ELSEVIER

Available online at www.sciencedirect.com

ScienceDirect

Linear Algebra and its Applications 421 (2007) 69–84

LINEAR ALGEBRA AND ITS APPLICATIONS

www.elsevier.com/locate/laa

Zero-preserving iso-spectral flows based on parallel sums

Kenneth R. Driessel [a,*], Alf Gerisch [b]

[a] *Mathematics Department, Colorado State University, Fort Collins, Colorado, USA*

[b] *Fachbereich Mathematik und Informatik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany*

Received 1 November 2005; accepted 4 July 2006

Available online 18 September 2006

Submitted by S. Kirkland

Abstract

Driessel [K.R. Driessel, Computing canonical forms using flows, Linear Algebra Appl. 379 (2004) 353–379] introduced the notion of quasi-projection onto the range of a linear transformation from one inner product space into another inner product space. Here we introduce the notion of quasi-projection onto the intersection of the ranges of two linear transformations from two inner product spaces into a third inner product space. As an application, we design a new family of iso-spectral flows on the space of symmetric matrices that preserves zero patterns. We discuss the equilibrium points of these flows. We conjecture that these flows generically converge to diagonal matrices. We perform some numerical experiments with these flows which support this conjecture. We also compare our zero-preserving flows with the Toda flow.

AMS classification: 15A18

Keywords: Iso-spectral flow; Group action; Orbit; Eigenvalues; Sparse matrix; Dynamical system; Ordinary differential equation; Vector field; Toda flow; Double bracket flow; QR algorithm; Differential geometry; Projection; Quasi-projection; Parallel sum; Harmonic mean

* Corresponding author.

E-mail addresses: driessel@math.colostate.edu (K.R. Driessel), gerisch@mathematik.uni-halle.de (A. Gerisch).

0024-3795/$ - see front matter

doi:10.1016/j.laa.2006.07.013

1. Introduction

Let Δ be a set of pairs (i, j) of integers between 1 and n which satisfies the following conditions: (1) for $i = 1, 2, \dots, n$, the diagonal pair (i, i) is in Δ, and (2) if the pair (i, j) is in Δ then so is the symmetric pair (j, i). We regard Δ as a (symmetric) sparsity **pattern of interest** of nonzero entries for matrices. In particular, let $\mathrm{Sym}(n)$ denote the vector space of symmetric, $n \times n$, real matrices and let $\mathrm{Sym}(\Delta)$ denote the subspace of $\mathrm{Sym}(n)$ consisting of the symmetric matrices which are zero outside the pattern Δ; in symbols,

$$\mathrm{Sym}(\Delta) := \{X \in \mathrm{Sym}(n) : X(i, j) \neq 0 \text{ implies } (i, j) \in \Delta\}.$$

In this paper we consider the following task: Find flows in the space $\mathrm{Sym}(\Delta)$ which preserve eigenvalues and converge to diagonal matrices. We can describe this task more precisely as follows: With an $n \times n$ symmetric matrix A, we associate the **iso-spectral surface**, $\mathrm{Iso}(A)$, of all symmetric matrices which have the same eigenvalues as A. By the spectral theorem, we have

$$\mathrm{Iso}(A) := \{QAQ^{\mathrm{T}} : Q \in O(n)\},$$

where $O(n)$ denotes the group of orthogonal matrices.

We shall use the Frobenius inner product on matrices; recall that it is defined by $\langle X, Y\rangle := \mathrm{Trace}(XY^{\mathrm{T}})$. With a symmetric matrix D, we associate a real-valued 'objective' function

$$f := \mathrm{Sym}(n) \to R : X \mapsto (1/2)\langle X - D, X - D\rangle.$$

Note that f is a measure of the distance from X to D. We shall consider the following constrained optimization problem:

Problem 1. Given $A \in \mathrm{Sym}(\Delta)$, minimize $f(X)$ subject to the constraints $X \in \mathrm{Iso}(A)$ and $X \in \mathrm{Sym}(\Delta)$.

In particular, we shall describe a flow on the surface $\mathrm{Iso}(A) \cap \mathrm{Sym}(\Delta)$ which solves this problem in the sense that it usually converges to a local minimum.

Here is a summary of the contents of this paper.

In the next section, we present some theoretical background material. Driessel [7] introduced the notion of quasi-projection onto the range of a linear transformation from one inner product space to another. In this section we introduce the notion of quasi-projection onto the intersection of the ranges of two linear transformations A and B from two inner product spaces into a third inner product space. We use the notation $!(A, B)$ to denote our quasi-projection operator. We show that $!(A, B) = 2A(A + B)^{+}B$ where the superscript $+$ denotes the Moore–Penrose pseudo inverse operation.

Remark. If A and B are invertible then

$$!(A, B) = 2A(A + B)^{-1}B = 2(A^{-1} + B^{-1})^{-1}.$$

This operator is called the "harmonic mean" of the operators A and B. See, for example, Kubo and Ando [11]. (Chandler Davis pointed out this reference to us.) They use the infix notation $A!B$ to denote the harmonic mean of A and B where A and B are positive operators on a Hilbert space. Anderson and Duffin [1] define the "parallel sum" of semi-definite matrices A and B by the formula $A(A + B)^{+}B$ and denote it by $A : B$. Most of the results in Section 2 appear in Anderson and Duffin [1], Anderson [2], Anderson and Schreiber [3], Anderson and Trapp [4]; we included our proofs in the interest of keeping the paper self-contained.

In Section 3, we describe an application of the quasi-projection method. In particular, we describe how we used this method to design a new flow corresponding to the optimization problem described above. We conjecture that this flow generically converges to a symmetric matrix E that commutes with D. Note that if we choose D to be a diagonal matrix with distinct diagonal entries then E commutes with D iff E is a diagonal matrix. (For background material on differential equations see, for example, Hirsch et al. [10].)

In Section 4, which is entitled "Numerical results", we describe our implementation of our iso-spectral zero-preserving flow in Matlab. We also describe several numerical experiments that we performed using this computer program.

In all our experiments this flow converges (sometimes slowly) to a diagonal matrix. Consequently these experiments provide evidence for the conjecture described above. We do not claim our program to be competitive with standard methods used to compute eigenvalues. But we hope our ideas will lead eventually to practical, competitive methods for finding eigenvalues of some classes of structured matrices.

This paper is a shortened version of Driessel and Gerisch [8]. In that paper, we show how quasi-projections arise by simplifying standard projections, and we indicate our geometric view of the Toda flow.

We want to sketch here the way we arrived at the quasi-projection equations. (For more detail see the first appendix of the long version of this paper mentioned above.) Let U, V and W be inner product spaces and let $L : U \to W$ and $M : V \to W$ be linear maps. Consider the following least squares problem: Given $c \in W$, find $u \in U$ and $v \in V$ such that $Lu = Mv$ and $\hat{c} := Lu$ is the vector in Range.$L \cap$ Range.M which is closest to c. Using the method of Lagrange multipliers leads to the following set of equations for u, v and λ (the Lagrange multiplier):

$$L^*Lu - L^*\lambda = L^*c, \quad M^*Mv + M^*\lambda = M^*c, \quad Lu = Mv.$$

If L and M are injective then we can rewrite these equations as follows:

$$w - P\lambda = Pc, \quad (P + Q)\lambda = (-P + Q)c,$$

where $w := Lu = Mv$, $P := L(L^*L)^{-1}L^*$ and $Q := M(M^*M)^{-1}M^*$. Note that P and Q are projections. If we replace P and Q by $A := LL^*$ and $B := MM^*$ we get the quasi-projection equations:

$$w - A\lambda = Ac, \quad (A + B)\lambda = (-A + B)c,$$

which appear at the beginning of the next section. Driessel [7] introduced the idea of simply dropping inverse maps like $(L^*L)^{-1}$ and $(M^*M)^{-1}$.

For another example of a structured iso-spectral flow see Fasino [9].

2. Quasi-projection onto the intersection of two subspaces

In this section we shall present some theoretical background material concerning quasi-projections. We shall apply this material in the next section. Let V be a finite-dimensional, real inner product space. We use $\langle x, y\rangle$ to denote the inner product of two elements of V. Let $A : V \to V$ and $B : V \to V$ be (self-adjoint) positive semi-definite linear operators on V. For any vector c in V, consider the following system of linear equations for u and λ in V:

$$u - A\lambda = Ac, \tag{q1}$$

$$(A + B)\lambda = (B - A)c. \tag{q2}$$

We call these equations the **quasi-projection equations** determined by A, B and c.

Remark. In this section we usually assume that A and B are two positive semi-definite operators on a finite-dimensional space. These assumptions simplify the analysis considerably. They will be obviously satisfied in the application considered below. However, many of the results in this section are true in more general settings.

Note that (q1) is equivalent to the following condition:

$$u = A(\lambda + c). \tag{eq1}$$

Hence u is in the range of A. Also note that (q2) is equivalent to the following condition:

$$A(\lambda + c) = B(-\lambda + c). \tag{eq2}$$

Hence u is also in the range of B. Thus we see that u is in the intersection of the range of A and the range of B.

Remark. We sometimes use $f.x$ or fx in place of $f(x)$ to indicate function application. We also use association to the left. For example, $D(\omega.A).I.K$ means evaluate ω at A to get a function, differentiate this function, evaluate the result at I to get a linear function, and finally evaluate at K. This notation is also used in Range.L and Kernel.L to denote range and kernel of an operator L.

We shall use the following lemma repeatedly.

Lemma 1. *If A and B are positive semi-definite operators then*

$$\text{Kernel}(A + B) = \text{Kernel}.A \cap \text{Kernel}.B,$$
$$\text{Range}(A + B) = \text{Range}.A + \text{Range}.B.$$

Proof. If $Az = Bz = 0$ then $(A + B)z = 0$. Now assume $(A + B)z = 0$. Then $0 = \langle z, (A + B)z\rangle = \langle z, Az\rangle + \langle z, Bz\rangle$. Since A and B are positive semi-definite, we get $0 = \langle z, Az\rangle = \langle z, Bz\rangle$ and hence $0 = Az = Bz$. The second equation of this lemma is obtained from the first one by taking orthogonal complements. $\square$

The following proposition shows that the vector u is uniquely determined by the quasi-projection equations.

Proposition 1 (Uniqueness). *Let A and B be positive semi-definite operators. For any $c \in V$, if (u_1, λ_1) and (u_2, λ_2) are solutions of the quasi-projection equations* (q1) *and* (q2) *then $u_1 = u_2$, $A\lambda_1 = A\lambda_2$ and $B\lambda_1 = B\lambda_2$.*

Proof. Let $u := u_1 - u_2$ and $\lambda := \lambda_1 - \lambda_2$. Then we have $u - A\lambda = 0$ and $(A + B)\lambda = 0$. By Lemma 1 we get $A\lambda = B\lambda = 0$. Then $u = A\lambda = 0$. $\square$

The following proposition shows that solutions of the quasi-projection equations always exist.

Proposition 2 (Existence). *Let A and B be positive semi-definite operators. For all $c \in V$, there exist u and λ in V satisfying the quasi-projection equations* (q1) *and* (q2).

Proof. It clearly suffices to show that there is a λ in V such that $(A+B)\lambda = (B-A)c$. In other words, we need to see that $(B-A)c \in \mathrm{Range}(A+B) = \mathrm{Range}.A + \mathrm{Range}.B$. For this we simply note $(B-A)c = A(-c) + Bc \in \mathrm{Range}.A + \mathrm{Range}.B$. $\square$

Let $!(A,B) : V \to V$ denote the linear operator on V which maps a vector c to the unique vector u which satisfies the following condition: There exists $\lambda \in V$, such that the pair (u,λ) satisfies the quasi-projection equations (q1) and (q2). We call the vector $u = \,!(A,B).c$ the **quasi-projection** of c onto the intersection of Range.A and Range.B. Following [1] we call $!(A,B)$ the **parallel sum** of A and B (even though there is a difference of a factor of 2).

For any linear map M between inner product spaces let M^* denote the **adjoint** map which is defined by the following condition: for all x in the domain of M and all y in the codomain of M, $\langle Mx, y\rangle = \langle x, M^*y\rangle$. The following proposition shows how quasi-projection behaves with respect to congruence.

Proposition 3 (Congruence). *Let $M : V \to V$ be any invertible linear map. Then $M(!(A,B))M^* = \,!(MAM^*, MBM^*)$.*

Proof. The pair of equations (eq1) and (eq2) is equivalent to the following pair:

$$Mu = MAM^*(M^*)^{-1}(c+\lambda),$$
$$MAM^*(M^*)^{-1}(c+\lambda) = MBM^*(M^*)^{-1}(c-\lambda).$$

Hence, for all c in V, we have

$$M(!(A,B))c = \,!(MAM^*, MBM^*)(M^*)^{-1}c. \qquad \square$$

Let U and V be inner product spaces and let $L : U \to V$ be a linear map. We use L^+ to denote the Moore–Penrose pseudo-inverse of L. (see, for example, [12]). We list the following properties of the pseudo-inverse

$$L^{*+} = L^{+*}, \quad LL^+L = L, \quad L^+LL^+ = L^+,$$

and note that LL^+ is the projection of V onto Range.L and L^+L is the projection of U onto Range.L^*.

Lemma 2. *Let A and B be positive semi-definite operators on an inner product space V. Then*

$$A = A(A+B)(A+B)^+ = A(A+B)^+(A+B)$$
$$= (A+B)(A+B)^+A = (A+B)^+(A+B)A.$$

Proof. Note that $P := (A+B)(A+B)^+ = (A+B)^+(A+B)$ is the projection of V onto the range of $A+B$. In particular, by Lemma 1, for all x in the range of A, we have $Px = x$. Also note that $V = \mathrm{Range}.A \oplus \mathrm{Kernel}.A$ since $(\mathrm{Range}.A)^\perp = \mathrm{Kernel}.A^* = \mathrm{Kernel}.A$.

Now consider any $x \in V$. Note that $PAx = Ax$ because Ax is in the range of A which is a subset of the range of $A+B$. Hence $A = PA$. Since A is self-adjoint we also have $A = AP$. $\square$

The following proposition is our main result concerning quasi-projections. We shall use it below to design zero-preserving flows.

Proposition 4 (Quasi-projection formulas). *Let A and B be positive semi-definite operators. Then the quasi-projection operator is given by the following formulas*:

$$!(A, B) = 2A(A + B)^+B = 2B(A + B)^+A.$$

Furthermore, the quasi-projection operator is positive semi-definite and

$$\mathrm{Range}(!(A, B)) = \mathrm{Range}.A \cap \mathrm{Range}.B,$$
$$\mathrm{Kernel}(!(A, B)) = \mathrm{Kernel}.A + \mathrm{Kernel}.B.$$

Proof

Claim. $!(A, B) = 2A(A + B)^+B$.

We take $\lambda := (A + B)^+(B - A)c$. This λ satisfies the quasi-projection equation (q2). Substituting in equation (q1), we get $u = !(A, B)c = (A(A + B)^+(B - A) + A)c$. Using Lemma 2, we get $A(A + B)^+(B - A) + A = 2A(A + B)^+B$.

Claim. $A(A + B)^+B = A - A(A + B)^+A$.

Using Lemma 2 again yields $A - A(A + B)^+A = A(A + B)^+(A + B) - A(A + B)^+A = A(A + B)^+B$.

Claim. *The map $A(A + B)^+B$ is self-adjoint.*

Use the previous claim and the fact that $(A + B)^+ = (A + B)^{*+} = (A + B)^{+*}$.

Claim. $A(A + B)^+B = B(A + B)^+A$.

Use the previous claim and $(A(A + B)^+B)^* = B(A + B)^+A$.

Claim. $\mathrm{Kernel}(!(A, B)) = \mathrm{Kernel}.A + \mathrm{Kernel}.B$.

By the formulas for the quasi-projection, we see that its kernel contains $\mathrm{Kernel}.A$ and $\mathrm{Kernel}.B$ and hence $\mathrm{Kernel}.A + \mathrm{Kernel}.B$. We need to prove the other inclusion; in other words, we want to see that the following statement is true:

$$\forall z \in \mathrm{Kernel}.(!(A, B)), \exists x, y \in V, z = x + y, Ax = 0, By = 0.$$

Consider any z satisfying $0 = !(A, B)z = 2A(A + B)^+Bz$. Take $x := (A + B)^+Bz$. Note $Ax = 0$. Using Lemma 2 again we also have $Bx = (A + B)x = (A + B)(A + B)^+Bz = Bz$. Hence $B(z - x) = 0$. We can take $y := z - x$.

Claim. $\mathrm{Range}(!(A, B)) = \mathrm{Range}.A \cap \mathrm{Range}.B$.

Take orthogonal complements of the previous claim.

Claim. *The map* $!(A, B)$ *is positive semi-definite.*

Note that the range of $A + B$ is an invariant subspace of $!(A, B)$. Clearly we only need to see that the restriction of $!(A, B)$ to this range is positive semi-definite. Consequently we assume that $V = \text{Range}(A + B)$. In this case we have $!(A, B) = 2A(A + B)^{-1}B = 2B(A + B)^{-1}A$. We now view A and B as matrices. Since $A + B$ is positive definite and A is self-adjoint, we can simultaneously diagonalize these two matrices by a congruence. (See, for example, [5].) In particular, there is an invertible matrix M and a diagonal matrix $D := \text{diag}(a_1^2, \ldots, a_n^2)$ such that $M(A + B)M^* = I$ and $MAM^* = D$. We see from these equations that $E := MBM^*$ is also a diagonal matrix; in particular, $E = \text{diag}(b_1^2, \ldots, b_n^2)$ where the b_i^2 are defined by $a_i^2 + b_i^2 := 1$. Now we have (by the formula for the quasi-projection operator):

$$\begin{aligned} M(!(A, B))M^* &= 2MAM^*(M(A + B)M^*)^{-1}MBM^* \\ &= 2\text{diag}(a_1^2 b_1^2, \ldots, a_n^2 b_n^2). \end{aligned}$$

Thus $M(!(A, B))M^*$ is positive semi-definite and hence $!(A, B)$ is positive semi-definite. □

3. An iso-spectral flow which preserves zeros

As above, let $\Delta \subseteq \{1, 2, \ldots, n\} \times \{1, 2, \ldots, n\}$ be a set of pairs (i, j) of indices which satisfy the following conditions for all $i, j = 1, 2, \ldots, n$:

$$(i, i) \in \Delta, \tag{nz1}$$

$$(i, j) \in \Delta \text{ implies } (j, i) \in \Delta. \tag{nz2}$$

Recall that we are using $\text{Sym}(n)$ to denote the vector space of symmetric $n \times n$ matrices and we are using $\text{Sym}(\Delta)$ to denote the subspace of $\text{Sym}(n)$ consisting of the symmetric matrices which are zero outside of Δ. The set Δ of pairs of indices represents the nonzero pattern of interest. The first condition on Δ implies that the diagonal matrices are a subspace of $\text{Sym}(\Delta)$. The second condition simply says that the pattern Δ is symmetric. We want to consider some iso-spectral flows on $\text{Sym}(\Delta)$.

We use $[X, Y] := XY - YX$ to denote the **commutator** of two square matrices. Note that if X is symmetric and K is skew-symmetric then $[X, K]$ is symmetric. Furthermore, we use $O(n)$ to denote the orthogonal group. For a symmetric matrix X, let

$$\omega.X := O(n) \to \text{Sym}(n) : Q \mapsto QXQ^{\text{T}}.$$

Then the image of $\omega.X$ is the iso-spectral surface, $\text{Iso}(X)$, determined by X. We can regard $\omega.X$ as a map from one manifold to another. In particular we can differentiate this map at the identity I to obtain the following linear map:

$$D(\omega.X).I = \text{Tan}.O(n).I \to \text{Tan}.\text{Sym}(n).X : K \mapsto [K, X].$$

The space tangent to $O(n)$ at the identity I may be identified with the skew-symmetric matrices; in symbols,

$$\text{Tan}.O(n).I = \text{Skew}(n) := \{K \in R^{n\times n} : K^{\text{T}} = -K\}.$$

(See, for example, Curtis [6].) Clearly we can also identify Tan.Sym$(n).X$ with Sym(n). Hence, we define a map $l.X$ as a linear map from Skew(n) to Sym(n) by

$$l.X := D(\omega.X).I = \mathrm{Skew}(n) \to \mathrm{Sym}(n) : K \mapsto [K, X].$$

It is not hard to prove that the space tangent to Iso(X) at X is the image of the linear map $D(\omega.X).I$; in symbols,

$$\mathrm{Tan.Iso}(X).X = \{[K, X] : K \in \mathrm{Skew}(n)\}.$$

(For details see Warner [13, Chapter 3: Lie groups, Section: homogeneous manifolds].)

Recall that we are using the Frobenius inner product on n-by-n matrices: $\langle X, Y\rangle := \mathrm{Trace}(XY^{\mathrm{T}})$. We list a few properties of this inner product: $\langle XY, Z\rangle = \langle X, ZY^{\mathrm{T}}\rangle = \langle Y, X^{\mathrm{T}}Z\rangle$ and $\langle [X, Y], Z\rangle = \langle X, [Z, Y^{\mathrm{T}}]\rangle = \langle Y, [X^{\mathrm{T}}, Z]\rangle$.

The adjoint $(l.X)^*$ of $l.X$ is the following map:

$$(l.X)^* = \mathrm{Sym}(n) \to \mathrm{Skew}(n) : Y \mapsto [Y, X]$$

since, for every symmetric matrix Y and every skew-symmetric matrix K, $\langle [K, X], Y\rangle = \langle K, [Y, X]\rangle$. The composition of $l.X$ with its adjoint is a "double bracket":

$$(l.X)(l.X)^* = \mathrm{Sym}(n) \to \mathrm{Sym}(n) : Y \mapsto [[Y, X], X].$$

Note that for any $Y \in \mathrm{Sym}(n)$, we have that $(l.X)(l.X)^*.Y$ is tangent to the iso-spectral surface Iso(X) at X.

We shall also use the map $m : \mathrm{Sym}(n) \to \mathrm{Sym}(\Delta)$ which is defined as follows: For any symmetric matrix Y, let $m.Y$ denote the matrix defined by $m.Y(i, j) := Y(i, j)$ if (i, j) is in Δ and $m.Y(i, j) := 0$ if (i, j) is not in Δ. Note that m is the orthogonal projection of Sym(n) onto Sym(Δ). In particular, we have $m = m^* = m^2$.

We want to consider vector fields on Sym(Δ) which are iso-spectral. We can obtain such vector fields by quasi-projection. Let $v : \mathrm{Sym}(n) \to \mathrm{Sym}(n)$ be any smooth map on Sym(n). From v we can obtain an iso-spectral vector field on Sym(Δ) by quasi-projection as follows. For any symmetric matrix X, let $\rho.X := !(A.X, B.X)$ be the quasi-projection map determined by $A.X := (l.X)(l.X)^*$ and $B.X := m$. Since these latter two linear maps are positive semi-definite, the results of the last section apply here. We shall use those results without explicitly citing particular propositions. In particular, note that for any symmetric matrix Y, the symmetric matrix $\rho.X.Y$ is in the intersection of the range of $(l.X)(l.X)^*$ and m; in symbols,

$$\rho.X.Y \in \mathrm{Tan.Iso}(X).X \cap \mathrm{Sym}(\Delta).$$

We have the following iso-spectral vector field on Sym(Δ):

$$\mathrm{Sym}(\Delta) \to \mathrm{Sym}(\Delta) : X \mapsto \rho.X(v.X).$$

The corresponding differential equation is $X' = \rho.X(v.X)$. We can rewrite this differential equation as a differential (linear) algebraic equation as follows:

$$X' = (l.X)(l.X)^*(\lambda + v.X),$$
$$(l.X)(l.X)^*(\lambda + v.X) = m(-\lambda + v.X).$$

Note that the second of these equations is a linear equation for the unknown symmetric matrix λ. The vector field is determined by solving this second equation for λ and substituting the solution into the first equation.

Using the formulas for $l.X$ and $(l.X)^*$, we get

$$(l.X)(l.X)^*(\lambda + v.X) = [[\lambda + v.X, X], X].$$

Substituting this simplification into the differential algebraic equation, we get

$$X' = [[\lambda + v.X, X], X],$$
$$[[\lambda + v.X, X], X] = m(-\lambda + v.X).$$

We now turn our attention to a specific flow. This flow is determined by the optimization problem (Problem 1) that we mentioned in the introduction. We shall see that we can solve this problem by finding a vector field on $\mathrm{Sym}(\Delta)$ associated with the objective function f which is iso-spectral. We obtain $X - D$ for the gradient of f at X, in symbols $\nabla f.X = X - D$. We can get an iso-spectral vector field by orthogonal projection of $\nabla f.X$ onto the intersection $\mathrm{Tan.Iso}(X).X \cap \mathrm{Sym}(\Delta)$. We prefer to quasi-project instead. We simply substitute the negative of the gradient into the formulas given above. We get the following system:

$$X' = [[\lambda + D, X], X], \tag{de1}$$
$$[[\lambda + D, X], X] = -m(\lambda + X - D). \tag{de2}$$

We call the flow generated by this system the **quasi-projected gradient flow** determined by the objective function f. We summarize the properties of this flow in the following proposition.

Proposition 5. *Let D be a symmetric matrix. Then the system* (de1) *and* (de2) *generating the quasi-projected gradient flow has the following properties*:

(i) *The quasi-projected gradient flow preserves eigenvalues and the nonzero pattern of interest.*
(ii) *The function $f(X) := (1/2)\langle X - D, X - D\rangle$ is non-increasing along solutions of this system.*
(iii) *A point $E \in \mathrm{Sym}(\Delta)$ is an equilibrium point of this system iff it satisfies the conditions*

$$[\lambda + D, E] = 0, \quad \textit{and} \tag{e1}$$
$$m(\lambda + E - D) = 0 \tag{e2}$$

for some symmetric matrix λ.
(iv) *If a matrix $E \in \mathrm{Sym}(\Delta)$ commutes with D then E is an equilibrium point of this system.*

Proof. (i) That this flow preserves eigenvalues and the nonzero pattern of interest is clear from the discussion above. The vector field was chosen to have these properties. In particular, the vector field preserves the nonzero pattern because $X' = -m(\lambda + X - D)$ has the nonzero pattern of interest. Also the vector field preserves eigenvalues because $X' = [[\lambda + D, X], X]$ is tangent to the iso-spectral surface $\mathrm{Iso}(X)$ at X.

(ii) Let $X(t)$ be any solution of the differential equation. Then, since the quasi-projection operator $\rho.X =!((l.X)(l.X)^*, m)$ is positive semi-definite, we have

$$\begin{aligned}(f(X))' &= \langle \nabla f.X, X'\rangle = \langle \nabla f.X, \rho.X(-\nabla f.X)\rangle \\ &= -\langle \nabla f.X, \rho.X(\nabla f.X)\rangle \leqslant 0.\end{aligned}$$

(iii) Let $E \in \mathrm{Sym}(\Delta)$ satisfy conditions (e1) and (e2). Then clearly $[[\lambda + D, E], E] = [0, E] = 0$ and E is an equilibrium point of the system (de1), (de2). On the other hand, if $E \in \mathrm{Sym}(\Delta)$ is an equilibrium point then (de1) implies $[[\lambda + D, E], E] = 0$ and (de2) implies (e2). We then also get

$$0 = \langle [[\lambda + D, E], E], \lambda + D\rangle = \langle [\lambda + D, E], [\lambda + D, E]\rangle,$$

which implies (e1).

(iv) Take $\lambda := D - E$. Then (e2) is trivially satisfied and for (e1) we have

$$[\lambda + D, E] = [2D - E, E] = 2[D, E] = 0. \qquad \square$$

Remark. We should say a few words about convergence of this system. (We intend to discuss convergence more fully in a future paper.) Note that the map $\omega.A$ is a smooth map from $O(n)$ onto $\mathrm{Iso}(A)$. Hence $\mathrm{Iso}(A)$ is compact since $O(n)$ is compact. From part (i) of the proposition, we then see that every solution starting in the iso-spectral surface $\mathrm{Iso}(A)$ remains in that surface and is entire. (In particular,"blowup" is not possible.) Again using compactness, we see that every such solution has ω-limit points. If the equilibrium points on the iso-spectral surface are isolated (which we expect is usually true) then every solution that starts in the iso-spectral surface tends to an equilibrium point.

Note that if D is a diagonal matrix with distinct diagonal entries and E is a symmetric matrix then E commutes with D iff E is a diagonal matrix. It follows from part (iv) of the theorem that diagonal E is an equilibrium point of the quasi-projected gradient flow determined by D. In 2001 we conjectured that diagonal matrices were the only equilibrium points of this flow. In 2005 Bryan Shader found a counterexample to that conjecture. Here is a counterexample.

Example. Let a and b be real non-zero parameters and consider the non-diagonal, symmetric matrix

$$E := \begin{pmatrix} 0 & a & 0 \\ a & 0 & b \\ 0 & b & 0 \end{pmatrix}.$$

The matrix E has the distinct eigenvalues 0 and $\pm\sqrt{a^2 + b^2}$.

We set Δ as the non-zero pattern of E. We show, by suitably defining matrices D and λ, that E is an equilibrium point of the quasi-projected gradient flow, i.e. satisfies conditions (e1) and (e2).

Let y and z be real parameters and take $\lambda + D := yE + zE^2$. This clearly gives $[\lambda + D, E] = 0$, i.e. condition (e1) is satisfied. Furthermore,

$$\begin{aligned} m(\lambda + E - D) &= m(\lambda + D + E - 2D) = m((y + 1)E + zE^2) - 2D \\ &= (y + 1)E + z \cdot \mathrm{diag}(E^2) - 2D, \end{aligned}$$

where

$$E^2 = \begin{pmatrix} a^2 & 0 & ab \\ 0 & a^2 + b^2 & 0 \\ ab & 0 & b^2 \end{pmatrix} \quad \text{and} \quad \mathrm{diag}(E^2) = \begin{pmatrix} a^2 & 0 & 0 \\ 0 & a^2 + b^2 & 0 \\ 0 & 0 & b^2 \end{pmatrix}.$$

Now, by choosing $y = -1$ and defining $D := \frac{1}{2}z \cdot \mathrm{diag}(E^2)$, we arrive at $m(\lambda + E - D) = 0$, i.e. condition (e2) is satisfied. Furthermore, if $z \neq 0$ and $|a| \neq |b|$ then D has the required distinct diagonal entries.

A numerical experiment shows that the equilibrium point E with $a := 1$ and $b := 2$ and $z := 2$ is not stable.

We now conjecture that if D is a diagonal matrix with distinct diagonal entries then diagonal matrices are the only *stable* equilibrium points of the quasi-projected gradient flow determined by D.

4. Numerical results

We have implemented the quasi-projected gradient flow in a Matlab program. This flow is iso-spectral and preserves zeros as discussed in the previous section. In our implementation we assume that $\mathrm{Range}((l.X)(l.X)^* + m) = \mathrm{Sym}(n)$. This is generic behavior for the set of symmetric matrices with distinct eigenvalues as is shown in the following (long) remark.

Remark. A set S in a topological space T is called *nowhere-dense* if the interior of its closure is empty. A set $S \subset T$ is called *generic* if it is open and dense. Note that if S is closed then it is nowhere-dense iff $T \backslash S$ is generic.

Let V be a (finite-dimensional) vector space over the reals R and $f : V \to R$ a real-valued function on V. If $f(x)$ is a polynomial in the components of x with respect to some basis for V then f has this property for every choice of basis and we say that f is a *polynomial function*. In the following we use the standard topology on V.

Proposition. *Let $f : V \to R$ be a polynomial function. If f is not the zero polynomial then the variety*, $\mathrm{Variety}(f) := \{x \in V : f(x) = 0\}$, *of f is nowhere-dense.*

Proof. Note that the variety is closed. Suppose that the variety is not nowhere-dense. Then f vanishes on an open subset of V. It follows that f is identically 0. □

Here is an application involving determinants. Consider the determinant function $\det : R^{n\times n} \to R$. The set $\{M \in R^{n\times n} : \det .M = 0\}$ is nowhere-dense and closed. Hence the set of non-singular $n \times n$ matrices is generic in the set of $n \times n$ matrices.

Let V and W be vector spaces and let $f : V \to W$ be a map. Then f is a *polynomial map* if the components $f_i(x)$, $i = 1, \dots, \dim(W)$, with respect to some basis for W are polynomial functions. Note that the composition of two polynomial maps is a polynomial map.

Above we introduced the assumption that the map $(A.X + m) : \mathrm{Sym}(n) \to \mathrm{Sym}(n)$ with $A.X = (l.X)(l.X)^* = [[\cdot, X], X]$ is invertible for given $X \in \mathrm{Sym}(n)$. Here we show that this is generic behavior if X has distinct eigenvalues. Hence, consider the map $A.X := \mathrm{Sym}(n) \to \mathrm{Lin}(\mathrm{Sym}(n) \to \mathrm{Sym}(n)) : X \mapsto (Y \mapsto [[Y, X], X])$.

Proposition. *The set* $\{X \in \mathrm{Sym}(n) : \mathrm{Range}(A.X + m) = \mathrm{Sym}(n)\}$ *is generic in* $\mathrm{Sym}(n)$.

Proof. Consider the polynomial function $\mathrm{Sym}(n) \to R$ defined by $X \mapsto \det(A.X + m)$. (Here det is regarded as a real-valued function on the space of linear maps $\mathrm{Lin}(\mathrm{Sym}(n) \to \mathrm{Sym}(n))$.) Note that A and m are polynomial maps.) We show below that this function is not the zero function. Then we have that $\{X \in \mathrm{Sym}(n) : \det(A.X + m) = 0\}$ is nowhere-dense in $\mathrm{Sym}(n)$. Since this set is also closed we have that

$$\{X \in \mathrm{Sym}(n) : \mathrm{Range}(A.X + m) = \mathrm{Sym}(n)\}$$
$$= \mathrm{Sym}(n)\backslash\{X \in \mathrm{Sym}(n) : \det(A.X + m) = 0\}$$

is generic. To complete the proof, we show that the function $X \mapsto \det(A.X + m)$ is not the zero function. Take $X = D := \mathrm{diag}(d_1, \ldots d_n)$ where the d_i are distinct. Then $A.D.Y(i, j) = (d_i - d_j)^2 Y(i, j)$. Furthermore, the range of m includes the diagonal matrices. These properties together show that $\mathrm{Range}(A.D + m) = \mathrm{Sym}(n)$ and hence $\det(A.D + m) \neq 0$. This is the end of our long remark concerning generic sets. □

We solve numerically for $t > 0$ the initial value problem for $X(t)$ given by

$$X' = g(X) := 2m((l.X)(l.X)^* + m)^{-1}(l.X)(l.X)^*.(D - X), \quad X(0) = X_0,$$

where $X_0 \in \mathrm{Sym}(\Delta)$ (Δ is defined by the nonzero pattern of X_0 and kept constant) and D is the diagonal matrix, $D := \mathrm{diag}(1, 2, \ldots, n)$. We refer to this flow as the **Zero flow** in the discussion of the examples and in the figures below.

The assumption on the ranges of $(l.X)(l.X)^*$ and m guarantees the existence of the inverse in the right-hand side of the differential equation. This assumption is not satisfied in general as the following example demonstrates.

Example. Let X be the circulant matrix with -2 on the diagonal and 1 on the first sub- and super-diagonal (and the corresponding corner entries). The pattern Δ is defined as the nonzero pattern of X. Now let Y be any circulant matrix with nonzero pattern completely outside of Δ, i.e. $m.Y = 0$. If $n = 4$ this is, for instance, achieved by selecting Y as the matrix with ones on second sub- and super-diagonal. Since circulant matrices commute with each other, and by the choice of the nonzero pattern of Y we have $((l.X)(l.X)^* + m)Y = 0$. Thus Y is a non-trivial element in the kernel of the map and hence the inverse does not exist.

By construction of the flow, the matrix $g(X(t)) \in \mathrm{Sym}(\Delta)$ for all $t \geqslant 0$ and when integrating the differential equation we ignore all matrix elements outside the pattern Δ (these remain zero for all $t > 0$). Therefore the dimension of our differential equation is reduced to the cardinality of Δ which may be significant less than n^2. (We have currently not taken into account the symmetry of the matrices.) However, we remark that we obtain intermediate matrices, when evaluating the expression for $g(X(t))$ from the right to the left, which can have nonzero entries outside of Δ.

For the numerical solution of the initial value problem we employ Matlab's explicit Runge–Kutta method of order 4(5) (`ode45`) with absolute and relative tolerance requirement set to 10^{-13}. These very stringent accuracy requirements reflect the fact that we are currently interested in very accurate solutions to the initial value problem and not (yet) in competitive numerical schemes for the solution of sparse eigenvalue problems. Therefore, the cost of the numerical computations are not considered in the following.

During the course of integration we monitor two characteristic quantities of the flow.

1. The relative departure of the matrix $X(t)$ from the iso-spectral surface associated with the initial matrix X_0. In particular, we define

$$d_{\mathrm{ev}}(t) := \frac{\|\mathrm{ev}(X_0) - \mathrm{ev}(X(t))\|}{\|\mathrm{ev}(X_0)\|},$$

where $\mathrm{ev}(X)$ is the vector of sorted eigenvalues of X. This quantity measures the quality of the time integration and should be approximately constant in time and near the machine accuracy (10^{-14}).

2. The relative size of the off-diagonal elements of $X(t)$ (with respect to X_0). In particular, we define

$$d_{\mathrm{off}}(t) := \frac{\|X(t) - \mathrm{diag}(X(t))\|_{\mathrm{F}}}{\|X_0 - \mathrm{diag}(X_0)\|_{\mathrm{F}}},$$

where $\mathrm{diag}(X)$ is the matrix containing the diagonal part of X and $\|\cdot\|_{\mathrm{F}}$ is the Frobenius norm. This quantity measures the convergence of the flow to a diagonal steady state and in conjunction with a constant value of $d_{\mathrm{ev}}(t)$ the convergence to the diagonal matrix with elements corresponding to the eigenvalues of X_0.

We compare the Zero flow with the "double-bracket (DB) flow". That is, we also numerically solve the initial value problem

$$X' = h(X) := [[D, X], X], \quad X(0) = X_0,$$

where $X_0 \in \mathrm{Sym}(n)$ and D is the same diagonal matrix as above. This flow is also iso-spectral and converges to a diagonal matrix steady state with the eigenvalues of X_0 on the diagonal. (See Driessel [7].) It does not preserve the zero pattern of the initial matrix X_0 and considerable fill-in can appear. The double-bracket flow coincides with the Toda flow if X_0 is a tridiagonal matrix.

We consider three different kinds of initial data in the next three subsections.

4.1. Example 1

Here the initial value X_0 is a symmetric, tridiagonal random matrix of dimension 6:

$$X_0 := \begin{pmatrix} 0.87 & 1.23 & 0 & 0 & 0 & 0 \\ 1.23 & 1.67 & 0.62 & 0 & 0 & 0 \\ 0 & 0.62 & 0.25 & 1.17 & 0 & 0 \\ 0 & 0 & 1.17 & 0.79 & 1.87 & 0 \\ 0 & 0 & 0 & 1.87 & 1.92 & 1.63 \\ 0 & 0 & 0 & 0 & 1.63 & 1.8 \end{pmatrix}.$$

We note that the DB flow preserves the tridiagonal pattern but we do not exploit this fact in our implementation.

We simulate the solution with this initial value until $t = 60$ for both flows. The maximum value of $d_{\mathrm{ev}}(t) \approx 7 \times 10^{-14}$ for the Zero flow and $\approx 2 \times 10^{-14}$ for the DB flow. This shows that for both flows the eigenvalues of the initial matrix are preserved up to machine accuracy in the numerical solution. In Fig. 1, we plot the monitored values of $d_{\mathrm{off}}(t)$ for both flows. We observe that both converge to zero and that this happens slightly faster for the DB flow initially but later the Zero flow converges faster and reaches machine accuracy before the DB flow. The results of this example show that for tridiagonal matrices the Toda flow is different than our zero flow.

4.2. Example 2

In this example the initial value X_0 is a symmetric random matrix of dimension 10 with a random zero pattern:

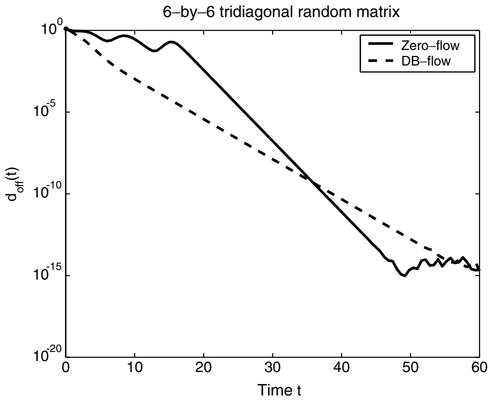

Fig. 1. Convergence history of the off-diagonal elements of the solution of Example 1 for the Zero and the DB flow.

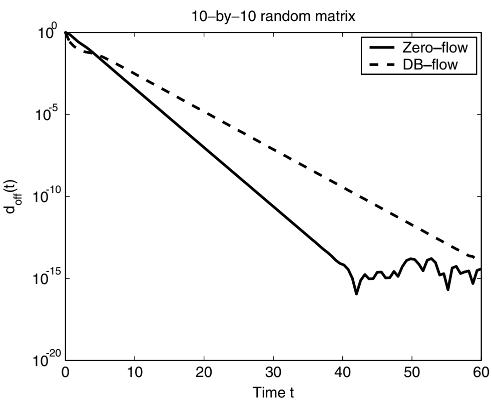

Fig. 2. Convergence history of the off-diagonal elements of the solution of Example 2 for the Zero and the DB flow.

$$X_0 := \begin{pmatrix} 1.7 & 0 & 0 & 0 & 0 & 0 & 1.92 & 0 & 0.48 & 1.25 \\ 0 & 1.16 & 1.16 & 0.91 & 1.56 & 0 & 0 & 1.69 & 0 & 0 \\ 0 & 1.16 & 0.48 & 0 & 0.90 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.91 & 0 & 0.66 & 0.88 & 0 & 0.93 & 1.25 & 0 & 1.39 \\ 0 & 1.56 & 0.9 & 0.88 & 0.3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.94 & 1.49 & 0.37 & 0.88 & 0 \\ 1.92 & 0 & 0 & 0.93 & 0 & 1.49 & 1.12 & 0.67 & 0.4 & 0 \\ 0 & 1.69 & 0 & 1.25 & 0 & 0.37 & 0.67 & 1.1 & 0 & 1.54 \\ 0.48 & 0 & 0 & 0 & 0 & 0.88 & 0.4 & 0 & 0.44 & 1.05 \\ 1.25 & 0 & 0 & 1.39 & 0 & 0 & 0 & 1.54 & 1.05 & 1.2 \end{pmatrix}.$$

We simulate the solution with this initial value until $t = 60$ for both flows. The maximum value of $d_{\mathrm{ev}}(t) \approx 2 \times 10^{-14}$ for the Zero flow and $\approx 6 \times 10^{-15}$ for the DB flow. This shows that for both flows the eigenvalues of the initial matrix are preserved up to machine accuracy in the numerical solution. In Fig. 2, we plot the monitored values of $d_{\mathrm{off}}(t)$ for both flows. We observe that both converge to zero and that this happens slightly faster for the Zero flow.

4.3. Example 3

In the third example we consider tridiagonal matrices which arise when one discretizes the boundary value problem $u_{xx} = 0, u(0) = u(1) = 0$ by standard second-order central differences. Let $T_n := \text{tridiag}(1, -2, 1) \in \text{Sym}(n)$ and $\tilde{T}_n := (n + 1)^2 T_n$. Hence $\tilde{T}_n$ corresponds to the discretization matrix of the boundary value problem on an equidistant grid with grid width $h := 1/(n + 1)$. The eigenvalues of both, T_n and $\tilde{T}_n$, are distinct and negative. We present results for the four cases $X_0 = T_5, T_{10}, \tilde{T}_5$, and $\tilde{T}_{10}$ in Fig. 3.

We run these experiments to different final times as can be seen in the plots. We note that the values of $d_{\text{ev}}(t)$ are in the range 10^{-15} to 10^{-13} for all values of t considered. Again this demonstrates that the numerical solution does only insignificantly drift off the iso-spectral surface associated with the initial matrix. Both the Zero flow and the DB flow converge to the diagonal matrix containing the eigenvalues of the initial data. However, whereas the Zero flow does so much faster than the DB flow for the matrices T_n, the situation is the opposite for the scaled

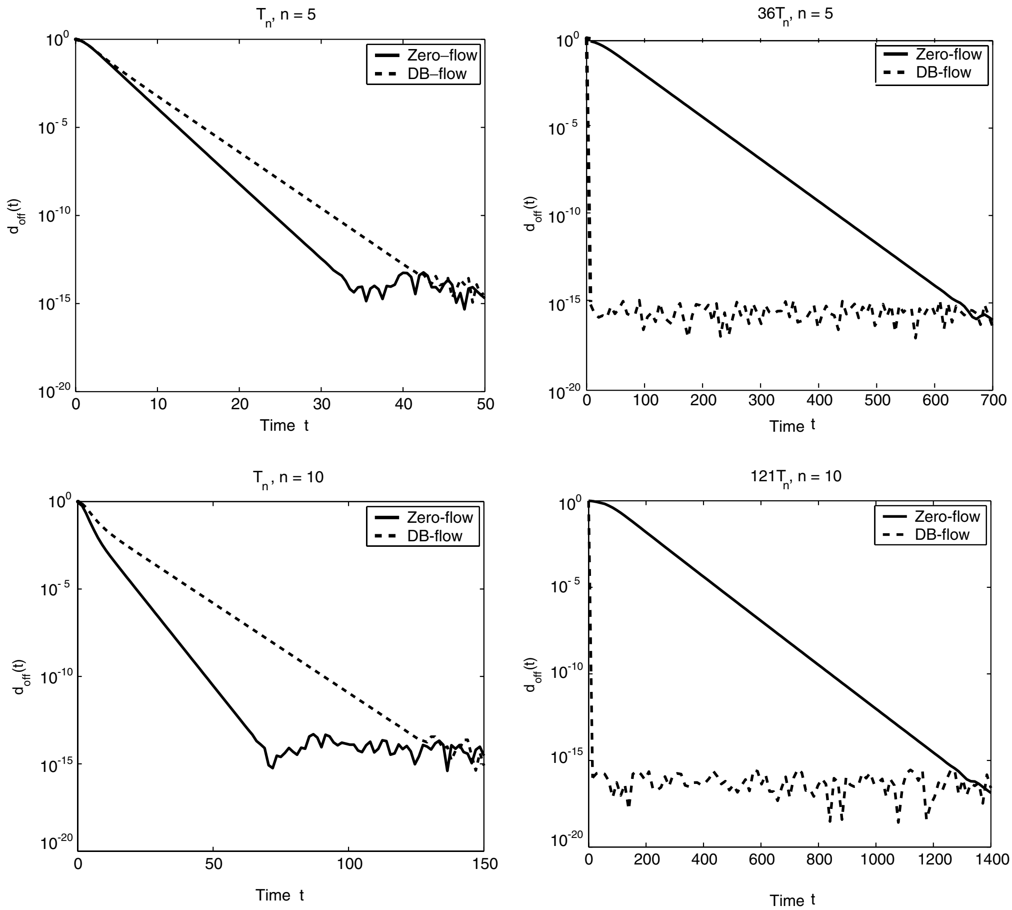

Fig. 3. Convergence history of the off-diagonal elements of the solutions of Example 3 for the Zero and the DB flow for initial conditions $X_0 = T_5$ (top left), $X_0 = \tilde{T}_5 = 36T_5$ (top right), $X_0 = T_{10}$ (bottom left), and $X_0 = \tilde{T}_{10} = 121T_{10}$ (top right).

matrices $\tilde{T}_n$. The change in the convergence speed of the DB flow for different initial matrices T_n and $\tilde{T}_n$ is precisely explained by the following proposition.

Proposition 6. *If $X(t)$ is the solution of the double-bracket flow with initial value X_0 then $cX(ct)$ is the solution of the double-bracket flow with initial value cX_0, $c > 0$.*

Proof. We can write $h(cX) = [[D, cX], cX] = c^2[[D, X], X] = c^2h(X)$. This relation gives the desired scaling result. $\square$

We have not analyzed how scaling affects the Zero flow.

Acknowledgments

We wrote most of this paper during the Fall of 2001 while visiting the Fields Institute for Research in Mathematical Sciences in Toronto, Ontario. We wish to thank all the people at the institute who extended hospitality to us during this pleasant visit, especially Ken Jackson (one of the organizers of the Thematic Year on Numerical and Computational Challenges in Science and Engineering at the Institute) and Ken Davidson (head of the institute). In addition to these people, we wish to thank colleagues who discussed iso-spectral flows with us during this visit and offered advice and encouragement: Chandler Davis (University of Toronto), Itamar Halevy (University of Toronto), Peter Miegom (Fields Institute), and John Pryce (Cranfield University, UK).

Further, Alf Gerisch acknowledges financial support from the Fields Institute for Research in Mathematical Sciences and the University of Guelph.

In 2003 and 2006, we received constructive comments from referees. We thank them. In particular, the earlier referee suggested that we compare projections and quasi-projections. We added an appendix to the longer version Gerisch and Driessel [8] of our paper (based on our research notes of 2001) in which we make such a comparison.

References

[1] W.N. Anderson Jr., R.J. Duffin, Series and parallel addition of matrices, J. Math. Anal. Appl. 26 (1969) 576–594.
[2] W.N. Anderson Jr., Shorted operators, SIAM J. Appl. Math. 20 (1971) 520–525.
[3] W.N. Anderson Jr., M. Schreiber, The infimum of two projections, Acta Sci. Math. 33 (1972) 165–168.
[4] W.N. Anderson Jr., G.E. Trapp, Shorted operators II, SIAM J. Appl. Math. 28 (1975) 60–71.
[5] R. Bellman, Introduction to Matrix Analysis, McGraw-Hill, 1970.
[6] M.L. Curtis, Matrix Groups, Springer-Verlag, 1984.
[7] K.R. Driessel, Computing canonical forms using flows, Linear Algebra Appl. 379 (2004) 353–379.
[8] K.R. Driessel, A. Gerisch, Zero-preserving iso-spectral flows based on parallel sums, 2006. arxiv:math.GM/0605243. Available from: <http://arxiv.org>.
[9] D. Fasino, Iso-spectral flows on displacement structured matrix spaces, in: D. Bini, E. Tyrtyshnikov, P. Yalamov (Eds.), Structured Matrices: Recent Developments in Theory and Computation, Nova Science Publisher Inc., 2001.
[10] M.W. Hirsch, S. Smale, R.L. Devaney, Differential Equations, Dynamical Systems & An Introduction to Chaos, second ed., Elsevier, 2004.
[11] K. Kubo, T. Ando, Means of positive linear operators, Mathematische Annalen 246 (1980) 205–224.
[12] C. Lawson, R. Hanson, Solving Least Squares Problems, Prentice-Hall, Inc., 1974.
[13] F.W. Warner, Foundations of Differential Manifolds and Lie Groups, Springer-Verlag, 1983.