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# Gradient Flows Computing the $C$-numerical Range with Applications in NMR Spectroscopy ⋆

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**Abstract.** In this paper gradient flows on unitary matrices are studied that maximize the real part of the $C$-numerical range of an arbitrary complex $n \times n$-matrix $A$. The geometry of the $C$-numerical range can be quite complicated and is only partially understood. A numerical discretization scheme of the gradient flow is presented that converges to the set of critical points of the cost function. Special emphasis is taken on a situation arising in NMR spectroscopy where the matrices $C$, $A$ are nilpotent and the $C$-numerical range is a circular disk in the complex plane around the origin.

**Key words:** $C$-numerical range, Optimization, Gradient flows, Discretization, NMR spectroscopy, Nilpotent matrices

## 1. Introduction

The $C$-numerical range and the $C$-numerical radius were introduced by Goldberg and Straus [9] as generalisations of the classical numerical range $W(A)$ and radius $r(A)$, respectively. Let $U(n, \mathbb{C})$ denote the compact Lie group of all unitary complex $n \times n$-matrices $U \in \mathbb{C}^{n\times n}$ satisfying $UU^\dagger = I_n$, where $U^\dagger = \overline{U}^\top$ denotes Hermitian conjugate, i.e., complex conjugate transpose. For arbitrary complex matrices $C$, $A \in \mathbb{C}^{n\times n}$ the *$C$-numerical range* of $A$ is the subset of the complex plane defined as

$$W(C, A) := \left\{ \operatorname{tr}(C^\dagger U A U^\dagger) \middle| U \in U(n, \mathbb{C}) \right\}. \tag{1}$$

Unlike the usual numerical range $W(A)$ of $A$, where $C$ is a rank one Hermitian projection operator and $W(A)$ is convex, the geometry of the $C$-numerical range can be quite complicated and is only partially understood. See, e.g., the special issue [1] for a collection of papers on the $C$-numerical range.

From (1) it is easily seen that $W(C, A)$ is invariant under unitary similarities of $A$ and $C$. Furthermore, $W(C, A)$ is the continuous image of $U(n, \mathbb{C})$ and therefore

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is compact and connected. Moreover, $W(C, A)$ is star like with respect to the point $(\operatorname{tr} C^\dagger)(\operatorname{tr} A)/n$ (see [6]).

In general, $W(C, A)$ is not convex but even if it is, then sharp estimates on the size of $W(C, A)$ are unknown. It is therefore desirable to develop numerical methods that enable one to find sharp bounds on the size of $W(C, A)$. A natural measure of the size of $W(C, A)$ is the so-called *C-numerical radius* of $A$

$$r_C(A) := \max\left\{|\operatorname{tr}(C^\dagger U A U^\dagger)| \middle| U \in U(n, \mathbb{C})\right\}. \tag{2}$$

Thus $r_C(A)$ is the smallest radius of disks centered at the origin containing $W(C, A)$. An upper bound for the $C$-numerical radius $r_C(A)$ is due to von Neumann, see [9, 18], as

$$r_C(A) \leq \|A\|_C, \tag{3}$$

where

$$\|A\|_C = \max_{V,W} \left|\operatorname{tr}(V A W C^\dagger)\right| \leq \sum_i \sigma_i(A)\sigma_i(C), \qquad V, W \in U(n, \mathbb{C}) \tag{4}$$

denotes the *C-spectral norm*, and $\sigma_i(A)$ and $\sigma_i(C)$ denote the singular values of $A$ and $C$ ordered in descending magnitude, respectively. Equality is reached if $A$ and $C$ are normal. Alternatively, one can consider the smallest sizes of rectangular boxes containing $W(C, A)$. This leads to the problem of finding the smallest/largest real and imaginary parts of points in the $C$-numerical range, i.e., the boundary points of the compact intervals

$$\begin{aligned} \Re(W(C, A)) &:= \{\Re(\operatorname{tr}(C^\dagger U A U^\dagger))|U \in U(n, \mathbb{C})\}, \\ \Im(W(C, A)) &:= \{\Im(\operatorname{tr}(C^\dagger U A U^\dagger))|U \in U(n, \mathbb{C})\}. \end{aligned} \tag{5}$$

In [2] the boundary $\partial W(C, A)$ of the $C$-numerical range for normal $A$ and $C$ is studied. The authors classify points of $\partial W(C, A)$ by regularity, i.e., via their degree of smoothness. Except for the heuristic approach outlined in [8] there is to the best of our knowledge no reported constructive method for computing $\partial W(C, A)$ in the general case.

Since

$$\Im(W(C, A)) = \Re(W(\mathrm{i}C, A)), \quad \mathrm{i} := \sqrt{-1}$$

we focus on the task of optimizing the smooth function

$$\begin{aligned} f : U(n, \mathbb{C}) &\to \mathbb{R}, \\ f(U) &= \Re(\operatorname{tr}(C^\dagger U A U^\dagger)). \end{aligned} \tag{6}$$

We approach the problem of optimizing the function $f$ by designing a suitable gradient flow, see also [8] for a similar approach. A discretization of the gradient flow is given that leads to a numerical algorithm of finding the critical points of $f$.

A complete theory is available for Hermitian matrices $C$, $A$ (see [10]). For arbitrary matrices $C$, $A$ the function $f$ may have local minima or local maxima and therefore the gradient algorithm may not always converge to the global maximum. Thus a general critical point analysis of $f$ is difficult and currently out of reach. Nevertheless, the gradient flow approach leads to further insights and may provide, e.g., sometimes good estimates for the maximum, which are hard to achieve otherwise. We illustrate this by studying the gradient flow for special choices of nilpotent matrices $C$, $A$.

The maximization task for $f$ as a means to assess $r_C(A)$ also arises in a natural way in physics: It amounts to maximizing the generalised quantum mechanical expectation value governing the signal intensity in coherent ensemble spectroscopy. Here we show that our methods lead to state of the art theoretical bounds in nuclear magnetic resonance (NMR) spectroscopy. See [5, 8] for parallel efforts to tackle related problems.

First, while recalling some definitions of quantum mechanics we relate the generalised notions of a quantum mechanical expectation value and the $C$-numerical range. In cases relevant to the dynamics of spin-1/2 particles, the aim is to determine its extremal point, the $C$-numerical radius, see (2).

### (I) QUANTUM MECHANICS OF CLOSED SYSTEMS

Usually, a state of a closed quantum system is represented by a *state vector* $\psi(t)$, i.e., by an element of a Hilbert space $\mathcal{H}$. In multi-body problems, the total Hilbert space is composed by taking the tensor product over all the single particle ones $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots$. A quantum mechanical *observable* $X = X^\dagger$ is a linear selfadjoint operator on $\mathcal{H}$, and its *expectation value* $\langle X \rangle$ then takes the form of a scalar product on $\mathcal{H}$, the linear functional $\langle X \rangle_\psi = \langle \psi | X\psi \rangle$.

Moreover, if $U(t) \in U(\mathcal{H})$ is a one-parameter group of unitary operators on a Hilbert space $\mathcal{H}$, then there is a linear self-adjoint operator $H$ on $\mathcal{H}$ called the *Hamiltonian* which generates the unitary group by $U(t) = \mathrm{e}^{-\mathrm{i}tH}$ (Stone's theorem). This accounts for the deterministic part of quantum mechanical time evolution solving Schrödinger's equation of motion

$$\mathrm{i}\frac{\partial}{\partial t}\ \psi(t) = H\ \psi(t) \tag{7}$$

by $U(t) = \mathrm{e}^{-\mathrm{i}tH}$ such as to give

$$\psi(t) = U(t)\ \psi(0). \tag{8}$$

### (II) QUANTUM MECHANICS OF ENSEMBLES

In ensembles or in open quantum systems, a state is represented by a selfadjoint non-negative linear operator normalised to a trace of one: it is called a *density*

*operator* $D$ [19]. Then $D = D^\dagger \geq 0$ (i.e., the scalar product $\langle\psi|D\psi\rangle \geq 0$ for all $\psi \in \mathcal{H}$) and $\operatorname{tr} D = 1$. If $D^2 = D$ then $D$ represents a *pure state*, otherwise a *non-pure state*. Only pure states can be written as dyadic products $|\psi\rangle\langle\psi|$, whereas non-pure ones are non-trivial convex (i.e., trace-preserving) linear combinations of pure ones (giving coherent superpositions). Non-pure states are generic in open quantum systems or ensembles.

Nevertheless, the immediate analogue to Schrödinger's equation of motion reads

$$\mathrm{i}\frac{\partial}{\partial t}\, D(t) = [H, D(t)] \tag{9}$$

with the solution

$$D(t) = U(t)\, D(0)\, U(t)^\dagger. \tag{10}$$

Hamiltonian time evolution is reversible; it induces an automorphism on the algebra of observables.

### (III) RELATION TO C-NUMERICAL RANGE

In view of later applications, we now generalise the traditional concepts of expection values $\langle X\rangle_D = \operatorname{tr}(UDU^\dagger X)$ and substitute the selfadjoint operators $D$, $X$ by two elements $A$, $C$ that are no longer necessarily selfadjoint. $A$ and $C$ may thus collect 'some experimentally relevant terms' from states $D$ or observables $X$. The generalised expectation value $\langle C\rangle_A = \operatorname{tr}(UAU^\dagger C^\dagger)$ then is an element of the C-numerical range of A, the largest absolute value of which is the $C$-numerical radius of A.

In physical terms, the $C$-numerical radius determines the largest (absolute) generalised expectation value. Therefore it is of important significance to the experimentalist: It specifically defines the maximum achievable projection under unitary transfer of signal-relevant components $A$ from a given initial quantum state onto the signal-relevant components $C^\dagger$ of a given observable.

As already mentioned above, little is known when it comes to explicitely calculating either the $C$-numerical radius $r_C(A)$ or $\Re(\operatorname{tr}(C^\dagger UAU^\dagger))$ for non-normal complex square matrices $A, C$, see also [12], as occuring in problems of physics. Then the maximum transfer determined by $\max_{U(n,\mathbb{C})} \Re(\operatorname{tr}(C^\dagger UAU^\dagger))$ (respectively, $r_C(A)$) can actually be obtained, provided the entire pertinent special unitary group is generated by experimentally accessible system Hamiltonians. It can be shown constructively that under mild conditions, this is the case in spin-1/2 systems [15]. So, for optimizing experiments in many kinds of coherent ensemble spectroscopy, the knowledge of maximum values is of considerable interest.

We emphasize that the matrices $A$ and $C$ in our application are always finite dimensional. For the NMR applications we have in mind only $N$-spin-1/2 systems are relevant, i.e., the matrices $A, C \in \mathbb{C}^{2^N \times 2^N}$.

## 2. Gradient flows for the $C$-numerical range

Before analyzing the specific situation of interest in NMR spectroscopy, we first derive some general results concerning the $C$-numerical range for arbitrary matrices. Thus let $C$, $A$ be arbitrary and

$$W(C, A) := \{\mathrm{tr}\,(C^\dagger U A U^\dagger) | U \in U(n, \mathbb{C})\}. \tag{11}$$

Recall that the set $U(n, \mathbb{C})$ of complex unitary matrices is a compact connected Lie group of real dimension $n^2$. The tangent space of $U(n, \mathbb{C})$ at an element $U$ is

$$T_U U(n, \mathbb{C}) = \{\Omega U | \Omega^\dagger = -\Omega\}. \tag{12}$$

In particular, the tangent space of $U(n, \mathbb{C})$ at the identity element $I$ is the Lie algebra

$$\mathfrak{u}(n, \mathbb{C}) := \{\Omega \in \mathbb{C}^{n\times n} | \Omega^\dagger = -\Omega\} \tag{13}$$

of all skew-Hermitian matrices. In the sequel, we will endow $U(n, \mathbb{C})$ with its bi-invariant Riemannian metric defined on the tangent spaces $T_U U(n, \mathbb{C})$ as

$$\langle \Omega_1 U, \Omega_2 U\rangle := \Re(\mathrm{tr}\,(\Omega_1^\dagger \Omega_2)). \tag{14}$$

The next lemma characterizes the critical points of the map $q : U(n, \mathbb{C}) \to \mathbb{R}^2$ with image $q(U(n, \mathbb{C})) = W(C, A)$

$$\begin{aligned} q &: U(n, \mathbb{C}) \to \mathbb{R}^2, \\ U &\mapsto \Big(\Re(\mathrm{tr}\,(C^\dagger U A U^\dagger)), \Im(\mathrm{tr}\,(C^\dagger U A U^\dagger))\Big), \end{aligned} \tag{15}$$

for fixed but arbitrary square and complex matrices $A, C$.

LEMMA 2.1 *[7].Let $q$ be def ined by (15). Then*
*(a) The tangent map* $\mathrm{D}q(U) : T_U U(n, \mathbb{C}) \to \mathbb{R}^2$ *is given by*

$$\mathrm{D}q(U)(\Omega U) = \Big(\Re(\mathrm{tr}\,(\Omega[B, C^\dagger]), \Im(\mathrm{tr}\,(\Omega[B, C^\dagger]))\Big),$$

*where* $\Omega U \in T_U U(n, \mathbb{C})$, $\Omega = -\Omega^\dagger$, *and* $B := U A U^\dagger$.
*(b) The rank of $q$ at $U$ is*

$$\mathrm{rk}_U(q) = \dim \mathrm{lin}\,(W([B, C^\dagger])),$$

*where* $\mathrm{lin}\,(S)$ *denotes the linear subspace of* $\mathbb{R}^2$ *generated by the subset* $S \subset \mathbb{R}^2$ *and* $W(Z)$ *is the classical numerical range defined by*

$$W(Z) := \{x^\dagger Z x | x \in \mathbb{C}^n, \|x\| = 1\}.$$

□

COROLLARY 2.1 *Sharp points in $W(C, A)$, i.e., the values $q(U)$ of critical points $U$ having rank zero derivative are characterized by* $[UAU^\dagger, C^\dagger] = 0$. □

We now investigate a measure of size of the $C$-numerical range.

## 2.1. EUCLIDEAN DISTANCE FUNCTION

For any $U \in U(n, \mathbb{C})$ the Euclidean distance between $C$ and $UAU^\dagger$ is

$$\|C - UAU^\dagger\|^2 = \|C\|^2 + \|A\|^2 - 2\Re(\text{tr}\,(C^\dagger UAU^\dagger)), \tag{16}$$

where here and in the sequel $\|\cdot\|$ always means the Frobenius norm, i.e., $\|C\| = \sqrt{\text{tr}\,(CC^\dagger)}$. Thus minimizing the distance between $C$ and $UAU^\dagger$ is the same as maximizing the trace function $f : U(n, \mathbb{C}) \to \mathbb{R}$, defined by (6). Let

$$X = X_+ + X_- = \frac{X + X^\dagger}{2} + \frac{X - X^\dagger}{2} \tag{17}$$

denote the unique decomposition of $X \in \mathbb{C}^{n\times n}$ into Hermitian part $X_+$ and skew-Hermitian part $X_-$. Let

$$[A, B] := AB - BA \tag{18}$$

denote the commutator. Then

$$[A, B]_- = \frac{[A, B] + [A^\dagger, B^\dagger]}{2}. \tag{19}$$

The gradient flow appearing in the next theorem has been first used in [8] as a means to optimize $f$.

THEOREM 2.1 *The gradient flow of $f : U(n, \mathbb{C}) \to \mathbb{R}$ defined by (6) with respect to the bi-invariant Riemannian metric (14) is given from the gradient*

$$\text{grad}\, f(U) = [C^\dagger, UAU^\dagger]_- U \tag{20}$$

*as*

$$\begin{aligned} \dot{U} &= \text{grad}\, f(U) \\ &= [C^\dagger, UAU^\dagger]_- U \\ &= \tfrac{1}{2}(C^\dagger UA + CUA^\dagger - UAU^\dagger C^\dagger U - UA^\dagger U^\dagger CU). \end{aligned} \tag{21}$$

*Every solution of (21) exists in $U(n, \mathbb{C})$ for all $t \in \mathbb{R}$ and converges for $t \to \pm\infty$ to a critical point. The critical points of $f$ are characterized as*

$$[C^\dagger, UAU^\dagger] = [C^\dagger, UAU^\dagger]^\dagger. \tag{22}$$

**Proof.** The Fréchet derivative of $f$ at $U \in U(n,\mathbb{C})$ is the linear map on the tangent space $T_U U(n,\mathbb{C})$ defined by

$$\begin{aligned} \mathrm{D}f(U)(\Omega U) &= \Re(\mathrm{tr}\,(C^\dagger[\Omega, UAU^\dagger])) \\ &= \Re(\mathrm{tr}\,([UAU^\dagger, C^\dagger]\Omega)) \\ &= \mathrm{tr}\,([C^\dagger, UAU^\dagger]_-^\dagger \Omega) \end{aligned} \tag{23}$$

and therefore

$$\mathrm{grad}\, f(U) = [C^\dagger, UAU^\dagger]_- U \tag{24}$$

is the gradient. By compactness of $U(n,\mathbb{C})$ the solution of (21) exists for all $t \in \mathbb{R}$ and converges to the set of critical points. Since grad $f$ is a real analytic gradient vector field the pointwise convergence of (21) follows from a result by Łojasiewicz [14]. The result follows. □

Note that the gradient flow (21) tends to maximize the trace function $f : U(n,\mathbb{C}) \to \mathbb{R}$. Moreover, if $C = C^\dagger$ and $A = A^\dagger$ are both Hermitian then the gradient flow simplifies to

$$\dot{U} = [C, UAU^\dagger]U. \tag{25}$$

In this case critical points are characterized as,

$$[C, UAU^\dagger] = 0 \tag{26}$$

because $[C, UAU^\dagger]_- = [C, UAU^\dagger]$ holds. In this simpler situation a complete phase portrait analysis of the gradient flow can be given; see [3] and [10]. The general case studied here is, however, more complicated and not fully understood. If only $C = C^\dagger$ is Hermitian then the flow is seen as equal to

$$\begin{aligned} \dot{U} &= [C^\dagger, U(A + A^\dagger)U^\dagger]_- U \\ &= [C, U(A + A^\dagger)U^\dagger]_- U \\ &= \tfrac{1}{2}\Big([C, U(A + A^\dagger)U^\dagger] - [C, U(A + A^\dagger)U^\dagger]^\dagger\Big)U \\ &= [C, U(A + A^\dagger)U^\dagger]U \end{aligned} \tag{27}$$

and we are reduced to the fully Hermitian case.

Stability properties of the critical points of (21) are expressed in terms of the eigenvalues of the Hessian. To determine the Hessian of $f : U(n,\mathbb{C}) \to \mathbb{R}$ at a critical point $U_\infty \in U(n,\mathbb{C})$, with $A_\infty := U_\infty A U_\infty^\dagger$, one has to compute the second derivative of

$$\phi(t) = \Re(\mathrm{tr}\,(C^\dagger \mathrm{e}^{t\Omega} A_\infty \mathrm{e}^{-t\Omega})) \tag{28}$$

at $t = 0$ for arbitrary $\Omega \in \mathfrak{u}(n,\mathbb{C})$:

$$\phi''(0) = \Re(\mathrm{tr}\,(C^\dagger[\Omega, [\Omega, A_\infty]])). \tag{29}$$

We compute the Hessian bilinear form by the familar polarization process from the quadratic form (29). A straight forward computation shows the following result.

PROPOSITION 2.1 *Let $U_\infty \in U(n,\mathbb{C})$ be a critical point of $f : U(n,\mathbb{C}) \to \mathbb{R}$, $A_\infty := U_\infty A U_\infty^\dagger$, and let*

$$S : \mathfrak{u}(n,\mathbb{C}) \to \mathfrak{u}(n,\mathbb{C})$$

*be the self-adjoint operator defined as*

$$S(\Omega) := [[\Omega, A_\infty], C^\dagger] + [C, [A_\infty^\dagger, \Omega]] + [[\Omega, C], A_\infty^\dagger] + [A_\infty, [C^\dagger, \Omega]].$$

*Then the Hessian of $f$ at $U_\infty$ is given as the symmetric bilinear form*

$$H_f(\Omega_1, \Omega_2) = \frac{1}{4}\mathrm{tr}\,(\Omega_1 S(\Omega_2)).$$

*Moreover,*

$$\frac{1}{2}S(\Omega) = [[\Omega, A_\infty], C^\dagger]_- + [[\Omega, C], A_\infty^\dagger]_-.$$

□

## 3. Discretization

We now aim at a suitable step size selection to derive an implementable numerical integration scheme for the above differential equation. Standard numerical integration methods such as, e.g., the Euler method are not applicable here as they do not preserve the unitary nature of the solution. The discretization we propose is similar as in [8]

$$U_{k+1} = \exp(\alpha_k [C^\dagger, U_k A U_k^\dagger]_-) U_k \tag{30}$$

yet with a specific step size $\alpha_k \geq 0$ to be determined. See [4, 10] for similar step size selection schemes in different contexts.

THEOREM 3.1 *Let*

$$\alpha_k := \frac{\left\| [C^\dagger, U_k A U_k^\dagger]_- \right\|^2}{\left\| [C^\dagger, [C^\dagger, U_k A U_k^\dagger]_-] \right\| \cdot \left\| [U_k A U_k^\dagger, [C^\dagger, U_k A U_k^\dagger]_-] \right\|}. \tag{31}$$

*Then (30) converges to the set of critical points of $f$.*

**Proof.** For $\Omega := [C^\dagger, B]_-$, $B := U_k A U_k^\dagger$ let

$$\phi(t) := \Re(\mathrm{tr}\,(C^\dagger \mathrm{e}^{t\Omega} B \mathrm{e}^{-t\Omega})). \tag{32}$$

The derivative of $\phi$ is

$$\phi'(t) = \Re(\mathrm{tr}\,([\mathrm{e}^{t\Omega} B \mathrm{e}^{-t\Omega}, C^\dagger]\Omega)) \tag{33}$$

with

$$\begin{aligned} \phi'(0) &= \Re(\mathrm{tr}\,([B, C^\dagger]\Omega)) \\ &= \mathrm{tr}\,([B, C^\dagger]_-\Omega) \\ &= -\mathrm{tr}\,(\Omega^2) \\ &= \|\Omega\|^2 \\ &= \|[C^\dagger, B]_-\|^2 \\ &\geq 0 \end{aligned} \tag{34}$$

and $\phi'(0) = 0$ if and only if $U_k$ is a critical point of $f$. Moreover,

$$\phi''(t) = \Re(\mathrm{tr}\,([C^\dagger, \Omega][\Omega, \mathrm{e}^{t\Omega}B\mathrm{e}^{-t\Omega}])). \tag{35}$$

Therefore, since $\mathrm{e}^{t\Omega}$ is unitary, we have for all $t$

$$\begin{aligned} |\phi''(t)| &\leq \left\|[C^\dagger, \Omega]\right\| \cdot \left\|[\Omega, \mathrm{e}^{t\Omega}B\mathrm{e}^{-t\Omega}]\right\| \\ &= \left\|[C^\dagger, \Omega]\right\| \cdot \left\|\mathrm{e}^{t\Omega}[\Omega, B]\mathrm{e}^{-t\Omega}\right\| \\ &= \left\|[C^\dagger, \Omega]\right\| \cdot \left\|[\Omega, B]\right\|. \end{aligned} \tag{36}$$

By the Mean Value Theorem this implies

$$|\phi'(t) - \phi'(0)| \leq \sup_{0\leq\tau\leq t} |\phi''(\tau)| \cdot t. \tag{37}$$

That is, for

$$t \leq \alpha_k := \frac{\|\Omega\|^2}{\left\|[C^\dagger, \Omega]\right\| \cdot \left\|[\Omega, B]\right\|} \tag{38}$$

then by (36)

$$\begin{aligned} |\phi'(t) - \phi'(0)| &\leq \left\|[C^\dagger, \Omega]\right\| \cdot \left\|[\Omega, B]\right\| \cdot t \\ &\leq \|\Omega\|^2 \\ &= \phi'(0). \end{aligned} \tag{39}$$

This shows that

$$\phi'(t) \geq 0 \quad \text{for} \quad t \in [0, \alpha_k] \tag{40}$$

and therefore $\phi$ is monotonically increasing on $[0, \alpha_k]$. Thus

$$\phi(\alpha_k) \leq \phi(t_*), \tag{41}$$

i.e.,

$$\begin{aligned} 0 &\leq \phi(\alpha_k) - \phi(0) \\ &\leq \phi(t_*) - \phi(0) \end{aligned} \tag{42}$$

with

$$t_* := \arg\max\{\phi(t) | t \geq 0\} \in [0, \infty). \tag{43}$$

Since $e^{t\Omega}$ stays in the compact set $U(n, \mathbb{C})$, $t_*$ exists (although it need not be finite). The result now follows from a familar Lyapunov-type argument, as explained in section 2.3 of [10]. □

In particular the above result holds for all step sizes $0 \leq \alpha \leq \alpha_k$. Thus upper bounds on the denominator in $\alpha_k$ lead to more conservative step size selection schemes.

COROLLARY 3.1 *Convergence of (30) holds for the step size*

$$\alpha_k^* = \frac{\left\| [C^\dagger, U_k A U_k^\dagger]_- \right\|}{2\|A\| \cdot \left\| [C^\dagger, [C^\dagger, U_k A U_k^\dagger]_-] \right\|} \tag{44}$$

*and in particular for the constant step size*

$$\alpha_k^{**} = \frac{1}{4\|A\| \cdot \|C\|}. \tag{45}$$

**Proof.** From

$$\begin{aligned} \left\| [B, \Omega] \right\| &\leq 2\|B\| \cdot \|\Omega\| \\ &= 2\|A\| \cdot \|\Omega\| \end{aligned} \tag{46}$$

we obtain

$$\begin{aligned} \alpha_k^* &= \frac{\|\Omega\|}{2\|A\| \cdot \left\| [C^\dagger, \Omega] \right\|} \\ &\leq \frac{\|\Omega\|^2}{\left\| [C^\dagger, \Omega] \right\| \cdot \left\| [\Omega, B] \right\|} \\ &= \alpha_k. \end{aligned} \tag{47}$$

and similarly

$$\alpha_k^{**} \leq \alpha_k^*. \qquad \square$$

Recently, many of the existing numerical integration schemes which are usually formulated with respect to $\mathbb{R}^n$ were generalized to the Lie group case. That is, if instead on $\mathbb{R}^n$ the solution of a system of ordinary differential equations (ODE) is a smooth curve on a *Lie group*, these new methods also produce iterates living

on the same Lie group. For many applications higher order methods are a good choice, especially if one is interested not only in an equilibrium point of an ODE but also in an approximation of the whole trajectory. Therefore, for our purpose it is completely sufficient to use a first order method, i.e., (30). Higher order methods will have better approximation properties but will be in general slower due to greater computational complexity. For recent work and additional information on Lie methods for numerical integration schemes see [11].

## 4. Special Nilpotent Matrices

In this section, motivated by recent results in NMR spectroscopy of so-called $I_n S$-*spin systems*, see [8] and [15], we consider the optimization task for $f$ defined by (6) for special choices of nilpotent matrices $C$, $A$.

For any $n \in \mathbb{N}$ consider the recursively defined nilpotent $(2^{n+1} \times 2^{n+1})$-matrices

$$\begin{aligned} C_n &:= \begin{bmatrix} 0 & 0 \\ I_{2^n} & 0 \end{bmatrix}, \qquad C_0 := \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \\ A_n &:= \begin{bmatrix} N_n & 0 \\ 0 & N_n \end{bmatrix}, \\ N_n &:= \begin{bmatrix} N_{n-1} & 0 \\ I_{2^{n-1}} & N_{n-1} \end{bmatrix}, \quad N_0 := 0. \end{aligned} \tag{48}$$

Here and in the sequel zero entries stand for zero matrices of appropriate order and $I_n$ stands for the $(n \times n)$-identity matrix. Thus for $n = 1, 2, 3$ we have

$$C_1 = \left[\begin{array}{cc|cc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{array}\right], \quad A_1 = \left[\begin{array}{cc|cc} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{array}\right], \tag{49}$$

$$C_2 = \left[\begin{array}{c|c} 0 & 0 \\ \hline I_4 & 0 \end{array}\right], \quad A_2 = \left[\begin{array}{c|c} \begin{matrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{matrix} & 0 \\ \hline 0 & \begin{matrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{matrix} \end{array}\right], \tag{50}$$

$$C_3 = \left[\begin{array}{c|c} 0 & 0 \\ \hline I_8 & 0 \end{array}\right],$$

$$A_3 = \left[\begin{array}{c|c|c|c} \begin{matrix} 0&0&0&0\\ 1&0&0&0\\ 1&0&0&0\\ 0&1&1&0 \end{matrix} & 0 & 0 & 0 \\ \hline I_4 & \begin{matrix} 0&0&0&0\\ 1&0&0&0\\ 1&0&0&0\\ 0&1&1&0 \end{matrix} & 0 & 0 \\ \hline 0 & 0 & \begin{matrix} 0&0&0&0\\ 1&0&0&0\\ 1&0&0&0\\ 0&1&1&0 \end{matrix} & 0 \\ \hline 0 & 0 & I_4 & \begin{matrix} 0&0&0&0\\ 1&0&0&0\\ 1&0&0&0\\ 0&1&1&0 \end{matrix} \end{array}\right]. \tag{51}$$

Hence,

$$C_n = \begin{bmatrix} 0 & 0 \\ I_{2^n} & 0 \end{bmatrix}, \quad A_n = \left[\begin{array}{c|c} A_{n-1} + C_{n-1} & 0 \\ \hline 0 & A_{n-1} + C_{n-1} \end{array}\right]. \tag{52}$$

LEMMA 4.1 *For* $C = \left[\begin{smallmatrix} 0 & 0 \\ I & 0 \end{smallmatrix}\right]$ *and* $A$ *arbitrary but square the* $C$*-numerical range* $W(C, A)$ *is a circular disk around the origin, i.e.,*

$$W(C, A) = \mathrm{e}^{\mathrm{i}\theta} W(C, A)$$

*for all* $\theta \in \mathbb{R}$.

**Proof.** Note that $C$ is of the so-called block-shift form, therefore Theorem 2.1. in [13] can be applied. □

The critical points of $f : U(2^{n+1}, \mathbb{C}) \to \mathbb{R}$, defined by (6) can be characterized in a somewhat more explicit way.

LEMMA 4.2 *Let* $C = C_n$ *as in (48) and* $A$ *arbitrary but square. Let* $B := UAU^\dagger$ *with* $U \in U(2^{n+1}, \mathbb{C})$. $U$ *is a critical point for* $f$ *if and only if*

$$B = UAU^\dagger = \begin{bmatrix} B_1 & B_2 \\ H & B_1 \end{bmatrix} \tag{53}$$

*with* $H = H^\dagger$ *Hermitian.*

**Proof.** By (22)

$$\begin{aligned} [C^\dagger, B] &= \begin{bmatrix} 0 & I_n \\ 0 & 0 \end{bmatrix} \begin{bmatrix} B_1 & B_2 \\ B_3 & B_4 \end{bmatrix} - \begin{bmatrix} B_1 & B_2 \\ B_3 & B_4 \end{bmatrix} \begin{bmatrix} 0 & I_n \\ 0 & 0 \end{bmatrix} \\ &= \begin{bmatrix} B_3 & B_4 - B_1 \\ 0 & -B_3 \end{bmatrix} \end{aligned}$$

is Hermitian. Therefore $B_4 = B_1$ and $B_3 = B_3^\dagger$ must hold. □

Note that there exists an orthogonal permutation matrix $P$ such that

$$\begin{aligned} PA_nP^\dagger &= P\begin{bmatrix} N_n & 0 \\ 0 & N_n \end{bmatrix} P^\dagger \\ &= P\begin{bmatrix} N_{n-1} & 0 & 0 & 0 \\ I_{2^{n-1}} & N_{n-1} & 0 & 0 \\ 0 & 0 & N_{n-1} & 0 \\ 0 & 0 & I_{2^{n-1}} & N_{n-1} \end{bmatrix} P^\dagger \\ &= \left[\begin{array}{cc|cc} N_{n-1} & 0 & \multicolumn{2}{c}{\multirow{2}{*}{$0$}} \\ 0 & N_{n-1} & & \\ \hline \multicolumn{2}{c|}{\multirow{2}{*}{$I_{2^n}$}} & N_{n-1} & 0 \\ & & 0 & N_{n-1} \end{array}\right]. \end{aligned} \tag{54}$$

COROLLARY 4.1 *For $C = C_n$ and $A = A_n$ the permutation matrix $P$ defined by (54) is a critical point of*
*(a) the map $q : U(2^{n+1}, \mathbb{C}) \to \mathbb{R}^2$, defined by (15),*
*(b) the cost function $f : U(2^{n+1}, \mathbb{C}) \to \mathbb{R}$, defined by (6).*

**Proof.** Note that $[PA_nP^\dagger, C_n^\dagger] = \begin{bmatrix} -I_{2^n} & 0 \\ 0 & I_{2^n} \end{bmatrix}$. From

$$\operatorname{lin} W(X) = \mathrm{i}\operatorname{tr}(X \cdot u(2^{n+1}, \mathbb{C}))$$

it follows that

$$\operatorname{lin} W([PA_nP^\dagger, C_n^\dagger]) = \mathrm{i}\operatorname{tr}\left(\begin{bmatrix} -I_{2^n} & 0 \\ 0 & I_{2^n} \end{bmatrix} \cdot u(2^{n+1}, \mathbb{C})\right).$$

But any skew-Hermitian matrix has purely imaginary diagonal entries and therefore

$$\dim \operatorname{lin} W\left(\left[PA_nP^\dagger, C_n^\dagger\right]\right) = 1 < 2.$$

Part (b) follows since $PA_nP^\dagger$ has the form (53). □

Now we apply Lemma 2.1 to the case $C = \begin{bmatrix} 0 & 0 \\ I & 0 \end{bmatrix}$. By Lemma 4.1 $W(C, A)$ is a disk around 0. By Corollary 2.1 the derivative of $q$ at $U$ has rank zero if and only if $[C^\dagger, UAU^\dagger] = 0$ holds. Defining

$$B = \begin{bmatrix} B_1 & B_2 \\ B_3 & B_4 \end{bmatrix} := UAU^\dagger,$$

then $[C^\dagger, B] = 0$ is equivalent to $B_1 = B_4$ and $B_3 = 0$, i.e.,

$$B = \begin{bmatrix} B_1 & B_2 \\ 0 & B_1 \end{bmatrix}.$$

Consequently, $\operatorname{tr}(C^\dagger B) = 0$. That is, we have proved

LEMMA 4.3 *For $n$ even let $C = \begin{bmatrix} 0 & 0 \\ I_{n/2} & 0 \end{bmatrix}$ and let $q : U(n, \mathbb{C}) \to \mathbb{R}^2$, defined by (15). Then any rank zero critical point $U$ of $q$ has critical value $q(U) = 0$.* □

The next result shows that critical values of $q$ form circles in $\mathbb{R}^2$.

THEOREM 4.1 *For $n$ even let $C = \begin{bmatrix} 0 & 0 \\ I_{n/2} & 0 \end{bmatrix}$ and let $q : U(n, \mathbb{C}) \to \mathbb{R}^2$, defined by (15). Let $U$ be a rank one critical point of $q$ with critical value $q(U)$. Then for all $\phi \in \mathbb{R}$*

$$e^{i\phi} q(U)$$

*is also a critical value.*

**Proof.** For arbitrary $X \in \mathbb{C}^{n\times n}$ it holds

$$\begin{aligned} \text{lin } W(X) &= i \,\text{tr}\,(X \cdot \mathfrak{u}(n, \mathbb{C})) \\ &= \left\{ i \,\text{tr}\,(XV i\Lambda V^\dagger) \,\middle|\, V \in U(n, \mathbb{C}),\ \Lambda = \text{diag}\,(\lambda_1, .., \lambda_n),\ \lambda_1, .., \lambda_n \in \mathbb{R} \right\}. \end{aligned}$$

Therefore, $\dim \text{lin } W(X) = 1$ is equivalent to saying that the diagonal entries $y_{ii} \in \mathbb{C}$ of $Y = (y_{ij}) := V^\dagger X V$ for all $V \in U(n, \mathbb{C})$ are elements of one and the same real one-dimensional subspace of $\mathbb{R}^2 \cong \mathbb{C}$. Now assume $\dim \text{lin } W(X) = 1$. Hence, there exists an $\alpha \in \mathbb{R}$ such that for all $V \in U(n, \mathbb{C})$ the diagonal entries $e^{i\alpha} y_{ii}$ of the matrix $e^{i\alpha} Y$ are real. Decompose $e^{i\alpha} Y = (e^{i\alpha} Y)_+ + (e^{i\ alpha} Y)_-$ into Hermitian and skew-Hermitian part. Consequently, for all $V \in U(n, \mathbb{C})$ the diagonal entries of $(e^{i\alpha} Y)_- = (e^{i\alpha} Y - e^{-i\alpha} Y^\dagger)/2$ have to be zero, i.e., the skew-Hermitian part itself has to be zero, i.e., $e^{i\alpha} Y = (e^{i\alpha} Y)_+ = e^{-i\alpha} Y^\dagger$ is Hermitian. Now set $X = [B, C^\dagger]$ with $B = \begin{bmatrix} B_1 & B_2 \\ B_3 & B_4 \end{bmatrix} := U A U^\dagger$. Then

$$e^{i\alpha} X = e^{i\alpha} \begin{bmatrix} -B_3 & B_1 - B_4 \\ 0 & B_3 \end{bmatrix}$$

is also Hermitian. Hence $e^{i\alpha} B_3 = e^{-i\alpha} B_3^\dagger$ and $B_1 = B_4$. Therefore $B$ has the structure

$$B = \begin{bmatrix} B_1 & B_2 \\ e^{-i\alpha} K & B_1 \end{bmatrix} \quad \text{with} \quad K = K^\dagger = e^{i\alpha} B_3.$$

An easy calculation shows that if $U$ is critical of rank one with critical value $q(U) = e^{-i\alpha} \text{tr}\, K$ then for all $\phi \in \mathbb{R}$

$$\begin{bmatrix} e^{-i\phi/2} I_{n/2} & 0 \\ 0 & e^{i\phi/2} I_{n/2} \end{bmatrix} U$$

is also a rank one critical point with critical value $e^{i(\phi-\alpha)} \text{tr}\, K$. The result follows.□
The following Theorem gives upper bounds for $\Re\,(\text{tr}\,(C_n^\dagger U A_n U^\dagger))$ for any $n \in \mathbb{N}$.

THEOREM 4.2 *For $A_n, C_n$, defined by (48) and for all $U \in U(2^{n+1}, \mathbb{C})$ it holds*

$$\Re\,(\mathrm{tr}\,(C_n^\dagger U A_n U^\dagger)) \le 2(n-m)\binom{n}{m}$$

*where $m = n/2$ if $n$ is even and $m = (n-1)/2$ if $n$ is odd.*

**Proof.** Define for all $n \in \mathbb{N}_0$

$$F_n := \begin{bmatrix} 0 & I_{2^n} \\ I_{2^n} & 0 \end{bmatrix}, \quad G_n := \mathrm{i}\begin{bmatrix} 0 & I_{2^n} \\ -I_{2^n} & 0 \end{bmatrix}, \tag{55}$$

and for all $n \in \mathbb{N}$ recursively

$$X_n := \begin{bmatrix} X_{n-1} + F_{n-1} & 0 \\ 0 & X_{n-1} + F_{n-1} \end{bmatrix}, \quad X_0 := 0_2\,, \tag{56}$$

$$Y_n := \begin{bmatrix} Y_{n-1} + G_{n-1} & 0 \\ 0 & Y_{n-1} + G_{n-1} \end{bmatrix}, \quad Y_0 := 0_2\,. \tag{57}$$

By induction on $n$ it is easily seen that for all $n \in \mathbb{N}$

$$C_n = \frac{1}{2}(F_n + \mathrm{i}\,G_n)$$

$$A_n = \frac{1}{2}(X_n + \mathrm{i}\,Y_n)$$

coincide with the formerly defined matrices $A_n, C_n$, see (48). That is, we get for all $n \in \mathbb{N}$ the unique additive decomposition of $A_n$ and $C_n$, respectively, into Hermitian and skew-Hermitian parts. Consequently,

$$\Re\,\mathrm{tr}\,(C_n^\dagger U A_n U^\dagger) = \frac{1}{4}\mathrm{tr}\,(F_n U X_n U^\dagger + G_n U Y_n U^\dagger). \tag{58}$$

Now we compute the eigenvalues of $X_n$ and $Y_n$, respectively. Let

$$\pi_n(\lambda) := \det(\lambda I - X_n)$$

be the characteristic polynomial of $X_n$. By definition (56) of $X_n$

$$\pi_n(\lambda) := \det(\lambda I - F_{n-1} - X_{n-1})^2.$$

But

$$\begin{aligned} \det(\lambda I - F_{n-1} - X_{n-1}) &= \det\begin{bmatrix} \lambda I - F_{n-2} - X_{n-2} & I \\ I & \lambda I - F_{n-2} - X_{n-2} \end{bmatrix} \\ &= \det\left((\lambda I - F_{n-2} - X_{n-2})^2 - I\right) \\ &= \det\left(\lambda I - I - F_{n-2} - X_{n-2}\right) \cdot \\ &\qquad \det\left(\lambda I + I - F_{n-2} - X_{n-2}\right). \end{aligned}$$

Therefore,

$$\begin{aligned}\det(\lambda I - F_{n-1} - X_{n-1})^2 &= \det\left((\lambda-1)I - F_{n-2} - X_{n-2})\right)^2 \cdot \\ &\qquad \det\left((\lambda+1)I - F_{n-2} - X_{n-2})\right)^2 \\ &= \pi_{n-1}(\lambda-1)\cdot\pi_{n-1}(\lambda+1),\end{aligned}$$

i.e.,

$$\pi_n(\lambda) = \pi_{n-1}(\lambda-1)\cdot\pi_{n-1}(\lambda+1).$$

By induction on $n$ we get

LEMMA 4.4 *The eigenvalues of $X_n$, or equivalently, the roots of $\pi_n(\lambda)$ are given as*

$$n-2k, \qquad k = 0, 1, \ldots, n,$$

*each occuring with multiplicity*

$$2\binom{n}{k},$$

*respectively.* □

By the same arguments the eigenvalues of $Y_n$ can be computed. In fact, it turns out that the spectrum of $Y_n$ and the spectrum of $X_n$ are identical. From the definition of $F_n$ and $G_n$, see (55), it is easily seen that the spectrum of $F_n$ and the spectrum of $G_n$ are also identical, the eigenvalues being $\pm 1$, each with multiplicity $2^n$.

Now we are in the position to compute the maximum values

$$\max_{U\in U(2^{n+1},\mathbb{C})} \operatorname{tr}(F_n U X_n U^\dagger)$$

and

$$\max_{U\in U(2^{n+1},\mathbb{C})} \operatorname{tr}(G_n U Y_n U^\dagger),$$

respectively. By the hermiticity of the matrices $F_n, G_n, X_n$, and $Y_n$ it is a well known fact that these maximum values are just the sum of the pairwise products of the eigenvalues of $G_n$ and $Y_n$, (respectively, $F_n$ and $X_n$), provided that they are

ordered similarly by their magnitude. Therefore,

$$\begin{aligned}\max_{U\in U(2^{n+1},\mathbb{C})} \operatorname{tr}(F_n U X_n U^\dagger) &= \max_{U\in U(2^{n+1},\mathbb{C})} \operatorname{tr}(G_n U Y_n U^\dagger)\\ &= 2\sum_{k=0}^{m} 2\tbinom{n}{k}(n-2k)\\ &= 4\sum_{k=0}^{m} n\left(\tbinom{n-1}{k}-\tbinom{n-1}{k-1}\right)\\ &= 4n\tbinom{n-1}{m}\\ &= 4(n-m)\tbinom{n}{m}\end{aligned}.$$

Now, it is a priori not evident (and in general wrong) that this maximum value is *simultaneously* attained, i.e., that there exists a unitary matrix, say $\widetilde{U}\in U(2^{n+1},\mathbb{C})$, such that

$$\operatorname{tr}(F_n\widetilde{U}X_n\widetilde{U}^\dagger)=\operatorname{tr}(G_n\widetilde{U}Y_n\widetilde{U}^\dagger)=4(n-m)\binom{n}{m}.$$

Nevertheless, we at least obtain the estimate

$$\begin{aligned}\max_{U\in U(2^{n+1},\mathbb{C})} \Re\left(\operatorname{tr}(C_n^\dagger U A_n U^\dagger)\right) &= \tfrac{1}{4}\max_{U\in U(2^{n+1},\mathbb{C})} \operatorname{tr}(F_n\widetilde{U}X_n\widetilde{U}^\dagger + G_n\widetilde{U}Y_n\widetilde{U}^\dagger)\\ &\le 2(n-m)\tbinom{n}{m}\end{aligned}$$

as claimed. □

COROLLARY 4.2 *For $n=1,2$ the upper bounds of Theorem 4.2 are sharp ones, i.e.,*

*(a)* $\max_{U\in U(4,\mathbb{C})} \Re\left(\operatorname{tr}(C_1^\dagger U A_1 U^\dagger)\right)=2,$

*(b)* $\max_{U\in U(8,\mathbb{C})} \Re\left(\operatorname{tr}(C_2^\dagger U A_2 U^\dagger)\right)=4.$

**Proof.** Using the orthogonal permutation matrix $P$ defined by (54) the maximum value is attained for $n=1,2$. □

Our next result yields an upper bound on $\max_{U\in U(2^{n+1},\mathbb{C})} \Re\left(\operatorname{tr}(C_n^\dagger U A_n U^\dagger)\right)$ which is independent of $n$ for sufficiently large $n$. We first need a lemma.

LEMMA 4.5 *For $A_n$ and $C_n$ as defined in (48) it holds*

$$\|C_n\|^2=2^n,\qquad \|A_n\|^2=n2^n.$$

**Proof.** One has

$$\|C_n\|^2 = \operatorname{tr} I_{2^n} = 2^n.$$

Also

$$\begin{aligned}\|A_n\|^2 &= 2\|A_{n-1} + C_{n-1}\|^2 \\ &= 2\|A_{n-1}\|^2 + 2\|C_{n-1}\|^2 + 4\operatorname{tr}(A_{n-1}^\top C_{n-1}).\end{aligned}$$

Since

$$C_{n-1} = \begin{bmatrix} 0 & 0 \\ I_{2^{n-1}} & 0 \end{bmatrix}, \quad A_{n-1}^\top = \begin{bmatrix} A_{n-2}^\top + C_{n-2}^\top & 0 \\ 0 & A_{n-2}^\top + C_{n-2}^\top \end{bmatrix},$$

we see that $\operatorname{tr}(A_{n-1}^\top C_{n-1}) = 0$ and therefore

$$\|A_n\|^2 = 2\|A_{n-1}\|^2 + 2^n, \quad \|A_0\|^2 := 0.$$

Thus

$$\|A_n\|^2 = \sum_{k=0}^{n-1} 2^k 2^{n-k} = n2^n.$$

□

From Theorem 4.2 and Lemma 4.5 we have

$$\frac{\max\limits_{U \in U(2^{n+1},\mathbb{C})} \Re\,(\operatorname{tr}(C_n^\dagger U A_n U^\dagger))}{\|A_n\| \cdot \|C_n\|} \leq \frac{2(n-m)nm}{\sqrt{n}2^n} =: k_n.$$

Let $n := 2m$ be even. By Stirling's formula

$$n! \approx \sqrt{2\pi n}\left(\frac{n}{\mathrm{e}}\right)^n.$$

Thus

$$\begin{aligned} k_{2m} &= \frac{2m\binom{2m}{m}}{\sqrt{2m}\,2^{2m}} \\ &= \sqrt{2m}\,2^{-2m}\frac{(2m)!}{m!m!} \\ &\approx \sqrt{2m}\,2^{-2m}\frac{\sqrt{2\pi 2m}}{\sqrt{2\pi m}\sqrt{2\pi m}}\frac{\left(\frac{2m}{\mathrm{e}}\right)^{2m}}{\left(\frac{m}{\mathrm{e}}\right)^{2m}} \\ &= 2^{-2m}\sqrt{\frac{2}{\pi}}\,2^{2m} \\ &= \sqrt{\frac{2}{\pi}} < 1. \end{aligned}$$

Thus for $n$ sufficiently large the upper bound

$$k_n \approx \sqrt{\frac{2}{\pi}}.$$

These bounds improve the SVD upper bounds (3) already known, see e.g., [8] and references cited therein. For $n \leq 3$ they are also reported in [17]. The fully Hermitian case appeared already in [16].

### 4.1. STEP SIZE SELECTIONS REVISITED

We have seen that the step size

$$\alpha_k = \frac{\left\| [C^\dagger, U_k A U_k^\dagger]_- \right\|^2}{\left\| [C^\dagger, [C^\dagger, U_k A U_k^\dagger]_-] \right\| \cdot \left\| [U_k A U_k^\dagger, [C^\dagger, U_k A U_k^\dagger]_-] \right\|}. \tag{59}$$

guarantees convergence. Consider the nilpotent matrices $A_n$ and $C_n$ as in (48). For the block partioned matrices

$$B^{(k)} := U_k A U_k^\dagger = \begin{bmatrix} B_{11}^{(k)} & B_{12}^{(k)} \\ B_{21}^{(k)} & B_{22}^{(k)} \end{bmatrix},$$

the step size (59) is rewritten as

$$\alpha_k = \frac{\left\| [C^\dagger, B^{(k)}]_- \right\|^2}{\left\| [C^\dagger, [C^\dagger, B^{(k)}]_-] \right\| \cdot \left\| [B^{(k)}, [C^\dagger, B^{(k)}]_-] \right\|}. \tag{60}$$

Now

$$\begin{aligned} \left\| [C^\dagger, B^{(k)}]_- \right\|^2 &= \left\| \begin{bmatrix} (B_{21}^{(k)})_- & B_{22}^{(k)} - B_{11}^{(k)} \\ -(B_{22}^{(k)} - B_{11}^{(k)})^\dagger & -(B_{21}^{(k)})_- \end{bmatrix} \right\|^2 \\ &= 2\|(B_{21}^{(k)})_-\|^2 + 2\|B_{22}^{(k)} - B_{11}^{(k)}\|^2. \end{aligned}$$

Also

$$\begin{aligned} \left\| [C^\dagger, [C^\dagger, B^{(k)}]_-] \right\| &= \left\| \begin{bmatrix} -(B_{22}^{(k)} - B_{11}^{(k)})^\dagger & -2(B_{21}^{(k)})_- \\ 0 & (B_{22}^{(k)} - B_{11}^{(k)})^\dagger \end{bmatrix} \right\| \\ &= \sqrt{2\|B_{22}^{(k)} - B_{11}^{(k)}\|^2 + 4\|(B_{21}^{(k)})_-\|^2}. \end{aligned}$$

But

$$\left\| [B^{(k)}, [C^\dagger, B^{(k)}]_-] \right\| \leq 2\|A\| \cdot \|[C^\dagger, B^{(k)}]_-\|.$$

Thus convergence still holds for

$$\frac{\left\|[C^\dagger, B^{(k)}]_-\right\|}{2\|A\| \cdot \left\|[C^\dagger, [C^\dagger, B^{(k)}]_-]\right\|} = \frac{1}{2\|A\|}\sqrt{\frac{2\|(B_{21}^{(k)})_-\|^2 + 2\|B_{22}^{(k)} - B_{11}^{(k)}\|^2}{4\|(B_{21}^{(k)})_-\|^2 + 2\|B_{22}^{(k)} - B_{11}^{(k)}\|^2}}$$

and hence for the lower bound

$$\frac{1}{2\sqrt{2}\,\|A\|}.$$

Consequently, using Lemma 4.5, we have proved

THEOREM 4.3 *Let $A_n$ and $C_n$ as in (48). Then for the constant step size*

$$\alpha^{***} = \frac{1}{\sqrt{n2^{n+3}}} \tag{61}$$

*the algorithm*

$$U_{k+1} = \mathrm{e}^{\alpha^{***}[C^\dagger, U_k A U_k^\dagger]_-} U_k$$

*converges to the set of critical points of $f(U) = \Re\,\mathrm{tr}\,(C^\dagger U A U^\dagger)$.* □

REMARK 4.1 *For all $n \in \mathbb{N}$ with $n \geq 2$ it holds $\alpha^{**} \leq \alpha^{***}$.* □

We conclude with the following conjecture that gives the prospective maximal values of the cost function.

CONJECTURE 4.1 *For $A_n, C_n$, defined by (48) the gradient flow of the function $\Re(\mathrm{tr}\,(C_n^\dagger U A_n U^\dagger))$ converges to the following maximal values $f_n^{\max}$:*

| $n$ | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| $f_n^{\max}$ | 2 | 4 | $4(1+\sqrt{3})$ | $8(1+\sqrt{3})$ | $16(1+\sqrt{3})+4\sqrt{5}$ | $32(1+\sqrt{3})+8\sqrt{5}$ |

For numerical illustration, we compare the values from the above Conjecture with the more conservative estimate given in Theorem 4.2 as well as with the even rougher upper bound by the $C$-spectral norm of $A$ (see Eq. 4) mentioned in the introduction.

| $n$ | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| $f_n^{\max}$ | 2 | 4 | 10.9282 | 21.8564 | 52.6571 | 105.3142 |
| $f_n^{\text{Th.4.2}} = 2\ (n-m)\binom{n}{m}$ | 2 | 4 | 12 | 24 | 60 | 120 |
| $f_n^{\text{SVD}} = \|A_n\|_{C_n}$ | 2 | 5.6569 | 12.9282 | 29.1117 | 66.5067 | 142.2638 |

## 5. Numerical experiments

In this section we present a few numerical experiments. We apply our discretization method (30) to maximize the function $f : U(2^{n+1}, \mathbb{C}) \to \mathbb{R}$, defined by (6) to the above special case of nilpotent matrices. For $n = 1$ the matrices $A_1$ and $C_1$, defined by (49), are unitarily similar, so we disregard this case. For $n = 2, \ldots, 6$ see the recursive definition (48) of the matrices $A_n$ and $C_n$, respectively. Initial unitary matrices $U_0$ are chosen by computing the QR-decomposition of a randomly generated complex matrix. Each plot combines the trajectories of five different initial values. Experiments with the step sizes $\alpha_k$, $\alpha_k^*$, and $\alpha^{***}$, defined by (31), (44), and (61), respectively, are reported below. The function

$$\text{cost} := f_n^{\max} - \Re(\text{tr}\,(C_n^\dagger U_k A_n U_k^\dagger))$$

is plotted on a logarithmic scale against the number of iterations. The values of $f_n^{\max}$ for $n = 2, \ldots, 6$ are taken from Conjecture 4.1. Figure 1 shows experiments with the adaptive step size (31). The contents of Figure 2 are simulations with the more conservative step size selection of (44), whereas the last figure shows the relatively slow convergence of the constant step size defined by (61). The termination criteria we used for the several plots can be seen from the following table.

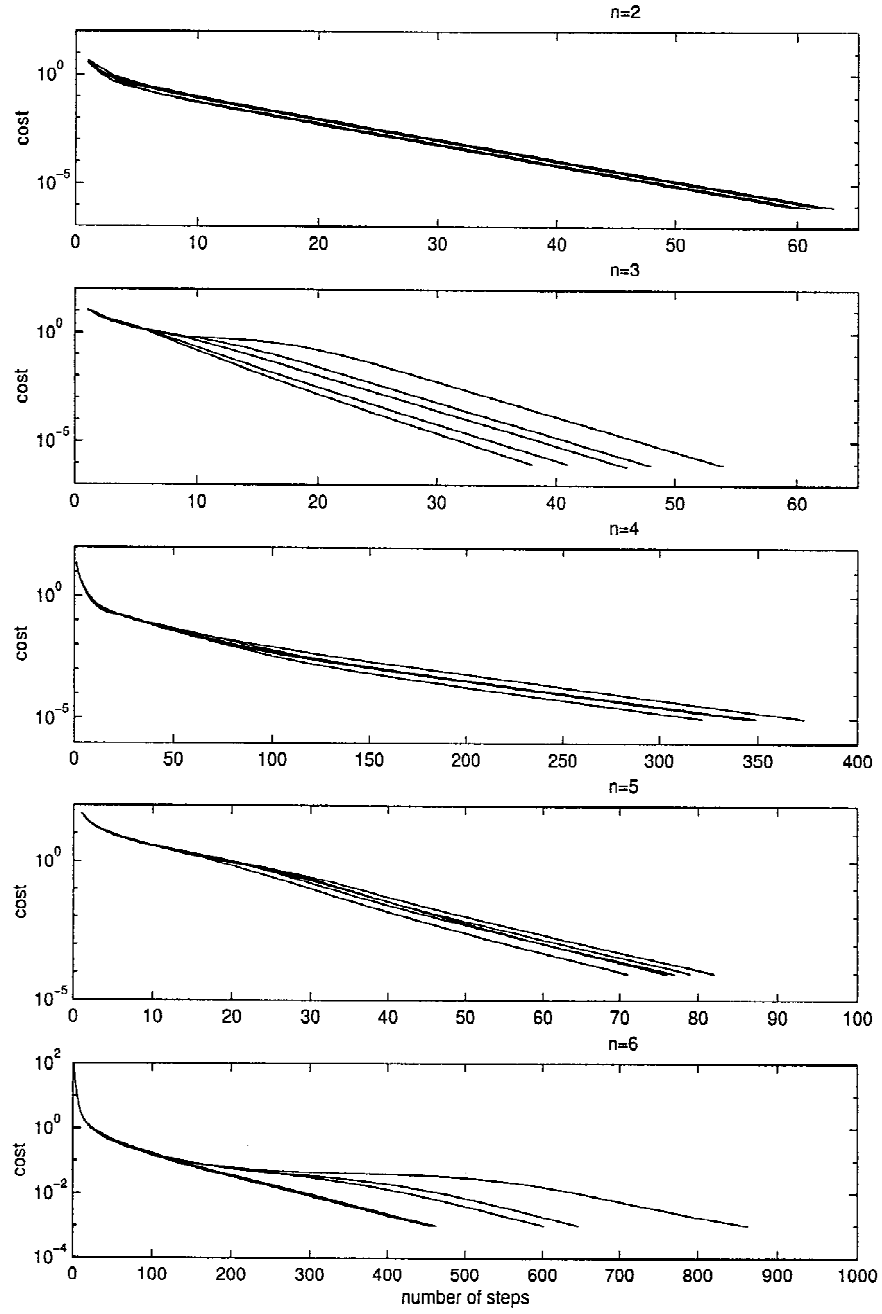


*Figure 1.* Minimization of the function cost $:= f_n^{\max} - \Re(\mathrm{tr}\,(C_n^\dagger U_k A_n U_k^\dagger))$ by discretization of the associated gradient flow using the adaptive step size $\alpha_k$, defined by (31).

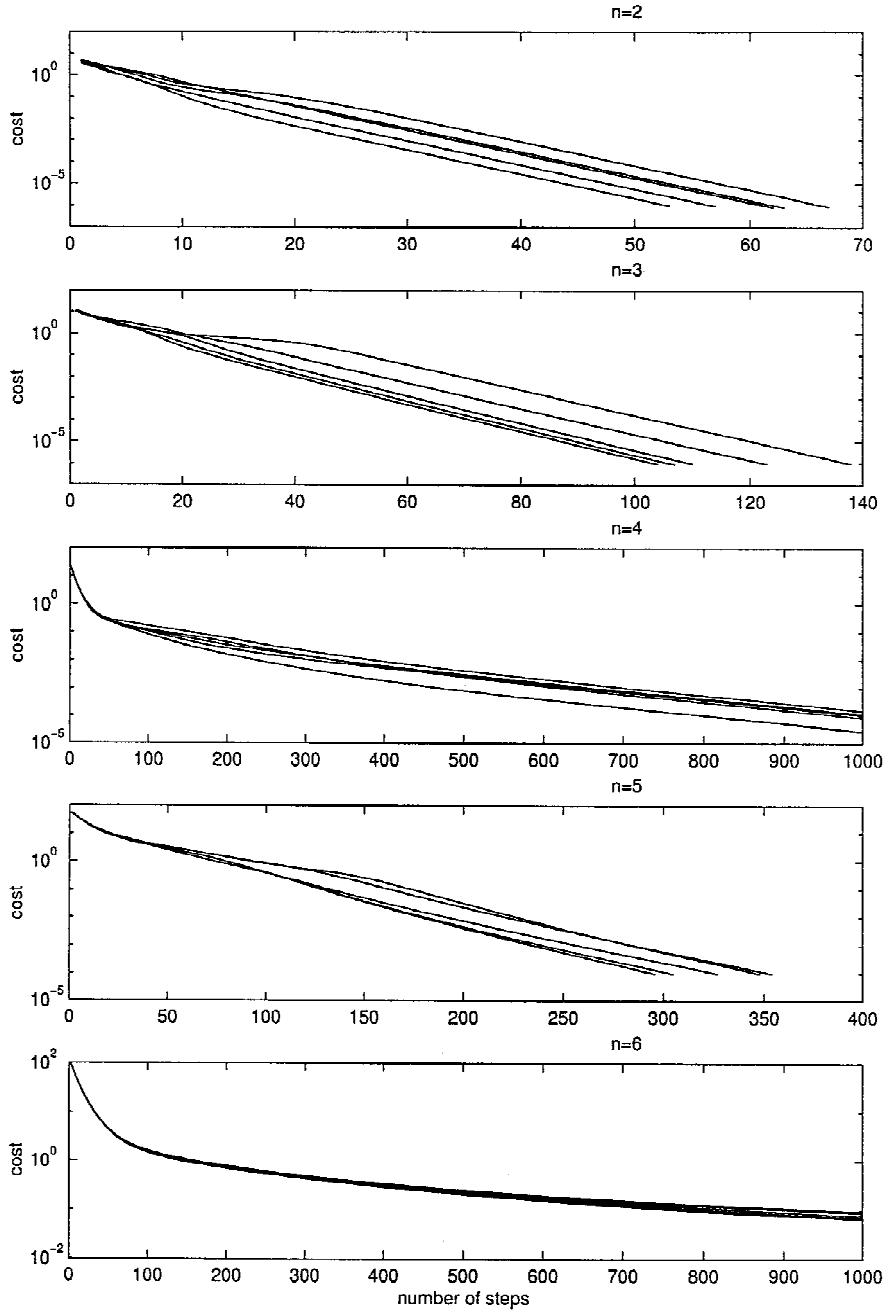


*Figure 2.* Minimization of the function cost $:= f_n^{\max} - \Re(\mathrm{tr}\,(C_n^\dagger U_k A_n U_k^\dagger))$ by discretization of the associated gradient flow using the adaptive step size $\alpha_k^*$, defined by (44).

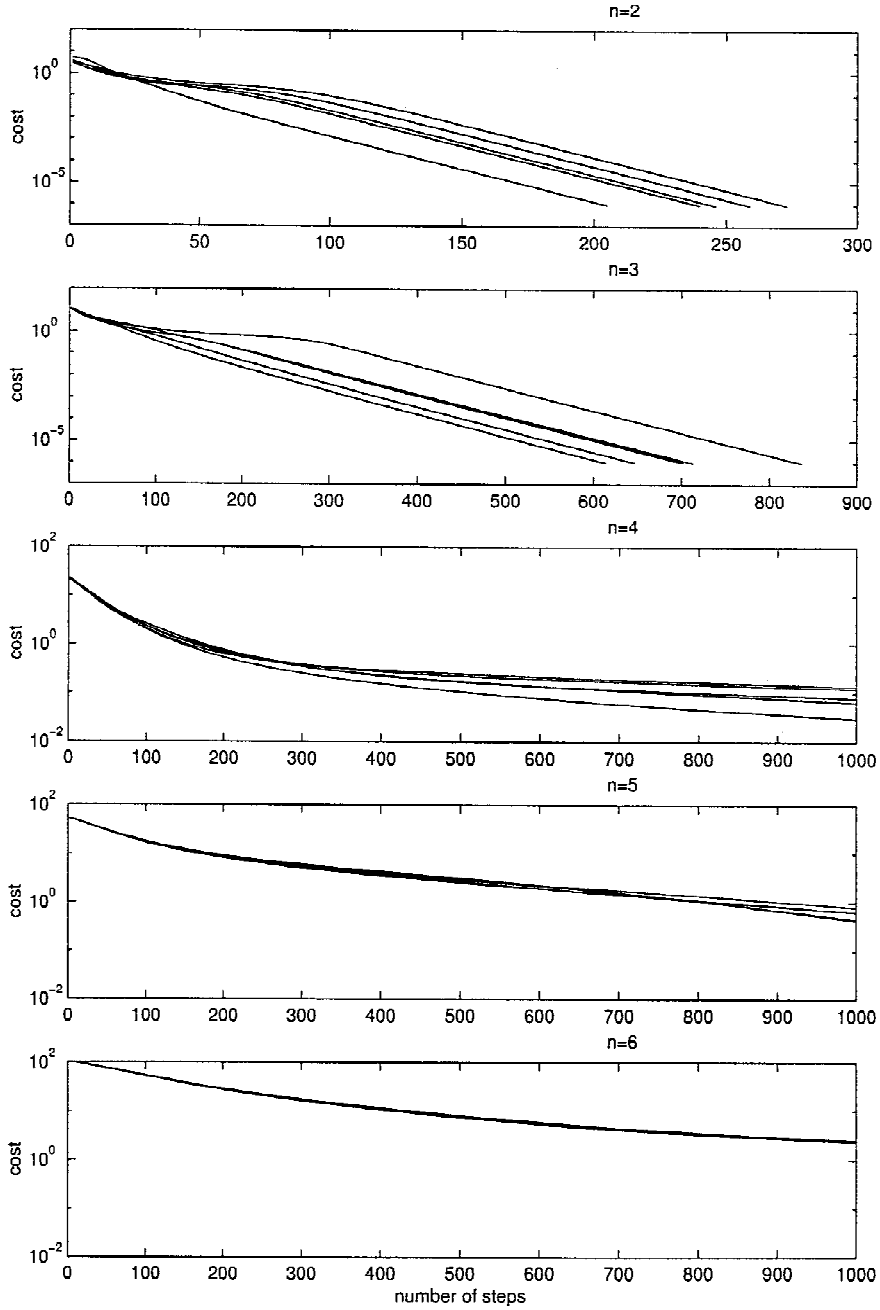


*Figure 3.* Minimization of the function cost $:= f_n^{\max} - \Re(\mathrm{tr}\,(C_n^\dagger U_k A_n U_k^\dagger))$ by discretization of the associated gradient flow using the constant step size defined by (61).

| Number of I–Spins | Termination Criterion | | |
|---|---|---|---|
| $n$ | cost | or: | no. of steps $k$ |
| 2 | $< 10^{-6}$ | | $> 1000$ |
| 3 | $< 10^{-6}$ | | $> 1000$ |
| 4 | $< 10^{-5}$ | | $> 1000$ |
| 5 | $< 10^{-4}$ | | $> 1000$ |
| 6 | $< 10^{-3}$ | | $> 1000$ |

In all figures plotted points are joined by linear interpolation. The number of iterations seems to be typical in each case. The plots document linear convergence to a maximum as one would expect for a gradient-like method.

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