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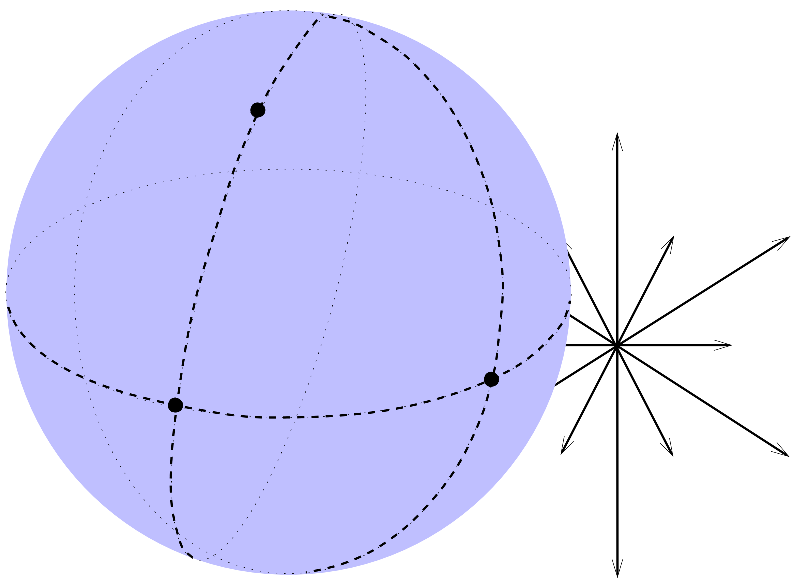
A Lie Algebraic Approach to the Symmetric Eigenvalue Problem



Jacobi-type Methods on Semisimple Lie Algebras

A Lie Algebraic Approach to Numerical Linear Algebra

Dissertation zur Erlangung des naturwissenschaftlichen Doktorgrades der Bayerischen Julius-Maximilians-Universität Würzburg

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1. Gutachter: Prof. Dr. Uwe Helmke

2. Gutachter: Priv. Doz. Dr. Knut Hüper

Tag der mündlichen Prüfung:

Für meine Eltern
Sabina und Klaus

mein Kind
Maximilian

und meine liebe Frau
Simone

Vorwort

Die vorliegende Dissertation entstand während meiner Tätigkeit als wissenschaftlicher Mitarbeiter an der Fakultät für Mathematik und Informatik der Universität Würzburg. Ihr Anspruch ist es, einem Teilbereich der numerischen Mathematik eine Sprache näherzubringen, die in ganz natürlicher Art und Weise viele Eigenwert- und Matrixfaktorisierungsprobleme vereint. Diese Sprache der Lie Theorie hat seit langem schon Einzug erhalten in große Bereiche der Physik und es ist nahezu erstaunlich, dass ihre mannigfaltigen Ergebnisse nicht schon früher Anwendungen in der numerischen Linearen Algebra fanden. In dieser Arbeit sollen in einem behutsamen Schritt Lie algebraische Methoden zu neuen Erkenntnissen und interessanten Resultaten rund um das symmetrische Eigenwertproblem bis hin zur symplektischen Singulärwertzerlegung und den damit verbundenen Jacobi-Verfahren führen. Sie ist in diesem Sinne eine natürliche Fortsetzung meiner Diplomarbeit ,,Das Jacobi-Verfahren auf kompakten Lie Algebren", die ich ebenfalls unter der Betreuung von Herrn Prof. Dr. Helmke am Lehrstuhl II des mathematischen Instituts der Universität Würzburg anfertigen durfte. An dieser Stelle möchte ich mich recht herzlich bei ihm für die fachliche und moralische Unterstützung bedanken. Er ließ mir die nötige Freiheit bei meiner Forschung und war stets behilflich, als sich das ein oder andere Problem als knifflig erwies. Desweiteren danke ich den lieben Sekretärinnen Karin Krumpholz und Ingrid Böhm und meinen Kollegen und Freunden Jochen Trumpf, Knut Hüper, Jens Jordan, Christian Lageman, Markus Baumann und Gunther Dirr, die jederzeit für eine familiäre und entspannte Atmosphäre sorgten und so manchen Stress vergessen machten. Besonders, und das meine ich wortwörtlich, möchte ich dabei Herrn Gunther Dirr hervorheben. Ohne sein geduldiges Zuhören, seinen messerscharfen Verstand und den damit verbundenen hilfreichen – mitunter auch fachlichen – Diskussionen und Gesprächen wäre diese Arbeit nicht möglich gewesen. Mein Dank gilt ebenfalls meinen Eltern, die mich von jeher in meinen Entscheidungen bestärkten und deren Zuspruch mir immer Motivation und Sicherheit auch während meines Studiums gaben. Zu guter Letzt möchte ich meiner Frau Simone herzlichst danken – für das Verständnis, das sie meiner Arbeit entgegenbringt und für ihre liebevolle Art und Fürsorge. Sie und mein kleiner Sohn Maximilian geben mir stets Kraft und Geborgenheit – oder anders gesagt: Wenn ich während der Erstellung dieser Dissertation ein Akku gewesen wäre, wären sie meine Aufladestation gewesen.

Publikationsliste

Die folgenden Arbeiten habe ich im Rahmen meiner Tätigkeit als wissenschaftlicher Mitarbeiter veröffentlicht.

- M. Kleinsteuber, U. Helmke, and K. Hüper. *Jacobi's Algorithm on Compact Lie-Algebras.* SIAM J. Matrix Anal. Appl. 26(1): 42–69, 2004.

- G. Dirr, U. Helmke, and M. Kleinsteuber. *Time optimal factorizations on compact Lie groups.* Proc. Appl. Math. Mech. 4: 664-665, 2004.

- G. Dirr, U. Helmke, and M. Kleinsteuber. *Lie algebra representations, nilpotent matrices, and the C-numerical range.* to appear in Linear Algebra Appl.

- G. Dirr, U. Helmke, K. Hüper, M. Kleinsteuber, and Y. Liu. *Spin Dynamics: A Paradigm for Time Optimal Control on Compact Lie Groups.* to appear in J. Global Optimization.

The most exciting phrase to hear in science, the one that heralds new discoveries, is not "Eureka!" but "That's funny..."

– Isaac Asimov –

Contents

Introduction

Structured eigenvalue and singular value problems play an important role in applied mathematics and the engineering sciences. They frequently arise in areas such as control theory and signal processing, where e.g. optimal control and signal estimation tasks require the fast computation of eigenvalues for Hamiltonian and symmetric matrices, respectively. We refer to [7] for an extensive list of structured eigenvalue problems and relevant literature. Such problems cannot be easily solved using standard software packages, as these eigenvalue algorithms do not necessarily preserve the underlying matrix structures and therefore may suffer by accumulation of rounding errors or numerical instabilities. In constrast, structure preserving eigenvalue methods have the potential of combining memory savings with high accuracy requirements and therefore are the methods of choice. Most of the previous approaches to structured problems have been on a case-to-case basis, by trying to adapt either known solution methods or software packages to each individual problem. However, such an ad–hoc approach is bound to fail if the problem of interest cannot be easily reformulated as a standard problem from numerical linear algebra. Thus a more flexible kind of algorithm is needed, that enables one to tackle whole classes of interesting eigenvalue problems. Clearly, one cannot expect to find one method that works for all structured problems. Nevertheless, it seems reasonable to develop methods that allow a unified approach to sufficiently rich classes of interesting eigenvalue problems.

The structure preserving Jacobi-type methods, proposed and studied in this thesis, are of this kind. Their inherent parallelizability, cf. [4], and high computational accuracy, cf. [13, 51] makes them also useful for large scale matrix computations. In contrast to earlier work, we extend the classical concept of a Jacobi-algorithm towards a new, unified Lie algebraic approach to structured eigenvalue problems, where structure of a matrix is defined by being an element of a Lie algebra (or of a suitably defined sub-structure). Specifically, we focus on a generalization of the well-known symmetric eigenvalue (EVD) and singular value decompositions (SVD) to classes of matrices that can be endowed with a Lie algebraic structure. The associated normal form problems therefore provide a natural generalization of the symmetric EVD into a Lie algebraic setting and include a large number of interesting structured eigenvalue problems.

The Jacobi algorithm for diagonalizing real symmetric or complex Hermitian matrices is a classical eigenvalue method from numerical linear algebra, cf. [25]. The original version of the algorithm has been first proposed by Jacobi (1846) in [43], who successively applied elementary rotations in a plane (later also called Jacobi or Givens rotations), that produce the largest decrease in the distance to diagonality, by annihilating the off-diagonal element with the largest absolute value. Modern approaches follow the same idea, but use cyclic sweep strategies to minimize the sum of squares of off-diagonal entries. Such cyclic sweep strategies are more efficient than Jacobi's original approach, as one avoids the time consuming search for the largest off-diagonal element.
Variants of the Jacobi algorithm have been applied to various structured eigenvalue problems, including e.g. the real skew-symmetric eigenvalue problem, [26, 42, 54], computations of the singular value decomposition [46], non-symmetric eigenvalue problems [9, 16, 61, 65], complex symmetric eigenproblems [17], and the computation of eigenvalues of normal matrices [24]. For extensions to different types of generalized eigenvalue problems, we refer to [11, 66]. For applications of Jacobi–type methods to problems in systems theory, see [32, 33, 34].
A characteristic feature of all known Jacobi-type methods is that they act to minimize the distance to diagonality while preserving the eigenvalues. Thus different measures to diagonality can be used to design different types of Jacobi algorithms. Conventional Jacobi algorithms, like classical cyclic Jacobi algorithms for symmetric matrices, Kogbetliantz's method for the SVD, cf. [46], methods for the skew-symmetric EVD, cf. [26], and for the Hamiltonian EVD, cf. [48], as well as recent methods for the perplectic EVD, cf. [49] all foot on reducing the sum of squares of off-diagonal entries (the so-called off-norm). Although local quadratic convergence to the diagonalization has been shown in some of these cases, at least for generic situations, the analysis of such conventional Jacobi methods becomes considerably more complicate for clustered eigenvalues. This difficulty is unavoidable for conventional Jacobi methods and is due to the fact, that the to be minimized off-norm function has a complicated critical point structure and several global minima. Thus this difficulty might be remedied by a better choice of cost function that measures the distance to diagonality. In fact, Brockett's trace function turns out to be a more appropriate distance measure than the off-norm function. In [6], R.W. Brockett showed that the gradient flow of the trace function can be used to diagonalize a symmetric matrix and simultaneously sort the eigenvalues. This trace function also appeared in the early work of J. von Neumann on the classification of unitarily invariant norms. It has been also considered by e.g. M.T. Chu, [12] associated with gradient methods for matrix factorizations, and subsequently by many others. For a systematic critical point analysis of the trace function in a Lie group setting, we refer to the early work of Duistermaat, Kolk and Varadarajan, cf. [15]. See also [62] for more recent results on this topic in the framework of reductive Lie groups.
K. Hüper, in his Ph.D. thesis [42], has been the first who realized, that Brockett's

trace function can be effectively used to design a new kind of Jacobi algorithm for symmetric matrix diagonalization, that automatically sorts the eigenvalues in any prescribed order. This so-called *Sort-Jacobi algorithm* uses Givens rotations that do not only annihilate the off-diagonal element, but also sort the two corresponding elements on the diagonal. The idea of combining sorting with eigenvalue computations can be carried over to the SVD, too; cf. [42]. It is this automatic sorting property that distinguishes the Sort-Jacobi algorithm from the known conventional schemes and leads both to improved convergence properties as well as to a simplified theory. In fact, numerical simulations by Hüper have shown that the Sort-Jacobi algorithm for the symmetric EVD and the SVD has considerably better convergence properties than the conventional cyclic Jacobi schemes and Kogbetliantz's method, respectively, cf. [42]. Moreover, local quadratic convergence has been proven for matrices with distinct eigenvalues and singular values, respectively. These theoretical and practical advantages of the Sort-Jacobi method will be confirmed by results in this thesis as well.

The main achievements of this thesis are the following:

- **Unified treatment of Jacobi-type algorithms on semisimple Lie algebras**. This includes both conventional Jacobi methods as well as Sort-Jacobi methods, with unified local quadratic convergence proofs for arbitrary regular elements and sweep strategies.

- **A new type of cyclic sweeps**. The new class of special cyclic sweeps is introduced for which local quadratic convergence is shown for arbitrary irregular elements of a Lie algebra.

- **New classes of structured eigenvalue problems**. We present a unified convergence theory of the algorithms, including so far unstudied cases such as the symplectic SVD, Takagi's factorization and an eigenvalue problem in an exceptional Lie algebra of (7×7)-matrices.

We now give a more detailed description. To the best of the author's knowledge, Wildberger [67] has been the first who proposed a generalization of the (non-cyclic) classical Jacobi algorithm on arbitrary compact Lie algebras. Wildberger showed that suitable Lie algebraic generalizations of the Givens rotations act as minimizing the appropriate generalization of the off-norm function. Thus he succeeded in proving global convergence of the algorithm, however, did not prove local quadratic convergence. The well–known classification of compact Lie algebras shows that this approach essentially includes structure preserving Jacobi-type methods for the real skew-symmetric, the complex skew-Hermitian, the real skew-symmetric Hamiltonian, the complex skew-Hermitian Hamiltonian eigenvalue problem, and some exceptional cases. Following [67], one can treat the above mentioned problems on the same footing, meaning that the description and analysis of the Jacobi method can be carried out simultaneously.

(i)	symmetric/Hermitian EVD
(ii)	skew-symmetric EVD
(iii)	real/complex SVD
(iv)	real symmetric/skew-symmetric Hamiltonian EVD
(v)	Hermitian $\mathbb{R}$-Hamiltonian EVD
(vi)	perplectic EVD
(vii)	Takagi's Factorization
(viii)	symplectic SVD
(xi)	Hermitian $\mathbb{C}$-Hamiltonian EVD
(x)	Hermitian Quaternion EVD
(xi)	a Takagi-like factorization
(xii)	some exceptional cases.

Table 1: Normal form problems considered in this thesis.

Wildberger's work has been subsequently extended by Kleinsteuber et.al. [44], where local quadratic convergence for general cyclic Jacobi schemes is shown to hold for arbitrary regular elements in a compact Lie algebra. In this thesis we present a systematic account of Jacobi-type algorithms that contains the previous results on compact Lie algebras as a special case. Thus, we propose and analyze both the classical Jacobi algorithm (reducing the off-norm) as well as the Sort-Jacobi algorithm (optimizing the trace function) for a large class of structured matrices that essentially include the normal form problems quoted in Table 1. These cases arise from the known classification of simple Lie algebras. A list of the different Lie algebra structures considered here can be found in Table 4.1 in Chapter 4. Cyclic Jacobi-type methods for some of the above cases have been discussed earlier, e.g. for types (i) see [21, 42], (ii) see [26, 42, 54], (iii) see [42, 46], (iv) see [18], (v) see [9], and (vi) see [49]. Thus we achieve a simultaneous generalization of all this prior work. Note that the methods proposed in this thesis exclusively use one-parameter transformations and therefore slightly differ from the algorithms in [9, 18, 26, 42, 54], where block Jacobi methods

are used, i.e. multiparameter transformations that annihilate more than one pair of off-diagonal elements at the same time.
Lie theory provides us both with a unified treatment and a coordinate free approach of Jacobi-type methods. In particular, it allows a formulation of Jacobi methods that is independent of the underlying matrix representation. Together with the above specific matrix cases, *all* isomorphic types can be simultaneously treated. If a class of matrices is known to be isomorphic to one of the cases listed above, then, by a straightforward re-definition of terms, a Jacobi-type algorithm is obtained together with appropriate convergence results. Thus we can completely avoid the often tiring case-by-case analysis. Let us give two examples to illustrate this process.
Recently, a Jacobi method for the eigenvalue problem of so-called perplectic matrices has been introduced, [49]. The Lie algebra of the *perskew-symmetric matrices*

$$\{A \in \mathbb{R}^{n\times n} \mid A^\top R + RA = 0\}, \quad \text{where } R := \begin{bmatrix} & & 1 \\ & \cdot^{\cdot^{\cdot}} & \\ 1 & & \end{bmatrix}$$

is isomorphic to $\mathfrak{so}(k,k)$ if $n = 2k$ and to $\mathfrak{so}(k+1,k)$ if $n = 2k+1$. The symmetric perskew-symmetric EVD is therefore equivalent to the SVD of a real $(k \times k)$-matrix, $(k+1 \times k)$ respectively. Similarly, the skew-symmetric perskew-symmetric EVD, the symmetric persymmetric EVD and the skew-symmetric persymmetric EVD reduce to well-known normal form problems. cf. Section 4.2.
In systems theory, the *real* Lie algebra of $\mathbb{R}$-Hamiltonian matrices

$$\left\{ \begin{bmatrix} A & G \\ Q & -A^* \end{bmatrix}, A, G, Q \in \mathbb{C}^{n\times n}, G^* = G, H^* = H \right\}$$

plays an important role in linear optimal control and associated algebraic Riccati equations. This Lie algebra is equivalent to $\mathfrak{su}(n,n)$. Hence the diagonalization of a Hermitian $\mathbb{R}$-Hamiltonian matrix is equivalent to the SVD of a complex $(n\times n)$-matrix, cf. [8] and Section 4.5 for more details.
Let G be a semisimple Lie group and $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ be the Cartan decomposition of its Lie algebra. In this thesis, we propose a Jacobi–type method that "diagonalizes" an element $S \in \mathfrak{p}$ by conjugation with some $k \in K$, where $K \subset G$ is the Lie subgroup corresponding to $\mathfrak{k}$. Of course, if A is a Hermitian matrix, then iA is skew-Hermitian and therefore the Hermitian and the skew-Hermitian eigenvalue problem are equivalent. The same trick extends to arbitrary compact Lie algebras. In this sense it becomes clear that the present work immediately generalizes the corresponding results for compact Lie algebras in [44]. In fact, if $\mathfrak{k}$ is a compact semisimple Lie algebra, then $\mathfrak{g}_0 := \mathfrak{k} \oplus i\mathfrak{k}$ is the Cartan decomposition of $\mathfrak{g}_0$. Thus the analysis of Jacobi-type methods on compact Lie algebras appears as a special case of our result.
The coordinate free approach forces one to formulate the basic characteristics of the algorithm in an abstract way, thus enabling one to develop the essential features of Jacobi algorithms. In particularly, the local convergence analysis for the algorithms

is in all the cases (i)-(xii) exactly the same and follows from one general convergence result. It turns out that for a local convergence analysis in these cases one has to distinguish (a) the regular case (roughly corresponding to pairwise distinct eigenvalues/singular values) and (b) the irregular case, where eigenvalues/singular values occur in clusters. The regular case is quite well understood and local quadratic convergence has been proven both for the conventional as well as for the Sort-Jacobi schemes; see e.g. [36, 42, 58, 68]. In constrast, the irregular case is more delicate and is best understood only for the symmetric EVD, where van Kempen showed locally quadratic convergence for a special cyclic scheme; [64]. The convergence properties of the Kogbetliantz method in the irregular case are treated in [19, 21, 27, 28, 55]. See also [2] and [10], where local quadratic convergence has been shown for the irregular case for an upper triangular matrix.
Our convergence analysis of Jacobi-type methods deviates from earlier work, by extending the elegant calculus approach first described in the Ph.D. thesis by K. Hüper, [42] and [40]. However, the analysis in [42], [40] is mainly restricted to the regular case; the convergence analysis in [42] in the irregular case is either incorrect or has at least major gaps. We prove local quadratic convergence for the Jacobi-methods in the general setting, including all cases (i)–(xii) for the regular as well as for the irregular case. The regular case is a rather straightforward generalization of the ideas in [42] and indeed local quadratic convergence is shown for any cyclic Jacobi scheme. In contrast the irregular case is more tricky. Simulations show that for certain structured EVDs, Jacobi-type methods for the irregular case converge much faster than for the regular case. For example, the special cyclic Jacobi for the symmetric EVD converges faster if the eigenvalues occur in clusters, cf. [64]. In contrast, Kogbetliantz's method for computing the SVD of an arbitrary real matrix becomes worse the closer the singular values are, cf. [10], and local quadratic convergence for Kogbetliantz's method has only been proven if the difference between two singular values is large enough. On the other hand, if one applies Kogbetliantz's algorithm to an upper triangular square matrix with clustered singular values, then Bai has shown that the algorithm converges quadratically, cf. [2]. Thus the special structure of matrices may have impact on the local convergence rate. Another crucial point here is the order in which the sweep directions are worked off. In the literature, local quadratic convergence in the irregular case is only proven for very special sweep strategies. We generalize the idea of van Kempen [64] to the Lie algebra context and propose a new class of *special cyclic sweeps* that ensure local quadratic convergence for the irregular cases in any of the above mentioned normal form problems (i)–(xii). It should be emphasized that our sweep strategy differs from that in the literature for the SVD, i.e. compared with Kogbetliantz's algorithm. Numerical experiments confirm that the proposed Sort-Jacobi method with special cyclic sweeps yields better convergence results than the established Jacobi methods. The advantage is the bigger, the more the element is irregular, i.e. the more the eigenvalues and singular values, respectively, are clustered, cf. Figure 1.

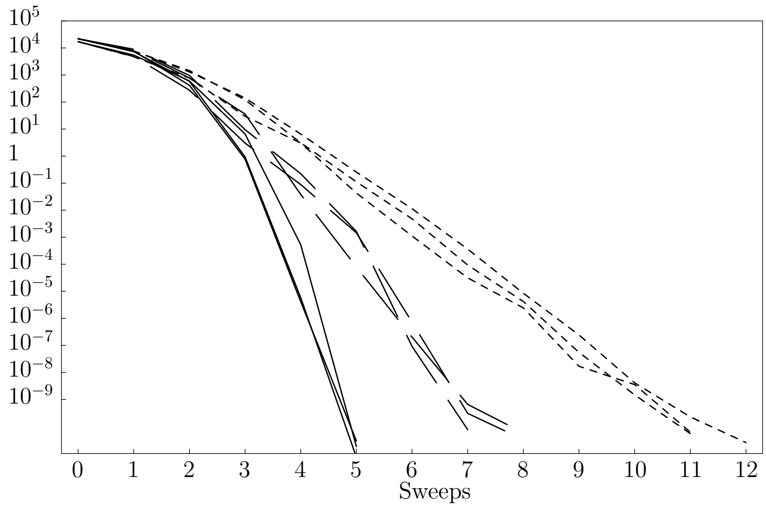

Figure 1: Convergence behavior for the real SVD of matrices with clustered singular values; stopping criterion: off-norm $< 10^{-10}$ (vertical axes); small dashed line = classical cyclic Kogbetliantz; large dashed line = sort Jacobi with classical cyclic sweeps, [42]; solid line = sort Jacobi with special cyclic sweeps. For details cf. Section 4.2.

This thesis is organized as follows. The first chapter summarizes basic definitions and facts on Lie algebras and Lie groups. We focus on reviewing the structure of semi-simple Lie algebras as they play a major role for our purposes. Since the so-called restricted-root space decomposition is of special importance in determining the sweep directions, it is explained in full detail. Chapter 2 deals with the analysis of abstract Jacobi-type methods on manifolds. These can be considered as abstract coordinate descent optimization methods and thus are useful not only for eigenvalue computations but for general constrained optimization tasks. Following [40], sufficient conditions for the cost function and the Jacobi directions are specified that ensure local quadratic convergence. The idea is that the optimization directions have to be mutually orthogonal with respect to the Hessian of the cost function at the critical point. We then specify the Jacobi method to the special case where the manifold is the K-adjoint orbit of an element $S \in \mathfrak{p}$. Under certain assumptions on the cost function (that are fulfilled for the trace function and the off-norm), we derive a sufficient condition for the sweep directions to be computed simultaneously. This result is expected to be useful in direction of parallel implementations of the algorithm. In Chapter 3 we study the proposed Lie algebraic generalization of the symmetric eigenvalue problem. We briefly discuss the Lie algebraic version of the classical off-norm function and the trace function whose respective optimization tasks give rise to a classical (off-norm) and a Sort-Jacobi algorithm (trace-function) on Lie algebras. The last part of this chapter is devoted to the local convergence analysis. While the regular case follows rather routinely from the results in Chapter 2, an excursion to the theory of abstract root systems is required for a rigorous treatment of the irregular case. Special cyclic sweeps are introduced for which we then prove local quadratic convergence in the irregular case. Applications to structured eigenvalue and singular value problems are discussed in Chapter 4. Numerical experiments are presented where the special cyclic sweep method is compared with other Jacobi methods. Moreover, the equivalence of some seemingly different normal forms and corresponding Jacobi algorithms is discussed. The algorithms from Chapter 3 are exemplified for the real and the symplectic SVD, for the real symmetric Hamiltonian EVD and for the case of the exceptional Lie algebra $\mathfrak{g}_2$.

Chapter 1

Background: Lie Groups and Lie Algebras

1.1 Preliminaries on Lie Algebras

We first recall some basic facts and definitions about Lie algebras. We follow mainly [45] and [31] and content ourselves by giving references to the proofs unless details are needed later on. Moreover, several examples are given in order to illustrate the concepts. For further details on Lie theory, see also [5], [14] or [39]. In the sequel, let $\mathbb{K}$ denote the fields $\mathbb{R}$, $\mathbb{C}$ of real or complex numbers, respectively.

Definition 1.1. A $\mathbb{K}$-vector space $\mathfrak{g}$ with a bilinear product

$$[\cdot,\cdot]\colon \mathfrak{g}\times\mathfrak{g}\longrightarrow\mathfrak{g},$$

is called a *Lie algebra* over $\mathbb{K}$ if

(i) $[X,Y]=-[Y,X]$ for all $X,Y\in\mathfrak{g}$

(ii) $[[X,Y],Z]+[[Y,Z],X]+[[Z,X],Y]=0$ (*Jacobi identity*).

Example 1.2. Let $\mathbb{K}=\mathbb{R}$ or $\mathbb{C}$. Classical Lie algebras are given for example by

$$\begin{aligned}
\mathfrak{sl}(n,\mathbb{K}) &:= \{X\in\mathbb{K}^{n\times n} \mid \mathrm{tr}X=0\}\\
\mathfrak{so}(n,\mathbb{K}) &:= \{X\in\mathbb{K}^{n\times n} \mid X^\top+X=0\}\\
\mathfrak{sp}(n,\mathbb{K}) &:= \{X\in\mathbb{K}^{2n\times 2n} \mid X^\top J+JX=0\},
\end{aligned}$$

where

$$J:=\begin{bmatrix}0 & I_n\\ -I_n & 0\end{bmatrix}$$

$(\cdot)^\top$ denotes transpose and I_n denotes the $(n\times n)$-identity matrix.

A Lie algebra $\mathfrak{g}$ over $\mathbb{R}$ ($\mathbb{C}$) is called *real* (*complex*). A *Lie subalgebra* $\mathfrak{h}$ is a $\mathbb{K}$-linear subspace of $\mathfrak{g}$ for which $[\mathfrak{h}, \mathfrak{h}] \subset \mathfrak{h}$ holds, where

$$[\mathfrak{h}_1, \mathfrak{h}_2] := \{[H_1, H_2] \mid H_1 \in \mathfrak{h}_1, H_2 \in \mathfrak{h}_2\}.$$

It is called an *ideal* of $\mathfrak{g}$, if $[\mathfrak{h}, \mathfrak{g}] \subset \mathfrak{h}$. A Lie algebra $\mathfrak{g}$ is called *simple*, if its only ideals are $\mathfrak{g}$ and $\{0\}$, it is called *abelian* if $[\mathfrak{g}, \mathfrak{g}] = 0$. In the sequel, $\mathfrak{g}$ is always assumed to be finite dimensional. Denote the *endomorphisms of* $\mathfrak{g}$, i.e. the $\mathbb{K}$-linear mappings $\mathfrak{g} \to \mathfrak{g}$ by $\mathrm{End}(\mathfrak{g})$ and let $GL(\mathfrak{g})$ denote the invertible endomorphisms. For any $X \in \mathfrak{g}$, the *adjoint transformation* is the linear map

$$\mathrm{ad}_X \colon \mathfrak{g} \longrightarrow \mathfrak{g}, \qquad Y \longmapsto [X, Y] \tag{1.1}$$

and

$$\mathrm{ad} \colon \mathfrak{g} \longrightarrow \mathrm{End}(\mathfrak{g}), \qquad Y \longmapsto \mathrm{ad}_Y \tag{1.2}$$

is called the *adjoint representation* of $\mathfrak{g}$.
By means of (1.1) and (1.2), the properties (i) and (ii) of Definition 1.1 are equivalent to

$$\mathrm{ad}_X Y = -\mathrm{ad}_Y X$$

and

$$\mathrm{ad}_{[X,Y]} = \mathrm{ad}_X \mathrm{ad}_Y - \mathrm{ad}_Y \mathrm{ad}_X,$$

respectively. It follows immediately from property (i) that $\mathrm{ad}_X X = 0$ for all $X \in \mathfrak{g}$. The subsequently defined bilinear form plays an essential role in Lie theory.

Definition 1.3. Let $\mathfrak{g}$ be a finite dimensional Lie algebra over $\mathbb{K}$. The symmetric bilinear form

$$\kappa \colon \mathfrak{g} \times \mathfrak{g} \longrightarrow \mathbb{K}, \qquad \kappa(X, Y) \longmapsto \mathrm{tr}(\mathrm{ad}_X \mathrm{ad}_Y) \tag{1.3}$$

is called the *Killing form* of $\mathfrak{g}$.

Example 1.4. Let $\mathbb{K} = \mathbb{R}$ or $\mathbb{C}$. Then the Killing form for the classical simple Lie algebras is given in the following.

$$\begin{array}{lcll} \mathfrak{sl}(n, \mathbb{K}) & : & \kappa(X, Y) = 2\, n\, \mathrm{tr}(XY) & \text{for } n \geq 2, \\ \mathfrak{so}(n, \mathbb{K}) & : & \kappa(X, Y) = (n-2)\mathrm{tr}(XY) & \text{for } n \geq 3, \\ \mathfrak{sp}(n, \mathbb{K}) & : & \kappa(X, Y) = 2(n+1)\mathrm{tr}(XY) & \text{for } n \geq 1, \end{array}$$

cf. [30], Section IV.2 or [20], VI.4. Note that in [30], the notation $\mathfrak{sp}(2n, \mathbb{K})$ is used instead of $\mathfrak{sp}(n, \mathbb{K})$.

A *Lie group* is defined as a group together with a manifold structure such that the group operations are smooth functions. For an arbitrary Lie group G, the tangent space $T_1 G$ at the unit element $1 \in G$ possesses a Lie algebraic structure. This tangent space is called the Lie algebra of the Lie group G, denoted by $\mathfrak{g}$. The tangent mapping of the conjugation mapping in G at 1,

$$\mathrm{conj}_x(y)\colon = xyx^{-1}, \quad x, y \in G,$$

is given by

$$\mathrm{Ad}_x\colon = T_1(\mathrm{conj}_x)\colon \mathfrak{g} \longrightarrow \mathfrak{g}$$

and leads to the so-called *adjoint representation* of G in $\mathfrak{g}$, given by

$$\mathrm{Ad}\colon x \longmapsto \mathrm{Ad}_x,$$

cf. [14], Section I.1. Considering now the tangent mapping of Ad at 1 leads to the adjoint transformation (1.1). If G is a matrix group, i.e. G consists of invertible real or complex matrices, then the elements of the corresponding Lie algebra can also be regarded as matrices, cf. [45], Section I.10. In this case the adjoint representation of $g \in G$ applied to $X \in \mathfrak{g}$ is given by

$$\mathrm{Ad}_g X = gXg^{-1}, \tag{1.4}$$

i.e., by the usual similarity transformation of matrices, and the adjoint transformation is given by

$$\mathrm{ad}_Y X = YX - XY.$$

Example 1.5. Some classical Lie groups are

$$\begin{array}{lll} SL(n,\mathbb{K}) & := \{g \in \mathbb{K}^{n\times n} \mid \det g = 1\} & \text{corresponding Lie algebra: } \mathfrak{sl}(n,\mathbb{K}), \\ SO(n,\mathbb{K}) & := \{g \in \mathbb{K}^{n\times n} \mid g^\top g = 1\} & \text{corresponding Lie algebra: } \mathfrak{so}(n,\mathbb{K}), \\ Sp(n,\mathbb{K}) & := \{g \in \mathbb{K}^{2n\times 2n} \mid g^\top J g = J\} & \text{corresponding Lie algebra: } \mathfrak{sp}(n,\mathbb{K}), \end{array}$$

where J is defined as in Example 1.2.

A basic property of the Killing form κ defined by (1.3) is its Ad-invariance, i.e.

$$\kappa(\mathrm{Ad}_g X, \mathrm{Ad}_g Y) = \kappa(X,Y) \qquad \text{for all } X, Y \in \mathfrak{g} \text{ and } g \in G. \tag{1.5a}$$

Differentiating this equation with respect to g immediately yields

$$\kappa(\mathrm{ad}_X Y, Z) = -\kappa(Y, \mathrm{ad}_X Z) \qquad \text{for all } X, Y, Z \in \mathfrak{g}. \tag{1.5b}$$

Property (1.5a) is just the special case of the following more general result. A *(Lie algebra-) automorphism* of $\mathfrak{g}$ is an invertible linear map φ with $\varphi[X,Y] = [\varphi X, \varphi Y]$. We denote the set of automorphisms of $\mathfrak{g}$ by $\mathrm{Aut}(\mathfrak{g})$.

Proposition 1.6. *The Killing form is invariant under automorphisms of $\mathfrak{g}$, i.e*

$$\kappa(X,Y) = \kappa(\varphi X, \varphi Y) \ \ \textit{for all } \varphi \in \mathrm{Aut}(\mathfrak{g}).$$

Proof. Let $\varphi \in \mathrm{Aut}(\mathfrak{g})$. Then we have for all $Z \in \mathfrak{g}$ that $\mathrm{ad}_{\varphi X} Z = [\varphi X, Z] = \varphi([X, \varphi^{-1} Z] = (\varphi \mathrm{ad}_X \varphi^{-1}) Z$ and hence

$$\begin{aligned}\kappa(\varphi X, \varphi Y) &= \mathrm{tr}(\mathrm{ad}_{\varphi X} \mathrm{ad}_{\varphi Y}) \\ &= \mathrm{tr}(\varphi(\mathrm{ad}_X)\varphi^{-1}\varphi(\mathrm{ad}_Y)\varphi^{-1}) \\ &= \kappa(X, Y),\end{aligned}$$

cf. [45], Prop. 1.119. □

Now since $\mathrm{Aut}(\mathfrak{g})$ is a closed subgroup of the general linear group $GL(\mathfrak{g})$ it is a Lie group and its Lie algebra is contained in $\mathrm{End}(\mathfrak{g})$. More precisely we have the following proposition.

Proposition 1.7. *The Lie algebra of* $\mathrm{Aut}(\mathfrak{g})$ *is given by*

$$\mathrm{Der}(\mathfrak{g}) := \{D \in \mathrm{End}(\mathfrak{g}) \mid D[X, Y] = [DX, Y] + [X, DY] \textit{ for all } X, Y \in \mathfrak{g}\}.$$

Moreover, the image of the adjoint representation $\mathrm{ad}(\mathfrak{g})$ *is a subalgebra of* $\mathrm{Der}(\mathfrak{g})$*.*

Any element $D \in \mathrm{Der}(\mathfrak{g})$ is called a *derivation* of $\mathfrak{g}$ and the image elements of $\mathrm{ad}(\mathfrak{g})$ are called *inner derivations.*

Proof. Cf. [45], Ch. I, Prop 1.120. □

An *analytic subgroup* H of a Lie group G is a connected subgroup where the inclusion mapping is smooth. The group of *inner automorphisms* $\mathrm{Int}(\mathfrak{g})$ of $\mathfrak{g}$ is defined as the analytic subgroup of $\mathrm{Aut}(\mathfrak{g})$ with Lie algebra $\mathrm{ad}(\mathfrak{g})$. Hence if for $X \in \mathfrak{g}$ we define the exponential map by

$$\exp\colon \mathrm{ad}(\mathfrak{g}) \longrightarrow GL(\mathfrak{g}), \quad \mathrm{ad}_X \longmapsto \sum_{k=0}^{\infty} \frac{1}{k!} \mathrm{ad}_X^k,$$

then

$$\mathrm{Int}(\mathfrak{g}) = \text{the group generated by } \{\exp(\mathrm{ad}_X) \mid X \in \mathfrak{g}\}. \tag{1.6}$$

Theorem 1.8. *If* $\mathfrak{g}$ *is the Lie algebra of a Lie group* G *and if* G_0 *denotes the identity component of* G*, then*

$$\mathrm{Int}(\mathfrak{g}) = \{\varphi \in \mathrm{Aut}(\mathfrak{g}) \mid \varphi = \mathrm{Ad}_g \textit{ for some } g \in G_0\}. \tag{1.7}$$

Proof. Since $\mathrm{Ad}\colon g \mapsto \mathrm{Ad}_g$ is a smooth homomorphism of Lie groups, cf. [45], Prop. 1.89, Ch. I, of G into $\mathrm{Aut}(\mathfrak{g})$, the group $\mathrm{Ad}(G)$ is a Lie subgroup of $\mathrm{Aut}(\mathfrak{g})$ with Lie algebra $\mathrm{ad}(\mathfrak{g})$. By definition, the analytic subgroup of $\mathrm{Aut}(\mathfrak{g})$ is $\mathrm{Int}(\mathfrak{g})$. Thus $\mathrm{Int}(\mathfrak{g})$ is the identity component of $\mathrm{Ad}(G)$ and equals therefore $\mathrm{Ad}(G_0)$. Cf. [45], Prop. 1.91, Ch. I, Sec. 10. □

According to Eqs. (1.6) and (1.7) we use the common notation

$$\mathrm{Ad}_{\exp X} := \exp(\mathrm{ad}_X).$$

In the case where $\mathfrak{g}$ is a Lie algebra of complex or real $(n \times n)$-matrices, then multiplication is defined on $\mathfrak{g}$ and for $X, Y \in \mathfrak{g}$ we have $\exp(X) = \sum_{k=0}^{\infty} \frac{X^k}{k!} \subset GL(n)$ and

$$\mathrm{Ad}_{\exp X} Y = \exp(X) Y \exp(-X).$$

Let $\mathfrak{k} \subset \mathfrak{g}$ be a Lie subalgebra. We denote by $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ the analytic subgroup of $\mathrm{Int}(\mathfrak{g})$ with Lie algebra $\mathrm{ad}(\mathfrak{k}) \subset \mathrm{End}(\mathfrak{g})$. Note that

$$\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k}) = \text{the group generated by } \{\exp(\mathrm{ad}_X) \mid X \in \mathfrak{k}\},$$

or, equivalently, if $\mathfrak{g}$ is the Lie algebra of a Lie group G and K is the analytic subgroup of G with Lie algebra $\mathfrak{k}$, we have

$$\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k}) = \{\varphi \in \mathrm{Int}(\mathfrak{g}) \mid \varphi = \mathrm{Ad}_k, k \in K\}. \tag{1.8}$$

Definition 1.9. A real finite dimensional Lie algebra $\mathfrak{g}$ is called *compact* if $\mathrm{Int}(\mathfrak{g})$ is compact. A subalgebra $\mathfrak{k} \subset \mathfrak{g}$ is called a *compactly embedded subalgebra* if $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ is compact.

Example 1.10. (a) If $\mathfrak{g}$ is an abelian Lie algebra, then $\mathrm{ad}_X \equiv 0$ for all $X \in \mathfrak{g}$. Therefore $\mathrm{Int}(\mathfrak{g}) = \{1\}$ and hence $\mathfrak{g}$ is a compact Lie algebra.

(b) Although the Lie subalgebra

$$\mathfrak{a} := \left\{ \begin{bmatrix} a & 0 \\ 0 & -a \end{bmatrix} \mid a \in \mathbb{R} \right\} \subset \mathfrak{sl}(2, \mathbb{R})$$

is abelian, it is not compactly embedded in $\mathfrak{sl}(2, \mathbb{R})$. Note that $\{1\} = \mathrm{Int}(\mathfrak{a}) \neq \mathrm{Int}_{\mathfrak{sl}(2,\mathbb{R})}(\mathfrak{a})$.

Since the map $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k}) \to \mathrm{Int}(\mathfrak{k})$, $\varphi \mapsto \varphi|_{\mathfrak{k}}$ is smooth, every compactly embedded Lie subalgebra is itself compact. The following proposition immediately involves more examples.

Proposition 1.11. *A real finite dimensional Lie algebra $\mathfrak{g}$ is compact if it is the Lie algebra of a compact Lie group.*

Proof. [45], Ch. IV, Prop. 4.23. □

Example 1.12. The following Lie algebras are compact, cf. [45], Section I.8.

$$\begin{aligned}
\mathfrak{so}(n, \mathbb{R}) &:= \{S \in \mathbb{R}^{n \times n} \mid S^\top = -S\} \\
\mathfrak{u}(n) &:= \{X \in \mathbb{C}^{n \times n} \mid X^* = -X\}, \\
\mathfrak{su}(n) &:= \{X \in \mathbb{C}^{n \times n} \mid X^* = -X, \mathrm{tr} X = 0\}, \\
\mathfrak{sp}(n) &:= \mathfrak{u}(2n) \cap \mathfrak{sp}(n, \mathbb{C}),
\end{aligned}$$

where $(\cdot)^*$ denotes conjugate transpose. They correspond to the Lie groups

$$\begin{aligned}
&SO(n,\mathbb{R}) := \{g \in \mathbb{R}^{n\times n} \mid g^\top g = 1\}\\
&U(n) := \{g \in \mathbb{C}^{n\times n} \mid g^* g = 1\},\\
&SU(n) := \{X \in \mathbb{C}^{n\times n} \mid g^* g = 1, \det g = 1\},\\
&Sp(n) := U(2n) \cap Sp(n,\mathbb{C}).
\end{aligned}$$

A compact Lie algebra $\mathfrak{g}$ admits a positive definite Ad-invariant bilinear form, cf. [45], Ch. IV., Prop. 4.24. This property is used to show that the Killing form on compact Lie algebras is negative semi-definite.

Proposition 1.13. *Let $\mathfrak{g}$ be a compact Lie algebra. Then the Killing form is negative semi-definite.*

Proof. [45], Ch. IV, Cor. 4.26. □

Although in general differently but equivalently defined in the literature, it proves to be convenient for our purposes to use Cartan's Criterion, cf. [45], Thm. 1.45, to define semisimple Lie algebras.

Definition 1.14. A finite dimensional Lie algebra is called *semisimple*, if its Killing form is nondegenerate.

Together with Proposition 1.13 this yields the following theorem.

Theorem 1.15. *A semisimple Lie algebra is compact if and only if its Killing form is negative definite. On the other hand, the Killing form of a Lie algebra $\mathfrak{g}$ is negative definite if and only if $\mathfrak{g}$ is compact and semisimple.*

Proof. Cf. [45], Ch. IV, Prop. 4.27. □

As another characterization of semisimple Lie algebras we have the following theorem.

Theorem 1.16. *The Lie algebra $\mathfrak{g}$ is semisimple if and only if*

$$\mathfrak{g} = \mathfrak{g}_1 \oplus \ldots \oplus \mathfrak{g}_m$$

with simple ideals $\mathfrak{g}_i$. This decomposition is unique. Moreover, every ideal $\mathfrak{i} \subset \mathfrak{g}$ is the sum of various $\mathfrak{g}_i$.

Proof. [45], Ch. I, Thm. 1.54. □

Example 1.17. (a) ([45], Section I.8.) The Lie algebras $\mathfrak{sl}(n,\mathbb{K})$, $\mathfrak{so}(n,\mathbb{K})$, $\mathfrak{sp}(n,\mathbb{K})$, cf. Example 1.2, and $\mathfrak{su}(n)$, $\mathfrak{sp}(n)$, cf. Example 1.12 are semisimple. Furthermore, let

$$I_{p,q} := \begin{bmatrix} I_p & 0 \\ 0 & -I_q \end{bmatrix}.$$

Then the following Lie algebras are also semisimple.

$$\begin{aligned}
\mathfrak{so}(p,q) &:= \{X \in \mathbb{R}^{(p+q)\times(p+q)} \mid X^\top I_{p,q} + I_{p,q}X = 0\}, \quad p+q \geq 3, \\
\mathfrak{su}(p,q) &:= \{X \in \mathbb{C}^{(p+q)\times(p+q)} \mid X^* I_{p,q} + I_{p,q}X = 0, \mathrm{tr}X = 0\}, \quad p+q \geq 2, \\
\mathfrak{sp}(n,\mathbb{R}) &:= \{X \in \mathbb{R}^{2n\times 2n} \mid X^\top J + JX = 0\}, \quad n \geq 1, \\
\mathfrak{so}^*(2n) &:= \{X \in \mathfrak{su}(n,n) \mid X^\top \begin{bmatrix} 0 & I_n \\ I_n & 0 \end{bmatrix} + \begin{bmatrix} 0 & I_n \\ I_n & 0 \end{bmatrix} X = 0\}, \quad n \geq 2.
\end{aligned}$$

(b) The Lie algebra $\mathfrak{u}(n)$ is not semisimple, because $\mathrm{ad}_\Lambda \equiv 0$ for all $\Lambda = \lambda I_n$, hence $\kappa(\Lambda, X) = 0$ for all $X \in \mathfrak{u}(n)$.

(c) For some Lie algebras, the Killing form is completely degenerated. They are in this sense the converse of semisimple Lie algebras. Consider the Lie algebra of real upper triangular matrices

$$\mathfrak{b} := \{X \in \mathbb{R}^{n\times n} \mid X \text{ is upper triangular }\}.$$

Then for arbitrary $X, Y, Z \in \mathfrak{b}$ we have

$$\mathrm{ad}_Y Z = \begin{bmatrix} 0 & & * \\ & \ddots & \\ 0 & & 0 \end{bmatrix}.$$

Hence $\mathrm{ad}_X \mathrm{ad}_Y$ is nilpotent and therefore $\kappa(X, Y) = 0$ for all $X, Y \in \mathfrak{b}$.

It is easy to see by Eq. (1.5b) that $\mathfrak{a}$ is an ideal in $\mathfrak{g}$ if and only if $\mathfrak{a}^\perp$ is an ideal, but in general, $\mathfrak{a} \cap \mathfrak{a}^\perp \neq \emptyset$. However, for semisimple Lie algebras we have the following proposition.

Proposition 1.18. *Let $\mathfrak{g}$ be a semisimple Lie algebra.*

(a) Then $[\mathfrak{g}, \mathfrak{g}] = \mathfrak{g}$. Furthermore if $\mathfrak{a}$ is an ideal in $\mathfrak{g}$, we have $\mathfrak{g} = \mathfrak{a} \oplus \mathfrak{a}^\perp$.

(b) The adjoint representation $\mathrm{ad}\colon \mathfrak{g} \longmapsto \mathrm{ad}(\mathfrak{g})$ is a Lie algebra isomorphism.

Proof. (a) This is an immediate consequence of Theorem 1.16, cf. also [45], Ch. I, Cor. 1.55. (b) Assume that $\mathrm{ad}_X = \mathrm{ad}_Y$; it follows that $\mathrm{ad}_{X-Y} \equiv 0$ and therefore for all $Z \in \mathfrak{g}$ one has $0 = \mathrm{tr}(\mathrm{ad}_{X-Y}\mathrm{ad}_Z) = \kappa(X - Y, Z)$. By semisimplicity of $\mathfrak{g}$ the Killing form is non degenerated. Hence $X = Y$. □

The following theorem establishes a relation between the Lie algebras $\mathrm{Der}(\mathfrak{g})$ and $\mathrm{ad}(\mathfrak{g})$.

Theorem 1.19. *If $\mathfrak{g}$ is semisimple, then $\mathrm{ad}(\mathfrak{g}) = \mathrm{Der}(\mathfrak{g})$, that is, every derivation is inner.*

Proof. Cf. [31], Ch. II, Prop. 6.4. $\square$

Lemma 1.20. *Let $\mathfrak{g}$ be semisimple and $X, Y \in \mathfrak{g}$. Then the inner automorphisms $\exp(t\mathrm{ad}_X)$ and $\exp(s\mathrm{ad}_Y)$ commute for all $t, s \in \mathbb{R}$ if and only if $[X, Y] = 0$.*

Proof. " $\Rightarrow$ " : Assume that $\exp(t\mathrm{ad}_X)\exp(s\mathrm{ad}_Y) = \exp(s\mathrm{ad}_Y)\exp(t\mathrm{ad}_X)$ for all $s, t \in \mathbb{R}$. Then differentiating both sides with respect to t and s yields for $t = s = 0$ that $\mathrm{ad}_X\mathrm{ad}_Y = \mathrm{ad}_Y\mathrm{ad}_X$. Since $[\mathrm{ad}_X, \mathrm{ad}_Y] = \mathrm{ad}_{[X,Y]}$ and by semisimplicity of $\mathfrak{g}$, this is equivalent to $[X, Y] = 0$, cf. Prop. 1.18.
" $\Leftarrow$ " : Assume that $[X, Y] = 0$. This is equivalent to $\mathrm{ad}_X\mathrm{ad}_Y = \mathrm{ad}_Y\mathrm{ad}_X$, implying $\mathrm{ad}_X^k\mathrm{ad}_Y^l = \mathrm{ad}_Y^l\mathrm{ad}_X^k$ for all $l, k \in \mathbb{N}$ and hence for all $n, m \in \mathbb{N}$ and $t, s \in \mathbb{R}$ the operators $\sum_{k=0}^n \frac{t^k}{k!}\mathrm{ad}_X^k$ and $\sum_{l=0}^m \frac{t^l}{l!}\mathrm{ad}_X^l$ commute. Passing to the limits yields the assertion. $\square$

1.2 Compact Real Forms of Complex Semisimple Lie Algebras

Let $\mathfrak{g}$ be a complex semisimple Lie algebra. We write $\mathfrak{g}^{\mathbb{R}}$ for $\mathfrak{g}$ if it is regarded as a real Lie algebra, i.e. by restricting the scalars and call $\mathfrak{g}^{\mathbb{R}}$ the *realification* of $\mathfrak{g}$. Note, that $\dim_{\mathbb{R}} \mathfrak{g}^{\mathbb{R}} = 2\dim_{\mathbb{C}} \mathfrak{g}$.

Proposition 1.21. *Let $\mathfrak{g}$ be a complex Lie algebra with Killing form $\kappa\colon \mathfrak{g}\times\mathfrak{g} \longrightarrow \mathbb{C}$. Denote by $\kappa_{\mathfrak{g}^{\mathbb{R}}}\colon \mathfrak{g}^{\mathbb{R}} \times \mathfrak{g}^{\mathbb{R}} \longrightarrow \mathbb{R}$ the Killing form on $\mathfrak{g}^{\mathbb{R}}$, i.e. $\mathfrak{g}$ regarded as a real vector space. Then*

$$\kappa_{\mathfrak{g}^{\mathbb{R}}} = 2\mathrm{Re}\kappa.$$

In particular, $\mathfrak{g}$ is semisimple if and only if $\mathfrak{g}^{\mathbb{R}}$ is semisimple.

Proof. Let $\{B_1, ..., B_n\}$ be a basis of the (complex) vector space $\mathfrak{g}$ and denote by $v_{\mathbb{R}}$ its real span. Every X in $\mathfrak{g}$ decomposes uniquely into $X = \mathrm{Re}X + \mathrm{i}\mathrm{Im}X$ with $\mathrm{Re}X, \mathrm{Im}X \in v_{\mathbb{R}}$ and moreover, $X \longmapsto (\mathrm{Re}X, \mathrm{Im}X) \in v_{\mathbb{R}} \times v_{\mathbb{R}}$ is an $\mathbb{R}$-linear vector space isomorphism. For every $\mathbb{C}$-linear operator $M\colon \mathfrak{g} \longrightarrow \mathfrak{g}$ one has

$$M(\mathrm{Re}X + \mathrm{i}\mathrm{Im}X) = \mathrm{Re}M(\mathrm{Re}X) - \mathrm{Im}M(\mathrm{Im}X) + \mathrm{i}(\mathrm{Im}M(\mathrm{Re}X) + \mathrm{Re}M(\mathrm{Im}X))$$

and hence

$$\iota\colon M \longmapsto \begin{bmatrix} \mathrm{Re}M & -\mathrm{Im}M \\ \mathrm{Im}M & \mathrm{Re}M \end{bmatrix}$$

isomorphically lifts every $\mathbb{C}$-linear operator on $\mathfrak{g}$ to an $\mathbb{R}$-linear operator on $v_{\mathbb{R}} \times v_{\mathbb{R}}$. It is easily seen, that

$$\iota(MN) = \iota(M)\iota(N) \quad \text{and} \quad \mathrm{tr}\iota(M) = 2\mathrm{Re}\mathrm{tr}M.$$

For the Killing form on $\mathfrak{g}$ we have $\kappa(X,Y) = \mathrm{tr}(\mathrm{ad}_X \mathrm{ad}_Y)$, while

$$\kappa_{\mathfrak{g}^{\mathbb{R}}}(X,Y) = \mathrm{tr}(\iota(\mathrm{ad}_X \mathrm{ad}_Y)) = 2\mathrm{Re}\kappa(X,Y).$$

Cf. [45], Ch. I, Sec. 8. □

Example 1.22. For the classical complex semisimple Lie algebras, the Killing form alters in the following way by realification.

Lie algebra $\mathfrak{g}$	(complex) Killing form	(real) Killing form of $\mathfrak{g}^{\mathbb{R}}$
$\mathfrak{sl}(n,\mathbb{C})$	$2n\mathrm{tr}(XY)$	$4n\mathrm{Retr}(XY)$
$\mathfrak{so}(n,\mathbb{C})$	$(n-2)\mathrm{tr}(XY)$	$2(n-2)\mathrm{Retr}(XY)$
$\mathfrak{sp}(n,\mathbb{C})$	$2(n+1)\mathrm{tr}(XY)$	$8(n+1)\mathrm{Retr}(XY)$

Let $\mathfrak{g}_0$ be a real Lie algebra. Then forming the tensor product with $\mathbb{C}$ yields a complex Lie algebra

$$\mathfrak{g}_0^{\mathbb{C}} := \mathfrak{g}_0 \otimes_{\mathbb{R}} \mathbb{C} = \mathfrak{g}_0 \oplus i\mathfrak{g}_0.$$

It is called the *complexification of* $\mathfrak{g}_0$.

Definition 1.23. Let $\mathfrak{g}$ be a complex Lie algebra. Then any real Lie algebra $\mathfrak{g}_0$ with the property

$$\mathfrak{g} = \mathfrak{g}_0 \oplus i\mathfrak{g}_0$$

is called a *real form* of $\mathfrak{g}$. The Lie algebra $\mathfrak{g}_0$ is said to be a *compact real form*, if it is a compact Lie algebra.

Note that $\dim_{\mathbb{C}} \mathfrak{g} = \dim_{\mathbb{R}} \mathfrak{g}_0$. If $\mathfrak{g}_0$ is a real form of the complex Lie algebra $\mathfrak{g}$, then an $\mathbb{R}$-basis of $\mathfrak{g}_0$ is also a $\mathbb{C}$-basis of $\mathfrak{g}$. Consequently, if $X, Y \in \mathfrak{g}_0$, then the matrix of $\mathrm{ad}_X \circ \mathrm{ad}_Y$ is the same for $\mathfrak{g}_0$ as it is for $\mathfrak{g}$ and the respective Killing forms are related by

$$\kappa_{\mathfrak{g}_0} = \kappa_{\mathfrak{g}}|_{\mathfrak{g}_0 \times \mathfrak{g}_0}. \tag{1.9}$$

Complexification preserves semisimplicity. Moreover, the following result holds.

Proposition 1.24. *Let $\mathfrak{g}$ be a complex Lie algebra with real form $\mathfrak{g}_0$. Then $\mathfrak{g}$ is semisimple if and only if $\mathfrak{g}_0$ is semisimple.*

Proof. [45], Ch. I, Cor. 1.53. □

Theorem 1.25. *If $\mathfrak{g}$ is a complex semisimple Lie algebra, then it has a compact real form. Moreover, if $\mathfrak{u}_0$ and $\mathfrak{u}_0'$ are two compact real forms of $\mathfrak{g}$ then they are conjugate, i.e. there exists an inner automorphism $\varphi \in \mathrm{Int}(\mathfrak{g})$ such that*

$$\mathfrak{u}_0' = \varphi \mathfrak{u}_0.$$

Proof. [45], Ch. VI, Thm. 6.11 and Cor. 6.20. □

Example 1.26. The compact real forms of the classical complex semisimple Lie algebras $\mathfrak{sl}(n,\mathbb{C})$, $\mathfrak{so}(n,\mathbb{C})$, and $\mathfrak{sp}(n,\mathbb{C})$ are given by $\mathfrak{su}(n), \mathfrak{so}(n,\mathbb{R})$, and $\mathfrak{sp}(n)$, respectively. All other compact real forms are obtained by conjugation with a fixed element in the corresponding group. For example, all compact real forms of $\mathfrak{sl}(n,\mathbb{C})$ are given by $\{sUs^{-1} \mid U \in \mathfrak{su}(n)\}$ with $s \in SL(n,\mathbb{C}) := \{g \in \mathbb{C}^{n\times n} \mid \det(g) = 1\}$.

The proof of Theorem 1.25 uses results on the so called Cartan involution and its resulting decomposition of a semisimple Lie algebra which will be the subject of the remainder of this chapter.

1.3 Cartan Decomposition of Semisimple Lie Algebras

The following definition applies only to real semisimple Lie algebras $\mathfrak{g}$. In the case where $\mathfrak{g}$ is complex we consider therefore its realification $\mathfrak{g}^{\mathbb{R}}$.

Definition 1.27. Let $\mathfrak{g}_0$ be a real semisimple Lie algebra. An involution $\theta \in \mathrm{Aut}(\mathfrak{g}_0)$, i.e. $\theta^2 = 1$, such that the symmetric bilinear form

$$B_\theta(X,Y) := -\kappa(X,\theta Y) \tag{1.10}$$

is positive definite is called a *Cartan involution*.

To see that the bilinear form (1.10) is symmetric, we use the invariance of the Killing form under automorphisms of $\mathfrak{g}$ and obtain

$$\begin{aligned} B_\theta(X,Y) &= -\kappa(X,\theta Y) = -\kappa(\theta X, \theta^2 Y) \\ &= -\kappa(Y,\theta X) = B_\theta(Y,X). \end{aligned}$$

Example 1.28. (a) By Example 1.4, the Killing form on $\mathfrak{sl}(n,\mathbb{C})$ is given by $2n\mathrm{tr}(XY)$. According to Proposition 1.21, the Killing form translates into

$$\kappa(X,Y) = 4n\mathrm{Re}\mathrm{tr}(XY)$$

if we regard $\mathfrak{sl}(n,\mathbb{C})$ as a real vector space. It is easily seen, that the map $\theta(X) := -X^*$ is an involution that respects brackets:

$$\theta[X,Y] = -[X,Y]^* = -[Y^*,X^*] = [-X^*,-Y^*] = [\theta(X),\theta(Y)].$$

Now since $\mathrm{Re}\mathrm{tr}(XY^*) = -\frac{1}{4n}\kappa(X,\theta Y)$ is an inner product on $\mathfrak{sl}(n,\mathbb{C})^{\mathbb{R}}$, the map θ is indeed a Cartan involution.

(b) Similar, for $n \geq 3$, the Killing form on $\mathfrak{so}(n, \mathbb{R})$ is, up to a factor dependent on n, equal to $\operatorname{tr}(XY)$. Since $\operatorname{tr}(XY^\top) = -\operatorname{tr}(XY)$ yields an inner product on $\mathfrak{so}(n, \mathbb{R})$, it follows that a Cartan involution is given by the identity mapping $\theta(X) = X$.

Cartan involutions for the complex case are given in the following proposition.

Proposition 1.29. *Let $\mathfrak{g}$ be a complex semisimple Lie algebra, $\mathfrak{u}_0$ a compact real form of $\mathfrak{g}$ and τ the conjugation of $\mathfrak{g}$ with respect to $\mathfrak{u}_0$, i.e.*

$$\tau \colon X + \mathrm{i}Y \longmapsto X - \mathrm{i}Y, \quad X, Y \in \mathfrak{u}_0.$$

Then τ is a Cartan involution of $\mathfrak{g}^{\mathbb{R}}$.

Proof. Let $Z = X + \mathrm{i}Y \in \mathfrak{g}$ with $X, Y \in \mathfrak{u}_0$. Using Eq. (1.9) we obtain

$$\begin{aligned} \kappa_{\mathfrak{g}}(Z, \tau Z) &= \kappa_{\mathfrak{g}}(X, X) + \kappa_{\mathfrak{g}}(Y, Y) \\ &= \kappa_{\mathfrak{u}_0}(X, X) + \kappa_{\mathfrak{u}_0}(Y, Y) < 0 \ \text{ if } Z \neq 0, \end{aligned}$$

because $\mathfrak{u}_0$ is compact and the Killing form of compact Lie algebras is negative definite, cf. Theorem 1.15. Proposition 1.21 yields

$$B_\tau(Z_1, Z_2) = -\kappa_{\mathfrak{g}^{\mathbb{R}}}(Z_1, \tau Z_2) = -2\mathrm{Re}\kappa_{\mathfrak{g}}(Z_1, Z_2)$$

is positive definite on $\mathfrak{g}^{\mathbb{R}}$, cf. [45], Ch. VI, Prop. 6.14. □

Theorem 1.30. *If $\mathfrak{g}_0$ is a real semisimple Lie algebra, then $\mathfrak{g}_0$ has a Cartan involution. Any two Cartan involutions of $\mathfrak{g}_0$ are conjugate via* $\operatorname{Int}(\mathfrak{g}_0)$.

Proof. [45], Ch. VI, Cor. 6.18 & 6.19. □

Example 1.31. We saw in Example 1.28 (a), that $\theta(X) := -X^*$ is a Cartan involution on the Lie algebra $\mathfrak{sl}(n, \mathbb{C})$. Now let $\mathrm{Ad}_g \in \operatorname{Int}(\mathfrak{g})$ with $g \in SL(n, \mathbb{C})$. Define $\widetilde{\theta} = \mathrm{Ad}_g \theta \mathrm{Ad}_g^{-1}$. Then

$$\widetilde{\theta} X = g(-(g^{-1}Xg)^*)g^{-1} = -gg^*X^*(gg^*)^{-1}.$$

On the other hand, noting that $d := gg^*$ is positive definite and by Example 1.4 we obtain

$$-\kappa(X, \widetilde{\theta}Y) = -4n\mathrm{Retr}(X\widetilde{\theta}Y) = 4n\mathrm{Retr}(XdY^*d^{-1}),$$

which indeed is an inner product. This shows in fact, that all Cartan involutions on $\mathfrak{sl}(n, \mathbb{C})$ are given by $\theta_d X = -dX^*d^{-1}$ with d positive definite.

It follows immediately by Proposition 1.29 and Theorem 1.30 that if $\mathfrak{g}$ is a complex semisimple Lie algebra, then the only Cartan involutions of $\mathfrak{g}^{\mathbb{R}}$ are the conjugations with respect to the compact real forms. By means of the Cartan involution, every semisimple Lie algebra decomposes into two vector spaces.

Definition 1.32 (Cartan Decomposition)**.** Let θ be a Cartan involution of a real semisimple Lie algebra $\mathfrak{g}_0$. Let

$$\begin{aligned}&\mathfrak{k}_0 \text{ denote the } +1\text{-eigenspace of } \theta \text{ and}\\ &\mathfrak{p}_0 \text{ denote the } -1\text{-eigenspace of } \theta.\end{aligned}$$

Then

$$\mathfrak{g}_0 = \mathfrak{k}_0 \oplus \mathfrak{p}_0 \tag{1.11}$$

is called a *Cartan decomposition* of $\mathfrak{g}_0$.

Theorem 1.33. *Let $\mathfrak{g}_0$ be a real semisimple Lie algebra and $\mathfrak{g}_0 = \mathfrak{k}_0 \oplus \mathfrak{p}_0$ a Cartan decomposition of $\mathfrak{g}_0$. Then*

(a) $[\mathfrak{k}_0, \mathfrak{k}_0] \subseteq \mathfrak{k}_0$, $[\mathfrak{k}_0, \mathfrak{p}_0] \subseteq \mathfrak{p}_0$ and $[\mathfrak{p}_0, \mathfrak{p}_0] \subseteq \mathfrak{k}_0$.

(b) The Cartan decomposition is orthogonal with respect to the Killing form and the positive definite form B_θ.

(c) The Killing form is negative definite on $\mathfrak{k}_0$ and positive definite on $\mathfrak{p}_0$.

(d) The Lie subalgebra $\mathfrak{k}_0$ is maximal compactly imbedded in $\mathfrak{g}_0$.

Proof. (a) Let $X, Y \in \mathfrak{k}_0$, then $\theta[X,Y] = [\theta X, \theta Y] = [X,Y]$. The other bracket relations are proved analogously. (b) Let $X \in \mathfrak{k}_0$ and $Y \in \mathfrak{p}_0$. Then $\mathrm{ad}_X \mathrm{ad}_Y \mathfrak{k}_0 \subseteq \mathfrak{p}_0$ and $\mathrm{ad}_X \mathrm{ad}_Y \mathfrak{p}_0 \subseteq \mathfrak{k}_0$. Therefore $\mathrm{tr}(\mathrm{ad}_X \mathrm{ad}_Y) = 0$. Since $\theta Y = -Y$, also $B_\theta(X,Y) = 0$. (c) Let $X \in \mathfrak{k}$. The positive definiteness of B_θ yields

$$0 < B_\theta(X,X) = -\kappa(X, \theta X) = -\kappa(X,X).$$

(d) Cf. [31], Ch. III, Prop. 7.4. $\square$

Note that in (a), semisimplicity of $\mathfrak{g}$ implies that $[\mathfrak{k}_0, \mathfrak{p}_0] = \mathfrak{p}_0$. In fact, by Proposition 1.18, we have

$$\mathfrak{g} = [\mathfrak{k}_0 \oplus \mathfrak{p}_0, \mathfrak{k}_0 \oplus \mathfrak{p}_0] \subseteq [\mathfrak{k}_0, \mathfrak{k}_0] + [\mathfrak{p}_0, \mathfrak{p}_0] + [\mathfrak{k}_0, \mathfrak{p}_0].$$

Therefore

$$[\mathfrak{k}_0, \mathfrak{k}_0] + [\mathfrak{p}_0, \mathfrak{p}_0] = \mathfrak{k} \quad \text{and} \quad [\mathfrak{k}_0, \mathfrak{p}_0] = \mathfrak{p}_0.$$

Example 1.34. (a) On compact, semisimple Lie algebras, the Killing form is negative definite by Theorem 1.15. The Cartan decomposition and hence the Cartan involution are therefore trivial.

(b) Corresponding to the Cartan involution $\theta X = -X^\top$, the Cartan decomposition of $\mathfrak{sl}(n,\mathbb{R})$ is given by

$$\mathfrak{sl}(n,\mathbb{R}) = \mathfrak{so}(n,\mathbb{R}) \oplus \{P \in \mathbb{R}^{n\times n} \mid P^\top = P, \mathrm{tr}P = 0\}.$$

Note that for $n = 2$ we have the strict inclusion $[\mathfrak{so}(2,\mathbb{R}), \mathfrak{so}(2,\mathbb{R})] = 0 \subsetneq \mathfrak{so}(2,\mathbb{R})$.

(c) Corresponding to the Cartan involution $\theta X = -X^*$, the Cartan decomposition of $\mathfrak{sl}(n, \mathbb{C})$ is given by

$$\mathfrak{sl}(n, \mathbb{C}) = \mathfrak{su}(n) \oplus \{P \in \mathbb{C}^{n \times n} \mid P^* = P, \mathrm{tr} P = 0\}.$$

(d) Corresponding to the Cartan involution $\theta X = -X^*$, the Cartan decomposition of $\mathfrak{su}(p, q)$ is given by

$$\mathfrak{su}(p, q) = \left\{ \begin{bmatrix} S_1 & 0 \\ 0 & S_2 \end{bmatrix} \right\} \oplus \left\{ \begin{bmatrix} 0 & B \\ B^* & 0 \end{bmatrix} \right\},$$

where $S_1^* = -S_1 \in \mathbb{C}^{p \times p}$, $S_2^* = -S_2 \in \mathbb{C}^{q \times q}$, $\mathrm{tr}(S_1) + \mathrm{tr}(S_2) = 0$ and $B \in \mathbb{C}^{p \times q}$.

As a kind of converse to Theorem 1.33 a decomposition $\mathfrak{g}_0 = \mathfrak{k}_0 \oplus \mathfrak{p}_0$ of a semisimple real Lie algebra $\mathfrak{g}_0$ such that the Killing form is negative definite on $\mathfrak{k}_0$ and positive definite on $\mathfrak{p}_0$ and such that the bracket relations $[\mathfrak{k}_0, \mathfrak{k}_0] \subseteq \mathfrak{k}_0$, $[\mathfrak{k}_0, \mathfrak{p}_0] \subseteq \mathfrak{p}_0$ and $[\mathfrak{p}_0, \mathfrak{p}_0] \subseteq \mathfrak{k}_0$ hold, determines a Cartan involution θ by defining

$$\theta := \begin{cases} +1 & \text{on } \mathfrak{k}_0 \\ -1 & \text{on } \mathfrak{p}_0. \end{cases}$$

Corollary 1.35 (Weyl unitary trick). *If $\mathfrak{g}_0 = \mathfrak{k}_0 \oplus \mathfrak{p}_0$ is a Cartan decomposition of a semisimple Lie algebra $\mathfrak{g}_0$, then $\mathfrak{k}_0 \oplus \mathrm{i}\mathfrak{p}_0$ is a compact real form of $(\mathfrak{g}_0)^{\mathbb{C}}$*

Proof. We have $(\mathfrak{k}_0 \oplus \mathrm{i}\mathfrak{p}_0)^{\mathbb{C}} = (\mathfrak{k}_0 \oplus \mathrm{i}\mathfrak{p}_0) \oplus \mathrm{i}(\mathfrak{k}_0 \oplus \mathrm{i}\mathfrak{p}_0) = (\mathfrak{g}_0)^{\mathbb{C}}$. The Killing form is negative definite on $\mathfrak{k}_0 \oplus \mathrm{i}\mathfrak{p}_0$, and therefore $\mathfrak{k}_0 \oplus \mathrm{i}\mathfrak{p}_0$ is a compact Lie algebra. □

Lemma 1.36. *Let $\mathfrak{g}_0$ be a real semisimple Lie algebra with Cartan involution θ and define adjoint $(\cdot)^\dagger$ relative to the inner product B_θ (1.10) of $\mathfrak{g}_0$. Then*

$$(\mathrm{ad}_X)^\dagger = -\mathrm{ad}_{\theta X} \quad \textit{for all } X \in \mathfrak{g}_0.$$

Proof. A simple computation yields

$$\begin{aligned} B_\theta(\mathrm{ad}_{\theta X} Y, Z) &= -\kappa(\mathrm{ad}_{\theta X} Y, \theta Z) = \kappa(Y, [\theta X, \theta Z]) \\ &= \kappa(Y, \theta[X, Z]) = -B_\theta(Y, \mathrm{ad}_X Z) \\ &= -B_\theta((\mathrm{ad}_X)^\dagger Y, Z) \quad \text{for all} \quad X, Y, Z \in \mathfrak{g}_0. \end{aligned}$$

□

Theorem 1.37. *Let $\mathfrak{g}_0$ be a real semisimple Lie algebra with Cartan involution θ. Then $\mathfrak{g}_0$ is isomorphic to a Lie algebra of real matrices that is closed under transposition and the isomorphism can be chosen such that θ is carried to negative transpose.*

Proof. Let θ be a Cartan involution of $\mathfrak{g}_0$ and denote by B_θ the inner product (1.10). Since $\mathfrak{g}_0$ is semisimple, $\mathfrak{g}_0 \cong \mathrm{ad}_{\mathfrak{g}_0}$ by Proposition 1.18. Now choose an orthonormal basis $\mathcal{B} = \{b_1, ..., b_N\}$ of $\mathfrak{g}_0$ with respect to B_θ. Then

$$\{M \in \mathbb{R}^{N \times N} \mid M \text{ is matrix representation of } \mathrm{ad}_X \in \mathrm{ad}_{\mathfrak{g}_0} \text{ with respect to } \mathcal{B}\}$$

is the required Lie algebra. It is closed under transpose, because of Lemma 1.36 and the fact that $\mathfrak{g}_0$ is closed under θ, cf. [45], Ch. VI, Prop. 6.28. □

1.4 Cartan-Like Decompositions

We saw in Example 1.34 (a), that the Cartan involution is trivial on compact semisimple Lie algebras. Nevertheless, every compact semisimple Lie algebra decomposes in an analogous way such that the algorithms developed in Chapter 2 can easily be adopted.

Definition 1.38. Let $\mathfrak{u}_0 = \mathfrak{k}_0 \oplus \mathfrak{p}_0$ be a compact semisimple Lie algebra and let the vector spaces $\mathfrak{k}_0$ and $\mathfrak{p}_0$ fulfill the relations

$$[\mathfrak{k}_0, \mathfrak{k}_0] \subset \mathfrak{k}_0, \quad [\mathfrak{k}_0, \mathfrak{p}_0] \subset \mathfrak{p}_0, \quad \text{and} \quad [\mathfrak{p}_0, \mathfrak{p}_0] \subset \mathfrak{k}_0. \tag{1.12}$$

Then the decomposition $\mathfrak{u}_0 = \mathfrak{k}_0 \oplus \mathfrak{p}_0$ is called a *Cartan-like decomposition* of $\mathfrak{u}_0$.

It is conceivable to define Cartan-like decompositions for arbitrary, not necessarily compact, semisimple Lie algebras. However, we restrict ourselves to the above definition because Proposition 1.40 then yields a one-to-one correspondence of Cartan-like and Cartan decompositions and the theory in the subsequent chapters can easily be adopted. This is not the case if we accept Cartan-like decompositions for noncompact Lie algebras.

Example 1.39. For a non trivial example consider the compact Lie algebra $\mathfrak{so}(4,\mathbb{R})$ and let $I_{2,2} := \begin{bmatrix} I_2 & \\ & -I_2 \end{bmatrix}$ and $I_{3,1} := \begin{bmatrix} I_3 & \\ & -I_1 \end{bmatrix}$. The involutions $\theta_1 := I_{2,2}(\cdot)I_{2,2}$ and $\theta_2 = I_{3,1}(\cdot)I_{3,1}$ yield the Cartan-like decompositions

$$\mathfrak{so}(4,\mathbb{R}) = \left\{ \begin{bmatrix} S_1 & 0 \\ 0 & S_2 \end{bmatrix} \mid S_1, S_2 \in \mathfrak{so}(2,\mathbb{R}) \right\} \oplus \left\{ \begin{bmatrix} 0 & B \\ -B^\top & 0 \end{bmatrix} \mid B \in \mathbb{R}^{2\times 2} \right\},$$

$$\mathfrak{so}(4,\mathbb{R}) = \left\{ \begin{bmatrix} S_3 & 0 \\ 0 & 0 \end{bmatrix} \mid S_3 \in \mathfrak{so}(3,\mathbb{R}) \right\} \oplus \left\{ \begin{bmatrix} 0 & b \\ -b^\top & 0 \end{bmatrix} \mid b \in \mathbb{R}^{3} \right\},$$

respectively.

The above example shows that two Cartan-like decompositions and their corresponding involutions of a compact Lie algebra need not be isomorphic in the sense of Theorem 1.30. Nevertheless, the following proposition shows the correspondence of Cartan-like decompositions of compact semisimple Lie algebras and the Cartan decompositions of real semisimple Lie algebras. It is in some sense the converse result to Corollary 1.35.

Proposition 1.40. *Let $\mathfrak{u}_0$ be a compact and semisimple Lie algebra und let $\mathfrak{u}_0 = \mathfrak{k}_0 \oplus \mathfrak{p}_0$ be a Cartan-like decomposition. Then $\mathfrak{g}_0 := \mathfrak{k}_0 \oplus i\mathfrak{p}_0$ is a semisimple real Lie algebra with Cartan decomposition $\mathfrak{g}_0 = \mathfrak{k}_0 \oplus i\mathfrak{p}_0$.*

Proof. Both, $\mathfrak{u}_0$ and $\mathfrak{g}_0$ are real forms of the complex Lie algebra $\mathfrak{u} := \mathfrak{u}_0 \oplus \mathrm{i}\mathfrak{u}_0$, defined as the complexification of $\mathfrak{u}_0$. Hence, as $\mathfrak{u}_0$ is semisimple, so are $\mathfrak{u}$ and $\mathfrak{g}_0$ by Proposition 1.24. Now let $X \in \mathfrak{p}_0$. By the negative definiteness of the Killing form on $\mathfrak{u}_0$ we have $0 > \kappa(X, X) = -\kappa(\mathrm{i}X, \mathrm{i}X)$ and hence $\kappa > 0$ on $\mathrm{i}\mathfrak{p}$. Moreover, $[\mathfrak{k}, \mathfrak{k}] \subset \mathfrak{k}, [\mathrm{i}\mathfrak{p}, \mathfrak{k}] \subset \mathrm{i}\mathfrak{p}$, and $[\mathrm{i}\mathfrak{p}, \mathrm{i}\mathfrak{p}] \subset \mathfrak{k}$. Therefore $\mathfrak{g}_0 = \mathfrak{k}_0 \oplus \mathrm{i}\mathfrak{p}_0$ is indeed a Cartan decomposition. □

According to Proposition 1.40, in abuse of language, Cartan-like decompositions of a compact Lie algebra $\mathfrak{u}_0$ are sometimes called Cartan decompositions of $\mathfrak{u}_0$.

1.5 The Structure of Semisimple Lie Algebras

We shall see that an understanding of the structure of semisimple Lie algebras will be the crucial point to develop structure preserving Jacobi-type methods for normal form problems of matrices. In this section, the so-called *restricted-root space decomposition* of a semisimple Lie algebra is explained and examples are given that exhibit the correspondence between the root space decomposition and the off-diagonal entries of symmetric matrices.

Let $\mathfrak{g}$ be a semisimple Lie algebra, θ a Cartan involution and $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ the corresponding Cartan decomposition. By finite dimensionality of $\mathfrak{p}$, there exists a maximal abelian subspace $\mathfrak{a} \subset \mathfrak{p}$. We shall see later on, that any two maximal abelian subspaces $\mathfrak{a}, \mathfrak{a}' \subset \mathfrak{p}$ are conjugate in the sense that there exists a $\varphi \in \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ such that $\mathfrak{a} = \varphi\mathfrak{a}'$. In particular, for every $X \in \mathfrak{p}$ there exists a $\varphi \in \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ such that $\varphi X \in \mathfrak{a}$. This generalizes the well-known fact that any real symmetric matrix is orthogonal diagonalizable and any Hermitian matrix is unitarily diagonalizable.

Let $H \in \mathfrak{a}$. Then $\theta H = -H$, since $H \in \mathfrak{p}$. By Lemma 1.36 we have $(\mathrm{ad}_H)^\dagger = -\mathrm{ad}_{\theta H} = \mathrm{ad}_H$. Moreover, if $H_1, H_2 \in \mathfrak{a}$ then

$$\mathrm{ad}_{H_1}\mathrm{ad}_{H_2}X = [H_1, [H_2, X]] = -[X, [H_1, H_2]] - [H_2, [X, H_1]] = \mathrm{ad}_{H_2}\mathrm{ad}_{H_1}X$$

for all $X \in \mathfrak{g}$. Hence the set $\{\mathrm{ad}_H \mid H \in \mathfrak{a}\}$ is a commuting family of self-adjoint transformations of $\mathfrak{g}$. Therefore $\mathfrak{g}$ decomposes orthogonally into the simultaneous eigenspaces of these commuting operators. Let $\mathcal{X}$ be a (simultaneous) eigenspace and denote by $\lambda(H)$ the corresponding eigenvalue of ad_H. Then $\lambda(H) \in \mathbb{R}$ since ad_H is self-adjoint. For $s, t \in \mathbb{R}$ and $X \in \mathcal{X}$ it follows by the identity

$$\lambda(tH_1 + sH_2)X = \mathrm{ad}_{tH_1+sH_2}X = t\mathrm{ad}_{H_1}X + s\mathrm{ad}_{H_2}X = (t\lambda(H_1) + s\lambda(H_2))X$$

that $\lambda\colon \mathfrak{a} \longrightarrow \mathbb{R}$ is linear. This motivates the following definition. We denote by $\mathfrak{a}^* := \{\nu\colon \mathfrak{a} \to \mathbb{R} \mid \nu \text{ is linear}\}$ the dual space of $\mathfrak{a}$.

Definition 1.41. Let $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ be a Cartan decomposition of a semisimple Lie algebra $\mathfrak{g}$ and let $\mathfrak{a} \subset \mathfrak{p}$ be a maximal abelian subalgebra. For $\lambda \in \mathfrak{a}^*$, let

$$\mathfrak{g}_\lambda := \{X \in \mathfrak{g} \mid \mathrm{ad}_H X = \lambda(H)X \text{ for all } H \in \mathfrak{a}\}. \tag{1.13}$$

If $\lambda \neq 0$ and $\mathfrak{g}_\lambda \neq 0$, the vector space $\mathfrak{g}_\lambda$ is called *restricted-root space* and λ is called *restricted root*. The set of restricted roots is denoted by Σ. A vector $X \in \mathfrak{g}_\lambda$ is called a *restricted-root vector*.

We summarize the above results.

Theorem 1.42 (Restricted-root space decomposition)**.** *Let $\mathfrak{g}$ be a semisimple Lie algebra with Cartan involution θ and corresponding Cartan decomposition $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$. Let $\mathfrak{a} \subset \mathfrak{p}$ be maximal abelian, denote by Σ the set of restricted roots and for $\lambda \in \Sigma$ let $\mathfrak{g}_\lambda$ denote the corresponding restricted-root space. Then $\mathfrak{g}$ decomposes orthogonally with respect to B_θ, cf. Eq. (1.10), into*

$$\mathfrak{g} = \mathfrak{g}_0 \oplus \sum_{\lambda \in \Sigma} \mathfrak{g}_\lambda \tag{1.14}$$

and $\mathfrak{g}_0 = \mathfrak{z}_{\mathfrak{k}}(\mathfrak{a}) \oplus \mathfrak{a}$, where $\mathfrak{z}_{\mathfrak{k}}(\mathfrak{a}) := \{X \in \mathfrak{k} \mid [X, H] = 0$ for all $H \in \mathfrak{a}\}$ denotes the centralizer of $\mathfrak{a}$ in $\mathfrak{k}$. Furthermore, for $\lambda, \mu \in \Sigma \cup \{0\}$, we have

(a) $[\mathfrak{g}_\lambda, \mathfrak{g}_\mu] \subseteq \begin{cases} \mathfrak{g}_{\lambda+\mu} & \text{if } \lambda + \mu \in \Sigma \cup \{0\} \\ 0 & \text{else.} \end{cases}$

(b) $\theta \mathfrak{g}_\lambda = \mathfrak{g}_{-\lambda}$, *and hence* $\lambda \in \Sigma \iff -\lambda \in \Sigma$.

Proof. The decomposition (1.14) of $\mathfrak{g}$ follows since the set $\{\mathrm{ad}_H \mid H \in \mathfrak{a}\}$ is a commuting family of self-adjoint transformations of $\mathfrak{g}$. To proof (a), we simply apply the Jacobi identity. Let $X \in \mathfrak{g}_\lambda, Y \in \mathfrak{g}_\mu$ and $H \in \mathfrak{a}$. Then

$$[H, [X, Y]] = -[Y, [H, X]] - [X, [Y, H]] = \lambda(H)[X, Y] + \mu(H)[X, Y] = (\lambda+\mu)(H)[X, Y].$$

Hence if $[X, Y] \neq 0$, then $\lambda + \mu$ has to be a restricted root. Since $\theta H = -H$, part (b) follows by

$$[H, \theta X] = \theta[\theta H, X] = -\theta[H, X] = -\lambda(H)\theta X.$$

Now let $X \in \mathfrak{z}_{\mathfrak{k}}(\mathfrak{a}) \oplus \mathfrak{a}$. Then $[H, X] = 0 \cdot X$ for all $H \in \mathfrak{a}$ and therefore $\mathfrak{g}_0 = \mathfrak{z}_{\mathfrak{k}}(\mathfrak{a}) \oplus \mathfrak{a}$. As $\mathfrak{a} \subset \mathfrak{p}$ and $\mathfrak{z}_{\mathfrak{k}}(\mathfrak{a}) \subset \mathfrak{k}$, this decomposition is orthogonal by the orthogonality of the Cartan decomposition. To show the orthogonality of (1.14) note that

$$\begin{aligned} \lambda(H) B_\theta(X, Y) &= -\kappa(\mathrm{ad}_H X, \theta Y) = \kappa(X, \mathrm{ad}_H \theta Y) = \kappa(X, \theta \mathrm{ad}_{\theta H} Y) \\ &= -\kappa(X, \theta \mathrm{ad}_H Y) = -\kappa(X, \mu(H)\theta Y) = \mu(H) B_\theta(X, Y), \end{aligned}$$

for all $H \in \mathfrak{a}$ and hence $B_\theta(X, Y) = 0$. Cf. [45], Ch. VI, Prop. 6.40. $\square$

According to Equation (1.14), we decompose an element $X \in \mathfrak{g}$ into

$$X = X_0 + \sum_{\lambda \in \Sigma} X_\lambda. \tag{1.15}$$

Remark 1.43. Similar to the above, it is possible to decompose complex semisimple Lie algebras into a maximal abelian subalgebra and the so called *root spaces* (in contrast to *restricted*-root spaces), cf. [45], Sec. 1, Ch. II. In this context, the term *Cartan subalgebra* arises. Note, that although a Cartan subalgebra is related to the maximal abelian subspace $\mathfrak{a} \subset \mathfrak{p}$, they do not coincide. A further investigation is not relevant for our purposes and we refer to the literature. The word *restricted* roots is due to the fact, that they are the nonzero restrictions to $\mathfrak{a}$ of the (ordinary) roots of the complexification $\mathfrak{g}^{\mathbb{C}}$. Cf. [45], Ch. VI, Prop. 6.47 and the subsequent remark.

Remark 1.44. Note that the restricted-root space decomposition can be equivalently computed via the eigenspaces of a single operator ad_H for a generic element $H \in \mathfrak{a}$ with pairwise distinct roots. Such elements are dense in $\mathfrak{a}$ since they are obtained by omitting from $\mathfrak{a}$ the finitely many hyperplanes $\{H \in \mathfrak{a} \mid \lambda_i(H) - \lambda_j(H) = 0\}$, $\lambda_i \neq \lambda_j$. Let $\mathcal{E}_\mu$ denote an eigenspace of ad_H with eigenvalue μ. By definition of the restricted-root spaces it must hold $\mathcal{E}_\mu = \bigoplus \mathfrak{g}_{\lambda_i}$ for some $\lambda_i \in \Sigma \cup \{0\}$. Assume now that $\mathcal{E}_\mu$ contains at least two restricted-root spaces, say $\mathfrak{g}_{\lambda_1}$ and $\mathfrak{g}_{\lambda_2}$. Then it follows $\mu = \lambda_1(H) = \lambda_2(H)$ which is a contradiction to the choice of H.

Restricted-root spaces are orthogonal with respect to the Killing form as long as the corresponding restricted roots do not add up to zero.

Corollary 1.45. *Let $\lambda, \mu \in \Sigma \cup \{0\}$ and $\lambda \neq -\mu$. Then $\kappa(\mathfrak{g}_\lambda, \mathfrak{g}_\mu) = 0$.*

Proof. Let $X \in \mathfrak{g}_\lambda, Y \in \mathfrak{g}_\mu$ and $H \in \mathfrak{a}$, then we have

$$\mu(H)\kappa(X,Y) = \kappa(\mathrm{ad}_H X, Y) = -\kappa(X, \mathrm{ad}_H Y) = -\lambda(H)\kappa(X,Y), \quad \text{for all } H \in \mathfrak{a},$$

implying that $\kappa(X,Y) = 0$. □

We see in particular, that $\kappa(X,Y) = 0$ if $X, Y \in \mathfrak{g}_\lambda$, $\lambda \neq 0$. The restricted-root spaces and the corresponding roots for the real simple Lie algebras are explicitly given in Chapter 4 and in the Appendix. For now we content ourselves with a very simple example.

Example 1.46. By Example 1.34 (b), the Cartan decomposition of $\mathfrak{sl}(3,\mathbb{R}) = \mathfrak{k} \oplus \mathfrak{p}$ is given by

$$\mathfrak{k} = \{\Omega \in \mathbb{R}^{3\times 3} \mid \Omega^\top = -\Omega\}, \quad \mathfrak{p} = \{X \in \mathbb{R}^{3\times 3} \mid \mathrm{tr} X = 0, X^\top = X\}.$$

A maximal abelian subalgebra in $\mathfrak{p}$ is, for example, the Lie algebra of diagonal matrices

$$\mathfrak{a} = \{H \in \mathfrak{p} \mid H \text{ is diagonal}\}.$$

We have $\mathfrak{z}_{\mathfrak{k}}(\mathfrak{a}) = 0$ and therefore by Theorem 1.42, the only subspace where $\{\mathrm{ad}_H \mid H \in \mathfrak{a}\}$ acts trivial is $\mathfrak{g}_0 = \mathfrak{a}$. It is easily seen, that

$$\mathbb{R}\begin{bmatrix}0&1&0\\0&0&0\\0&0&0\end{bmatrix}, \mathbb{R}\begin{bmatrix}0&0&1\\0&0&0\\0&0&0\end{bmatrix}, \mathbb{R}\begin{bmatrix}0&0&0\\0&0&1\\0&0&0\end{bmatrix}, \mathbb{R}\begin{bmatrix}0&0&0\\1&0&0\\0&0&0\end{bmatrix}, \mathbb{R}\begin{bmatrix}0&0&0\\0&0&0\\1&0&0\end{bmatrix}, \mathbb{R}\begin{bmatrix}0&0&0\\0&0&0\\0&1&0\end{bmatrix},$$

are (one-dimensional) invariant subspaces of $\{\mathrm{ad}_H \mid H \in \mathfrak{a}\}$. Parameterizing

$$\mathfrak{a} = \left\{ \begin{bmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_3 \end{bmatrix} \;\Big|\; a_1, a_2, a_3 \in \mathbb{R}, \sum_{i=1}^{3} a_i = 0 \right\}.$$

yields the corresponding roots

$$\lambda_{12}(H) = a_1 - a_2;\ \lambda_{13}(H) = a_1 - a_3;\ \lambda_{23}(H) = a_2 - a_3;$$

$$\lambda_{21}(H) = a_2 - a_1;\ \lambda_{31}(H) = a_3 - a_1;\ \lambda_{32}(H) = a_3 - a_2.$$

respectively.

Lemma 1.47. *The set*

$$\mathfrak{a}_{\mathrm{reg}} := \{H \in \mathfrak{a} \mid \lambda(H) \neq 0 \text{ for all } \lambda \in \Sigma\} \tag{1.16}$$

is open and dense in $\mathfrak{a}$. *Moreover,* $\mathfrak{z}_{\mathfrak{g}}(H) = \mathfrak{g}_0$ *if* $H \in \mathfrak{a}_{\mathrm{reg}}$.

Proof. We have $\mathfrak{a}_{\mathrm{reg}} = \mathfrak{a} \setminus \Big(\bigcup_{\lambda \in \Sigma} \lambda^{-1}(0) \Big)$. There are only finitely many restricted roots and therefore only finitely many hyperplanes $\lambda^{-1}(0)$. Thus the first part of the lemma follows. For the second part, let $X \in \mathfrak{z}_{\mathfrak{g}}(H)$ and decompose X according to (1.15). Then

$$0 = [H, X] = [H, X_0 + \sum_{\lambda \in \Sigma} X_\lambda] = \sum_{\lambda \in \Sigma} \lambda(H) X_\lambda$$

and hence $\lambda(H)X_\lambda = 0$ for all $\lambda \in \Sigma$. Since by assumption $\lambda(H) \neq 0$, we must have $X_\lambda = 0$. Cf. [45], Ch. VI., Lemma 6.50. □

Theorem 1.48. *If* $\mathfrak{a}, \mathfrak{a}' \subset \mathfrak{p}$ *are maximal abelian, then there exists a* $\varphi_0 \in \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ *such that* $\varphi_0 \mathfrak{a}' = \mathfrak{a}$. *Consequently, for every* $X \in \mathfrak{p}$ *there exists a* $\varphi_0 \in \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ *such that* $\varphi_0 X \in \mathfrak{a}$ *and* $\mathfrak{p} = \bigcup_{\varphi \in \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})} \mathfrak{a}$.

Proof. Let $H_r \in \mathfrak{a}$ and $H_r' \in \mathfrak{a}'$ be regular elements. Choose by compactness of $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$, cf. Theorem 1.33(d), $\varphi_0 \in \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ such that

$$h\colon \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k}) \longrightarrow \mathbb{R}, \quad h(\varphi) = \kappa(\varphi H_r', H_r)$$

is minimized. Therefore, the derivation at φ_0 vanishes, i.e.

$$Dh(\varphi_0)\mathrm{ad}_\Omega \varphi_0 = \kappa(\mathrm{ad}_\Omega \varphi_0 H_r', H_r) = \kappa(\Omega, [\varphi_0 H_r', H_r]) = 0 \quad \text{for all } \Omega \in \mathfrak{k}.$$

Since $[\varphi_0 H_r', H_r] \in \mathfrak{k}$ and κ is negative definite on $\mathfrak{k}$, it follows $[\varphi_0 H_r', H_r] = 0$ and by Lemma 1.47 $\varphi_0 H_r' \in \mathfrak{z}_{\mathfrak{g}}(H_r) \cap \mathfrak{p} = \mathfrak{g}_0 \cap \mathfrak{p} = \mathfrak{a}$. Since $\mathfrak{a}$ is abelian and $\varphi_0 H_r' \in \mathfrak{a}$, we have

$$\mathfrak{a} \subseteq \mathfrak{z}_{\mathfrak{p}}(\varphi_0 H_r') = \varphi_0 \mathfrak{z}_{\mathfrak{p}}(H_r') = \varphi_0 \mathfrak{a}'.$$

Equality must hold because $\mathfrak{a}$ is maximal abelian in $\mathfrak{p}$. Now for every $X \in \mathfrak{p}$ extend $\mathbb{R}X$ to a maximal abelian subspace $\mathfrak{a}' \subset \mathfrak{p}$. Then $\varphi_0 \mathfrak{a}' = \mathfrak{a}$ as above and the assertion follows. Cf. [45], Ch. VI, Thm. 6.51. □

An element $X \in \mathfrak{p}$ is called *regular*, if it is $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$-conjugate to a regular element.
By Theorem 1.48 it follows that if G is a Lie group with semisimple Lie algebra $\mathfrak{g}$ and $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ is its Cartan decomposition and K denotes the maximal compact analytic subgroup $K \subset G$ corresponding to $\mathfrak{k}$, then for any $X \in \mathfrak{p}$ there exists $k_0 \in K$ such that $\mathrm{Ad}_{k_0} X \in \mathfrak{a}$. Therefore, Theorem 1.48 generalizes the well-known fact that every Hermitian matrix is unitarily similar to a real diagonal matrix.
Let λ be a restricted root and denote by $H_\lambda \in \mathfrak{a}$ its dual, i.e.

$$\lambda(H) = \kappa(H_\lambda, H) \quad \text{for all } H \in \mathfrak{a}.$$

Lemma 1.49. *Let $X_\lambda \in \mathfrak{g}_\lambda \setminus \{0\}$ and $H_\lambda \in \mathfrak{a}$ as above. Then*

$$[X_\lambda, \theta X_\lambda] = \kappa(X_\lambda, \theta X_\lambda) H_\lambda \quad \textit{and} \quad \kappa(X_\lambda, \theta X_\lambda) < 0.$$

Proof. By Theorem 1.42 we have $[X_\lambda, \theta X_\lambda] \in \mathfrak{g}_0$ and $\theta[X_\lambda, \theta X_\lambda] = -[X_\lambda, \theta X_\lambda]$, and hence $[X_\lambda, \theta X_\lambda] \in \mathfrak{g}_0 \cap \mathfrak{p} = \mathfrak{a}$. For $H \in \mathfrak{a}$ we compute

$$\begin{aligned} \kappa([X_\lambda, \theta X_\lambda], H) &= \kappa(X_\lambda, [\theta X_\lambda, H]) = \lambda(H)\kappa(X_\lambda, \theta X_\lambda) \\ &= \kappa(H_\lambda, H)\kappa(X_\lambda, \theta X_\lambda) = \kappa(\kappa(X_\lambda, \theta X_\lambda)H_\lambda, H). \end{aligned} \tag{1.17}$$

The first statement now follows by the nondegeneracy of κ on $\mathfrak{a}$. For the second statement, note that $\kappa(X_\lambda, \theta X_\lambda) = -B_\theta(X_\lambda, X_\lambda) < 0$, since B_θ is an inner product. Cf. [45], Ch. VI, Prop. 6.52. □

Let $E_\lambda \in \mathfrak{g}_\lambda$ be normalized such that

$$T_\lambda := [E_\lambda, \theta E_\lambda] = -\frac{2}{|\lambda|^2} H_\lambda. \tag{1.18}$$

Furthermore define

$$\Omega_\lambda := E_\lambda + \theta E_\lambda \quad \text{and} \quad \overline{\Omega}_\lambda := E_\lambda - \theta E_\lambda. \tag{1.19}$$

Note that

$$\begin{gathered} \Omega_\lambda \in \mathfrak{k}, \quad \overline{\Omega}_\lambda \in \mathfrak{p}, \quad \kappa(\overline{\Omega}_\lambda, \overline{\Omega}_\lambda) = \frac{2}{|\lambda|^2}, \\ \kappa(\Omega_\lambda, \Omega_\lambda) = -\frac{2}{|\lambda|^2}, \quad \lambda(T_\lambda) = -2. \end{gathered} \tag{1.20}$$

The normalization (1.18) of E_λ is only unique up to multiplication with ± 1.

Example 1.50. Consider the case where $\mathfrak{g} := \mathfrak{sl}(n, \mathbb{R})$ and the Cartan involution yields the decomposition into skew symmetric and symmetric matrices with the diagonal as the maximal abelian subalgebra. Denote by X_{ij} the (i, j)-entry of the matrix X. Then the roots are given by

$$\lambda_{ij}(H) = H_{ii} - H_{jj}, \quad i \neq j.$$

Recall that the Killing form κ is given by $\kappa(X,Y) = 2n\mathrm{tr}(XY)$. Therefore,

$$H_{\lambda_{ij}} = \frac{1}{2n}(e_ie_i^\top - e_je_j^\top)$$

where e_i denotes the i-th standard basis vector and

$$\lambda_{ij}(H_{\lambda_{ij}}) = |\lambda_{ij}|^2 = \frac{1}{n}.$$

Hence $T_{\lambda_{ij}} = -e_ie_i^\top + e_je_j^\top$ and $E_{\lambda_{ij}} = \pm e_ie_j^\top$. Depending on the choice of $E_{\lambda_{ij}}$, either $\Omega_{\lambda_{ij}} = e_ie_j^\top - e_je_i^\top$ or $\Omega_{\lambda_{ij}} = e_je_i^\top - e_ie_j^\top$.

Define

$$\begin{aligned} \mathfrak{k}_\lambda &:= \{X + \theta X \mid X \in \mathfrak{g}_\lambda\} \subset \mathfrak{k}, \\ \mathfrak{p}_\lambda &:= \{X - \theta X \mid X \in \mathfrak{g}_\lambda\} \subset \mathfrak{p}. \end{aligned} \tag{1.21}$$

Then for every element $Y_\lambda = X_\lambda + \theta X_\lambda \in \mathfrak{k}_\lambda$ the corresponding element in $\mathfrak{p}_\lambda$ is denoted by $\overline{Y}_\lambda := X_\lambda - \theta X_\lambda$.
The following lemma will prove to be useful.

Lemma 1.51. *Let $H \in \mathfrak{a}$ and $Y_\lambda \in \mathfrak{k}_\lambda$. Then*

$$[H, \overline{Y}_\lambda] = \lambda(H)Y_\lambda, \quad [H, Y_\lambda] = \lambda(H)\overline{Y}_\lambda \quad \textit{and} \quad [Y_\lambda, \overline{Y}_\lambda] \in \mathfrak{a}.$$

Proof. By definition $Y_\lambda = X_\lambda + \theta X_\lambda$ and $\overline{Y}_\lambda = X_\lambda - \theta X_\lambda$ with $X_\lambda \in \mathfrak{g}_\lambda$ and hence, by Theorem 1.42, $\theta X_\lambda \in \mathfrak{g}_{-\lambda}$. Therefore,

$$\begin{aligned} [H, \overline{Y}_\lambda] &= [H, X_\lambda] - [H, \theta X_\lambda] = \lambda(H)X_\lambda - (-\lambda(H))\theta X_\lambda = \lambda(H)Y_\lambda, \\ [H, Y_\lambda] &= [H, X_\lambda] + [H, \theta X_\lambda] = \lambda(H)X_\lambda - \lambda(H)\theta X_\lambda = \lambda(H)\overline{Y}_\lambda. \end{aligned}$$

The last assertion follows by the Jacobi-identity. Namely let $H \in \mathfrak{a}$ be a regular element. Then

$$[H, [Y_\lambda, \overline{Y}_\lambda]] = -[\overline{Y}_\lambda, [H, Y_\lambda]] + [Y_\lambda, [H, \overline{Y}_\lambda]] = -\lambda(H)[\overline{Y}_\lambda, \overline{Y}_\lambda] + \lambda(H)[Y_\lambda, Y_\lambda] = 0.$$

Now, by Theorem 1.33, $[Y_\lambda, \overline{Y}_\lambda] \in \mathfrak{p}$ and hence, since it commutes with H, $[Y_\lambda, \overline{Y}_\lambda] \in \mathfrak{a}$. □

For given $X_1, ..., X_k \in \mathfrak{g}$, denote by $\langle X_1, ..., X_k\rangle_{LA}$ the subalgebra of $\mathfrak{g}$ generated by the X_i's, i.e.

$$\langle X_1, ..., X_k\rangle_{LA} := \bigcap\{\mathfrak{h} \subset \mathfrak{g} \mid \mathfrak{h} \text{ is subalgebra and } X_1, ..., X_k \in \mathfrak{h}\}.$$

Proposition 1.52. *The Lie algebra $\langle E_\lambda, \theta E_\lambda, T_\lambda\rangle_{LA}$ is isomorphic to $\mathfrak{sl}(2,\mathbb{R})$. More precisely, the following relations hold.*

(a) $[E_\lambda, \theta E_\lambda] = T_\lambda, \quad [E_\lambda, T_\lambda] = 2E_\lambda$ *and* $[\theta E_\lambda, T_\lambda] = -2\theta E_\lambda$.

(b) $[\Omega_\lambda, \overline{\Omega}_\lambda] = -2T_\lambda, \quad [\Omega_\lambda, T_\lambda] = 2\overline{\Omega}_\lambda$ *and* $[\overline{\Omega}_\lambda, T_\lambda] = 2\Omega_\lambda$.

Proof. The first commutator relation holds by definition of T_λ. Furthermore, keeping in mind that $\lambda(T_\lambda) = -2$, one has $[E_\lambda, T_\lambda] = -\lambda(T_\lambda)E_\lambda = 2E_\lambda$. The remaining commutator relations are easily computed analogously. Then a Lie algebra isomorphism is given via

$$E_\lambda \longmapsto \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \qquad -\theta E_\lambda \longmapsto \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \quad \text{and hence} \quad -T_\lambda \longmapsto \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{1.22}$$

Cf. [45], Ch. VI, Prop. 6.52. □

Since $\mathfrak{k}_\lambda$ and $\mathfrak{p}_\lambda$ involve $\mathfrak{g}_\lambda$ as well as $\mathfrak{g}_{-\lambda}$, we introduce a notion of positivity for the roots in order to avoid notational ambiguity.

Definition 1.53. An element $l \in \mathfrak{a}^* \setminus \{0\}$ is called *positive*, if

(a) exactly one of l and $-l$ is positive,

(b) the sum of positive elements is positive, and any positive multiple of a positive element is positive.

We denote the set of positive restricted roots by Σ^+.

Theorem 1.42 assures that $\lambda \in \Sigma$ if and only if $-\lambda \in \Sigma$ and that Σ is finite. Thus a set of positive roots can be obtained for example by a hyperplane through the origin in $\mathfrak{a}^*$ that does not contain any root and defining all roots on one side to be positive. Hence partitioning Σ into $\Sigma^+ \cup \Sigma^-$, where $\Sigma^- := \Sigma \setminus \Sigma^+$ is the set of *negative roots*, is not unique. Positivity allows us to specify decomposition (1.15) for elements in $\mathfrak{k}$ and $\mathfrak{p}$. To do so, let $\mathfrak{g}_\lambda$ be a restricted-root space and let $\{E_\lambda^{(i)}, i = 1, ..., \dim \mathfrak{g}_\lambda\}$ be an orthogonal basis of $\mathfrak{g}_\lambda$, each element normalized according to Eq. (1.18). Furthermore, define analogously to Eq. (1.19)

$$\Omega_\lambda^{(i)} := E_\lambda^{(i)} + \theta E_\lambda^{(i)}, \qquad \overline{\Omega}_\lambda^{(i)} := E_\lambda^{(i)} - \theta E_\lambda^{(i)}.$$

Denote by

$$\mathrm{p}\colon \mathfrak{g} \longrightarrow \mathfrak{g}_0 \tag{1.23}$$

the orthogonal projection onto $\mathfrak{g}_0 = \mathfrak{a} \oplus \mathfrak{z}_{\mathfrak{k}}(\mathfrak{a})$.

Lemma 1.54. *Let $r := \dim \mathfrak{g}_\lambda$. The set*

$$\mathcal{B}_{\mathfrak{k}} := \bigcup_{\lambda \in \Sigma^+} \{\Omega_\lambda^{(i)}, i = 1, ..., r\} \tag{1.24}$$

is an orthogonal basis of $\mathfrak{z}_{\mathfrak{k}}(\mathfrak{a})^\perp \cap \mathfrak{k}$ and

$$\mathcal{B}_{\mathfrak{p}} := \bigcup_{\lambda \in \Sigma^+} \{\overline{\Omega}_\lambda^{(i)}, i = 1, ..., r\} \tag{1.25}$$

is an orthogonal basis of $\mathfrak{a}^\perp \cap \mathfrak{p}$. In particular, every $X \in \mathfrak{p}$ and $Y \in \mathfrak{k}$ decomposes orthogonally into

$$X = X_0 + \sum_{\lambda \in \Sigma^+} \sum_{i=1}^{r} c_\lambda^{(i)} \overline{\Omega}_\lambda^{(i)}, \qquad Y = Y_0 + \sum_{\lambda \in \Sigma^+} \sum_{i=1}^{r} d_\lambda^{(i)} \Omega_\lambda^{(i)}, \tag{1.26}$$

where $X_0 := \mathrm{p}(X) \in \mathfrak{a}$, $Y_0 := \mathrm{p}(Y) \in \mathfrak{z}_{\mathfrak{k}}(\mathfrak{a})$ and

$$c_\lambda^{(i)} := \frac{\kappa(X, \overline{\Omega}_\lambda^{(i)})}{\kappa(\overline{\Omega}_\lambda^{(i)}, \overline{\Omega}_\lambda^{(i)})}, \qquad d_\lambda^{(i)} := \frac{\kappa(Y, \Omega_\lambda^{(i)})}{\kappa(\Omega_\lambda^{(i)}, \Omega_\lambda^{(i)})}.$$

Proof. The lemma is a direct consequence of Eq. (1.15). □

This lemma yields immediately the following dimension formula.

Corollary 1.55. *We have the dimension formula*

$$\dim \mathfrak{k} - \dim \mathfrak{z}_{\mathfrak{k}}(\mathfrak{a}) = \dim \mathfrak{p} - \dim \mathfrak{a}. \tag{1.27}$$

1.6 Weyl Chambers and the Weyl Group

Consider the set of regular elements $\mathfrak{a}_{\mathrm{reg}}$ defined in Eq. (1.16). By construction, it consists of finitely many connected components, the so called *Weyl chambers*. These are open, convex cones of $\mathfrak{a}$. Denote by

$$C^+ := \{H \in \mathfrak{a} \mid \lambda(H) > 0 \text{ for all } \lambda \in \Sigma^+\}$$

the Weyl chamber consisting of all elements with positive roots greater than zero. C^+ is called the *fundamental Weyl chamber* and we write $C^- := -C^+$ for the Weyl chamber that lies across from C^+.

Example 1.56. Consider the root-space decomposition of $\mathfrak{sl}(3, \mathbb{R})$ as discussed in Example 1.46. Here, $\mathfrak{a}$ is two dimensional and the hyperplanes $\lambda^{-1}(0)$ are straight lines, partitioning $\mathfrak{a}$ into six Weyl chambers, cf. Fig. 1.1 and 1.2 subsequently in this section.

The following proposition shows that reflections on the hyperplanes $\lambda^{-1}(0)$ with $\lambda \in \Sigma$ can be realized by some automorphisms in $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$.

Proposition 1.57. *Let $\Omega_\lambda, \overline{\Omega}_\lambda$ and T_λ be defined as in Eqs. (1.18) and (1.19) respectively. Then*

$$\exp(\mathrm{ad}_{\frac{\pi}{2}\Omega_\lambda})(\mathfrak{a}) \subset \mathfrak{a}$$

and $\exp(\mathrm{ad}_{\frac{\pi}{2}\Omega_\lambda})$ acts as the reflection on the hyperplane $\lambda^{-1}(0)$.

Proof. To show that $\exp(\mathrm{ad}_{\frac{\pi}{2}\Omega_\lambda})$ leaves the hyperplane $\lambda^{-1}(0)$ pointwise fixed, let $H_0 \in \lambda^{-1}(0)$, i.e. $\lambda(H_0) = 0$. Then

$$\exp(\mathrm{ad}_{\frac{\pi}{2}\Omega_\lambda})H_0 = \sum_{n=0}^{\infty} \frac{\mathrm{ad}^n_{\frac{\pi}{2}\Omega_\lambda} H_0}{n!} = H_0,$$

because $[\Omega_\lambda, H_0] = -\lambda(H_0)\overline{\Omega}_\lambda = 0$. Now let $H \in \mathfrak{a}$ be arbitrary. Since $\lambda^{-1}(0)$ is a hyperplane with codimension one and since $T_\lambda \notin \lambda^{-1}(0)$, we can write $H = H_0 + tT_\lambda$ for some $t \in \mathbb{R}$ and $H_0 \in \lambda^{-1}(0)$. Moreover, $\exp(\mathrm{ad}_{\frac{\pi}{2}\Omega_\lambda})H = H_0 + t\exp(\mathrm{ad}_{\frac{\pi}{2}\Omega_\lambda})T_\lambda$ and therefore it remains to show that $\exp(\mathrm{ad}_{\frac{\pi}{2}\Omega_\lambda})$ changes the sign of T_λ. To do this, note that by Proposition 1.52 we have

$$\mathrm{ad}_{\frac{\pi}{2}\Omega_\lambda} T_\lambda = \pi\overline{\Omega}_\lambda \quad \text{and} \quad \mathrm{ad}^2_{\frac{\pi}{2}\Omega_\lambda} T_\lambda = -\pi^2 T_\lambda.$$

Therefore

$$\begin{aligned}
\exp(\mathrm{ad}_{\frac{\pi}{2}\Omega_\lambda})T_\lambda &= \sum_{n=0}^{\infty} \frac{\mathrm{ad}^n_{\frac{\pi}{2}\Omega_\lambda} T_\lambda}{n!} \\
&= \sum_{n=0}^{\infty} \frac{\mathrm{ad}^{2n}_{\frac{\pi}{2}\Omega_\lambda} T_\lambda}{(2n)!} + \sum_{n=0}^{\infty} \frac{\mathrm{ad}^{2n+1}_{\frac{\pi}{2}\Omega_\lambda} T_\lambda}{(2n+1)!} \\
&= \sum_{n=0}^{\infty} \frac{(-\pi^2)^n T_\lambda}{(2n)!} + \sum_{n=0}^{\infty} \frac{(-\pi^2)^n \pi\overline{\Omega}_\lambda}{(2n+1)!} \\
&= (\cos\pi)T_\lambda + (\sin\pi)\overline{\Omega}_\lambda = -T_\lambda,
\end{aligned}$$

and hence the assertion follows, cf. [45], Ch. VI, Prop. 6.52 (c). □

Definition 1.58. Denote the *centralizer* and the *normalizer* of $\mathfrak{a}$ in $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ by

$$Z(\mathfrak{a}) := \{\varphi \in \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k}) \mid \varphi H = H \text{ for all } H \in \mathfrak{a}\},$$

$$N(\mathfrak{a}) := \{\varphi \in \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k}) \mid \varphi H \in \mathfrak{a} \text{ for all } H \in \mathfrak{a}\},$$

respectively. Then the factor group $W = N(\mathfrak{a})/Z(\mathfrak{a})$ is called the *Weyl group* of $\mathfrak{g}$.

Proposition 1.59. *The Weyl group is finite.*

Proof. Both $N(\mathfrak{a})$ and $Z(\mathfrak{a})$ are closed subgroups of $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ and hence compact. Obviously, $\mathfrak{z}_{\mathfrak{k}}(\mathfrak{a})$ is the Lie algebra of $Z(\mathfrak{a})$ and contained in the Lie algebra $\mathfrak{n}$ of $N(\mathfrak{a})$. Now let Y in $\mathfrak{n}$ be given. Then $\mathrm{Ad}_{\exp(tY)}H \in \mathfrak{a}$ for all t and $H \in \mathfrak{a}$ and hence $[Y, H] \in \mathfrak{a}$ for all $H \in \mathfrak{a}$. But then $[Y, H] = 0$ since

$$\kappa([Y, H], [Y, H]) = -\kappa([H, [H, Y]], Y) = 0$$

and κ is positive definite on $\mathfrak{p}$. Therefore we conclude that $Y \in \mathfrak{z}_{\mathfrak{k}}(\mathfrak{a})$. Thus $N(\mathfrak{a})$ and $Z(\mathfrak{a})$ have the same Lie algebra. It follows that W is 0-dimensional and compact, hence finite. Cf. [31], Ch. VII, Prop. 2.1. $\square$

Proposition 1.57 shows, that the reflections $\{\exp(\mathrm{ad}_{\frac{\pi}{2}\Omega_\lambda}) \mid \lambda \in \Sigma\}$ are contained in N. It can be deduced from the following theorem, that they generate the Weyl group.

Theorem 1.60. *(a) Each $s \in W$ permutes the Weyl chambers.*

(b) The Weyl group is simply transitive on the set of Weyl chambers, i.e. if C_1, C_2 are Weyl chambers and $H \in C_1$, then there exists a $s \in W$ such that $sH \in C_2$ and $s' \in W$ with $s'H \in C_1$ implies $s' = id$.

Proof. (a) Let $s \in W$ and $H \in \mathfrak{a}$ and let $E_\lambda \in \mathfrak{g}_\lambda$ be an arbitrary restricted-root vector. We have

$$[H, sE_\lambda] = s[s^{-1}H, E_\lambda] = \lambda(s^{-1}H)sE_\lambda.$$

Hence $\lambda \circ s^{-1}$ is again a restricted root (corresponding to the restricted-root space $s\mathfrak{g}_\lambda$) and therefore W permutes the Weyl chambers. (b) We first show that W is transitive. Denote by $||\cdot||$ the norm on $\mathfrak{a}$, induced by the inner product B_θ. Let H_1 and H_2 be in different Weyl chambers, i.e. there exists a restricted root λ such that the line segment $\overline{H_1H_2}$ intersects the hyperplane $\lambda^{-1}(0)$. If $\exp(\mathrm{ad}_{\frac{\pi}{2}\Omega_\lambda})$ is defined as in Proposition 1.57, i.e. the reflection on the hyperplane $\lambda^{-1}(0)$, then a simple geometric argument shows that

$$||H_1 - H_2|| > ||H_1 - \exp(\mathrm{ad}_{\frac{\pi}{2}\Omega_\lambda})H_2||.$$

Now W is finite and hence there exists $s_0 \in W$ such that $||H_1 - s_0H_2||$ is minimal, which implies with the foregoing consideration, that H_1 and s_0H_2 must lie in the same Weyl chamber. Now to the "simple"-part. Suppose that an element $s \in W$ maps the Weyl chamber C into itself. For $H_0 \in C$ define $H := H_0 + sH_0 + ... + s^{N-1}H_0$, where N is the order of s. Then $sH = H$ and by convexity of C we have $H \in C$. In particular, H is a regular element and its centralizer in $\mathfrak{g}$ is $\mathfrak{g}_0 = \mathfrak{a} \oplus \mathfrak{z}_{\mathfrak{k}}(\mathfrak{a})$. Let $\mathfrak{u} := \mathfrak{k} \oplus i\mathfrak{p}$ the compact real form of $\mathfrak{g}^{\mathbb{C}}$ and denote by $U := \mathrm{Int}(\mathfrak{u})$ the inner automorphisms of $\mathfrak{u}$. Then $\mathrm{Int}_{\mathfrak{g}^{\mathbb{C}}}(\mathfrak{k}) \subset U$ and in particular $s \in U$. Let

$$\gamma(t) := \exp(\mathrm{ad}_{tiH})$$

denote the one parameter subgroup in U that is generated by iH. Since U is compact, its closure $\overline{\gamma(t)}$ is a torus and we denote its Lie algebra by $\mathfrak{s}$. The element s is in the centralizer of this torus, denoted by $Z_U(\overline{\gamma(t)})$. It remains to show, cf. Definition 1.58, that every member of $Z_U(\overline{\gamma(t)})$ centralizes $\mathfrak{a}$. Since the centralizer of a torus in a compact connected Lie group is itself connected, cf. [45], Ch. IV., Cor. 4.51, it suffices to show that the Lie algebra $\mathfrak{z}_\mathfrak{u}(\mathfrak{s})$ centralizes $\mathfrak{a}$. Then

$$\mathfrak{z}_\mathfrak{u}(\mathfrak{s}) = \mathfrak{u} \cap \mathfrak{z}_{\mathfrak{g}^\mathbb{C}}(\mathfrak{s}) = \mathfrak{u} \cap \mathfrak{z}_{\mathfrak{g}^\mathbb{C}}(H) = \mathfrak{u} \cap (\mathfrak{g}_0 \oplus \mathrm{i}\mathfrak{g}_0) = \mathrm{i}\mathfrak{a} \oplus \mathfrak{z}_\mathfrak{k}(\mathfrak{a})$$

and therefore the assertion follows. Cf. [31], Ch. VII, Thm. 2.12. & [45], Ch. VI., Thm. 6.57. □

Proposition 1.61. *Let $\varphi \in \mathrm{Int}_\mathfrak{g}(\mathfrak{k})$, $H \in \mathfrak{a}$ and $\varphi H \in \mathfrak{a}$. Then there exists a Weyl group element $s \in W$ such that $\varphi H = sH$.*

Proof. Analogously as in the proof of the previous Theorem, let $\mathfrak{u} = \mathfrak{k} \oplus \mathrm{i}\mathfrak{p}$ be the compact real form of the complexification of $\mathfrak{g}$ and denote $U := \mathrm{Int}(\mathfrak{u})$ the inner automorphisms of $\mathfrak{u}$. Let $H \in \mathfrak{a}$ and $\varphi \in \mathrm{Int}_\mathfrak{g}(\mathfrak{k})$ such that $\varphi H \in \mathfrak{a}$. Then the centralizer of H in U is a closed subgroup of U, cf. [31], Ch. IV, Cor. 4.51. We denote it by $Z_U(H)$ and its Lie algebra by

$$\mathfrak{z}_\mathfrak{u}(H) = \mathfrak{z}_\mathfrak{u}(H) \cap \mathfrak{k} \oplus \mathfrak{z}_\mathfrak{u}(H) \cap \mathrm{i}\mathfrak{p}.$$

The subspaces $\mathrm{i}\mathfrak{a}$ and $\varphi^{-1}\mathrm{i}\mathfrak{a}$ are maximal abelian in $\mathfrak{z}_\mathfrak{u}(H) \cap \mathrm{i}\mathfrak{p}$. Let $H_r \in \mathfrak{a}$ be a regular element and fix some $X \in \mathfrak{z}_\mathfrak{u}(H) \cap \mathrm{i}\mathfrak{p}$. The function $\phi \mapsto \kappa(\mathrm{i}H_r, \phi X), \phi \in Z_U(H) \cap \mathrm{Int}_\mathfrak{g}(\mathfrak{k})$ is real and attains its minimum since the group $Z_U(H) \cap \mathrm{Int}_\mathfrak{g}(\mathfrak{k})$ is compact. Denote this minimum by z_0. Then

$$\frac{d}{dt}\kappa(\mathrm{i}H_r, \mathrm{Ad}_{\exp(tT)} z_0 X)\Big|_{t=0} = 0$$

for all $T \in \mathfrak{z}_\mathfrak{u}(H) \cap \mathfrak{k}$. It follows that

$$\kappa(\mathrm{i}H_r, [T, z_0X]) = -\kappa([\mathrm{i}H_r, z_0X], T) = 0$$

for each $T \in \mathfrak{z}_\mathfrak{u}(H) \cap \mathfrak{k}$. Since $[\mathrm{i}H_r, z_0X] \in \mathfrak{z}_\mathfrak{u}(H) \cap \mathfrak{k}$ we conclude that $[\mathrm{i}H_r, z_0X] = 0$, implying $z_0X \in \mathrm{i}\mathfrak{a}$. In particular, let $X = H_r'$ where $H_r' \in \varphi^{-1}\mathrm{i}\mathfrak{a}$ whose centralizer in $\mathrm{i}\mathfrak{p}$ is $\varphi^{-1}\mathrm{i}\mathfrak{a}$. Then it follows that $H_r' \in z_0^{-1}\mathrm{i}\mathfrak{a}$ and so

$$z_0^{-1}\mathrm{i}\mathfrak{a} = \varphi^{-1}\mathrm{i}\mathfrak{a}.$$

Consequently φz_0^{-1} is in the normalizer of $\mathfrak{a}$ and the restriction of φz_0^{-1} to $\mathfrak{a}$ is the desired element $s \in W$. Cf. [31], Ch. VII, Prop. 2.2. □

Proposition 1.61 implies that the $\mathrm{Int}_\mathfrak{g}(\mathfrak{k})$-*adjoint orbit* of $S \in \mathfrak{p}$

$$\mathcal{O}(S) = \{\varphi S \mid \varphi \in \mathrm{Int}_\mathfrak{g}(\mathfrak{k})\}, \tag{1.28}$$

intersects $\mathfrak{a}$ in only finitely many points. The following corollary specifies this result. It is preceded by a Lemma.

Lemma 1.62. *Let $H \in \mathfrak{a}$ be an irregular element. Denote the subgroup of W generated by the reflections on the hyperplanes $\{\lambda^{-1}(0) \mid \lambda(H) = 0\}$ by*

$$Z_W(H) := \langle \exp(\mathrm{ad}_{\frac{\pi}{2}\Omega_\lambda}) \mid \lambda(H) = 0 \rangle.$$

Then $Z_W(H)$ acts simply transitively on the set of adjacent Weyl chambers of H.

Proof. The proof adapts the idea of the proof of Theorem 1.60. Consider that H_1 and H_2 lie in two different Weyl chambers C_1 and C_2 adjacent to H. Then the line $\overline{H_1 H_2}$ intersects a hyperplane $\lambda^{-1}(0)$ with $\lambda(H) = 0$. Now the same argument as in Theorem 1.60 yields that there exists an $s_0 \in Z_W(H)$ such that H_1 and $s_0 H_2$ lie in the same Weyl chamber. The fact that $Z_W(H)$ acts *simply* transitive follows by Theorem 1.60. □

Corollary 1.63. *The Weyl orbit of an element $H \in \mathfrak{a}$ intersects any closure of a Weyl chamber in exactly one point, i.e. let C be a Weyl chamber, $\overline{C}$ its closure and $W \cdot H := \{sH \mid s \in W\}$ the Weyl orbit of H. Then*

$$\#(W \cdot H \cap \overline{C}) = 1.$$

Proof. Let $s \in W$ be a Weyl group element and let C_0 be a Weyl chamber. First note, that H is regular if and only if sH is regular, or more precisely, by Theorem 1.60, s permutes the roots, hence

$$\#\{\lambda \in \Sigma^+ \mid \lambda(H) = 0\} = \#\{\lambda \in \Sigma^+ \mid \lambda(sH) = 0\}. \tag{1.29}$$

We have to show that $H, sH \in \overline{C}$ implies $H = sH$, so assume that s is not the identity. The Weyl group is simply transitive on the Weyl chambers, hence if H is regular, i.e. $H \in C_0$, there is nothing more to show. Now assume that H is not regular and sH as well as H lie in $\overline{C_0}$. Since $s^{-1}(C_0)$ is adjacent to H and since also C_0 is adjacent to H it follows by Lemma 1.62 that $s^{-1} \in Z_W(H)$. But all elements in $Z_W(H)$ leave H fixed and it follows $sH = H$. □

The phenomenon of Corollary 1.63 is illustrated in Fig. 1.1 and 1.2. We also give the appropriate example.

Example 1.64. Consider again the root-space decomposition of $\mathfrak{sl}(3, \mathbb{R})$ as discussed in Example 1.46. Let $H_1, H_2 \in \mathfrak{a}$ be given as

$$H_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad \text{and} \quad H_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix}.$$

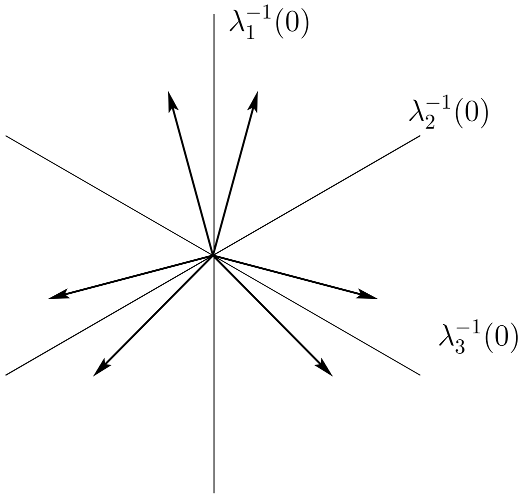

Figure 1.1: Weyl orbit of a regular element.

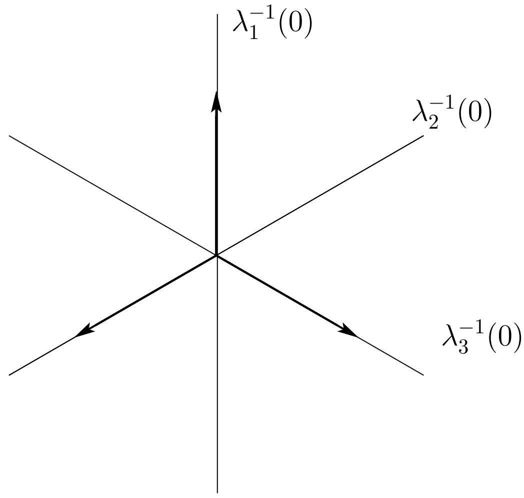

Figure 1.2: Weyl orbit of an irregular element.

H_1 is regular whereas H_2 is not. The order of the Weyl group is $\#W = 6$. All diagonal matrices that are similar to H_1, H_2 respectively, are given by

$$W \cdot H_1 = \left\{ \pm H_1, \pm \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \pm \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \right\}$$

$$W \cdot H_2 = \left\{ H_2, \begin{bmatrix} 1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} -2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \right\}.$$

There is an interesting connection between the Weyl orbit of an element $H \in \mathfrak{a}$ and its adjoint orbit, firstly derived by B. Kostant in 1973. His theorem is a generalization of the well-known theorem of Horn (1951) [37] and the later theorems of Sing [59] and Thompson [63] (1976,1977).

Theorem 1.65 (Kostant's convexity theorem). *Let $H \in \mathfrak{a}$ and let $\mathcal{O}(H) = \{\varphi H \mid \varphi \in \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})\}$ be the adjoint orbit of H. Furthermore denote by $\overline{W \cdot H}$ the convex hull of the Weyl orbit of H and let $\mathrm{p}\colon \mathfrak{p} \longrightarrow \mathfrak{a}$ be the orthogonal projection. Then*

$$\overline{W \cdot H} = \mathrm{p}(\mathcal{O}(H)).$$

Proof. Cf. [47]. □

Chapter 2

Generalized Jacobi Method: Coordinate Descent on Manifolds

Jacobi-type algorithms and cyclic coordinate descent methods can be regarded as optimization tasks on smooth manifolds, see [32]. Suppose we want to compute a local minimum of a smooth cost function

$$f\colon M \longrightarrow \mathbb{R}$$

on an n-dimensional manifold M. Following [32], in [41] a Jacobi-type method on M is defined by specifying smooth maps

$$r_i\colon \mathbb{R} \times M \longrightarrow M \quad (t, X) \longmapsto r_i(t, X), \quad i = 1, ..., m$$

with $r_i(0, X) = X$. Restricting the function f to $r_1(\mathbb{R}, X) \subset M$ and searching for the minimum of the restricted function yields (if it exists!) an element $X_1 \in M$. If we repeat this procedure and restrict f to $r_2(\mathbb{R}, X_1)$, another element $X_2 \in M$ is obtained. Thus proceeding recursively, a sequence of elements $X_k \in M$ is obtained by defining the $(k+1)$-st element X_{k+1} as the result of minimizing f along $r_1(\mathbb{R}, X_k)$. We will be more precise in Section 2.2. The above formulation of a Jacobi-type method is sufficiently general to contain both the classical Jacobi method for diagonalizing a Hermitian matrix as well as the so-called cyclic coordinate descent method known from optimization theory. Under additional assumptions on the above algorithm local quadratic convergence has been shown in [41].

There are several possibilities to specify a Jacobi-type method. The problem with the above proposed method is that it is not well defined at every step. Moreover, for a local convergence analysis quite severe assumptions have to be made. Throughout this thesis, we therefore follow a slightly different approach and instead of searching for a global minimum of the restricted cost function we are searching for a *local* minimum. We shall see that this condition is sufficient for the algorithm to be well defined in a neighborhood of a nondegenerate minimum of f.

This chapter is organized as follows. After a short summary of basic facts and definitions from global analysis, an abstract construction of cyclic Jacobi-type algorithms is given and, following [41], the local convergence properties are investigated. Subsequently, we focus on a special situation where Jacobi-type methods on the compact orbit of a Lie algebra element $S \in \mathfrak{p}$

$$M = \mathcal{O}(S) = \{\varphi S \mid \varphi \in \operatorname{Int}_{\mathfrak{g}}(\mathfrak{k})\}, \quad S \in \mathfrak{p}, \tag{2.1}$$

under the group action of $\operatorname{Int}_{\mathfrak{g}}(\mathfrak{k})$ are considered. Here $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ is a Cartan decomposition of $\mathfrak{g}$. Note, that if G is a Lie group, $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ is the Cartan decomposition of its Lie algebra and $K \subset G$ is the analytic subgroup with Lie algebra $\mathfrak{k}$, then $\operatorname{Ad}(K) = \operatorname{Int}_{\mathfrak{g}}(\mathfrak{k})$, cf. Eq. (1.8). In the case where G is a group of matrices, Eq. (2.1) reads as

$$\mathcal{O}(S) = \{kSk^{-1} \mid k \in K\}.$$

We investigate the orbit of one parameter subgroups in $\mathcal{O}(S)$ and deduce sufficient conditions for a Jacobi algorithm to be globally well defined. Furthermore, a result on parallelizability for these algorithms is given under some assumptions on the underlying cost function.

2.1 Preliminaries on Differential Geometry

We recall some basic facts and definitions on global analysis, cf. [35]. Let M be a smooth manifold of dimension n. A *curve* through $x \in M$ is a smooth map

$$\gamma \colon I \longrightarrow M,$$

where $I \subset \mathbb{R}$ is an open interval containing 0 and $\gamma(0) = x$. Let U be a neighborhood of x and let $\phi \colon U \longrightarrow \mathbb{R}^n$ be a chart. Then

$$\phi \circ \gamma \colon I \longrightarrow \phi(U) \subset \mathbb{R}^n$$

is differentiable. Two curves γ_1 and γ_2 through $x \in M$ are said to be *equivalent*, if $(\phi \circ \gamma_1)'(0) = (\phi \circ \gamma_2)'(0)$ holds for some and therefore any chart ϕ. This defines an equivalence relation on the set of all curves through x. A *tangent vector* at x is then an equivalence class $\xi := [\gamma]$ of a curve γ and the *tangent space* T_xM is the set of all tangent vectors. It can be shown to be an n-dimensional real vector space.

Example 2.1. Let $\mathfrak{g}$ be a Lie algebra and let $\operatorname{Int}(\mathfrak{g})$ be the group of inner automorphisms of $\mathfrak{g}$. Let $\mathfrak{h} \subset \mathfrak{g}$ be a Lie subalgebra. Given an arbitrary Lie algebra element $S \in \mathfrak{g}$ and setting $H := \operatorname{Int}_{\mathfrak{g}}(\mathfrak{h})$, we denote by

$$\mathcal{O}_H(S) := \{\varphi S \mid \varphi \in H\}$$

the *adjoint orbit of* S. Recall that

$$\mathrm{Int}_{\mathfrak{g}}(\mathfrak{h}) = \text{ group generated by } \{\exp(\mathrm{ad}_X) \mid X \in \mathfrak{h}\}.$$

To avoid unnecessary notation we drop the subscription H if no confusion is expected. As a representative of an equivalence class $[\gamma]$ of curves through $Y \in \mathcal{O}(S)$ we choose $\gamma_X(t) = \exp(t\mathrm{ad}_X)Y$, $X \in \mathfrak{h}$. Thus the tangent space of $\mathcal{O}(S)$ at Y is given by

$$T_Y\mathcal{O}(S) = \{\gamma_X'(0) \mid X \in \mathfrak{h}\} = \{[X,Y] \mid X \in \mathfrak{h}\} = \mathrm{ad}_Y(\mathfrak{h}).$$

Now let M, N be manifolds and let

$$f\colon M \longrightarrow N$$

be smooth. If γ is a curve through $x \in M$, then $f \circ \gamma$ is a curve through $f(x) \in N$ and equivalent curves through x are mapped to equivalent curves through $f(x)$. We can therefore define the *derivative* of f at $x \in M$ as the linear map

$$Df(x)\colon T_xM \longrightarrow T_{f(x)}N$$

given by $Df(x)[\gamma] = [f \circ \gamma]$ for all tangent vectors $[\gamma] \in T_xM$. If $f\colon M \longrightarrow \mathbb{R}$ is a smooth real valued function, we identify $T_y(\mathbb{R}) = \mathbb{R}$ for all $y \in \mathbb{R}$ and define a *critical point* of f as a point $x \in M$ such that $Df(x)\xi = 0$ for all $\xi \in T_xM$. The *Hessian* of f at a critical point x then is the symmetric bilinear form

$$\begin{aligned} &\mathsf{H}_f(x)\colon T_xM \times T_xM \longrightarrow \mathbb{R}, \\ &(\xi_1,\xi_2) \longmapsto \tfrac{1}{2}\Big(\mathsf{H}_f(x)(\xi_1+\xi_2,\xi_1+\xi_2) - \mathsf{H}_f(x)(\xi_1,\xi_1) - \mathsf{H}_f(x)(\xi_2,\xi_2)\Big), \end{aligned} \tag{2.2}$$

where

$$\mathsf{H}_f(x)([\gamma],[\gamma]) := (f \circ \gamma)''(0). \tag{2.3}$$

It can be shown that this definition is independent of the choice of the representative γ only if $\gamma(0)$ is a critical point of f. The Hessian is therefore only well defined at critical points of f. A critical point is *nondegenerate*, if its Hessian is nondegenerate. If x is a local maximum (minimum), then $\mathsf{H}_f(x)$ is negativ (positive) semidefinite. On the other hand, if $\mathsf{H}_f(x)$ is negative (positive) definite, then x is a local maximum (minimum).

2.2 Abstract Jacobi-Type Algorithms

In this section a Jacobi-type algorithm on manifolds is presented that is well–defined on a neighborhood of a nondegenerate local minimum of the cost function. Furthermore, some necessary conditions for local quadratic convergence of the algorithm are proposed.

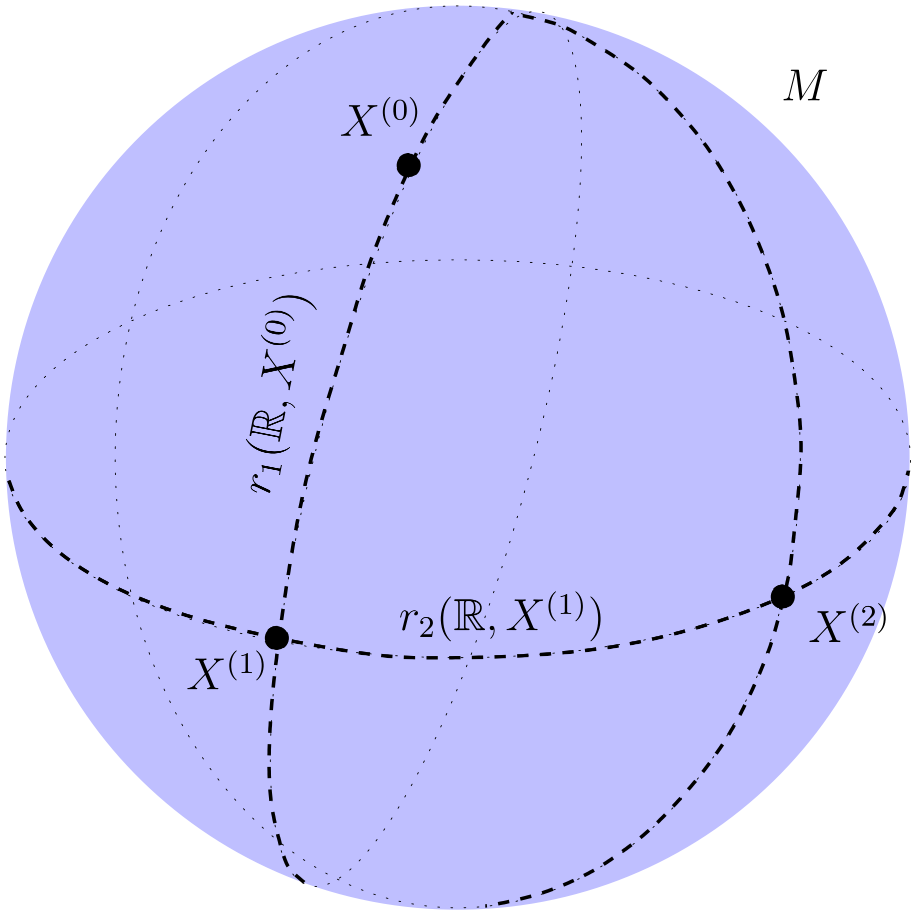

Figure 2.1: Illustration of the Jacobi sweep.

Let M denote a smooth manifold and let $f\colon M \longrightarrow \mathbb{R}$ be the considered cost function. For $i = 1, ..., m$ let

$$r_i\colon \mathbb{R} \times M \longrightarrow M \quad (t, X) \longmapsto r_i(t, X), \quad i = 1, ..., m,$$

be smooth with $r_i(0, X) = X$. Note, that $r_i{}'(0, X) := \frac{d}{dt}|_{t=0} r_i(t, X) \in T_X M$ for all $i = 1, ..., m$.

Starting from an arbitrary point $X \in M$, we search in a predetermined direction to find the nearest local minimum of the restricted cost function. This minimum is the initial point for a subsequent minimization along the next predetermined direction and so on, cf. Figure 2.1 for an illustration of the idea. Explicitly, the algorithm is given as follows.

Algorithm 2.2 (abstract Jacobi sweep)**.** Suppose that for all $i = 1, ..., m$ and $X \in M$ not both sets

$$\mathcal{T}^{(i)}(X)^+ := \{t \geq 0 \mid t \text{ is local minimum of } f \circ r_i(t, X)\},$$

$$\mathcal{T}^{(i)}(X)^- :\ = \{t < 0 \mid t \text{ is local minimum of } f \circ r_i(t, X)\}$$

are empty. Let $\mathcal{T}^{(i)}(X) := \mathcal{T}^{(i)}(X)^+ \cup \mathcal{T}^{(i)}(X)^-$ and define the *step size* as

$$t_*^{(i)}(X) := \begin{cases} \underset{\mathrm{t}\in\mathcal{T}^{(\mathrm{i})}(\mathrm{X})}{\arg\min} |\mathrm{t}| & \text{if } \inf \mathcal{T}^{(i)}(X)^+ \neq \sup \mathcal{T}^{(i)}(X)^- \\ \inf \mathcal{T}^{(i)}(X)^+ & \text{else,} \end{cases} \tag{2.4}$$

i.e. $t_*^{(i)}(X)$ is the element of $\mathcal{T}^{(i)}(X)$ with smallest absolute value and in the case of two possibilities, the positive one. A *sweep* is defined as a map

$$s\colon M \longrightarrow M$$

that is explicitly given as follows. Let $X_k^{(0)} := X$.

$$\begin{aligned}
X_k^{(1)} &:= r_1\left(t_*^{(1)}\left(X_k^{(0)}\right), X_k^{(0)}\right)\\
X_k^{(2)} &:= r_2\left(t_*^{(2)}\left(X_k^{(1)}\right), X_k^{(1)}\right)\\
X_k^{(3)} &:= r_3\left(t_*^{(3)}\left(X_k^{(2)}\right), X_k^{(2)}\right)\\
&\ \ \vdots\\
X_k^{(n)} &:= r_m\left(t_*^{(m)}\left(X_k^{(n-1)}\right), X_k^{(m-1)}\right)
\end{aligned}$$

and set now $s(X) := X_k^{(n)}$.

Note that although, by construction, $\mathcal{T}^{(i)}(X)$ consists only of local minima, this need not be true for $t_*^{(i)}(X)$. However, since f is smooth, $t_*^{(i)}(X)$ is always a critical point of $t \mapsto f \circ r_i(t, X)$.

Remark 2.3. Note that in complete analogy it is possible to formulate a sweep that searches for local maxima instead of minima. In fact, in a later chapter such an optimization task is implemented. Nevertheless, in the sequel we restrict the theory to the *minimization task*. It is straightforward to see that all subsequent results on Jacobi methods remain valid for *maximization tasks*, too.

The Jacobi algorithm consists of iterating sweeps.

Algorithm 2.4 (Jacobi Algorithm)**.**

1. Assume that we already have $X_0, X_1, ..., X_k \in M$ for some $k \in \mathbb{N}$.
2. Put $X_{k+1} :\ = s(X_k)$ and continue with the next sweep.

Clearly, Algorithm 2.2 is only well defined if the sets $\mathcal{T}^{(i)}(X)$ are not empty. This is ensured in a neighborhood of a nondegenerate minimum of f. To see this we apply the following lemma for a fixed integer i.

Lemma 2.5. *Let $Z \in M$ be a local minimum of the smooth cost function $f\colon M \longrightarrow \mathbb{R}$ and denote $\xi_i := r_i'(0, Z) \in T_Z M$. Suppose that the Hessian*

$$\mathsf{H}_f(Z)\colon T_Z M \times T_Z M \longrightarrow \mathbb{R}$$

satisfies $\mathsf{H}_f(Z)(\xi_i, \xi_i) \neq 0$. Then the step size selections $t_*^{(i)}(X)$ in Algorithm 2.2 are well defined and smooth in a neighborhood of Z. In this case

$$Dt_*^{(i)}(Z)(\,\cdot\,) = -\frac{\mathsf{H}_f(Z)(\xi_i,\,\cdot\,)}{\mathsf{H}_f(Z)(\xi_i, \xi_i)}.$$

Proof. The main argument is the Implicit Function Theorem, cf. [1], Theorem 2.5.7. Define the C^∞-function

$$\psi\colon \mathbb{R} \times M \longrightarrow \mathbb{R}, \quad \psi(t, X) := \frac{\mathrm{d}}{\mathrm{d}t}\left(f \circ r_i(t, X)\right).$$

By the chain rule we have

$$\psi(t, X) = Df\left(r_i(t, X)\right) r_i'(t, X). \tag{2.5}$$

Since Z is a local minimum of $f\left(r_i(t, X)\right)$ it follows that

$$\psi(0, Z) = 0.$$

Differentiating ψ with respect to the first variable yields

$$\frac{d}{dt}\psi(t, X)\Big|_{(0,Z)} = \frac{d^2}{dt^2} f \circ r_i(t, X)\Big|_{(0,Z)} = \mathsf{H}_f(Z)(\xi_i, \xi_i) \neq 0 \tag{2.6}$$

by assumption, where $\xi_i := r_i'(0, Z) \in T_Z M$. Now the Implicit Function Theorem yields that there exists a neighborhood U' of X and a unique smooth function

$$\varphi\colon U' \longrightarrow \mathbb{R}$$

such that $\psi(\varphi(X), X) = 0$ for all $X \in U'$. Since $\psi(t_*^{(i)}(Z), Z) = 0$, it follows from the uniqueness of φ that there exists a suitable neighborhood $U \subset U'$ of X such that

$$\varphi(X) = t_*^{(i)}(X) \quad \text{for all } X \in U.$$

Thus $t_*^{(i)}$ is well defined and smooth in a neighborhood of Z. Now let $\xi \in T_Z M$. Differentiating ψ with respect to the second variable yields together with Eq. (2.5)

$$\begin{aligned} D_X\psi(t, X)\Big|_{t=0, X=Z}\xi &= D_X\Big(\frac{d}{dt} f \circ r_i(t, X)\Big)\Big|_{t=0, X=Z}\xi \\ &= D_X\big(Df(X) r_i'(0, X)\big)\Big|_{X=Z}\xi \\ &= \mathsf{H}_f(Z)(\xi_i, \xi). \end{aligned}$$

Since $\psi(t_*^{(i)}(X), X) = 0$ for all $X \in U$,

$$0 = D\psi(t_*^{(i)}(X), X)\Big|_{X=Z}\xi = \frac{d}{dt}\psi(t_*^{(i)}(Z), Z) \circ Dt_*^{(i)}(Z)\xi + D_X\psi(t_*^{(i)}(Z), Z)\xi$$

and the assertion follows. □

Under some additional assumptions, Algorithm 2.4 is locally quadratic convergent to a local minimum of the cost function.

Definition 2.6. Let M be an n-dimensional manifold and let $s\colon M \longrightarrow M$. We say that the iterative algorithm defined by $X_{k+1} = s(X_k)$ is *locally quadratic convergent to* $Z \in M$ if Z is a fixed point of s and there exists a neighborhood U of Z, a chart $\phi\colon U \to \phi(U) \subset \mathbb{R}^n$ with $\phi(Z) := q$ and a constant $K \in \mathbb{R}$ such that

(a) $s(U) \subset U$,

(b) $||\phi \circ s \circ \phi^{-1}(p) - q|| \leq K||p - q||^2$ for all $p \in \phi(U)$.

Lemma 2.7. *Let ϕ and U be as above. For every neighborhood $W \subset U$ of Z there exists a neighborhood $W' \subset W$ such that $s(W') \subset W'$.*

Proof. By part (b) of the above definition,

$$||\phi \circ s(X) - \phi(Z)|| \leq K||\phi(X) - \phi(Z)||^2 \quad \text{for all } X \in U.$$

Now let $W \subset U$ be a neighborhood of Z and let

$$W' := \{X \in W \mid K||\phi(X) - \phi(Z)|| < 1\}.$$

Then W' is also a neighborhood of Z and $s(W') \subset W'$ because

$$K||\phi \circ s(X) - \phi(Z)|| \leq K^2||\phi(X) - \phi(Z)||^2 < 1$$

for all $X \in W'$. □

Definition 2.6 is independent of the chosen chart, because if $\psi\colon U' \to \psi(U')$ is another chart, by Lemma 2.7 we can assume without loss of generality that $U' \subset U$ and $s(U') \subset U'$. Assume furthermore without loss of generality that U' is compact. Then for all $X \in U'$ we have

$$\begin{aligned}||\psi \circ s(X) - \psi(Z)|| &= ||\psi \circ \phi^{-1} \circ \phi \circ s(X) - \psi \circ \phi^{-1} \circ \phi(Z)||\\ &\leq KK_1||\phi(X) - \phi(Z)||^2\\ &= KK_1||\phi \circ \psi^{-1} \circ \psi(X) - \phi \circ \psi^{-1} \circ \psi(Z)||\\ &\leq KK_1K_2||\psi(X) - \psi(Z)||^2,\end{aligned}$$

where

$$K_1 = \sup_{p \in \phi(U')} ||D(\psi \circ \phi^{-1})(p)||, \quad K_2 = \sup_{p' \in \psi(U')} ||D(\phi \circ \psi^{-1})(p')||.$$

If $M \subset E$ is a submanifold of a real N-dimensional normed vector space, then this definition of local quadratic convergence is compatible with any norm on E.

Lemma 2.8. *Let $M \subset E$ be an n-dimensional submanifold of a real N-dimensional vector space E and let $||\cdot||_E$ be any norm on E. The iterative algorithm induced by $s\colon M \longrightarrow M$ is locally quadratic convergent to $Z \in M$ if and only if there exists a neighborhood $U \subset E$ of Z and a constant L such that*

$$||s(X) - Z||_E \le L||X - Z||_E^2 \quad \textit{for all } X \in U \cap M.$$

Proof. We may assume without loss of generality that $E = \mathbb{R}^N$. Let $U \subset \mathbb{R}^N$ be a compact neighborhood of Z and let ϕ be a *submanifold chart*, i.e. $\phi\colon U \to \mathbb{R}^N, \phi(X) \in \mathbb{R}^n \times \{0\}$ for all $X \in U \cap M$.
"$\Rightarrow$": Assume that the algorithm is locally quadratic convergent. Then

$$\begin{aligned}
||s(X) - Z||_E &= ||\phi^{-1} \circ \phi \circ s(X) - \phi^{-1} \circ \phi(Z)||_E \\
&\le \underbrace{\sup_{y \in \phi(U)} ||D\phi^{-1}(y)||}_{:=K_1} \cdot ||\phi \circ s(X) - \phi(Z)|| \\
&\le K_1 K||\phi(X) - \phi(Z)||^2 \\
&\le K_1 K(\sup_{X \in U} ||D\phi(X)||)^2 ||X - Z||_E^2.
\end{aligned}$$

"$\Leftarrow$": The converse direction is shown analogously. Restrict a chart ϕ by Lemma 2.7 to a suitable compact neighborhood $U' \cap M$ of Z with $U' \subset U$. Then

$$\begin{aligned}
||\phi \circ s(X) - \phi(Z)|| &\le \underbrace{\sup_{x \in U \cap M} ||D\phi(x)||}_{:=K_1} \cdot ||s(X) - Z||_E \\
&\le K_1 L||X - Z||_E^2 \\
&\le K_1 L(\sup_{y \in \phi(U \cap M)} ||D\phi^{-1}(y)||)^2 ||\phi(X) - \phi(Z)||^2 \text{ for all } X \in U' \cap M.
\end{aligned}$$

□

Lemma 2.9. *Let $s\colon M \to M$ be twice continuously differentiable in a neighborhood $U \subset M$ of Z and let Z be a fixed point of the algorithm. Then the derivative of s at Z vanishes if and only if the algorithm induced by s is locally quadratic convergent to Z.*

Proof. Without loss of generality we may assume that $U \subset \mathbb{R}^n$.
"$\Leftarrow$": Assume that

$$||s(X) - Z|| = ||s(X) - s(Z)|| \le K||X - Z||^2.$$

By definition of the derivative

$$\frac{||s(X) - s(Z) - Ds(Z)(X - Z)||}{||X - Z||} = o(||X - Z||)$$

it follows immediately that $Ds(Z) = 0$.
"$\Rightarrow$": Now let $Ds(Z) = 0$. Then Taylor's Theorem yields

$$s(X) = s(Z) + Ds(Z)(X - Z) + \tfrac{1}{2}D^2 f(\xi)(X - Z, X - Z),$$

with $\xi \in \overline{XZ}$, the connecting line of X and Z. Now using that $s(Z) = Z$, it follows

$$||s(X) - Z|| \leq \sup_{X \in \overline{U}} ||D^2 s(X)|| \cdot ||X - Z||^2.$$

This also implies the existence of a neighborhood $U' \subset U$ with $s(U') \subset U'$. Thus the algorithm induced by s converges quadratically fast to Z. $\square$

Part (b) of the following theorem is according to a result in [41].

Theorem 2.10. *Let M be an n-dimensional manifold, let Z be a local minimum of the smooth cost function $f\colon M \longrightarrow \mathbb{R}$ with nondegenerate Hessian $\mathsf{H}_f(Z)$ and assume that $\xi_i := r_i'(0, Z) \neq 0$ for all $i = 1, ..., m$.*

(a) Then a sweep, cf. Algorithm 2.2, is well defined in a neighborhood of Z.

(b) If furthermore $\{\xi_i \mid i = 1, ..., m\}$ is a basis of $T_Z M$ (implying $m = n$) and $\mathsf{H}_f(Z)(\xi_i, \xi_j) = 0$ for $i \neq j$, then Algorithm 2.4 is locally quadratic convergent to Z.

Proof. We apply Lemma 2.5 to show that Algorithm 2.19 defines a smooth function on M in a neighborhood of Z. Moreover, under the assumption that $\mathsf{H}_f(\xi_i, \xi_j) = 0$ for $i \neq j$, its first derivative vanishes. Then Lemma 2.9 will complete the proof.
(a) One basic step within a sweep (cf. Algorithm 2.18) is given by

$$r_i\colon M \longrightarrow M, \quad r_i(X) = r_i(t_*^{(i)}(X), X)$$

and one sweep is the composition

$$s(X) = r_n \circ ... \circ r_1(X).$$

Since the Hessian at Z is positive definite, Lemma 2.5 implies that $t_*^{(i)}$ is well defined and smooth in a neighborhood of Z for all i, and hence so is r_i and therefore s, because Z is a fixed point of every r_i.
(b) Now let $\xi \in T_Z M$ denote an arbitrary tangent space element. The derivative of r_i in Z is given by

$$\begin{aligned} Dr_i(Z)\xi &= D\left(r_i(t_*^{(i)}(X), X)\Big|_{X=Z} \right) \xi \\ &= Dr_i(t, X)|_{(t,X)=(t_*^{(i)}(Z), Z)} \circ D(t_*^{(i)}(X), \mathrm{id})|_{X=Z}\xi \\ &= Dt_*^{(i)}(Z)\xi_i + \xi \end{aligned}$$

since $t_*^{(i)}(Z) = 0$. By Lemma 2.5 therefore

$$Dr_i(Z)\xi = \xi - \frac{\mathsf{H}_f(Z)(\xi_i, \xi)}{\mathsf{H}_f(Z)(\xi_i, \xi_i)}\xi_i.$$

Thus $Dr_i(Z)$ is a projection operator that – by orthogonality of the ξ_i's with respect to H_f – maps ξ into $(\mathbb{R}\xi_i)^\perp$. The composition of these projection operators is the zero map. Since Z is a fixed point of Algorithm 2.18, i.e. $r_i(Z) = Z$ for all $i = 1, ..., n$, we conclude

$$Ds(Z) = D(r_n \circ ... \circ r_1)(Z) = 0.$$

Consequently, Algorithm 2.18 defines a smooth sweep map on a neighborhood of Z with vanishing derivative. Therefore, Lemma 2.9 implies that the algorithm is locally quadratic convergent to Z. □

2.3 Jacobi-Type Algorithms on the $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$-Orbit

In order to specialize the abstract Jacobi-type method given in the last section to the case where M is the compact orbit $\mathcal{O}(S)$, cf. Eq. (2.1), we need to have a closer look at the one parameter subgroups in $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ and the corresponding orbits of an element $S \in \mathfrak{p}$. The obtained results will also prove useful in the subsequent chapter, where the generalization of the symmetric eigenvalue problem is considered.

2.3.1 One Parameter Subgroups in $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$

We first show that $\mathcal{O}(S)$ is a compact submanifold in $\mathfrak{p}$. By Theorem 1.33, $\mathfrak{k}$ is compactly imbedded in $\mathfrak{g}$ and therefore the group $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ is compact. Now for $S \in \mathfrak{p}$ consider the orbit

$$\mathcal{O}(S) := \{\varphi S \mid \varphi \in \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})\}.$$

Note, that if G is a matrix Lie group with Lie algebra $\mathfrak{g}$ and K is the analytic subgroup corresponding to $\mathfrak{k}$, then

$$\mathcal{O}(S) = \{kSk^{-1} \mid k \in K\}.$$

Proposition 2.11. *Let $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ be a Cartan decomposition of the semisimple Lie algebra $\mathfrak{g}$ and let $S \in \mathfrak{p}$. Then the orbit $\mathcal{O}(S)$ is a compact submanifold of the real vector space $\mathfrak{p}$.*

Proof. Every element $\varphi \in \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ is given by $\exp(\mathrm{ad}_\Omega)$ for some $\Omega \in \mathfrak{k}$ and hence, if θ denotes the Cartan involution,

$$\theta(\varphi S) = \sum_{k=0}^{\infty} \frac{1}{k!}\theta \mathrm{ad}_\Omega^k S = -\varphi S,$$

because $\mathrm{ad}_\Omega^k S \in \mathfrak{p}$ for all $k \in \mathbb{N}$, cf. Theorem 1.33 (a). Therefore, the compact group $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ operates on $\mathfrak{p}$ and thus has compact orbits $\mathcal{O}(S)$. □

Now fix a maximal abelian subalgebra $\mathfrak{a} \subset \mathfrak{p}$ and let

$$\mathfrak{g} = \mathfrak{g}_0 \oplus \sum_{\lambda \in \Sigma} \mathfrak{g}_\lambda$$

be the associated restricted-root space decomposition, cf. Theorem 1.42. For any restricted root $\lambda \in \Sigma$ let $\Omega_\lambda \in \mathfrak{k}_\lambda$ and $\overline{\Omega}_\lambda \in \mathfrak{p}_\lambda$ be the normalized vectors defined in (1.19), i.e.

$$\Omega_\lambda := E_\lambda + \theta E_\lambda \quad \text{and} \quad \overline{\Omega}_\lambda := E_\lambda - \theta E_\lambda, \tag{2.7}$$

with $E_\lambda \in \mathfrak{g}_\lambda$ normalized such that

$$T_\lambda := [E_\lambda, \theta E_\lambda] = -\frac{2}{|\lambda|^2} H_\lambda. \tag{2.8}$$

Here, $H_\lambda \in \mathfrak{a}$ denotes as usual the dual to λ with respect to the Killing form. For any $\lambda \in \Sigma$ consider the one parameter subgroup

$$\varphi_\lambda \colon \mathbb{R} \longrightarrow \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k}), \quad \varphi_\lambda(t) = \mathrm{Ad}_{\exp t\Omega_\lambda}. \tag{2.9}$$

An important fact is that the image of $\mathbb{R}$ under φ_λ is closed in $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$. Thus since $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ is compact, it is also compact.

Lemma 2.12. *The one–parameter subgroups $\varphi_\lambda(\mathbb{R})$ are isomorphic to the circle $S^1 := \{e^{it} \mid t \in \mathbb{R}\}$.*

Proof. Let $\mathfrak{u} = \mathfrak{k} \oplus i\mathfrak{p}$ be the compact real form of the complexification of $\mathfrak{g}$ and denote $U := \mathrm{Int}(\mathfrak{u})$ the inner automorphims of $\mathfrak{u}$. Correspondingly,

$$\mathfrak{s} := \langle \Omega_\lambda, i\overline{\Omega}_\lambda, iT_\lambda \rangle_{LA} \subset \mathfrak{u}$$

is the compact real form of the complexification of the Lie algebra $\langle \Omega_\lambda, \overline{\Omega}_\lambda, T_\lambda \rangle_{LA}$. Consider now the closure of $\varphi_\lambda(\mathbb{R})$ in $\mathrm{Int}(\mathfrak{g})$. Since $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ is compact, $\overline{\varphi_\lambda(\mathbb{R})} \subset \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$. Moreover, $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ is a closed subset of U and hence $\varphi_\lambda(\mathbb{R})$ is closed in $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ if and only if it is closed in U. By Proposition 1.52, the Lie algebra $\mathfrak{s}$ is isomorphic to $\mathfrak{su}(2)$. Since $\mathfrak{u}$ is semisimple, Proposition 1.18 implies that $\mathrm{ad}(\mathfrak{s})$ is isomorphic to $\mathfrak{su}(2)$. The analytic subgroup $S \subset U$ with Lie algebra $\mathrm{ad}(\mathfrak{s})$ is closed in U, because U is compact and $\mathrm{ad}(\mathfrak{s})$ is semisimple, cf. [53], Corollary 2. Therefore the closure $\overline{\varphi_\lambda(\mathbb{R})}$ is contained in S. Since every compact abelian analytic Lie group is a torus, cf. [45], Ch. I.12, Corollary 1.103,

$$\overline{\varphi_\lambda(\mathbb{R})} = S^1 \times \ldots \times S^1.$$

On the other hand, for dimensional reasons, the only torus contained in S is S^1, so $\overline{\varphi_\lambda(\mathbb{R})} = S^1$. Therefore

$$\overline{\varphi_\lambda(\mathbb{R})} = \varphi_\lambda(\mathbb{R}),$$

since both Lie groups are connected and have the same Lie algebra and are therefore identical, cf. [31], Ch. II, Thm. 2.1. Thus $\varphi_\lambda(\mathbb{R}) = S^1$. $\square$

The topological properties of the adjoint orbits of elements $X \in \mathfrak{g}$ are given in the following corollary.

Corollary 2.13. *Let $Y \in \mathfrak{k}_\lambda$ and let $X \in \mathfrak{g}$ be arbitrary. Then the following holds.*

(a) $\mathrm{Ad}_{\exp \mathbb{R}Y} X = X$ *if and only if* $[Y, X] = 0$.

(b) If $[Y, X] \neq 0$, *then* $\mathrm{Ad}_{\exp \mathbb{R}Y} X$ *is closed curve.*

Proof. Part (a) is easily seen by taking the derivatives at $t = 0$ on both sides of the equation $\mathrm{Ad}_{\exp tY} X = X$. Part (b) follows immediately from Lemma 2.12. □

For our purposes, it is of particular interest to consider the orthogonal projection of the one-parameter orbit $\mathrm{Ad}_{\exp \mathbb{R}\Omega_\lambda} X$ onto the maximal abelian subalgebra $\mathfrak{a} \subset \mathfrak{p}$. In the next theorem, a parametrization of the resulting curve is given.

Theorem 2.14. *Let $\mathfrak{g}$ be a semisimple Lie algebra with Cartan decomposition $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$. Let $X \in \mathfrak{p}$ and $T_\lambda, \Omega_\lambda, \overline{\Omega}_\lambda$ be as in Eq. (2.7). Denote by $\mathrm{p} \colon \mathfrak{p} \longrightarrow \mathfrak{a}$ the orthogonal projection onto $\mathfrak{a}$ and let*

$$c_\lambda := \frac{\kappa(X, \overline{\Omega}_\lambda)}{\kappa(\overline{\Omega}_\lambda, \overline{\Omega}_\lambda)}$$

be the $\overline{\Omega}_\lambda$-coefficient of X. Then

$$\mathrm{p}\left(\mathrm{Ad}_{\exp t\Omega_\lambda} X\right) = X_0 + g(t) T_\lambda,$$

where $X_0 := \mathrm{p}(X)$ and g is defined by

$$g \colon \mathbb{R} \longrightarrow \mathbb{R}, \quad t \longmapsto \tfrac{1}{2}\lambda(X_0)\Big(1 - \cos(2t)\Big) - c_\lambda \sin(2t). \tag{2.10}$$

The proof of Theorem 2.14 is based on the following two lemmas.

Lemma 2.15. *Let $n \in \mathbb{N}_0$ and $T_\lambda, \Omega_\lambda, \overline{\Omega}_\lambda$ as in Eq. (2.7). The following identities hold.*

(a) $\mathrm{ad}_{\Omega_\lambda}^{2n+1} \overline{\Omega}_\lambda = (-1)^n 2^{2n+1} (-T_\lambda)$,

(b) $\mathrm{ad}_{\Omega_\lambda}^{2n} T_\lambda = (-1)^n 2^{2n} T_\lambda$.

Proof. (a) The first formula is shown by induction. By Proposition 1.52 it is valid for $n = 0$. Assume it is true for n. Then

$$\mathrm{ad}_{\Omega_\lambda}^{2n+3} \overline{\Omega}_\lambda = -2\mathrm{ad}_{\Omega_\lambda}^{2n+2} T_\lambda = -4\mathrm{ad}_{\Omega_\lambda}^{2n+1} \overline{\Omega}_\lambda = (-1)^{n+1} 2^{2n+3} (-T_\lambda),$$

and the formula is shown for $n + 1$. (b) The second identity follows from (a) by a straightforward calculation. It is clearly true for $n = 0$. Now let $n > 1$. Then

$$\mathrm{ad}_{\Omega_\lambda}^{2n} T_\lambda = 2\mathrm{ad}_{\Omega_\lambda}^{2n-1} \overline{\Omega}_\lambda = 2(-1)^{n-1} 2^{2n-1} (-T_\lambda) = (-1)^n 2^{2n} T_\lambda.$$

The result follows. □

Lemma 2.16. *Let λ, μ be positive restricted roots with $\lambda \neq \mu$. Let $\overline{\Omega}_\lambda \in \mathfrak{p}_\lambda$ and $\Omega_\mu \in \mathfrak{k}_\mu$. Then $\mathrm{p}(\mathrm{ad}^k_{\Omega_\mu}\overline{\Omega}_\lambda) = 0$ for all $k \in \mathbb{N}$.*

Proof. The proof is done by induction, separately for the even and the odd case. The assumption is clearly true for $n = 0$ and $n = 1$ by Theorem 1.42. Now let $H \in \mathfrak{a}$ be arbitrary. Then, by the induction hypothesis,

$$\begin{aligned}\kappa(\mathrm{ad}^k_{\Omega_\mu}\overline{\Omega}_\lambda, H) &= \mu(H)\kappa(\mathrm{ad}^{k-1}_{\Omega_\mu}\overline{\Omega}_\lambda, \overline{\Omega}_\mu) = \mu(H)\kappa(\mathrm{ad}^{k-2}_{\Omega_\mu}\overline{\Omega}_\lambda, [\overline{\Omega}_\mu, \Omega_\mu]) \\ &= \mu(H)\kappa(\mathrm{ad}^{k-2}_{\Omega_\mu}\overline{\Omega}_\lambda, 2T_\mu) = 0,\end{aligned}$$

as $T_\mu \in \mathfrak{a}$. This completes the proof. □

Proof of Theorem 2.14. For all $t \in \mathbb{R}$ we have the identity, cf. [45], I.10, Proposition 1.91,

$$\mathrm{Ad}_{\exp t\Omega_\lambda} X = \exp(\mathrm{ad}_{t\Omega_\lambda})X = \sum_{k=0}^{\infty} \frac{t^k}{k!}\mathrm{ad}^k_{\Omega_\lambda} X. \tag{2.11}$$

It is shown that, if we decompose $X \in \mathfrak{p}$ according to Eq. (1.26), then the only summands in Eq. (2.11) that affect the projection onto $\mathfrak{a}$ are X_0 and $c_\lambda\overline{\Omega}_\lambda$. First, assume that $\overline{\Omega}'_\lambda, \overline{\Omega}_\lambda \in \mathfrak{p}_\lambda$ and $\kappa(\overline{\Omega}_\lambda, \overline{\Omega}'_\lambda) = 0$. Then, by Lemma 1.51 we have for all $H \in \mathfrak{a}$ that

$$0 = \lambda(H)\kappa(\overline{\Omega}_\lambda, \overline{\Omega}'_\lambda) = \kappa(\overline{\Omega}_\lambda, [H, \Omega'_\lambda]) = \kappa([\Omega'_\lambda, \overline{\Omega}_\lambda], H)$$

and hence $[\Omega'_\lambda, \overline{\Omega}_\lambda]$ is contained in $\mathfrak{a}^\perp$. Therefore, Theorem 1.42 implies that $[\Omega'_\lambda, \overline{\Omega}_\lambda] \in \mathfrak{p}_{2\lambda}$ if $2\lambda \in \Sigma$ and is zero otherwise. For $\mu \neq \lambda$ we can apply Lemma 2.16. Hence using Lemma 1.51 and Proposition 1.52, we obtain

$$\begin{aligned}\mathrm{p}\left(\mathrm{Ad}_{\exp t\Omega_\lambda} X\right) &= \mathrm{p}\left(\sum_{k=0}^{\infty} \frac{t^k}{k!}\mathrm{ad}^k_{\Omega_\lambda} X\right) = \mathrm{p}\left(\sum_{k=0}^{\infty} \frac{t^k}{k!}\mathrm{ad}^k_{\Omega_\lambda}(X_0 + c_\lambda\overline{\Omega}_\lambda)\right) = \\ &= X_0 + \mathrm{p}\left(\sum_{k=1}^{\infty} \frac{t^k}{k!}\mathrm{ad}^{k-1}_{\Omega_\lambda}[\Omega_\lambda, X_0]\right) + c_\lambda\,\mathrm{p}\left(\sum_{k=1}^{\infty} \frac{t^k}{k!}\mathrm{ad}^k_{\Omega_\lambda}\overline{\Omega}_\lambda\right) = \\ &= X_0 - \lambda(X_0)\,\mathrm{p}\left(\sum_{k=1}^{\infty} \frac{t^k}{k!}\mathrm{ad}^{k-1}_{\Omega_\lambda}\overline{\Omega}_\lambda\right) + c_\lambda\,\mathrm{p}\left(\sum_{k=1}^{\infty} \frac{t^k}{k!}\mathrm{ad}^k_{\Omega_\lambda}\overline{\Omega}_\lambda\right) = \\ &= X_0 - \lambda(X_0)\sum_{k=0}^{\infty} \frac{t^{2k+2}}{(2k+2)!}\mathrm{ad}^{2k+1}_{\Omega_\lambda}\overline{\Omega}_\lambda + c_\lambda\sum_{k=0}^{\infty} \frac{t^{2k+1}}{(2k+1)!}\mathrm{ad}^{2k+1}_{\Omega_\lambda}\overline{\Omega}_\lambda.\end{aligned}$$

By Lemma 2.15, the last sum simplifies to

$$\begin{aligned}\sum_{k=0}^{\infty} \frac{t^{2k+1}}{(2k+1)!}\mathrm{ad}^{2k+1}_{\Omega_\lambda}\overline{\Omega}_\lambda &= -\sum_{k=0}^{\infty} \frac{t^{2k+1}}{(2k+1)!}(-1)^k 2^{2k+1} T_\lambda \\ &= -\sum_{k=0}^{\infty}(-1)^k \frac{(2t)^{2k+1}}{(2k+1)!}T_\lambda = -\sin(2t)T_\lambda.\end{aligned}$$

Furthermore,

$$\sum_{k=0}^{\infty} \frac{t^{2k+2}}{(2k+2)!}\mathrm{ad}_{\Omega_\lambda}^{2k+1}\overline{\Omega}_\lambda = -\sum_{k=0}^{\infty} \frac{t^{2k+2}}{(2k+2)!}(-1)^k 2^{2k+1} T_\lambda.$$

Now we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\sum_{k=0}^{\infty} \frac{t^{2k+2}}{(2k+2)!}(-1)^k 2^{2k+1} = \sum_{k=0}^{\infty}(-1)^k \frac{(2t)^{2k+1}}{(2k+1)!} = \sin(2t),$$

and

$$\sum_{k=0}^{\infty} \frac{t^{2k+2}}{(2k+2)!}(-1)^k 2^{2k+1} = \tfrac{1}{2}(1-\cos(2t)),$$

and therefore

$$\mathrm{p}\left(\mathrm{Ad}_{\exp t\Omega_\lambda} X\right) = X_0 + \tfrac{1}{2}\lambda(X_0)(1-\cos(2t))T_\lambda - c_\lambda \sin(2t) T_\lambda.$$

□

As can be seen from Theorem 2.14, the torus algebra component varies along the orbit of the one–parameter group $\mathrm{Ad}_{\exp t\Omega_\lambda}$. In the next lemma we analyze this variation in more precise terms by discussing the function (2.10).

Lemma 2.17. *The function $g(t) = \frac{1}{2}\lambda(X_0)(1-\cos(2t)) - c_\lambda \sin(2t)$ is π-periodic and is either constant or possesses on $(-\frac{\pi}{2}, \frac{\pi}{2}]$ exactly one minimum $t_{\min}$ and one maximum $t_{\max}$. In this case*

$$\begin{aligned} \sin 2t_{\min} &= \frac{2c_\lambda}{\sqrt{4c_\lambda^2 + \lambda(X_0)^2}}, & \cos 2t_{\min} &= \frac{\lambda(X_0)}{\sqrt{4c_\lambda^2 + \lambda(X_0)^2}}, \\ \sin 2t_{\max} &= -\sin 2t_{\min}, & \cos 2t_{\max} &= -\cos 2t_{\min}, \end{aligned} \tag{2.12}$$

and $g(t_{\min}) = \frac{1}{2}\lambda(X_0) - \frac{1}{2}\sqrt{4c_\lambda^2 + \lambda(X_0)^2}$ and $g(t_{\max}) = \frac{1}{2}\lambda(X_0) + \frac{1}{2}\sqrt{4c_\lambda^2 + \lambda(X_0)^2}$.

Proof. The first assertion is trivial and we only need to prove Eqs. (2.12). Substituting $v := \sin 2t$ and $u := \cos 2t$ into the function $g(t) = \frac{1}{2}\lambda(X_0)\Big(1-\cos(2t)\Big) - c_\lambda \sin(2t)$, leads to the following optimization task.

$$\begin{aligned} \text{Minimize/Maximize} \quad & \tfrac{1}{2}\lambda(X_0)(1-u) - c_\lambda v \\ \text{subject to} \quad & u^2 + v^2 = 1. \end{aligned} \tag{2.13}$$

We use the Lagrangian multiplier method to find the solutions. Let

$$L_m(u,v) := \tfrac{1}{2}\lambda(X_0)(1-u) - c_\lambda v + m(u^2+v^2-1)$$

be the Lagrangian function with multiplier m. By assumption, $g(t)$ is not constant and therefore the system of equations

$$\begin{aligned} D_u L_m(u,v) = &\quad -\tfrac{1}{2}\lambda(X_0) + 2mu &= 0 \\ D_v L_m(u,v) = &\quad -c_\lambda + 2mv &= 0 \\ &\quad u^2 + v^2 &= 1 \end{aligned}$$

has exactly the two solutions

$$\begin{aligned} (u_1, v_1, m_1) &= \left(\frac{\lambda(X_0)}{\sqrt{4c_\lambda^2 + \lambda(X_0)^2}}, \frac{2c_\lambda}{\sqrt{4c_\lambda^2 + \lambda(X_0)^2}}, \tfrac{1}{2}\sqrt{4c_\lambda^2 + \lambda(X_0)^2} \right) \quad \text{and} \\ (u_2, v_2, m_2) &= \left(-\frac{\lambda(X_0)}{\sqrt{4c_\lambda^2 + \lambda(X_0)^2}}, -\frac{2c_\lambda}{\sqrt{4c_\lambda^2 + \lambda(X_0)^2}}, -\tfrac{1}{2}\sqrt{4c_\lambda^2 + \lambda(X_0)^2} \right). \end{aligned} \tag{2.14}$$

An inspection of the Hessian of $L_{m_i}(u_i, v_i)$ for $i = 1, 2$ and noting that $(u_1, v_1) = -(u_2, v_2)$ completes the proof. The last assertion is proven by a straightforward computation. □

2.3.2 The Algorithm

We specify the Jacobi algorithm 2.4 in more concrete form for the optimization task of a smooth cost function

$$f \colon \mathcal{O}(S) \longrightarrow \mathbb{R}$$

on the compact orbit $\mathcal{O}(S)$. We take advantage of the results of the previous section and use the $\Omega_\lambda \in \mathfrak{k}_\lambda$, cf. Eq. (2.7), arising from the restricted-root space decomposition in order to determine the search directions. This guarantees that the algorithm is globally well defined.

Algorithm 2.18 (Jacobi sweep)**.** Let $X \in \mathcal{O}(S)$ and let $\mathcal{B} := \{\Omega_1, ..., \Omega_m\} \subset \mathfrak{k}$ where every Ω_i lies in $\mathfrak{k}_{\lambda_i}$ for some restricted root λ_i. We can assume without loss of generality that the Ω_i are normalized according to Eq. (2.7). Define for $\Omega \in \mathcal{B}$ the search directions

$$r_\Omega \colon\ \mathcal{O}(S) \times \mathbb{R} \longrightarrow \mathcal{O}(S), \quad (X, t) \longmapsto \mathrm{Ad}_{\exp t\Omega} X. \tag{2.15}$$

A sweep on $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ is the map

$$s \colon \mathcal{O}(S) \longrightarrow \mathcal{O}(S),$$

explicitly given as follows. Set $X_k^{(0)} := X$.

$$X_k^{(1)} := r_{\Omega_1}\left(X_k^{(0)}, t_*^{(1)}\left(X_k^{(0)}\right)\right)$$

$$X_k^{(2)} := r_{\Omega_2}\left(X_k^{(1)}, t_*^{(2)}\left(X_k^{(1)}\right)\right)$$

$$X_k^{(3)} := r_{\Omega_3}\left(X_k^{(2)}, t_*^{(3)}\left(X_k^{(2)}\right)\right)$$

$$\vdots$$

$$X_k^{(m)} := r_{\Omega_m}\left(X_k^{(m-1)}, t_*^{(m)}\left(X_k^{(m-1)}\right)\right),$$

where $t_*^{(i)}$ is defined in Algorithm 2.2. Now set $s(X) := X_k^{(m)}$.

The Jacobi algorithm consists of iterating sweeps.

Algorithm 2.19 (Jacobi Algorithm)**.**

1. Assume that we already have $X_0, X_1, ..., X_k \in \mathcal{O}(S)$ for some $k \in \mathbb{N}$.
2. Put $X_{k+1} := s(X_k)$ and continue with the next sweep.

Remark 2.20. Note, that by construction, a Jacobi sweep does not work in directions $\Omega \in \mathfrak{z}_{\mathfrak{k}}(\mathfrak{a})$.

Theorem 2.21. *Algorithm 2.19 is well defined, for any start value $X \in \mathcal{O}(S)$ and all iteration steps. Assume that f is smooth and $Z \in \mathcal{O}(S)$ is a nondegenerate local minimum of f. Then the Jacobi algorithm is locally quadratic convergent to Z, provided $\{[Z, \Omega] \mid \Omega \in \mathcal{B}\}$ is a basis of $T_Z\mathcal{O}(S)$ (implying $m = \dim \mathcal{O}(S)$) that is orthogonal with respect to the Hessian $\mathsf{H}_f(Z)$.*

Proof. The first part of the theorem follows from Corollary 2.13, that assures, that the cost function restricted to orbits of one parameter groups $\mathrm{Ad}_{\exp t\Omega}$ is periodic, since $\Omega \in \mathfrak{k}_\lambda$. By continuity of f, the step size and therefore Algorithm 2.18 is well defined. For the second part recall that the tangent space $T_Z\mathcal{O}(S)$ is given by

$$T_Z\mathcal{O}(S) = \mathrm{ad}_Z\mathfrak{k},$$

cf. Example 2.1. The assertion now follows by Theorem 2.10. □

In the rest of this chapter we give some brief ideas on the issue of parallelizability of the Jacobi-algorithm. This is linked to the possibility of achieving simultaneous minimization for the Jacobi sweep 2.18 in certain directions. For $\Omega \in \mathfrak{k}_\lambda$, we assume that the step-size selection t_* along $\mathrm{Ad}_{\exp t\Omega}X$ only depends on the $\overline{\Omega}$-component of X and on $\lambda(X_0)$. Although this seems quite restrictive, it includes the classical cyclic Jacobi and the Sort-Jacobi methods for the Lie algebraic generalization of the symmetric eigenvalue problem. The following theorem generalizes the results in [25], Section 8.4.

Lemma 2.22. *Let λ, μ be restricted roots such that neither $\lambda + \mu$ nor $\lambda - \mu$ are restricted roots or zero. Let H_μ denote the dual to μ. Then*

$$\lambda(H_\mu) = 0.$$

Proof. Let $E_\lambda \in \mathfrak{g}_\lambda$ be defined as in Eq. (1.18). Then

$$\lambda(H_\mu)\kappa(E_\lambda, \theta E_\lambda) = \kappa([H_\mu, E_\lambda], \theta E_\lambda) = \kappa(H_\mu, [E_\lambda, \theta E_\lambda) = -\frac{2}{|\lambda|^2}\kappa(H_\mu, H_\lambda) = 0,$$

by Proposition 3.20 (e). The assumption follows since $\kappa(E_\lambda, \theta E_\lambda) = -B_\theta(E_\lambda, E_\lambda) < 0$. □

Theorem 2.23 (Parallelizability)**.** *Suppose that for all $X \in \mathcal{O}(S)$ the step-size t_* in Algorithm 2.18 along $\mathrm{Ad}_{\exp t\Omega} X$ only depends on the $\overline{\Omega}$-component of X and the corresponding root of $X_0 := \mathrm{p}(X) \in \mathfrak{a}$. Then the line search in Ω_1- and Ω_2-direction can be done simultaneously if $\lambda + \mu \notin \Sigma \cup \{0\}$ and $\lambda - \mu \notin \Sigma \cup \{0\}$.*

Proof. Let $\Omega_1 \in \mathfrak{k}_\lambda$ and $\Omega_2 \in \mathfrak{k}_\mu$ such that neither $\lambda + \mu$ nor $\lambda - \mu$ is a restricted root or zero. The line search can be done simultaneously if and only if the transformations $\mathrm{Ad}_{\exp t\Omega_1}$, $t \in \mathbb{R}$, do neither affect the $\overline{\Omega}_2$-component of elements $X \in \mathfrak{p}$, nor the corresponding root of its projection onto $\mathfrak{a}$, i.e. $\mu(X_0)$. The $\overline{\Omega}_2$-component of $X \in \mathfrak{g}$ is not affected by transformations $\mathrm{Ad}_{\exp t\Omega_1}$ if and only if

$$\kappa(\mathrm{Ad}_{\exp t\Omega_1} X, \overline{\Omega}_2) = \kappa(X, \overline{\Omega}_2) \qquad \text{for all } t \in \mathbb{R}.$$

Differentiating with respect to t and using the ad-invariance of the Killing form yields

$$-\kappa(\mathrm{Ad}_{\exp t\Omega_1} X, [\Omega_1, \overline{\Omega}_2]) = 0 \qquad \text{for all } t \in \mathbb{R},$$

hence a sufficient condition for not affecting the $\overline{\Omega}_2$-component is that

$$[\Omega_1, \overline{\Omega}_2] = 0. \tag{2.16}$$

Now let $\Omega_1 = E_\lambda + \theta E_\lambda$ and $\overline{\Omega}_2 = E_\mu - \theta E_\mu$. If $\lambda + \mu$ and $\lambda - \mu$ are not in $\Sigma \cup \{0\}$, it follows from Theorem 1.42 that

$$[\Omega_1, \overline{\Omega}_2] = [E_\lambda, E_\mu] - [E_\lambda, \theta E_\mu] + [\theta E_\lambda, E_\mu] - [\theta E_\lambda, \theta E_\mu] = 0.$$

To see that $\mu\big(\mathrm{p}(\mathrm{Ad}_{\exp t\Omega_1} X)\big) = \mu(X_0)$ for all $t \in \mathbb{R}$, we equivalently have by orthogonality of p that

$$\kappa\big(\mathrm{Ad}_{\exp t\Omega_1} X, H_\mu\big) = \mu(X_0) \qquad \text{for all } t \in \mathbb{R}.$$

The same argument as above yields the sufficient condition

$$0 = [\Omega_1, H_\mu] = \lambda(H_\mu)\overline{\Omega}_1.$$

But this holds true since by Corollary 2.22, we have $\lambda(H_\mu) = 0$ indeed. □

An example from [25], explained in our more general Lie-algebraic context, will help to illustrate the previous proof.

Example 2.24 ([25], Section 8.4.). Consider the task of annihilating the off-diagonal entries of a real symmetric (8×8)-matrix X successively by elementary Givens rotations in order to diagonalize it. In this case, the 28 sweep directions are given by

$$\Omega_{ij} = E_{ij} - E_{ji}, 1 \leq i < j \leq 8,$$

where E_{ij} has (ij)-entry 1 and zeros elsewhere. Note, that the Givens rotations are just given by $\exp(t\Omega_{ij})$ and the conjugation by $\mathrm{Ad}_{\exp(t\Omega_{ij})}$, cf. Eq. (1.4). According to [25], Section 8.4., throughout one sweep, the following elementary rotations can be done simultaneously.

1. $\{\Omega_{12}, \Omega_{34}, \Omega_{56}, \Omega_{78}\}$ 2. $\{\Omega_{14}, \Omega_{26}, \Omega_{38}, \Omega_{57}\}$ 3. $\{\Omega_{16}, \Omega_{48}, \Omega_{27}, \Omega_{35}\}$
4. $\{\Omega_{18}, \Omega_{67}, \Omega_{45}, \Omega_{23}\}$ 5. $\{\Omega_{17}, \Omega_{58}, \Omega_{36}, \Omega_{24}\}$ 6. $\{\Omega_{15}, \Omega_{37}, \Omega_{28}, \Omega_{46}\}$
7. $\{\Omega_{13}, \Omega_{25}, \Omega_{47}, \Omega_{68}\}$

In the Lie algebraic setting, this reads as follows. Consider the Cartan decomposition of $\mathfrak{sl}(8, \mathbb{R})$ into skew-symmetric and symmetric matrices, and fix the diagonal matrices as the maximal abelian subalgebra $\mathfrak{a} \subset \mathfrak{p}$, cf. Examples 1.34 and 1.50. The positive roots are given by $\lambda_{ij}(H) = H_{ii} - H_{jj}, i < j$, $H \in \mathfrak{a}$, and the corresponding subspaces $\mathfrak{k}_{\lambda_{ij}}$ have real dimension one and are

$$\mathfrak{k}_{\lambda_{ij}} = \mathbb{R}\Omega_{ij}.$$

The step size $t_*^{(ij)}$ only depends on the $\overline{\Omega_{ij}}$-component of X, i.e. its (i,j)-entry and the root of its projection to $\mathfrak{a}$, i.e. $X_{ii} - X_{jj}$. Hence we can apply Theorem 2.23 and it is easy to check that within one of the seven sets given above, neither $\lambda_{ij} + \lambda_{kl}$ nor $\lambda_{ij} - \lambda_{kl}$ is a root or zero for $(i,j) \neq (k,l)$.

Chapter 3

Jacobi-Type Eigenvalue Methods

In this chapter we apply the results from Chapter 2 and investigate Jacobi-type methods for structured singular value and eigenvalue problems on Lie algebras. We consider the optimization of two basic functions, the off-norm function and the trace function. Their optimization on the $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ orbit leads us to two basic versions of a Lie algebraic generalization of the symmetric eigenvalue problem:

(I) the conventional cyclic Jacobi method (reducing the off-norm)

(II) the cyclic Sort-Jacobi method (maximizing the trace function).

The proposed algorithms are sufficiently general to include the symmetric, skew-symmetric and Hermitian eigenvalue problem, the real and complex singular value decomposition, the real and complex Hamiltonian eigenvalue problem and some– to our knowledge– new structured eigenvalue problems. Table 4.1 in Chapter 4 contains an overview of the specific eigenvalue and singular value problems to which our theory applies. We shall see that both algorithms are locally quadratic convergent for regular Lie algebra elements, i.e. in the case corresponding to pairwise distinct eigenvalues and singular values, respectively. Moreover, in this regular case, *any* cyclic Jacobi method is shown to be locally quadratically convergent. The irregular case turns out to be more delicate and local quadratic convergence cannot be guaranteed for arbitrary cyclic sweeps. Thus, *special* sweep methods are needed to ensure local quadratic convergence. This was already noted in [64] where local convergence for a special cyclic scheme for the conventional Jacobi method on symmetric matrices is discussed. Moreover, as also noted by [64], a special ordering of the diagonal entries of the element that converges to diagonal form is required as well. This additional assumption is quite restrictive, as the to-be-optimized off-norm function in the conventional cyclic Jacobi method possesses several global minima, all corresponding to different diagonalizations. In contrast, the proposed trace function in the Sort–Jacobi method has only one local and global maximum at the diagonalizations. It turns out that this optimal diagonalization fulfills the ordering condition in a natural way. We interpret this as a clear indication, that the natural way of looking at the symmetric

EVD is to maximize the trace function instead of minimizing the familiar off-norm function from the numerical linear algebra literature. Thus Sort-Jacobi algorithm is *the* proper Jacobi method for structured eigenvalue problems, an insight that has also been supported by numerical experiments, cf. [42].

3.1 The Generalized Off-Norm and the Classical Cyclic Jacobi

The conventional way to choose a cost function for diagonalization of a symmetric matrix $S = (S_{ij}) \in \mathbb{R}^{n\times n}$ is via the so-called off-norm on the symmetric similarity orbit, i.e.

$$\mathrm{off}\colon \{kSk^\top \mid k \in SO(n,\mathbb{R})\} \longrightarrow \mathbb{R}, \quad \mathrm{off}(X) := \sum_{i<j} X_{ij}^2.$$

All its global minima correspond to diagonalizations of S. In general, this function possesses a continuum of maxima and saddle points, cf. [42] or Example 3.6 for the Hermitian case. In this section we show that the off-norm is defined on an arbitrary semisimple Lie algebra and we will compute its critical points. Moreover, we characterize the maxima and minima, cf. [62]. Implementing the cyclic Jacobi method proposed in Section 2.3.2 with the off-norm as cost function f leads to the classical cyclic Jacobi and is thus a Lie algebraic generalization of the classical cyclic Jacobi methods for the symmetric, skew-symmetric and Hermitian EVD as well as for Kogbetliantz's algorithm for computing the singular values of a matrix.

Let $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ be a Cartan decomposition of a semisimple Lie algebra $\mathfrak{g}$ with corresponding Cartan involution θ. Let $S \in \mathfrak{p}$ and denote as before the adjoint orbit of S under $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ by

$$\mathcal{O}(S) := \{\varphi S \mid \varphi \in \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})\}.$$

Let $\mathfrak{a} \subset \mathfrak{p}$ be maximal abelian and recall that $\mathfrak{g}$ is the orthogonal direct sum

$$\mathfrak{g} = \mathfrak{g}_0 \oplus \sum_{\lambda\in\Sigma} \mathfrak{g}_\lambda, \tag{3.1}$$

with respect to the inner product B_θ, cf. Eq. (1.10), where

$$\mathfrak{g}_0 = \mathfrak{a} \oplus \mathfrak{z}_{\mathfrak{k}}(\mathfrak{a}) \tag{3.2}$$

is the orthogonal direct sum of the maximal abelian subspace in $\mathfrak{p}$ and the centralizer of $\mathfrak{a}$ in $\mathfrak{k}$, cf. Theorem 1.42. Let

$$\mathrm{p}\colon \mathfrak{g} \longrightarrow \mathfrak{g}_0, \quad X \longmapsto X_0, \tag{3.3}$$

denote the orthogonal projection onto $\mathfrak{g}_0$ with respect to B_θ. According to (3.1), we write

$$X = X_0 + \sum_{\lambda\in\Sigma} X_\lambda \tag{3.4}$$

for $X \in \mathfrak{g}$. Then obviously $\mathrm{p}(X) \in \mathfrak{a}$ whenever $X \in \mathfrak{p}$. Note, that $B_\theta|_{\mathfrak{p}} = \kappa|_{\mathfrak{p}}$ denotes the restriction of the Killing–form κ, cf. Theorem 1.33.

Definition 3.1. Let $S \in \mathfrak{p}$ and let κ denote the Killing-form. The smooth function

$$f\colon \mathcal{O}(S) \longrightarrow [0,\infty), \quad X \longmapsto \kappa(X - X_0, X - X_0), \tag{3.5}$$

is called the *off-norm function* on the adjoint orbit $\mathcal{O}(S)$.

Note that for $\mathfrak{g} := \mathfrak{sl}(n,\mathbb{C})$ the Cartan decomposition is given by $\mathfrak{g} = \mathfrak{su}(n) \oplus \mathfrak{p}$ where

$$\mathfrak{p} = \{S \in \mathfrak{sl}(n,\mathbb{C}) \mid S^* = S\}$$

denotes the set of Hermitian matrices of trace zero. Therefore, in this case the off-norm function coincides, up to a positive constant that depends on n, with the usual off-norm, i.e. the sum of squares of the absolute values of the off-diagonal entries.
We proceed by characterizing the critical points and the Hessian of the off-norm function.

Proposition 3.2. *(a) The following statements are equivalent.*

(i) *$X \in \mathcal{O}(S)$ is a critical point of the off-norm function* (3.5)*.*

(ii) $[X_0, X] = 0$*.*

(iii) *For each $\lambda \in \Sigma$, either $\lambda(X_0) = 0$ or $X_\lambda = 0$.*

(b) Let X be a critical point of the off-norm (3.5) *and let $\xi = \mathrm{ad}_\Omega X \in T_X\mathcal{O}(S)$ be an arbitrary element of the tangent space at X. Then the Hessian at X is given by*

$$\mathsf{H}_f(X)(\xi,\xi) = 2\kappa\Big(\mathrm{ad}_\Omega X, \mathrm{ad}_\Omega X_0 - \mathrm{p}(\mathrm{ad}_\Omega X)\Big). \tag{3.6}$$

Proof. (a) For $\Omega \in \mathfrak{k}$ and $X \in \mathfrak{p}$ let

$$\gamma\colon \mathbb{R} \longrightarrow \mathcal{O}(S), \quad t \longmapsto \mathrm{Ad}_{\exp(t\Omega)} X,$$

be a smooth curve through X. By orthogonality of the restricted-root space decomposition (3.1) and the Ad-invariance of κ we compute the derivative of the cost function:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\Big(f \circ \gamma(t)\Big)\Big|_{t=0} &= 2\kappa\Big(\mathrm{ad}_\Omega X - \mathrm{p}(\mathrm{ad}_\Omega X), X - X_0\Big) \\
&= 2\kappa\Big(-\mathrm{ad}_X \Omega, X - X_0\Big) - 2\kappa\Big(\mathrm{p}(\mathrm{ad}_X\Omega), X - X_0\Big) \\
&= 2\kappa\Big(\Omega, \mathrm{ad}_X(X - X_0)\Big) \\
&= 2\kappa\Big(\Omega, \mathrm{ad}_{X_0} X\Big).
\end{aligned}$$

The Killing form is negative definite on $\mathfrak{k}$, cf. Theorem 1.33, and therefore

$$Df(X) = 0 \iff [X_0, X] = 0.$$

By decomposing X according to Eq. (1.26) and using the property, that $\mathrm{ad}_H Y = \lambda(H)Y$ whenever $H \in \mathfrak{a}$ and $Y \in \mathfrak{g}_\lambda$, one has

$$[X_0, X] = 0 \iff \lambda(X_0)X_\lambda = 0 \text{ for all } \lambda \in \Sigma.$$

(b) Let X be a critical point of the cost function (3.5). Again, the Ad-invariance of the Killing form and the orthogonality of the restricted-root space decomposition is used to compute the Hessian.

$$\begin{aligned}
&\frac{\mathrm{d}^2}{\mathrm{d}t^2}\Big(f \circ \gamma(t)\Big)\Big|_{t=0} \\
= \;& 2\frac{\mathrm{d}}{\mathrm{d}t}\kappa\Big(\mathrm{ad}_\Omega \mathrm{Ad}_{\exp(t\Omega)}X - \mathrm{p}(\mathrm{ad}_\Omega \mathrm{Ad}_{\exp(t\Omega)}X), \mathrm{Ad}_{\exp(t\Omega)}X - \mathrm{p}(\mathrm{Ad}_{\exp(t\Omega)}X)\Big)\Big|_{t=0} \\
= \;& 2\kappa\Big(\mathrm{ad}_\Omega^2 X - \mathrm{p}(\mathrm{ad}_\Omega^2 X), X - X_0\Big) + 2\kappa\Big(\mathrm{ad}_\Omega X - \mathrm{p}(\mathrm{ad}_\Omega X), \mathrm{ad}_\Omega X - \mathrm{p}(\mathrm{ad}_\Omega X)\Big) \\
= \;& -2\kappa\Big(\mathrm{ad}_\Omega^2 X, X - X_0\Big) + 2\underbrace{\kappa\Big(\mathrm{p}(\mathrm{ad}_\Omega^2 X), X - X_0\Big)}_{=0} - 2\kappa\Big(\mathrm{ad}_\Omega X, \mathrm{ad}_\Omega X - \mathrm{p}(\mathrm{ad}_\Omega X)\Big) \\
& +2\underbrace{\kappa\Big(\mathrm{p}(\mathrm{ad}_\Omega X), \mathrm{ad}_\Omega X - \mathrm{p}(\mathrm{ad}_\Omega X)\Big)}_{=0} \\
= \;& -2\kappa\Big(\mathrm{ad}_\Omega X, -\mathrm{ad}_\Omega X + \mathrm{ad}_\Omega X_0 + \mathrm{ad}_\Omega X - \mathrm{p}(\mathrm{ad}_\Omega X)\Big) \\
= \;& 2\kappa\Big(\mathrm{ad}_\Omega X, \mathrm{ad}_\Omega X_0 - \mathrm{p}(\mathrm{ad}_\Omega X)\Big).
\end{aligned}$$

□

The next two lemmas provide information about the restriction of the Hessian to one dimensional subspaces of the tangent space $T_X\mathcal{O}(S)$ at a critical point X. Sufficient conditions for a critical point will be given such that there exist one dimensional subspaces of $T_X\mathcal{O}(S)$, where the restriction of the Hessian is negative, resp. positive definite. These results imply that the local minima, and local maxima respectively, of the off-norm (3.5) are global.

Lemma 3.3. *Let X be a critical point of the off-norm (3.5) and let $\mu \in \Sigma$ be a restricted root such that $\mu(X_0) \neq 0$. Let E_μ be a restricted-root vector in $\mathfrak{g}_\mu \setminus \{0\}$ and let $\Omega_\mu := E_\mu + \theta E_\mu \in \mathfrak{k}_\mu$. Then*

$$\mathsf{H}_f(X)(\mathrm{ad}_{\Omega_\mu}X, \mathrm{ad}_{\Omega_\mu}X) > 0.$$

Proof. Decomposing $X \in \mathfrak{p}$ according to Eq. (1.26) into

$$X = X_0 + \sum_{\lambda \in \Sigma^+} (X_\lambda - \theta X_\lambda)$$

together with Lemma 1.51 yields $\operatorname{ad}_{\Omega_\mu}(X_\lambda - \theta X_\lambda) \in \mathfrak{a}^\perp$ for all λ with $\lambda \neq \pm\mu$. By assumption, X is a critical point of the cost function (3.5) and therefore $\mu(X_0) \neq 0$, implying by Proposition 3.2 that $X_\mu = X_{-\mu} = 0$. Hence

$$\mathrm{p}\left(\operatorname{ad}_{\Omega_\mu}(X_\lambda - \theta X_\lambda)\right) = 0 \quad \text{for all } \lambda \in \Sigma^+$$

and therefore $\mathrm{p}(\operatorname{ad}_{\Omega_\mu} X) = 0$. Let $\overline{\Omega}_\mu := E_\mu - \theta E_\mu \in \mathfrak{p}_\mu$. Again, by using Lemma 1.51 and the fact that $[\overline{\Omega}_\mu, \Omega_\mu] \in \mathfrak{a}$, cf. Proposition 1.52, we can explicitly compute the restriction of the Hessian.

$$\begin{aligned}
&\mathsf{H}_f(X)(\operatorname{ad}_{\Omega_\mu} X, \operatorname{ad}_{\Omega_\mu} X) = \\
&\quad = \kappa\Big(\operatorname{ad}_{\Omega_\mu} X, \operatorname{ad}_{\Omega_\mu} X_0 - \mathrm{p}(\operatorname{ad}_{\Omega_\mu} X)\Big) \\
&\quad = \kappa\Big(\operatorname{ad}_{\Omega_\mu} X_0 + \sum_{\lambda \in \Sigma^+} \operatorname{ad}_{\Omega_\mu}(X_\lambda - \theta X_\lambda), \operatorname{ad}_{\Omega_\mu} X_0\Big) \\
&\quad = \mu(X_0)^2 \kappa\Big(\overline{\Omega}_\mu, \overline{\Omega}_\mu\Big) + \sum_{\lambda \in \Sigma^+} \kappa\Big(X_\lambda - \theta X_\lambda, [\overline{\Omega}_\mu, \Omega_\mu]\Big) \\
&\quad = \mu(X_0)^2 \kappa\Big(\overline{\Omega}_\mu, \overline{\Omega}_\mu\Big) \ > \ 0.
\end{aligned}$$

□

Lemma 3.4. *Let X be a critical point of the off-norm* (3.5) *and let $\lambda \in \Sigma$ such that $X_\lambda \neq 0$. Let E_λ be a vector in $\mathfrak{g}_\lambda$ such that $E_\lambda \notin (\mathbb{R}X_\lambda)^\perp$ and let $\Omega_\lambda := E_\lambda + \theta E_\lambda \in \mathfrak{k}$. Then*

$$\mathsf{H}_f(X)(\operatorname{ad}_{\Omega_\lambda} X, \operatorname{ad}_{\Omega_\lambda} X) \ < 0.$$

Proof. This proof runs similar to the proof of Lemma 3.3. Since X is a critical point and by assumption $X_\lambda \neq 0$, it follows from Proposition 3.2 that $\lambda(X_0) = 0$. Hence

$$\operatorname{ad}_{\Omega_\lambda} X_0 = -\lambda(X_0) E_\lambda + \lambda(X_0)\theta E_\lambda = 0.$$

We compute the restriction of the Hessian.

$$\begin{aligned}
&\mathsf{H}_f(X)(\operatorname{ad}_{\Omega_\lambda} X, \operatorname{ad}_{\Omega_\lambda} X) = \\
&\quad = \kappa\Big(\operatorname{ad}_{\Omega_\lambda} X_0 + \sum_{\mu \in \Sigma^+} \operatorname{ad}_{\Omega_\lambda}(X_\mu - \theta X_\mu), \operatorname{ad}_{\Omega_\lambda} X_0 - \mathrm{p}(\operatorname{ad}_{\Omega_\lambda} X)\Big) \\
&\quad = -\kappa\Big(\mathrm{p}\Big(\sum_{\mu \in \Sigma^+} \operatorname{ad}_{\Omega_\lambda}(X_\mu - \theta X_\mu)\Big), \sum_{\mu \in \Sigma^+} \mathrm{p}(\operatorname{ad}_{\Omega_\lambda}(X_\mu - \theta X_\mu))\Big) \\
&\quad = -\kappa\Big(\operatorname{ad}_{\Omega_\lambda}(X_\lambda - \theta X_\lambda), \operatorname{ad}_{\Omega_\lambda}(X_\lambda - \theta X_\lambda)\Big) \leq 0,
\end{aligned}$$

because κ is positive definite on $\mathfrak{p}$. It remains to show that strict inequality holds, i.e. $\mathrm{ad}_{\Omega_\lambda}(X_\lambda - \theta X_\lambda) \neq 0$. Therefore, let $H \in \mathfrak{a}$ with $\lambda(H) \neq 0$. By Corollary 1.45 we have

$$\begin{aligned}
\kappa(H, \mathrm{ad}_{\Omega_\lambda}(X_\lambda - \theta X_\lambda)) &= \lambda(H)\kappa(E_\lambda - \theta E_\lambda, X_\lambda - \theta X_\lambda) \\
&= \lambda(H)\Big(\kappa(-\theta E_\lambda, X_\lambda) - \kappa(E_\lambda, \theta X_\lambda)\Big) \\
&= \lambda(H)\Big(B_\theta(X_\lambda, E_\lambda) + B_\theta(E_\lambda, X_\lambda)\Big) \\
&= 2\lambda(H)B_\theta(X_\lambda, E_\lambda) \neq 0,
\end{aligned}$$

since $E_\lambda \notin (\mathbb{R}X_\lambda)^\perp$, hence $\mathrm{ad}_{\Omega_\lambda}(X_\lambda - \theta X_\lambda) \neq 0$. □

The following proposition is a consequence of the last two lemmas.

Proposition 3.5. *(a) The local minima of the off-norm function* (3.5) *are global minima. The set of the minima is $\mathcal{O}(S) \cap \mathfrak{a}$. In particular, there are only finitely many minima.*

(b) The local maxima of the off-norm function (3.5) *are global maxima. The set of the maxima is $\mathcal{O}(S) \cap \mathfrak{a}^\perp$, where $\mathfrak{a}^\perp$ denotes the orthogonal complement of $\mathfrak{a}$ with respect to B_θ.*

Proof. (a) The set of global minima of (3.5) is exactly the intersection of $\mathcal{O}(S)$ with the maximal abelian subspace $\mathfrak{a}$ in $\mathfrak{p}$. By Corollary 1.63 the cardinality $|\mathcal{O}(S) \cap \mathfrak{a}|$ is finite. Suppose $\widetilde{X}$ is a local minimum but not global, i.e. $f(\widetilde{X}) > 0$. Then there exists $\lambda \in \Sigma$ such that $\widetilde{X}_\lambda \neq 0$ and if $\Omega_\lambda := X_\lambda + \theta X_\lambda$ then

$$\mathsf{H}_f(\widetilde{X})(\mathrm{ad}_{\Omega_\gamma}\widetilde{X}, \mathrm{ad}_{\Omega_\gamma}\widetilde{X}) \geq 0,$$

since $\widetilde{X}$ is a local minimum. On the other hand, since $X_\lambda \notin \mathbb{R}X_\lambda^\perp$, Lemma 3.4 yields

$$\mathsf{H}_f(\widetilde{X})(\mathrm{ad}_{\Omega_\gamma}\widetilde{X}, \mathrm{ad}_{\Omega_\gamma}\widetilde{X}) < 0$$

and we obtain a contradiction.
(b) Suppose $\widetilde{X}$ is a local maximum. Hence the restriction of the Hessian to any one–dimensional subspace of the tangent space $T_{\widetilde{X}}\mathcal{O}(S)$ cannot be positive definite. In particular for the subspaces $\mathbb{R}\mathrm{ad}_{\Omega_\lambda}\widetilde{X}$ one has

$$\mathsf{H}_f(\widetilde{X})(\mathrm{ad}_{\Omega_\lambda}\widetilde{X}, \mathrm{ad}_{\Omega_\lambda}\widetilde{X}) \leq 0.$$

Hence by Lemma 3.3, $\lambda(\widetilde{X}_0) = 0$ for all $\lambda \in \Sigma$. Since Σ contains a basis of the dual space $\mathfrak{a}^*$, it follows $\widetilde{X}_0 = 0$. The Ad-invariance of the Killing form yields

$$f(\widetilde{X}) = \kappa(\widetilde{X} - \widetilde{X}_0, \widetilde{X} - \widetilde{X}_0) = \kappa(\widetilde{X}, \widetilde{X}) = \kappa(S, S).$$

Therefore all local maxima lie in the same level set and by compactness of the orbit $\mathcal{O}(S)$ they have to be global maxima. □

Although the set of minima is finite, this is in general not true for the set of saddle points or maxima. Even more so, the set of critical points may have a complicated geometric structure. Thus the off-norm has a lot of critical points which are of no significance to the diagonalization task. It is this property that makes the off-norm function a rather unsuitable cost function for eigenvalue computations.

Example 3.6. Let $\mathfrak{g} = \mathfrak{sl}(3, \mathbb{C})$ and let a Cartan decomposition be given by $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ with

$$\mathfrak{k} = \mathfrak{su}(3) \quad \text{and} \quad \mathfrak{p} = \{S \in \mathfrak{sl}(3, \mathbb{C}) \mid S^* = S\},$$

and fix a maximal abelian subspace $\mathfrak{a} \subset \mathfrak{p}$ via $\mathfrak{a} = \{H \in \mathfrak{p} \mid H \text{ is diagonal}\}$. Let $S \in \mathfrak{p}$ be given by

$$S = \begin{bmatrix} 1 & & \\ & 0 & \\ & & -1 \end{bmatrix}.$$

It follows from Proposition 3.5 that a (global) maximum $\widetilde{Z}$ of the cost function f (3.5) has zero diagonal. Therefore $\widetilde{Z}$ has the structure

$$\widetilde{Z} = \begin{bmatrix} 0 & x_1 + \mathrm{i}x_2 & x_3 + \mathrm{i}x_4 \\ x_1 - \mathrm{i}x_2 & 0 & x_5 + \mathrm{i}x_6 \\ x_3 - \mathrm{i}x_4 & x_5 - \mathrm{i}x_6 & 0 \end{bmatrix}, \quad x_i \in \mathbb{R},\ i = 1, ..., 6. \tag{3.7}$$

The characteristic polynomial is an invariant on the adjoint orbit and $Z \in \mathfrak{p}$ is unitary similar to S if and only if the characteristic polynomial of Z coincides with that of S. The three coefficients of the characteristic polynomial give the conditions

$$\text{(i) } \det \widetilde{Z} = 0, \quad \text{(ii) } \operatorname{tr} \widetilde{Z}\widetilde{Z}^* = 2 \quad \text{(iii) } \operatorname{tr} \widetilde{Z} = 0.$$

Hence the set of all maxima is the intersection of the orbit $\mathcal{O}(S)$ with the set of all matrices with structure given in Eq. (3.7). Condition (iii) gives no further information about the x_i's, but expressing (i) and (ii) in terms of the x_i's yields

$$\begin{array}{lll} \text{(i)} & x_1x_3x_5 + x_2x_4x_5 - x_2x_3x_6 + x_1x_4x_6 & = 0, \\ \text{(ii)} & x_1^2 + x_2^2 + x_3^2 + x_4^2 + x_5^2 + x_6^2 - 2 & = 0. \end{array} \tag{3.8}$$

The following argument shows that the set of solutions of (3.8) is not a manifold. Let $\phi : \mathbb{R}^6 \longrightarrow \mathbb{R}^2$ be given by

$$\phi(x_1, ..., x_6) = \begin{bmatrix} x_1x_3x_5 + x_2x_4x_5 - x_2x_3x_6 + x_1x_4x_6 \\ x_1^2 + x_2^2 + x_3^2 + x_4^2 + x_5^2 + x_6^2 - 2 \end{bmatrix}. \tag{3.9}$$

Let $\mathcal{M}$ denote the set of solution of (3.8). Then $\mathcal{M} = \phi^{-1}(0)$ and obviously $z^* := (\sqrt{2}, 0, 0, 0, 0, 0)$ solves (3.8). Suppose $\mathcal{M}$ is a manifold. Let

$$\begin{aligned} \gamma_1(t) &:= \sqrt{2}(\cos t, \sin t, 0, 0, 0, 0), \\ \gamma_2(t) &:= \sqrt{2}(\cos t, 0, \sin t, 0, 0, 0), \\ &\ \vdots \\ \gamma_5(t) &:= \sqrt{2}(\cos t, 0, 0, 0, 0, \sin t) \end{aligned}$$

denote the smooth curves with $\gamma_i(t) \subset \mathcal{M}$ for all $t \in \mathbb{R}$ and $\gamma_i(0) = z^*$, $i = 1, ..., 5$. The tangent space $T_{z^*}\mathcal{M}$ contains at least 5 linear independent vectors, so $\mathcal{M}$ has to be at least 5 dimensional. But it is easy to see that in any neighborhood of z^* there are points z with rank $D\phi(z) = 2$, hence $\phi^{-1}(z)$ is locally a 4 dimensional manifold. Therefore $\mathcal{M}$ cannot be a manifold.

For a further concretization of Algorithms 2.18 and 2.19 for minimizing the off-norm function (3.5), we derive explicit formulas for the sine and cosine of the step-size t_*. These formulas extend known formulas for symmetric matrices to our Lie algebraic setting.

Theorem 3.7. *Let f denote the off-norm function (3.5) and let $\Omega_\lambda \in \mathfrak{k}_\lambda$ be normalized as in Eq. (2.7). Denote by t_* the local minimum of $t \mapsto f(\mathrm{Ad}_{\exp t\Omega_\lambda} X)$ with smallest absolute value, according to Algorithm 2.2. Then*

$$\tan 2t_* = \frac{1}{\tau},$$

where $\tau := \frac{\lambda(X_0)}{2c_\lambda}$ and hence

$$\tan t_* = \min\{-\tau + \sqrt{1+\tau^2}, -\tau - \sqrt{1+\tau^2}\}.$$

Consequently,

$$\cos t_* = \frac{1}{\sqrt{1+\tan t_*^2}}, \qquad \sin t_* = \cos t_* \tan t_*.$$

Proof. Minimizing the off-norm

$$f(X) = \kappa(X - X_0, X - X_0) = \kappa(X, X) - \kappa(X_0, X_0)$$

on the adjoint orbit is, by the Ad-invariance of the Killing form, equivalent to maximizing $\kappa(X_0, X_0)$. Theorem 2.14 yields therefore that

$$\text{minimize} \quad f(\mathrm{Ad}_{\exp t\Omega_\lambda} X) \text{ with respect to } t$$

is equivalent to

$$\text{maximize} \quad g(t)(g(t) - \lambda(X_0)) \text{ with respect to } t, \tag{3.10}$$

where $g(t) = \frac{1}{2}\lambda(X_0)(1 - \cos 2t) - c_\lambda \sin 2t$. Now by Lemma 2.17, the values of $g(t)$ lie symmetric around $\frac{1}{2}\lambda(X_0)$ and therefore Eq. (3.10) is solved for $t = t_{\min}$ and $t = t_{\max}$ with $t_{\min}, t_{\max}$ as in Lemma 2.17. In any case $t_* = \pi$ if $\lambda(X_0) = 0$ and

$$\tan 2t_* = \frac{\sin 2t_{\min}}{\cos 2t_{\min}} = \frac{\sin 2t_{\max}}{\cos 2t_{\max}} = \frac{2c_\lambda}{\lambda(X_0)}$$

if $\lambda(X_0) \neq 0$. Now a standard trigonometric argument implies that $\tan t_* = 0$ if $c_\lambda = 0$ and $\tan t_* = -\tau \pm \sqrt{1+\tau^2}$ with $\tau = \frac{\lambda(X_0)}{2c_\lambda}$ if $c_\lambda \neq 0$. Since t_* is chosen to have minimal absolute value

$$\tan t_* = \min\{-\tau + \sqrt{1+\tau^2}, -\tau - \sqrt{1+\tau^2}\}.$$

The remaining assertions follow immediately. □

We close this section with the explicit cyclic Jacobi algorithm. For the general local convergence analysis we refer to Section 3.3. By comparison with the classical cyclic Jacobi algorithm on e.g. symmetric matrices it is seen that our formulas are direct generalizations of those for e.g. symmetric matrices, cf. [25].

Algorithm 3.8. For a given matrix $X \in \mathfrak{p}$, the following algorithm computes $(\sin t_*, \cos t_*)$ such that

$$\widetilde{X} := \mathrm{Ad}_{\exp t_* \Omega_\lambda} X$$

has no $\overline{\Omega}_\lambda$-component. Note that in the case where $\mathfrak{g}$ is a Lie algebra of matrices

$$\widetilde{X} = \exp(t_* \Omega_\lambda) X \exp(-t_* \Omega_\lambda).$$

ALGORITHM 3.8. PARTIAL STEP OF CLASSICAL JACOBI SWEEP.

function: $(\cos t_*, \sin t_*) = \text{classic.elementary.rotation}(X, \lambda)$
    Set $c_\lambda := \overline{\Omega}_i$-coefficient of X.
    Set $X_0 := \mathrm{p}(X)$.
    if $c_\lambda \neq 0$
        Set $\tau := \frac{\lambda(X_0)}{2c_\lambda}$.
        Set $\tan t_* := \min\{-\tau + \sqrt{1-\tau^2}, -\tau - \sqrt{1-\tau^2}\}$.
        Set $\cos t_* := 1/\sqrt{1+\tan t_*^2}$.
        Set $\sin t_* := \tan t_* \cos t_*$.
    else
        Set $(\cos t_*, \sin t_*) := (1, 0)$.
    endif
end classic.elementary.rotation

Remark 3.9. The algorithm is designed to compute $(\cos t_*, \sin t_*)$ of the step size t_*. Depending on the underlying matrix representation, however, it may happen that the elementary rotation $\mathrm{Ad}_{\exp t\Omega_\lambda}$ involves entries of the type $(\cos rt, \sin rt)$, cf. for example Section 4.6. In this case it is advisable to use standard trigonometric arguments to compute $\cos rt_*$, $\sin rt_*$ respectively, by means of $\cos t_*, \sin t_*$.

Let $d(X) := ||X - X_0||^2$ denote the squared distance from X to the maximal abelian subalgebra $\mathfrak{a}$. This coincides, up to a constant, with the off-norm function.

Algorithm 3.10. Given a Lie algebra element $S \in \mathfrak{p}$ and a tolerance $tol > 0$, the following algorithm overwrites S by φS where $\varphi \in \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ and $d(\varphi S) \leq tol$.

Algorithm 3.10. Classical Jacobi Algorithm.
Set $\varphi :=$ identity.
while $d(S) > tol$
  for $i = 1 : N$
    $(\cos t_*, \sin t_*) :=$ classical.elementary.rotation(S, λ_i).
    $\varphi := \mathrm{Ad}_{\exp t_* \Omega_i} \circ \varphi$.
    $S := \varphi S$.
  endfor
endwhile

3.2 The Generalized Trace Function and the Cyclic Sort-Jacobi

We have seen in the last section that the off-norm possesses undesired continua of critical points which are of no significance to the diagonalization task. An alternative – and more appropriate – approach is the following. Consider the trace function

$$X \longmapsto \mathrm{tr}(NX), \quad N = \mathrm{diag}(1, 2, ..., n),$$

on a similarity orbit of symmetric matrices, introduced by Brockett [6] for symmetric matrix diagonalization. This function has only finitely many critical points, with a unique local minimum and a unique local maximum. Moreover, the critical points coincide with the diagonal orbit elements and the (local) maximum and the (local) minimum are respectively characterized by an ordering property on the eigenvalues. This ordering will be of crucial interest when discussing the rate of convergence for irregular elements, i.e. in the case of multiple eigenvalues, a fact that van Kempen already noticed when investigating the convergence behavior of the special cyclic Jacobi method for symmetric matrices in 1966, cf. [64]. In the sequel, we will generalize these facts and results to the same Lie algebraic setting as in the previous section.
Thus let $\mathfrak{g}$ denote a semisimple Lie algebra with a Cartan decomposition. Denote by $C^- \subset \mathfrak{a}$ the negative of the fundamental Weyl chamber C^+ and let $N \in C^-$ be a regular element. Let $\mathcal{O}(S)$ denote the $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$-adjoint orbit of an element $S \in \mathfrak{p}$. It is shown in this section that the element $Z \in \mathcal{O}(S)$ with minimal distance to N lies in the closure of the Weyl chamber C^- and as such is our "diagonalization with ordered eigenvalues" of S. We illustrate the idea in Figure 3.1, where the projection of $\mathcal{O}(S)$

is drawn as a convex set in accordance with the convexity theorem of Kostant, cf. Theorem 1.65.

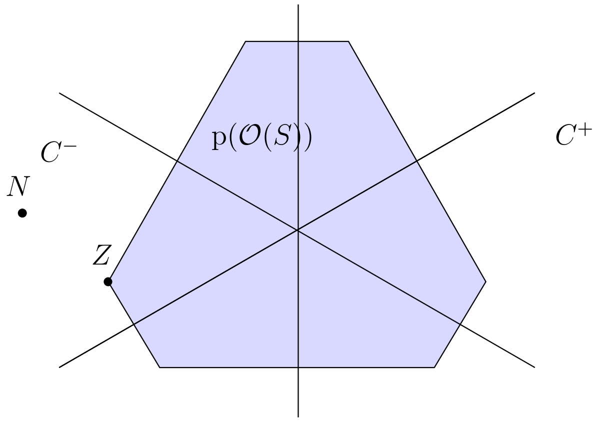

Figure 3.1: Motivation of the cost function.

Our goal is to minimize the distance function

$$\mathcal{O}(S) \longrightarrow \mathbb{R}, \quad X \longrightarrow B_\theta(X-N, X-N), \tag{3.11}$$

where $N \in C^-$, i.e. $\lambda(N) < 0$ for all $\lambda \in \Sigma^+$. This simplifies to

$$\begin{aligned} B_\theta(X-N, X-N) &= \kappa(X-N, X-N) = \kappa(X,X) + \kappa(N,N) - 2\kappa(X,N) \\ &= \kappa(S,S) + \kappa(N,N) - 2\kappa(X,N) \end{aligned}$$

because of $B_\theta|_\mathfrak{p} = \kappa|_\mathfrak{p}$ and the Ad-invariance of κ. Minimizing function (3.11) is therefore equivalent to maximizing the following function.

Definition 3.11. Let $S \in \mathfrak{p}$ and let $N \in \mathfrak{a}$ with $\lambda(N) < 0$ for all $\lambda \in \Sigma^+$. Let κ denote the Killing form. The *trace function* is given by

$$f\colon\ \mathcal{O}(S) \longrightarrow \mathbb{R}, \quad X \longmapsto \kappa(X, N). \tag{3.12}$$

An analysis of this Lie algebraic generalization of the function that R.W. Brockett discussed in [6] shows, that it has only finitely many critical points: the intersections of $\mathcal{O}(S)$ with $\mathfrak{a}$. This fact has been also noted by Bloch, Brockett and Ratiu in [3], where the trace function is studied on compact Lie algebras. For us, the trace function serves as a very suitable cost function in order to formulate Sort-Jacobi-type methods for a large variety of normal form problems, cf. Chapter 4. Furthermore, we obtain an easy-to-implement formula for the step size and prove local quadratic convergence.

Proposition 3.12. *(a) X is a critical point of the trace function* (3.12) *if and only if $X \in \mathfrak{a}$. In particular, there are only finitely many critical points.*

(b) *The trace function* (3.12) *has exactly one maximum, say Z, and one minimum, say $\widetilde{Z}$, and $\lambda(Z) \leq 0$, $\lambda(\widetilde{Z}) \geq 0$ for all $\lambda \in \Sigma^+$.*

Proof. (a) To compute the critical points, let $\Omega \in \mathfrak{k}$ and denote by $\xi = \mathrm{ad}_\Omega X$ an arbitrary tangent vector in $T_X\mathcal{O}(S)$. The ad-invariance of κ yields

$$Df(X)\xi = \kappa(\xi, N) = \kappa(\mathrm{ad}_\Omega X, N) = \kappa(\Omega, \mathrm{ad}_X N).$$

The Killing form is negative definite on $\mathfrak{k}$ and hence

$$Df(X) = 0 \quad \Longleftrightarrow \quad [X, N] = 0.$$

Since N is a regular element, it follows $X \in \mathfrak{a}$, cf. Lemma 1.47. From Corollary 1.63 it follows that $|\mathcal{O}(S) \cap \mathfrak{a}|$ is finite. (b) We compute the Hessian H_f at the critical points X. Denote by Ω_λ the $\mathfrak{k}_\lambda$-component of Ω. Then

$$\begin{aligned} \mathsf{H}_f(X)(\xi,\xi) &= \kappa(\mathrm{ad}_\Omega^2 X, N) = -\kappa(\mathrm{ad}_\Omega X, \mathrm{ad}_\Omega N) \\ &= -\sum_{\lambda \in \Sigma^+} \lambda(X)\,\lambda(N)\,\kappa(\Omega_\lambda, \Omega_\lambda). \end{aligned} \tag{3.13}$$

By assumption, $\lambda(N) < 0$ for all $\lambda \in \Sigma^+$, so by positive definiteness of κ on $\mathfrak{p}$ a necessary condition for a local maximum Z is that $\lambda(Z) \leq 0$ for all $\lambda \in \Sigma^+$. We know by Corollary 1.63 that the orbit $\mathcal{O}(S)$ intersects the closure of the Weyl chamber

$$C^- = \{H \in \mathfrak{a} \mid \lambda(H) < 0 \text{ for all } \lambda \in \Sigma^+\}$$

exactly once. Hence Z is the only local maximum of the function and by compactness of $\mathcal{O}(S)$ it is the unique global maximum. A similar argument proves the existence of a unique minimum, having all positive roots greater or equal to zero. □

We restrict the trace function (3.12) to the orbits of one-parameter subgroups in order to explicitly compute the step size t_*, cf. Eq. (2.5). Therefore, let $E_\lambda \in \mathfrak{g}_\lambda$ be a restricted-root vector that is normalized to

$$\lambda([E_\lambda, \theta E_\lambda]) = -2.$$

Let $\overline{\Omega}_\lambda := E_\lambda - \theta E_\lambda$, $\Omega_\lambda = E_\lambda + \theta E_\lambda$, $X \in \mathfrak{p}$ and consider the orbit of X under the adjoint action of the one parameter subgroup $\mathrm{Ad}_{\exp(t\Omega_\lambda)}$.

Theorem 3.13. *Let f be the trace function (3.12), $\Omega_\lambda \in \mathfrak{k}_\lambda$ as defined above and $X \in \mathfrak{p}$. Let*

$$c_\lambda = \frac{\kappa(X, \overline{\Omega}_\lambda)}{\kappa(\overline{\Omega}_\lambda, \overline{\Omega}_\lambda)}$$

be the $\overline{\Omega}_\lambda$-coefficient of X. Then *(a)* $f\left(\mathrm{Ad}_{\exp t\Omega_\lambda} X\right) = \kappa(X_0, N) - \dfrac{2\lambda(N)}{|\lambda|^2} g(t)$, *where* $g(t) = \frac{1}{2}\lambda(X_0)(1 - \cos(2t)) - c_\lambda \sin(2t)$.

(b) Let $t_* \in (-\frac{\pi}{2}, \frac{\pi}{2}]$ *be the (local) maximum of* $f\left(\mathrm{Ad}_{\exp t\Omega_\lambda} X\right)$*. Then*

$$\cos 2t_* = -\frac{\lambda(X_0)}{\sqrt{4c_\lambda^2 + \lambda(X_0)^2}}, \qquad \sin 2t_* = -\frac{2c_\lambda}{\sqrt{4c_\lambda^2 + \lambda(X_0)^2}}.$$

and hence

$$\cos t_* = \sqrt{\frac{1+\cos 2t_*}{2}}, \qquad \sin t_* = \begin{cases} \sqrt{\frac{1-\cos 2t_*}{2}} & \textit{if } \sin 2t_* \geq 0 \\ -\sqrt{\frac{1-\cos 2t_*}{2}} & \textit{if } \sin 2t_* < 0. \end{cases}$$

(c) $\lambda\left(\mathrm{p}\left(\mathrm{Ad}_{\exp t_*\Omega_\lambda} X\right)\right) = -\frac{1}{2}\sqrt{4c^2 + \lambda(X_0)^2} \leq 0.$

Proof. (a) The orthogonality of the projection $\mathrm{p}\colon \mathfrak{p} \longrightarrow \mathfrak{a}$ yields

$$f(X) = \kappa(X, N) = \kappa(\mathrm{p}(X), N).$$

Let $T_\lambda = [E_\lambda, \theta E_\lambda]$ be defined as in Eq. (1.18). By Theorem 2.14,

$$\begin{aligned} f\left(\mathrm{Ad}_{\exp t\Omega_\lambda} X\right) &= \kappa(X_0 + g(t)T_\lambda, N) \\ &= \kappa(X_0, N) - \frac{2\lambda(N)}{|\lambda|^2} g(t), \end{aligned} \tag{3.14}$$

where $g(t) = \frac{1}{2}\lambda(X_0)(1 - \cos(2t)) - c_\lambda \sin(2t)$ and the last identity holds since by definition $T_\lambda = -\frac{2}{|\lambda|^2} H_\lambda$. (b) Since by assumption $\lambda(N) < 0$, the second statement now follows immediately by Lemma 2.17 and a standard trigonometric argument. (c) follows immediately by Lemma 2.17. □

We present a Matlab-like pseudo code for the algorithm on semisimple Lie algebras. Note that in Chapter 4, the algorithm is exemplified in several cases.
Let $\mathfrak{g}$ be a semisimple Lie algebra with Cartan involution θ, corresponding Cartan decomposition $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ and $\mathfrak{a} \subset \mathfrak{p}$ a maximal abelian subalgebra. Let $\lambda \in \Sigma^+$ be a positive restricted root and let $\mathfrak{g}_\lambda$ be the corresponding restricted-root space. Let $E_\lambda \in \mathfrak{g}_\lambda$ be normalized to

$$\lambda([E_\lambda, \theta E_\lambda]) = -2, \tag{3.15}$$

cf. Eq. (1.18). Denote $\Omega_\lambda = E_\lambda + \theta E_\lambda$ and $\overline{\Omega}_\lambda = E_\lambda - \theta E_\lambda$. The orthogonal projection onto $\mathfrak{a}$ is denoted by p.

Algorithm 3.14. For a given $X \in \mathfrak{p}$, the following algorithm computes

$$(\sin t_*, \cos t_*, \sin 2t_*, \cos 2t_*),$$

such that

$$\widetilde{X} := \mathrm{Ad}_{\exp t_* \Omega_\lambda} X$$

has no $\overline{\Omega}_\lambda$-component and such that $\lambda(\widetilde{X}_0) \leq 0$. Note that in the case where $\mathfrak{g}$ is a Lie algebra of matrices

$$\widetilde{X} = \exp(t_* \Omega_\lambda) X \exp(-t_* \Omega_\lambda).$$

Algorithm 3.14. Partial Step of Jacobi Sweep.
function: $(\cos t_*, \sin t_*, \cos 2t_*, \sin 2t_*) = \text{elementary.rotation}(X, \lambda)$
  Set $c_\lambda := \overline{\Omega}_i$-coefficient of X.
  Set $X_0 := \mathrm{p}(X)$.
  Set $dis := \sqrt{\lambda(X_0)^2 + 4c_\lambda^2}$.
  if $dis \neq 0$
    Set $(\cos 2t_*, \sin 2t_*) := -\dfrac{1}{dis}\,(\lambda(X_0), 2c_\lambda)$.
  else
    Set $(\cos 2t_*, \sin 2t_*) := (1, 0)$.
  endif
  Set $\cos t_* := \sqrt{\frac{1+\cos 2t_*}{2}}$.
  if $\sin 2t_* \geq 0$
    Set $\sin t_* = \sqrt{\frac{1-\cos 2t_*}{2}}$.
  else
    Set $\sin t_* = -\sqrt{\frac{1-\cos 2t_*}{2}}$.
  endif
end elementary.rotation

Remark 3.15. The algorithm is designed to compute $(\cos t_*, \sin t_*, \cos 2t_*, \sin 2t_*)$ of the step size t_* since this is natural by the chosen normalization of the sweep directions Ω_i, cf. Eq. (1.19). Nevertheless, depending on the underlying matrix representation, it may happen that $\mathrm{Ad}_{\exp t\Omega_\lambda}$ involves entries of the type $(\cos rt, \sin rt)$ with $r \neq 1, 2$. In this case it is advisable to use standard trigonometric arguments to compute $\cos rt_*$, $\sin rt_*$ respectively, by means of $\cos t_*, \sin t_*, \cos 2t_*, \sin 2t_*$.

Denote by $d(X) := ||X - X_0||^2$ the squared distance from X to the maximal abelian subalgebra $\mathfrak{a}$. This coincides up to a constant with the off-norm.

Algorithm 3.16. Given a Lie algebra element $S \in \mathfrak{p}$ and a tolerance $tol > 0$, the following algorithm overwrites S by φS where $\varphi \in \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ and $d(\varphi S) \leq tol$.

ALGORITHM 3.16. SORT-JACOBI ALGORITHM.
Set $\varphi :=$ identity.
while $d(S) > tol$
  for $i = 1 : N$
    $(\cos t_*, \sin t_*, \cos 2t_*, \sin 2t_*) :=$ elementary.rotation(S, λ_i).
    $\varphi := \mathrm{Ad}_{\exp t_* \Omega_i} \circ \varphi$.
    $S := \varphi S$.
  endfor
endwhile

3.3 Local Quadratic Convergence

We have seen in Chapter 2 that local quadratic convergence for the Algorithm 2.19 optimizing a function f is guaranteed if the search directions form an orthogonal basis with respect to the Hessian at the fixed point Z, cf. Theorem 2.10. As we shall see in the first part of this section, this is the case for both the off-norm and the trace function, at least in the regular case. However, this holds no longer true in the case of clustered eigenvalues/singular values, and then another approach is needed. Therefore, it is necessary to gain a deeper understanding of the restricted-root systems, because they are the crucial ingredient to formulate a special ordering of the sweep directions that will ensure local quadratic convergence.

3.3.1 The Regular Case

We show that both the classical Jacobi algorithm 3.10 and the Sort-Jacobi algorithm 3.16 are locally quadratic convergent to a minimum of the off-norm function and the maximum of the trace function, respectively, if the element is regular, i.e. has all roots different to zero. In this case the order of optimizing along the different directions is irrelevant. We begin with the off-norm function.

Theorem 3.17. *Let f denote the off-norm function (3.5) and let Z be a minimum of f. Assume, that Algorithm 2.18 is implemented with pairwise orthogonal sweep directions $\Omega_i \in \mathfrak{k}_\lambda$, $i = 1, ..., \dim \mathfrak{g}_\lambda$. If Z is regular, then Algorithm 2.19 reducing f is locally quadratic convergent to Z.*

Proof. By Theorem 2.21, all we have to show is that (a) the Hessian of f in Z is nondegenerate and that (b) the set

$$\mathcal{B} := \{\mathrm{ad}_Z \Omega_i \mid i = 1, ..., m\}, \quad m = \sum_{\lambda \in \Sigma^+} \dim \mathfrak{k}_\lambda,$$

with $\Omega_i \in \mathfrak{k}_\lambda$ for suitable $\lambda \in \Sigma^+$ is orthogonal with respect to the Hessian of f at Z and $0 \notin \mathcal{B}$. (a) Let $\xi = \mathrm{ad}_\Omega Z \in T_Z\mathcal{O}(S)$ be an arbitrary tangent vector in $T_Z\mathcal{O}(S)$. By Propositions 3.2 and 3.5,

$$\mathsf{H}_f(Z)(\xi, \xi) = 2\kappa(\mathrm{ad}_\Omega Z, \mathrm{ad}_\Omega Z - \mathrm{p}(\mathrm{ad}_\Omega Z)).$$

Since $Z \in \mathfrak{a}$ and $\Omega \in \mathfrak{k}$ we have $\mathrm{ad}_\Omega Z \in \mathfrak{a}^\perp$ and hence $\mathrm{p}(\mathrm{ad}_\Omega Z) = 0$. Therefore

$$\mathsf{H}_f(Z)(\mathrm{ad}_\Omega Z, \mathrm{ad}_\Omega Z) = 2\kappa(\mathrm{ad}_\Omega Z, \mathrm{ad}_\Omega Z).$$

Since κ is positive definite on $\mathfrak{p}$, $\mathsf{H}_f(Z)$ is nondegenerate. (b) Now $\mathrm{ad}_Z\Omega_i = \lambda(Z)\overline{\Omega_i}$ for $\Omega_i \in \mathfrak{k}_\lambda$ and since by assumption Z is regular, i.e. $\lambda(Z) \neq 0$ for all $\lambda \in \Sigma$, 0 is not contained in $\mathcal{B}$. As Ω_i belongs to, say $\mathfrak{k}_\lambda$ and Ω_j to, say $\mathfrak{k}_\mu$, we can write $\Omega_i = E_\lambda + \theta E_\lambda$ and $\Omega_j = \widetilde{E}_\mu + \theta \widetilde{E}_\mu$. Orthogonality of E_λ and $\widetilde{E}_\mu$ is immediate by Theorem 1.42 if $\lambda \neq \mu$. If $\lambda = \mu$, this holds also true because the orthogonality of Ω_i and Ω_j implies

$$0 = B_\theta(\Omega_i, \Omega_j) = 2B_\theta(E_\lambda, \widetilde{E}_\lambda) + 2B_\theta(E_\lambda, \theta\widetilde{E}_\lambda).$$

The last term vanishes again by Theorem 1.42 since $\theta\widetilde{E}_\lambda \in \mathfrak{g}_{-\lambda}$. Hence

$$\mathsf{H}_f(Z)(\mathrm{ad}_{\Omega_i} Z, \mathrm{ad}_{\Omega_j} Z) = 2\kappa\big(\lambda(Z)(E_\lambda - \theta E_\lambda), \mu(Z)(\widetilde{E}_\mu - \theta\widetilde{E}_\mu)\big) = 0,$$

and therefore $\mathcal{B}$ is a basis of $T_Z\mathcal{O}(S)$ that is orthogonal with respect to the Hessian $\mathsf{H}_f(Z)$. □

We now derive the analogous result for the Sort-Jacobi algorithm 2.19. I.e. the Jacobi algorithm for maximizing the trace function converges locally quadratically fast to the maximum Z in the regular case, provided the sweep directions $\Omega_i \in \mathfrak{k}_\lambda$ are chosen to be orthogonal. Again, the order in working off the different elementary rotations is irrelevant.

Theorem 3.18. *Denote by f the trace function (3.12) and let Z be a maximum of f. Assume, that Algorithm 2.18 is implemented with pairwise orthogonal sweep directions $\Omega_i \in \mathfrak{k}_\lambda$, $i = 1, ..., \dim \mathfrak{g}_\lambda$. If Z is a regular element, then Algorithm 2.19 maximizing f is locally quadratic convergent to Z.*

Proof. By Theorem 2.10, it remains to show that the Hessian of f in Z is nondegenerate and that for the sweep directions Ω_i, the set $\{[Z, \Omega_i]\}$ forms a basis of $T_Z\mathcal{O}(S)$ that is orthogonal with respect to the Hessian of f. The Hessian is given by

$$\mathsf{H}_f(Z)(\xi, \xi) = \kappa(\mathrm{ad}_\Omega^2 Z, N) = -\kappa(\mathrm{ad}_Z\Omega, \mathrm{ad}_N\Omega),$$

cf. the proof of Proposition 3.12. For the sweep directions Ω_i we have $[Z, \Omega_i] = \lambda(Z)\overline{\Omega_i}$ for $\Omega_i \in \mathfrak{k}_\lambda$ and since by assumption Z is regular, $[Z, \Omega_i] \neq 0$ for all Ω_i. Orthogonality with respect to the Hessian is shown in a straightforward way, since for $\Omega_i = E_\lambda + \theta E_\lambda$ and $\Omega_j = E_\mu + \theta E_\mu$ the orthogonality of the Ω_i implies for $i \neq j$

$$\mathsf{H}_f(Z)(\mathrm{ad}_Z\Omega_i, \mathrm{ad}_Z\Omega_j) = \tfrac{1}{2}\big(\lambda(Z)\ \mu(N) + \lambda(N)\mu(Z)\big)\ \kappa(\overline{\Omega}_i, \overline{\Omega}_j) = 0.$$

□

3.3.2 On Abstract Root Systems

We briefly summarize those results on abstract root systems that are necessary for our proposes and refer to [45], Section II.5, for further details. The connection to restricted-root systems is explained. Let V be a finite dimensional real vector space with inner product $\langle\cdot,\cdot\rangle$ and norm squared $|\cdot|^2$. A subset $\Sigma \subset V$ is called an *abstract root system in V* if

(a) $0 \notin \Sigma$ and Σ is finite;

(b) the linear span of Σ is V;

(c) for $\alpha \in \Sigma$, the reflections

$$s_\alpha \colon V \longrightarrow V, \quad x \longmapsto x - \frac{2\langle x, \alpha\rangle}{|\alpha|^2}$$

carry Σ into itself;

(d) $\dfrac{2\langle \beta, \alpha\rangle}{|\alpha|^2}$ is an integer for $\alpha, \beta \in \Sigma$.

The following proposition motivates the investigation of abstract root systems.

Proposition 3.19. *The set $\{H_\lambda \mid \lambda(H) = B_\theta(H, H_\lambda)$ for all $H \in \mathfrak{a}, \lambda \in \Sigma\}$ is an abstract root system in $\mathfrak{a}$ and the set of restricted-roots Σ is an abstract root system in $\mathfrak{a}^*$, where the inner product $\langle\cdot,\cdot\rangle$ on $\mathfrak{a}^*$ is induced by B_θ.*

Proof. [45], Ch. VI, Sec. 5, Cor. 6.53. □

Examples of root systems can therefore be found in Example 1.46 and in Chapter 4. An abstract root system is said to be *reduced*, if $\alpha \in \Sigma$ implies $2\alpha \notin \Sigma$. For example, the restricted-root system (4.25) is not reduced if $p > q$. The root α is called *reduced*, if $\frac{1}{2}\alpha$ is not a root.

Proposition 3.20. *Let $\alpha \in \Sigma$ and $\beta \in \Sigma \cup \{0\}$.*

(a) Then $-\alpha \in \Sigma$.

(b) If α is reduced, then $\pm\alpha, \pm 2\alpha$, and 0 are the only members of $\Sigma \cup \{0\}$ proportional to α. ($\pm 2\alpha$ cannot occur if Σ is reduced.)

(c) One has

$$\frac{2\langle \alpha, \beta\rangle}{|\alpha|^2} \in \{0, \pm 1, \pm 2, \pm 3, \pm 4\},$$

and ± 4 occurs only in a nonreduced system with $\beta = 2\alpha$.

(d) If α and β are nonproportional and $|\alpha| \leq |\beta|$, then

$$\frac{2\langle\alpha,\beta\rangle}{|\beta|^2} \in \{0, \pm 1\}.$$

(e) If $\langle\alpha,\beta\rangle > 0$, then $\alpha - \beta$ is a root or zero. If $\langle\alpha,\beta\rangle < 0$, then $\alpha + \beta$ is a root or zero. Consequently, if neither $\alpha + \beta$ nor $\alpha - \beta$ are in $\Sigma \cup \{0\}$, then $\langle\alpha,\beta\rangle = 0$.

Proof. (a) This is immediate since $s_\alpha(\alpha) = -\alpha$. (b) Let $\alpha, c\alpha \in \Sigma$. Then both, $2\langle c\alpha,\alpha\rangle/|\alpha|^2$ and $2\langle\alpha, c\alpha\rangle/|c\alpha|^2$ are integers, implying that $2/c$ and $c/2$ are integers. since α is reduced, $c \neq \frac{1}{2}$ and hence the only possibilities are $c = \pm 1$ or $c = \pm 2$. If Σ is reduced, the latter case cannot occur. (c) We may assume that $\beta \neq 0$. The Cauchy-Schwarz inequality yields

$$\left| \frac{2\langle\alpha,\beta\rangle}{|\alpha|^2} \frac{2\langle\alpha,\beta\rangle}{|\beta|^2} \right| \leq 4$$

and equality only holds if $\beta = c\alpha$, cf. part (b). Otherwise $\frac{2\langle\alpha,\beta\rangle}{|\alpha|^2}$ and $\frac{2\langle\alpha,\beta\rangle}{|\beta|^2}$ are two integers whose product is less than or equal to three and the assertion follows. (d) The following inequality of integers

$$\left| \frac{2\langle\alpha,\beta\rangle}{|\alpha|^2} \right| \geq \left| \frac{2\langle\alpha,\beta\rangle}{|\beta|^2} \right|$$

together with the fact that their product is less than or equal to 3, cf. proof of (c), yields the assertion. (e) We may assume that α and β are not proportional. Assume that $|\alpha| \leq |\beta|$. Then $s_\beta(\alpha) = \alpha - \frac{2\langle\alpha,\beta\rangle}{|\beta|^2}\beta$ must be $\alpha - \beta$ by (d) and the first statement follows. For the second statement replace α by $-\alpha$. The last assertion then is an immediate consequence. Cf. [45], Sec. II.5, Prop. 2.48. □

Now let $\Sigma^+ \subset \Sigma$ be a set of positive roots defined analogously as in Definition 1.53. A root $\alpha \in \Sigma^+$ is called *simple*, if it is not the sum of two positive roots. We denote the set of simple roots by Π. The following result holds.

Proposition 3.21. *With $l = \dim V$, there are l simple roots $\alpha_1, ..., \alpha_l$ and they form a basis of V. Furthermore, any $\beta \in \Sigma^+$ can be written as*

$$\beta = \sum_{i=1}^{l} c_i \alpha_i, \quad \textit{with non-negative integers } c_i.$$

Proof. Cf. [45], Ch. II, Sec. 5, Prop. 2.49. □

Proposition 3.21 allows to introduce an ordering on V that is compatible with the already introduced notion of positivity in the sense that all positive roots are greater than 0, cf. Corollary 3.23.

Definition 3.22 (lexicographic ordering)**.** Let $\{\alpha_1, ..., \alpha_l\} = \Pi$ be the set of simple roots and let

$$x = \sum_{i=1}^{l} x_i \alpha_i.$$

We say that $x > 0$ if there exists an index k such that $x_1 = ... = x_{k-1} = 0$ and $x_k > 0$. Furthermore, we define $x > y :\Longleftrightarrow x - y > 0$.

It is clear that the introduced ordering depends on the enumeration of the simple roots. We denote the set of simple roots by $(\Pi, >)$, if Π is endowed with an enumeration that determines $>$. Furthermore, we equivalently write $\alpha < \beta$ if $\beta > \alpha$.

Corollary 3.23. *The restricted-root λ is contained in Σ^+ if and only if $\lambda > 0$.*

Proof. The lemma is an immediate consequence of Proposition 3.21 and the above definition. □

Now let $\mathfrak{g}$ be a semisimple Lie algebra with Cartan decomposition $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ and let $\mathfrak{a} \subset \mathfrak{p}$ be maximal abelian. Let $(\Pi, >)$ be the simple roots of the positive restricted-roots Σ^+. Note that $\alpha_1 < \alpha_2 < ... < \alpha_{\max}$ by definition of $>$. Let

$$\mathfrak{g}^{\alpha_k} := \langle \mathfrak{g}_{\pm\alpha_k}, \mathfrak{g}_{\pm\alpha_{k-1}}, ..., \mathfrak{g}_{\pm\alpha_1} \rangle_{LA}$$

denote the Lie subalgebra of $\mathfrak{g}$ generated by the restricted-root spaces $\mathfrak{g}_{\alpha_i}$ and $\mathfrak{g}_{-\alpha_i}$, $1 \leq i \leq k$. By Theorem 1.42 it is immediate to see that

$$\mathfrak{g}^{\alpha_k} = \sum_{\{\lambda \in \Sigma \mid \lambda = \sum_{i=1}^{k} c_i \alpha_i\}} \mathfrak{g}_\lambda \oplus \mathfrak{g}_0^{\alpha_k}, \tag{3.16}$$

with $\mathfrak{g}_0^{\alpha_k} := \mathfrak{g}_0 \cap \mathfrak{g}^{\alpha_k}$. Moreover, $\mathfrak{g}^{\alpha_k}$ is semisimple with Cartan decomposition

$$\mathfrak{g}^{\alpha_k} = (\mathfrak{g}^{\alpha_k} \cap \mathfrak{k}) \oplus (\mathfrak{g}^{\alpha_k} \cap \mathfrak{p}).$$

The restricted-root space decomposition of $\mathfrak{g}^{\alpha_k}$ is given by Eq. (3.16). We denote the set of the corresponding restricted roots by

$$\Sigma_k := \Sigma(\mathfrak{g}^{\alpha_k}) = \{\lambda \in \Sigma \mid \lambda = \sum_{i=1}^{k} c_i \alpha_i\}.$$

Obviously the inclusions

$$\mathfrak{g}^{\alpha_1} \subset \mathfrak{g}^{\alpha_2} \subset ... \subset \mathfrak{g}^{\alpha_{\max}} \subset \mathfrak{g} \tag{3.17}$$

and

$$\Sigma_1 \subset \Sigma_2 \subset ... \subset \Sigma_{\max} = \Sigma. \tag{3.18}$$

hold. We further use the notation

$$\Sigma_i^+ := \Sigma_i \cap \Sigma^+.$$

Example 3.24. Consider the Lie algebra $\mathfrak{g} = \mathfrak{sl}(4, \mathbb{R})$. The restricted-root space decomposition is analogously to Example 1.46 if we choose

$$\mathfrak{a} = \left\{ \begin{bmatrix} a_1 & & \\ & \ddots & \\ & & a_4 \end{bmatrix} \mid \sum_{i=1}^{4} a_i = 0 \right\}$$

as the maximal abelian subspace in $\mathfrak{p}$. The restricted roots are given by $H \mapsto \pm(a_i - a_j)$, $1 \leq i < j \leq 4$, $H \in \mathfrak{a}$. For simplicity of notation we shortly write $a_i - a_j$ instead of $H \mapsto a_i - a_j$. It is easy to see that $\Sigma^+ := \{\pm(a_i - a_j), 1 \leq i < j \leq 4\}$ is a possible choice for the positive roots. Then, the simple system is given by $\Pi = \{a_1 - a_2, a_2 - a_3, a_3 - a_4\}$. Now let $\alpha_1 := a_3 - a_4, \alpha_2 := a_2 - a_3, \alpha_3 := a_1 - a_2$, then

$$\mathfrak{g}^{\alpha_1} \cong \mathfrak{sl}(2, \mathbb{R}), \quad \mathfrak{g}^{\alpha_2} \cong \mathfrak{sl}(3, \mathbb{R}) \quad \text{and } \mathfrak{g}^{\alpha_3} = \mathfrak{sl}(4, \mathbb{R})$$

and

$$\Sigma_1^+ = \{\alpha_1\}, \quad \Sigma_2^+ = \{\alpha_2, \alpha_2 + \alpha_1\} \cup \Sigma_1^+, \quad \Sigma_3^+ = \{\alpha_3, \alpha_3 + \alpha_2, \alpha_3 + \alpha_1\} \cup \Sigma_2^+, \quad \Sigma_4^+ = \Sigma^+.$$

Proposition 3.25. *Let $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ be a Cartan decomposition of $\mathfrak{g}$ and denote by $\alpha_{\max}$ the greatest simple root. Then*

$$\mathfrak{g}^{\alpha_{\max}} = \mathfrak{p} \oplus [\mathfrak{p}, \mathfrak{p}] = \langle \mathfrak{p} \rangle_{LA} \tag{3.19}$$

and $\mathfrak{g}^{\alpha_{\max}}$ is an ideal in $\mathfrak{g}$.

Proof. The second equality of Eq. (3.19) is obvious, since Theorem 1.33 (a) implies $[\mathfrak{p}, [\mathfrak{p}, \mathfrak{p}]] \subset \mathfrak{p}$. To see the first equality, note that the inclusion $\mathfrak{p} \oplus [\mathfrak{p}, \mathfrak{p}] \subset \mathfrak{g}^{\alpha_{\max}}$ holds, since $\mathfrak{p} \subset \mathfrak{g}^{\alpha_{\max}}$ by Theorem 1.42. Now choose a basis $\mathcal{C} = \{E_\lambda^{(1)}, ..., E_\lambda^{(\dim \mathfrak{g}_\lambda)} \mid \lambda \in \Sigma^+\}$ of

$$\sum_{\lambda \in \Sigma^+} \mathfrak{g}_\lambda.$$

Then, by Proposition 1.52 (a), $\langle \mathcal{C} \cup \theta\mathcal{C} \rangle_{LA} = \mathfrak{g}^{\alpha_{\max}}$ and part (b) of 1.52 implies that $\mathfrak{g}^{\alpha_{\max}} \subset \langle \mathfrak{p} \rangle_{LA}$. The fact that $\mathfrak{g}^{\alpha_{\max}}$ is an ideal in $\mathfrak{g}$ follows now from Eq. (3.19). We have

$$[\mathfrak{g}, \mathfrak{p} \oplus [\mathfrak{p}, \mathfrak{p}]] = [\mathfrak{k} \oplus \mathfrak{p}, \mathfrak{p} \oplus [\mathfrak{p}, \mathfrak{p}]] \subset [\mathfrak{k}, \mathfrak{p}] \oplus [\mathfrak{k}, [\mathfrak{p}, \mathfrak{p}]] \oplus [\mathfrak{p}, \mathfrak{p}] \oplus [\mathfrak{p}, [\mathfrak{p}, \mathfrak{p}]].$$

Now using the Jacobi-identity, we obtain $[\mathfrak{k}, [\mathfrak{p}, \mathfrak{p}]] \subset [\mathfrak{p}, [\mathfrak{k}, \mathfrak{p}]] \subset [\mathfrak{p}, \mathfrak{p}]$ and the proof is complete. □

Corollary 3.26. *If $\mathfrak{g}$ is simple with nontrivial Cartan decomposition $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$, then $\mathfrak{g} = \mathfrak{g}^{\alpha_{\max}}$.*

Proof. By Proposition 3.25, $\mathfrak{g}^{\alpha_{\max}}$ is an ideal. Since $0 \neq \mathfrak{p} \subset \mathfrak{g}^{\alpha_{\max}}$, it can not be trivial, hence $\mathfrak{g} = \mathfrak{g}^{\alpha_{\max}}$. □

The abstract root system Σ is said to be *irreducible*, if it does not decompose into a nontrivial disjoint union $\Sigma = \Sigma' \cup \Sigma''$ such that every elements of Σ' are orthogonal to every elements of Σ''. Otherwise it is called *reducible*. One can show that the root system of a complex semisimple Lie algebra $\mathfrak{g}$ is irreducible if and only if $\mathfrak{g}$ is simple, cf. [45], Ch. II, Sec. 5, Prop. 2.44. This is in general not true for real semisimple Lie algebras and their restricted roots, as the following example shows.

Example 3.27. Let $\mathfrak{g} = \mathfrak{so}(3,\mathbb{R}) \oplus \mathfrak{sl}(3,\mathbb{R})$. Then $\mathfrak{g}$ is semisimple but not simple and its Cartan decomposition yields $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ with

$$\mathfrak{k} = \mathfrak{so}(3,\mathbb{R}) \oplus \mathfrak{so}(3,\mathbb{R}), \quad \mathfrak{p} = \mathfrak{k}^{\perp},$$

and the maximal abelian subspace $\widetilde{\mathfrak{a}} = 0 \oplus \mathfrak{a} \subset \mathfrak{p}$ with $\mathfrak{a}$ given as in Example 1.46. The restricted-root system however is the same as in Example 1.46, hence irreducible.

Nevertheless, we have the following result for restricted-root systems.

Proposition 3.28. *Let Σ be the restricted-root system of a semisimple Lie algebra $\mathfrak{g}$ with nontrivial Cartan decomposition $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$. Then Σ is irreducible, if and only if $\mathfrak{g}^{\alpha_{\max}}$ is simple.*

For the proof we follow the line of [45], Ch. II, Prop. 2.44.

Proof. "$\Rightarrow$". We have seen in Proposition 3.25, that $\mathfrak{g}^{\alpha_{\max}}$ is an ideal in $\mathfrak{g}$. Assume that $\mathfrak{g}^{\alpha_{\max}}$ is semisimple but not simple, i.e. $\mathfrak{g}^{\alpha_{\max}}$ decomposes into two nontrivial ideals $\mathfrak{g}^{\alpha_{\max}} = \mathfrak{g}' \oplus \mathfrak{g}''$. Let $\lambda \in \Sigma$ and decompose $X \in \mathfrak{g}_\lambda$ accordingly to $X = X' + X''$. For any $H \in \mathfrak{a}$ one has

$$0 = [H,X] - \lambda(H)X = ([H,X'] - \lambda(H)X') + ([H,X''] - \lambda(H)X'').$$

Both terms on the right are separately equal to zero since $\mathfrak{g}' \cap \mathfrak{g}'' = \{0\}$ and therefore X' and X'' are both in the restricted-root space $\mathfrak{g}_\lambda$. Suppose now that $X' \neq 0$. From Lemma 1.49 it follows that $[X', \theta X'] = cH_\lambda$ with $c < 0$. Furthermore, $[X', \theta X'] \in \mathfrak{g}'$, and hence

$$0 = [X'', [X', \theta X']] = [X'', cH_\lambda] = c|\lambda|^2 X'',$$

implying $X'' = 0$. Hence $\mathfrak{g}_\lambda \subset \mathfrak{g}'$ and by defining

$$\Sigma' := \{\lambda \in \Sigma \mid \mathfrak{g}_\lambda \subset \mathfrak{g}'\}, \quad \Sigma'' := \{\lambda \in \Sigma \mid \mathfrak{g}_\lambda \subset \mathfrak{g}''\},$$

we get $\Sigma = \Sigma' \cup \Sigma''$ disjointly. To prove mutual orthogonality, let $\lambda' \in \Sigma'$, $X \in \mathfrak{g}_{\lambda'} \setminus \{0\}$ and $\lambda'' \in \Sigma''$, $Y \in \mathfrak{g}_{\lambda''} \setminus \{0\}$. We have

$$\lambda'(H_{\lambda''})X = [H_{\lambda''}, X] \subseteq [H_{\lambda''}, \mathfrak{g}'] = [[Y, \theta Y], \mathfrak{g}'] \subseteq [\mathfrak{g}'', \mathfrak{g}'] = \{0\}.$$

"$\Leftarrow$". Suppose that Σ is reducible, i.e. $\Sigma = \Sigma' \cup \Sigma''$. Then $\mathfrak{g}^{\alpha_{\max}} = \mathfrak{g}' \oplus \mathfrak{g}''$ as vector spaces with

$$\mathfrak{g}' := \langle \mathfrak{g}_\lambda \mid \lambda \in \Sigma' \rangle_{LA}, \quad \mathfrak{g}'' = \langle \mathfrak{g}_\lambda \mid \lambda \in \Sigma'' \rangle_{LA}$$

by Eq. (3.16). It remains to show that $\mathfrak{g}'$ and $\mathfrak{g}''$ are ideals in $\mathfrak{g}^{\alpha_{\max}}$. Therefore, let $X \in \mathfrak{g}_{\lambda''} \subset \mathfrak{g}''$. For any $H_{\lambda'} \in \mathfrak{g}' \cap \mathfrak{a}$ we have

$$[H_{\lambda'}, X] = \lambda''(H_{\lambda'})X = 0,$$

by the assumed orthogonality of λ' and λ''. Also, if $[\mathfrak{g}_{\lambda'}, \mathfrak{g}_{\lambda''}] \neq 0$, then by Theorem 1.42, $\lambda' + \lambda''$ would be a root, neither orthogonal to λ', nor to λ'' in contradiction to the orthogonal decomposition of Σ, hence

$$[\mathfrak{g}_{\lambda'}, \mathfrak{g}_{\lambda''}] = 0.$$

It follows that $[\mathfrak{g}', \mathfrak{g}_{\lambda''}] = 0$. Since $[\mathfrak{g}', \mathfrak{a}] \subset [\mathfrak{g}']$ and since $\mathfrak{g}'$ is a subalgebra of $\mathfrak{g}^{\alpha_{\max}}$, we conclude that $\mathfrak{g}'$ is an ideal of $\mathfrak{g}^{\alpha_{\max}}$. An analogous proof yields that $\mathfrak{g}''$ is an ideal of $\mathfrak{g}^{\alpha_{\max}}$. □

3.3.3 The Irregular Case

Before we elaborate on the Lie algebraic tools necessary to handle the irregular case in full generality, we first discuss the rather well understood real symmetric EVD with multiple eigenvalues [64].

Let $S = S^\top \in \mathbb{R}^{n \times n}$. The *Special Cyclic Jacobi Method* annihilates the off-diagonal entries of S in the natural order, i.e. the entries $(1,2), (1,3), ..., (1,n), (2,3), ...(2,n), ...,$ $(n-1,n)$ are annihilated successively, as shown in Fig. 3.2.

$$\begin{bmatrix} \circ & \star & \circ & \circ & \circ \\ \star & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \star & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \star & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \star & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \star & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \circ & \star \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \star & \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow$$

$$\begin{bmatrix} \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \star & \circ & \circ \\ \circ & \star & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \star & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \star & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow \ldots \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \star \\ \circ & \circ & \circ & \star & \circ \end{bmatrix}$$

Figure 3.2: Special cyclic sweep for the symmetric EVD.

Van Kempen investigated the local convergence behavior for the Special Cyclic Jacobi Method in the case where S has eigenvalues of multiplicities greater than one [64]. This special Jacobi method reduces the off-norm and for the local quadratic convergence analysis he had to require that the diagonal elements of S which converge to the same eigenvalue occupy successive positions on the diagonal. This property can not be ensured for methods that minimize the off-norm since *all* diagonalizations are

(global) minima. In contrast, for the trace function (i.e. Sort-Jacobi methods) the maximum is unique and fulfills this condition a priori, cf. Proposition 3.12.
Although in this chapter we adopt the ideas of van Kempen, the proof of our main theorem is based on a more geometric approach involving the results of Chapter 2.
Since every semisimple Lie algebra is the direct sum of simple ones, cf. Theorem 1.16, we can restrict without loss of generality the analysis of the convergence behavior for the irregular case to simple Lie algebras.
Let Σ be a restricted-root system arising from a Cartan decomposition $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ of a simple Lie algebra $\mathfrak{g}$. Let $\Sigma^+ \subset \Sigma$ be a set of positive roots and let $\Pi \subset \Sigma^+$ be the simple roots of Σ^+. Define an ordering in Σ in the sense of Definition 3.22 that is determined by some enumeration of the simple roots. We will further make use of the notation established in the previous subsection.

Definition 3.29 (SCS-condition). Let Σ be a restricted-root system of the simple Lie algebra $\mathfrak{g}$ (Hence Σ is irreducible, cf. Corollary 3.26 and Proposition 3.28). Assume that the simple system $\Pi = \{\alpha_1, ..., \alpha_{\max}\}$ admits an enumeration such that

(I) for every k and every $j \leq k$ there exists a $\lambda = \sum_{i=1}^{k} c_i \alpha_i \in \Sigma_k^+ \setminus \Sigma_{k-1}^+$ with $c_j \neq 0$;

(II) if $\lambda, \mu \in \Sigma_k^+ \setminus \Sigma_{k-1}^+$ and $\lambda = \sum_{i=1}^{k} c_i \alpha_i < \mu = \sum_{i=1}^{k} d_i \alpha_i$ then $c_j \neq 0$ implies $d_j \neq 0$ for all $j = 1, ..., k$.

In this case we say that $(\Pi, >)$ satisfies the ***S****pecial-*__*C*__*yclic-*__*S*__*weep*-condition.

Example 3.30. Consider Example 3.24. It is easy to see that the proposed enumeration satisfies the SCS-condition. In fact, for $\mathfrak{g} = \mathfrak{sl}(n, \mathbb{R})$ with the usual Cartan decomposition (see Appendix A.1) and with simple root system

$$\Pi = \{a_1 - a_2, a_2 - a_3, ..., a_{n-1} - a_n\}$$

there are several enumerations that satisfy the SCS-condition.

(a) Let $\alpha_i := a_i - a_{i+1}$, $1 \leq i \leq n-1 =: \max$. Then all positive roots are given by $a_k - a_{l+1} = \sum_{i=k}^{l} \alpha_l$, $1 \leq k \leq l \leq n-1$ and

$$\Sigma_1^+ = \{\alpha_1\},\ \Sigma_2^+ \setminus \Sigma_1^+ = \{\alpha_2, \alpha_2 + \alpha_1\}, ...$$

$$..., \Sigma_k^+ \setminus \Sigma_{k-1}^+ = \left\{ \sum_{i=l}^{k} \alpha_i \mid 1 \leq l \leq k \right\}.$$

Hence SCS-condition (I) is fulfilled. SCS-condition (II) also holds because if $\lambda, \mu \in \Sigma_k^+ \setminus \Sigma_{k-1}^+$ with $\lambda < \mu$, then $\mu = \lambda + \tilde{\lambda}$ for a suitable $\tilde{\lambda} \in \Sigma^+$.

(b) An analogous argument as in (a) shows that reversing the enumeration in (a), i.e. defining $\alpha_i = a_{n-i} - a_{n-i+1}$, $1 \leq i \leq n-1 =: \max$, also satisfies the SCS-condition.

(c) Consider now the case $n = 5$. We define

$$\alpha_1 := a_2 - a_3,\ \alpha_2 := a_3 - a_4,\ \alpha_3 := a_1 - a_2,\ \alpha_4 := a_4 - a_5.$$

This yields

$$\begin{aligned}
&\Sigma_1^+ = \{\alpha_1\},\\
&\Sigma_2^+ \setminus \Sigma_1^+ = \{\alpha_2, \alpha_1 + \alpha_2\},\\
&\Sigma_3^+ \setminus \Sigma_2^+ = \{\alpha_3, \alpha_3 + \alpha_1, \alpha_3 + \alpha_1 + \alpha_2\},\\
&\Sigma_4^+ \setminus \Sigma_3^+ = \{\alpha_4, \alpha_4 + \alpha_2, \alpha_4 + \alpha_1 + \alpha_2, \alpha_4 + \alpha_1 + \alpha_2 + \alpha_3\}
\end{aligned}$$

and hence the SCS-condition is fulfilled.

Example 3.31. Let $\mathfrak{g} = \mathfrak{so}(3,3)$ with Cartan decomposition as in Section 4.2. The positive restricted roots are given by

$$\Sigma^+ = \{a_1 \pm a_2, a_1 \pm a_3, a_2 \pm a_3\},$$

cf. Eq. (4.8) and the set of simple roots is

$$\Pi = \{a_1 - a_2, a_2 - a_3, a_2 + a_3\}.$$

Let

$$\alpha_1 := a_1 - a_2, \quad \alpha_2 := a_2 - a_3, \quad \text{and} \quad \alpha_3 := a_2 + a_3,$$

then $\Sigma^+ = \{\alpha_1, \alpha_2, \alpha_3, \alpha_1 + \alpha_2, \alpha_1 + \alpha_3, \alpha_1 + \alpha_2 + \alpha_3\}$ and $(\Pi, >)$ satisfies the SCS-condition. In fact, we have

$$\begin{aligned}
&\Sigma_1^+ = \{\alpha_1\},\\
&\Sigma_2^+ \setminus \Sigma_1^+ = \{\alpha_2, \alpha_2 + \alpha_1\},\\
&\Sigma_3^+ \setminus \Sigma_2^+ = \{\alpha_3, \alpha_3 + \alpha_1, \alpha_3 + \alpha_1 + \alpha_2\},
\end{aligned}$$

whereas an enumeration

$$\alpha_1 := a_2 + a_3, \quad \alpha_2 := a_2 - a_3, \quad \text{and} \quad \alpha_3 := a_1 - a_2,$$

violates for $k = 2$ condition (I) in Definition 3.29, because

$$\begin{aligned}
&\Sigma_1^+ = \{\alpha_1\},\\
&\Sigma_2^+ \setminus \Sigma_1^+ = \{\alpha_2\},\\
&\Sigma_3^+ \setminus \Sigma_2^+ = \{\alpha_3, \alpha_3 + \alpha_1, \alpha_3 + \alpha_2, \alpha_1 + \alpha_2 + \alpha_3\}.
\end{aligned}$$

Example 3.32. Let $\mathfrak{g} = \mathfrak{su}(m,2)$, $m > 2$, with Cartan decomposition as in Appendix A.7. The positive restricted roots are given by

$$\Sigma^+ = \{a_1, a_2, a_1 \pm a_2, 2a_1, 2a_2\}.$$

The set of simple roots is given by

$$\Pi = \{a_2, a_1 - a_2\}.$$

Choosing $\alpha_1 := a_2$ and $\alpha_2 := a_1 - a_2$ yields $\Sigma^+ = \{\alpha_1 + \alpha_2, \alpha_1, \alpha_2 + 2\alpha_1, \alpha_2, 2\alpha_2 + 2\alpha_1, 2\alpha_1\}$. and the SCS-condition is satisfied because

$$\Sigma_1^+ = \{\alpha_1, 2\alpha_1\}, \quad \Sigma_2^+ \setminus \Sigma_1^+ = \{\alpha_2, \alpha_2 + \alpha_1, \alpha_2 + 2\alpha_1, 2\alpha_2 + 2\alpha_1\}.$$

However, the enumeration $\alpha_1 := a_1 - a_2$, $\alpha_2 := a_2$ yields $\Sigma^+ = \{\alpha_1 + \alpha_2, \alpha_2, \alpha_1 + 2\alpha_2, \alpha_1, 2\alpha_1 + 2\alpha_2, 2\alpha_2\}$ and leads to a violation of condition (II) in Definition 3.29, because $\Sigma_1^+ = \{\alpha_1\}$ and $\Sigma_2^+ \setminus \Sigma_1^+$ contains the elements

$$\alpha_2 < \alpha_1 + \alpha_2 < 2\alpha_2 < 2\alpha_2 + \alpha_1 < 2\alpha_2 + 2\alpha_1.$$

Note, that by Proposition 3.28, condition (I) in Definition 3.29 is only meaningful for simple $\mathfrak{g}^{\alpha_{\max}}$, which is guaranteed by Corollary 3.26 if we restrict to simple Lie algebras $\mathfrak{g}$. In fact, assume that the restricted-root system Σ of $\mathfrak{g}^{\alpha_{\max}}$ is reducible and decomposes into $\Sigma = \Sigma' \cup \Sigma''$. Let $\Pi = \Pi' \cup \Pi''$ be the union of the corresponding simple root systems and let $<$ be induced by an arbitrary enumeration of Π. We can assume without loss of generality that the smallest simple root α_1 lies in Π'. Then for the smallest root α_j in Π'' we have

$$\Sigma_j^+ \setminus \Sigma_{j-1}^+ \subset \{k\alpha_j, \mid k \in \mathbb{N}\}, \tag{3.20}$$

since every positive root $\lambda \in \Sigma^+$ is a linear combination of either elements of Π' or of Π''. Thus SCS-condition (I) is violated.
In order to distinguish different cyclic schemes for the Jacobi sweep in Algorithm 2.18, we introduce the following notation.

Definition 3.33. Let $\lambda_1, ..., \lambda_k \in \Sigma^+$ be different positive restricted roots. Denote the elementary rotations in Algorithm 2.18 as before by

$$r_\Omega(X) = \mathrm{Ad}_{\exp t_*(X)\Omega} X, \tag{3.21}$$

where Ω lies in some $\mathfrak{k}_\lambda$, cf. Eq. (2.15). Then

$$\widetilde{s} := r_{\Omega_k} \circ r_{\Omega_{k-1}} \circ ... \circ r_{\Omega_1}$$

is called a *partial sweep of type* $(\lambda_1, ..., \lambda_k)$, if the Ω_i are orthogonal with respect to B_θ and if the elementary rotations are successively applied in an order such that

$$\begin{aligned}
&\{\Omega_1, ..., \Omega_{r_1}\} \text{ is a basis of } \mathfrak{k}_{\lambda_1},\\
&\{\Omega_{r_1+1}, ..., \Omega_{r_1+r_2}\} \text{ is a basis of } \mathfrak{k}_{\lambda_2},\\
&\qquad\vdots\\
&\{\Omega_{r_1+...+r_{k-1}}, ..., \Omega_m\} \text{ is a basis of } \mathfrak{k}_{\lambda_k},
\end{aligned}$$

where $m = \sum_{\lambda\in\Sigma^+} \dim \mathfrak{k}_\lambda$.

The following definition now generalizes the special cyclic Jacobi method for the symmetric eigenvalue problem [21].

Definition 3.34 (Special Cyclic Sweep). Let Σ^+ be a set of positive roots and let $(\Pi, >)$ satisfy the SCS-condition 3.29.

(a) A *special k-th row sweep* $s_k^\sharp$ is a partial sweep of type $(\lambda_1, ..., \lambda_n)$ with $\{\lambda_i \mid i = 1, ..., n\} = \Sigma_k^+ \setminus \Sigma_{k-1}^+$ and $\lambda_1 < \lambda_2 < ... < \lambda_n < \alpha_{k+1}$. Note, that $\lambda_1 = \alpha_k$.

(b) A *special sweep for* $\mathfrak{g}^{\alpha_k}$ is a partial sweep that consists of special row sweeps ordered as
$$s_k := s_1^\sharp \circ s_2^\sharp \circ ... \circ s_k^\sharp.$$

(c) A *special cyclic sweep* is an entire sweep that consists of special row sweeps ordered as
$$s_{\max} = s_1^\sharp \circ s_2^\sharp \circ ... \circ s_{\max}^\sharp.$$

Note, that any special cyclic sweep always starts with the special row sweep $s_{\max}^\sharp$.

Example 3.35. According to Example 3.30, the respective enumerations yield the following cyclic methods.

(a) Enumeration 3.30 (a) leads to a column-wise annihilation of the off-diagonal entries. The special k-th row sweep here consists of rotations corresponding to the $(n-k+1)$-th column.

$$\begin{bmatrix} \circ&\circ&\circ&\circ&\circ\\ \circ&\circ&\circ&\circ&\circ\\ \circ&\circ&\circ&\circ&\circ\\ \circ&\circ&\circ&\circ&\star\\ \circ&\circ&\circ&\star&\circ \end{bmatrix} \to \begin{bmatrix} \circ&\circ&\circ&\circ&\circ\\ \circ&\circ&\circ&\circ&\circ\\ \circ&\circ&\circ&\circ&\star\\ \circ&\circ&\circ&\circ&\circ\\ \circ&\circ&\star&\circ&\circ \end{bmatrix} \to \begin{bmatrix} \circ&\circ&\circ&\circ&\circ\\ \circ&\circ&\circ&\circ&\star\\ \circ&\circ&\circ&\circ&\circ\\ \circ&\circ&\circ&\circ&\circ\\ \circ&\star&\circ&\circ&\circ \end{bmatrix} \to \begin{bmatrix} \circ&\circ&\circ&\circ&\star\\ \circ&\circ&\circ&\circ&\circ\\ \circ&\circ&\circ&\circ&\circ\\ \circ&\circ&\circ&\circ&\circ\\ \star&\circ&\circ&\circ&\circ \end{bmatrix} \to$$

$$\begin{bmatrix} \circ&\circ&\circ&\circ&\circ\\ \circ&\circ&\circ&\circ&\circ\\ \circ&\circ&\circ&\star&\circ\\ \circ&\circ&\star&\circ&\circ\\ \circ&\circ&\circ&\circ&\circ \end{bmatrix} \to \begin{bmatrix} \circ&\circ&\circ&\circ&\circ\\ \circ&\circ&\circ&\star&\circ\\ \circ&\circ&\circ&\circ&\circ\\ \circ&\star&\circ&\circ&\circ\\ \circ&\circ&\circ&\circ&\circ \end{bmatrix} \to \ldots \to \begin{bmatrix} \circ&\star&\circ&\circ&\circ\\ \star&\circ&\circ&\circ&\circ\\ \circ&\circ&\circ&\circ&\circ\\ \circ&\circ&\circ&\circ&\circ\\ \circ&\circ&\circ&\circ&\circ \end{bmatrix}$$

(b) Here, we obtain the special cyclic sweep for the symmetric eigenvalue problem as described at the beginning of this subsection, cf. Figure 3.2.

(c) Ordering (c) yields a sweep consisting of combined row- and column-wise annihilating of the off-diagonal elements.

$$\begin{bmatrix} \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \star \\ \circ & \circ & \circ & \star & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \star \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \star & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \star \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \star & \circ & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \circ & \star \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \star & \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow$$

$$\begin{bmatrix} \circ & \star & \circ & \circ & \circ \\ \star & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \star & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \star & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \star & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \star & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \star & \circ \\ \circ & \circ & \star & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow$$

$$\begin{bmatrix} \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \star & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \star & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \star & \circ & \circ \\ \circ & \star & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ \end{bmatrix}$$

We can now state and prove the main result of this section. Using special cyclic sweeps in the irregular case, the classical Jacobi as well as the Sort-Jacobi converge locally quadratic.

Theorem 3.36 (Local quadratic convergence for classical and Sort-Jacobi)**.** *Let $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ be the Cartan decomposition of a simple Lie algebra $\mathfrak{g}$ and let $S \in \mathfrak{p}$. Let $f\colon \mathcal{O}(S) \to \mathbb{R}$ denote either the off-norm (3.5) or the trace function (3.12), respectively. Let $Z \in \mathfrak{a}$ with $\lambda(Z) \leq 0$ for all $\lambda \in \Sigma^+$ be a minimum of the off-norm or the maximum of the trace function, respectively. Then the classical algorithm 2.19 reducing the off-norm, as well as the Sort-Jacobi algorithm maximizing the trace function, are locally quadratic convergent to Z, provided that special cyclic sweeps are used. This holds true even for irregular elements.*

Remark 3.37. Since every semisimple Lie algebra decomposes orthogonally into simple ideals, cf. Theorem 1.16, the above result straightforwardly yields locally quadratic convergent cyclic Jacobi methods for general semisimple Lie algebras, namely by considering each simple ideal independently.

The proof of the above theorem splits into several lemmas. Let $||\cdot||$ denote the norm on $\mathfrak{p}$ induced by the inner product B_θ. The following lemma states that minimizing along the $\mathrm{Ad}_{\exp t\Omega}$ orbit of an element $X \in \mathfrak{p}$ does not change the distance to $Z \in \mathfrak{a}$ if $[\Omega, Z] = 0$.

Lemma 3.38. *Let $\Omega \in \mathfrak{k}_\lambda$ and let $Z \in \mathfrak{a}$ with $\lambda(Z) = 0$. Then $\mathrm{Ad}_{\exp t\Omega}(Z) = Z$ for all $t \in \mathbb{R}$. Consequently,*

$$||r_\Omega(X, t) - Z|| = ||X - Z||,$$

if r_Ω is defined as in Eq. (3.21).

Proof. Since $\Omega = X_\lambda + \theta X_\lambda$ for some restricted-root vector $X_\lambda \in \mathfrak{g}_\lambda$ and $\lambda(Z) = 0$, we have $\mathrm{ad}_\Omega Z = 0$ and therefore

$$\mathrm{Ad}_{\exp t\Omega} Z = \sum_{k=0}^{\infty} \frac{t^k}{k!} \mathrm{ad}_\Omega^k Z = Z.$$

Furthermore, the Ad-invariance of the Killing form κ yields for all $t \in \mathbb{R}$ that

$$\begin{aligned} ||r_\Omega(X, t) - Z||^2 &= -\kappa(r_\Omega(X, t) - Z, \theta(r_\Omega(X, t) - Z)) \\ &= \kappa(\mathrm{Ad}_{\exp t\Omega} X - Z, \mathrm{Ad}_{\exp t\Omega} X - Z) \\ &= \kappa(\mathrm{Ad}_{\exp t\Omega}(X - Z), \mathrm{Ad}_{\exp t\Omega}(X - Z)) = ||X - Z||^2. \end{aligned}$$

□

Let

$$\mathrm{p}_k \colon \mathfrak{g} \longrightarrow \mathfrak{g}^{\alpha_k} \tag{3.22}$$

be the orthogonal projection onto $\mathfrak{g}^{\alpha_k}$ and let

$$\mathrm{p}_k^\sharp \colon \mathfrak{g} \longrightarrow \mathfrak{g}^{\alpha_k} \cap (\mathfrak{g}^{\alpha_{k-1}})^\perp \tag{3.23}$$

be the orthogonal projection onto $\mathfrak{g}^{\alpha_k} \cap (\mathfrak{g}^{\alpha_{k-1}})^\perp$. We sometimes use the abbreviate notation $\mathrm{p}_k^\sharp(X) =: X_k^\sharp$ and $\mathrm{p}_k(X) =: X_k$.

Example 3.39. Consider the Lie algebra $\mathfrak{sl}(4, \mathbb{R})$ with an ordering on the simple roots as in Example 3.30 (a). Let

$$H := \begin{bmatrix} -2 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \in \mathfrak{a}.$$

Then

$$\mathrm{p}_1(H) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}, \quad \mathrm{p}_2(H) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 7/3 & 0 & 0 \\ 0 & 0 & -2/3 & 0 \\ 0 & 0 & 0 & -5/3 \end{bmatrix},$$

$$\mathrm{p}_1^\sharp(H) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}, \quad \mathrm{p}_2^\sharp(H) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 7/3 & 0 & 0 \\ 0 & 0 & -7/6 & 0 \\ 0 & 0 & 0 & -7/6 \end{bmatrix}.$$

Lemma 3.40. *Let* p_k, $\mathrm{p}_k^\sharp$ *be as above and* $H \in \mathfrak{a}$. *Then*

(a) $\lambda(H_k^\sharp) = 0$ *if* $\lambda \in \Sigma_{k-1}$,

(b) $\lambda(H) = \lambda(\mathrm{p}_k(H))$ *if* $\lambda \in \Sigma_k$.

Proof. Let $\lambda \in \Sigma_k$ and denote by $H_\lambda \in \mathfrak{a}$ the element that is dual to λ, i.e. $\lambda(H) = B_\theta(H_\lambda, H)$ for all $H \in \mathfrak{a}$. Then by Lemma 1.49

$$H_\lambda \in \mathbb{R} \cdot [E_\lambda, \theta E_\lambda]$$

and hence $H_\lambda \in \mathfrak{g}^{\alpha_k}$. (a) Let $\lambda \in \Sigma_{k-1}$. Then $H_\lambda \in \mathfrak{g}^{\alpha_{k-1}}$ and

$$\lambda(H_k^\sharp) = B_\theta(H_\lambda, H_k^\sharp) = 0.$$

(b) Now let $\lambda \in \Sigma_k$. Then $H_\lambda \in \mathfrak{g}^{\alpha_k}$ and the orthogonality of p_k yields

$$\lambda(H) = B_\theta(H_\lambda, H) = B_\theta(H_\lambda, \mathrm{p}_k(H)) = \lambda(\mathrm{p}_k(H)).$$

□

Lemma 3.41. *Let* $X \in \mathfrak{p}$, $\varphi = \mathrm{Ad}_{\exp Y} \in \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k} \cap \mathfrak{g}^{\alpha_{k-1}})$, *i.e.* $Y \in \mathfrak{k} \cap \mathfrak{g}^{\alpha_{k-1}}$, *and* $H \in \mathfrak{a}$. *Then*

$$||\varphi(X) - H_k^\sharp|| = ||X - H_k^\sharp||.$$

Proof. Lemma 3.40 (a) yields that $\lambda(H_k^\sharp) = 0$ for all $\lambda \in \Sigma_{k-1}$. Now decomposing Y into its $\mathfrak{k}_\lambda$ components we get

$$[Y, H_k^\sharp] = 0$$

and the assertion follows analogously to Lemma 3.38. □

Lemma 3.42. *Let* $s = s_1^\sharp \circ s_2^\sharp \circ \ldots \circ s_{\max}^\sharp$ *be a special cyclic sweep. Let* $0 \neq Z \in \mathfrak{a}$ *with* $\lambda(Z) \leq 0$ *for all* $\lambda \in \Sigma^+$. *Let* $\alpha_m \in \Pi$ *be the smallest simple root such that* $\alpha_m(Z) < 0$. *Then* $\lambda(Z) = 0$ *for all* λ *involved in* $s_k^\sharp$ *if* $k < m$. *Moreover, the following holds.*

(I) If $k \geq m$, *then there exists a* $\lambda \in \Sigma_k^+ \setminus \Sigma_{k-1}^+$ *such that* $\lambda(Z) \neq 0$.

(II) Let $\lambda, \mu \in \Sigma_k^+ \setminus \Sigma_{k-1}^+$ *be two roots involved in* $s_k^\sharp$. *If* $\lambda(Z) < 0$, *then* $\mu(Z) < 0$ *for all* $\mu \geq \lambda$.

Proof. Condition 3.29 (I) assures that there exists a $\lambda = \sum_{i=1}^k c_i\alpha_i \in \Sigma_k^+ \setminus \Sigma_{k-1}^+$ with $c_m \neq 0$. Since $c_i \geq 0$ for all $i = 1, \ldots, k$, Proposition 3.21 yields

$$\lambda(Z) = \sum_{i=1}^k c_i\alpha_i \leq c_m\alpha_m(Z) < 0.$$

Now let $\lambda_0 = \sum_{i=1}^k c_i\alpha_i \in \Sigma_k^+ \setminus \Sigma_{k-1}^+$ be the smallest root such that $\lambda_0(Z) < 0$. Then there exists an index j such that $c_j > 0$. Let $\lambda_0 < \mu = \sum_{i=1}^k d_i\alpha_i$. Condition 3.29 (II) yields $d_j > 0$ and hence $\mu(Z) < 0$. □

Lemma 3.43. *Let $T_Z\mathcal{O}(S)$ denote the tangent space of $\mathcal{O}(S)$ at $Z \in \mathfrak{a}$ with $\lambda(Z) \leq 0$ for all $\lambda \in \Sigma^+$ and let p_k be defined as in Eq. (3.22). Then*

$$\mathrm{p}_k(T_Z\mathcal{O}_S) = \{[\Omega, \mathrm{p}_k(Z)] \mid \Omega \in \mathfrak{k}_\lambda \textit{ with } \lambda \in \Sigma_k, \lambda(Z) \neq 0\}.$$

Furthermore,

$$\mathcal{B} := \{\Omega_i \mid \Omega_i \textit{ lies in some } \mathfrak{k}_\lambda \textit{ for } i = 1, ..., \nu\} \subset \mathfrak{k}$$

is an orthogonal basis of $\sum\limits_{\{\lambda \mid \lambda(Z)<0\}} \mathfrak{k}_\lambda$ *if and only if*

$$\{\overline{\Omega}_i \mid \Omega_i \textit{ lies in some } \mathfrak{k}_\lambda \textit{ for } i = 1, ..., \nu\} \subset \mathfrak{p}$$

is an orthogonal basis of $\mathrm{p}_k(T_Z\mathcal{O}_S)$.

Proof. We have

$$T_Z\mathcal{O}(S) = \mathrm{ad}_Z\mathfrak{k} = \mathrm{ad}_Z\left(\sum_{\lambda\in\Sigma^+} \mathfrak{k}_\lambda + \mathfrak{z}_\mathfrak{k}(\mathfrak{a})\right) = \mathrm{ad}_Z\left(\sum_{\{\lambda\mid\lambda(Z)<0\}} \mathfrak{k}_\lambda\right),$$

since $[Z, \mathfrak{k}_\lambda] = 0$ if $\lambda(Z) = 0$. Furthermore $[Z, \mathfrak{k}_\lambda] \subset \mathfrak{p}_\lambda$ by Lemma 1.51, thus

$$T_Z\mathcal{O}(S) = \sum_{\{\lambda\mid\lambda(Z)<0\}} \mathfrak{p}_\lambda$$

and

$$\mathrm{p}_k(T_Z\mathcal{O}(S)) = \sum_{\lambda\in\Sigma_k^+, \lambda(Z)<0} \mathfrak{p}_\lambda = \{[\Omega, \mathrm{p}_k(Z)] \mid \Omega \in \mathfrak{k}_\lambda \text{ with } \lambda \in \Sigma_k, \lambda(Z) \neq 0\},$$

where the last equality holds because $\mathfrak{p}_\lambda = \lambda(\mathrm{p}_k(Z))\mathfrak{p}_\lambda = [\mathrm{p}_k(Z), \mathfrak{k}_\lambda]$. The last assertion follows since for $\lambda(Z) \neq 0$ and Ω_i, $\Omega_j \in \mathfrak{k}_\lambda$

$$B_\theta(\Omega_i, \Omega_j) = 0 \iff \lambda(Z)^2 B_\theta(\overline{\Omega}_i, \overline{\Omega}_j) = 0 \iff B_\theta([Z, \Omega_i], [Z, \overline{\Omega}_j]) = 0.$$

□

We will finally introduce some further notation. For every $X \in \mathfrak{p}$, the optimal step size selection $t_*^{(i)}(X)$ gives rise to an inner automorphism

$$r_{\Omega_i}(\cdot, t_*^{(i)}(X)) = \mathrm{Ad}_{\exp t_*^{(i)}(X)}$$

that obviously depends on X. Hence every (partial) sweep s yields an inner automorphism that depends on the initial point X. We will indicate this dependence by writing

$$s(X) = s^X(X).$$

Of course it makes sense to apply the transformation s^X to any other element in $\mathfrak{g}$. The following lemma shows that the transformation induced by the special sweep for $\mathfrak{g}^{\alpha_k}$ only depends on the $\mathfrak{g}^{\alpha_k}$-component of the underlying element X.

Lemma 3.44. *Let s_k be the special Jacobi sweep for $\mathfrak{g}^{\alpha_k}$ for minimizing the off-norm or maximizing the trace function, respectively. Let p_k denote the orthogonal projection onto $\mathfrak{g}^{\alpha_k}$. Then*

$$s_k(X) = s_k^{\mathrm{p}_k(X)}(X)$$

for all $X \in \mathfrak{p}$.

Proof. The special sweep s_k only consists of rotations $r_\Omega(X) = \mathrm{Ad}_{\exp t_*(X)\Omega} X$ with $\Omega \in \mathfrak{k}_\lambda$, $\lambda \in \Sigma_k$. For the tasks of minimizing the off-norm or maximizing the trace function, respectively, $t_*(X)$ only depends on the $\overline{\Omega}$-component of X and $\lambda(X_0)$, cf. Theorem 3.7 and Theorem 3.13. Now $\lambda(X_0) = \lambda(\mathrm{p}_k(X_0))$ by Lemma 3.40 and the assertion follows. □

We are now ready to prove the main theorem.

Proof of Theorem 3.36. The proof follows the idea of van Kempen [64]. Roughly spoken, it is an inductive proof over the "blocks" $\mathfrak{g}^{\alpha_k}$.
So let $\mathfrak{g}$ be a simple Lie algebra. Let $\Pi = \{\alpha_1, ..., \alpha_{\max}\}$ be the set of simple roots and assume that $(\Pi, >)$ satisfies the SCS-condition 3.29. Furthermore, denote by $Z \in \mathfrak{a}$ the minimum of the off-norm, maximum of the trace function respectively, with $\lambda(Z) \leq 0$ for all $\lambda \in \Sigma^+$. We show by induction that there exists a neighborhood $U(Z)$ of Z such that if $X \in U(Z) \cap \mathcal{O}(S)$ the estimate

$$||s_k(\mathrm{p}_k(X)) - \mathrm{p}_k(Z)|| \leq K||X - Z||^2, \quad \text{for all } X \in U(Z) \cap \mathcal{O}(S) \tag{3.24}$$

holds. Now denote by α_m the smallest simple root such that $\alpha_m(Z) < 0$. We can assume without loss of generality that such an α_m exists, because if not, then $\lambda(Z) = 0$ for all $\lambda \in \Sigma$ and hence $Z = 0$ implying that $\mathcal{O}(S) = \{0\}$. Let us see that Eq. (3.24) holds true for α_m. Therefore, recall that

$$s_m = s_1^\sharp \circ ... \circ s_m^\sharp$$

and that the roots λ involved in s_{m-1} are Σ_{m-1}^+ and the roots involved in $s_m^\sharp$ are given by $\Sigma_m^+ \setminus \Sigma_{m-1}^+$. Now let

$$\lambda = \sum_{i=1}^{m-1} c_i \alpha_i \in \Sigma_{m-1}^+ \quad \text{and} \quad \mu = d_m \alpha_m + \sum_{i=1}^{m-1} d_i \alpha_i \in \Sigma_m^+ \setminus \Sigma_{m-1}^+, \;\; d_m > 0.$$

Since by assumption, $\alpha_i(Z) = 0$ for all $i < m$, it follows that $\lambda(Z) = 0$ and $\mu(Z) = d_m \alpha_m(Z) < 0$. Therefore with $X_m := \mathrm{p}_m(X)$ Lemma 3.38 implies

$$||s_m(X_m) - Z_m|| = ||s_{m-1} \circ s_m^\sharp(X_m) - Z_m|| = ||s_m^\sharp(X_m) - Z_m||. \tag{3.25}$$

We now follow the idea of the proof of Theorem 2.10 and consider the function

$$s_m^\sharp \circ \mathrm{p}_m \colon \mathcal{O}(S) \longrightarrow \mathfrak{p}.$$

One step within $s_m^\sharp$ is given by

$$r_i(X_m) = r_{\Omega_i}(X_m, t_*^{(i)}(X_m)) = \mathrm{Ad}_{\exp t_*^{(i)}(X_m)\Omega_i} X_m$$

with $\Omega_i \in \mathfrak{k}_\mu$. For the classical case,

$$t_*^{(i)}(X_m) = \tfrac{1}{2}\arctan\left(\tfrac{2c_\mu}{\mu((X_m)_0)}\right),$$

cf. Theorem 3.7, and for the Sort-Jacobi

$$t_*^{(i)}(X_m) = \tfrac{1}{2}\arcsin\left(-\tfrac{2c_\mu}{\sqrt{c_\mu^2+\mu((X_m)_0)^2}}\right),$$

cf. Theorem 3.13. Now since $\mu(Z) = \mu(Z_m) < 0$, there exists a neighborhood $U \subset \mathcal{O}(S)$ of Z and a $\delta > 0$ such that $\mu((X_m)_0) < -\delta$. Hence the step size selections t_* and therefore $s_m^\sharp \circ \mathrm{p}_m$ is differentiable in U. We show that its derivative at Z vanishes and use a Taylor series argument to complete the initial induction step. By Lemma 3.43,

$$\{\mathrm{ad}_{\Omega_i}\, \mathrm{p}_k(Z) \mid \Omega_i \in \mathfrak{k}_\lambda \text{ with } \lambda \in \Sigma_k, \lambda(Z) \neq 0\}$$

is an orthogonal basis of $\mathrm{p}_k(T_Z\mathcal{O}(S))$. For the derivative we have

$$D(s_m^\sharp \circ \mathrm{p}_m)(Z)\xi = Ds_m^\sharp(\mathrm{p}_m(Z))\,\mathrm{p}_m(\xi)$$

and the derivative of each elementary rotation $r_{\Omega_i}(t_*^{(i)}(X), X)$ is explicitly computed analogously to the proof of Theorem 2.10. Lemma 2.5 yields

$$Dt_*^{(i)}(\mathrm{p}_m(Z))(\xi) = -\frac{\mathsf{H}_f(\mathrm{p}_m(Z))(\xi_i, \xi)}{\mathsf{H}_f(\mathrm{p}_m(Z))(\xi_i, \xi)},$$

where H_f is the Hessian of the off-norm, the trace function at $\mathrm{p}_m(Z)$ respectively.

$$\begin{aligned} Dr_i(\mathrm{p}_m(Z))\xi &= D\left(r_i(t_*^{(i)}(X), X)\Big|_{X=\mathrm{p}_m(Z)}\right)\xi \\ &= Dr_i(t, X)|_{(t,X)=(t_*^{(i)}(\mathrm{p}_m(Z)),\mathrm{p}_m(Z))} \circ D(t_*^{(i)}(X), \mathrm{id})|_{X=\mathrm{p}_m(Z)}\xi \\ &= Dt_*^{(i)}(\mathrm{p}_m(Z))\xi_i + \xi \end{aligned}$$

since $t_*^{(i)}(\mathrm{p}_m(Z)) = 0$ and hence

$$Dr_i(\mathrm{p}_m(Z))\xi = \xi - \frac{\mathsf{H}_f(\mathrm{p}_m(Z))(\xi_i, \xi)}{\mathsf{H}_f(\mathrm{p}_m(Z))(\xi_i, \xi_i)}\xi_i.$$

For both, the Hessian of the off-norm, cf. Eq. (3.6) and the Hessian of the trace function, cf. Eq. (3.13), $Dr_i(\mathrm{p}_m(Z))$ is an orthogonal projector onto $(\mathbb{R}\cdot[\Omega_i, \mathrm{p}_m(Z)])^\perp$. Since $\mathrm{p}_m(Z)$ is a fixed point of every r_i (because every element in $\mathfrak{a}$ is), one has

$$Ds_m(\mathrm{p}_m(Z))\,\mathrm{p}_m(\xi) = 0.$$

Hence by Lemma 2.9, there exists a neighborhood $U(Z)$ of Z and a constant K such that

$$||s_m^\sharp \circ \mathrm{p}_m(X) - \mathrm{p}_m(Z)|| \leq K||X-Z||^2.$$

The initial induction step is done, since now by Eq. (3.25) it follows

$$||s_m(\mathrm{p}_m(X)) - \mathrm{p}_m(Z)|| = ||s_m^\sharp \circ \mathrm{p}_m(X) - \mathrm{p}_m(Z)|| \leq K||X-Z||^2.$$

Assume now that the assertion (3.24) is true for α_{k-1} with $k-1 \geq m$. Partition the special sweep s_k into $s_k =: s_{k-1} \circ s_k^\sharp$. Substituting $\widetilde{X} := s_k^\sharp(\mathrm{p}_k(X))$ and using Lemma 3.44 for the second equality we obtain

$$\begin{aligned}
||s_k(\mathrm{p}_k(X)) - \mathrm{p}_k(Z)|| &= ||s_{k-1}(\widetilde{X}) - \mathrm{p}_k(Z)|| \\
&= ||s_{k-1}^{\mathrm{p}_{k-1}(\widetilde{X})}(\mathrm{p}_{k-1}(\widetilde{X}) + \widetilde{X}_k^\sharp) - \mathrm{p}_{k-1}(Z) - Z_k^\sharp|| \\
&\leq ||s_{k-1}^{\mathrm{p}_{k-1}(\widetilde{X})}(\mathrm{p}_{k-1}(\widetilde{X})) - \mathrm{p}_{k-1}(Z)|| + ||s_{k-1}^{\mathrm{p}_{k-1}(\widetilde{X})}(\widetilde{X}_k^\sharp) - Z_k^\sharp|| \\
&= ||s_{k-1}(\mathrm{p}_{k-1}(\widetilde{X})) - \mathrm{p}_{k-1}(Z)|| + ||\widetilde{X}_k^\sharp - Z_k^\sharp||,
\end{aligned} \tag{3.26}$$

where the last equality holds by Lemma 3.41, since $s_{k-1}^{\mathrm{p}_{k-1}(\widetilde{X})} \in \mathrm{Int}_{\mathfrak{g}}(\mathfrak{g}^{\alpha_{k-1}} \cap \mathfrak{k})$. Applying the induction hypothesis, it remains to analyze the summand

$$||\widetilde{X}_k^\sharp - Z_k^\sharp|| = ||\,\mathrm{p}_k^\sharp \circ s_k^\sharp(X) - \mathrm{p}_k^\sharp(Z)||.$$

By Lemma 3.42, $s_k^\sharp$ is a special row sweep of type

$$(\lambda_1, .., \lambda_{\nu-1}, \lambda_\nu, ..., \lambda_m)$$

where $\lambda_i(Z) = 0$ if $1 \leq i < \nu$ and $\lambda_i(Z) < 0$ for $\nu \leq i$. Hence

$$s_k^\sharp = g \circ b, \tag{3.27}$$

where b is either the identity or a partial sweep of type $(\lambda_1, .., \lambda_{\nu-1})$ and g is a partial sweep of type $(\lambda_\nu, ..., \lambda_m)$. By Lemma 3.38, $b(X) =: \widehat{X}$ is contained in a ball around Z if and only if X is contained in the same ball. It therefore suffices to examine $||\,\mathrm{p}_k^\sharp \circ g(\widehat{X}) - \mathrm{p}_k^\sharp \circ g(Z)||$. Now $[\Omega_i, Z] \neq 0$ for all Ω_i involved in g and hence by Lemma 2.5, $\mathrm{p}_k^\sharp \circ g$ is differentiable in a neighborhood $\widehat{U}(Z)$ of Z, that is assumed without loss of generality to be a ball. For the derivative in Z we have

$$D(\mathrm{p}_k^\sharp \circ g)(Z)\xi = \mathrm{p}_k^\sharp \circ Dg(Z)\xi,$$

and analogously to the proof of Theorem 2.10, $Dr_i(Z)$ is an orthogonal projector onto $(\mathbb{R} \cdot [\Omega_i, Z])^\perp$ if r_i is an elementary rotation of g for both, the classical Jacobi and the Sort-Jacobi. The remaining components of ξ are annihilated by the projection $\mathrm{p}_\sharp$. Since Z is a fixed point of every rotation, one has

$$\mathrm{p}_\sharp \circ Dg(Z)\xi = 0.$$

Hence again by Taylor's Theorem there exists a constant L such that

$$|| \, \mathrm{p}_k^\sharp \circ g(\widehat{X}) - \mathrm{p}_k^\sharp \circ g(Z)|| \leq L||\widehat{X} - Z||^2 \text{ for all } \widehat{X} \in \widehat{U}(Z).$$

Now choose a ball $V(Z) \subset U(Z) \cap \widehat{U}(Z)$. Applying the induction hypothesis to Eq. (3.26), we obtain for all $X \in V(Z)$ that

$$||s_k(\mathrm{p}_k(X)) - \mathrm{p}_k(Z)|| \leq (K + L)||X - Z||^2.$$

The proof is complete for $k = \max$. □

Remark 3.45. Not every restricted-root system admits an enumeration such that the SCS-condition 3.29 is satisfied. For example this is the case for the root system D_q if $q > 3$ defined in the next Chapter, cf. Eq. (4.8). Nevertheless, we are able to introduce an ordering on D_q such that the above proof can be adapted, cf. Corollary 4.5. Note therefore, that the SCS-conditions (I), (II) are used only in Eq. (3.27):

(I) To guarantee that $s_k^\sharp$ contains *at least* one rotation r_Ω with $[\Omega, Z] \neq 0$;

(II) To guarantee that for the sweep $s_k^\sharp$ of type $(\lambda_1, ..., \lambda_s)$ there exists an index ν such that $\lambda_i(Z) < 0$ for all $i \geq \nu i$.

Although (I) and (II) are exactly the conditions we need for the proof, they are not suitable for defining special cyclic sweeps since these conditions depend on Z and in general Z is unknown before starting the algorithm.

Chapter 4

Applications to Structured Singular Value and Eigenvalue Problems

4.1 Generalities

In this chapter we discuss in detail how some of the well known normal form problems from numerical linear algebra fit into the developed Lie algebraic setting. In Table 4.1 we present an overview of the Cartan decompositions of simple Lie algebras and the corresponding matrix factorizations. The Sort-Jacobi algorithm from the previous section is specified for the real and symplectic singular value decomposition, for the real symmetric Hamiltonian EVD and for one exceptional case. It is straightforward to implement a Sort-Jacobi algorithm with special cyclic sweeps for all cases with a restricted-root space decomposition, as in the appendix. Each of the examples is of course only one representative of the corresponding isomorphism class. By knowledge of the isomorphism, it is then straightforward to adapt the presented algorithm in order to obtain structure preserving Jacobi-type methods for the isomorphic classes. Stronger than isomorphic is the following definition.

Definition 4.1. Two Lie algebras $\mathfrak{g}, \mathfrak{g}' \subset \mathbb{C}^{n\times n}$ are *equivalent*, if there exists an invertible $g \in \mathbb{C}^{N\times N}$ such that $g\mathfrak{g}g^{-1} = \mathfrak{g}'$.

If $\mathfrak{g}$ and $\mathfrak{g}'$ are semisimple with $g\mathfrak{g}g^{-1} = \mathfrak{g}'$, then their Cartan decompositions transform in the same way, i.e. if $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ is the Cartan decomposition of $\mathfrak{g}$, then $g\mathfrak{k}g^{-1} \oplus g\mathfrak{p}g^{-1}$ yields the Cartan decomposition of $\mathfrak{g}'$. This means, that to every row in Table 4.1, there correspond *infinitely many* structured eigenvalue problems, and as is often not recognized in the literature, seemingly "different" structured eigenvalue problems can be equivalent. We mention three examples.

Example 4.2. • The Lie algebra of the *perskew-symmetric matrices*

$$\{A \in \mathbb{R}^{n\times n} \mid A^\top R + RA = 0\}, \quad \text{where } R := \begin{bmatrix} & & 1 \\ & \cdot^{\cdot^{\cdot}} & \\ 1 & & \end{bmatrix} \tag{4.1}$$

is equivalent to $\mathfrak{so}(k,k)$ if $n = 2k$ and to $\mathfrak{so}(k+1,k)$ if $n = 2k+1$. The symmetric perskew-symmetric EVD is therefore equivalent to the SVD of a real $(k \times k)$-matrix, $(k+1 \times k)$ respectively, cf. Section 4.2.

- Takagi's factorization is equivalent to the symmetric Hamiltonian EVD, cf. Section 4.3.

- In systems theory, the *real* Lie algebra

$$\mathfrak{g} := \left\{ \begin{bmatrix} A & G \\ Q & -A^* \end{bmatrix}, A, G, Q \in \mathbb{C}^{n\times n}, G^* = G, H^* = H \right\} \tag{4.2}$$

plays an important role in linear optimal control and associated algebraic Riccati equations. We refer to $\mathfrak{g}$ as the set of $\mathbb{R}$-*Hamiltonian matrices* in order to avoid confusion with the *complex* Lie algebra $\mathfrak{sp}(n,\mathbb{C})$, whose elements are called, following the established convention in mathematics, *(complex or* $\mathbb{C}$*)-Hamiltonian*. The Lie algebra $\mathfrak{g}$ is equivalent to $\mathfrak{su}(n,n)$ and hence the diagonalization of a Hermitian $\mathbb{R}$-Hamiltonian matrix is equivalent to the SVD of a complex $(n\times n)$-matrix, cf. Section 4.5.

Note, that different choices for the maximal abelian subalgebra $\mathfrak{a}$ do only appear to lead to different eigenvalue problems, since they are all conjugate to each other, cf. Theorem 1.48. Furthermore, we can apply our results to the symplectic singular value decomposition and a structured eigenvalue problem, arising by considering a Cartan decomposition of a real form of the exceptional Lie algebra $\mathfrak{g}_2$. To our knowledge, the corresponding Sort-Jacobi-algorithms are new.
For the numerical simulations we randomly generate matrices with prescribed structure and eigenvalues. This is done in the following way.

Algorithm 4.3. Let $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ be a Cartan decomposition and let $\mathfrak{a} \subset \mathfrak{p}$ be maximal abelian. Let $\mathcal{B} = \{\Omega_1, ..., \Omega_N\}$ be the set of sweep directions as given in Algorithm 2.18, and let $Z \in \mathfrak{a}$. The following algorithm generates a random matrix $S \in \mathcal{O}(Z)$, the $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$-adjoint orbit of Z.

Algorithm 4.3. Random initial point.
function: $S = \text{random.element}(Z)$
Set $g :=$ identity matrix.

$\mathfrak{g}$	$\mathfrak{k}$	$\mathfrak{p}$	Matrix Factorization
$\mathfrak{sl}(n,\mathbb{R})$	$\mathfrak{so}(n,\mathbb{R})$	$S \in \mathbb{R}^{n\times n}$, $S = S^\top$, $\mathrm{tr}S = 0$	symmetric EVD
$\mathfrak{sl}(n,\mathbb{C})$	$\mathfrak{su}(n)$	$S \in \mathbb{C}^{n\times n}$, $S = S^*$, $\mathrm{tr}S = 0$	Hermitian EVD
$\mathfrak{so}(n,\mathbb{C})$	$\mathfrak{so}(n,\mathbb{R})$	$\Psi \in \mathrm{i}\mathbb{R}^{n\times n}$, $\Psi = -\Psi^\top$	skew-symmetric EVD (up to multiplication with i)
$\mathfrak{su}^*(2n)$	$\mathfrak{sp}(n)$	$P := \begin{bmatrix} S & \Psi^* \\ \Psi & \overline{S} \end{bmatrix}, S, \Psi \in \mathbb{C}^{n\times n}$, $\mathrm{tr}S = 0, S = S^*, \Psi = -\Psi^\top$	Hermitian Quaternion EVD, i.e. $uPu^* = \begin{bmatrix} \Lambda & \\ & \Lambda \end{bmatrix}, \mathrm{tr}\Lambda = 0, \Lambda$ real diagonal, $u \in Sp(n)$
$\mathfrak{so}(p,q)$	$\mathfrak{so}(p,\mathbb{R}) \oplus \mathfrak{so}(q,\mathbb{R})$	$\begin{bmatrix} 0 & B \\ B^\top & 0 \end{bmatrix}, B \in \mathbb{R}^{p\times q}$	real SVD, cf. Sec. 4.2
$\mathfrak{su}(p,q)$	$\mathfrak{s}(\mathfrak{u}(p) \oplus \mathfrak{u}(q))$	$\begin{bmatrix} 0 & B \\ B^* & 0 \end{bmatrix}, B \in \mathbb{C}^{p\times q}$	complex SVD, Hermitian $\mathbb{R}$-Hamiltonian EVD, cf. Sec. 4.5
$\mathfrak{so}^*(2n)$	$\mathfrak{u}(n)$	$\begin{bmatrix} 0 & B \\ B^* & 0 \end{bmatrix}, B \in \mathbb{C}^{n\times n}, B = -B^\top$	Takagi-like factorization, i.e. $uBu^\top = \begin{bmatrix} 0 & x_1 & & & \\ -x_1 & 0 & & & \\ & & \ddots & & \\ & & & 0 & x_n \\ & & & -x_n & 0 \end{bmatrix}, x_i \in \mathbb{R}, u \in U(n)$

Table 4.1: Classical Cartan-decompositions and corresponding matrix factorizations, Part I.

$\mathfrak{g}$	$\mathfrak{k}$	$\mathfrak{p}$	Matrix Factorization
$\mathfrak{sp}(n,\mathbb{R})$	$\mathfrak{u}(n)$	$\begin{bmatrix} S & C \\ C & -S \end{bmatrix}, S, C \in \mathbb{R}^{n\times n}, S = S^\top, C = C^\top$	symmetric Hamiltonian EVD Takagi's factorization, cf. Sec. 4.3
$\mathfrak{sp}(n,\mathbb{C})$	$\mathfrak{sp}(n)$	$P := \begin{bmatrix} S & C \\ \overline{C} & -\overline{S} \end{bmatrix}, S, C \in \mathbb{C}^{n\times n}, S = S^*, C = C^\top$	Hermitian $\mathbb{C}$-Hamiltonian EVD
$\mathfrak{sp}(p,q)$, $p \geq q$	$\mathfrak{sp}(p) \oplus \mathfrak{sp}(q)$	$\begin{bmatrix} & & B & -\overline{F} \\ & & F & \overline{B} \\ B^* & F^* & & \\ -F^\top & B^\top & & \end{bmatrix}, B, F \in \mathbb{C}^{p\times q}$	symplectic SVD, cf. Sec. 4.4, i.e. $u \begin{bmatrix} B & -\overline{F} \\ F & \overline{B} \end{bmatrix} v^* = \begin{bmatrix} \Sigma & 0 \\ 0 & \Sigma \end{bmatrix},$ $\Sigma = \left[\begin{array}{ccc} & 0 & \\ \hline a_1 & & 0 \\ & \ddots & \\ 0 & & a_n \end{array}\right] \in \mathbb{R}^{p\times q}, u \in Sp(p), v \in Sp(q)$
$\mathfrak{g}_2$	$\mathfrak{su}(2) \oplus \mathfrak{su}(2)$	$\begin{bmatrix} 0 & \sqrt{2}b^\top & -\sqrt{2}b^\top \\ \sqrt{2}b & S & B \\ -\sqrt{2}b & -B & -S \end{bmatrix}, b = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix},$ $B = \begin{bmatrix} 0 & -b_3 & b_2 \\ b_3 & 0 & -b_1 \\ -b_2 & b_1 & 0 \end{bmatrix}, b_i \in \mathbb{R}, S \in \mathbb{R}^{3\times 3},$ $\mathrm{tr} S = 0, S = S^\top$	cf. Section 4.6

Table 4.2: Classical Cartan-decompositions and corresponding matrix factorizations, Part II.

Set $S := Z$
for $l = 1 : 3$
  for $k = 1 : N$
    Set $t :=$ Real Random number out of $[-\pi, \pi]$.
    Set $S := \exp(t\Omega_k).S.\exp(-t\Omega_k)$.
  endfor
  Set l=l+1.
endfor

All subsequent experiments are performed with three different randomly chosen initial points, plotted in one single diagram. As a measure of how far an element $X \in \mathfrak{p}$ is away from diagonalization, we always evaluate $d(X) = ||X - X_0||^2$, a multiple of the off-norm. The value of d is plotted against the vertical axis. For a better visualisation, the values of the off-norm at each sweep are connected with a line. All simulations are done using MATHEMATICA 5.2. There are essentially three observations for the numerical experiments.

- The Sort-Jacobi consistently shows a faster convergence behavior than the classical Jacobi method.
- Special cyclic sweeps yield better convergence than arbitrary sweeps, especially for the irregular case.
- For special cyclic sweeps, the convergence is the faster, the more the element is irregular, i.e. the fewer clusters appear.

4.2 The Singular Value Decomposition of a Real Matrix

We illustrate how a Jacobi-type method for the singular value decomposition fits into the Lie algebraic setting, developed in the previous chapters. We apply the algorithm of Section 3.2 to the standard representation of the simple Lie algebra $\mathfrak{so}(p,q)$, where we assume that $p \geq q$. Let

$$\mathfrak{so}(p,q) = \{X \in \mathfrak{sl}(p+q,\mathbb{R}) \mid X^\top I_{p,q} + I_{p,q}X = 0\},$$

where

$$I_{p,q} = \begin{bmatrix} I_p & \\ & -I_q \end{bmatrix}$$

and I_p denotes the $(p \times p)$-identity matrix. The Cartan involution

$$\theta : \mathfrak{so}(p,q) \longrightarrow \mathfrak{so}(p,q), \quad X \longmapsto I_{p,q} X I_{p,q} \tag{4.3}$$

leads to the Cartan decomposition

$$\mathfrak{so}(p,q) = \mathfrak{k} \oplus \mathfrak{p}, \tag{4.4}$$

where the (+1)-eigenspace of θ is given by

$$\mathfrak{k} = \left\{ \begin{bmatrix} S_1 & 0 \\ 0 & S_2 \end{bmatrix} \mid -S_1^\top = S_1 \in \mathbb{R}^{p\times p}, -S_2^\top = S_2 \in \mathbb{R}^{q\times q} \right\} \tag{4.5}$$

and the (−1)-eigenspace of θ is given by

$$\mathfrak{p} = \left\{ \begin{bmatrix} 0 & B \\ B^\top & 0 \end{bmatrix} \mid B \in \mathbb{R}^{p\times q} \right\}. \tag{4.6}$$

We fix a maximal abelian subalgebra in $\mathfrak{p}$ as

$$\mathfrak{a} := \left\{ \begin{bmatrix} 0 & B \\ B^\top & 0 \end{bmatrix} \mid B = \begin{bmatrix} & 0 & \\ \hline a_1 & & 0 \\ & \ddots & \\ 0 & & a_q \end{bmatrix} \in \mathbb{R}^{p\times q} \right\}. \tag{4.7}$$

A set of positive restricted roots is given by the linear functionals

$$\boxed{\begin{aligned} &a_i - a_j, \quad 1 \le i < j \le q, \\ &a_i + a_j, \quad 1 \le i < j \le q. \end{aligned}} \tag{4.8a}$$

Moreover, in the case where $p > q$, we have additionally the restricted roots

$$\boxed{a_i, \quad 1 \le i \le q.} \tag{4.8b}$$

The restricted-root system is said to be of type D_q if $p = q$ and of type B_q if $p > q$. The root systems are illustrated in Fig. 4.1 and 4.2 for the case $q = 2$.
Consider first the case where $p > q$. A simple system is given by

$$\Pi_{B_q} = \{a_i - a_{i+1} \mid 1 \le i < q\} \cup \{a_q\}. \tag{4.9}$$

The following Proposition specifies an ordering on Π_{B_q} such that the SCS-condition is satisfied.

Proposition 4.4. *Let $\alpha_i := a_i - a_{i+1}$, $i = 1, ..., q-1$ and let $\alpha_q := a_q$. Then $(\Pi_{B_q}, >)$ satisfies the SCS-condition 3.29 if $>$ is defined by*

$$\alpha_i > \alpha_j, \quad \textit{if } i < j.$$

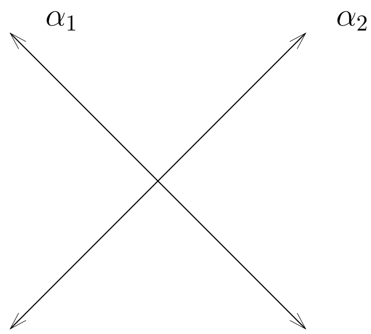

Figure 4.1: The root system D_2 with simple roots α_1, α_2.

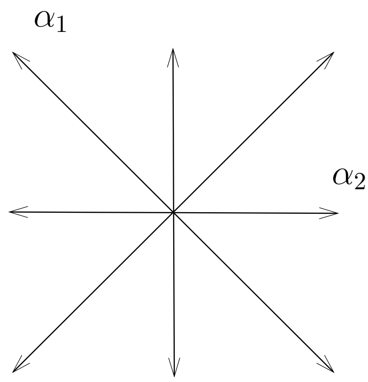

Figure 4.2: The root system B_2 with simple roots α_1, α_2.

Note, that the notation slightly differs from the notation in the previous chapter. Here, α_1 is the largest and α_q is the smallest root.

Proof. In terms of the simple roots α_i, the positive restricted roots are

$$a_i - a_j = \sum_{k=i}^{j-1} \alpha_k, \quad a_i = \sum_{k=i}^{q} \alpha_k, \quad a_i + a_j = \sum_{k=i}^{q} \alpha_k + \sum_{k=j}^{q} \alpha_k. \tag{4.10}$$

Therefore the sets $\Sigma_k^+ \setminus \Sigma_{k-1}^+$ are given by

$$\begin{aligned}
\Sigma_{\max}^+ \setminus \Sigma_{\max-1}^+ &: a_1 - a_2 < \dots < a_1 - a_q < a_1 < a_1 + a_q < \dots < a_1 + a_2 \\
&\ \vdots \\
\Sigma_k^+ \setminus \Sigma_{k-1}^+ &: a_k - a_{k+1} < \dots < a_k - a_q < a_k < a_k + a_q < \dots < a_k + a_{k+1} \\
&\ \vdots \\
\Sigma_1^+ &: a_q.
\end{aligned}$$

By Equation (4.10) it can easily be checked that $(\Pi_{B_q}, >)$ satisfies the SCS-condition. □

Now let $p = q$. Although Example 3.31 shows that for $p = q = 3$ an ordering on the simple roots exists such that the SCS-condition is fulfilled, this does not hold for $p > 3$. Nevertheless, we are able to introduce an ordering such that the resulting sweep yields local quadratic convergence. A simple system is given by

$$\Pi_{D_q} = \{a_i - a_{i+1} \mid 1 \leq i < q\} \cup \{a_{q-1} + a_q\}. \tag{4.11}$$

Let $\alpha_i := a_i - a_{i+1}$, $i = 1, ..., q-2$ let $\alpha_{q-1} := a_{q-1} + a_q$ and let $\alpha_q := a_{q-1} - a_q$. In terms of the simple roots α_i, the positive restricted roots are

$$\begin{aligned}
a_i - a_j &= \sum_{k=i}^{j-2} \alpha_k, \text{ for } i \geq q-2 \\
a_i - a_q &= \sum_{k=i}^{j-2} \alpha_k + \alpha_q \\
a_{q-1} + a_q &= \alpha_{q-1}, \\
a_i + a_q &= \sum_{k=i}^{q-1} \alpha_k, \text{ for } i \geq q-2, \\
a_i + a_{q-1} &= \sum_{k=i}^{q} \alpha_k, \\
a_i + a_j &= \sum_{k=1}^{q} \alpha_k + \sum_{k=j}^{q-2} \alpha_k, \text{ for } j \geq q-2.
\end{aligned} \tag{4.12}$$

If we define the ordering on Π_{D_q} by

$$\alpha_i > \alpha_j, \quad \text{if } i < j, \tag{4.13}$$

the sets $\Sigma_k^+ \setminus \Sigma_{k-1}^+$ are given by

$$\begin{aligned}
\Sigma_{\max}^+ \setminus \Sigma_{\max-1}^+ &: a_1 - a_2 < ... < a_1 - a_q < a_1 + a_q < ... < a_1 + a_2 \\
&\vdots \\
\Sigma_k^+ \setminus \Sigma_{k-1}^+ &: a_k - a_{k+1} < ... < a_k - a_q < a_k + a_q < ... < a_k + a_{k+1} \\
&\vdots \\
\Sigma_2^+ \setminus \Sigma_1^+ &: a_{q-1} + a_q \\
\Sigma_1^+ &: a_{q-1} - a_q.
\end{aligned}$$

Corollary 4.5. *Let $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ be the Cartan decomposition of a simple Lie Algebra with restricted-root system D_q. Let $Z \in \mathfrak{a}$ with $\lambda(Z) \leq 0$ for all $\lambda \in \Sigma^+$ be a minimum of the off-norm, the maximum of the trace-function respectively. Let $(\Pi_{D_q}, >)$ be ordered as above and let $s_k^\sharp$ by a partial sweep of type $(\lambda_1, ..., \lambda_n)$ with $\{\lambda_1, ..., \lambda_n\} = \Sigma_k^+ \setminus \Sigma_{k-1}^+$ and $\lambda_1 < ... < \lambda_n$. Let*

$$s = s_1^\sharp \circ s_2^\sharp \circ ... \circ s_{\max}^\sharp.$$

Then s yields local quadratic convergence to Z for the classical as well as for the Sort-Jacobi Algorithm 3.10 and 3.16, even for irregular elements.

Proof. We adapt the proof of Theorem 3.36 and use the notation established therein. The crucial point in adapting the proof is to note that neither $\alpha_q - \alpha_{q-1} = -2a_q$ nor $\alpha_q + \alpha_{q-1} = 2a_{q-1}$ is a root or zero and hence, by Theorem 2.23, the respective elementary rotations commute. The same holds true for rotations corresponding to the roots $a_k + a_q$ and $a_k - a_q$ for $k \geq 3$. Hence

$$s = s_1^\sharp \circ s_2^\sharp \circ ... \circ s_{\max}^\sharp = s_2^\sharp \circ s_1^\sharp \circ \widetilde{s}_3^\sharp ... \circ \widetilde{s}_{\max}^\sharp,$$

where $\widetilde{s}_k^\sharp$ are sweeps of type

$$(a_k - a_{k+1}, ..., a_k + a_q, a_k - a_q, ..., a_k + a_{k+1}),$$

Hence we can assume without loss of generality by a possibly re-enumeration of the simple roots that if α_m denotes the smallest root such that $\alpha_m(Z) < 0$ the following holds.

(I) If $k \geq m$, then there exists a $\lambda \in \Sigma_k^+ \setminus \Sigma_{k-1}^+$ such that $\lambda(Z) \neq 0$.

(II) Let $\lambda, \mu \in \Sigma_k^+ \setminus \Sigma_{k-1}^+$ be two roots involved in $s_k^\sharp$. If $\lambda(Z) < 0$, then $\mu(Z) < 0$ for all $\mu \geq \lambda$.

Using this result to obtain Eq. (3.27), the proof of Theorem 3.36 adapts straightforwardly. □

The corresponding restricted-root spaces are given below. For the roots $a_i \pm a_j$, the restricted-root spaces are of real dimension 1 and are nonzero only in the 16 entries corresponding to row and column indices $p-i+1, p-j+1, p-i+1+q, p-j+1+q$. They are

$$\mathfrak{g}_{a_i - a_j} = \mathbb{R} \cdot \frac{1}{2} \begin{bmatrix} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} & \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ \\ \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} & \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \end{bmatrix}, \quad \mathfrak{g}_{a_i + a_j} = \mathbb{R} \cdot \frac{1}{2} \begin{bmatrix} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} & \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \\ \\ \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} & \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \end{bmatrix}. \tag{4.14}$$

The above basis vectors are all normalized in the sense of Eq. (3.15). The restricted-root spaces for the roots $H \longmapsto a_i$ only exist if $p > q$ and have real dimension $p - q$. They are nonzero only in the entries corresponding to row and column indices $1, ..., p-q, p-q+i, p+i$, where they are

$$\mathfrak{g}_{a_i} = \left\{ \begin{bmatrix} 0 & v & -v \\ -v^\top & 0 & 0 \\ -v^\top & 0 & 0 \end{bmatrix} | v \in \mathbb{R}^{p-q} \right\}. \tag{4.15}$$

An orthogonal basis of $\mathfrak{g}_{a_i}$, normalized in the sense of Eq. (3.15), is given by

$$\begin{bmatrix} 0 & \begin{bmatrix} 1 & -1 \end{bmatrix} \\ \begin{bmatrix} -1 \\ -1 \end{bmatrix} & 0 \end{bmatrix} \tag{4.16}$$

Using the results in Section 3.2, we are now ready to introduce a Jacobi-type algorithm that computes the SVD of a real matrix B. Figure 4.3 illustrates the SCS-sweep method for the real SVD.

$$\begin{bmatrix} \circ & \circ & \circ & \circ \\ \circ & \ast & \circ & \circ \\ \ast & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \circ \\ \circ & \circ & \ast & \circ \\ \circ & \circ & \circ & \circ \\ \ast & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \ast \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \ast & \circ & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \star & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow$$

$$\begin{bmatrix} \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \bullet \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \bullet & \circ & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \circ \\ \circ & \circ & \bullet & \circ \\ \circ & \circ & \circ & \circ \\ \bullet & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \circ \\ \circ & \bullet & \circ & \circ \\ \bullet & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \ast & \circ \\ \circ & \ast & \circ & \circ \\ \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow$$

$$\begin{bmatrix} \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \ast \\ \circ & \circ & \circ & \circ \\ \circ & \ast & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \star & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \bullet \\ \circ & \circ & \circ & \circ \\ \circ & \bullet & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \bullet & \circ \\ \circ & \bullet & \circ & \circ \\ \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow$$

$$\begin{bmatrix} \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \ast \\ \circ & \circ & \ast & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \star & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \bullet \\ \circ & \circ & \bullet & \circ \end{bmatrix} \longrightarrow \begin{bmatrix} \circ & \circ & \circ & \star \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \end{bmatrix}.$$

Figure 4.3: Special cyclic sweep for the SVD. $\star$: annihilating, $\bullet$: symmetrizing, $\ast$: skew-symmetrizing.

According to Theorem 3.36, this algorithm is locally quadratic convergent for any element, including irregular ones, since we use special cyclic sweeps. The proposed code is admittedly not optimal in the sense that matrices are used that occur with twice the size that is in fact needed. An implementation with bisected matrices is straightforward and is omitted here.

Algorithm 4.6. Denote by X_{ij} the (i, j)-entry of the matrix X. In a first step we generate the sweep directions $\Omega_i \in \mathfrak{k}_\lambda$ with corresponding $\lambda(i)$ and $\overline{\Omega}_i$-coefficient $c(i)$. Let $E_{ij} \in \mathbb{R}^{p+q}$ the matrix with (i, j)- entry 1 and zeros elsewhere and define $\Psi_{ij} := E_{ij} - E_{ji}$.

Algorithm 4.6. real SVD - sweep directions and SCS order.
function: $(\Omega_1, \lambda(1), c(1), ..., \Omega_N, \lambda(N), c(N), N) = \text{generate.directions}(p, q)$
Set $k := 1$
for $i = 1 : q$
  for $j = i + 1 : q$
    Set $\Omega_k := \Psi_{p-q+i,p-q+j} + \Psi_{p+i,p+j}$.
    Set $\lambda_k := E_{p-q+i,p+i} - E_{p-q+j,p+j}$.
    Set $c(k) := \frac{1}{2}(E_{p-q+i,p+j} + E_{p-q+j,p+i})$.
    Set $k = k + 1$, $j = j + 1$.
  endfor
  for $h = 1 : p - q$
    Set $\Omega_k := 2\Psi_{h,p-q+i}$.
    Set $\lambda_k := E_{p-q+i,p+i}$.
    Set $c(k) := -\frac{1}{2}E_{h,p+i}$.
    Set $k = k + 1$, $h = h + 1$.
  endfor
  for $j = q : i + 1$
    Set $\Omega_k := \Psi_{p-q+i,p-q+j} - \Psi_{p+i,p+j}$.
    Set $\lambda_k := E_{p-q+i,p+i} + E_{p-q+j,p+j}$.
    Set $c(k) := \frac{1}{2}(-E_{p-q+i,p+j} + E_{p-q+j,p+i})$.
    Set $k = k + 1$, $j = j - 1$.
  endfor
endfor
Set $N := k - 1$.
end generate.directions

Let $B \in \mathbb{R}^{p \times q}$ and $S := \begin{bmatrix} 0 & B \\ B^\top & 0 \end{bmatrix}$. Let $\omega_i(\cos t, \sin t, \cos 2t, \sin 2t) = \exp t\Omega_i$ denote the elementary rotations. A sweep is explicitly given by the following algorithm. It constructs the transformed $S_{\text{new}} = uSu^\top$ and the transformation $u = \begin{bmatrix} v_1 & 0 \\ 0 & v_2 \end{bmatrix}$.

function: $(S_{\text{new}}, u_{\text{new}}) = \text{scs.sweep}(S, u)$
Set $(S_{\text{new}}, u_{\text{new}}) = (S, u)$
Set $(\Omega_1, \lambda(1), c(1), ..., \Omega_N, \lambda(N), c(N), N) = \text{generate.directions}(p, q)$.
for $i = 1 : N$
  Set $c := \operatorname{tr}(c(i)S)$, $\lambda := \operatorname{tr}(\lambda(i)S)$, $dis := \lambda^2 + 4c^2$
  if $dis \neq 0$

Set $(cos2t_*, sin2t_*) := -\dfrac{1}{dis}(\lambda, 2c)$.

else

Set $(cos2t_*, sin2t_*) := (1, 0)$.

endif

Set $cost_* := \sqrt{\frac{1+cos2t_*}{2}}$.

if $sin2t_* \geq 0$

Set $sint_* = \sqrt{\frac{1-cos2t_*}{2}}$.

else

Set $sint_* = -\sqrt{\frac{1-cos2t_*}{2}}$.

endif

Set $S_{\text{new}} := \omega_i(cost_*, sint_*, cos2t_*, sin2t_*)S_{\text{new}}\omega_i(cost_*, sint_*, cos2t_*, sin2t_*)^\top$

Set $u_{\text{new}} := \omega_i(cost_*, sint_*, cos2t_*, sin2t_*)u$.

end scs.sweep

It is now straightforward to implement the Sort-Jacobi algorithm with special cyclic sweeps for computing the SVD of a given matrix $B \in \mathbb{R}^{p\times q}$. Let $\mathfrak{p}$ be defined as in Eq. (4.6). We use the function $d\colon \mathfrak{p} \longrightarrow \mathbb{R}^+$, $X \longmapsto ||X - X_0||^2$ as a measure for the distance of an element in X to $\mathfrak{a}$. Given a matrix $S = \begin{bmatrix} 0 & B \\ B^\top & 0 \end{bmatrix}$ and a tolerance $tol > 0$, this algorithm overwrites S by $uSu^\top$ where $u = \begin{bmatrix} v_1 & 0 \\ 0 & v_2 \end{bmatrix}$ and $d(uSu^\top) \leq tol$.

Set $u :=$ identity matrix.

while $d(S) > tol$

Set $(S, u) = \text{scs.sweep}(S, u)$.

endwhile

The above algorithm differs in two essential points from the algorithm that Kogbetliantz proposed in [46] and that seems to be used still in many applications. While Kogbetliantz's method minimizes the off-norm, our approach minimizes the trace function and therefore sorts the singular values. The Sort-Jacobi methods have already been discussed in [42] for the real SVD and the symmetric EVD and it has been observed there, that they have a better convergence behavior than the classical methods. The second difference is the order in which the sweep directions are worked off. The special cyclic sweep has been introduced as a generalization of the special cyclic sweep for symmetric matrices, cf. [21], and has been needed in order to prove local quadratic convergence for irregular elements. However, in the above case of the singular value decomposition of a non-symmetric matrix it yields a sweep method that

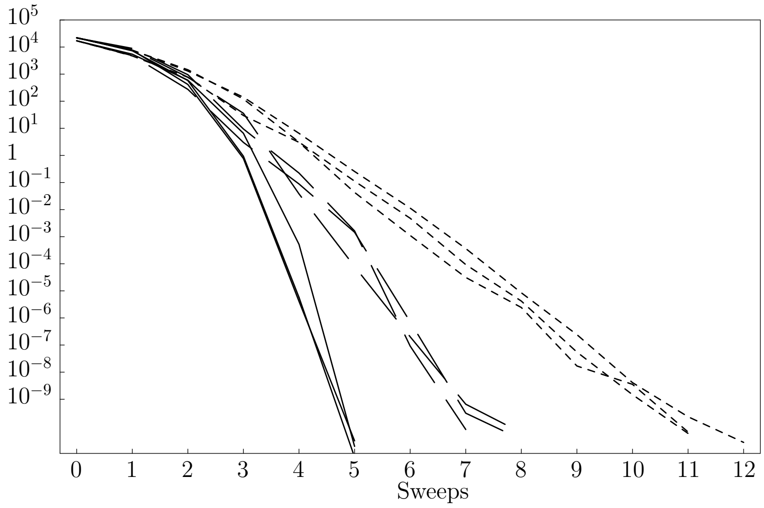

Figure 4.4: Convergence behavior for the real SVD of three (65×50)-matrices with clustered singular values at $30, 10, 5, 0$; stopping criterion: off-norm $< 10^{-10}$; small dashed line = classical cyclic Kogbetliantz; large dashed line = sort Jacobi with classical cyclic sweeps; solid line = Sort-Jacobi with special cyclic sweeps.

does *not* correspond to the sweep order proposed in [21], [42] and [46]. In Fig. 4.4 we compare the classical cyclic Kogbetliantz, the Sort-Jacobi method with classical sweep order and the Sort-Jacobi with special cyclic sweeps. All three methods have been applied to the same, randomly generated (65×50)-matrices with clustered singular values at $30, 10, 5$ and 0. The off-norm is labeled at the vertical axis. Kogbetliantz's classical method shows the worst convergence behavior. Slightly better is Hüper's Sort-Jacobi algorithm with standard sweeps, [42]. The sort Jacobi with special cyclic sweeps exhibits the best convergence behavior. Here, the matrix is almost diagonalized after 5 sweeps, whereas with the usual Kogbetliantz method, the off-norm after five sweeps is of order $\sim 10^1$. The advantage of the special cyclic sweeps increases the bigger the matrix and the bigger the clusters of the singular values are.

An interesting special case is the computation of the SVD of a triangular matrix, since the problem of computing the singular values can be reduced to that case by a previous QR-decomposition, cf. [25], of the rectangular matrix. In this case, Kogbetliantz's method is known to converge locally quadratic, cf. [2], and preserves the triangular structure, cf. [29]. Comparisons between Kogbetliantz's method and the method proposed here show that although our method does not preserve the triangular structure, it is faster convergent. The advantage over the Kogbetliantz method is apparent for matrices of size greater than $\sim (30 \times 30)$. Fig. 4.5 illustrates the convergence behavior for an upper triangular (50×50)-matrix with clustered singular values at $0, 5, 10, 30$.

As mentioned at the beginning of this chapter, the symmetric perskew-symmetric

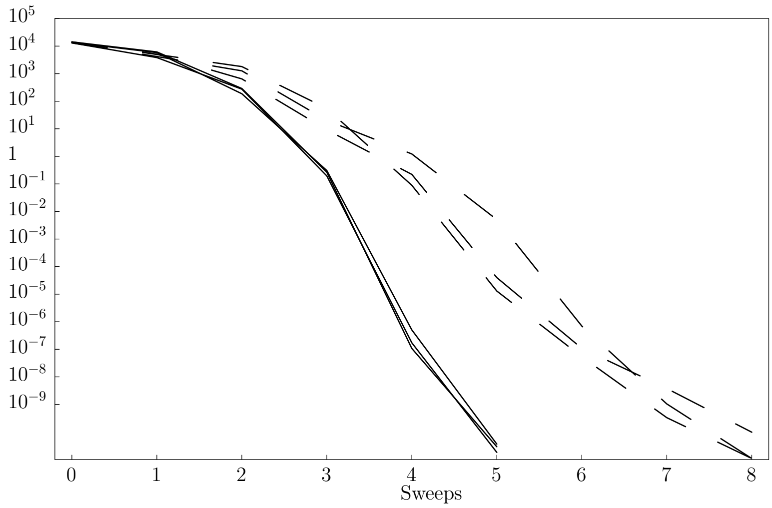

Figure 4.5: Convergence behavior for the real SVD of three (50×50)-matrices with clustered singular values at $30, 10, 5, 0$ in upper triangular form; stopping criterion: off-norm $< 10^{-10}$; dashed line = classical cyclic Kogbetliantz; solid line = Sort-Jacobi with special cyclic sweeps.

eigenvalue problem, cf. [49], is equivalent to the real SVD. For the subsequent discussion, we restrict ourselves to the case where the regarded matrices are of size $(2k+1) \times (2k+1)$. The even case is treated analogously. More precisely, if $R \in \mathbb{R}^{(2k+1)\times(2k+1)}$ is defined as in Eq. (4.1), then

$$gRg^\top = \begin{bmatrix} I_{k+1} & \\ & -I_k \end{bmatrix}, \quad \text{with orthogonal } g = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & & & \cdots & & 0 & 1 \\ 0 & \ddots & & & & & \iddots & 0 \\ & & 1 & 0 & 1 & & & \\ \vdots & & 0 & \sqrt{2} & 0 & & & \vdots \\ & & -1 & 0 & 1 & & & \\ 0 & \iddots & & & & & \ddots & 0 \\ -1 & 0 & & & \cdots & & 0 & 1 \end{bmatrix}. \tag{4.17}$$

The same conjugation $g(\cdot)g^\top$ yields the equivalence between the Lie algebra of perskew-symmetric matrices and $\mathfrak{so}(k+1,k)$. Similarly, the Cartan decomposition of perskew-symmetric matrices is given by $\mathfrak{k}' \oplus \mathfrak{p}'$ with $\mathfrak{k}' = g^\top \mathfrak{k} g$ and $\mathfrak{p}' = g^\top \mathfrak{p} g$, where $\mathfrak{k}$ and $\mathfrak{p}$ are defined by (4.5), (4.6). If $\mathfrak{a}' \subset \mathfrak{p}'$ is chosen to be the set of diagonal matrices and $\mathfrak{a}$ is defined as in Eq. (4.7), then

$$\mathfrak{a}' = g^\top v \mathfrak{a} v^\top g, \quad \text{where } v = \begin{bmatrix} J_k & 0 \\ 0 & I_k \end{bmatrix},$$

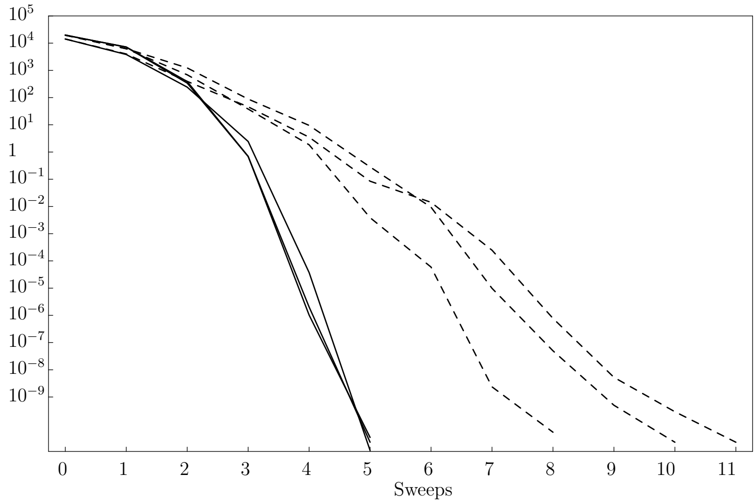

Figure 4.6: Convergence behavior for the symmetric perskew-symmetric EVD for three (101×101)-matrices with clustered singular values at $0, \pm 5, \pm 10, \pm 30$. small dashed line = algorithm proposed in [49]; solid line = sort Jacobi with special cyclic sweeps.

with

$$J_k = \begin{bmatrix} & & 1 \\ & \cdot^{\cdot^{\cdot}} & \\ 1 & & \end{bmatrix} \text{ if } k \text{ is odd} \quad \text{and} \quad J_k = \begin{bmatrix} & & & -1 \\ & & 1 & \\ & \cdot^{\cdot^{\cdot}} & & \\ 1 & & & \end{bmatrix} \text{ if } k \text{ is even.}$$

With these transformations it is easily seen that the proposed algorithm in [49] for the symmetric perskew-symmetric eigenvalue problem is in fact nothing else than Kogbetliantz's algorithm for a real $(k+1) \times k$-matrix with the only difference that the sweep order differs. Nevertheless, the used order is not a special cyclic sweep. We compare the algorithm proposed in [49] with the one that is obtained by using a Sort-Jacobi with special cyclic sweeps. The result is illustrated in Fig. 4.6. Again. the advantage of the sort Jacobi with special cyclic sweeps is the bigger, the bigger the clusters of the eigenvalues are. Note that the same transformation $g(\cdot)g^\top$ with g defined as in Eq. (4.17) yields the equivalence between the skew-symmetric perskew-symmetric EVD and the skew symmetric EVD of two independent $(k \times k)$, $(k+1 \times k+1)$-matrices respectively; the symmetric persymmetric EVD and the symmetric EVD of two independent $(k \times k)$, $(k+1 \times k+1)$-matrices respectively; the skew-symmetric persymmetric EVD and the real SVD of a $(k+1 \times k)$-matrix.

4.3 The Real Symmetric Hamiltonian EVD & Takagi's Factorization

We demonstrate in this section how the real Symmetric Hamiltonian EVD can be derived as a special case of the ideas developed in the previous chapter. In [18], the authors use a Jacobi-type method that is based on the direct solution of a 4×4 subproblem. We will not follow this approach and restrict ourselves to optimization along one-parameter subgroups. By Theorem 2.23, Ch. 2, it is clear which optimization directions can be grouped together in order to achieve parallelizability. Moreover, we prove that the real symmetric Hamiltonian EVD is equivalent to Takagi's Factorization of a complex symmetric matrix, i.e. given a complex symmetric matrix $B \in \mathbb{C}^{n\times n}$, find a unitary matrix $u \in U(n)$ such that $uBu^\top$ is real and diagonal, cf. [38] Sec. 4.4.
The set of real Hamiltonian matrices forms a real and semisimple Lie algebra, namely

$$\mathfrak{sp}(n,\mathbb{R}) = \left\{ \begin{bmatrix} A & B \\ C & -A^\top \end{bmatrix},\ B^\top = B, C^\top = C, A \in \mathbb{R}^{n\times n} \right\}. \tag{4.18}$$

By Example 1.4, the Killing form on $\mathfrak{sp}(n,\mathbb{R})$ is $\kappa(X,Y) = 2(n+1)\mathrm{tr}(XY)$. Therefore, $\theta := -(\cdot)^\top$ yields a Cartan involution since

$$B_\theta(X,Y) = -\kappa(X,\theta Y) = 2(n+1)\mathrm{tr}(XY^\top)$$

is an inner product. The corresponding Cartan decomposition is given by $\mathfrak{sp}(n,\mathbb{R}) = \mathfrak{k} \oplus \mathfrak{p}$ with

$$\begin{aligned} \mathfrak{k} &= \left\{ \begin{bmatrix} \Psi & B \\ -B & \Psi \end{bmatrix},\ B^\top = B, \Psi^\top = -\Psi \in \mathbb{R}^{n\times n} \right\}, \\ \mathfrak{p} &= \left\{ \begin{bmatrix} S & C \\ C & -S \end{bmatrix},\ C^\top = C, S^\top = S \in \mathbb{R}^{n\times n} \right\}. \end{aligned} \tag{4.19}$$

Hence $\mathfrak{p}$ consists of all symmetric Hamiltonian matrices of size $2n \times 2n$. Note, that $\mathfrak{k}$ is isomorphic to $\mathfrak{u}(n)$ via the Lie algebra isomorphism

$$\iota\colon X + \mathrm{i}Y \longmapsto \begin{bmatrix} X & Y \\ -Y & X \end{bmatrix}, \qquad X,Y \in \mathbb{R}^{n\times n}.$$

and the same mapping also yields a Lie group isomorphism

$$\iota\colon U(n) \longrightarrow \mathbb{R}^{2n\times 2n}, \quad u \longmapsto \begin{bmatrix} \mathrm{Re}u & \mathrm{Im}u \\ -\mathrm{Im}u & \mathrm{Re}u \end{bmatrix}.$$

As a maximal abelian subalgebra in $\mathfrak{p}$ we choose the diagonal matrices, i.e.

$$\mathfrak{a} = \left\{ \begin{bmatrix} \Lambda & \\ & -\Lambda \end{bmatrix}, \Lambda = \mathrm{diag}(a_1, ..., a_n) \right\}. \tag{4.20}$$

The equivalence of the real Symmetric Hamiltonian EVD and Takagi's Factorization is stated in the following proposition. The two normal form problems can be carried over to one another via conjugation by a fixed matrix.

Proposition 4.7. *Let $\mathfrak{p}$ be defined as in Eq. (4.19), let $\mathfrak{a}$ be as in Eq. (4.20) and let* $\begin{bmatrix} S & C \\ C & -S \end{bmatrix} \in \mathfrak{p}$*. Then*

$$\iota(u) \begin{bmatrix} S & C \\ C & -S \end{bmatrix} \iota(u^*) \in \mathfrak{a}$$

if and only if $u(S - \mathrm{i}C)u^\top$ is real and diagonal.

Proof. Let $g_0 \in U(2n)$ be defined by

$$g_0 := \frac{1}{\sqrt{2}} \begin{bmatrix} \mathrm{i}I_n & I_n \\ I_n & \mathrm{i}I_n \end{bmatrix}$$

and let $u \in U(n)$. Then we have

$$g_0 \iota(u) g_0^{-1} = \begin{bmatrix} \mathrm{Re}u + \mathrm{i}\mathrm{Im}u & 0 \\ 0 & \mathrm{Re}u - \mathrm{i}\mathrm{Im}u \end{bmatrix} = \begin{bmatrix} u & 0 \\ 0 & \overline{u} \end{bmatrix}.$$

Therefore for symmetric $S, C \in \mathbb{R}^{n \times n}$ and real diagonal Λ we have

$$\begin{aligned}
&\iota(u) \begin{bmatrix} S & C \\ C & -S \end{bmatrix} \iota(u^*) = \begin{bmatrix} \Lambda & 0 \\ 0 & -\Lambda \end{bmatrix} \quad \Longleftrightarrow \\
&g_0 \iota(u) g_0^{-1} g_0 \begin{bmatrix} S & C \\ C & -S \end{bmatrix} g_0^{-1} g_0 \iota(u^*) g_0^{-1} = g_0 \begin{bmatrix} \Lambda & 0 \\ 0 & -\Lambda \end{bmatrix} g_0^{-1} \quad \Longleftrightarrow \\
&\begin{bmatrix} u & 0 \\ 0 & \overline{u} \end{bmatrix} \begin{bmatrix} 0 & C + \mathrm{i}S \\ C - \mathrm{i}S & 0 \end{bmatrix} \begin{bmatrix} u^* & 0 \\ 0 & u^\top \end{bmatrix} = \begin{bmatrix} 0 & \mathrm{i}\Lambda \\ -\mathrm{i}\Lambda & 0 \end{bmatrix} \quad \Longleftrightarrow \\
&u(C + \mathrm{i}S)u^\top = \mathrm{i}\Lambda \quad \Longleftrightarrow \quad u(S - \mathrm{i}C)u^\top = \Lambda.
\end{aligned}$$

□

Proposition 4.7 justifies that we restrict our discussion to the real symmetric Hamiltonian case. As a set of positive restricted roots we choose

$$\boxed{\begin{aligned} &a_i - a_j, \quad 1 \le i < j \le n, \\ &a_i + a_j, \quad 1 \le i \le j \le n. \end{aligned}} \tag{4.21}$$

The restricted roots form a root system that is called to be of type C_n. It is illustrated in Fig. 4.8 for the case $n = 2$. A simple system is given by

$$\Pi_{C_q} = \{a_i - a_{i+1} \mid 1 \le i < n\} \cup \{2a_n\}. \tag{4.22}$$

An ordering that satisfies the SCS-condition is given by the following Proposition.

Proposition 4.8. *Let $\alpha_i := a_i - a_{i+1}$, $i = 1, ..., n-1$ and let $\alpha_n := 2a_n$. Then $(\Pi_{C_n}, >)$ satisfies the SCS-condition 3.29 if $>$ is defined by*

$$\alpha_i > \alpha_j, \quad \text{if } i < j.$$

Proof. In terms of the simple roots α_i, the restricted roots are

$$a_i - a_j = \sum_{k=i}^{j-1} \alpha_k, \quad a_i + a_n = \sum_{k=i}^{n} \alpha_k, \quad a_i + a_j = \sum_{k=i}^{n} \alpha_k + \sum_{k=j}^{n-1} \alpha_k \text{ for } j > n. \tag{4.23}$$

Therefore the sets $\Sigma_k^+ \setminus \Sigma_{k-1}^+$ are given by

$$\begin{aligned}
\Sigma_{\max}^+ \setminus \Sigma_{\max-1}^+ &: a_1 - a_2 < ... < a_1 - a_n < a_1 + a_n < ... < a_1 + a_2 < 2a_1 \\
&\vdots \\
\Sigma_k^+ \setminus \Sigma_{k-1}^+ &: a_k - a_{k+1} < ... < a_k - a_n < a_k + a_n < ... < a_k + a_{k+1} < 2a_k \\
&\vdots \\
\Sigma_1^+ &: 2a_n.
\end{aligned}$$

Again with Eq. (4.23) it can easily be checked that $(\Pi_{C_n}, >)$ satisfies the SCS-condition. ☐

All restricted-root spaces are of real dimension one and have the following form. For $\mathfrak{g}_{a_i - a_j}$, all entries are zero except the (i,j)- and the $(n+j, n+i)$-entry. If $i < j$, the entries of $\mathfrak{g}_{a_i + a_j}$ all vanish except the $(i, n+j)$- and the $(j, n+i)$-entries. For $\mathfrak{g}_{2a_i}$ the only nonzero entry is at $(n+i, i)$.

$$\mathfrak{g}_{a_i - a_j} = \mathbb{R} \cdot \begin{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} & \\ & \begin{bmatrix} 0 & 0 \\ -1 & 0 \end{bmatrix} \end{bmatrix}, \qquad \mathfrak{g}_{a_i + a_j} = \mathbb{R} \cdot \begin{bmatrix} & \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} & \end{bmatrix},$$
$$\mathfrak{g}_{2a_i} = \mathbb{R} \cdot \begin{bmatrix} & \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} & \end{bmatrix}. \tag{4.24}$$

It is straightforward to check that the above basis vectors are all normalized in the sense of Eq. (3.15). An implementation of the algorithm of Section 3.2 has been done analogously to the previous section. Figure 4.7 illustrates the case where the initial points are randomly generated (120×120)-symmetric Hamiltonian matrices, all with the same spectrum, clustered at $0, \pm 3, \pm 5$ and ± 10. The squared distance to $\mathfrak{a}$, i.e. $||X - \mathrm{p}(X)||^2$ is labeled at the vertical axis. The special cyclic sweep yields quadratic convergence, while a sweep method whose order has randomly been chosen before starting the experiment (and has not been modified throughout choosing the three randomly initial points) indicates rather linear convergence.

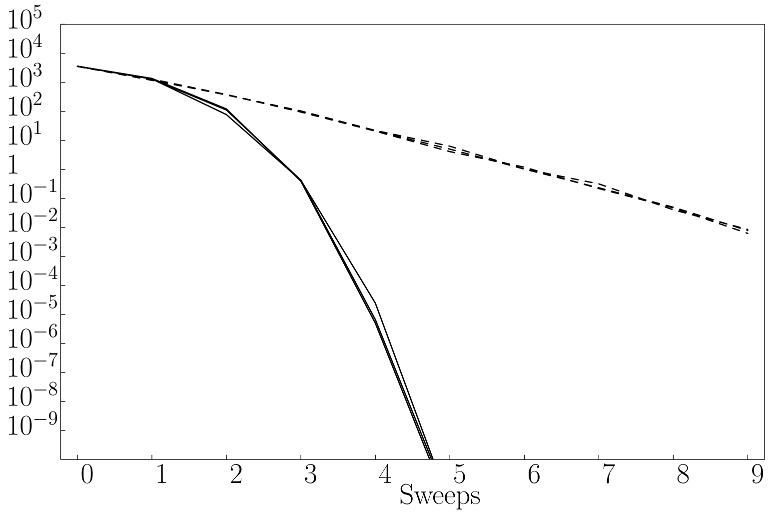

Figure 4.7: Convergence behavior for the real symmetric Hamiltonian EVD of three (120×120)-matrices with clustered singular values at $0, \pm 3, \pm 5, \pm 10$. dashed line = sort Jacobi with a randomly chosen sweep method; solid line = sort Jacobi with special cyclic sweeps; stopping criterion: off-norm $< 10^{-10}$.

4.4 The Symplectic Singular Value Decomposition

Consider the real simple Lie algebra

$$\mathfrak{sp}(p,q) := \left\{ \begin{bmatrix} A & -\overline{E} & B & -\overline{F} \\ E & \overline{A} & F & \overline{B} \\ B^* & F^* & D & -\overline{H} \\ -F^\top & B^\top & H & \overline{D} \end{bmatrix}, \right.$$
$$\left. A^* = -A, D^* = -D, E = E^\top, H = H^\top, B, F \in \mathbb{C}^{p\times q} \right\}.$$

The above Lie algebra is a real form of $\mathfrak{sp}(p+q,\mathbb{C})$ and hence its Killing form is given by $\kappa(X,Y) = 2(p+q+1)\operatorname{tr}(XY)$, cf. Eq. (1.9) together with Example 1.4. Hence a Cartan involution is given by $\theta = -(\cdot)^*$ and the corresponding Cartan decomposition is $\mathfrak{sp}(p,q) = \mathfrak{k} \oplus \mathfrak{p}$ with

$$\mathfrak{k} = \left\{ \begin{bmatrix} \begin{matrix} A & -\overline{E} \\ E & \overline{A} \end{matrix} & 0 \\ 0 & \begin{matrix} D & -\overline{H} \\ H & \overline{D} \end{matrix} \end{bmatrix} A^* = -A, D^* = -D, E = E^\top, H = H^\top \right\},$$

$$\mathfrak{p} = \left\{ \begin{bmatrix} 0 & \begin{matrix} B & -\overline{F} \\ F & \overline{B} \end{matrix} \\ \begin{matrix} B^* & F^* \\ -F^\top & B^\top \end{matrix} & 0 \end{bmatrix} B, F \in \mathbb{C}^{p\times q} \right\}.$$

As a maximal abelian subspace in $\mathfrak{p}$ we fix

$$\mathfrak{a} := \left\{ \begin{bmatrix} 0 & 0 & \Lambda & 0 \\ 0 & 0 & 0 & \Lambda \\ \Lambda^\top & 0 & 0 & 0 \\ 0 & \Lambda^\top & 0 & 0 \end{bmatrix} \mid \Lambda = \left[\begin{array}{ccc} & 0 & \\ \hline a_1 & & 0 \\ & \ddots & \\ 0 & & a_q \end{array}\right] \in \mathbb{R}^{p\times q} \right\}.$$

The restricted roots form a root system of type $(BC)_q$ if $p > q$ and of type C_q if $p = q$. The root systems are illustrated in Fig. 4.8 and 4.9 for the case that $q = 2$. A set of positive restricted roots is given by the linear functionals

$$\boxed{\begin{array}{ll} a_i - a_j, & 1 \leq i < j \leq q, \\ \\ a_i + a_j, & 1 \leq i \leq j \leq q. \end{array}} \tag{4.25a}$$

Moreover, in the case where $p > q$, we have

$$\boxed{a_i, \quad 1 \leq i \leq q.} \tag{4.25b}$$

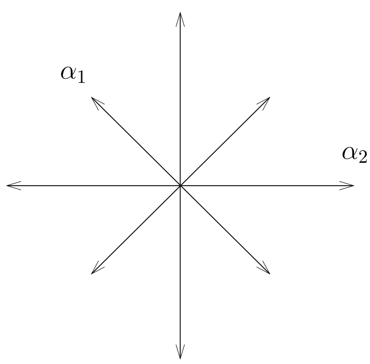

Figure 4.8: The root system C_2 with simple roots α_1, α_2.

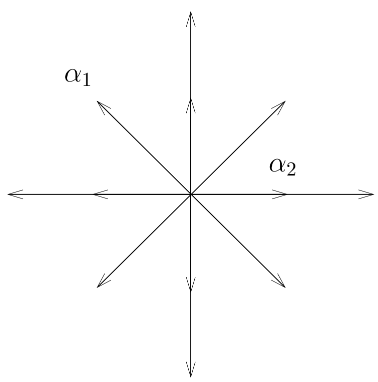

Figure 4.9: The root system $(BC)_2$ with α_1, α_2 simple.

For the root system $(BC)_q$ and the above choice of positive roots, the set of simple roots is given by

$$\Pi_{(BC)_q} = \{a_i - a_{i+1} \mid 1 \leq i < q\} \cup \{a_q\}.$$

Proposition 4.9. *Let $\alpha_i := a_i - a_{i+1}$, $i = 1, ..., q-1$ and let $\alpha_q := a_q$. Then $(\Pi_{(BC)_q}, >)$ satisfies the SCS-condition 3.29 if $>$ is defined by*

$$\alpha_i > \alpha_j, \quad \textit{if } i < j.$$

Proof. In terms of the simple roots α_i, the restricted roots are

$$a_i - a_j = \sum_{k=i}^{j-1} \alpha_k, \quad a_i = \sum_{k=i}^{q} \alpha_k, \quad a_i + a_j = \sum_{k=i}^{q} \alpha_k + \sum_{k=j}^{q} \alpha_k. \tag{4.26}$$

Therefore the sets $\Sigma_k^+ \setminus \Sigma_{k-1}^+$ are given by

$$\begin{aligned}
\Sigma_{\max}^+ \setminus \Sigma_{\max-1}^+ &: a_1 - a_2 < \ldots < a_1 - a_q < a_1 < a_1 + a_q < \ldots < a_1 + a_2 < 2a_1 \\
&\vdots \\
\Sigma_k^+ \setminus \Sigma_{k-1}^+ &: a_k - a_{k+1} < \ldots < a_k - a_q < a_k < a_k + a_q < \ldots < 2a_k \\
&\vdots \\
\Sigma_1^+ &: a_q < 2a_q.
\end{aligned}$$

Together with Eq. (4.26) it can easily be checked that $(\Pi_{(BC)_q}, >)$ satisfies the SCS-condition. $\square$

Now if $p = q$, the restricted roots are of type C_q as in the previous section. A simple system is given by Π_{C_q}, defined as in Eq. (4.22) and Proposition 4.8 yields an ordering such that $(\Pi_{C_q}, >)$ satisfies the SCS-condition. Relative to $\mathfrak{a}$, the restricted-root spaces are as follows. For the roots $H \longmapsto a_i \pm a_j$, $i < j$, the restricted-root spaces are of real dimension 4 and are nonzero only in the 32 entries corresponding to row and column indices $p-q+i, 2p-q+i, 2p+i, 2p+q+i, p-q+j, 2p-q+j, 2p+j, 2p+q+j$. They are

$$\mathfrak{g}_{a_i - a_j} = \left\{ \begin{bmatrix} \begin{bmatrix} 0 & z \\ -\overline{z} & 0 \end{bmatrix} & \begin{bmatrix} 0 & w \\ w & 0 \end{bmatrix} & \begin{bmatrix} 0 & z \\ \overline{z} & 0 \end{bmatrix} & \begin{bmatrix} 0 & w \\ -w & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & -\overline{w} \\ -\overline{w} & 0 \end{bmatrix} & \begin{bmatrix} 0 & \overline{z} \\ -z & 0 \end{bmatrix} & \begin{bmatrix} 0 & -\overline{w} \\ \overline{w} & 0 \end{bmatrix} & \begin{bmatrix} 0 & \overline{z} \\ z & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & z \\ \overline{z} & 0 \end{bmatrix} & \begin{bmatrix} 0 & w \\ -w & 0 \end{bmatrix} & \begin{bmatrix} 0 & z \\ -\overline{z} & 0 \end{bmatrix} & \begin{bmatrix} 0 & w \\ w & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & -\overline{w} \\ \overline{w} & 0 \end{bmatrix} & \begin{bmatrix} 0 & \overline{z} \\ z & 0 \end{bmatrix} & \begin{bmatrix} 0 & -\overline{w} \\ -\overline{w} & 0 \end{bmatrix} & \begin{bmatrix} 0 & \overline{z} \\ -z & 0 \end{bmatrix} \end{bmatrix} \middle| w, z \in \mathbb{C} \right\} \tag{4.27}$$

and

$$\mathfrak{g}_{a_i+a_j} = \left\{ \begin{bmatrix} \begin{bmatrix} 0 & z \\ -\overline{z} & 0 \end{bmatrix} & \begin{bmatrix} 0 & w \\ w & 0 \end{bmatrix} & \begin{bmatrix} 0 & -z \\ \overline{z} & 0 \end{bmatrix} & \begin{bmatrix} 0 & -w \\ -w & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & -\overline{w} \\ -\overline{w} & 0 \end{bmatrix} & \begin{bmatrix} 0 & \overline{z} \\ -z & 0 \end{bmatrix} & \begin{bmatrix} 0 & \overline{w} \\ \overline{w} & 0 \end{bmatrix} & \begin{bmatrix} 0 & -\overline{z} \\ z & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & z \\ -\overline{z} & 0 \end{bmatrix} & \begin{bmatrix} 0 & w \\ w & 0 \end{bmatrix} & \begin{bmatrix} 0 & -z \\ \overline{z} & 0 \end{bmatrix} & \begin{bmatrix} 0 & -w \\ -w & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & -\overline{w} \\ -\overline{w} & 0 \end{bmatrix} & \begin{bmatrix} 0 & \overline{z} \\ -z & 0 \end{bmatrix} & \begin{bmatrix} 0 & \overline{w} \\ \overline{w} & 0 \end{bmatrix} & \begin{bmatrix} 0 & -\overline{z} \\ z & 0 \end{bmatrix} \end{bmatrix} \middle| w, z \in \mathbb{C} \right\}. \tag{4.28}$$

The restricted-root spaces for the roots $H \longmapsto 2a_i$ have real dimension 3 and are nonzero only in the entries corresponding to row and column indices $p-q+i, 2p-q+i, 2p+i, 2p+q+i$, where they are

$$\mathfrak{g}_{2a_i} = \left\{ \begin{bmatrix} \mathrm{i}x & z & -\mathrm{i}x & -z \\ -\overline{z} & -\mathrm{i}x & \overline{z} & \mathrm{i}x \\ \mathrm{i}x & z & -\mathrm{i}x & -z \\ -\overline{z} & -\mathrm{i}x & \overline{z} & \mathrm{i}x \end{bmatrix} \middle| x \in \mathbb{R}, z \in \mathbb{C} \right\}. \tag{4.29}$$

The restricted-root spaces for the roots $H \longmapsto a_i$, which only exist if $p > q$, have real dimension $4(p-q)$ and are nonzero only in the entries corresponding to row and column indices $1, ..., p-q, p+1, ..., 2p-q, 2p-q+i, 2p+i, 2p+q+i$, where they are

$$\mathfrak{g}_{a_i} = \left\{ \begin{bmatrix} 0 & v & 0 & w & -v & -w \\ -v^* & 0 & w^\top & 0 & 0 & 0 \\ 0 & -\overline{w} & 0 & \overline{v} & \overline{w} & -\overline{v} \\ -w^* & 0 & -v^\top & 0 & 0 & 0 \\ -v^* & 0 & w^\top & 0 & 0 & 0 \\ -w^* & 0 & -v^\top & 0 & 0 & 0 \end{bmatrix} \middle| v, w \in \mathbb{C}^{p-q} \right\}. \tag{4.30}$$

For the sake of completeness, we also specify the centralizer of $\mathfrak{a}$ in $\mathfrak{k}$ which is given by

$$\mathfrak{z}_{\mathfrak{k}}(\mathfrak{a}) = \left\{ \begin{bmatrix} Z_1 & 0 & Z_2 & 0 & 0 & 0 \\ 0 & \Gamma & 0 & \Xi & 0 & 0 \\ -\overline{Z_2} & 0 & \overline{Z_1} & 0 & 0 & 0 \\ 0 & -\overline{\Xi} & 0 & -\Gamma & 0 & 0 \\ 0 & 0 & 0 & 0 & \Gamma & \Xi \\ 0 & 0 & 0 & 0 & -\overline{\Xi} & -\Gamma \end{bmatrix}, Z_1, Z_2 \in \mathbb{C}^{(p-q)\times(p-q)}, Z_1 = -Z_1^*, \right.$$
$$\left. Z_2 = Z_2^\top, \Gamma = \begin{bmatrix} \mathrm{i}x_1 & & \\ & \ddots & \\ & & \mathrm{i}x_q \end{bmatrix}, \Xi = \begin{bmatrix} z_1 & & \\ & \ddots & \\ & & z_q \end{bmatrix}, x_i \in \mathbb{R}, z_i \in \mathbb{C} \right\}. \tag{4.31}$$

In the sequel we specify an algorithm to compute the symplectic SVD. According to Theorem 3.36, this algorithm is locally quadratic convergent for any element since we use Special Cyclic Sweeps. Again, the proposed code has a more instructive character. It can easily be improved for implementation. To give an idea how the special cyclic sweeps look like for the symplectic SVD, we firstly generate the sweep directions $\Omega_i \in \mathfrak{k}_\lambda$ with corresponding $\lambda(i)$ and $\overline{\Omega}_i$-coefficient $c(i)$.

Algorithm 4.10. Denote by X_{ij} the (i,j) entry of the matrix X. Let $E_{ij} \in \mathbb{R}^{2(p+q)}$ the matrix with (i,j)- entry 1 and zeros elsewhere and define $\Psi_{ij} := E_{ij} - E_{ji}$ and $\overline{\Psi} := E_{ij} + E_{ji}$.

Algorithm 4.10. symplectic SVD - Sweep directions and SCS-order.
function: $(\Omega_1, \lambda(1), c(1), ..., \Omega_N, \lambda(N), c(N), N) = \text{gen.sympl.svd.directions}(p,q)$
Set $k := 1$
for $i = 1 : q$
  for $j = i+1 : q$
    Set $\Omega_k := \Psi_{p-q+i,p-q+j} + \Psi_{2p-q+i,2p-q+j} + \Psi_{2p+i,2p+j} + \Psi_{2p+q+i,2p+q+j}$.
    Set $\lambda_k := E_{2p+i,p-q+i} - E_{2p+j,p-q+j}$.
    Set $c(k) := \frac{1}{2}(E_{2p+j,p-q+i} + E_{2p+i,p-q+j})$, $k := k+1$.
    Set $\Omega_k := \mathrm{i}\overline{\Psi}_{p-q+i,p-q+j} - \mathrm{i}\overline{\Psi}_{2p-q+i,2p-q+j} + \mathrm{i}\overline{\Psi}_{2p+i,2p+j} - \mathrm{i}\overline{\Psi}_{2p+q+i,2p+q+j}$.
    Set $\lambda_k := E_{2p+i,p-q+i} - E_{2p+j,p-q+j}$.
    Set $c(k) := \frac{\mathrm{i}}{2}(E_{2p+i,p-q+j} - E_{2p+j,p-q+i})$, $k := k+1$.
    Set $\Omega_k := \Psi_{p-q+i,2p-q+j} - \Psi_{2p-q+i,p-q+j} + \Psi_{2p+i,2p+q+j} - \Psi_{2p+q+i,2p+j}$.
    Set $\lambda_k := E_{2p+i,p-q+i} - E_{2p+j,p-q+j}$.
    Set $c(k) := \frac{1}{2}(E_{2p+q+j,p-q+i} - E_{2p+q+i,p-q+j})$, $k := k+1$.
    Set $\Omega_k := \mathrm{i}\overline{\Psi}_{p-q+i,2p-q+j} + \mathrm{i}\overline{\Psi}_{2p-q+i,p-q+j} + \mathrm{i}\overline{\Psi}_{2p+i,2p+q+j} + \mathrm{i}\overline{\Psi}_{2p+q+i,2p+j}$.
    Set $\lambda_k := E_{2p+i,p-q+i} - E_{2p+j,p-q+j}$.
    Set $c(k) := \frac{\mathrm{i}}{2}(E_{2p+q+i,p-q+j} - E_{2p+q+j,p-q+i})$, $k := k+1$, $j := j+1$.
  endfor
  for $h = 1 : p-q$
    Set $\Omega_k := 2(\Psi_{h,p-q+i} + \Psi_{p+h,2p-q+i})$.
    Set $\lambda_k := E_{2p+i,p-q+i}$.
    Set $c(k) := -\frac{1}{2}E_{2p+i,h}$, $k := k+1$.
    Set $\Omega_k := -2\mathrm{i}\overline{\Psi}_{h,p-q+i} + 2\mathrm{i}\overline{\Psi}_{p+h,2p-q+i}$.
    Set $\lambda_k := E_{2p+i,p-q+i}$.
    Set $c(k) := -\frac{\mathrm{i}}{2}E_{2p+i,h}$, $k := k+1$.
    Set $\Omega_k := 2(\Psi_{h,2p-q+i} - \Psi_{p+h,p-q+i})$.
    Set $\lambda_k := E_{2p+i,p-q+i}$.
    Set $c(k) := -\frac{1}{2}E_{2p+q+i,h}$, $k := k+1$.
    Set $\Omega_k := 2\mathrm{i}(\overline{\Psi}_{h,2p-q+i} + \overline{\Psi}_{p+h,p-q+i})$.
    Set $\lambda_k := E_{2p+i,p-q+i}$.

Set $c(k) := \frac{\mathrm{i}}{2} E_{2p+q+i,h}$, $k := k+1$, $h := h+1$.
endfor
for $j = q : i+1$
Set $\Omega_k := \Psi_{p-q+i,p-q+j} + \Psi_{2p-q+i,2p-q+j} - \Psi_{2p+i,2p+j} - \Psi_{2p+q+i,2p+q+j}$.
Set $\lambda_k := E_{2p+i,p-q+i} + E_{2p+j,p-q+j}$.
Set $c(k) := -\frac{1}{2}(E_{2p+j,p-q+i} - E_{2p+i,p-q+j})$, $k := k+1$.
Set $\Omega_k := \mathrm{i}\overline{\Psi}_{p-q+i,p-q+j} - \mathrm{i}\overline{\Psi}_{2p-q+i,2p-q+j} - \mathrm{i}\overline{\Psi}_{2p+i,2p+j} + \mathrm{i}\overline{\Psi}_{2p+q+i,2p+q+j}$.
Set $\lambda_k := E_{2p+i,p-q+i} + E_{2p+j,p-q+j}$.
Set $c(k) := \frac{\mathrm{i}}{2}(E_{2p+i,p-q+j} + E_{2p+j,p-q+i})$, $k := k+1$.
Set $\Omega_k := \Psi_{p-q+i,2p-q+j} - \Psi_{2p-q+i,p-q+j} - \Psi_{2p+i,2p+q+j} + \Psi_{2p+q+i,2p+j}$.
Set $\lambda_k := E_{2p+i,p-q+i} + E_{2p+j,p-q+j}$.
Set $c(k) := -\frac{1}{2}(E_{2p+q+j,p-q+i} + E_{2p+q+i,p-q+j})$, $k := k+1$.
Set $\Omega_k := \mathrm{i}\overline{\Psi}_{p-q+i,2p-q+j} + \mathrm{i}\overline{\Psi}_{2p-q+i,p-q+j} - \mathrm{i}\overline{\Psi}_{2p+i,2p+q+j} - \mathrm{i}\overline{\Psi}_{2p+q+i,2p+j}$.
Set $\lambda_k := E_{2p+i,p-q+i} + E_{2p+j,p-q+j}$.
Set $c(k) := \frac{\mathrm{i}}{2}(E_{2p+q+i,p-q+j} + E_{2p+q+j,p-q+i})$, $k := k+1$, $j := j-1$.
endfor
Set $\Omega_k = 2\mathrm{i}(E_{p-q+i,p-q+i} - E_{2p-q+i,2p-q+i} - E_{2p+i,2p+i} + E_{2p+q+i,2p+q+i})$.
Set $\lambda_k = 2E_{2p+i,p-q+i}$.
Set $c(k) = \frac{\mathrm{i}}{2} E_{2p+i,p-q+i}$; $k := k+1$.
Set $\Omega_k = 2(\Psi_{p-q+i,2p-q+i} - \Psi_{2p+i,2p+q+i})$.
Set $\lambda_k = 2E_{2p+i,p-q+i}$.
Set $c(k) = -\frac{1}{2} E_{2p+q+i,p-q+i}$; $k := k+1$.
Set $\Omega_k = 2\mathrm{i}(\Psi_{p-q+i,2p-q+i} - \Psi_{2p+i,2p+q+i})$.
Set $\lambda_k = 2E_{2p+i,p-q+i}$.
Set $c(k) = \frac{\mathrm{i}}{2} E_{2p+q+i,p-q+i}$; $k := k+1$; $i := i+1$.
endfor
Set $N := k-1$.
end gen.sympl.svd.directions

Let $\widetilde{B} := \begin{bmatrix} B & -\overline{F} \\ F & \overline{B} \end{bmatrix}$ be given with $B, F \in \mathbb{C}^{p\times q}$ and $S := \begin{bmatrix} 0 & \widetilde{B} \\ \widetilde{B}^* & 0 \end{bmatrix}$. Let

$$\omega_i(\cos t, \sin t, \cos 2t, \sin 2t) = \exp t\Omega_i$$

denote the elementary rotations. A sweep is explicitly given by the following algorithm. It computes the transformed $S_{\text{new}} = uSu^*$ and the transformation $u = \begin{bmatrix} v_1 & 0 \\ 0 & v_2 \end{bmatrix} \in Sp(p) \times Sp(q)$.

function: $(S_{\text{new}}, u_{\text{new}}) = \text{scs.sweep.sympl.SVD}(S, u)$

Set $(S_{\text{new}}, u_{\text{new}}) = (S, u)$
Set $(\Omega_1, \lambda(1), c(1), ..., \Omega_N, \lambda(N), c(N), N) = \text{gen.sympl.svd.directions}(p, q)$.
for $i = 1 : N$
  Set $c := \text{Retr}(c(i)S)$, $\lambda := \text{Retr}(\lambda(i)S)$, $dis := \lambda^2 + 4c^2$
  if $dis \neq 0$
    Set $(cos2t_*, sin2t_*) := -\frac{1}{dis}(\lambda, 2c)$.
  else
    Set $(cos2t_*, sin2t_*) := (1, 0)$.
  endif
  Set $cost_* := \sqrt{\frac{1+cos2t_*}{2}}$.
  if $sin2t_* \geq 0$
    Set $sint_* = \sqrt{\frac{1-cos2t_*}{2}}$.
  else
    Set $sint_* = -\sqrt{\frac{1-cos2t_*}{2}}$.
  endif
  Set $S_{\text{new}} := \omega_i(cost_*, sint_*, cos2t_*, sin2t_*) S_{\text{new}} \omega_i(cost_*, sint_*, cos2t_*, sin2t_*)^*$
  Set $u_{\text{new}} := \omega_i(cost_*, sint_*, cos2t_*, sin2t_*)u$.
end scs.sweep.sympl.svd

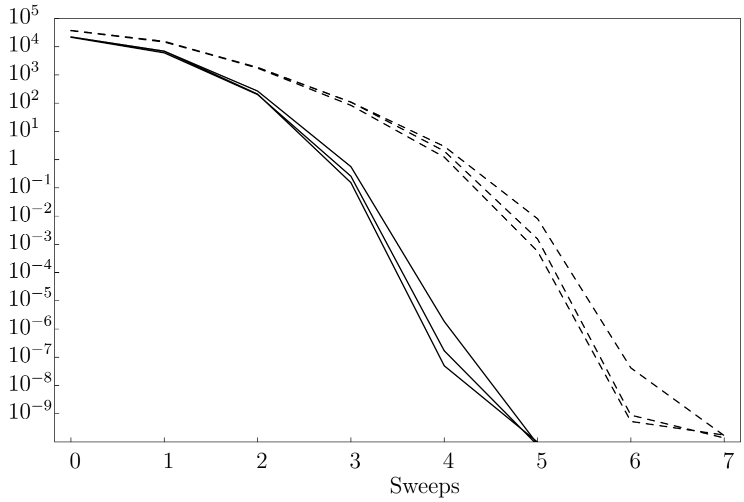

Figure 4.10: Sort-Jacobi with special cyclic sweeps for the symplectic SVD of a complex 70×60-matrix. solid line = irregular element with symplectic singular values clustered at $0, \pm 5, \pm 10, \pm 30$; dashed line = regular element with symplectic singular values $1, ..., 30$.

The implementation of the Sort-Jacobi algorithm for computing the symplectic SVD is now straightforward as in Section 4.2. We skip the details.

An implementation of the above algorithm shows the typical behavior for the sort Jacobi with special cyclic sweeps, namely that irregular elements converge faster than regular ones. Figure 4.10 illustrates the convergence for complex $\widetilde{B}$ of size 70×60 with (symplectic) singular values clustered at $0, \pm 5, \pm 10, \pm 30$ and with (symplectic) singular values $1, ..., 30$.

4.5 A Note on the Complex SVD and the Complex $\mathbb{R}$-Hamiltonian EVD

To the author's knowledge, R. Byers has been the first to propose a structure preserving Jacobi algorithm for the $\mathbb{R}$-Hamiltonian EVD, [9]. His work followed the idea of G.W. Stewart who presented a Jacobi algorithm to compute the Schur form for arbitrary complex matrices, [61]. Byers' algorithm was improved in [8] for non-normal $\mathbb{R}$-Hamiltonian matrices and C. Mehl further extended the algorithm in [8] to Hermitian pencils, cf. [52]. As pointed out in [8], the algorithm becomes Kogbetliantz's method if the $\mathbb{R}$-Hamiltonian matrix is Hermitian. For the comparison with the Sort-Jacobi with special cyclic sweeps we refer therefore to Section 4.2. Again we shall see that the method proposed here performs equally well if the pairwise difference of the absolute value of the eigenvalues is sufficiently large, i.e. if the matrix is a regular element in the sense of Eq. (1.16). However, for clustered eigenvalues the method in [8] (applied to Hermitian matrices) seems to converge only linearly, while the Sort-Jacobi with special cyclic sweeps is much faster – even faster than in the regular case.
The following proposition clarifies the equivalence of the Hermitian $\mathbb{R}$-Hamiltonian EVD and the SVD of a complex matrix of half the size.

Proposition 4.11. *Let u, v in $U(n)$ and let $B, C \in \mathbb{C}^{n \times n}$ be Hermitian. Then $u(B - \mathrm{i}C)v^*$ is real diagonal if and only if*

$$\begin{bmatrix} u+v & -\mathrm{i}(u-v) \\ \mathrm{i}(u-v) & u+v \end{bmatrix} \begin{bmatrix} B & C \\ C & -B \end{bmatrix} \begin{bmatrix} u+v & -\mathrm{i}(u-v) \\ \mathrm{i}(u-v) & u+v \end{bmatrix}^*$$

is real diagonal.

Proof. Let $g_0 = \frac{1}{2}\begin{bmatrix} I_n + \mathrm{i}I_n & I_n + \mathrm{i}I_n \\ -I_n + \mathrm{i}I_n & I_n - \mathrm{i}I_n \end{bmatrix} \in U(2n)$ and let $\iota(\cdot) := g_0(\cdot)g_0^*$ denote conjugation by g_0. Let $\Lambda \in \mathbb{R}^{n\times n}$ be diagonal. Then

$$\begin{aligned}
&u(B-\mathrm{i}C)v^* = \Lambda \quad\iff\\
&\begin{bmatrix} u & 0\\ 0 & v\end{bmatrix}\begin{bmatrix} 0 & B-\mathrm{i}C\\ B+\mathrm{i}C & 0\end{bmatrix}\begin{bmatrix} u & 0\\ 0 & v\end{bmatrix}^* = \begin{bmatrix} 0 & \Lambda\\ \Lambda & 0\end{bmatrix} \quad\iff\\
&\iota\left(\begin{bmatrix} u & 0\\ 0 & v\end{bmatrix}\right)\iota\left(\begin{bmatrix} 0 & B-\mathrm{i}C\\ B+\mathrm{i}C & 0\end{bmatrix}\right)\iota\left(\begin{bmatrix} u & 0\\ 0 & v\end{bmatrix}\right)^* = \iota\left(\begin{bmatrix} 0 & \Lambda\\ \Lambda & 0\end{bmatrix}\right) \quad\iff\\
&\frac{1}{4}\begin{bmatrix} u+v & -\mathrm{i}(u-v)\\ \mathrm{i}(u-v) & u+v\end{bmatrix}\begin{bmatrix} B & C\\ C & -B\end{bmatrix}\begin{bmatrix} u+v & -\mathrm{i}(u-v)\\ \mathrm{i}(u-v) & u+v\end{bmatrix}^* = \begin{bmatrix} \Lambda & 0\\ 0 & -\Lambda\end{bmatrix}.
\end{aligned}$$

Cf. also [8]. □

4.6 The Exceptional Case $\mathfrak{g}_2$

We examine now a rather exotic looking case that leads to a new structured eigenvalue problem and its corresponding Sort-Jacobi algorithm. It is not isomorphic to any of the cases discussed above. The complex semisimple Lie algebra $\mathfrak{g}_2$ is a 14-dimensional Lie algebra that is isomorphic to the Lie algebra of derivations of the complex octonians, cf. [22], Lecture 22. We introduce its standard representation following J.E. Humphreys, [39], Section 19, and deduce two structured EVDs, one arising from the real form $\mathfrak{g}_{2,0}$ and another one by using its adjoint representation.
Let the complex semisimple Lie algebra $\mathfrak{g}_2$ be defined as

$$\begin{aligned}
\mathfrak{g}_2 := \Bigg\{ &\begin{bmatrix} 0 & \sqrt{2}b^\top & \sqrt{2}c^\top\\ -\sqrt{2}c & M & B\\ -\sqrt{2}b & C & -M^\top\end{bmatrix} \;\Bigg|\; b = \begin{bmatrix} b_1\\ b_2\\ b_3\end{bmatrix}, B = \begin{bmatrix} 0 & -b_3 & b_2\\ -b_3 & 0 & -b_1\\ -b_2 & b_1 & 0\end{bmatrix},\\
&c = \begin{bmatrix} c_1\\ c_2\\ c_3\end{bmatrix}, C = \begin{bmatrix} 0 & -c_3 & c_2\\ -c_3 & 0 & -c_1\\ -c_2 & c_1 & 0\end{bmatrix}, b_i, c_i \in \mathbb{C}, M \in \mathbb{C}^{3\times 3}, \mathrm{tr}M = 0 \Bigg\}.
\end{aligned} \tag{4.32}$$

Note, that $\mathfrak{g}_2$ is a 14-dimensional Lie subalgebra of the 21-dimensional Lie algebra

$$\mathfrak{o}(7) := \left\{X \in \mathbb{C}^{7\times 7} \mid XF + FX^\top = 0\right\}, \tag{4.33}$$

where $F = \begin{bmatrix} 1 & 0 & 0\\ 0 & 0 & I_3\\ 0 & I_3 & 0\end{bmatrix}$ and that $\mathfrak{o}(7)$ is equivalent to the standard representation of $\mathfrak{so}(7,\mathbb{C})$, i.e.

$$g_0\mathfrak{o}(7)g_0^{-1} = \mathfrak{so}(7,\mathbb{C}), \quad \text{with} \quad g_0 = \frac{\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}}{\sqrt{2}}\begin{bmatrix} \sqrt{2}\mathrm{e}^{-\mathrm{i}\frac{\pi}{4}} & 0 & 0\\ 0 & I_3 & -\mathrm{i}I_3\\ 0 & -\mathrm{i}I_3 & I_3\end{bmatrix}. \tag{4.34}$$

Now consider the real Lie algebra

$$\mathfrak{g}_{2,0} := \left\{ \begin{bmatrix} 0 & \sqrt{2}b^\top & \sqrt{2}c^\top \\ -\sqrt{2}c & M & B \\ -\sqrt{2}b & C & -M^\top \end{bmatrix} \;\middle|\; b = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}, B = \begin{bmatrix} 0 & -b_3 & b_2 \\ b_3 & 0 & -b_1 \\ -b_2 & b_1 & 0 \end{bmatrix}, \right.$$
$$\left. c = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix}, C = \begin{bmatrix} 0 & -c_3 & c_2 \\ c_3 & 0 & -c_1 \\ -c_2 & c_1 & 0 \end{bmatrix}, b_i, c_i \in \mathbb{R}, M \in \mathbb{R}^{3\times 3}, \mathrm{tr}M = 0 \right\}. \tag{4.35}$$

Obviously, $\mathfrak{g}_{2,0}$ is a real form of $\mathfrak{g}$. We work with the following basis of $\mathfrak{g}_{2,0}$. Let E_{ij} denote the (7×7)-matrix with (i,j)-entry 1 and 0 elsewhere.

$$\begin{aligned}
&X_1 := \sqrt{2}(E_{16} - E_{31}) + E_{54} - E_{72}; && X_2 := E_{23} - E_{65};\\
&X_3 := \sqrt{2}(E_{15} - E_{21}) + E_{73} - E_{64}; && X_4 := \sqrt{2}(E_{14} - E_{71}) + E_{35} - E_{26};\\
&X_5 := E_{34} - E_{76}; && X_6 := E_{24} - E_{75};\\
&Y_i := -X_i^\top, \quad i = 1, ..., 6; &&\\
&H_1 := \begin{bmatrix} 0&0&0&0&0&0&0\\ 0&1&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&-1&0&0&0\\ 0&0&0&0&-1&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&1 \end{bmatrix}; && H_2 := \begin{bmatrix} 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&1&0&0&0&0\\ 0&0&0&-1&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&-1&0\\ 0&0&0&0&0&0&1 \end{bmatrix}.
\end{aligned} \tag{4.36}$$

The commutator relations of these basis elements is listed in Table 4.3. By help of the Killing form we compute the Cartan involution and the corresponding Cartan decomposition of $\mathfrak{g}_{2,0}$.

Proposition 4.12. *The Killing form on $\mathfrak{g}_2$ and on $\mathfrak{g}_{2,0}$ is given by*

$$\kappa_{\mathfrak{g}_2}(X,Y) = 4\mathrm{tr}(XY), \quad \kappa_{\mathfrak{g}_{2,0}}(X,Y) = 4\mathrm{tr}(XY). \tag{4.37}$$

Proof. Using the commutator relations of the basis (4.36) as listed in Table 4.3, one can easily construct matrix representations of the adjoint operators $\mathrm{ad}_{X_i}, \mathrm{ad}_{Y_i}, \mathrm{ad}_{H_j} \in \mathbb{C}^{14\times 14}$. It is straightforward to check that for all $Z, \widetilde{Z} \in \{X_1, ..., X_6, Y_1, ..., Y_6, H_1, H_2\}$ the relation

$$\kappa(Z, \widetilde{Z}) = \mathrm{tr}(\mathrm{ad}_Z \circ \mathrm{ad}_{\widetilde{Z}}) = 4\mathrm{tr}(Z\widetilde{Z})$$

holds. Hence for arbitrary $X \in \mathfrak{g}_2$ we have $\kappa(X,X) = 4\mathrm{tr}(X^2)$. The claim now follows by linearizing

$$\begin{aligned}
4\mathrm{tr}(X^2) + 4\mathrm{tr}(Y^2) + 8\mathrm{tr}(XY) &= 4\mathrm{tr}((X+Y)^2) = \\
&= \kappa(X+Y, X+Y) = \kappa(X,X) + \kappa(Y,Y) + 2\kappa(X,Y).
\end{aligned}$$

$[\cdot,\cdot]$	H_1	H_2	X_1	Y_1	X_2	Y_2	X_3	Y_3	X_4	Y_4	X_5	Y_5	X_6	Y_6
H_1	0	0	0	0	X_2	$-Y_2$	X_3	$-Y_3$	X_4	$-Y_4$	X_5	$-Y_5$	$2X_6$	$-2Y_6$
H_2	0	0	X_1	$-Y_1$	$-X_2$	Y_2	0	0	X_4	$-Y_4$	$2X_5$	$-2Y_5$	X_6	$-Y_6$
X_1	0	$-X_1$	0	H_1-2H_2	$-X_3$	0	$-2X_4$	$3Y_2$	$-3X_5$	$2Y_3$	0	Y_4	0	0
Y_1	0	Y_1	$-H_1+2H_2$	0	0	$-Y_3$	$3X_2$	$-2Y_4$	$2X_3$	$-3Y_5$	X_4	0	0	0
X_2	$-X_2$	X_2	X_3	0	0	$-H_1+H_2$	0	$-Y_1$	0	0	X_6	0	0	$-Y_5$
Y_2	Y_2	$-Y_2$	0	Y_3	H_1-H_2	0	$-X_1$	0	0	0	0	Y_6	$-X_5$	0
X_3	$-X_3$	0	$2X_4$	$-3X_2$	0	X_1	0	$-2H_1+H_2$	$-3X_6$	$-2Y_1$	0	0	0	Y_4
Y_3	Y_3	0	$-3Y_2$	$2Y_4$	Y_1	0	$2H_1-H_2$	0	$-2X_1$	$-3Y_6$	0	0	X_4	0
X_4	$-X_4$	$-X_4$	$3X_5$	$-2X_3$	0	0	$3X_6$	$2X_1$	0	$-H_1-H_2$	0	$-Y_1$	0	$-Y_3$
Y_4	Y_4	Y_4	$-2Y_3$	$3Y_5$	0	0	$2Y_1$	$3Y_6$	H_1+H_2	0	$-X_1$	0	$-X_3$	0
X_5	$-X_5$	$-2X_5$	0	$-X_4$	$-X_6$	0	0	0	0	X_1	0	$-H_2$	0	Y_2
Y_5	Y_5	$2Y_5$	$-Y_4$	0	0	$-Y_6$	0	0	Y_1	0	H_2	0	X_2	0
X_6	$-2X_6$	$-X_6$	0	0	0	X_5	0	$-X_4$	0	X_3	0	$-X_2$	0	$-H_1$
Y_6	$2Y_6$	Y_6	0	0	Y_5	0	$-Y_4$	0	Y_3	0	$-Y_2$	0	H_1	0

Table 4.3: Lie bracket table for $\mathfrak{g}_2$.

□

Corollary 4.13. *A Cartan involution on* $\mathfrak{g}_{2,0}$ *is given by* $\theta(X) = -X^\top$. *Correspondingly, the Cartan decomposition is* $\mathfrak{g}_{2,0} = \mathfrak{k}_0 \oplus \mathfrak{p}_0$ *with*

$$\mathfrak{k}_0 = \mathfrak{g}_{2,0} \cap \mathfrak{so}(7, \mathbb{R}), \quad \mathfrak{p}_0 = \{X \in \mathfrak{g}_{2,0} \mid X^\top = X\}. \tag{4.38}$$

Proof. For $\theta = -(\cdot)^\top$, the bilinear form

$$B_\theta(X, Y) = -\kappa(X, \theta Y) = 4\mathrm{tr}(XY^\top)$$

is an inner product of $\mathfrak{g}_{2,0}$. Therefore θ is a Cartan involution. It is clear that if $\mathfrak{k}_0$ and $\mathfrak{p}_0$ are chosen as in Eq. (4.38) and $\Omega \in \mathfrak{k}_0$, $\overline{\Omega} \in \mathfrak{p}_0$, one has

$$\theta\Omega = \Omega \quad \text{and} \quad \theta\overline{\Omega} = -\overline{\Omega}.$$

□

Note that $\mathfrak{k}_0$ defined in Eq. (4.38) is isomorphic to $\mathfrak{su}(2) \oplus \mathfrak{su}(2)$, cf. [45], Section VI.10. With respect to the maximal abelian subspace

$$\mathfrak{a} := \{a_1 H_1 + a_2 H_2 \mid a_i \in \mathbb{R}\} \subset \mathfrak{p}_0,$$

we can choose the set of positive restricted roots by

$$\boxed{\begin{array}{lll} \lambda_1 := a_2, & \lambda_2 := a_1 - a_2, & \lambda_3 := a_1, \\ \lambda_4 := a_1 + a_2, & \lambda_5 := a_1 + 2a_2, & \lambda_6 := 2a_1 + a_2. \end{array}} \tag{4.39}$$

The restricted roots are illustrated in Figure 4.11.

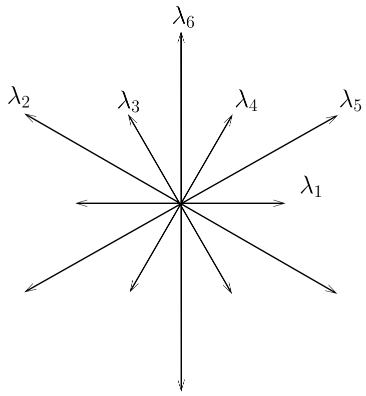

Figure 4.11: The root system of type G_2.

The corresponding restricted-root spaces are given by

$$\mathfrak{g}_{\lambda_i} = \mathbb{R}X_i, \quad \mathfrak{g}_{-\lambda_i} = \mathbb{R}Y_i, \quad i = 1, ..., 6. \tag{4.40}$$

Note that

$$\lambda_3 = \lambda_1 + \lambda_2, \quad \lambda_4 = 2\lambda_1 + \lambda_2, \quad \lambda_5 = 3\lambda_1 + \lambda_2, \quad \lambda_6 = 3\lambda_1 + 2\lambda_2, \tag{4.41}$$

and therefore

$$\Pi = \{\lambda_1, \lambda_2\} \tag{4.42}$$

is the simple system.

Lemma 4.14. *Both orderings $\lambda_1 < \lambda_2$ and $\lambda_2 < \lambda_1$ of Π satisfy the SCS-condition 3.29.*

Proof. Let us first consider $\lambda_1 < \lambda_2$. By Eq. (4.41), we obtain the ordering

$$\begin{aligned} \Sigma_1^+ : &\quad \lambda_1 \\ \Sigma_2^+ \setminus \Sigma_1^+ : &\quad \lambda_2 < \lambda_2 + \lambda_1 < \lambda_2 + 2\lambda_1 < \lambda_2 + 3\lambda_1 < 2\lambda_2 + 3\lambda_1. \end{aligned}$$

In the case where $\lambda_2 < \lambda_1$ the ordering is

$$\begin{aligned} \Sigma_1^+ : &\quad \lambda_2 \\ \Sigma_2^+ \setminus \Sigma_1^+ : &\quad \lambda_1 < \lambda_1 + \lambda_2 < 2\lambda_1 + \lambda_2 < 3\lambda_1 + \lambda_2 < 3\lambda_1 + 2\lambda_2. \end{aligned}$$

In both cases, the SCS-condition 3.29 is fulfilled. □

We now present a Jacobi algorithm that diagonalizes an element $S \in \mathfrak{p}_0$, preserving the special structure of $\mathfrak{p}_0$. Note, that for $i = 1, ..., 6$ we have $\theta X_i = Y_i$ and the $X_i \in \mathfrak{g}_{\lambda_i}$ are normalized such that

$$\lambda_i([X_i, \theta X_i]) = \lambda_i[X_i, Y_i] = -2, \quad \text{for all } i = 1, ..., 6.$$

Let

$$\Omega_i := X_i + \theta X_i = X_i + Y_i \in \mathfrak{k}_0.$$

Then the elementary structure preserving rotations are given by

$$\exp(t\Omega_1) = \begin{bmatrix} \cos 2t & 0 & \frac{\sin 2t}{\sqrt{2}} & 0 & 0 & \frac{\sin 2t}{\sqrt{2}} & 0 \\ 0 & \cos t & 0 & 0 & 0 & 0 & \sin t \\ -\frac{\sin 2t}{\sqrt{2}} & 0 & \frac{1}{2} + \frac{1}{2}\cos 2t & 0 & 0 & -\frac{1}{2} + \frac{1}{2}\cos 2t & 0 \\ 0 & 0 & 0 & \cos t & -\sin t & 0 & 0 \\ 0 & 0 & 0 & \sin t & \cos t & 0 & 0 \\ -\frac{\sin 2t}{\sqrt{2}} & 0 & -\frac{1}{2} + \frac{1}{2}\cos 2t & 0 & 0 & \frac{1}{2} + \frac{1}{2}\cos 2t & 0 \\ 0 & -\sin t & 0 & 0 & 0 & 0 & \cos t \end{bmatrix},$$

$$\exp(t\Omega_2) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \cos t & \sin t & 0 & 0 & 0 & 0 \\ 0 & -\sin t & \cos t & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cos t & \sin t & 0 \\ 0 & 0 & 0 & 0 & -\sin t & \cos t & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

$$\exp(t\Omega_3) = \begin{bmatrix} \cos 2t & \frac{\sin 2t}{\sqrt{2}} & 0 & 0 & \frac{\sin 2t}{\sqrt{2}} & 0 & 0 \\ -\frac{\sin 2t}{\sqrt{2}} & \frac{1}{2} + \frac{1}{2}\cos 2t & 0 & 0 & -\frac{1}{2} + \frac{1}{2}\cos 2t & 0 & 0 \\ 0 & 0 & \cos t & 0 & 0 & 0 & -\sin t \\ 0 & 0 & 0 & \cos t & 0 & \sin t & 0 \\ -\frac{\sin 2t}{\sqrt{2}} & -\frac{1}{2} + \frac{1}{2}\cos 2t & 0 & 0 & \frac{1}{2} + \frac{1}{2}\cos 2t & 0 & 0 \\ 0 & 0 & 0 & -\sin t & 0 & \cos t & 0 \\ 0 & 0 & \sin t & 0 & 0 & 0 & \cos t \end{bmatrix},$$

$$\exp(t\Omega_4) = \begin{bmatrix} \cos 2t & 0 & 0 & \frac{\sin 2t}{\sqrt{2}} & 0 & 0 & \frac{\sin 2t}{\sqrt{2}} \\ 0 & \cos t & 0 & 0 & 0 & -\sin t & 0 \\ 0 & 0 & \cos t & 0 & \sin t & 0 & 0 \\ -\frac{\sin 2t}{\sqrt{2}} & 0 & 0 & \frac{1}{2} + \frac{1}{2}\cos 2t & 0 & 0 & -\frac{1}{2} + \frac{1}{2}\cos 2t \\ 0 & 0 & -\sin t & 0 & \cos t & 0 & 0 \\ 0 & \sin t & 0 & 0 & 0 & \cos t & 0 \\ -\frac{\sin 2t}{\sqrt{2}} & 0 & 0 & -\frac{1}{2} + \frac{1}{2}\cos 2t & 0 & 0 & \frac{1}{2} + \frac{1}{2}\cos 2t \end{bmatrix},$$

$$\exp(t\Omega_5) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \cos t & \sin t & 0 & 0 & 0 \\ 0 & 0 & -\sin t & \cos t & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \cos t & \sin t \\ 0 & 0 & 0 & 0 & 0 & -\sin t & \cos t \end{bmatrix},$$

$$\exp(t\Omega_6) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \cos t & 0 & \sin t & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & -\sin t & 0 & \cos t & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cos t & 0 & \sin t \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -\sin t & 0 & \cos t \end{bmatrix}.$$

The Jacobi algorithm from Section 3.2 explicitly reads as follows. Denote by X_{ij} the (i, j)-entry of the matrix X.

ALGORITHM G_2(I). PARTIAL STEP OF JACOBI SWEEP.

function: $(cost_*, sint_*, cos2t_*, sin2t_*) = \text{elementary.rotation}(X, \lambda_i)$

Do Case

Case i=1

Set $c := X_{45}$, $\lambda := X_{33}$.

Case i=2

Set $c := X_{32}$, $\lambda := X_{22} - X_{33}$.

Case i=3
Set $c := X_{73}$, $\lambda := X_{22}$.
Case i=4
Set $c := X_{35}$, $\lambda := X_{77}$.
Case i=5
Set $c := X_{34}$, $\lambda := X_{22} + 2X_{33}$.
Case i=6
Set $c := X_{24}$, $\lambda := 2X_{22} + X_{33}$.
End Case
Set $dis := \lambda^2 + 4c^2$.
if $dis \neq 0$
Set $(cos2t_*, sin2t_*) := -\frac{1}{dis}(\lambda, 2c)$.
else
Set $(cos2t_*, sin2t_*) := (1, 0)$.
endif
Set $cost_* := \sqrt{\frac{1+cos2t_*}{2}}$.
if $sin2t_* \geq 0$
Set $sint_* = \sqrt{\frac{1-cos2t_*}{2}}$.
else
Set $sint_* = -\sqrt{\frac{1-cos2t_*}{2}}$.
endif
end elementary.rotation

As usual we denote by subscribing 0 the projection of X onto $\mathfrak{a}$. Let $d\colon \mathfrak{p}_0 \longrightarrow \mathbb{R}^+$, $X \longmapsto \operatorname{tr}(X - X_0)^2$ be the squared distance of an element in $\mathfrak{p}_0$ to $\mathfrak{a}$. Given a matrix $S \in \mathfrak{p}_0$ and a tolerance $tol > 0$, this algorithm overwrites S by kSk^{-1} where $k \in \exp(\mathfrak{k}_0)$ and $d(kSk^{-1}) \leq tol$.

Algorithm G_2(II). Jacobi Algorithm.
Set $k :=$ identity matrix.
while $d(S) > tol$
for $i = 1 : 6$
$(cost_*, sint_*, cos2t_*, sin2t_*) :=$ elementary.rotation(S, λ_i).
$u := \exp(t_* \Omega_i)$.
$S := uSu^{-1}$.
$k := uk$.
endfor
endwhile

The regular element

$$S_{reg} = \begin{bmatrix} 0 & -3.17415 & -3.90421 & -4.63169 & 3.17415 & 3.90421 & 4.63169 \\ -3.17415 & 0.993208 & 3.14172 & 2.55770 & 0 & 3.27510 & -2.76069 \\ -3.90421 & 3.14172 & 3.224433 & -1.97516 & -3.27510 & 0 & 2.24446 \\ -4.63169 & 2.55770 & -1.97516 & -4.23754 & 2.76069 & -2.24446 & 0 \\ 3.17415 & 0 & -3.27510 & 2.76069 & -0.993208 & -3.14172 & -2.5577 \\ 3.90421 & 3.27510 & 0 & -2.24446 & -3.14172 & -3.24433 & 1.97516 \\ 4.63169 & -2.76069 & 2.24446 & 0 & -2.5577 & 1.97516 & 4.23754 \end{bmatrix}$$

is almost diagonalized after 3 sweeps (off-norm $< 10^{-10}$). It converges to the diagonal matrix

$$Z_{reg} = \operatorname{diag}\Big[\ 0, -9.12818, -1.97129, 11.0995, 9.12818, 1.97129, -11.0995\ \Big].$$

Irregular elements show the same convergence behavior. In all simulations, at most 3 sweeps were required to diagonalize (off-norm $< 10^{-10}$) a given irregular element.
It is also possible to construct in a complete analogous way an algorithm that works on the adjoint representation of $\mathfrak{g}_{2,0}$. By the commutating relations in Table 4.6, we obtain representing matrices of $\mathrm{ad}_{X_i}, \mathrm{ad}_{Y_i}, \mathrm{ad}_{H_j} \in \mathbb{R}^{14\times 14}$, $i = 1, ..., 6$ and $j = 1, 2$. We will further denote these matrices by $\widetilde{X}_i, \widetilde{Y}_i$ and $\widetilde{H}_j$, respectively. In this setting, the representation of $\mathfrak{g}_2$ and the corresponding Cartan decomposition is given by

$$\widetilde{\mathfrak{g}}_2 = \widetilde{\mathfrak{k}} \oplus \widetilde{\mathfrak{p}},$$

with

$$\widetilde{\mathfrak{k}} := \langle \widetilde{X}_i + \widetilde{Y}_i \mid i = 1, ..., 6\rangle \quad \text{and} \quad \widetilde{\mathfrak{p}} := \langle \widetilde{X}_i - \widetilde{Y}_i \mid i = 1, ..., 6\rangle \oplus \widetilde{\mathfrak{a}},$$

where $\widetilde{\mathfrak{a}}$ is the maximal abelian subspace in $\widetilde{\mathfrak{p}}$. Note, that $\widetilde{\mathfrak{p}}$ does not – unlike $\mathfrak{p}_0$ – consist of symmetric matrices. Its structure is given in Figure 4.12. It is not surprising that the algorithm works with the same speed on $\widetilde{\mathfrak{p}}_0$ as in the standard irreducible representation $\mathfrak{p}_0$. All simulations show that a given matrix in $\widetilde{\mathfrak{p}}_0$ is diagonalized in at most 3 sweeps (off-norm $< 10^{-10}$) .

$$
\begin{bmatrix}
0 & 0 & a & a & -b & -b & -2c & -2c & -d & -d & 0 & 0 & -2e & -e \\
0 & 0 & -2a & -2a & b & b & c & c & -d & -d & 0 & -e & 0 & 0 \\
0 & -a & h2 & 0 & 0 & c & b & 2d & 2c & e & d & 0 & 0 & 0 \\
0 & -a & 0 & -h2 & -c & 0 & -2d & -b & 0 & -2c & 0 & -d & 0 & 0 \\
-b & b & 0 & -3c & h1-h2 & 0 & -3a & 0 & 0 & 0 & 0 & -e & 0 & 0 \\
-b & b & 3c & 0 & 0 & -h1+h2 & 0 & 3a & 0 & 0 & 2e & 0 & 0 & e \\
-c & 0 & b & -2d & -a & 0 & h1 & 0 & -2a & e & 0 & 0 & d & 0 \\
-c & 0 & 2d & -b & 0 & a & 0 & -h1 & -2e & 2a & 0 & 0 & 0 & -d \\
-d & -d & 2c & -e & 0 & 0 & -2a & -e & h1+h2 & 0 & -a & 0 & -c & 0 \\
-d & -d & 0 & -2c & 0 & 0 & 2e & 2a & 0 & -h1-h2 & 0 & a & 0 & c \\
-e & -2e & 3d & 0 & 0 & e & 0 & 0 & -3a & 0 & h1+2h2 & 0 & b & 0 \\
0 & 0 & 0 & -3d & -2e & 0 & 0 & 0 & 0 & 3a & 0 & -h1-2h2 & 0 & -b \\
-2e & -e & 0 & 0 & -e & 0 & 3d & 0 & -3c & 0 & b & 0 & 2h1+h2 & 0 \\
-4e & -2e & 0 & 0 & 0 & 0 & 0 & -3d & 0 & 3c & 0 & -b & 0 & -2h1-h2
\end{bmatrix}
$$

Figure 4.12: Structure of $\widetilde{\mathfrak{p}}$.

Chapter 5

Conclusion and Outlook

A Lie algebraic generalization of the classical and the Sort-Jacobi algorithm for diagonalizing a symmetric matrix has been proposed. The coordinate free setting provides new insights in the nature of Jacobi-type methods and allows a unified treatment of several structured eigenvalue and singular value problems, including so far unstudied normal form problems. Local quadratic convergence has been shown for both types of Jacobi methods with a fully comprehension of the regular and irregular case. New sweep methods have been introduced that generalize the special cyclic sweep for symmetric matrices and ensure local quadratic convergence also for irregular elements. The new sweep methods yield faster convergence behavior than the previously known cyclic schemes.

Although the symmetric EVD is perhaps the easiest and mostly understood structured eigenvalue problem, the global convergence in the general setting is still to be analyzed. Furthermore, an investigation of the so-called block-Jacobi methods in combination with the special cyclic sweeps should lead to further efficient algorithms.

The obtained results suggest that the Lie algebraic setting is very well suited to investigate eigenvalue problems with a certain structure and their algorithms. With our approach, many cases can be subsumed and the abstraction to the Lie algebraic level allows to focus on the essential features of the problem. It is therefore reasonable to expect that further steps in this direction have the potential to yield new significant results in numerical linear algebra. We give two examples.

- Several algorithms exist that construct a Hermitian matrix with prescribed diagonal entries and eigenvalues. A generalization of this *Hermitian inverse eigenvalue problem* to the normal form problems treated in this thesis should be straightforward: Let $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ be the Cartan decomposition of a semisimple Lie algebra and fix a maximal abelian subalgebra $\mathfrak{a} \in \mathfrak{p}$. Then for given $H_0, H_1 \in \mathfrak{a}$ construct, an element $\varphi \in \mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$ such that $\mathrm{p}(\varphi H_1) = H_2$. Here, two approaches are thinkable. Either the adaption of the finite-step algorithms treated in the literature or a Jacobi-type method minimizing a suitable cost on $\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$.

- For the *nonsymmetric eigenvalue problem*, there is no satisfactory theory for Jacobi-type methods available. A main challenge from the author's point of view is to tackle the nonsymmetric eigenvalue problem for matrices with a certain Lie algebraic structure. For given $X \in \mathfrak{g}$ find a transformation $\varphi \in \mathrm{Int}(\mathfrak{g})$ such that φX lies in a Cartan subalgebra of $\mathfrak{g}$. A first question to ask is whether and for what elements such a φ exists. Viewing the nonsymmetric eigenvalue problem in terms of an optimization task as in Chapter 2, it is evident where further difficulties lie. For example, the $\mathrm{Int}(\mathfrak{g})$-orbit of X is in general not compact and the same holds true for the orbits of one-parameter subgroups. Hence the Jacobi algorithm has to be modified such that it is well defined. Furthermore, finding a suitable cost function such that optimizing over the one-parameter subgroups yields at least a locally efficient algorithm is another challenge. One possible approach here follows the idea of optimizing *two* function alternately. One that minimizes the distance to normality, using hyperbolic transformations, and another function that reduces the distance to the Cartan subalgebra by using orthogonal rotations.

Appendix A

Restricted-Root Space Decompositions for the Classical Simple Lie Algebras

According to Table 4.1, we present the restricted-root space decompositions and the restricted roots of the classical simple Lie algebras that have not been treated yet in Chapter 4. With these ingredients, it is straightforward to implement Jacobi-type methods according to the algorithms developed so far in order to obtain satisfactory results for the corresponding eigenvalue- and singular value decompositions.

A.1 $\mathfrak{sl}(n,\mathbb{R})$ and the Real Symmetric EVD

- matrix factorization:

$$u \in SO(n,\mathbb{R}), B = B^\top \in \mathbb{R}^{n\times n}, \quad uBu^\top = \begin{bmatrix} a_1 & & \\ & \ddots & \\ & & a_n \end{bmatrix} \in \mathbb{R}^{n\times n}.$$

- underlying Lie algebra: $\mathfrak{sl}(n,\mathbb{R}) = \{X \in \mathbb{R}^{n\times n} \mid \mathrm{tr}X = 0\}$.

- Cartan involution, Killing form: $\theta = -(\cdot)^\top$, $\kappa(X,Y) = 2n\mathrm{tr}(XY)$.

- Cartan decomposition:

$$\mathfrak{k} = \mathfrak{so}(n,\mathbb{R}) = \{X \in \mathbb{R}^{n\times n} \mid X = -X^\top\},$$

$$\mathfrak{p} = \{B \in \mathbb{R}^{n\times n} \mid B = B^\top, \mathrm{tr}B = 0\}.$$

- maximal abelian subalgebra in $\mathfrak{p}$:

$$\mathfrak{a} = \left\{ \begin{bmatrix} a_1 & & \\ & \ddots & \\ & & a_n \end{bmatrix} \mid a_i \in \mathbb{R}, \sum_{i=1}^{n} a_i = 0 \right\}.$$

(dim $\mathfrak{a} = n-1$)

- restricted roots: type A_{n-1}, i.e.

$$\boxed{\pm(a_i - a_j), \quad 1 \leq i < j \leq n.}$$

- SCS-ordering: $(\Pi_{A_{n-1}}, >)$ with

$\Pi_{A_{n-1}} = \{a_1 - a_2, a_2 - a_3, ..., a_{n-1} - a_n\}$ and $a_{n-1} - a_n < ... < a_2 - a_3 < a_1 - a_2$.

- restricted-root spaces for positive roots:

$$\mathfrak{g}_{a_i - a_j} = \mathbb{R}E_{ij},$$

where E_{ij} has (i,j)-entry 1 and zeros elsewhere.

- the centralizer of $\mathfrak{a}$ in $\mathfrak{k}$: $\mathfrak{z}_{\mathfrak{k}}(\mathfrak{a}) = 0$.

A.2 $\mathfrak{sl}(n, \mathbb{C})$ and the Hermitian EVD

- matrix factorization:

$$u \in SU(n), B = B^* \in \mathbb{C}^{n\times n}, \quad uBu^* = \begin{bmatrix} a_1 & & \\ & \ddots & \\ & & a_n \end{bmatrix} \in \mathbb{R}^{n\times n}.$$

- underlying Lie algebra: $\mathfrak{sl}(n, \mathbb{C}) = \{X \in \mathbb{C}^{n\times n} \mid \mathrm{tr}X = 0\}$.

- Cartan involution, Killing form: $\theta = -(\cdot)^*$, $\kappa(X,Y) = 2n\mathrm{tr}(XY)$.

- Cartan decomposition:

$$\mathfrak{k} = \mathfrak{su}(n) = \{X \in \mathbb{C}^{n\times n} \mid X = -X^*\},$$
$$\mathfrak{p} = \{B \in \mathbb{C}^{n\times n} \mid B = B^*, \mathrm{tr}B = 0\}.$$

- maximal abelian subalgebra in $\mathfrak{p}$:

$$\mathfrak{a} = \left\{ \begin{bmatrix} a_1 & & \\ & \ddots & \\ & & a_n \end{bmatrix} \mid a_i \in \mathbb{R}, \sum_{i=1}^{n} a_i = 0 \right\}.$$

  $(\dim \mathfrak{a} = n-1)$

- restricted roots: type A_{n-1}, cf. Section A.1.
- SCS-ordering: cf. Section A.1.
- restricted-root spaces for positive roots:

$$\mathfrak{g}_{a_i - a_j} = \mathbb{C}E_{ij},$$

  where E_{ij} has (i,j)-entry 1 and zeros elsewhere.

- the centralizer of $\mathfrak{a}$ in $\mathfrak{k}$: $\mathfrak{z}_{\mathfrak{k}}(\mathfrak{a}) = \mathrm{i}\mathfrak{a}$.

A.3 $\mathfrak{so}(n,\mathbb{C})$ and the Real Skew-Symmetric EVD

Let $n = 2k$ or $n = 2k+1$, respectively.

- matrix factorization:

$$u \in SO(2k,\mathbb{R}), B = -B^\top \in \mathbb{R}^{2k\times 2k}, \quad uBu^\top = \begin{bmatrix} 0 & a_1 & & & \\ -a_1 & 0 & & & \\ & & \ddots & & \\ & & & 0 & a_k \\ & & & -a_k & 0 \end{bmatrix},$$

  and $u \in SO(2k+1,\mathbb{R}), B = -B^\top \in \mathbb{R}^{(2k+1)\times(2k+1)}$,

$$uBu^\top = \begin{bmatrix} 0 & a_1 & & & & \\ -a_1 & 0 & & & & \\ & & \ddots & & & \\ & & & 0 & a_k & \\ & & & -a_k & 0 & \\ & & & & & 0 \end{bmatrix}.$$

- underlying Lie algebra: $\mathfrak{so}(n,\mathbb{C}) = \{X \in \mathbb{C}^{n\times n} \mid X = -X^\top\}$.
- Cartan involution, Killing form: $\theta = -(\cdot)^*$, $\kappa(X,Y) = (n-2)\mathrm{tr}(XY)$.

- Cartan decomposition:

$$\mathfrak{k} = \mathfrak{so}(n,\mathbb{R}),$$
$$\mathfrak{p} = \mathrm{i}\mathfrak{so}(n,\mathbb{R}).$$

- maximal abelian subalgebra in $\mathfrak{p}$:

$$\mathfrak{a} = \mathrm{i}\left\{ \begin{bmatrix} 0 & a_1 & & & \\ -a_1 & 0 & & & \\ & & \ddots & & \\ & & & 0 & a_k \\ & & & -a_k & 0 \end{bmatrix} \mid a_i \in \mathbb{R} \right\},$$

$$\mathfrak{a} = \mathrm{i}\left\{ \begin{bmatrix} 0 & a_1 & & & & \\ -a_1 & 0 & & & & \\ & & \ddots & & & \\ & & & 0 & a_k & \\ & & & -a_k & 0 & \\ & & & & & 0 \end{bmatrix} \mid a_i \in \mathbb{R} \right\},$$

respectively. ($\dim \mathfrak{a} = k$)

- restricted roots: type D_k if $n = 2k$, cf. Eq. (4.8a); type B_k if $n = 2k+1$, cf. Eq. (4.8).
- SCS-ordering: cf. Proposition 4.4 and Corollary 4.5.
- restricted-root spaces for positive roots:

For the roots $a_i \pm a_j, i < j$, the restricted-root spaces have real dimension 2 and are nonzero only in the 8 entries corresponding to row and column indices $2i-1, 2i, 2j-1, 2j$ where they are

$$\mathfrak{g}_{a_i - a_j} = \left\{ \begin{bmatrix} & \begin{bmatrix} z & \mathrm{i}z \\ -\mathrm{i}z & z \end{bmatrix} \\ \begin{bmatrix} -z & \mathrm{i}z \\ -\mathrm{i}z & -z \end{bmatrix} & \end{bmatrix} | z \in \mathbb{C} \right\},$$

$$\mathfrak{g}_{a_i + a_j} = \left\{ \begin{bmatrix} & \begin{bmatrix} z & -\mathrm{i}z \\ -\mathrm{i}z & -z \end{bmatrix} \\ \begin{bmatrix} -z & \mathrm{i}z \\ \mathrm{i}z & z \end{bmatrix} & \end{bmatrix} | z \in \mathbb{C} \right\}.$$

The restricted-root spaces for the roots a_i, which only exist if $N = 2n+1$, have real dimension 2 and are nonzero only in the entries corresponding to row and column indices $2i-1, 2i, 2n+1$, where they are

$$\mathfrak{g}_{a_i} = \left\{ \begin{bmatrix} & \begin{bmatrix} z \\ \mathrm{i}z \end{bmatrix} \\ \begin{bmatrix} -z & -\mathrm{i}z \end{bmatrix} & 0 \end{bmatrix} \mid z \in \mathbb{C} \right\}.$$

- the centralizer of $\mathfrak{a}$ in $\mathfrak{k}$: $\mathfrak{z}_{\mathfrak{k}}(\mathfrak{a}) = \mathrm{i}\mathfrak{a}$.

A.4 $\mathfrak{sp}(n,\mathbb{C})$ and the Hermitian Hamiltonian EVD

- matrix factorization: $u \in Sp(n), S, C \in \mathbb{C}^{n\times n}, S = S^*, C = C^\top$

$$u \begin{bmatrix} S & C \\ \overline{C} & -\overline{S} \end{bmatrix} u^* = \begin{bmatrix} \Lambda & 0 \\ 0 & -\Lambda \end{bmatrix}, \quad \Lambda = \begin{bmatrix} a_1 & & \\ & \ddots & \\ & & a_n \end{bmatrix} \in \mathbb{R}^{n\times n}.$$

- underlying Lie algebra: $\mathfrak{sp}(n,\mathbb{C}) = \{X \in \mathbb{C}^{2n\times 2n} \mid X^\top J + JX = 0\}$, where $J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}$.

- Cartan involution, Killing form: $\theta = -(\cdot)^*$, $\kappa(X,Y) = 2(n+1)\mathrm{tr}(XY)$.

- Cartan decomposition:

$$\mathfrak{k} = \mathfrak{sp}(n),$$

$$\mathfrak{p} = \left\{ \begin{bmatrix} S & C \\ \overline{C} & -\overline{S} \end{bmatrix}, S, C \in \mathbb{C}^{n\times n}, S = S^*, C = C^\top \right\}.$$

- maximal abelian subalgebra in $\mathfrak{p}$:

$$\mathfrak{a} := \left\{ \begin{bmatrix} \Lambda & 0 \\ 0 & -\Lambda \end{bmatrix} \mid \Lambda = \begin{bmatrix} a_1 & & \\ & \ddots & \\ & & a_n \end{bmatrix} \in \mathbb{R}^{n\times n} \right\}.$$

($\dim \mathfrak{a} = n$)

- restricted roots: type C_n

- SCS-ordering: cf. Proposition 4.8.

- restricted-root spaces for positive roots:

  The restricted-root spaces all have real dimension 2 and are given by

$$\mathfrak{g}_{a_i-a_j} = \mathbb{C}(E_{i,j} - E_{j+n,i+n}), \quad \mathfrak{g}_{a_i+a_j} = \mathbb{C}(E_{i,j+n} + E_{j,i+n}), \quad i < j,$$
$$\mathfrak{g}_{2a_i} = \mathbb{C}E_{i,i+n}.$$

- the centralizer of $\mathfrak{a}$ in $\mathfrak{k}$: $\mathfrak{z}_{\mathfrak{k}}(\mathfrak{a}) = \mathrm{i}\mathfrak{a}$.

A.5 $\mathfrak{su}^*(2n)$ and the Hermitian Quaternion EVD

- matrix factorization: $u \in Sp(n), S, \Psi \in \mathbb{C}^{n\times n}, S = S^*, \Psi = -\Psi^\top$,

$$u \begin{bmatrix} S & \Psi^* \\ \Psi & \overline{S} \end{bmatrix} u^* = \begin{bmatrix} \Lambda & 0 \\ 0 & \Lambda \end{bmatrix}, \quad \Lambda = \begin{bmatrix} a_1 & & \\ & \ddots & \\ & & a_n \end{bmatrix} \in \mathbb{R}^{n\times n}.$$

- underlying Lie algebra: $\mathfrak{su}^*(2n) = \left\{ \begin{bmatrix} A & -\overline{B} \\ B & \overline{A} \end{bmatrix} A, B \in \mathbb{C}^{n\times n} \mid \mathrm{tr}A + \mathrm{tr}\overline{A} = 0 \right\}$.

  $\mathfrak{su}^*(2n)$ is a real form of $\mathfrak{sl}(2n,\mathbb{C})$; we have the isomorphism $\mathfrak{su}^*(2n) \cong \mathfrak{sl}(n,\mathbb{H})$, cf. [45], Section I.8.

- Cartan involution, Killing form: $\theta = -(\cdot)^*$, $\kappa(X,Y) = 4n\mathrm{tr}(XY)$.

- Cartan decomposition:

$$\mathfrak{k} = \mathfrak{sp}(n),$$
$$\mathfrak{p} = \left\{ \begin{bmatrix} S & \Psi^* \\ \Psi & \overline{S} \end{bmatrix} \mid S = S^*, \Psi = -\Psi^\top, \mathrm{tr}S = 0 \right\}.$$

- maximal abelian subalgebra in $\mathfrak{p}$:

$$\mathfrak{a} := \left\{ \begin{bmatrix} \Lambda & 0 \\ 0 & \Lambda \end{bmatrix}, \quad \Lambda = \begin{bmatrix} a_1 & & \\ & \ddots & \\ & & a_n \end{bmatrix} \in \mathbb{R}^{n\times n}, \sum_{i=1}^n a_i = 0 \right\}.$$

  $(\dim \mathfrak{a} = n-1)$

- restricted roots: type A_{n-1}, cf. Section A.1.

- SCS-ordering: cf. Section A.1.

- restricted-root spaces for positive roots:

  The restricted-root spaces for the roots $a_i - a_j$ have real dimension 4 and are nonzero only in the 4 entries corresponding to row and column indices $i, n+i, j, n+j$ where they are

$$\mathfrak{g}_{a_i-a_j} = \left\{ \begin{bmatrix} \begin{bmatrix} 0 & z \\ 0 & 0 \end{bmatrix} & \begin{bmatrix} 0 & w \\ 0 & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & \overline{w} \\ 0 & 0 \end{bmatrix} & \begin{bmatrix} 0 & \overline{z} \\ 0 & 0 \end{bmatrix} \end{bmatrix} \mid v, z \in \mathbb{C} \right\}.$$

- the centralizer of $\mathfrak{a}$ in $\mathfrak{k}$:

$$\mathfrak{z}_{\mathfrak{k}}(\mathfrak{a}) = \left\{ \begin{bmatrix} \mathrm{i}\Lambda & \Gamma \\ -\overline{\Gamma} & -\mathrm{i}\Lambda \end{bmatrix} \mid \Lambda = \begin{bmatrix} a_1 & & \\ & \ddots & \\ & & a_n \end{bmatrix} \in \mathbb{R}^{n\times n}, \right.$$
$$\left. \Gamma = \begin{bmatrix} z_1 & & \\ & \ddots & \\ & & z_n \end{bmatrix} \in \mathbb{C}^{n\times n} \right\}.$$

A.6 $\mathfrak{so}^*(2n)$ and a Takagi-Like Factorization

Let $n = 2k$ or $n = 2k+1$, respectively.

- matrix factorization:

$$u \in U(2k), B = -B^\top \in \mathbb{C}^{2k\times 2k}, \quad uBu^\top = \begin{bmatrix} 0 & a_1 & & & \\ -a_1 & 0 & & & \\ & & \ddots & & \\ & & & 0 & a_k \\ & & & -a_k & 0 \end{bmatrix},$$

and $u \in U(2k+1), B = -B^\top \in \mathbb{C}^{(2k+1)\times(2k+1)}$,

$$uBu^\top = \begin{bmatrix} 0 & a_1 & & & & \\ -a_1 & 0 & & & & \\ & & \ddots & & & \\ & & & 0 & a_k & \\ & & & -a_k & 0 & \\ & & & & & 0 \end{bmatrix}.$$

- underlying Lie algebra:

$$\mathfrak{so}^*(2n) = \left\{ \begin{bmatrix} \Psi & B \\ -\overline{B} & \overline{\Psi} \end{bmatrix} \mid B, \Psi \in \mathbb{C}^{n \times n}, B = -B^\top, \Psi = -\Psi^* \right\}.$$

- Cartan involution, Killing form: $\theta = -(\cdot)^*$, $\kappa(X,Y) = (2n-2)\mathrm{tr}(XY)$.

- Cartan decomposition:

$$\mathfrak{k} = \left\{ \begin{bmatrix} \Psi & 0 \\ 0 & \overline{\Psi} \end{bmatrix} \mid \Psi = -\Psi^* \right\} \cong \mathfrak{u}(n),$$

$$\mathfrak{p} = \left\{ \begin{bmatrix} 0 & B \\ -\overline{B} & 0 \end{bmatrix} \mid B = -B^\top \right\}.$$

- maximal abelian subalgebra in $\mathfrak{p}$:

$$\mathfrak{a} = \left\{ \begin{bmatrix} 0 & \Lambda \\ -\Lambda & 0 \end{bmatrix} \mid \Lambda = \begin{bmatrix} 0 & a_1 & & & \\ -a_1 & 0 & & & \\ & & \ddots & & \\ & & & 0 & a_k \\ & & & -a_k & 0 \end{bmatrix} \mid a_i \in \mathbb{R} \right\},$$

$$\mathfrak{a} = \left\{ \begin{bmatrix} 0 & \Lambda \\ -\Lambda & 0 \end{bmatrix} \mid \Lambda = \begin{bmatrix} 0 & a_1 & & & & \\ -a_1 & 0 & & & & \\ & & \ddots & & & \\ & & & 0 & a_k & \\ & & & -a_k & 0 & \\ & & & & & 0 \end{bmatrix} \mid a_i \in \mathbb{R} \right\},$$

respectively. ($\dim \mathfrak{a} = k$)

- restricted roots: type C_k if $n = 2k$, type $(BC)_k$ if $n = 2k+1$.

- SCS-ordering: cf. Propositions 4.8 and 4.9.

- restricted-root spaces for positive roots:

  For the roots $a_i \pm a_j, i < j$, the restricted-root spaces have real dimension 4 and are nonzero only in the 16 entries corresponding to row and column indices

$2i-1, 2i, n+2i-1, n+2i, 2j-1, 2j, n+2j-1, n+2j$ where they are

$$\mathfrak{g}_{a_i-a_j} = \left\{ \begin{bmatrix} & \begin{bmatrix} z & w \\ -\overline{w} & \overline{z} \end{bmatrix} & & \begin{bmatrix} -w & z \\ -\overline{z} & -\overline{w} \end{bmatrix} \\ \begin{bmatrix} z & w \\ -\overline{w} & \overline{z} \end{bmatrix} & & \begin{bmatrix} w & \overline{z} \\ -\overline{z} & \overline{w} \end{bmatrix} & \\ & \begin{bmatrix} \overline{w} & -z \\ \overline{z} & w \end{bmatrix} & & \begin{bmatrix} \overline{z} & \overline{w} \\ -w & z \end{bmatrix} \\ \begin{bmatrix} -\overline{w} & -\overline{z} \\ z & -w \end{bmatrix} & & \begin{bmatrix} \overline{z} & \overline{w} \\ -w & z \end{bmatrix} & \end{bmatrix} \middle| z, w \in \mathbb{C} \right\},$$

$$\mathfrak{g}_{a_i+a_j} = \left\{ \begin{bmatrix} & \begin{bmatrix} z & w \\ \overline{w} & -\overline{z} \end{bmatrix} & & \begin{bmatrix} w & -z \\ -\overline{z} & -\overline{w} \end{bmatrix} \\ \begin{bmatrix} -\overline{z} & -w \\ -\overline{w} & z \end{bmatrix} & & \begin{bmatrix} -w & \overline{z} \\ z & \overline{w} \end{bmatrix} & \\ & \begin{bmatrix} -\overline{w} & \overline{z} \\ z & w \end{bmatrix} & & \begin{bmatrix} \overline{z} & \overline{w} \\ w & -z \end{bmatrix} \\ \begin{bmatrix} \overline{w} & -z \\ -\overline{z} & -w \end{bmatrix} & & \begin{bmatrix} -z & -\overline{w} \\ -w & \overline{z} \end{bmatrix} & \end{bmatrix} \middle| z, w \in \mathbb{C} \right\}.$$

The restricted-root spaces for the roots $2a_i$ have real dimension 1 and are nonzero only in the 8 entries corresponding to row and column indices $2i-1, 2i, n+2i-1, n+2i$ where they are

$$\mathfrak{g}_{2a_i} = \mathbb{R} \cdot \begin{bmatrix} \begin{bmatrix} \mathrm{i} & 0 \\ 0 & \mathrm{i} \end{bmatrix} & \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix} & \begin{bmatrix} -\mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{bmatrix} \end{bmatrix}.$$

The restricted-root spaces for the roots a_i only occur if $n = 2k+1$. The have real dimension 4 and are nonzero only in the entries corresponding to row and column indices $2i-1, 2i, n+2i-1, n+2i, n, 2n$ where they are

$$\mathfrak{g}_{a_i} = \left\{ \begin{bmatrix} & \begin{bmatrix} z \\ w \end{bmatrix} & & \begin{bmatrix} \overline{w} \\ -\overline{z} \end{bmatrix} \\ \begin{bmatrix} -\overline{z} & -\overline{w} \end{bmatrix} & & \begin{bmatrix} -\overline{w} & \overline{z} \end{bmatrix} & \\ & \begin{bmatrix} -w \\ z \end{bmatrix} & & \begin{bmatrix} \overline{z} \\ \overline{w} \end{bmatrix} \\ \begin{bmatrix} w & -z \end{bmatrix} & & \begin{bmatrix} -z & -w \end{bmatrix} & \end{bmatrix} \middle| z, w \in \mathbb{C} \right\}.$$

- the centralizer of $\mathfrak{a}$ in $\mathfrak{k}$:

$$\mathfrak{z}_{\mathfrak{k}}(\mathfrak{a}) = \left\{ \begin{bmatrix} \Gamma & \\ & \overline{\Gamma} \end{bmatrix} \mid \Gamma = \begin{bmatrix} \begin{bmatrix} \mathrm{i}x_1 & z_1 \\ -\overline{z_1} & -\mathrm{i}x_1 \end{bmatrix} & & \\ & \ddots & \\ & & [\mathrm{i}x_{2k+1}] \end{bmatrix} \right\}.$$

A.7 $\mathfrak{su}(p,q)$ and the Complex SVD

We assume without loss of generality that $p \geq q$.

- matrix factorization:

$$B \in \mathbb{C}^{p\times q}, u \in U(p), v \in U(q), \det u \cdot \det v = 1; \quad uBv^* = \begin{bmatrix} & 0 & \\ \hline 0 & & a_q \\ & \iddots & \\ a_1 & & 0 \end{bmatrix}.$$

- underlying Lie algebra:

$$\mathfrak{su}(p,q) = \{X \in \mathfrak{sl}(p+q,\mathbb{C}) \mid X^* I_{p,q} + I_{p,q} X = 0\}.$$

- Cartan involution, Killing form: $\theta = -(\cdot)^*$, $\kappa(X,Y) = 2(p+q)\mathrm{tr}(XY)$.
- Cartan decomposition:

$$\mathfrak{k} = \left\{ \begin{bmatrix} S_1 & 0 \\ 0 & S_2 \end{bmatrix} \mid -S_1^* = S_1 \in \mathbb{C}^{p\times p}, -S_2^* = S_2 \in \mathbb{C}^{q\times q}, \mathrm{tr}(S_1) + \mathrm{tr}(S_2) = 0 \right\},$$

$$\mathfrak{p} = \left\{ \begin{bmatrix} 0 & B \\ B^* & 0 \end{bmatrix} \mid B \in \mathbb{C}^{p\times q} \right\}.$$

- maximal abelian subalgebra in $\mathfrak{p}$:

$$\mathfrak{a} := \left\{ \begin{bmatrix} 0 & B \\ B^* & 0 \end{bmatrix} \mid B = \begin{bmatrix} & 0 & \\ \hline 0 & & a_q \\ & \iddots & \\ a_1 & & 0 \end{bmatrix} \in \mathbb{R}^{p\times q} \right\}.$$

  ($\dim \mathfrak{a} = q$)

- restricted roots: type C_q for $p = q$; type $(BC)_q$ for $p > q$.
- SCS-ordering: cf. Propositions 4.8 and 4.9.

- restricted-root spaces for positive roots:

  For the roots $a_i \pm a_j$, $i < j$, the restricted-root spaces are of real dimension 2 and are nonzero only in the 16 entries corresponding to row and column indices $p-j+1, p-i+1, p+i, p+j$, where they are

$$\mathfrak{g}_{a_i-a_j} = \left\{ \begin{bmatrix} \begin{bmatrix} 0 & z \\ -\overline{z} & 0 \end{bmatrix} & \begin{bmatrix} -z & 0 \\ 0 & -\overline{z} \end{bmatrix} \\ \begin{bmatrix} -\overline{z} & 0 \\ 0 & -z \end{bmatrix} & \begin{bmatrix} 0 & -\overline{z} \\ z & 0 \end{bmatrix} \end{bmatrix} | z \in \mathbb{C} \right\},$$

$$\mathfrak{g}_{a_i+a_j} = \left\{ \begin{bmatrix} \begin{bmatrix} 0 & z \\ -\overline{z} & 0 \end{bmatrix} & \begin{bmatrix} -z & 0 \\ 0 & \overline{z} \end{bmatrix} \\ \begin{bmatrix} -\overline{z} & 0 \\ 0 & z \end{bmatrix} & \begin{bmatrix} 0 & \overline{z} \\ -z & 0 \end{bmatrix} \end{bmatrix} | z \in \mathbb{C} \right\}.$$

  The restricted-root spaces for the roots $2a_i$ have real dimension 1 and are nonzero only in the entries corresponding to row and column indices $p-i+1, p+i$. They are

$$\mathfrak{g}_{2a_i} = \left\{ \begin{bmatrix} -\mathrm{i}x & \mathrm{i}x \\ -\mathrm{i}x & \mathrm{i}x \end{bmatrix} | x \in \mathbb{R} \right\}.$$

  The restricted-root spaces for the roots a_i, which only exist if $p > q$, have real dimension $2(p-q)$ and are nonzero only in the entries corresponding to row and column indices $1, ..., p-q, p-i+1, p+i$. They are

$$\mathfrak{g}_{a_i} = \left\{ \begin{bmatrix} 0 & v & -v \\ -v^* & 0 & 0 \\ -v^* & 0 & 0 \end{bmatrix} | v \in \mathbb{C}^{p-q} \right\}.$$

- the centralizer of $\mathfrak{a}$ in $\mathfrak{k}$:

$$\mathfrak{z}_{\mathfrak{k}}(\mathfrak{a}) = \left\{ \begin{bmatrix} Z & 0 & 0 \\ 0 & \Gamma & 0 \\ 0 & 0 & \widetilde{\Gamma} \end{bmatrix} | Z \in \mathbb{C}^{(p-q)\times(p-q)}, \Gamma = \begin{bmatrix} \mathrm{i}x_1 & & \\ & \ddots & \\ & & \mathrm{i}x_q \end{bmatrix}, \right.$$
$$\left. \widetilde{\Gamma} = \begin{bmatrix} \mathrm{i}x_q & & \\ & \ddots & \\ & & \mathrm{i}x_1 \end{bmatrix} \right\} \cap \mathfrak{su}(p+q).$$

  We have $\mathfrak{z}_{\mathfrak{k}}(\mathfrak{a}) \cong \mathfrak{su}(p-q) \oplus \mathbb{R}^q$.

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Index of Notation

$\mathfrak{z}_{\mathfrak{k}}(\mathfrak{a})$	centralizer of $\mathfrak{a}$ in $\mathfrak{k}$	24
κ	Killing form	10
$\langle X_1, ..., X_k \rangle_{LA}$	subalgebra generated by the X_i	28
$\overline{\Omega}_\lambda$	normalized vector in $\mathfrak{p}$; $\overline{\Omega}_\lambda = E_\lambda - \theta E_\lambda$	28
p_k	orthogonal projection onto $\mathfrak{g}^{\alpha_k}$	81
$\mathrm{p}_k^\sharp$	orthogonal projection onto $\mathfrak{g}^{\alpha_k} \cap (\mathfrak{g}^{\alpha_{k-1}})^\perp$	81
θ	Cartan involution	18
$r_i(X)$	elementary rotation	44
s_k	partial special cyclic sweep	79
$s_k^\sharp$	special k-th row sweep	79
$t_*^{(i)}(X)$	step size from X in i-direction	40
$\mathrm{Aut}(\mathfrak{g})$	automorphisms of $\mathfrak{g}$	11
$\mathrm{Der}(\mathfrak{g})$	derivations of $\mathfrak{g}$	12
$\mathrm{End}(\mathfrak{g})$	endomorphisms of $\mathfrak{g}$	10
$\mathrm{Int}(\mathfrak{g})$	inner automorphisms of $\mathfrak{g}$	12
$\mathrm{Int}_{\mathfrak{g}}(\mathfrak{k})$	subgroup of $\mathrm{Int}(\mathfrak{g})$ with Lie algebra $\mathrm{ad}(\mathfrak{k})$	13

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