JACOBI'S ALGORITHM ON COMPACT LIE ALGEBRAS

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Abstract. A generalization of the cyclic Jacobi algorithm is proposed that works in an arbitrary compact Lie algebra. This allows, in particular, a unified treatment of Jacobi algorithms on different classes of matrices, such as, e.g., skew-symmetric or skew-Hermitian Hamiltonian matrices. Wildberger has established global, linear convergence of the algorithm for the classical Jacobi method on compact Lie algebras. Here we prove local quadratic convergence for general cyclic Jacobi schemes.

1. Introduction. The Jacobi algorithm for diagonalizing real symmetric or complex Hermitian matrices is a well known eigenvalue method from numerical linear algebra [14]. The classical version of the algorithm has been first proposed by Jacobi (1846),[24], who successively applied Givens rotations that produce the largest decrease in the distance to diagonality. In contrast, modern approaches use cyclic sweep strategies to minimize the sum of squares of off-diagonal entries. Cyclic sweep strategies are more efficient than Jacobi's original approach, as one avoids the time consuming search for the largest off-diagonal element. Moreover, cyclic strategies are known to be well suited for parallel computing.

Variants of the Jacobi algorithm have been applied to various structured eigenvalue problems, including e.g. the real skew-symmetric eigenvalue problem, [16, 23, 29], SVD computations [26], non-symmetric eigenvalue problems [3, 6, 7, 33, 35], complex symmetric eigenproblems [8], and normal matrices [13]. For applications to different types of generalized eigenvalue problems, we refer to [2, 4, 15, 36]. For Jacobi methods applied to systems theory, see [19, 18].

The starting point for this paper is the Jacobi algorithm for the real skew-symmetric eigenvalue problem. For previous work in this direction, see [29], and more recently [16, 23] as well as the related papers [9, 27]. They all have in common that some kind of a block Jacobi method is used, i.e., multi-parameter transformations that annihilate more than one pair of off-diagonal elements at the same time. In contrast, our approach exclusively uses one-parameter transformations.

Since the set of skew-symmetric matrices forms a Lie algebra it is not too surprising that the Jacobi algorithm can be extended to a general Lie algebraic setting. Wildberger [37] was the first who proposed a generalization of the classical Jacobi algorithm to arbitrary compact Lie algebras. The classification of compact Lie algebras shows that this approach essentially includes (i) the real skew-symmetric, (ii) the complex skew-Hermitian, (iii) the real skew-symmetric Hamiltonian, (iv) the complex skew-Hermitian Hamiltonian eigenvalue problem, and (v) some exceptional cases. One might think that an algorithm for case (i) is also appropriate for case (iii), analogously for (ii) and (iv). However, to stay within the corresponding Lie algebra requires that the transformations are structure preserving and therefore it is necessary to distinguish these four cases. Nevertheless, following Wildberger, one can treat the above mentioned problems (i)–(v) on the same footing, meaning that the description and analysis of the Jacobi method can be carried out simultaneously for all four problems. This is exactly what is done in this paper, with an emphasis on establishing local quadratic convergence. There are several advantages of such an abstract approach. First, the theory is independent of any special coordinate representation of

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the underlying Lie algebra. This coordinate-free approach forces one to formulate the basic features of the algorithm in an abstract way, thus enabling one to work out the essential features of Jacobi algorithms. Moreover, the local convergence analysis for the numerical algorithm is in all these cases exactly the same. Our convergence analysis extends that described in the Ph.D. thesis by the third author, [23], where elementary tools from global analysis were first used to prove local quadratic convergence for Jacobi-type methods. Questions of global convergence will not be discussed in this paper, albeit we expect that the ideas behind the proof of global convergence presented in [34] can be adopted. Instead, we restrict to local convergence properties.

The reader may have noticed that the real symmetric eigenvalue problem does not exactly fit into the framework developed in this paper, as the set of real symmetric matrices does not form a Lie algebra. In contrast, the Hermitian eigenvalue problem does. The reason is simply that the set of complex Hermitian matrices is isomorphic, up to multiplication with $\sqrt{-1}$, with the compact Lie algebra of skew-Hermitian matrices. Of course, this process does not work for real symmetric matrices and therefore requires a different approach to that of this paper.

The paper is organized as follows. Basic definitions and results on Lie algebras appear in Section 2. Furthermore, the structure of compact Lie algebras is discussed and examples are given. In Section 3 we discuss a cost function which can be regarded as the natural generalization of the familiar sum of squares function of off-diagonal entries. The critical points and the Hessian of this off-norm function are computed. The Jacobi algorithm on compact Lie algebras is formulated in Section 4. Explicit formulas for the step size selections are given in section 5. The main result, namely the local quadratic convergence of the Jacobi algorithm, is presented in Section 6. Finally, Section 7 presents a pseudo code of the algorithm and Section 8 includes some numerical experiments for the set of skew-Hermitian, Hamiltonian matrices.

2. Preliminaries on Lie Algebras. The purpose of this section is to recall some basic facts and definitions about compact Lie algebras. For further information see e.g. [1], [5], or [25]. In the sequel, let $\mathbb{K}$ denote the fields $\mathbb{R}$, $\mathbb{C}$ of real or complex numbers, respectively.

DEFINITION 2.1. *A $\mathbb{K}$-vector space $\mathfrak{g}$ with a bilinear product*

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

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 2.2. 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

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

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 subspace of $\mathfrak{g}$ for which $[\mathfrak{h}, \mathfrak{h}] \subset \mathfrak{h}$ holds. In the sequel, $\mathfrak{g}$ is always assumed to be a finite dimensional Lie algebra. For any $X \in \mathfrak{g}$, the *adjoint transformation* is the linear map

$$\mathrm{ad}_X : \mathfrak{g} \longrightarrow \mathfrak{g}, \qquad Y \longmapsto [X,Y] \tag{2.1}$$

and

$$\mathrm{ad} : \mathfrak{g} \longrightarrow \mathrm{End}(\mathfrak{g}), \qquad Y \longmapsto \mathrm{ad}_Y \tag{2.2}$$

is called the *adjoint representation* of $\mathfrak{g}$. Note that properties (i) and (ii) of Definition 2.1 read $\mathrm{ad}_X Y = -\mathrm{ad}_Y X$ 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 $X \in \mathfrak{g}$.

DEFINITION 2.3. *Let $\mathfrak{g}$ be a finite dimensional Lie algebra over $\mathbb{K}$. The symmetric bilinear form*

$$\kappa : \mathfrak{g} \times \mathfrak{g} \longrightarrow \mathbb{K}, \qquad \kappa(X,Y) \longmapsto \mathrm{tr}(\mathrm{ad}_X \circ \mathrm{ad}_Y) \tag{2.3}$$

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

Let $\mathbb{K} = \mathbb{R}$ or $\mathbb{C}$. Then

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

cf. [17], p.221 or [10], VI,4. Note that in [17], 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 in G at 1,

$$\mathrm{conj}_x(y) := xyx^{-1}$$

leads to the so-called *adjoint representation* of G

$$\mathrm{Ad} : G \times \mathfrak{g} \longrightarrow \mathfrak{g},$$

cf. [5], p. 2. Considering now the tangent mapping of Ad with respect to g at 1 leads to the adjoint transformation (2.1). If G is a matrix group, then the elements of the corresponding Lie algebra can also be regarded as matrices, cf. [25], p. 53. In this case the adjoint representation of $g \in G$ applied to $X \in \mathfrak{g}$ is given by

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

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

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

A basic property of the Killing form κ defined by (2.3) is its Ad-invariance, i.e.

$$\kappa(\mathrm{Ad}_g X, \mathrm{Ad}_g Y) = \kappa(X,Y) \qquad \text{for all } X, Y \in \mathfrak{g}, g \in G. \tag{2.4a}$$

Differentiating the left side of this equation with respect to g gives

$$\mathrm{D}\kappa(\mathrm{Ad}_g X, \mathrm{Ad}_g Y) \cdot gZ = \kappa(\mathrm{Ad}_g(\mathrm{ad}_Z X), \mathrm{Ad}_g Y) + \kappa(\mathrm{Ad}_g X, \mathrm{Ad}_g(\mathrm{ad}_Z Y)),$$

where $gZ \in T_g G$ is in the tangent space of G at g. Therefore, using (2.4a) we get

$$\kappa(\mathrm{ad}_X Y, Z) = -\kappa(Y, \mathrm{ad}_X Z) \qquad \text{for all} X, Y, Z \in \mathfrak{g}. \tag{2.4b}$$

DEFINITION 2.4. *A real finite dimensional Lie algebra* $\mathfrak{g}$ *is called* compact *if there exists a compact Lie group with Lie algebra* $\mathfrak{g}$.

Example 2.5. The following Lie algebras are compact, cf. [25], pp. 33,36 & 66ff.

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

A finite dimensional Lie algebra $\mathfrak{g}$ admits a positive definite Ad-invariant bilinear form, cf. [25], p. 196, Prop. 4.24. This property is used to show that the Killing form on compact Lie algebras is negative semidefinite (cf. [25], p. 197, Corollary 4.26).

A Lie algebra $\mathfrak{g}$ is called *Abelian* if $[\mathfrak{g}, \mathfrak{g}] = 0$. Let $\mathfrak{t} \subset \mathfrak{g}$ denote a maximal Abelian subalgebra of the compact Lie algebra $\mathfrak{g}$. Such a subalgebra is called *torus algebra* and the dual space is denoted as $\mathfrak{t}^*$. The Maximal Torus Theorem, cf. [5], p. 152, states that any two torus algebras, say $\mathfrak{t}, \mathfrak{t}'$, of a compact Lie algebra are conjugate, i.e., there exists a $g \in G$, such that

$$\mathrm{Ad}_g \mathfrak{t} = \mathfrak{t}'.$$

Moreover, for a given $X \in \mathfrak{g}$ and a fixed torus algebra $\mathfrak{t}$ there exists $g \in G$ such that

$$\mathrm{Ad}_g X \in \mathfrak{t}.$$

The Maximal Torus Theorem therefore generalizes the well known fact that any skew-symmetric matrix is unitarily diagonalizable over $\mathbb{C}$.

To define the Jacobi algorithm one needs a set of optimizing directions in a compact Lie algebra. This is given by the *Real Root Space Decomposition*, which is an important tool in analyzing the structure of Lie algebras. For the remainder of this section, the root space decomposition of a compact Lie algebra is explained. Example 2.8 illustrates the correspondence between the root space decomposition and the off-diagonal entries of a skew-Hermitian matrix.

LEMMA 2.6. *Let* $\mathfrak{g}$ *be a compact Lie algebra and* $X \in \mathfrak{g}$. *Then*

$$\mathrm{ad}_X^* = -\mathrm{ad}_X \quad \textit{for all } X \in \mathfrak{g},$$

where adjoint $(\cdot)^*$ *is defined relative to the* Ad-*invariant inner product on* $\mathfrak{g}$.

Proof. Denote by B the Ad-invariant inner product on $\mathfrak{g}$, cf. [25], p. 197, Corollary 4.26. Let $X, Y, Z \in \mathfrak{g}$. Then it holds

$$B(\mathrm{ad}_X Y, Z) = B(Y, -\mathrm{ad}_X Z) = B(-\mathrm{ad}_X^* Y, X). \quad \square$$

Now fix a maximal Abelian subalgebra $\mathfrak{t} \subset \mathfrak{g}$. For $T_1, T_2 \in \mathfrak{t}$, it holds $\mathrm{ad}_{T_1}\mathrm{ad}_{T_2} = \mathrm{ad}_{T_2}\mathrm{ad}_{T_1}$ and hence

$$\{\mathrm{ad}_T \mid T \in \mathfrak{t}\}$$

has a simultaneous eigenspace decomposition. Let X denote a simultaneous eigenvector of ad_T for all $T \in \mathfrak{t}$. By Lemma 2.6 ad_T possesses only purely imaginary eigenvalues and hence one has $\mathrm{ad}_T^2 X = -(\alpha(T))^2 X$, with $\alpha \in \mathfrak{t}^*$. To fix notation, a notion of positivity on $\mathfrak{t}^*$ is introduced. This can be done for example via lexicographic ordering, cf. [25], p. 109. For $\alpha > 0$, we write

$$\mathfrak{g}_\alpha = \{X \in \mathfrak{g} \mid (\mathrm{ad}_T)^2 X = -(\alpha(T))^2 X \text{ for all } T \in \mathfrak{t}\}.$$

If $\mathfrak{g}_\alpha \neq 0$, we call $\mathfrak{g}_\alpha$ a *real root space* and α a *root*. The set of all positive roots is denoted by $\Sigma^+ \subset \mathfrak{t}^*$. Note that our notation slightly differs from that in the literature. E.g., Duistermaat and Kolk [5] denote the real root spaces by $(\mathfrak{g}_\alpha \oplus \mathfrak{g}_{-\alpha}) \cap \mathfrak{g}$ where $\mathfrak{g}_\alpha, \mathfrak{g}_{-\alpha}$ are the complex root spaces of the complexification of $\mathfrak{g}$.

We summarize the above results.

PROPOSITION 2.7. **(Real Root Space Decomposition)** *Let $\mathfrak{g}$ be a compact Lie algebra and let Σ^+ denote the set of positive roots. Then $\mathfrak{g}$ decomposes orthogonally with respect to the Killing form into*

$$\mathfrak{g} = \mathfrak{t} \oplus \sum_{\alpha \in \Sigma^+} \mathfrak{g}_\alpha. \tag{2.5}$$

Each real root space $\mathfrak{g}_\alpha$ is of real dimension 2. It has an orthonormal basis $\{E_\alpha, F_\alpha\}$ with respect to κ such that for any $T \in \mathfrak{t}$ and $\alpha \in \Sigma^+$ (see Figure 2.1):

(i) $\mathrm{ad}_T E_\alpha = \alpha(T) F_\alpha$,
(ii) $\mathrm{ad}_T F_\alpha = -\alpha(T) E_\alpha$.

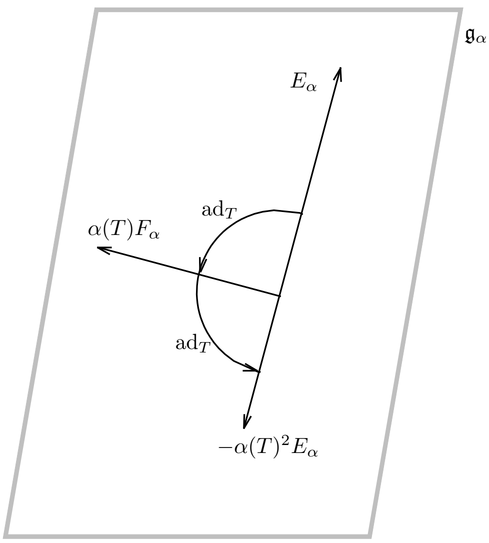

FIG. 2.1. Action of ad_T in the real root space $\mathfrak{g}_\alpha$ with respect to an orthogonal basis $\{E_\alpha, F_\alpha\}$.

Proof. The first part is not proven and the reader is referred to [5], p. 146 and [25], p. 96, Proposition 2.21. Let $E_\alpha \in \mathfrak{g}_\alpha$ arbitrary and let $T \in \mathfrak{t}$ with $\alpha(T) \neq 0$. Set

$$F_\alpha := \frac{1}{\alpha(T)} \mathrm{ad}_T E_\alpha.$$

Then $F_\alpha \neq 0$ since $\mathrm{ad}_T^2 E_\alpha = -\alpha(T)^2 E_\alpha \neq 0$ and $\kappa(F_\alpha, E_\alpha) = 0$ because

$$\kappa(\mathrm{ad}_T E_\alpha, E_\alpha) = \kappa(E_\alpha, -\mathrm{ad}_T E_\alpha) = -\kappa(\mathrm{ad}_T E_\alpha, E_\alpha). \quad \square$$

In the sequel, the following notation will be convenient. For $a, b \in \mathbb{R}$ and $X = aE_\alpha + bF_\alpha \in \mathfrak{g}_\alpha$ define

$$\overline{X} := -bE_\alpha + aF_\alpha. \tag{2.6}$$

Example 2.8. Let $\mathrm{i} := \sqrt{-1}$. Let $\mathfrak{g} = \mathfrak{su}(3, \mathbb{C})$ and fix a torus algebra $\mathfrak{t}$ by

$$\mathfrak{t} = \left\{ \begin{bmatrix} \mathrm{i}x_1 & 0 & 0 \\ 0 & \mathrm{i}x_2 & 0 \\ 0 & 0 & \mathrm{i}x_3 \end{bmatrix} \;\middle|\; x_1, x_2, x_3 \in \mathbb{R}, \sum_{k=1}^{3} x_k = 0 \right\}.$$

Then the real root spaces and the corresponding roots turn out to be

$$\mathfrak{g}_{\alpha_1} = \left\{ \begin{bmatrix} 0 & \lambda + \mathrm{i}\nu & 0 \\ -\lambda + \mathrm{i}\nu & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \;\middle|\; \lambda, \nu \in \mathbb{R} \right\}, \ \alpha_1 \left(\begin{bmatrix} \mathrm{i}x_1 & 0 & 0 \\ 0 & \mathrm{i}x_2 & 0 \\ 0 & 0 & \mathrm{i}x_3 \end{bmatrix} \right) = x_1 - x_2,$$

$$\mathfrak{g}_{\alpha_2} = \left\{ \begin{bmatrix} 0 & 0 & \lambda + \mathrm{i}\nu \\ 0 & 0 & 0 \\ -\lambda + \mathrm{i}\nu & 0 & 0 \end{bmatrix} \;\middle|\; \lambda, \nu \in \mathbb{R} \right\}, \ \alpha_2 \left(\begin{bmatrix} \mathrm{i}x_1 & 0 & 0 \\ 0 & \mathrm{i}x_2 & 0 \\ 0 & 0 & \mathrm{i}x_3 \end{bmatrix} \right) = x_1 - x_3,$$

$$\mathfrak{g}_{\alpha_3} = \left\{ \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \lambda + \mathrm{i}\nu \\ 0 & -\lambda + \mathrm{i}\nu & 0 \end{bmatrix} \;\middle|\; \lambda, \nu \in \mathbb{R} \right\}, \ \alpha_3 \left(\begin{bmatrix} \mathrm{i}x_1 & 0 & 0 \\ 0 & \mathrm{i}x_2 & 0 \\ 0 & 0 & \mathrm{i}x_3 \end{bmatrix} \right) = x_2 - x_3. \quad \square$$

The way real root spaces of a compact Lie algebra are related to each other is similar to the way complex root spaces of a complex semisimple Lie algebra ([25], p. 96) are related. We write $\alpha > \beta$ if $\alpha - \beta$ is positive.

LEMMA 2.9. *Let $\mathfrak{g}_\alpha$ and $\mathfrak{g}_\beta$ be real root spaces of the compact Lie algebra $\mathfrak{g}$. Without loss of generality assume $\alpha > \beta$. Then*

$$[\mathfrak{g}_\alpha, \mathfrak{g}_\beta] = \mathfrak{g}_{\alpha+\beta} \oplus \mathfrak{g}_{\alpha-\beta}$$

holds, where

$$\mathfrak{g}_{\alpha+\beta} := 0, \qquad \text{if} \quad \alpha + \beta \notin \Sigma^+,$$
$$\mathfrak{g}_{\alpha-\beta} := 0, \qquad \text{if} \quad \alpha - \beta \notin \Sigma^+.$$

Proof. Direct consequence of the definition of real root spaces ([5], p. 146) and the relations between complex root spaces ([25], p. 88, Proposition 2.5). $\square$

We need the following lemmata for further calculation.

LEMMA 2.10. *Let $\{E_\gamma, F_\gamma\}$ be a basis of the real root space $\mathfrak{g}_\gamma$ as in Proposition 2.7. Then $T_\gamma := [E_\gamma, F_\gamma]$ lies in the maximal torus algebra $\mathfrak{t}$ and moreover, $\gamma(T_\gamma) > 0$.*

Proof. By the Jacobi identity and Proposition 2.7 for an arbitrary $H \in \mathfrak{t}$ it holds

$$\mathrm{ad}_H[E_\gamma, F_\gamma] = 0.$$

Hence, $[E_\gamma, F_\gamma] \in \mathfrak{t}$. Now let $X = x\, E_\gamma + y\, F_\gamma$ with $(x, y) \in \mathbb{R}^2 - \{0\}$ and let B be a positive definite bilinear Ad-invariant form on $\mathfrak{g}$, cf. [25], p. 196. Moreover, cf. (2.6),

$$\begin{aligned}
\gamma([E_\gamma, F_\gamma])B\Big(\overline{X}, \overline{X}\Big) &= B\Big(\overline{X}, \mathrm{ad}_{[E_\gamma,F_\gamma]}X\Big) \\
&= -y\; B\Big(E_\gamma, x\; \mathrm{ad}_{E_\gamma}\mathrm{ad}_{F_\gamma}E_\gamma - y\; \mathrm{ad}_{F_\gamma}\mathrm{ad}_{E_\gamma}F_\gamma\Big) \\
&\quad +x\; B\Big(F_\gamma, x\; \mathrm{ad}_{E_\gamma}\mathrm{ad}_{F_\gamma}E_\gamma - y\; \mathrm{ad}_{F_\gamma}\mathrm{ad}_{E_\gamma}F_\gamma\Big) \\
&= -y\; B\Big(E_\gamma, -y\; \mathrm{ad}_{F_\gamma}\mathrm{ad}_{E_\gamma}F_\gamma\Big) + x\; B\Big(F_\gamma, x\; \mathrm{ad}_{E_\gamma}\mathrm{ad}_{F_\gamma}E_\gamma\Big) \\
&= y^2\; B\Big(\mathrm{ad}_{E_\gamma}F_\gamma, \mathrm{ad}_{E_\gamma}F_\gamma\Big) + x^2\; B\Big(\mathrm{ad}_{E_\gamma}F_\gamma, \mathrm{ad}_{E_\gamma}F_\gamma\Big) > 0,
\end{aligned}$$

since $[E_\gamma, F_\gamma] \neq 0$. □

LEMMA 2.11. *For arbitrary $H \in \mathfrak{t}$ and any* Ad*-invariant bilinear form $(\cdot,\cdot)$ it holds*

$$\Big(H, T_\gamma\Big) = \frac{\gamma(H)}{\gamma(T_\gamma)}\Big(T_\gamma, T_\gamma\Big) \qquad \textit{for all } \gamma \in \Sigma^+.$$

Proof. We use the definition of T_γ, cf. Lemma 2.10. Let $H \in \mathfrak{t}$. Then

$$\begin{aligned}
\gamma(T_\gamma)\Big(H, \mathrm{ad}_{E_\gamma}F_\gamma\Big) &= \gamma(T_\gamma)\Big(\mathrm{ad}_H E_\gamma, F_\gamma\Big) \\
&= \gamma(H)\gamma(T_\gamma)\Big(F_\gamma, F_\gamma\Big) \\
&= \gamma(H)\Big(\mathrm{ad}_{[E_\gamma,F_\gamma]}E_\gamma\;,\; F_\gamma\Big) \\
&= \gamma(H)\Big(-\,\mathrm{ad}_{E_\gamma}\mathrm{ad}_{E_\gamma}F_\gamma\;,\; F_\gamma\Big) \\
&= \gamma(H)\Big(T_\gamma, T_\gamma\Big). \quad □
\end{aligned}$$

3. A Cost Function. Since Jacobi-type methods can be considered as optimization algorithms, [21, 22], it is instrumental to make a thorough analysis of the cost function we want to minimize. For the Jacobi algorithm, one considers the so-called off-norm function of a square matrix $X = (x_{ij})$, defined as the sum of squares of all its off-diagonal elements

$$\mathrm{off} : \mathbb{R}^{n\times n} \longrightarrow [0, \infty), \qquad \mathrm{off}(X) = \sum_{i\neq j} x_{ij}^2.$$

In this section, a generalization of the off-norm of matrices is discussed. The set of critical points is computed as well as the Hessian. These calculations are essential steps towards the analysis of the local convergence properties of our algorithm.

Let G be a compact Lie group with compact Lie algebra $\mathfrak{g}$ and real root space decomposition (2.5). Let κ denote the Killing form on $\mathfrak{g}$. Denote by

$$\mathrm{p} : \mathfrak{g} \longrightarrow \mathfrak{t} \tag{3.1}$$

the orthogonal projection on $\mathfrak{t}$ with respect to κ. Any $X \in \mathfrak{g}$ decomposes into

$$X = X_0 + \sum_{\alpha \in \Sigma^+} X_\alpha$$

corresponding to (2.5), with $X_0 := \mathrm{p}(X)$. For a given $S \in \mathfrak{g}$ let

$$\mathcal{O}_S := \Big\{ \mathrm{Ad}_g S \mid g \in G \Big\}$$

denote the *adjoint orbit of* S. A cost function is defined as

$$f : \mathcal{O}_S \longrightarrow [0, \infty), \qquad X \longmapsto -\kappa\Big(X - X_0, X - X_0\Big). \tag{3.2a}$$

By negative semidefiniteness of κ on $\mathfrak{g}$, f is nonnegative. By orthogonality of the root space decomposition (2.5), it holds

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

and $\kappa(X, X) = \kappa(S, S)$ is constant along the orbit $\mathcal{O}_S$, cf. (2.4a). Moreover, by Proposition 2.7 and Lemma 3.1(ii), the cost function defined by (3.2a) is equal to

$$f(X) = -\kappa(S, S) - 2 \sum_{\alpha \in \Sigma^+} \alpha^2(X_0). \tag{3.2b}$$

This shows that f is the natural generalization of the off-norm function on a compact Lie algebra.

We now analyze the cost function (3.2a) in detail. The following result summarizes two properties that will be needed for subsequent calculations. Recall that $X_0 = \mathrm{p}(X)$ by definition.

LEMMA 3.1. *Let $\mathfrak{g}$ be a compact Lie algebra with fixed maximal torus algebra $\mathfrak{t} \subset \mathfrak{g}$. Let* p *be as in* (3.1) *and $X, Y \in \mathfrak{g}$. Then the following holds:*

(i) $\mathrm{p}(\mathrm{ad}_Y X_0) = 0$,

(ii) $\kappa\Big(Y_0, X - X_0\Big) = 0$.

Proof. By linearity of the adjoint transformation (2.4b) and by the root space decomposition (2.5) of $\mathfrak{g}$ it holds

$$\mathrm{ad}_Y X_0 = \mathrm{ad}_{Y_0} X_0 + \sum_{\alpha \in \Sigma^+} \mathrm{ad}_{Y_\alpha} X_0.$$

The summand $\mathrm{ad}_{Y_\alpha} X_0$ lies in $\mathfrak{g}_\alpha$ for all $\alpha \in \Sigma^+$ and $\mathrm{ad}_{Y_0} X_0 = 0$ holds. Hence $\mathrm{ad}_Y X_0$ has no $\mathfrak{t}$-component and therefore

$$\mathrm{p}(\mathrm{ad}_Y X_0) = 0.$$

Statement (ii) is a direct consequence of (3.1). □

THEOREM 3.2. *Let κ be the Killing form on the compact Lie algebra $\mathfrak{g}$, $S \in \mathfrak{g}$ arbitrary and* p *as in* (3.1). *Let*

$$f : \mathcal{O}_S \longrightarrow [0, \infty), \qquad X \longmapsto -\kappa\Big(X - \mathrm{p}(X), X - \mathrm{p}(X)\Big)$$

as above.

(a) *The following statements are equivalent:*
(i) $X \in \mathcal{O}_S$ *is a critical point of* f,
(ii) $\mathrm{ad}_{X_0} X = 0$,
(iii) $\alpha(X_0)\ X_\alpha = 0$ *for all* $\alpha \in \Sigma^+$.

(b) *Let* Z *be a critical point of* f *and let* $\mathrm{ad}_H Z \in T_Z\mathcal{O}_S$ *be an arbitrary element of the tangent space at* Z*. Then the Hessian of* f *at* Z *is*

$$\begin{aligned} \mathsf{H}_f(Z): \quad T_Z\mathcal{O}_S \times T_Z\mathcal{O}_S &\longrightarrow \mathbb{R}, \\ (\mathrm{ad}_H Z, \mathrm{ad}_H Z) &\longmapsto -2\kappa\Big(\mathrm{ad}_H Z, \mathrm{ad}_H Z_0 - \mathrm{p}(\mathrm{ad}_H Z)\Big). \end{aligned}$$

Proof. (a) For arbitrary $H, X \in \mathfrak{g}$ let $\gamma : \mathbb{R} \longrightarrow \mathcal{O}_S,\quad \gamma(t) = \mathrm{Ad}_{\exp(tH)} X$, be a smooth curve through X. The derivative of the cost function (3.2a) at X can be calculated in the following way. By Lemma 3.1 and the Ad-invariance of the Killing form κ (2.4b) we have

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

Hence

$$Df(X) \equiv 0 \quad \Longleftrightarrow \quad \mathrm{ad}_{X_0} X \in \mathrm{rad}_\kappa,$$

where rad_κ denotes the radical of the Killing form κ.

On compact Lie algebras, the radical rad_κ coincides with the center of $\mathfrak{g}$ ([5], p. 148) and therefore $\mathrm{ad}_{X_0} X$ has to coincide with its projection on $\mathfrak{t}$. Using Lemma 3.1 again, one obtains $\mathrm{ad}_{X_0} X = 0$. Hence for a critical point X it holds

$$\sum_{\alpha \in \Sigma^+} \mathrm{ad}_{X_0} X_\alpha = 0$$

$$\Longleftrightarrow$$

$$\mathrm{ad}_{X_0} X_\alpha = 0 \quad \text{for all } \alpha \in \Sigma^+$$

$$\Longleftrightarrow$$

$$\alpha(X_0) \cdot X_\alpha = 0 \quad \text{for all } \alpha \in \Sigma^+.$$

(b) By a simple but lengthy computation, for arbitrary $H \in \mathfrak{g}$ and $\gamma(t) :=$

$\mathrm{Ad}_{\exp(tH)}Z$, it follows

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\Big(f\circ\gamma\Big)(t)\Big|_{t=0}$$

$$= -\frac{\mathrm{d}^2}{\mathrm{d}t^2}\kappa\Big(\mathrm{Ad}_{\exp(tH)}Z - \mathrm{p}(\mathrm{Ad}_{\exp(tH)}Z), \mathrm{Ad}_{\exp(tH)}Z - \mathrm{p}(\mathrm{Ad}_{\exp(tH)}Z)\Big)\Big|_{t=0}$$

$$= -2\frac{\mathrm{d}}{\mathrm{d}t}\kappa\Big(\mathrm{ad}_H\mathrm{Ad}_{\exp(tH)}Z - \mathrm{p}(\mathrm{ad}_H\mathrm{Ad}_{\exp(tH)}Z), \mathrm{Ad}_{\exp(tH)}Z - \mathrm{p}(\mathrm{Ad}_{\exp(tH)}Z)\Big)\Big|_{t=0}$$

$$= -2\kappa\Big(\mathrm{ad}_H^2 Z - \mathrm{p}(\mathrm{ad}_H^2 Z), Z - Z_0\Big) - 2\kappa\Big(\mathrm{ad}_H Z - \mathrm{p}(\mathrm{ad}_H Z), \mathrm{ad}_H Z - \mathrm{p}(\mathrm{ad}_H Z)\Big)$$

$$= -2\kappa\Big(\mathrm{ad}_H Z, -\mathrm{ad}_H Z + \mathrm{ad}_H Z_0\Big) - 2\kappa\Big(\mathrm{ad}_H Z, \mathrm{ad}_H Z - \mathrm{p}(\mathrm{ad}_H Z)\Big)$$

$$= -2\kappa\Big(\mathrm{ad}_H Z, \mathrm{ad}_H Z_0 - \mathrm{p}(\mathrm{ad}_H Z)\Big). \quad \square$$

Note that for any $\xi \in T_Z\mathcal{O}_S$ in the tangent space at a critical point Z, elements $H \in \mathfrak{g}$ satisfying $\xi = \mathrm{ad}_H Z$ are not uniquely determined. That is $\xi = \mathrm{ad}_H Z = \mathrm{ad}_{H+C} Z$ whenever $[C, Z] = 0$. Nevertheless,

$$\kappa\Big(\mathrm{ad}_{H+C} Z, \mathrm{ad}_{H+C} Z_0 - \mathrm{p}(\mathrm{ad}_{H+C} Z)\Big) = \kappa\Big(\mathrm{ad}_H Z, \mathrm{ad}_H Z_0 - \mathrm{p}(\mathrm{ad}_H Z)\Big)$$

holds. Thus the selection of elements H with $\xi = \mathrm{ad}_H Z$ does not affect the validity of the expression for the Hessian.

The next two lemmata contain information about the restriction of the Hessian to one dimensional subspaces of $T_Z\mathcal{O}_S$. It turns out that, whenever the critical point Z is not a global minimum, there exists a one dimensional subspace of $T_Z\mathcal{O}_S$ on which the restriction of the Hessian is negative definite. Hence the cost function possesses only global minima. A similar argument shows that the local maxima of the cost function are global. One concludes that all other critical points are saddle points.

LEMMA 3.3. *Let $\beta \in \Sigma^+$ be a real root, $\Omega \neq 0$ an arbitrary element of the real root space $\mathfrak{g}_\beta$ and let $Z \in \mathcal{O}_S$ denote a critical point of the cost function* (3.2a)*. Let $Z_0 \in \mathfrak{t}$ denote the torus algebra component of Z. Then:*

$$\beta(Z_0) \neq 0 \qquad \textit{implies} \qquad \mathsf{H}_f(Z)\Big(\mathrm{ad}_\Omega Z, \mathrm{ad}_\Omega Z\Big) > 0.$$

Proof. Let $\beta(Z_0) \neq 0$. Then $Z_\beta = 0$ by Theorem 3.2. As $\mathrm{ad}_\Omega Z_\alpha$ has no torus algebra component for $\alpha \neq \beta$, one obtains

$$\mathrm{p}(\mathrm{ad}_\Omega Z_\alpha) = 0 \qquad \text{for all } \alpha \in \Sigma^+.$$

Moreover, $\mathrm{ad}_\Omega Z_\alpha$ lies for any $\alpha \in \Sigma^+$ in the orthogonal complement of $\mathfrak{g}_\beta$ (cf. Lemma 2.9) and therefore

$$\kappa\left(\sum_{\alpha\in\Sigma^+} \mathrm{ad}_\Omega Z_\alpha, \mathrm{ad}_\Omega Z_0\right) = -\kappa\left(\sum_{\alpha\in\Sigma^+} \mathrm{ad}_\Omega Z_\alpha, \mathrm{ad}_{Z_0}\Omega\right) = 0$$

also holds. We compute the restriction of the Hessian evaluated at Z to the subspace $\mathbb{R} \cdot \mathrm{ad}_\Omega Z$.

$$\frac{1}{2}\mathsf{H}_f(Z)(\mathrm{ad}_\Omega Z, \mathrm{ad}_\Omega Z) = -\kappa\Big(\mathrm{ad}_\Omega Z_0, \mathrm{ad}_\Omega Z_0\Big) - \kappa\left(\sum_{\alpha\in\Sigma^+} \mathrm{ad}_\Omega Z_\alpha, \mathrm{ad}_\Omega Z_0\right)$$
$$= -\kappa\Big(\mathrm{ad}_\Omega Z_0, \mathrm{ad}_\Omega Z_0\Big)$$
$$= -\beta(Z_0)^2\kappa\Big(\Omega, \Omega\Big) > 0. \qquad \square$$

LEMMA 3.4. *Let $\gamma \in \Sigma^+$ be a real root, let $\{\Omega_1, \Omega_2\}$ be some basis of $\mathfrak{g}_\gamma$, and let $Z \in \mathcal{O}_S$ be a critical point of the cost function defined by* (3.2a). *Then:*

$$Z_\gamma \neq 0 \qquad \textit{implies} \qquad \mathsf{H}_f(Z)(\mathrm{ad}_{\Omega_j} Z, \mathrm{ad}_{\Omega_j} Z) < 0$$

for either $j = 1$ or $j = 2$.

Proof. Let $\Omega \in \{\Omega_1, \Omega_2\}$ such that $\Omega \notin \mathbb{R} \cdot Z_\gamma$. By Theorem 3.2, $\gamma(Z_0) = 0$ and therefore, cf. (2.6),

$$\mathrm{ad}_\Omega Z_0 = -\mathrm{ad}_{Z_0}\Omega = \pm\gamma(Z_0)\overline{\Omega} = 0.$$

The Hessian restricted to the subspace $\mathbb{R} \cdot \mathrm{ad}_\Omega Z$ is

$$\frac{1}{2}\mathsf{H}_f(Z)(\mathrm{ad}_\Omega Z, \mathrm{ad}_\Omega Z) = \kappa\left(\sum_{\alpha\in\Sigma^+} \mathrm{ad}_\Omega Z_\alpha, \sum_{\alpha\in\Sigma^+} \mathrm{p}(\mathrm{ad}_\Omega Z_\alpha)\right)$$
$$= \kappa\left(\sum_{\alpha\in\Sigma^+} \mathrm{p}(\mathrm{ad}_\Omega Z_\alpha), \sum_{\alpha\in\Sigma^+} \mathrm{p}(\mathrm{ad}_\Omega Z_\alpha)\right)$$
$$= \kappa\Big(\mathrm{ad}_\Omega Z_\gamma, \mathrm{ad}_\Omega Z_\gamma\Big) < 0,$$

cf. Lemma 2.10. $\square$

As a consequence of the last two lemmata we obtain

PROPOSITION 3.5.

(i) *The local minima of the cost function* (3.2a) *are global minima. The set of the minima is $\mathcal{O}_S \cap \mathfrak{t}$.*

(ii) *The local maxima of the cost function* (3.2a) *are global maxima. The set of the maxima is $\mathcal{O}_S \cap \mathfrak{t}^\perp$ where $\mathfrak{t}^\perp$ denotes the orthogonal complement of $\mathfrak{t}$ with respect to κ.*

Proof. (i) Let Z be a local minimum of (3.2a), then

$$\mathsf{H}_f(Z)(\mathrm{ad}_\Omega Z, \mathrm{ad}_\Omega Z) \geq 0 \quad \text{for all } \Omega \in \mathfrak{g}.$$

By Lemma 3.4,

$$Z_\gamma = 0 \quad \text{for all } \gamma \in \Sigma^+.$$

Hence $\mathrm{p}(Z) = Z$ and $f(Z) = 0$.

(ii) Now let Z be a local maximum of (3.2a), then

$$\mathsf{H}_f(Z)(\mathrm{ad}_\Omega Z, \mathrm{ad}_\Omega Z) \leq 0 \quad \text{for all } \Omega \in \mathfrak{g}.$$

By Lemma 3.3,

$$\gamma(Z_0) = 0 \quad \text{for all } \gamma \in \Sigma^+. \tag{3.3}$$

By comparing (3.3) with (3.2b) it follows that $f(Z) = -\kappa(S,S)$ and therefore Z is a global maximum of f. It follows immediately from Equation (3.3) that $Z_0 \in \mathfrak{z}_\mathfrak{g}$, the center of $\mathfrak{g}$, and hence $Z \in \mathfrak{t}^\perp$. Note that $\mathfrak{t} \cap \mathfrak{t}^\perp = \mathfrak{z}_\mathfrak{g}$. □

The next theorem characterizes the critical points of the cost function (3.2a).

THEOREM 3.6.

(a) *A critical point Z of* (3.2a) *is a saddle point if and only if*

$$0 < f(Z) < -\kappa(S,S).$$

(b) *The set of minima of the cost function* (3.2a) *is finite.*

Proof. (a) Direct consequence of Proposition 3.5.

(b) The set of minima of the cost function (3.2a) is exactly the intersection of $\mathcal{O}_S$ with the torus algebra $\mathfrak{t}$. By Weyl's Covering Theorem ([5], p. 153, Section 3.7), we conclude that $|\mathcal{O}_S \cap \mathfrak{t}|$ is finite. □

4. The Algorithm. As mentioned in the introduction, a Lie algebraic version of the classical Jacobi algorithm has already been published by Wildberger, cf. [37]. Proceeding from the real root space decomposition (2.5) of a compact Lie algebra $\mathfrak{g}$, Wildberger decomposes a given $Z \in \mathfrak{g}$ into torus algebra and root space components $Z = Z_0 + \sum_\alpha Z_\alpha$. He shows the existence of a sequence of Lie algebra elements $(Z^{(1)}, Z^{(2)}, ...)$, for which the following holds.

(i) $Z^{(k+1)} = \mathrm{Ad}_{g_k} Z^{(k)}$ where g_k only depends on $Z_\alpha^{(k)}$ and α is chosen such that $||Z_\alpha^{(k)}|| = \max_{\gamma \in \Sigma^+} ||Z_\gamma^{(k)}||$,

(ii) $Z^{(k+1)}$ has no $\mathfrak{g}_\alpha$ component,

(iii) the sequence $(Z^{(k)})$ converges to some torus algebra element.

The method described in [37] uses only $SU(2,\mathbb{C})$ transformations in a non-cyclic manner which is completely analogous to Jacobi's original approach based on orthogonal transformations to annihilate the off-diagonal elements having greatest modulus, cf. [24].

We extend this construction by formulating in full generality a cyclic Jacobi algorithm on compact Lie algebras. The algorithm proceeds as follows. Given closed one-parameter subgroups $G_1, ..., G_M$ of the compact Lie group G, the restriction of the cost function (3.2a) to the orbit of the initial point $Z \in \mathfrak{g}$ under the adjoint action of G_1 is minimized. Let $Z^{(1)} \in \mathrm{Ad}_{G_1} Z$ denote that minimum. The next step is done by minimizing the restriction of (3.2a) to $\mathrm{Ad}_{G_2} Z^{(1)}$ and so on until arriving at $Z^{(M)}$. This procedure is called a *sweep*, and iterating sweeps forms the algorithm.

More precisely, let N denote the number of real root spaces of $\mathfrak{g}$ and choose

$$\mathfrak{B} = \{\Omega_1, ..., \Omega_{2N}\} \tag{4.1}$$

as a basis of $\mathfrak{g}/\mathfrak{t}$ where for $i = 1, ..., N$, the set $\{\Omega_{2i-1}, \Omega_{2i}\}$ denotes orthogonal basis vectors of the real root space $\mathfrak{g}_{\alpha_i}$, cf. Proposition 2.7. For $\Omega \in \mathfrak{B}$ consider

$$r_\Omega : \mathcal{O}_S \times \mathbb{R} \longrightarrow \mathcal{O}_S, \qquad r_\Omega(X,t) := \mathrm{Ad}_{\exp(t\Omega)} X.$$

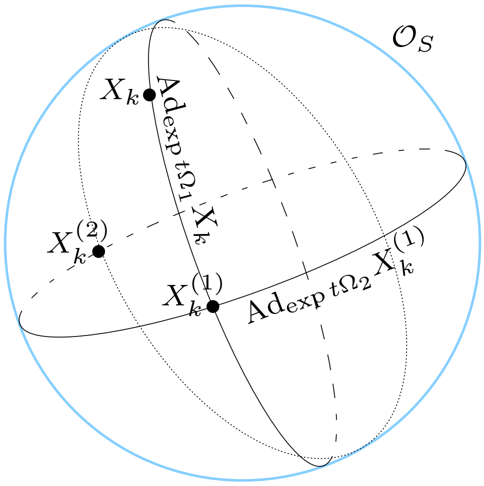

FIG. 4.1. Illustration of the first step of the cyclic Jacobi sweep.

Furthermore, *step size selections*, depending on $\Omega_i \in \mathfrak{B}, i = 1, ..., 2N$, are defined as

$$
t_*^{(i)} : \mathcal{O}_S \longrightarrow \mathbb{R},
$$

$$
t_*^{(i)}(X) := \begin{cases} 0, & \text{if } \left(f \circ \mathrm{Ad}_{\exp(t\Omega_i)}\right)(X) = f(X) \quad \text{for all } t \in \mathbb{R} \\ \arg\min_{t\in\mathbb{R}} \left(f \circ \mathrm{Ad}_{\exp(t\Omega_i)}\right)(X) & \text{otherwise.} \end{cases} \tag{4.2}
$$

To guarantee uniqueness, $\arg\min_{t\in\mathbb{R}} \left(f \circ \mathrm{Ad}_{\exp(t\Omega_i)}\right)(X)$ denotes that $t \in \mathbb{R}$ being of smallest absolute value. In case there are two such minimal values $\pm t$, we choose the positive solution $t > 0$. A more explicit formula for (4.2) is given in Section 5. Sweeps are defined as follows.

Cyclic Jacobi Sweep

$$
\begin{aligned}
X_k^{(1)} &:= r_{\Omega_1}\left(X_k^{(0)}, t_*^{(1)}\left(X_k^{(0)}\right)\right) \\
X_k^{(2)} &:= r_{\Omega_2}\left(X_k^{(1)}, t_*^{(2)}\left(X_k^{(1)}\right)\right) \\
&\vdots \\
X_k^{(2N)} &:= r_{\Omega_{2N}}\left(X_k^{(2N-1)}, t_*^{(2N)}\left(X_k^{(2N-1)}\right)\right).
\end{aligned} \tag{4.3}
$$

The Jacobi algorithm consists of iterating sweeps.

Jacobi's Algorithm

1. Let $X_0, X_1, ..., X_k \in \mathcal{O}_S$ be given for some $k \in \mathbb{N}$.
2. Set $X_k^{(0)} := X_k$ and define the sequence $X_k^{(1)}, ..., X_k^{(2N)}$ as in (4.3). (4.4)
3. Set $X_{k+1} := X_k^{(2N)}$ and continue with the next sweep.

Note that the smallest Lie algebra containing a root space is isomorphic to $\mathfrak{su}(2,\mathbb{C})$, see proof of Proposition 4.1. Therefore the Lie algebra $\mathfrak{g}$ is the (non direct) sum

$$\mathfrak{g} = \sum_N \mathfrak{su}(2,\mathbb{C}) + \mathfrak{z}_\mathfrak{g},$$

where $\mathfrak{z}_\mathfrak{g}$ denotes the center of $\mathfrak{g}$. Hence sweep operations can in principle be organized via $SU(2,\mathbb{C})$ suboperations minimizing simultaneously along the directions $\{\Omega_{2i-1}, \Omega_{2i}\}$ for $i = 1, ..., N$ as it has been done by Wildberger, [37]. Such an approach leads to so-called block-Jacobi methods as in each step the cost function restricted to a *two*-dimensional subset is minimized, cf. [21, 22], see also [27] for minimization over higher dimensional subsets. In this paper we do not follow this idea and restrict ourselves to the algorithm as described above.

Torus algebra directions $T \in \mathfrak{t}$ can be omitted from the minimization process as the cost function (3.2b) is constant along the orbits of the generated one-parameter groups, i.e.,

$$\mathrm{p}\Big(\mathrm{Ad}_{\exp(tT)} X\Big) = \mathrm{p}(X)$$

holds for all $T \in \mathfrak{t}$ and $t \in \mathbb{R}$, because Lemma 3.1 implies

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{p}\Big(\mathrm{Ad}_{\exp(tT)} X\Big) = \mathrm{p}\Big(\mathrm{ad}_T \mathrm{Ad}_{\exp(tT)} X\Big) = 0.$$

PROPOSITION 4.1. *Let $X_\alpha \in \mathfrak{g}_\alpha$ and $Y \in \mathfrak{g}$ arbitrary. Then*
(i) $\mathrm{Ad}_{\exp(\mathbb{R}\cdot X_\alpha)} Y \;\cong\; S^1$, *if* $[Y, X_\alpha] \neq 0$ *and*
(ii) $\mathrm{Ad}_{\exp(\mathbb{R}\cdot X_\alpha)} Y \;\cong\; \{1\}$, *if* $[Y, X_\alpha] = 0$.
Thus the cost function restricted to $\mathrm{Ad}_{\exp(\mathbb{R}\cdot X_\alpha)} Y$ *possesses at least one minimum and Algorithms* (4.3) *and* (4.4) *are therefore well defined.*

Proof. Let $X_\alpha \in \mathfrak{g}_\alpha - \{0\}$. The smallest Lie subalgebra containing $\mathfrak{g}_\alpha$ is

$$\langle \mathfrak{g}_\alpha \rangle := \bigcap_{\mathfrak{g}_\alpha \subset \mathfrak{h}} \{\mathfrak{h} \text{ is Lie subalgebra of } \mathfrak{g}\} = \mathfrak{g}_\alpha \oplus \mathbb{R} \cdot [X_\alpha, \overline{X_\alpha}],$$

cf. Lemma 2.10. Therefore $\langle \mathfrak{g}_\alpha \rangle$ is a three dimensional real vector space and it can easily be checked that $\langle \mathfrak{g}_\alpha \rangle$ and $\mathfrak{su}(2,\mathbb{C})$ are isomorphic as Lie algebras. Therefore, for any element $X \in \langle \mathfrak{g}_\alpha \rangle$, the closure of the one parameter group $\exp(\mathbb{R} \cdot X)$ is isomorphic to a torus in $SU(2,\mathbb{C})$. Any torus in $SU(2,\mathbb{C})$ is isomorphic to the circle group S^1, and hence

$$\exp(\mathbb{R} \cdot X) \;\cong\; S^1.$$

The assertion for the orbits follows immediately by the identity

$$\mathrm{Ad}_{\exp X} = \exp(\mathrm{ad}_X) \quad \text{for all } X \in \mathfrak{g},$$

cf. [5], p. 23, Theorem 1.5.2. □

5. More Explicit Description of the Algorithm. To derive a more explicit description of the algorithm, it is necessary to take a closer look at the cost function (3.2a).

For $\Omega, X \in \mathfrak{g}$ and $t \in \mathbb{R}$, it is well known (cf. [5], p. 23) that

$$\mathrm{Ad}_{\exp(t\Omega)}X = \exp(t\mathrm{ad}_\Omega)X = \sum_{k=0}^{\infty} \frac{1}{k!} t^k \mathrm{ad}_\Omega^k X. \tag{5.1}$$

The following convention is used to simplify notation. Let $\Omega \in \{E_\gamma, F_\gamma\}$ be one basis vector of the real root space $\mathfrak{g}_\gamma$ as in Proposition 2.7. Whenever "$\pm$" or "$\mp$" occurs in a formula, the upper sign stands for the case where $\Omega = E_\gamma$ while the lower one for the case where $\Omega = F_\gamma$. By Proposition 2.7 and Lemma 2.10 it holds

$$\mathrm{ad}_{\mathfrak{g}_\gamma}(\mathfrak{t}) \subset \mathfrak{g}_\gamma \quad \text{and} \quad \mathrm{ad}_{\mathfrak{g}_\gamma}(\mathfrak{g}_\gamma) \subset \mathfrak{t}. \tag{5.2}$$

Therefore, by projecting (5.1) onto the torus algebra, one obtains, cf. (2.6),

$$\begin{aligned} \mathrm{p}(\mathrm{Ad}_{\exp(t\Omega)}X) &= \sum_{k=0}^{\infty} \frac{1}{(2k)!} t^{2k} \ \mathrm{ad}_\Omega^{2k} \ X_0 + \sum_{k=0}^{\infty} \frac{1}{(2k+1)!} t^{2k+1} \ \mathrm{ad}_\Omega^{2k+1} \ c \cdot \overline{\Omega} \\ &= X_0 \mp \gamma(X_0) \cdot \sum_{k=0}^{\infty} \frac{1}{(2k+2)!} t^{2k+2} \ \mathrm{ad}_\Omega^{2k+1} \ \overline{\Omega} + \\ &\quad + c \cdot \sum_{k=0}^{\infty} \frac{1}{(2k+1)!} t^{2k+1} \ \mathrm{ad}_\Omega^{2k+1} \ \overline{\Omega}, \end{aligned}$$

where c denotes the $\overline{\Omega}$-coefficient of X. It is easily shown by induction that for all $k \in \mathbb{N}$

$$\mathrm{ad}_\Omega^{2k+1} \ \overline{\Omega} = \pm\Big(- \gamma(T_\gamma)\Big)^k \ T_\gamma \tag{5.3}$$

holds. A straightforward computation then leads to

$$\mathrm{p}(\mathrm{Ad}_{\exp(t\Omega)}X) = X_0 + g(t) \cdot T_\gamma, \tag{5.4}$$

where

$$g(t) := \frac{\gamma(X_0)}{\gamma(T_\gamma)} \cos\Big(\sqrt{\gamma(T_\gamma)} \cdot t\Big) - \frac{\gamma(X_0)}{\gamma(T_\gamma)} \pm \frac{c}{\sqrt{\gamma(T_\gamma)}} \sin\Big(\sqrt{\gamma(T_\gamma)} \cdot t\Big). \tag{5.5}$$

Because of Lemma 2.11 the cost function (3.2a), restricted to the orbit of a Lie algebra element $X \in \mathfrak{g}$ under the adjoint action of a one parameter group generated by some real root space element, is given by

$$f\Big|_{\mathrm{Ad}_{\exp(t\Omega)}X} = -\kappa(S,S) + \kappa\Big(X_0, X_0\Big) + \left(2g(t)\frac{\gamma(X_0)}{\gamma(T_\gamma)} + g(t)^2\right) \kappa\Big(T_\gamma, T_\gamma\Big). \tag{5.6}$$

From this expression we deduce an explicit formula for the step size selection (4.2). The following proposition and corollary are an adaptation of the results presented in Section 8.4.1 of [14] to the Lie algebra setting.

PROPOSITION 5.1. *Let $X \in \mathfrak{g}$ and $\Omega \in \{\Omega_1, ..., \Omega_{2N}\}$ as in* (4.1) *be a basis vector of the root space $\mathfrak{g}_\gamma$. Let f denote the cost function* (3.2a)*. Then, either*

$$f\Big|_{\mathrm{Ad}_{\exp(t\Omega)}X} \equiv f(X) \quad \textit{for all} \quad t \in \mathbb{R}$$

or

$$t \longmapsto f\Big|_{\mathrm{Ad}_{\exp(t\Omega)}X} \quad \textit{has periodicity} \quad \frac{\pi}{\sqrt{\gamma(T_\gamma)}}$$

and admits on

$$I := \left(-\frac{\pi}{2\sqrt{\gamma(T_\gamma)}}, \frac{\pi}{2\sqrt{\gamma(T_\gamma)}}\right]$$

exactly one minimum, namely at

$$t_*(X) = \begin{cases} \dfrac{\pi}{2\sqrt{\gamma(T_\gamma)}}, & \textit{if} \quad \gamma(X_0) = 0 \\ \\ \dfrac{1}{\sqrt{\gamma(T_\gamma)}} \arctan\left(\pm\dfrac{c\sqrt{\gamma(T_\gamma)}}{\gamma(X_0)}\right), & \textit{if} \quad \gamma(X_0) \neq 0, \end{cases} \tag{5.7}$$

where c denotes the $\overline{\Omega}$-coefficient of X.

Proof. The restricted cost function $f|_{\mathrm{Ad}_{\exp(t\Omega)}X}$ is constant if and only if $g(t)$ defined by (5.5) is constant, i.e.,

$$g'(t) \equiv 0$$
$$\Longleftrightarrow$$
$$\pm\, c\, \sqrt{\gamma(T_\gamma)}\, \cos\left(\sqrt{\gamma(T_\gamma)} \cdot t\right) - \gamma(X_0)\, \sin\left(\sqrt{\gamma(T_\gamma)} \cdot t\right) \equiv 0$$
$$\Longleftrightarrow$$
$$c = 0 \quad \text{and} \quad \gamma(X_0) = 0.$$

Now let $c \neq 0$. From the identity

$$g(t) + g\left(t + \frac{\pi}{\sqrt{\gamma(T_\gamma)}}\right) = -2\frac{\gamma(X_0)}{\gamma(T_\gamma)}$$

one obtains after some computation

$$f\Big(\mathrm{Ad}_{\exp\left(\left(t+\frac{\pi}{\sqrt{\gamma(T_\gamma)}}\right)\Omega\right)}X\Big) - f\Big(\mathrm{Ad}_{\exp(t\Omega)}X\Big) = 0.$$

Computing the zeros $\widetilde{t} \in \mathbb{R}$ of $\frac{\mathrm{d}}{\mathrm{d}t} f\Big(\mathrm{Ad}_{\exp(t\Omega)X}\Big)$ and the sign of the second derivative at $\widetilde{t}$ then completes the proof. □

Choosing the step size (5.7) in Ω-direction annihilates the $\overline{\Omega}$-component of X. More precisely we obtain

Corollary 5.2. *Let $X \in \mathfrak{g}$ and $\Omega \in \mathfrak{B} = \{\Omega_1, ..., \Omega_{2N}\}$ be a basis vector of the root space $\mathfrak{g}_\gamma$, see* (4.1)*. Denote by*

$$\mathrm{p}_{\overline{\gamma}} : \mathfrak{g} \longrightarrow \mathbb{R} \cdot \overline{\Omega}$$

the projection onto the subspace $\mathbb{R} \cdot \overline{\Omega} \subset \mathfrak{g}_\gamma$. Then

$$\mathrm{p}_{\overline{\gamma}}(\mathrm{Ad}_{\exp(t\Omega)} X) = \left(\mp \frac{\gamma(X_0)}{\sqrt{\gamma(T_\gamma)}} \sin\left(\sqrt{\gamma(T_\gamma)}\ t\right) + c \cos\left(\sqrt{\gamma(T_\gamma)}\ t\right)\right) \overline{\Omega},$$

where c denotes the $\overline{\Omega}$-coefficient of X. Consequently, choosing the step size $t_*(X)$ as in (5.7) *annihilates the $\overline{\Omega}$-component of X.*

Proof. We use again Equations (5.1) and (5.2) to deduce

$$\mathrm{p}_{\overline{\gamma}}(\mathrm{Ad}_{\exp(t\Omega)} X) = \sum_{k=0}^{\infty} \frac{1}{(2k+1)!} t^{2k+1}\ \mathrm{ad}_\Omega^{2k}\ \mathrm{ad}_\Omega X_0 + \sum_{k=0}^{\infty} \frac{1}{(2k)!} t^{2k}\ \mathrm{ad}_\Omega^{2k}\ c\, \overline{\Omega}.$$

It is easily seen by induction that $\mathrm{ad}_\Omega^{2k} \overline{\Omega} = (-\gamma(T_\gamma))^k \overline{\Omega}$ and it holds $\mathrm{ad}_\Omega X_0 = \mp\gamma(X_0)\overline{\Omega}$, hence

$$\begin{aligned}
\mathrm{p}_{\overline{\gamma}}(\mathrm{Ad}_{\exp(t\Omega)} X) &= \mp\,\gamma(X_0) \sum_{k=0}^{\infty} \frac{\left(\sqrt{\gamma(T_\gamma)}\ t\right)^{2k+1}}{(2k+1)!}\ \frac{(-1)^k}{\sqrt{\gamma(T_\gamma)}}\ \overline{\Omega} \\
&\quad + c \sum_{k=0}^{\infty} \frac{t^{2k}}{(2k)!}\ (-\gamma(T_\gamma))^k \overline{\Omega} \\
&= \left(\mp \frac{\gamma(X_0)}{\sqrt{\gamma(T_\gamma)}} \sin\left(\sqrt{\gamma(T_\gamma)}\ t\right) + c \cos\left(\sqrt{\gamma(T_\gamma)}\ t\right)\right) \overline{\Omega}.
\end{aligned}$$

The last statement follows from a simple calculation by substituting $t_*(X)$ into the last equation. ∎

Note, that the Ω-component of X is not affected by the transformation $\mathrm{Ad}_{\exp(t\Omega)} X$, thus the two minimization steps along the Ω- and $\overline{\Omega}$-directions can be done simultaneously.

6. Convergence Proof. We can now describe the main result of this paper. It is shown that the convergence of the Jacobi algorithm on compact Lie algebras is locally quadratically fast, provided the adjoint orbit $\mathcal{O}_S$ has maximal dimension. The dimension of $\mathcal{O}_S$ is equal to the dimension of the tangent space at $Z \in \mathcal{O}_S \cap \mathfrak{t}$. Now let $\alpha_1, ..., \alpha_k$ denote the roots for which

$$\alpha_i(Z) = 0, \qquad i = 1, ..., k$$

holds. Hence $\mathrm{ad}_Z \mathfrak{g}_{\alpha_i} = 0$ for $i = 1, ..., k$ and therefore

$$\ker\ \mathrm{ad}_Z = \mathfrak{t} \oplus \sum_i \mathfrak{g}_{\alpha_i}$$

and

$$\dim \mathcal{O}_S = \dim T_Z \mathcal{O}_S = \dim\{\mathrm{ad}_Z H \mid H \in \mathfrak{g}\} = \dim \mathfrak{g} - \dim \mathfrak{t} - 2k.$$

This formula for the dimension justifies

DEFINITION 6.1. *An element* $S \in \mathfrak{g}$ *is called* regular *if* $\dim \mathcal{O}_S = \dim \mathfrak{g} - \dim \mathfrak{t}$.

EXAMPLE: The set of skew-Hermitian $(n \times n)$-matrices forms the Lie algebra $\mathfrak{u}(n, \mathbb{C})$. Fix a maximal Abelian subalgebra

$$\mathfrak{t} = \{T \in \mathfrak{u}(n, \mathbb{C}) \mid T = \operatorname{diag}(\mathrm{i}t_1, ..., \mathrm{i}t_n), t_j \in \mathbb{R}\}.$$

The roots in this case turn out to be $\alpha(T) = \pm(t_i - t_j)$ for $i < j$. So the regular elements of $\mathfrak{u}(n, \mathbb{C})$ are exactly those matrices having pairwise distinct eigenvalues.

The set of regular elements in $\mathfrak{g}$ is connected, open, and dense (cf. [5], p. 118 Theorem 2.8.5 and p. 146). Therefore, the assumption in the following proposition is generically satisfied.

THEOREM 6.2 (MAIN THEOREM). *An element* $Z \in \mathcal{O}_S$ *is a fixed point of the algorithm if and only if* $\mathrm{p}(Z) = Z$ *holds. If* $S \in \mathfrak{g}$ *is a regular element, the convergence of the Jacobi algorithm* (4.4) *is locally quadratically fast.*

Proof.

The first statement of the theorem is implied by the following argument. Obviously, the only candidates for fixed points are critical points of the cost function. On the other hand by Lemma 3.4, the algorithm is stationary neither at saddle points nor at global maxima as in both cases there exists at least one Ω_i-direction leading downhill.

For the proof of the convergence property, we will show that a sweep is smooth in a neighborhood of a minimum $Z \in \mathcal{O}_S$ of the cost function (3.2a). Furthermore, its derivative vanishes at Z and hence a simple Taylor argument will finish the proof of the local quadratic convergence.

In a first step, the smoothness of the step size selections (4.2) is shown. Let N denote the number of real root spaces and let

$$I := \left(-\frac{\pi}{2\sqrt{\gamma(T_\gamma)}}, \frac{\pi}{2\sqrt{\gamma(T_\gamma)}}\right].$$

For $i = 1, ..., 2N$ define

$$\begin{aligned} \phi_i : I \times \mathcal{O}_S &\longrightarrow [0, \infty), & \phi_i(t, X) &= f(\mathrm{Ad}_{\exp(t\Omega_i)} X), \\ \psi_i : I \times \mathcal{O}_S &\longrightarrow \mathbb{R}, & \psi_i(t, X) &= \mathrm{D}_1 \phi_i(t, X), \end{aligned}$$

where D_k denotes the first derivative with respect to the k-th argument. By definition of $t_*^{(i)}$, see (4.2), it holds that

$$\psi_i\Big(t_*^{(i)}(X), X\Big) \equiv 0.$$

As in the proof of Lemma 3.3, one obtains for $\Omega_i \in \mathfrak{g}_\gamma$

$$\mathrm{D}_1 \psi_i(t, X)\Big|_{(0,Z)} = -2\gamma(Z)^2 \kappa(\Omega_i, \Omega_i) > 0.$$

This holds for all $\gamma \in \Sigma^+$ as S is a regular element. By continuity, $\mathrm{D}_1\psi_i(t, X)$ is greater than zero in a neighborhood of $(0, Z) \in I \times \mathcal{O}_S$. Hence the critical value

$$\phi_i(t_*^{(i)}(X), X)$$

is minimal for $X \in U$. This minimum is unique due to Proposition 5.1. Thus the Implicit Function Theorem implies that the functions $t_*^{(i)}$ (4.2) are smooth in a neighborhood U of Z, $i = 1, ..., 2N$.

Let $\xi \in T_Z\mathcal{O}_S = \mathrm{span}(\Omega_1, ..., \Omega_{2N})$, the tangent space of $\mathcal{O}_S$ at Z. Then

$$
\begin{aligned}
\mathrm{D}_2\psi_i(t, X)\Big|_{(0,Z)}\xi &= -2\mathrm{D}_2\kappa(\Omega_i, \mathrm{ad}_{Z_0}Z)\xi \\
&= -2\Big(\kappa(\mathrm{ad}_{\Omega_i}\xi_0, Z) + \kappa(\mathrm{ad}_{\Omega_i}Z_0, \xi)\Big) \\
&= -2\kappa(\mathrm{ad}_{\Omega_i}Z, \xi),
\end{aligned}
\tag{6.1}
$$

as $\xi_0 = \mathrm{p}(\xi) = 0$ and $Z_0 = \mathrm{p}(Z) = Z$. Any partial optimization step within a sweep is described by the mapping

$$
r_i : \mathcal{O}_S \longrightarrow \mathcal{O}_S, \quad X \longmapsto \mathrm{Ad}_{\exp\left(t_*^{(i)}(X)\Omega_i\right)}X.
$$

The derivative of r_i at Z acting on ξ is

$$
\begin{aligned}
\mathrm{D}r_i(Z)\xi &= \mathrm{Ad}_{\exp(t_*^{(i)}(Z)\Omega_i)}\xi + \Big(\mathrm{ad}_{\Omega_i}\mathrm{Ad}_{\exp(t_*^{(i)}(Z)\Omega_i)}(Z)\Big) \circ \mathrm{D}t_*^{(i)}(Z)\xi \\
&= \xi + \mathrm{ad}_{\Omega_i}(Z) \circ \mathrm{D}t_*^{(i)}(Z)\xi.
\end{aligned}
$$

By differentiating the equation

$$
\psi_i\Big(t_*^{(i)}(X), X\Big) \equiv 0
$$

with respect to X in direction ξ, one obtains by the chain rule

$$
\mathrm{D}\psi_i\Big(t_*^{(i)}(Z), Z\Big)\xi = \mathrm{D}_1\psi_i\Big(t_*^{(i)}(Z), Z\Big) \cdot \mathrm{D}t_*^{(i)}(Z)\xi + \mathrm{D}_2\psi_i\Big(t_*^{(i)}(Z), Z\Big)\xi = 0.
$$

Hence

$$
\mathrm{D}t_*^{(i)}(Z)\xi = -\frac{\mathrm{D}_2\psi_i\Big(t_*^{(i)}(Z), Z\Big)}{\mathrm{D}_1\psi_i\Big(t_*^{(i)}(Z), Z\Big)}\xi = -\frac{\kappa(\mathrm{ad}_{\Omega_i}Z, \xi)}{\gamma(Z)^2\kappa(\Omega_i, \Omega_i)}.
$$

The derivative for one partial step of the Jacobi sweep at Z therefore is

$$
\begin{aligned}
\mathrm{D}r_i(Z)\xi &= \xi - \mathrm{ad}_{\Omega_i}Z\frac{\kappa\Big(\mathrm{ad}_{\Omega_i}Z, \xi\Big)}{\gamma(Z)^2\kappa\Big(\Omega_i, \Omega_i\Big)} \\
&= \xi - \gamma(Z)\overline{\Omega}_i\frac{\kappa\Big(\gamma(Z)\overline{\Omega}_i, \xi\Big)}{\gamma(Z)^2\kappa\Big(\Omega_i, \Omega_i\Big)} \\
&= \xi - \overline{\Omega}_i\frac{\kappa\Big(\overline{\Omega}_i, \xi\Big)}{\kappa\Big(\Omega_i, \Omega_i\Big)},
\end{aligned}
$$

where $\Omega_i \in \mathfrak{g}_\gamma$. It is easily seen that $\mathrm{D}r_i(Z)$ is a projection that annihilates the $\overline{\Omega}_i$-component of $\xi \in T_Z\mathcal{O}_S$. By the chain rule and the fact that Z is a fixed point of each partial step, i.e., $r_i(Z) = Z$ for all i, one calculates the derivative of one entire sweep operation

$$s(X) := \big(r_{2n} \circ r_{2n-1} \circ \cdots \circ r_2 \circ r_1\big)(X),$$

evaluated at the fixed point Z as

$$\mathrm{D}s(Z)\xi = \big(\mathrm{D}r_{2n} \circ \cdots \circ \mathrm{D}r_1\big)(Z)\xi = 0, \quad \text{therefore} \quad \mathrm{D}s(Z) \equiv 0. \tag{6.2}$$

Now choose open, relatively compact neighborhoods U, V of Z in $\mathcal{O}_S$, such that $s(U) \subset V$. U, V are diffeomorphic to open subsets of $\mathbb{R}^{2N}$ where $2N = \dim \mathcal{O}_S$. Without loss of generality, we may assume that U, V are open, bounded subsets of $\mathbb{R}^{2N}$. Reformulating everything in local coordinates, from Taylor's theorem, using $\mathrm{D}s(Z) \equiv 0$, we obtain

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

Thus the sequence $(X_k)_{k\in\mathbb{N}}$ generated by the Jacobi algorithm converges quadratically fast to Z.
□

Theorem 6.2 generalizes the local convergence results for the Hermitian eigenvalue problem, [20]. Our proof applies to any cyclic method and is not restricted to what is called a row- or column wise cyclic method. The achieved shape of the "diagonalized" matrix need not necessarily be diagonal, but can be specified by the choice of the torus algebra. Furthermore, the theory is independent of choices of matrix representations of the underlying Lie algebra, hence a variety of structured matrix problems fit well into this setting. Several matrix representations of the classical Lie algebras can be found e.g. in [12].

7. Pseudo Code for the Algorithm. Here we present a Matlab-like pseudo code for the algorithm. Our formulation is sufficiently general such that one can easily adapt the algorithm to any compact Lie algebra. Note that in Section 8, the algorithm is examplified, using the Lie algebra $\mathfrak{sp}(n)$.

Let $\mathfrak{g}$ be a compact Lie algebra, $\mathfrak{t} \subset \mathfrak{g}$ a maximal Abelian subalgebra. Let a Lie algebra element $X \in \mathfrak{g}$ as well as a real root α be given. Denote by $\mathrm{p} : \mathfrak{g} \to \mathfrak{t}$ the orthogonal projection onto the torus algebra $\mathfrak{t}$. Let a basis of the corresponding root space $\mathfrak{g}_\alpha$ be $\{E_\alpha, F_\alpha\}$. Let this basis be normalized such that

$$\alpha(T_\alpha) = 1, \quad \text{where} \quad T_\alpha = [E_\alpha, F_\alpha]. \tag{7.1}$$

Then for $\Omega \in \{E_\alpha, F_\alpha\}$ the algorithm computes a pair $(\sin t, \cos t)$, such that $\exp(t\Omega) X \exp(-t\Omega)$ has no $\overline{\Omega}$-component. For the occurring $\pm$ signs see Section 5. Using standard trigonometric formulas, one obtains for the step size selections $t_*^{(i)}(X)$ (cf. Proposition 5.1) the identities

$$\sin t_*(X) = \pm \mathrm{sign}(\alpha(X_0)) \cdot \frac{c}{\sqrt{\alpha(X_0)^2 + c^2}},$$
$$\cos t_*(X) = \frac{|\alpha(X_0)|}{\sqrt{\alpha(X_0)^2 + c^2}},$$

where c denotes the $\overline{\Omega}$-coefficient of X and $X_0 = \mathrm{p}(X)$ is the orthogonal projection of X into the torus algebra.

Algorithm 1. Partial Step of Jacobi Sweep.

function: $(cos, sin) = \text{elementary.rotation}(X, \Omega)$

Set $c := \overline{\Omega}$-component of X.

Set $S_0 := \mathrm{p}(X)$.

if $\alpha(X_0) \neq 0$

$$\text{Set } (cos, sin) := \left(\frac{|\alpha(X_0)|}{\sqrt{\alpha(X_0)^2 + c^2}},\ \pm\text{sign}(\alpha(X_0)) \cdot \frac{c}{\sqrt{\alpha(X_0)^2 + c^2}} \right).$$

else

if $c \neq 0$

Set $(cos, sin) := (0, 1)$.

else

Set $(cos, sin) := (1, 0)$.

endif

endif

end elementary.rotation

Denote by N the number of real roots and let

$$\mathfrak{B} = \{\Omega_1, \Omega_2, ..., \Omega_{2N}\}$$

be a basis of $\mathfrak{g}/\mathfrak{t}$ as in (4.1) normalized as in (7.1). Denote the real root corresponding to the basis $\Omega_{2i-1}, \Omega_{2i}$ by α_i and let f denote the cost function (3.2a). Given a Lie algebra element $S \in \mathfrak{g}$ and a tolerance $tol > 0$, this algorithm overwrites S by gSg^{-1} where $g \in \exp(\mathfrak{g})$ and $f(gSg^{-1}) \leq tol$.

Algorithm 2. Jacobi Algorithm.

Set $g :=$ identity matrix.

while $f(S) > tol$

for $i = 1 : N$

$(cos, sin) := \text{elementary.rotation}(S, \Omega_{2i-1})$.

$r_1 := \exp(t_*(S)\Omega_{2i-1})$.

$S := r_1 S r_1^{-1}$.

$(cos, sin) := \text{elementary.rotation}(S, \Omega_{2i})$.

$r_2 := \exp(t_*(S)\Omega_{2i})$.

$S := r_2 S r_2^{-1}$.

$g := r_2^{-1} r_1^{-1} g$.

endfor

endwhile

Note that by choosing a suitable basis $\mathfrak{B}$, it is not necessary to compute the expressions $\exp(t_*(S)\Omega)$ but rather to construct the matrix r by replacing the required entries in the identity matrix by the computed *cos* or *sin*, respectively.

8. Numerical experiments. We illustrate the approach by considering the task of finding the eigenvalues of a skew-Hermitian, Hamiltonian matrix. As mentioned before, the set of skew-Hermitian, Hamiltonian matrices forms the compact Lie algebra $\mathfrak{sp}(n)$, see Example 2.5. This Lie algebra can be identified with the Lie algebra $\mathfrak{u}(n, \mathbb{H})$

of unitary quaternionic $(n \times n)$-matrices. Note that if λ is an eigenvalue of a Hamiltonian matrix, then so is $-\lambda$. Hence the eigenvalues of a skew-Hermitian, Hamiltonian matrix are purely imaginary and if $\mathrm{i}\lambda_k \neq 0$ is a (purely imaginary) eigenvalue, so is $-\mathrm{i}\lambda_k$. Although our previous theory is coordinate free and independent of the choice of matrix representations, choosing explicit descriptions for the Lie algebra elements, leads to different forms of the numerical algorithm. To illustrate this phenomenon, consider the Lie algebra $\mathfrak{sp}(n)$. $\mathfrak{sp}(n)$ has different isomorphic matrix representations, such as e.g.

$$\mathfrak{sp}(n) = \left\{ \begin{bmatrix} A & B \\ -\overline{B} & \overline{A} \end{bmatrix} \in \mathbb{C}^{2n\times 2n} \mid A^* = -A, B^\top = B \right\},$$

or as in the example below. There are various natural choices for a torus algebra of $\mathfrak{sp}(n)$, e.g.,

$$\begin{aligned} \mathfrak{t} &= \left\{ \begin{bmatrix} \mathrm{i}\Lambda & 0 \\ 0 & -\mathrm{i}\Lambda \end{bmatrix} \mid \Lambda \in \mathbb{R}^{n\times n} \text{ is diagonal} \right\} \\ \mathfrak{t}' &= \left\{ \begin{bmatrix} 0 & \Lambda \\ -\Lambda & 0 \end{bmatrix} \mid \Lambda \in \mathbb{R}^{n\times n} \text{ is diagonal} \right\} \\ \mathfrak{t}'' &= \left\{ \begin{bmatrix} 0 & \mathrm{i}\Lambda \\ \mathrm{i}\Lambda & 0 \end{bmatrix} \mid \Lambda \in \mathbb{R}^{n\times n} \text{ is diagonal} \right\}, \end{aligned}$$

leading to isomorphic variants of the eigenvalue problem. More matrix representations of classical Lie algebras can be found in [12].

As a computational example, we consider the eigenvalue problem for an isomorphic copy of $\mathfrak{sp}(n)$. Thus let

$$\begin{aligned} \mathfrak{g} = \Bigg\{ &\begin{bmatrix} A & B & C & D \\ -B & A & D & -C \\ -C & -D & A & B \\ -D & C & -B & A \end{bmatrix} ; A, B, C, D \in \mathbb{R}^{n\times n} \mid \\ &A^\top = -A, B^\top = B, C^\top = C, D^\top = D \Bigg\}. \end{aligned} \tag{8.1}$$

Note that $\mathfrak{g}$ is isomorphic to $\mathfrak{sp}(n)$ via the real Lie algebra isomorphism

$$\rho : \mathfrak{sp}(n) \longrightarrow \mathfrak{g}, \qquad X \longmapsto \begin{bmatrix} \mathrm{Re}X & \mathrm{Im}X \\ -\mathrm{Im}X & \mathrm{Re}X \end{bmatrix}. \tag{8.2}$$

Let $\otimes$ denote the Kronecker product. The torus algebra of $\mathfrak{g}$ is chosen as

$$\mathfrak{t} = \left\{ \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \otimes C_{\mathrm{diag}} \mid C_{\mathrm{diag}} \in \mathbb{R}^{n\times n} \text{ is diagonal} \right\}. \tag{8.3}$$

If $\pm\mathrm{i}\lambda_k$ are the eigenvalues of the skew-Hermitian, Hamiltonian matrix, the entries of the diagonal matrix C_{diag} in (8.3) consist of the λ_k's. Let $C_{\mathrm{diag}} = \mathrm{diag}(\lambda_1, ..., \lambda_n)$. With the assumptions above one computes the n^2 real roots as

$$\boxed{\begin{aligned}&\lambda_i - \lambda_j, \quad 1 \le i < j \le n,\\[1em]&\lambda_i + \lambda_j, \quad 1 \le i \le j \le n.\end{aligned}}$$

Hence the matrices are regular in the sense of Definition 6.1 if and only if the moduli of the λ_k's are pairwise distinct and $\lambda_k \neq 0$ for all k.

Let $E_{ij} \in \mathbb{R}^{n\times n}$ have (i,j)-entry equal to 1 and 0 elsewhere. As an orthogonal basis for the corresponding real root spaces that satisfies condition (7.1), choose

$$\mathfrak{B}_{\lambda_i-\lambda_j} = \left\{ \frac{1}{2}\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{bmatrix} \otimes (E_{ij}-E_{ji}),\ \frac{1}{2}\begin{bmatrix}0&0&1&0\\0&0&0&-1\\-1&0&0&0\\0&1&0&0\end{bmatrix} \otimes (E_{ij}+E_{ji}) \right\}$$

$$\mathfrak{B}_{\lambda_i+\lambda_j} = \left\{ \frac{1}{2}\begin{bmatrix}0&1&0&0\\-1&0&0&0\\0&0&0&1\\0&0&-1&0\end{bmatrix} \otimes (E_{ij}+E_{ji}),\ \frac{1}{2}\begin{bmatrix}0&0&0&1\\0&0&1&0\\0&-1&0&0\\-1&0&0&0\end{bmatrix} \otimes (E_{ij}+E_{ji}) \right\}$$

Then we obtain an ordered basis $\mathfrak{B}$ of $\mathfrak{sp}(n)/\mathfrak{t}$ as in (4.1) via

$$\mathfrak{B} = \bigcup_{1\le i<j\le n} \mathfrak{B}_{\lambda_i-\lambda_j} \cup \bigcup_{1\le i\le j\le n} \mathfrak{B}_{\lambda_i+\lambda_j} \tag{8.4}$$

Now let $X \in \mathfrak{g}$ in the chosen representation (8.1). Let Ω_k be the k-th element in $\mathfrak{B}$, cf. (8.4). Denote by $X_{[r,s]}$ the (r,s)-entry of X. Then the algorithms of Section 7 are explicitly as follows.

Algorithm 1'. Partial Step of Jacobi Sweep.

function: $(cos, sin) = \text{aux.func}(c)$
- **if** $c \neq 0$
  - Set $(cos, sin) := (0, 1)$.
- **else**
  - Set $(cos, sin) := (1, 0)$.
- **endif**

end aux.func

function: $(cos, sin) = \text{elementary.rotation}(X, \Omega_k)$
- **if** $1 \le k \le n^2 - n$
  - Set $\alpha(X_0) := X_{[i,2n+i]} - X_{[j,2n+j]}$.
  - **if** k is odd
    - Set $c := 2X_{[i,2n+j]}$.
    - **if** $\alpha(X_0) \neq 0$
      - Set $(cos, sin) := \left(\frac{|\alpha(X_0)|}{\sqrt{\alpha(X_0)^2 + c^2}},\ \text{sign}(\alpha(X_0)) \cdot \frac{c}{\sqrt{\alpha(X_0)^2 + c^2}} \right)$.
    - **else**
      - Set $(cos, sin) := \text{aux.func}(c)$.
    - **endif**
  - **else**

Set $c := 2X_{[i,j]}$.
if $\alpha(X_0) \neq 0$
Set $(cos, sin) := \left(\frac{|\alpha(X_0)|}{\sqrt{\alpha(X_0)^2 + c^2}}, \; -\text{sign}(\alpha(X_0)) \cdot \frac{c}{\sqrt{\alpha(X_0)^2 + c^2}} \right)$.
else
Set (cos, sin) :=aux.func(c).
endif
endif
else
Set $\alpha(X_0) := X_{[i,2n+i]} + X_{[j,2n+j]}$.
if k is odd
Set $c := 2X_{[i,3n+j]}$.
if $\alpha(X_0) \neq 0$
Set $(cos, sin) := \left(\frac{|\alpha(X_0)|}{\sqrt{\alpha(X_0)^2 + c^2}}, \; \text{sign}(\alpha(X_0)) \cdot \frac{c}{\sqrt{\alpha(X_0)^2 + c^2}} \right)$.
else
Set (cos, sin) :=aux.func(c).
endif
else
Set $c := 2X_{[i,n+j]}$.
if $\alpha(X_0) \neq 0$
Set $(cos, sin) := \left(\frac{|\alpha(X_0)|}{\sqrt{\alpha(X_0)^2 + c^2}}, \; -\text{sign}(\alpha(X_0)) \cdot \frac{c}{\sqrt{\alpha(X_0)^2 + c^2}} \right)$.
else
Set (cos, sin) :=aux.func(c).
endif
endif
endif
end elementary.rotation

Given a Lie algebra element $S \in \mathfrak{g}$ and a tolerance $tol > 0$, the following algorithm overwrites S by $gSg^\top$ where $g \in \exp(\mathfrak{g})$. Since the Killing form on $\mathfrak{g}$ is given by

$$\kappa(X, Y) = 4(n+1)\text{tr}(XY),$$

the cost function (3.2a) is

$$f(S) = -4(n+1)\text{tr}\Big((S - S_0)^2\Big),$$

where S_0 denotes the projection of S onto $\mathfrak{t}$.

Algorithm 2'. Jacobi Algorithm.
Set $g :=$ identity matrix.
while $f(S) > tol$
for $k = 1 : n^2$
$(cos, sin) :=$ elementary.rotation(S, Ω_k).
Set $r := \exp(t_*(S)\Omega_k)$.
Set $g := r^\top g$.

endfor
endwhile

Note that the matrix $\exp(t_*(S)\Omega_k)$ need not be calculated explicitly, but can easily be constructed as it holds

$$\exp\left(\begin{bmatrix} 0 & t \\ -t & 0 \end{bmatrix}\right) = \begin{bmatrix} \cos t & \sin t \\ -\sin t & \cos t \end{bmatrix},$$

and the Ω_k's only consists of such blocks.

Finally, some numerical experiments are presented which are compatible with local quadratic convergence. All simulations are done using Mathematica 4.0, cf. [38]. For a given torus algebra element T, the initial point S is generated in the following way. Let $\Omega_k \in \mathfrak{B}$, cf. (4.1), an ordered basis of $\mathfrak{g}$, where $n := 15$. Then $\dim \mathfrak{g} = 465$ real values $t_1, ..., t_{465} \in [-\pi, \pi]$ are chosen by using the Mathematica-command Random. A generic group element g is generated via

$$g = \prod_{k=1}^{465} \exp(t_k \Omega_k).$$

The initial point S is obtained by conjugating T with g, namely $S = gTg^\top$. Every experiment is done with three different randomly chosen initial points, plotted together in one diagram where the value of the cost function is on the vertical axes. The following simulations have been done.

Fig. 8.1	$C_{\text{diag}} = (1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15)$
Fig. 8.2	$C_{\text{diag}} = (96, 97, 97.5, 98, 98.5, 99, 99.5, 100, 100.5, 101, 101.5, 102, 102.5, 103, 104)$
Fig. 8.3	$C_{\text{diag}} = (0, 0, 0, 10, 10, 10, 20, 20, 20, 30, 30, 30, 40, 40, 50)$
Fig. 8.4	$C_{\text{diag}} = (99.9998, 100.001, 100.0002, 100.03, 100.002, 100.001, 99.997, -0.002, 0.01, 0.2, -0.03, -0.001, 0.01, 0.002, 0.0001)$

For the simulation in Fig. 8.2, the absolute values of all eigenvalues are close to 100. Nonregular elements show the same convergence behavior, cf. Fig. 8.3. Fig. 8.4 illustrates the convergence behavior of the algorithm in the case when there is a gap between the eigenvalues.

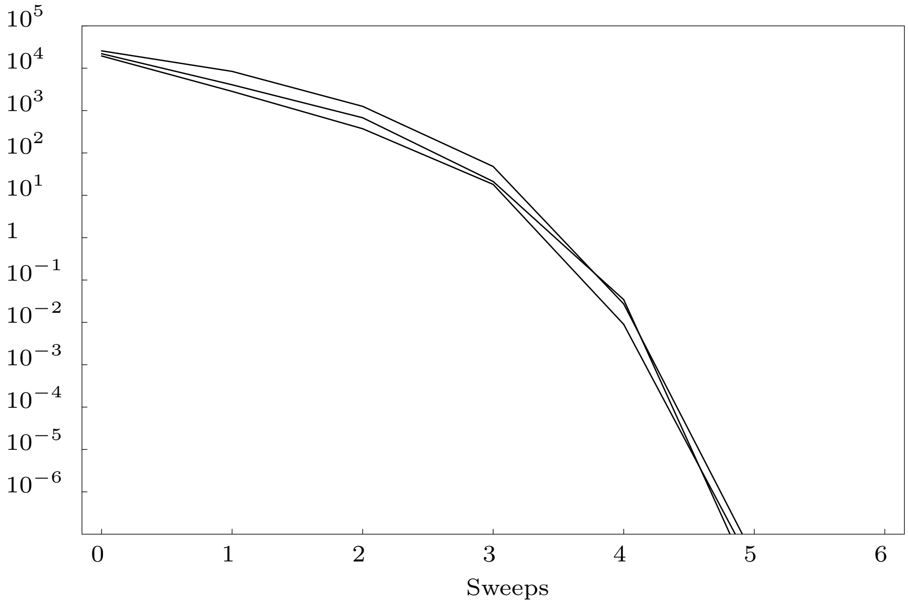

FIG. 8.1. *Convergence behavior for a regular element.* $\dim \mathfrak{g} = 465$, $f = -\kappa(X - X_0, X - X_0)$.

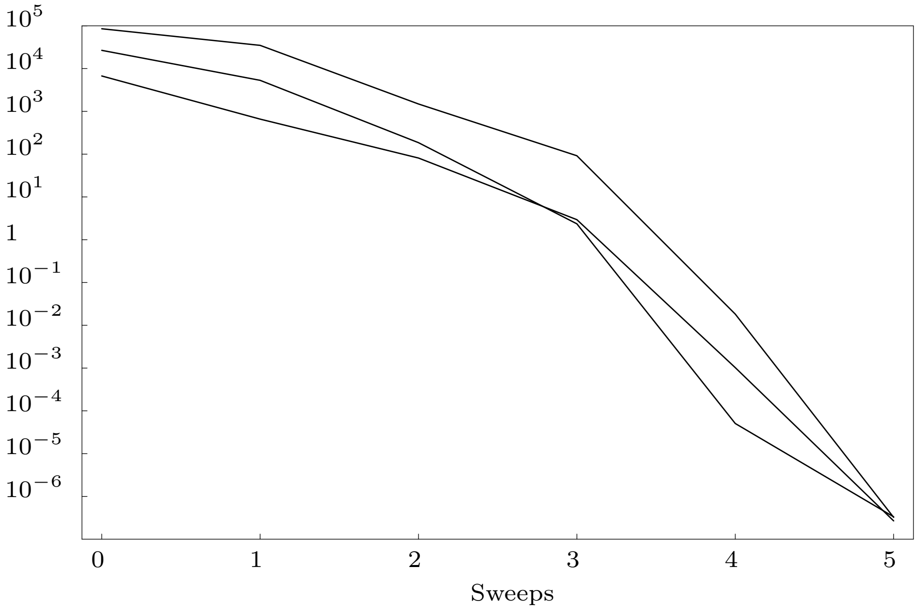

FIG. 8.2. *Convergence behavior for an element with eigenvalues near* 100, −100 *resp.* $\dim \mathfrak{g} = 465$, $f = -\kappa(X - X_0, X - X_0)$.

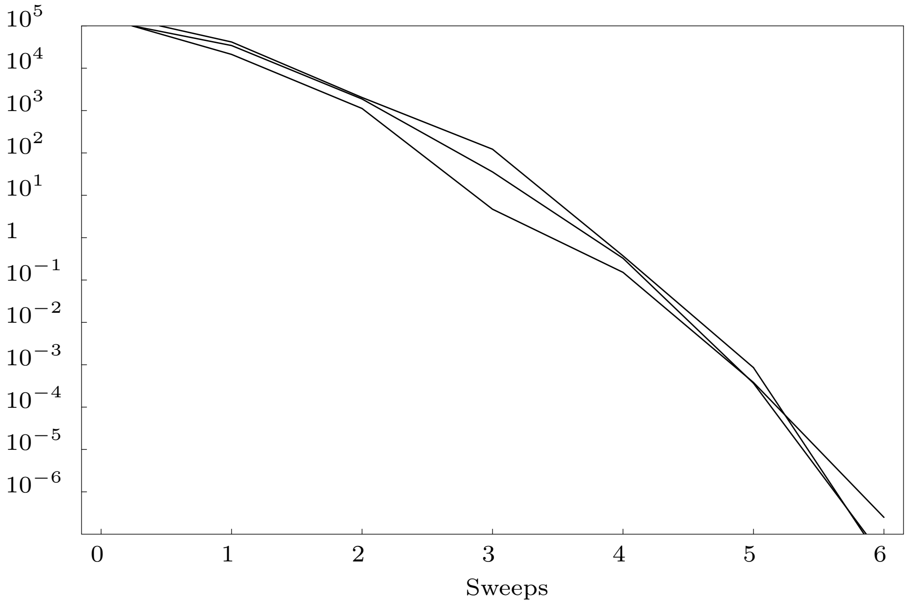

FIG. 8.3. *Convergence behavior for a nonregular element.* $\dim \mathfrak{g} = 465$, $f = -\kappa(X - X_0, X - X_0)$

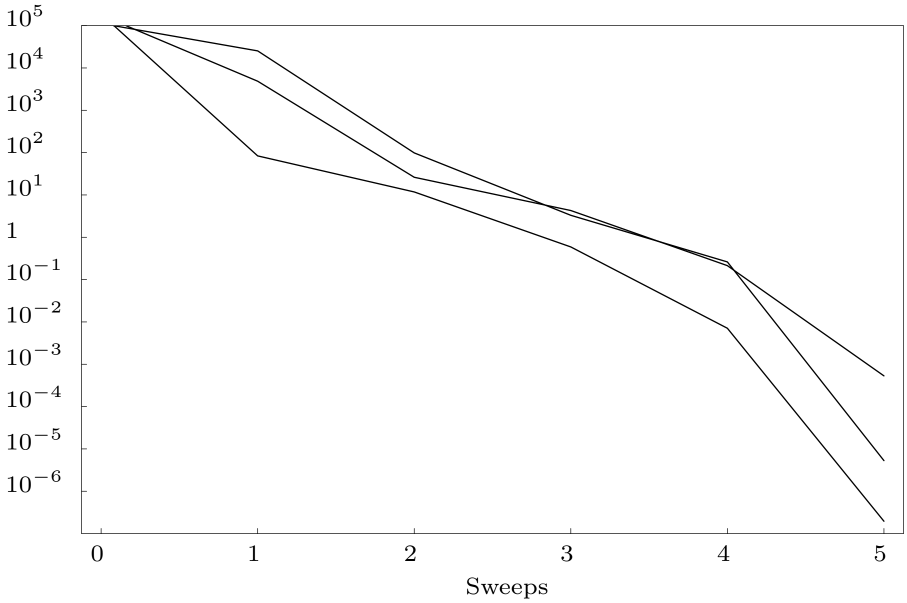

FIG. 8.4. *Convergence behavior for an element with a gap between great and small eigenvalues.* $\dim \mathfrak{g} = 465$, $f = -\kappa(X - X_0, X - X_0)$

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