A new constrained optimization model for solving the nonsymmetric stochastic inverse eigenvalue problem

Gabriele Steidl\textsuperscript{a} and Maximilian Winkler\textsuperscript{b}

\textsuperscript{a}Department of Mathematics, TU Berlin, Berlin, Germany; \textsuperscript{b}Department of Mathematics, Technische Universität Kaiserslautern, Kaiserslautern, Germany

ABSTRACT

The stochastic inverse eigenvalue problem aims to reconstruct a stochastic matrix from its spectrum. Recently, Zhao et al. [A geometric nonlinear conjugate gradient method for stochastic inverse eigenvalue problems. SIAM J Numer Anal. 2016;54(4):2015–2035] proposed a constrained optimization model on the manifold of so-called isospectral matrices and adapted a modified Polak-Ribière-Polyak conjugate gradient method to the geometry of this manifold. However, not every stochastic matrix is an isospectral one and the model in Zhao et al. is based on the assumption that for each stochastic matrix there exists a (possibly different) isospectral, stochastic matrix with the same spectrum. We are not aware of such a result in the literature, but prove the claim at least for 3 \times 3 matrices. In this paper, we suggest to extend the above model by considering matrices which differ from isospectral ones only by multiplication with a block diagonal matrix with 2 \times 2 blocks from the special linear group. First, we show that each stochastic matrix can be written in such a form. We prove that our model has a minimizer and show how the Polak–Ribiére–Polyak conjugate gradient method works on the corresponding more general manifold. We demonstrate by numerical examples that the new, more general method performs similarly as those in Zhao et al.

1. Introduction

Stochastic matrices arise in many applications and have recently got the author’s attention in a labelling approach in imaging science \cite{1, 2}. In this paper, we are interested in the inverse eigenvalue problem for stochastic matrices (StIEP) i.e. in finding a (nonsymmetric) stochastic matrix with this prescribed spectrum. Problems of this kind arise, e.g. in applied mechanics, molecular spectroscopy or control theory, see \cite{3, 4} and the references therein. StIEP is closely related to the problem of finding a matrix with nonnegative entries and prescribed spectrum, called NIEP. This is due to the fact that for any nonnegative matrix \( A \) with positive maximal eigenvalue \( \rho(A) \) and corresponding positive eigenvector \( u \), the
matrix $\rho(A)^{-1} \text{diag}(u)^{-1} A \text{diag}(u)$ is a stochastic one, see [4]. There exists a large literature on existence conditions of solutions of StIEP and NIEP for special settings. Sufficient conditions in case of a real-valued set of eigenvalues were first given in [5], continued by Perfect [6]. Karpelevic [7] completely characterized the set of points $\Theta_n$, which contains the eigenvalues of any stochastic $n \times n$ matrix. This does not mean that each $n$-tupel of real and complex conjugate points from $\Theta_n$ is the spectrum of a stochastic matrix. The complete statement of Karpelevic’s theorem is rather lengthy, see also [8, Theorem 1.8]. A shorter formulation can be found in [9] and a more constructive view was recently given in [10]. For further results, we refer to the survey papers [11, 12] and the monographs [4, 13]. However, the general question under which conditions on the eigenvalues a solution of StIEP exists, is still open.

Besides theoretical results, there exist certain numerical approaches to solve StIEP or NIEP. In [14, 15], stochastic matrices with given real-valued eigenvalues fulfilling additional assumptions are constructed explicitly with recursive algorithms. These assumptions are in particular fulfilled if all eigenvalues are positive with maximum 1. In [16], an alternating projection – like algorithm was proposed for solving NIEP without further assumptions on the eigenvalue set.

Another class of algorithms aims to minimize a certain cost function based on matrix factorizations using optimization methods which perform a descend on the underlying matrix manifolds. A first method in this direction was given by Chu [17], who treated the symmetric NIEP by solving for a given vector $\Lambda$ of eigenvalues

$$
\min_{Q,B} \frac{1}{2} \|B \circ Q - Q^T Q \text{diag}(\Lambda)\|_F^2 \quad \text{subject to } Q \in O(n), \quad B \in \mathbb{R}^{n,n},
$$

where $O(n)$ is the set of orthogonal matrices, $\circ$ denotes the componentwise product and $\| \cdot \|_F$ is the Frobenius norm. The above problem is manifold constrained in the variable $Q$ and a gradient flow with Riemannian gradient on $O(n)$ was applied. Extending the idea to not necessarily symmetric nonnegative matrices, a similar approach was developed later in [18]. After creating a real Jordan form $J(\Lambda)$ with the given real and imaginary parts of the eigenvalues, a gradient flow method for minimizing

$$
\min_{Q,B} \frac{1}{2} \|B \circ T - Q^T Q T^{-1}\|_F^2 \quad \text{subject to } T \in \text{GL}(n,\mathbb{R}), \quad B \in \mathbb{R}^{n,n},
$$

where $\text{GL}(n,\mathbb{R})$ denotes the (open) manifold of invertible $n \times n$ matrices, was proposed, where a singular value decomposition of the matrix $T$ is used to overcome the instabilities due to the matrix inverse. Apart from promising numerical results, the authors report several problems: the existence of a minimizer is unclear, there is no guarantee for the matrix $T$ to stay bounded during the algorithm, and for several choices of initial values it appears that $T$ converges to a singular matrix.

Recently, a model for solving StIEP also for nonsymmetric matrices together with a geometric optimization method, namely a conjugate gradient descent algorithm in a modified version of Polak–Ribiére–Polyak, was proposed by Zhao et al. [19]. The minimization is basically done over the product manifold of the orthogonal matrices and matrices with rows on the unit sphere of $\mathbb{R}^n$. The model is based on the assumption that StIEP has a solution if and only if the set of so-called isospectral matrices $\text{Iso}(\Lambda)$ associated to the given
vector of eigenvalues $\Lambda$ contains a stochastic matrix. While it is clear that the problem has a solution if $\text{Iso}(\Lambda)$ contains a stochastic matrix, the opposite direction is to the best of our knowledge not proved so far.

In this paper, we propose an extension of the model in [19] by special blockdiagonal matrices whose $2 \times 2$ blocks are special linear matrices and correspond to the complex conjugate eigenvalue pairs of the matrix. Our model has the advantage that every stochastic matrix can be written in the novel form which was not the case for isospectral matrices. We also use a geometric conjugate gradient algorithm for the minimization which performs on the manifold extended by the product of $\text{SL}(2)$ matrices. In contrast to [19], the Riemannian inner product of this manifold depends on the respective tangent space. Our method appears to be slightly slower than in the model [19], which is not surprising, since we have to minimize over more parameters. In general, StIEP remains a severely ill posed problem and the performance of all algorithms heavily depends on the distribution of the given eigenvalues.

The outline of this paper is as follows: in Section 2, we provide the preliminaries and motivate our model based on the fact that it is not clear if for any stochastic matrix there exists a (possibly different) isospectral, stochastic matrix with the same spectrum. Using the discrete Fourier transform, we prove that the above conjecture is at least correct for stochastic $3 \times 3$ matrices in Section 3. Here the reader may get an idea why its proof appears to be hard for arbitrary matrix sizes. In Section 4, we introduce our novel model based on those presented by Zhao et al. [19]. We prove that the new cost function has compact level sets which implies the existence of a (global) minimizer. We give a short introduction to conjugate gradient algorithms on manifolds in Section 5 and compute the required expressions for our special manifold in Section 6. We consider an additional parameter update step in linesearch which seems to accelerate the performance slightly for the model in [19] and is also needed in the convergence proof. Theorem 6.3 states a convergence result for the conjugate gradient method on our manifold. Since many, but not all parts of the proof follow the ideas in [19], we swap it to the appendix. In Section 7, we demonstrate by numerical experiments that our method is competitive with the one in [19], but slightly more costly.

2. Preliminaries

By Schur’s theorem we know that for every matrix $A \in \mathbb{C}^{n,n}$ there exists a unitary matrix $U \in \mathbb{C}^{n,n}$ such that $A = UBU^*$, where $B$ is an upper triangular matrix having the eigenvalues of $A$ on its diagonal. For real-valued matrices this result can be specified by the following theorem, see, e.g. [20, Theorems 2.3.1, 2.3.4]. Recall that the nonreal eigenvalues of a real-valued matrix appear in conjugate pairs. By $\text{O}(n)$ we denote the set of orthogonal $n \times n$ matrices.

**Theorem 2.1:** Let $A \in \mathbb{R}^{n,n}$ be an arbitrary matrix with real eigenvalues $\lambda_1, \ldots, \lambda_s$ and complex eigenvalues $\lambda_{s+1}, \ldots, \lambda_n \in \mathbb{C} \setminus \mathbb{R}$ appearing in conjugate pairs $\lambda_{s+2j} = \bar{\lambda}_{s+2j-1}$, $j = 1, \ldots, t$, $t = \lfloor n/2 \rfloor$. Let $\Lambda := (\lambda_1, \ldots, \lambda_n)^T$. Then the following holds true:

(i) There exists a real-valued, invertible matrix $T \in \mathbb{R}^{n,n}$ such that

$$A = T(D(\Lambda) + V)T^{-1},$$
where

\[
D(\Lambda) := \begin{pmatrix}
\lambda_1 & 0 & \ldots & \ldots & \ldots & 0 \\
0 & \lambda_2 & 0 & \ldots & \ldots & 0 \\
0 & 0 & \ddots & 0 & \ldots & 0 \\
0 & 0 & 0 & \lambda_s & 0 & \ldots & 0 \\
0 & 0 & 0 & 0 & \lambda_1^{[2]} & 0 & \ldots & 0 \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & 0 & 0 & 0 & 0 & \lambda_t^{[2]}
\end{pmatrix}
\]

with

\[
\lambda_j^{[2]} := \begin{pmatrix}
\text{Re}(\lambda_{s+2j}) & \text{Im}(\lambda_{s+2j}) \\
-\text{Im}(\lambda_{s+2j}) & \text{Re}(\lambda_{s+2j})
\end{pmatrix}, \quad j = 1, \ldots, t,
\]

and \(V \in V_t\). Here \(V_t\) denotes the set of upper triangular matrices with zeros on the diagonal and \(v_{s+2j-1,s+2j} = 0\) for all \(j = 1, \ldots, t\). If \(A\) has only real eigenvalues, then \(T\) can be chosen as an orthogonal matrix.

(ii) There exists a matrix \(Q \in O(n)\) such that

\[
A = Q(\tilde{D}(\Lambda) + V)Q^T
\]

with

\[
\tilde{D}(\Lambda) := \begin{pmatrix}
\lambda_1 & 0 & \ldots & \ldots & \ldots & 0 \\
0 & \lambda_2 & 0 & \ldots & \ldots & 0 \\
0 & 0 & \ddots & 0 & \ldots & 0 \\
0 & 0 & 0 & \lambda_s & 0 & \ldots & 0 \\
0 & 0 & 0 & 0 & \mu_1^{[2]} & 0 & \ldots & 0 \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & 0 & 0 & 0 & 0 & \mu_t^{[2]}
\end{pmatrix}
\]

where \(\mu_j^{[2]} \in \mathbb{R}^{2,2}\) is a matrix with eigenvalues \(\tilde{\lambda}_{s+2j}, \lambda_{s+2j}, j = 1, \ldots, t\) and \(V \in V_t\).

It is in general not possible to choose matrices \(\mu_j^{[2]}\) in Part (ii) of the theorem of the special form \(\lambda_j^{[2]}\) from Part (i), as the Example 3.1 in the next section shows. For a given vector

\[
\Lambda := (\lambda_1, \ldots, \lambda_n)^T, \lambda_1, \ldots, \lambda_s
\]

\(\in \mathbb{R}, \lambda_{s+1}, \ldots, \lambda_n \in \mathbb{C} \setminus \mathbb{R}, \lambda_{s+2j} = \tilde{\lambda}_{s+2j-1}, j = 1, \ldots, t,
\]

(1)
where \( t = (n - s)/2 \), let \( D(\Lambda) \) and \( \mathcal{V}_i \) be defined as in Theorem 2.1(i) and

\[
\text{Iso}(\Lambda) := \{A := Q(D(\Lambda) + V)Q^T : Q \in O(n), \, V \in \mathcal{V}_i\}.
\]

The set \( \text{Iso}(\Lambda) \) is known as set of isospectral matrices associated with \( \Lambda \). In the following, we will use \( \Lambda \) likewise as set of eigenvalues or as vector containing the eigenvalues, where the meaning becomes always clear from the context.

We are interested in the set of stochastic \( n \times n \) matrices

\[
S(n) := \{A \in \mathbb{R}^{n,n}_{\geq 0} : A1_n = 1_n\}
\]

\[
= \{S \circ S : \text{diag}(SS^T) = I_n, \, S \in \mathbb{R}^{n,n}\},
\]

where \( \circ \) denotes the componentwise product. For \( A \in S(n) \) we have \( A1_n = 1_n \), so that 1 is an eigenvalue of \( A \) with eigenvector \( 1_n \). Moreover, by the Frobenius–Perron theorem \([13, \text{Theorem 5.2.1}]\), all eigenvalues of \( A \) have absolute values not larger than 1.

We call a vector \( \Lambda \) whose nonreal components appear in conjugate pairs, self-conjugate. Given a self-conjugate vector \( \Lambda \) we are interested in finding a stochastic matrix having the components of \( \Lambda \) as eigenvalues. As already mentioned in the introduction, this problem has no solution for general self-conjugate vectors \( \Lambda \). In this paper, we examine the following problem:

\[(\text{StIEP}) \quad \text{Given a vector } \Lambda \text{ which entries are the eigenvalues of a stochastic matrix, find a stochastic matrix with these eigenvalues.}\]

**Remark 2.2:** In \([19]\), the authors claimed that (StIEP) has a solution if and only if \( \text{Iso}(\Lambda) \cap S(n) \neq \emptyset \). The authors develop a numerical algorithm to solve (StIEP) based on this claim. Clearly, if \( \text{Iso}(\Lambda) \cap S(n) \neq \emptyset \), then (StIEP) has a solution. However, we have not found a references that the converse is also true. In general, we do not know if it is possible that (StIEP) has a solution, but there is no solution with decomposition (2), i.e. \( \text{Iso}(\Lambda) \cap S(n) = \emptyset \).

At least for stochastic \( 3 \times 3 \) matrices there are some results in this direction which we summarize and partially prove in the next section.

### 3. Stochastic 3 \( \times \) 3 matrices

First, we give an example of a stochastic \( 3 \times 3 \) matrix which cannot be decomposed as in Theorem 2.1(ii) with \( \mu_1^{[2]} = \lambda_1^{[2]} \).

**Example 3.1:** Let \( A \in S(3) \cap \text{Iso}(\Lambda) \) with eigenvalue vector \( \Lambda = (1, \lambda, \lambda)^T, \, \lambda = \lambda_R + i\lambda_I, \, \lambda_I \neq 0 \). Then the matrix \( Q \in O(3) \) in the isospectral decomposition (2) of \( A \) has the normed eigenvector of \( A \) belonging to the eigenvalue 1 as first column, i.e. \( \pm \frac{1}{\sqrt{3}} 1_3 \). We denote the second column of \( Q \) by \( \sqrt{3}(q_1, q_2, q_3)^T \), where \( q_1 + q_2 + q_3 = 0 \) and \( q_1^2 + q_2^2 + q_3^2 = 1 \). Using the vector product of the first two columns of \( Q \in O(3) \), we conclude that,
up to sign changes of its columns, \( Q \) must have the form
\[
Q = \frac{1}{\sqrt{3}} \begin{pmatrix}
1 & \sqrt{3}q_1 & q_3 - q_2 \\
1 & \sqrt{3}q_2 & q_1 - q_3 \\
1 & \sqrt{3}q_3 & q_2 - q_1
\end{pmatrix} = \frac{1}{\sqrt{3}} \begin{pmatrix}
1 & \sqrt{3}q_1 & -q_1 - 2q_2 \\
1 & \sqrt{3}q_2 & 2q_1 + q_2 \\
1 & -\sqrt{3}(q_1 + q_2) & q_2 - q_1
\end{pmatrix}
\]
(3)
with
\[
q_1^2 + q_2^2 + q_1q_2 = \frac{1}{2}.
\]
Note that the last equation has a real solution if and only if \( q_2^2 \leq \frac{2}{3} \). Since \( A \in \text{Iso}(\Lambda) \), it holds
\[
Q^TAQ = \begin{pmatrix}
1 & u & v \\
0 & \lambda_R & \lambda_I \\
0 & -\lambda_I & \lambda_R
\end{pmatrix}
\]
for some \( u, v \in \mathbb{R} \), so that
\[
\sqrt{3}AQ = \begin{pmatrix}
1 & u + \sqrt{3}\lambda_R q_1 - \lambda_I (q_3 - q_2) & v + \sqrt{3}\lambda_I q_1 + \lambda_R (q_3 - q_2) \\
1 & u + \sqrt{3}\lambda_R q_2 - \lambda_I (q_1 - q_3) & v + \sqrt{3}\lambda_I q_2 + \lambda_R (q_1 - q_3) \\
1 & u + \sqrt{3}\lambda_R q_3 - \lambda_I (q_2 - q_1) & v + \sqrt{3}\lambda_I q_3 + \lambda_R (q_2 - q_1)
\end{pmatrix}.
\]
(4)
We want to show that the stochastic matrix
\[
A = \begin{pmatrix}
\frac{1}{2} & \frac{1}{2} & 0 \\
\frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\
1 & 0 & 0
\end{pmatrix}
\]
does not have a decomposition (2). The matrix \( A \) has the eigenvalues 1 and \( \frac{1}{12}(-1 \pm \sqrt{23}i) \).
Assume in the contrary that \( A \) has a decomposition (2). Comparison of the second and third columns of the matrices in (4) gives
\[
\frac{\sqrt{3}}{2}(q_1 + q_2) = u + \sqrt{3}\lambda_R q_1 - \lambda_I (q_3 - q_2),
\]
\[
0 = u + \sqrt{3}\lambda_R q_2 - \lambda_I (q_1 - q_3),
\]
\[
\sqrt{3}q_1 = u + \sqrt{3}\lambda_R q_3 - \lambda_I (q_2 - q_1),
\]
\[
\frac{1}{2}(q_1 - q_2) = v + \sqrt{3}\lambda_I q_1 + \lambda_R (q_3 - q_2),
\]
\[
0 = v + \sqrt{3}\lambda_I q_2 + \lambda_R (q_1 - q_3),
\]
\[
q_3 - q_2 = v + \sqrt{3}\lambda_I q_3 + \lambda_R (q_2 - q_1).
\]
(7)
Replacing \( u \) and \( v \) by applying the second and fourth equation and \( q_3 = -(q_1 + q_2) \), we get
\[
0 = q_1 \left( -\frac{1}{2} + \lambda_R + \sqrt{3}\lambda_I \right) + q_2 \left( -\frac{1}{2} - \lambda_R + \sqrt{3}\lambda_I \right),
\]
\[
0 = q_1 \left( -1 - \lambda_R + \sqrt{3}\lambda_I \right) - q_2 2\lambda_R,
\]
0 = q_1 \left( - \frac{1}{2} - 3\lambda_R + \sqrt{3}\lambda_I \right) + q_2 \left( \frac{1}{2} - 3\lambda_R - \sqrt{3}\lambda_I \right),
0 = q_1 \left( 1 - 3\lambda_R - \sqrt{3}\lambda_I \right) + q_2 \left( 2 - 2\sqrt{3}\lambda_I \right).

For \lambda_R = -\frac{1}{12} and \lambda_I = \frac{\sqrt{23}}{12} or \lambda_I = -\frac{\sqrt{23}}{12}, this linear system of equations has only the trivial solution \( q_1 = q_2 = 0 \). Since then \( q_3 \) is also zero, this contradicts the orthogonality of \( Q \).

Changing signs of the columns of \( Q \) would lead to three new cases in (6)–(7), namely the changes
\[ Q \rightarrow Q \text{ diag}(1, -1, 1) : u \rightarrow -u, \lambda_I \rightarrow -\lambda_I, \]
\[ Q \rightarrow Q \text{ diag}(1, -1, 1) : v \rightarrow -v, \lambda_I \rightarrow -\lambda_I, \]
\[ Q \rightarrow Q \text{ diag}(1, -1, -1) : u \rightarrow -u, v \rightarrow -v. \]

In all three cases, a simple variable substitution leads to the same final system of equations.

Next, let us characterize the spectra of stochastic 3 \times 3 matrices. The facts connected in the following theorem can be found in [21].

**Theorem 3.2:** A set \( \Lambda = \{\lambda_1, \lambda_2, \lambda_3\} \) with \( \Lambda = \tilde{\Lambda} \) is the spectrum of a matrix \( A \in \mathbb{R}^{3,3}_{\geq 0} \) if and only if
\[
\max_{1 \leq k \leq 3} |\lambda_k| \in \Lambda, \quad (8)
\]
\[
\text{tr}(A) = \lambda_1 + \lambda_2 + \lambda_3 \geq 0, \quad (9)
\]
\[
(\lambda_1 + \lambda_2 + \lambda_3)^2 \leq 3(\lambda_1^2 + \lambda_2^2 + \lambda_3^2). \quad (10)
\]

Note that for real-valued \( \lambda_k \), \( k = 1, 2, 3 \) the condition (10) is automatically fulfilled by the relation between arithmetic and geometric means. We further need the following auxiliary lemma.

**Lemma 3.3 ([13, Lemma 5.3.2]):** Let \( A \in \mathbb{R}^{n,n}_{\geq 0} \) with eigenvalues \{\lambda_1, \ldots, \lambda_n\} and spectral radius \( \lambda_1 \). Then there exists \( B \in \mathbb{R}^{n,n}_{\geq 0} \) with same eigenvalues such that
\[
B1_n = \lambda_1 1_n.
\]

Then we can simply deduce the following corollary.

**Corollary 3.4:** (i) Let \( \Lambda = \{\lambda_1, \lambda_2, \lambda_3\} \) with \( \lambda_2, \lambda_3 \in \mathbb{R} \). Then there exists \( A \in \mathcal{S}(3) \) with spectrum \( \Lambda \) if and only if \( \lambda_2, \lambda_3 \in [-1,1] \) and \( \lambda_2 + \lambda_3 \geq -1 \).

(ii) Let \( \Lambda = \{\lambda, \bar{\lambda}, \lambda\} \) with \( \lambda \notin \mathbb{R} \). Then there exists \( A \in \mathcal{S}(3) \) with spectrum \( \Lambda \) if and only if \( \lambda \in \Theta_3 \), where
\[
\Theta_3 := \{\lambda_R + i\lambda_I : \lambda_R \in [-\frac{1}{2},1], (\lambda_R - 1)^2 \geq 3\lambda_I^2\}
\]
\[
= \text{conv}\{1, \theta, \theta^2\}, \quad \theta = e^{-2\pi i/3} = -\frac{1}{2} - \frac{\sqrt{3}}{2}i.
\]
and \( \text{conv} \) denotes the convex hull.

The set \( \Theta_3 \cup \mathbb{I} \) is depicted in Figure 1.

**Proof:** (i) By Theorem 3.2, there exists a matrix \( A \in \mathbb{R}^{3,3}_{\geq 0} \) with spectrum \( \Lambda \) if and only if the two conditions in Part i) are fulfilled. Then we obtain the assertion by Lemma 3.3. (ii) Let \( \lambda_2 = \lambda_R + i\lambda_I, \lambda_I \neq 0 \). We prove that (8)–(10) hold true if and only if \( \lambda_2 \in \Theta_3 \). Then, the assertion follows again by Lemma 3.3.

For our setting we have that (8) is equivalent to \( |\lambda_2| \leq 1 \), (9) to \( \lambda_R \geq -\frac{1}{2} \), and (10) to

\[
(1 + 2\lambda_R)^2 \leq 3(1 + (\lambda_R + i\lambda_I)^2 + (\lambda_R - i\lambda_I)^2) = 6\lambda_R^2 - 6\lambda_I^2 + 3,
\]

i.e. \( \lambda_I^2 \leq \frac{1}{3}(\lambda_R - 1)^2 \). This yields the assertion. 

We will use the set of circulant \( n \times n \) matrices

\[
\{ \text{circ}(a) = a_0 I_n + a_1 P_n + \cdots + a_{n-1} P_n^{n-1} : a = (a_0, \ldots, a_{n-1})^T \in \mathbb{R}^n \}
\]

with the \( n \)th shift matrix

\[
P_n := \begin{pmatrix}
0_{n-1} & 1 \\
I_{n-1} & 0_{n-1}
\end{pmatrix}.
\]

Clearly, \( P_n \) is double stochastic. Note that the double stochastic matrices are the convex hull of the permutation matrices due to the Theorem of Birkhoff and Von Neumann. The circulant matrices can be diagonalized by the \( n \)th Fourier matrix \( F_n := (e^{-2\pi i jk/n})_{j,k=0}^{n-1} \), i.e.

\[
\text{circ}(a) = F_n^{-1} \text{diag}(F_n a) F_n
\]

see [22]. Note that \( F_n^{-1} = \frac{1}{n} F_n = \frac{1}{n} F_n^T \). Then it is easy to check the following lemma.
**Lemma 3.5:** Let \( n \in \mathbb{N} \) be odd, \( m = (n - 1)/2 \) and \( \Lambda = (1, \lambda_1, \ldots, \lambda_m, \bar{\lambda}_m, \ldots, \bar{\lambda}_1)^T \). Then the eigenvalues of \( B := \text{circ}(F_n^{-1}\Lambda) \) are the components of \( \Lambda \), \( B \) is real-valued and the rows of \( B \) sum up to 1.

**Proof:** By (11) the matrix \( B \) has the entries of \( \Lambda \) as eigenvalues. Further

\[
F_n^{-1}\Lambda = \frac{1}{n} \left( 1 + \sum_{j=1}^{m} (e^{2\pi ijk/n} \lambda_j + e^{-2\pi ijk/n} \bar{\lambda}_j) \right)_{k=0}^{n-1}
\]

is real-valued and

\[
1^T F_n^{-1}\Lambda = \frac{1}{n} \left( \sum_{k=0}^{n-1} e^{2\pi ijk/n} \right)_{j=0}^{n-1} \Lambda = (1, 0, \ldots, 0)^T \Lambda = 1. \quad \blacksquare
\]

Now we can prove the following proposition.

**Proposition 3.6:** For any \( A \in S(3) \), there exists a matrix \( B \in S(3) \) with the same eigenvalues which can be decomposed as in (2). If \( A \in S(3) \) has an eigenvalue \( \lambda = \lambda_R + i\lambda_I, \lambda_I \neq 0 \), then the matrix

\[
B = \text{circ}(F_3^{-1}(1, \lambda, \bar{\lambda})) \in S(3),
\]

has the same eigenvalues as \( A \) and possesses the decomposition

\[
B = Q \begin{pmatrix} 1 & 0 & 0 \\ 0 & \lambda_R & \lambda_I \\ 0 & -\lambda_I & \lambda_R \end{pmatrix} Q^T
\]

where \( Q \) is any matrix of the form (3).

**Proof:** (1) If the eigenvalues of \( A \) are real-valued, then the assertion follows from Theorem 2.1(i).

(2) Assume that the eigenvalues of \( A \) are the entries of the vector \( \Lambda = (1, \lambda, \bar{\lambda}) \). By Lemma 3.5, the matrix \( B \) is real-valued, has the same eigenvalues as \( A \) and its rows sum up to 1. Moreover, we have by Corollary 3.4(ii) that

\[
b := F_3^{-1} \left( \frac{1}{\lambda}, \frac{1}{\bar{\lambda}} \right) = \frac{1}{3} \begin{pmatrix} \lambda + \bar{\lambda} \\ \lambda + \bar{\lambda} \end{pmatrix} = \frac{1}{3} \begin{pmatrix} 1 + 2\lambda_R \\ 1 - \lambda_R - \sqrt{3}\lambda_I \end{pmatrix} \in \mathbb{R}^3 \geq 0.
\]

By straightforward computation, we obtain for \( Q \in O(3) \) as in (3) that

\[
Q^T P_3 Q = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}
\]

so that

\[
Q^T BQ = \begin{pmatrix} b_0 + b_1 + b_2 & 0 & 0 \\ 0 & b_0 - \frac{1}{2}(b_1 + b_2) & -\frac{\sqrt{3}}{2}(b_1 - b_2) \\ 0 & \frac{\sqrt{3}}{2}(b_1 - b_2) & b_0 - \frac{1}{2}(b_1 + b_2) \end{pmatrix}
\]
\[
\begin{pmatrix}
1 & 0 & 0 \\
0 & \lambda_R & \lambda_I \\
0 & -\lambda_I & \lambda_R
\end{pmatrix}.
\]

The matrix \(B\) in the above proposition is bistochastic. Finally, let us give an example of a stochastic matrix such that there does not exist a bistochastic matrix with the same eigenvalues.

**Example 3.7:** By Theorem 3.2 there exist stochastic matrices with eigenvalues \(\{1, 0, -1\}\), for example
\[
\begin{pmatrix}
0 & 1 & 0 \\
0 & 0 & 1 \\
0 & 1 & 0
\end{pmatrix}
\quad \text{or} \quad
\begin{pmatrix}
0 & 1 & 0 \\
1 & 0 & 0 \\
u & v & 0
\end{pmatrix}
\]
with \(u, v \geq 0\) and \(u + v = 1\).

However, there is no bistochastic matrix with these eigenvalues. Otherwise, it would have trace 0 and is therefore of the form
\[
B = \begin{pmatrix}
0 & a & 1 - a \\
1 - a & 0 & a \\
a & 1 - a & 0
\end{pmatrix}, \quad a \in [0, 1].
\]
The characteristic polynomial of \(B\) is \(-\lambda^3 + a^3 + (1 - a)^3 + 3a\lambda(1 - a)\). Since 0 is an eigenvalue, we get \(0 = a^3 + (1 - a)^3 = 1 - 3a + 3a^2\). This quadratic equation has no real-valued solution, which contradicts our assumption.

## 4. Old and new model

Throughout this section, let \(\lambda_1, \ldots, \lambda_s \in \mathbb{R}\) and conjugate pairs of complex numbers \(\lambda_{s+1}, \bar{\lambda}_{s+1}, \ldots, \lambda_n, \bar{\lambda}_n\) be given. Set \(t := \frac{n - s}{2}\). We define the vector \(\Lambda\) whose components are these numbers as in (1) and \(D(\Lambda)\) and \(\mathcal{V}_t\) as in Theorem 2.1(i).

Then the authors of [19] considered the optimization problem
\[
\min_{S, Q, V} \tilde{F}(S, Q, V) \quad \text{subject to } (S, Q, V) \in \tilde{M}_t
\]
where
\[
\tilde{F}(S, Q, V) := \frac{1}{2} \| S \circ S - Q(D(\Lambda) + V)Q^T \|_F^2,
\]
and
\[
\tilde{M}_t := \mathcal{O}B(n) \times O(n) \times \mathcal{V}_t,
\]
with
\[
\mathcal{O}B(n) := \{S \in \mathbb{R}^{n \times n} : \text{diag}(SS^T) = 1_n\}.
\]
Clearly, \(\mathcal{S}(n) = \{S \circ S : S \in \mathcal{O}B(n)\}\). By Zhao et al. [19], the level sets of \(\tilde{F}\) are compact, so that there exists a minimizer of \(\tilde{F}\).

However, as emphasized in Remark 2.2, even if \(\lambda_k, k = 1, \ldots, n\), are the eigenvalues of a stochastic matrix \(A\), this matrix may not be any solution (12). Even worse, it is not clear if
there exists any stochastic matrix such that the functional becomes zero. Therefore, we propose to consider an extended problem which is based on the following considerations. Let $\mu^{[2]} \in \mathbb{R}^{2,2}$ with eigenvalues $\lambda = \lambda_R \pm i\lambda_I, \lambda_I \neq 0$. Then there exists an invertible matrix $T \in \text{SL}(2)$ of determinant 1 such that

$$\mu^{[2]} = T\lambda^{[2]}T^{-1}, \quad \lambda^{[2]} = \begin{pmatrix} \lambda_R & \lambda_I \\ -\lambda_I & \lambda_R \end{pmatrix}. \quad (13)$$

Moreover, it follows from the QR decomposition of matrices that such a matrix $T$ can be uniquely decomposed as

$$T = Q_{\alpha,\beta}T_{\alpha,\beta}, \quad T_{\alpha,\beta} = \begin{pmatrix} \alpha & \beta \\ 0 & 1/\alpha \end{pmatrix}, \quad \alpha \in \mathbb{R}_{>0}, \beta \in \mathbb{R}, \ Q_{\alpha,\beta} \in \text{O}(2),$$

cf. [23]. We obtain

$$\mu^{[2]} = Q_{\alpha,\beta}T_{\alpha,\beta}\lambda^{[2]}T_{\alpha,\beta}^{-1}Q_{\alpha,\beta}^T, \quad T_{\alpha,\beta}^{-1} = \begin{pmatrix} 1/\alpha & -\beta \\ 0 & \alpha \end{pmatrix} = T_{\frac{1}{\alpha},-\beta}^{-1}.$$  

As a consequence we have by Theorem 2.1(ii) that every (stochastic) matrix with eigenvalues in $\Lambda$ can be written in the form

$$QT_{ab}(D(\Lambda) + V)T_{ab}^{-1}Q^T$$

with $Q \in \text{O}(n)$ and a blockdiagonal matrix

$$T_{ab} = \text{blockdiag}(I_s, T_{a_1b_1}, \ldots, T_{a_tb_t}),$$

where

$$a := (a_1, \ldots, a_t) \in \mathbb{R}_{>0}^t, \quad b := (b_1, \ldots, b_t) \in \mathbb{R}^t.$$  

**Example 4.1:** We continue Example 3.1. We have seen that the matrix $A$ in (5) does not have a decomposition (2), but can of course be decomposed as in (14) with $a \approx 0.81636$, $b = 0$ and

$$Q \approx \begin{pmatrix} 0.57735 & 0.78868 & 0.21132 \\ 0.57735 & -0.57735 & 0.57735 \\ 0.57735 & -0.21132 & 0.78868 \end{pmatrix}, \quad V \approx \begin{pmatrix} 1 & 0.42152 & 0.42834 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$  

Instead of problem (12), we consider $F : \mathbb{R}^{n,n} \times \mathbb{R}^{n,n} \times \mathbb{R}^{n,n} \times \mathbb{R}_{>0}^t \times \mathbb{R}^t \to \mathbb{R}$ defined by

$$F(S, Q, V, a, b) := \frac{1}{2} \| S \circ S - QT_{ab}(D(\Lambda) + V)T_{ab}^{-1}Q^T \|^2_F$$

and propose to solve

$$\min_{S, Q, V, a, b} F(S, Q, V, a, b) \quad \text{subject to } (S, Q, V, a, b) \in \mathcal{M}_t,$$  

where

$$\mathcal{M}_t := \mathcal{O}B(n) \times \text{O}(n) \times \mathcal{V}_t \times \mathbb{R}_{>0}^t \times \mathbb{R}^t.$$  

If the entries of $\Lambda$ are the eigenvalues of a stochastic matrix, then the minimum of $F$ is zero.
In the following proposition, bounded sets on the manifold $\mathcal{M}_t$ address boundedness w.r.t. the geodesic distance as introduced in Section 6.

**Proposition 4.2:** The function $F: \mathbb{R}^{n,n} \times \mathbb{R}^{n,n} \times \mathbb{R}^{n,n} \times \mathbb{R}_{>0}^t \times \mathbb{R}^t \to \mathbb{R}$ in (16) is lower level bounded, i.e.

$$\text{lev}_c F := \{ x = (S, Q, V, a, b) : F(x) \leq c \}$$

are bounded for all $c \in \mathbb{R}$, in particular the components of $a \in \mathbb{R}_{>0}^t$ are bounded away from zero. Then $\inf F$ is attained and the set of minimizers is compact.

**Proof:** By orthogonality of $Q$ we have

$$F(x) = \frac{1}{2} \| Q^T (S \circ S) Q - T_{ab}(D(\Lambda) + V) T_{ab}^{-1} \|_F^2 = \| Q^T (S \circ S) Q - (\tilde{D}(\Lambda, a, b) + \tilde{V}) \|_F^2,$$

where $\tilde{V} \in \mathcal{V}_t$ and

$$\tilde{D}(\Lambda, a, b) = \text{blockdiag}(\lambda_1, \ldots, \lambda_s, B_1, \ldots, B_t),$$

$$B_k := \begin{pmatrix} \lambda_{s+k,R} + \frac{b_k}{a_k} \lambda_{s+k,I} & (a_k^2 + b_k^2) \lambda_{s+k,I} \\ -a_k^2 \lambda_{s+k,I} & \lambda_{s+k,R} + \frac{b_k}{a_k} \lambda_{s+k,I} \end{pmatrix}, \quad k = 1, \ldots, t.$$

Since $\mathcal{O}B(n) \times \mathcal{O}(n)$ is compact, we know that $Q^T (S \circ S) Q$ has bounded entries. Therefore $F(X) \leq c$ implies that the entries of $\tilde{V}$ as well as those of $B_k, k = 1, \ldots, t$, are bounded. Since $\lambda_{s+k,I} \neq 0$, we obtain that $a_k^2 + b_k^2$ and $\frac{1}{a_k^2}$ are bounded, which implies that $|b_k|$ is bounded and $a_k$ is bounded from above and away from zero. In summary, the level sets of $F$ are bounded. Since $F$ is continuous, the rest of the claim follows by standard arguments from optimization, see, e.g. [24].

**Remark 4.3:** Two month after our ArXiv submission, Wang et al. [25] proposed a new model. Based on the standardization by Givens rotation, see [26, 27], they rewrote the matrix $\mu^{[2]}$ in (13) as

$$\mu^{[2]} = Q^{[2]} \begin{pmatrix} \lambda_R & d \\ -\lambda_I & \lambda_R \end{pmatrix} (Q^{[2]})^T, \quad d > 0$$

with an orthogonal $2 \times 2$ matrix $Q^{[2]}$. This can be seen as an alternative approach which avoids one parameter and we will consider it in our future work.

### 5. Geometric conjugate gradient algorithms

We want to find a minimizer of $F: \mathcal{M}_t \to \mathbb{R}$ by applying a CG algorithm.
5.1. CG algorithm on linear spaces

To this end, we start with briefly recalling the CG-algorithm to solve a linear system of equations \( Ax = b \) with a symmetric, positive definite matrix \( A \). The solution can be found by iteratively minimizing the functional

\[
 f(x) = \frac{1}{2} x^T A x - b^T x. \tag{17}
\]

The CG method is given in Algorithm 1.

\begin{algorithm}
\caption{CG algorithm for linear systems \( Ax = b \)}
\begin{algorithmic}
  \State \textbf{Input:} \( x^{(0)} \in \mathbb{R}^n \)
  \State \textbf{Initialization:} \( d^{(0)} = -g^{(0)} = - \nabla f(x^{(0)}) = b - Ax^{(0)} \)
  \For {\( k = 0, \ldots \) until a stopping criterion is reached,}
    \State \( \alpha^{(k)} = \frac{\langle -g^{(k)}, d^{(k)} \rangle}{\langle Ad^{(k)}, d^{(k)} \rangle} \)
    \State \( x^{(k+1)} = x^{(k)} + \alpha^{(k)} d^{(k)} \)
    \State \( g^{(k+1)} = \nabla f(x^{(k+1)}) = Ax^{(k+1)} - b \)
    \State \( \beta^{(k)} = \frac{\langle g^{(k+1)}, Ad^{(k)} \rangle}{\langle d^{(k)}, Ad^{(k)} \rangle} \)
    \State \( d^{(k+1)} = -g^{(k+1)} + \beta^{(k)} d^{(k)} \)
  \EndFor
\end{algorithmic}
\end{algorithm}

For the quadratic functional (17), the Hessian is given by \( \nabla^2 f(x^{(k)}) = A \). Further, it can be shown that \( \beta^{(k)} \) can be rewritten as

\[
 \beta^{(k)} = \frac{\langle g^{(k+1)}, g^{(k+1)} \rangle}{\langle g^{(k)}, g^{(k)} \rangle} \tag{18} \]

\[
 = \frac{\langle g^{(k+1)}, g^{(k+1)} - g^{(k)} \rangle}{\langle g^{(k)}, g^{(k)} \rangle}. \tag{19}
\]

The CG algorithms for minimizing an arbitrary two times differentiable function \( F : \mathbb{R}^n \rightarrow \mathbb{R} \) differ by the choice of \( \beta^{(k)} \) and \( \alpha^{(k)} \) in Algorithm 2. Note that the values (18) and (19) differ in the general case. For a good overview over different nonlinear CG algorithms see, e.g. [28].

\begin{algorithm}
\caption{Generic CG algorithm for two times differentiable functionals \( F : \mathbb{R}^n \rightarrow \mathbb{R} \)}
\begin{algorithmic}
  \State \textbf{Input:} \( x^{(0)} \in \mathbb{R}^n \)
  \State \textbf{Initialization:} \( d^{(0)} = -g^{(0)} = - \nabla F(x^{(0)}) \)
  \For {\( k = 0, \ldots \) until a stopping criterion is reached,}
    \State Choose a step size \( \alpha^{(k)} \)
    \State \( x^{(k+1)} = x^{(k)} + \alpha^{(k)} d^{(k)} \)
    \State \( g^{(k+1)} = \nabla F(x^{(k+1)}) \)
    \State \( d^{(k+1)} = -g^{(k+1)} + \beta^{(k)} d^{(k)} - \theta^{(k)} (g^{(k+1)} - g^{(k)}) \) for certain coefficients \( \beta^{(k)}, \theta^{(k)} \)
  \EndFor
\end{algorithmic}
\end{algorithm}
For $\theta^{(k)} = 0$ and
\[ \beta^{(k)} = \frac{\langle \nabla^2 F(x^{(k+1)})d^{(k)}, s^{(k+1)} \rangle}{\langle \nabla^2 F(x^{(k+1)})d^{(k)}, d^{(k)} \rangle}, \] (20)
the resulting algorithm was proposed by Daniel [29]. Using $\theta^{(k)} = 0$ and $\beta^{(k)}$ as in (18), we obtain the Fletcher-Reeves algorithm and $\beta^{(k)}$ as in (19) the Polak–Ribière–Polyak algorithm, cf. [30].

**Remark 5.1:** Actually, for well-definedness of the steps in Algorithm 2 with $\beta^{(k)}$ as in (20), a further assumption on $F$ is needed, for instance positive definiteness of $\nabla^2 F(x)$ for all $x \in \mathbb{R}^n$ is clearly sufficient. In the original work [29] it is even assumed that there are constants $a, A > 0$ such that it holds

\[ a\|\xi\|^2 \leq \langle \nabla^2 F(x)\xi, \xi \rangle \leq A\|\xi\|^2. \]

for all $x, \xi \in \mathbb{R}^n$.

Finally, the Polak–Ribière–Polyak algorithm can be modified by setting
\[ \theta^{(k)} = \frac{\langle g^{(k+1)}, d^{(k)} \rangle}{\|g^{(k)}\|^2}. \] (21)

This modified Polak–Ribière–Polyak algorithm will be our method of choice. It has the following properties whose brief proof we give for convenience, cf. [30, Theorem 2.1].

**Proposition 5.2:** For Algorithm 2 with update (19) and (21) the following holds true:

(i) If the step sizes $\alpha^{(k)}$ are generated by exact line search, i.e. $\alpha^{(k+1)} = \text{argmin}_\alpha F(x^{(k)} + \alpha d^{(k)})$, then $\theta^{(k)} = 0$ for all $k \in \mathbb{N}$, so that we obtain the usual Polak–Ribière–Polyak Algorithm.

(ii) Independently from the line search, $d^{(k)}$ is a descent direction at $x^{(k)}$ for all $k \in \mathbb{N}$.

**Proof:** (i) Since the line search is exact we have for the function $\alpha \mapsto F(x^{(k)} + \alpha d^{(k)})$ that

\[ 0 = \langle \nabla F(x^{(k)} + \alpha d^{(k)}), d^{(k)} \rangle = \langle \nabla F(x^{(k+1)}), d^{(k)} \rangle = \langle g^{(k+1)}, d^{(k)} \rangle. \]

(ii) For $k = 0$ it holds $d^{(0)} = -g^{(0)}$. For $k \geq 1$ we set $y^{(k)} := g^{(k+1)} - g^{(k)}$ and obtain

\[ \langle g^{(k+1)}, d^{(k+1)} \rangle = -\|g^{(k+1)}\|^2 + \beta^{(k)} \langle g^{(k+1)}, d^{(k)} \rangle - \theta^{(k)} \langle g^{(k+1)}, y^{(k)} \rangle \]
\[ = -\|g^{(k+1)}\|^2 + \frac{\langle g^{(k+1)}, y^{(k)} \rangle \langle g^{(k+1)}, d^{(k)} \rangle}{\|g^{(k)}\|^2} - \frac{(g^{k+1}, d^{(k)}) (g^{(k+1)}, y^{(k)})}{\|g^{(k)}\|^2} \]
\[ = -\|g^{(k+1)}\|^2 < 0. \]

**5.2. CG algorithms on manifolds**

Let $\mathcal{M}$ be a complete, connected $d$-dimensional Riemannian manifold with tangent space $T_x \mathcal{M}$ in $x \in \mathcal{M}$ and Riemannian metric $\| \cdot \|_x$. By $T\mathcal{M}$ we denote the tangent bundle of
The geometric version of the CG algorithm replaces the gradient/Hessian by the Riemannian gradient/Hessian $\nabla_M/\nabla^2_M$ on the manifold, and incorporate a vector transport $T$ between tangent spaces of the manifold in order to make the addition of the vectors $d^{(k)}$, which are in different tangent spaces, possible.

Recall that a map $\mathcal{R}: T_M \rightarrow M$ is called a retraction (on $M$), if

(i) $\mathcal{R}_x(0_x) = x$, where $0_x$ denotes the zero vector in $T_xM$, and
(ii) $D\mathcal{R}_x(0_x) = \text{id}_{T_xM}$ with the canonical identification $T_0(T_xM) = T_xM$.

In particular, on a complete manifold, the exponential map $\exp_x: T_xM \rightarrow M$ is a retraction. Fixing a retraction we can define a vector transport between tangent spaces.

A vector transport $T: T_M \times T_M \rightarrow T_M$ associated to a retraction $\mathcal{R}: T_M \rightarrow M$ is a smooth mapping defined by

$$((x, \theta), (x, \xi)) \mapsto (\mathcal{R}_x(\theta), T_{x, \theta} \xi)$$

with the following properties

(i) (Consistency) $T_{x, 0_x} \xi = \xi$ for all $\xi \in T_xM$.
(ii) (Linearity) $T_{x, \theta}(a\xi + b\zeta) = aT_{x, \theta} \xi + bT_{x, \theta} \zeta$ for all $\theta, \xi, \zeta \in T_xM, a, b \in \mathbb{R}$.

In particular, the parallel transport $P_{x, \theta}(\xi)$ along a geodesic starting at $x$ with tangent vector $\theta$ is a vector transport. A vector transport different from the parallel transport yields often computationally less expensive algorithms with similar convergence properties.

Now the modified Polak–Ribière–Polyak CG-algorithms on a manifold $M$ is given by Algorithm 3.

**Algorithm 3 Geometric Modified Polak–Ribièr–Polyak Algorithm (GMPRP)**

**Input:** initial point $x^{(0)} \in M$

**Initialization:** $g^{(0)} = \nabla_M F(x^{(0)}), d^{(0)} = -g^{(0)}, k = 0$

while $\|g^{(k)}\|_{x^{(k)}} > 0$ do

Find a steplength $\alpha^{(k)}$

$x^{(k+1)} = \mathcal{R}_{x^{(k)}}(\alpha^{(k)} d^{(k)})$

$g^{(k+1)} = \nabla_M F(x^{(k+1)})$

$y^{(k)} = g^{(k+1)} - T_{x^{(k)}, \alpha^{(k)} d^{(k)}} g^{(k)}$

$\tilde{d}^{(k)} = T_{x^{(k)}, \alpha^{(k)} d^{(k)}} d^{(k)}$

$\beta^{(k)} = \frac{\langle g^{(k+1)}, y^{(k)} \rangle_{x^{(k+1)}}}{\|g^{(k)}\|^2_{x^{(k)}}}$

$\theta^{(k)} = \frac{\langle g^{(k+1)}, \tilde{d}^{(k)} \rangle_{x^{(k+1)}}}{\|g^{(k)}\|^2_{x^{(k)}}}$

$d^{(k+1)} = -g^{(k+1)} + \beta^{(k)} \tilde{d}^{(k)} - \theta^{(k)} y^{(k)}$

$k = k + 1$

The geometric GMPRP algorithm has analogous properties as in the Euclidean setting.
Proposition 5.3: For Algorithm 3 the following holds true:

(i) If the step sizes \( \alpha^{(k)} \) are generated by an exact line search and parallel transport is chosen as vector transport, then it holds \( \theta^{(k)} = 0 \) for all \( k \in \mathbb{N} \).

(ii) Independently from the line search and the vector transport, \( d^{(k)} \) is a descent direction at \( x^{(k)} \) for all \( k \in \mathbb{N} \).

Proof: (i) In case of exact line search it holds

\[
\langle g^{(k+1)}, \tilde{d}^{(k)} \rangle_{x^{(k+1)}} = \langle \nabla_{\mathcal{M}} F(x^{(k+1)}), T_{x^{(k)}} \alpha^{(k)} d^{(k)} d^{(k)} \rangle_{x^{(k+1)}} = 0,
\]

cf. [31, p.131].

(ii) The assertions follow as in the proof of Proposition 5.2 by straightforward computation.

In the numerical part, we will determine \( \alpha^{(k)} \) by the Line Search Algorithm 4. This search was proposed in [19], but with another initial step size given by

\[
\tilde{\alpha}^{(0)} = \frac{\langle d, \nabla_{\mathcal{M}} F(X) \rangle_{X}}{\|Df(X)[d]\|_{F}^2}, \quad X \in \mathcal{M}, \ d \in T_{X}\mathcal{M}
\]

(22)

where \( f \) is the matrix function with \( F(X) = \|f(X)\|_{F}^2 \) and \( Df(X)[d] \) denotes the usual derivative in an euclidean space. In our numerical experiments we have observed that the initial Newton step size in Algorithm 4 with the approximated Hessian leads to less updates during linesearch than with initialization (22) and that this even compensates the fact that the Newton step size is more expansive to compute. We have approximated the Hessian by

\[
\nabla^2_{\mathcal{M}} F(x) d \approx \|d\| - \frac{\nabla_{\mathcal{M}} F(y_{x,d}(\frac{h}{\|d\|})) - \nabla_{\mathcal{M}} F(x)}{h}
\]

in our numerical examples. Note that, compared to the line search in [19], we have inserted an additional step which is required for (A5) in the convergence proof. In the proof of [19, Theorem 3.4] a constant initial stepsize \( \tilde{\alpha}^{(0)} \) or a similar step to our additional one is needed for the same reason. In Section 7 we compare the behaviour of both linesearch algorithms. Alternatively, we could use the classical Armijo Line Search with the same initial \( \tilde{\alpha}^{(0)} \). Indeed, we have also implemented this step size search algorithm, by it does not appear cheaper than the first one.

6. Special manifolds

In this section, we provide the quantities required in the CG algorithms for the special manifolds appearing in

\[
\mathcal{M}_t := \mathcal{O}B(n) \times \mathcal{O}(n) \times \mathcal{V}_t \times \mathbb{R}_{>0}^t \times \mathbb{R}^t.
\]

The spaces \( \mathcal{V}_t \) and \( \mathbb{R}^t \) are linear spaces, \( \mathcal{O}B(n) \) and \( \mathcal{O}(n) \) are smooth compact matrix manifolds of dimension \( n(n-1) \) with tangent spaces

\[
T_S\mathcal{O}B(n) = \{ \Xi \in \mathbb{R}^{n,n} : \text{diag}(S \Xi^T) = 0 \},
\]
$T_O(n) = Q \text{Skew}(n),$

where Skew$(n)$ denotes the linear space of $n \times n$ skew-symmetric matrices. Note that O$(n)$ is actually not a connected manifold, but can be split into the two connected components SO$(n)$ and $-\text{SO}(n)$ and since the functionals (12) and (15) are invariant under sign changes for $Q$, this fact is not of relevance for our algorithms. The manifolds $O_B(n)$ and $O(n)$ are isometrically embedded into $\mathbb{R}^{n^2}$ and the tangent spaces are equipped with the inner product

$$\langle \Xi_1, \Xi_2 \rangle_S = \text{tr} (\Xi_1^T \Xi_2), \quad \Xi_1, \Xi_2 \in T_S O_B(n),$$

$$\langle \Xi_1, \Xi_2 \rangle_Q = \text{tr} (\Xi_1^T \Xi_2), \quad \Xi_1, \Xi_2 \in T_O(n).$$

### Algorithm 4 (Line Search Algorithm)

**Parameters:** $0 < \tau < 1, 0 < \delta < 1$

**Input:** smooth function $F : \mathcal{M} \to [0, \infty)$, start point $x \in \mathcal{M}$, descent direction $d \in T_x \mathcal{M}$

**Output:** stepsize $\alpha^{(k)} = \tilde{\alpha}^{(l)}$

**Initialization:** $l = 0$,

$$\tilde{\alpha}^{(0)} = \begin{cases} 
\langle d, \nabla F(x) \rangle_x, & \langle d, \nabla^2 F(x) d \rangle_x \neq 0, \\
1, & \text{else}
\end{cases}$$

**while** $F(R_x(\tilde{\alpha}^{(l)} d)) - F(x) \geq -\delta \tilde{\alpha}^{(l)} \|d\|^2_x$ **do**

$$\tilde{\alpha}^{(l+1)} = \tau \tilde{\alpha}^{(l)}$$

$$l = l + 1$$

**Additional Step:**

if $l = 0$ then

**while** $F(R_x(\tilde{\alpha}^{(l)} d)) - F(x) < -\delta \tilde{\alpha}^{(l)} \|d\|^2_x$ **do**

$$\tilde{\alpha}^{(l+1)} = \tau^{-1} \tilde{\alpha}^{(l)}$$

$$l = l + 1$$

$$l = l - 1$$

In particular, these inner products are independent of $S$, resp. $Q$. The tangent space of the positive numbers at $a \in \mathbb{R}_{>0}^t$ is $T_a \mathbb{R}_{>0}^t = \mathbb{R}^t$ with inner product

$$\langle \xi^{(1)}, \xi^{(2)} \rangle_a = \frac{\xi^{(1)} \xi^{(2)}}{a^2}, \quad \xi^{(1)}, \xi^{(2)} \in \mathbb{R}^t, \quad \text{where the product (and quotients) of vectors is meant componentwise. Finally, we have for } x = (S, Q, V, a, b) \in \mathcal{M}_t \text{ that } T_x \mathcal{M}_t = T_S O_B(n) \times T_Q O(n) \times V \times \mathbb{R}^t \times \mathbb{R}^t \text{ with the Riemannian metric (24) on the fourth space and the Euclidean Riemannian metric on the other spaces (independent on the concrete } S, Q, V, b). \text{ The Riemannian gradient of}$$
$F$ requires the orthogonal projections of $\Xi \in \mathbb{R}^{n \times n}$ onto the tangent spaces which are given by

$$\Pi_{T_{S}O(n)}(\Xi) = \Xi - \text{diag}(S\Xi^{T})S,$$

$$\Pi_{T_{Q}O(n)}(\Xi) = Q_{\frac{1}{2}}(Q^{T}\Xi - \Xi^{T}Q).$$

Then we have the following lemma.

**Lemma 6.1:** The Riemannian gradient of $F = F(S, Q, V, a, b)$ in (16) reads as $\nabla_{M}F = (\nabla_{S}F, \nabla_{Q}F, \nabla_{V}F, \nabla_{a}F, \nabla_{b}F)$, where

$$\nabla_{S}F = \Pi_{T_{S}O(n)}(2S \circ H),$$

$$\nabla_{Q}F = \Pi_{T_{Q}O(n)}(-(H^{T}G + HG^{T})Q),$$

$$\nabla_{V}F = \Pi_{T_{V}D_{S}}(-T_{ab}^{T}Q^{T}GQ^{T}T_{ab}^{T}),$$

$$\nabla_{a}F = (Q^{T}(G^{T}H - HG^{T})Q_{ab}^{T} - \text{blockdiag}(0_{s+2(k-1)}, M_{ak}, 0_{2(t-k-1)})), $$

$$\nabla_{b}F = (Q^{T}(G^{T}H - HG^{T})Q_{ab}^{T} - \text{blockdiag}(0_{s+2(k-1)}, N, 0_{2(t-k-1)})), $$

for $k = 1, \ldots, t$, where $G := QT_{ab}(D(\Lambda) + V)_{ab}T_{ab}^{-1}Q^{T}$, $H := S \circ S - G$, and

$$N := \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad M_{\alpha} := \begin{pmatrix} \alpha^{2} & 0 \\ 0 & -1 \end{pmatrix}.$$

**Proof:** The computation of the first three Riemannian gradients is based on the fact that the Riemannian gradients are just orthogonal projections of the Euclidean gradients onto the respective tangent spaces and the Euclidean matrix gradients follow by straightforward computations.

The fourth and fifth Riemannian gradients can be directly obtained from the chain rule for computing matrix gradients, the fact that the mappings $f_{1} : \mathbb{R} \rightarrow \mathbb{R}^{2 \times 2}$ and $f_{2} : \mathbb{R}_{>0} \rightarrow \mathbb{S}_{L}(2)$ defined by

$$f_{1}(\beta) = \begin{pmatrix} \alpha & \beta \\ 0 & \frac{1}{\alpha} \end{pmatrix} \quad \text{and} \quad f_{2}(\alpha) = \begin{pmatrix} \alpha & \beta \\ 0 & \frac{1}{\alpha} \end{pmatrix}$$

have the differentials

$$Df_{1}(\beta) = N \quad \text{and} \quad Df_{2}(\alpha) = \frac{1}{\alpha^{2}}M_{\alpha},$$

respectively, and by regarding (24) in the computation of the fourth gradient. \hfill \blacksquare

For implementation, note that we can rewrite $\nabla_{a}F$ and $\nabla_{b}F$ as

$$\nabla_{a}F = a_{k}^{2}A_{s+2k-1,s+2k-1} - A_{s+2k,s+2k},$$

$$\nabla_{b}F = A_{s+2k-1,s+2k}$$

with $A := Q^{T}(G^{T}H - HG^{T})Q_{ab}^{T}$. 
Next we give retractions and corresponding transport maps for the involved manifolds. Since $V_t$ and $\mathbb{R}^t$ are linear spaces, we have

$$ R_V(ξ) = V + ξ, \quad R_bξ = b + ξ. $$

Retractions on $OB(n)$ follows from the retractions on the $(n - 1)$-sphere

$$ R_s(ξ) = \frac{s + ξ}{\|s + ξ\|_2}, \quad ξ \in T_sS^{n-1} $$

$$ \exp_s ξ = \cos(\|ξ\|)s + \frac{\sin(\|ξ\|)}{\|ξ\|}ξ $$

and are given by

$$ R_S(ξ) = (\text{diag}((S + ξ)(S + ξ)^T)^{-1/2})(S + ξ), \quad ξ \in T_SOB(n), $$

$$ \exp_S(ξ) = \cos(\text{diag}(ξ^T ξ)^{1/2})S + \sin(\text{diag}(ξ^T ξ)^{1/2}) \text{diag}(ξ^T ξ)^{-1/2} ξ, $$

which are both smooth mappings. For retractions on $O(n)$, recall that the sum of the identity matrix and any skew-symmetric matrix is invertible and that for an invertible matrix $A \in \mathbb{R}^{n,n}$, there is a unique matrix $Q \in O(n)$ and an upper diagonal matrix with positive diagonal entries $R \in \mathbb{R}^{n,n}$ such that $A = QR$. We denote the corresponding matrix $Q$ as $qf(A)$. Well-known retractions on $O(n)$ are given by

$$ R_Q(ξ) = Q qf(I + Q^T ξ) = qf(Q + ξ), \quad ξ \in T_QO(n), $$

$$ \exp_Q(ξ) = Q \text{Exp}(Q^T ξ), $$

see [32, Example 4.1.2], which are both smooth. Another retraction which we do not apply here is given via the Cayley transform, see also [32, Example 4.1.2].

Finally, we use as retraction on $\mathbb{R}_{>0}$ the exponential map

$$ R_{a_k}(ξ) = \exp_{a_k} ξ = a_k e^{ξ/a_k}, \quad ξ \in \mathbb{R}, $$

cf. [33, Theorem 2.14]. By straightforward computation one verifies that the geodesic distance on $\mathbb{R}_{>0}$ with inner product (24) is given by

$$ \text{dist}_{\mathbb{R}_{>0}}(a, \tilde{a}) = \|\log(a) - \log(\tilde{a})\|_2, $$

where the logarithm is meant componentwise.

For the vector transport we use as in [19],

$$ T_{S,Θ}ξ = \Pi_{T_{SΘ}OB(n)}(ξ), \quad Θ, ξ \in T_SOB(n), $$

$$ T_{Q,Θ}ξ = \Pi_{T_{QΘ}O(n)}(ξ), \quad Θ, ξ \in T_QO(n), $$

$$ T_{a_k,Θ}ξ = ξ, \quad Θ, ξ \in T_{a_k} \mathbb{R}_{>0}. $$

**Remark 6.2:** Alternatively we could apply the following parallel transport maps: The parallel transport of $ξ \in T_SOB(n)$ along geodesics in direction $Θ \in T_SOB(n)$ at $S \in OB(n)$
is determined row-wise by the parallel transport on the \((n-1)\)-sphere, see [34]:

\[
P_{s,\theta}(\xi) = \left( I_n + (\cos(\|\theta\|) - 1) \frac{\theta \theta^T}{\|\theta\|^2} - \sin(\|\theta\|) \frac{s\theta^T}{\|\theta\|} \right) \xi, \quad \xi \in T_s S^{n-1}.
\]

Further, we have

\[
P_{Q,\Theta}(\Xi) = Q \text{Exp} \left( \frac{Q^T \Theta}{2} \right) Q^T \Xi \text{Exp} \left( \frac{Q^T \Theta}{2} \right), \quad \Theta, \Xi \in T_Q O(n),
\]

\[
P_{a_k,\theta}(\xi) = e^{\theta/a_k} \xi = \frac{R_{a_k}(\theta)}{a_k} \xi, \quad \theta, \xi \in T_{a_k} \mathbb{R}_{>0}.
\]

In our numerical examples we have not seen advantages of the parallel transport over the vector transports in (25).

For our special manifold \(\mathcal{M} = \mathcal{M}_t\) have the following convergence result of Algorithm 3.

**Theorem 6.3:** Let \(x^{(k)}\) with \(x^{(k)} = (S^{(k)}, Q^{(k)}, V^{(k)}, a^{(k)}, b^{(k)}) \in \mathcal{M}_t\) be the sequence generated by Algorithm 3 and the Line Search Algorithm 4. If the algorithm does not stop with \(\|\nabla_{\mathcal{M}_t} F(x^{(k)})\|_{x^{(k)}} = 0\) in some step \(k_0\), then it holds

\[
\liminf_{k \to \infty} \|\nabla_{\mathcal{M}_t} F(x^{(k)})\|_{x^{(k)}} = 0.
\]

The proof was given for the manifold \(\tilde{\mathcal{M}}_t\) and the function \(\tilde{F}\) in [19]. The assertion can be shown for our more general setting in a similar way based on the fact that the linesearch algorithm ensures that the \(\{F(x^{(k)})\}\) is monotone decreasing and that by Proposition 4.2 the level sets \(\text{lev}_{F(x^{(k)})} F\) are bounded so that all iterates are in this compact set. For convenience we give the proof in the appendix.

**7. Numerical results**

results using Algorithm 3 with vector transport (25) and linesearch given by Algorithm 4 for minimizing

(I) model (12) from [19],

(II) our new model (16).

The algorithms were implemented in MATLAB R2019b and executed on a computer with Intel Core i5-7300U processor and 2 cores at 2.6 GHz/2712 MHz and 8 GB RAM.

In the linesearch of Algorithm 4, we set \(\delta = 10^{-4}\) and \(\tau = 0.5\) as it was also used in [19]. We set our initial stepsize to 1.4 in Method I if \(\|d\| < 10^{-5}\) in (23) or if \(\langle d, \nabla^2_{\mathcal{M}_t} F(x) d \rangle < 10^{-12}\) and in Method II to 1.6 if \(\|d\|_{x < 10^{-5}}\) or \(\langle d, \nabla^2_{\mathcal{M}_t} F(x) d \rangle_{x < 10^{-10}}\). We use the following initialization.
7.1. Initialization

For the initialization of the descent algorithm we use the MATLAB function \texttt{schur}, which computes a decomposition as in Theorem 2.1(ii), and choose
\[
\hat{S} = \text{rand}(n, n), \quad S^{(0)} = (\text{diag}(\hat{S}_1 n)^{-1} \hat{S})^{1/2} \in O(n),
\]
\[
[Q^{(0)}, \hat{V}] = \text{schur}(S^{(0)} \circ S^{(0)}, 'real'), \quad V^{(0)} = \Pi \hat{V}, \quad W = W \circ \hat{V}, \quad (26)
\]
where the square root is meant componentwise and
\[
W_{ij} = \begin{cases} 
0, & j \leq i \text{ or } i = j - 1, j = s + 2k, k \in \{1, \ldots, t\}, \\
1, & \text{otherwise}.
\end{cases}
\]

For model (16) we additionally set
\[
a^{(0)} = 1_t, \quad b^{(0)} = 0_t.
\]

We compare the eigenvalue sets using Algorithm 5.

\textbf{Algorithm 5} Greedy-type computation of a distance of eigenvalue sets

\begin{itemize}
  \item \textbf{Input:} Eigenvalue sets \(\Lambda, \tilde{\Lambda}\) with \(n\) elements
  \item \textbf{for} \(k = 1, \ldots, n\) \textbf{do}
  \begin{itemize}
    \item Choose \(\lambda' \in \Lambda, \tilde{\lambda}' \in \tilde{\Lambda}\) with \(|\lambda' - \tilde{\lambda}'| = \min\{|\lambda - \tilde{\lambda}| : \lambda \in \Lambda, \tilde{\lambda} \in \tilde{\Lambda}\}\)
    \item \(\Lambda = \Lambda \setminus \{\lambda'\}\)
    \item \(\tilde{\Lambda} = \tilde{\Lambda} \setminus \{\tilde{\lambda}'\}\)
    \item \(d(\Lambda, \tilde{\Lambda}) = \max(|\lambda' - \tilde{\lambda}'|, d(\Lambda, \tilde{\Lambda}))\)
  \end{itemize}
\end{itemize}

We consider two kind of numerical examples. The first one is similar to that proposed in [19, Example 5.1]. Here the number \(t\) of complex-conjugate eigenvalue pairs increases linearly in the dimension \(n\) of the vector space. In contrast to Method I, our algorithm has additionally to determine an increasing number of components of \(a\) and \(b\) in \(T_{ab}\). Our Method II appears to be slightly slower than the previous one. In the second example, we fix \(n\) and examine how the performance of the algorithm depends on the number \(t\) of complex-conjugate eigenvalue pairs. In the chosen setting, the problem becomes very ill-posed. Interestingly, both methods get closer to the prescribed eigenvalues as \(t\) grows.

7.2. Example with \(t \sim n\)

We start with a similar setting as in [19, Example 5.1]. The eigenvalues of a stochastic matrix \(A \in \mathbb{R}^{n,n}\) obtained by
\[
\tilde{A} = \text{rand}(n, n), \quad A = (\text{diag}(\tilde{A}_1 n)^{-1} \tilde{A})
\]
with the MATLAB built-in function \texttt{rand} are used as prescribed spectrum \(\Lambda\). For these matrices, the number \(t\) of pairs of complex conjugate eigenvalues is slightly below \(\frac{n}{2}\), see Figure 2, where we averaged over 10,000 samples.

We stop the iterations if the following criteria are fulfilled:
7.3. Stopping criterion

Method I is stopped, if

$$
\| S \circ S - Q(L + V)Q^T \|_F = \sqrt{2F(S, Q, V)} < 10^{-12}
$$

(28)

and Method II if

$$
\| S \circ S - PT_{ab}(L + V)T_{ab}^{-1}P^T \|_F = \sqrt{2F(S, Q, V, a, b)} < 10^{-12}.
$$

(29)

An alternative would be to stop the algorithms if the eigenvalues of the iterates are close enough to the prescribed eigenvalues in the distance measure of Algorithm 5. Nevertheless, Figure 3 indicates that the stopping criteria (28) and (29) yield basically the same eigenvalue distances. Besides, our stopping criteria are more convenient, since computation of eigenvalues becomes expensive if the dimension grows, and since the linesearch guarantees that the functional values decrease monotone, which is in general not the case for the eigenvalue distances.

We considered $n = 200, 400, 600, 800, 1000$ and compared the number of iterations, the runtime and the distance of the eigenvalues of the computed stochastic matrix from the given ones, where we averaged over 50 samples computed by (26) in each dimension.

Figure 2. Left: Number $t$ of pairs of complex conjugate eigenvalues of $A$ in (27) in dependence on the size $n \times n$ of $A$. Right: Histogram of $t$ for 10,000 samples and $n = 600$.

Figure 3. Comparison of Methods I and II.
Table 1. Iterations $k$ and Runtime in $s$ together with std error of the mean for 50 samples.

| $n$  | $k$          |        | $k$          |        | $k$          |        | $k$          |        | $k$          |        |
|------|--------------|--------|--------------|--------|--------------|--------|--------------|--------|--------------|--------|
| 200  | 273.5 ± 5.6  | 356.8 ± 8.7 | 407.8 ± 9.4  | 441 ± 10.3 | 510.1 ± 14.2 |
| 400  | 283.5 ± 6.0  | 364.5 ± 8.3 | 402.6 ± 10.6 | 473.3 ± 10.9 | 519.3 ± 13.2 |
| 600  | 4.9 ± 0.1    | 57.9 ± 0.6  | 168.8 ± 1.6  | 370.7 ± 3.6  | 757.2 ± 9.7  |
| 800  | 6.2 ± 0.1    | 69.0 ± 1.4  | 193.6 ± 3.9  | 456.5 ± 9.7  | 878.4 ± 18.5 |

Figure 3 shows that our new method performs slightly worse, which is not surprising since we have to minimize over more variables. The exact values of the runtime are shown in Table 1. Figure 4 depicts the decay of the target functionals in dependence on the number of iterations for $n \in \{200, 600, 1000\}$. We also show the corresponding two least square fitting lines. We observe that Method I and Method II both converge linearly with basically the same convergence rate and that the slope of the regression line grows with dimension $n$ in both cases.

Finally, we noticed that skipping the additional step in Algorithm 4 slightly reduces the computational effort in high dimensions for the model from [19] but without a real difference, while our model becomes slightly slower, see Figure 5. The corresponding values are also given in Table 5. Table 2 shows the number of linesearch updates required with and without the additional step, and Table 3 the number of functional evaluations. Note that in our implementation the evaluation of the gradient, which is only necessary one time in each outer iteration $k$ in the algorithm, is a more costly operation than a functional evaluation in a linesearch update. As reported in Tables 4 and 7, the parameter $a$ does not
Table 2. Linesearch updates in Algorithm 4.

|      | n = 200 | n = 400 | n = 600 | n = 800 | n = 1000 |
|------|---------|---------|---------|---------|----------|
| I    | 120.6   | 148.9   | 180.3   | 194.2   | 203.8    |
| II   | 139.9   | 176.1   | 200.5   | 231.2   | 245.9    |
| I without add. step | 26.8    | 33.0    | 40.7    | 44.6    | 56.6     |
| II without add step  | 52.9    | 60.6    | 66.5    | 69.6    | 73.9     |

Table 3. Number of functional evaluations in Algorithm 4.

|      | n = 200 | n = 400 | n = 600 | n = 800 | n = 1000 |
|------|---------|---------|---------|---------|----------|
| I    | 658.52  | 867.78  | 1001.8  | 1091.7  | 1234     |
| II   | 670     | 869.4   | 972.3   | 1141.1  | 1243.1   |
| I without add. step | 334.1   | 469.5   | 582.3   | 702.8   | 807.1    |
| II without add step  | 371.3   | 508.1   | 593.2   | 657.6   | 748.5    |

Table 4. Minimal component of the vector a over all iterations and executions.

|      | n = 200 | n = 400 | n = 600 | n = 800 | n = 1000 |
|------|---------|---------|---------|---------|----------|
| I    | 0.98    | 0.98    | 0.98    | 0.98    | 0.99     |
| II   | 0.97    | 0.97    | 0.98    | 0.97    | 0.98     |
| I with add. step | 0.98    | 0.98    | 0.98    | 0.98    | 0.99     |
| II with add. step | 0.97    | 0.97    | 0.98    | 0.97    | 0.98     |

Table 5. Iterations $k$ and runtime in s together with std error of the mean for 50 samples if the linesearch without additional step is applied.

|      | n = 200 | n = 400 | n = 600 | n = 800 | n = 1000 |
|------|---------|---------|---------|---------|----------|
| Iterations, I | 307.3 ± 2.8 | 436.5 ± 3.6 | 541.6 ± 5.5 | 658.2 ± 9.8 | 750.5 ± 14.3 |
| Iterations, II | 318.4 ± 6.2 | 448.0 ± 15.2 | 526.7 ± 6.9 | 587.9 ± 6.4 | 674.6 ± 9.7 |
| Runtime, I    | 4.1 ± 0.0 | 51.2 ± 0.3 | 161.9 ± 1.4 | 388.2 ± 5.1 | 762.4 ± 12.7 |
| Runtime, II   | 5.2 ± 0.1 | 62.5 ± 2.0 | 186.4 ± 2.0 | 413.4 ± 3.7 | 816.6 ± 11.0 |

decrease to zero during the algorithm, which implies nonsingularity of the transformation matrices $T_{a,b}$.

7.4. Example with prescribed numbers of complex eigenvalues

For given $t \in \{1, \ldots, \lfloor n/2 \rfloor\}$, $n \geq 3$, we want to prescribe $t$ complex conjugate and $s$ real eigenvalues of a stochastic matrix. The theorem of Karpelevic [7] determines only the set of points $\Theta_n \subset \mathbb{C}$ that are eigenvalues of any $n \times n$ stochastic matrix without characterizing the relation the eigenvalues of one stochastic matrix have to fulfill. In other words, not every self-conjugate set with entries from $\Theta_n$ is the spectrum of a stochastic matrix. We will make use of the following observation.

**Proposition 7.1:** Let $\Lambda = (1, \lambda_2, \ldots, \lambda_n)^T$ be a self-conjugate vector such that

$$|\lambda_k| \leq \frac{1}{2n}$$

for all $k = 2, \ldots, n$. Then there exists $A \in S(n)$ whose eigenvalues are the components of $\Lambda$. 

**Proof:** We have $\Theta_m \subseteq \Theta_{m+1}$, see [12]. By Corollary 3.4, it follows for $n \in \mathbb{N}$ and all $k = 2, \ldots, n$ that

$$\lambda_k \in B_{1/2n} \subseteq B_{1/2} \subseteq \Theta_3 \subseteq \Theta_n,$$

where $\Theta_r := \{z \in \mathbb{C} : |z| \leq r\}$. By Chu and Golub [4, Corollary 4.18] and [4, p. 98], there exists $A \in S(n)$ with eigenvalues from $\Lambda$ if $2n \max_{k=2, \ldots, n} |\lambda_k| \leq 1$, which is just fulfilled for our setting. □

We choose $s-1$ real eigenvalues according to the uniform distribution on $[-1/(2n), 1/(2n)]$ and $t$ pairs of conjugate complex eigenvalues according to the uniform distribution on $B_{1/(2n)}$ in the complex plane, which we simulate by

$$x, y = \text{randn}, \quad \lambda = \frac{(x + iy) \cdot \sqrt{\text{rand}}}{\sqrt{x^2 + y^2}},$$

cf. [35, Algorithm 2.5.4].

Then, by the above proposition, there exists a stochastic matrix with these eigenvalues. For larger $n$ the $n-1$ eigenvalues $\neq 1$ become rather small and problem (StIEP) is severely ill-posed. Hence, we only consider a small size of $n = 20$. We observed that for small $t$ the distance to the input eigenvalues oscillates although the value of the functional decreases, while for larger $t$, these oscillations became negligible. Therefore we stop the experiment after 3000 iterations and choose those matrix having the smallest eigenvalue distance from the given ones. Table 6 shows the minimal distance together with the corresponding iteration number $k$ for various $t$ averaged over 200 samples, respectively.

We observe that, as $t$ gets larger, better results are achieved. The iteration number and the eigenvalue distance appear to be rather independent of $t$ and the chosen method. The corresponding values from the stopping criterion are between $10^{-7}$ and $10^{-8}$, in particular the algorithms reach the minimal eigenvalue distance before they would have been stopped in the previous example (Table 7).

Using the exponential maps as retractions we see that the minimal eigenvalue distances are attained much earlier and that the eigenvalues become slightly less close, see Table 8. If the different retraction apart from the exponential map is chosen, both methods start to run into problems with descending, but only for values smaller than approx. $10^{-15}$ in the stopping criterion, i.e. much later than it is usually stopped, which is supposed to be due to rounding errors. Interestingly, this behaviour is never observed, if the exponential maps

| $t$ | 1     | 2     | 3     | 4     | 5     |
|-----|-------|-------|-------|-------|-------|
| I: eigenvalue distance | $4.0 \times 10^{-6}$ | $4.1 \times 10^{-6}$ | $3.9 \times 10^{-6}$ | $1.2 \times 10^{-7}$ | $8.7 \times 10^{-9}$ |
| I: iteration $k$ | 1548.9 | 1651.3 | 1506 | 1539.3 | 1607.1 |
| II: eigenvalue distance | $3.0 \times 10^{-6}$ | $7.7 \times 10^{-6}$ | $3.0 \times 10^{-6}$ | $1.4 \times 10^{-7}$ | $7.3 \times 10^{-9}$ |
| II: iteration $k$ | 1666.2 | 1617.5 | 1676.9 | 1512.1 | 1647.5 |
| $t$ | 6     | 7     | 8     | 9     |
| I: eigenvalue distance | $2.7 \times 10^{-10}$ | $3.1 \times 10^{-11}$ | $7.5 \times 10^{-12}$ | $9.0 \times 10^{-13}$ |
| I: iteration $k$ | 1634 | 1479.2 | 1580.5 | 1598.6 |
| II: eigenvalue distance | $2.7 \times 10^{-10}$ | $3.1 \times 10^{-11}$ | $7.0 \times 10^{-12}$ | $9.8 \times 10^{-13}$ |
| II: iteration $k$ | 1625.8 | 1551.5 | 1618.2 | 1587.7 |
are chosen as retractions. However, this is not an argument for choosing the exponential
map, since the problems in descending occur at a point where basically rounding errors are
minimized and we have observed that the choice of the exponential maps is more costly in
total. Besides, we have seen that the chosen retractions different from the exponential map
close to the eigenvalues in our experiment (see Tables 6 and 8).

Acknowledgements
The authors want to thank S. Neumayer (TU Berlin) for fruitful discussions. Funding by the German
Research Foundation (DFG) within the project STE 571/16-1 is gratefully acknowledged.

Disclosure statement
No potential conflict of interest was reported by the author(s).

Funding
Funding by the German Research Foundation (DFG) within the project STE 571/16-1 is gratefully
acknowledged.

References
[1] Åström F, Petra S, Schmitzer B, et al. Image labeling by assignment. J Math Imaging Vis.
2017;58(2):211–238.
[2] Bergmann R, Fitschen JH, Persch J, et al. Iterative multiplicative filters for data labeling. Int J
Comput Vis. 2017;123(3):435–453.
[3] Cacace F, Germani A, Manes C. Karpelevich theorem and the positive realization of matrices.
In: 2019 IEEE 58th Conference on Decision and Control (CDC). IEEE; 2019. p. 6074–6079.
[4] Chu M, Golub G. Inverse eigenvalue problems: theory, algorithms, and applications. New York:
Oxford University Press; 2005.
[5] Suleimanova H. Stochastic matrices with real characteristic numbers. In: Doklady Akad. Nauk
SSSR (NS). Vol. 66; 1949. p. 343–345.
[6] Perfect H. Methods of constructing certain stochastic matrices. Duke Math J. 1953;20(3):
395–404.

Table 7. Minimal component of the vector a over all iterations and executions (min) and average over
all executions (average).
\[
\begin{array}{cccccccccc}
\hline
 t & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\
\hline
\text{II: min} & 0.94 & 0.96 & 0.75 & 0.92 & 0.91 & 0.92 & 0.93 & 0.88 & 0.77 \\
\text{II: average} & 1.0 & 0.99 & 0.99 & 0.99 & 0.99 & 0.99 & 0.99 & 0.99 & 0.98 \\
\hline
\end{array}
\]

Table 8. Corresponding results as in Table 6 if the exponential maps as retraction are chosen.
\[
\begin{array}{cccccccccc}
\hline
 t & 1 & 2 & 3 & 4 & 5 \\
\hline
\text{I: eigenvalue distance} & 4.2 \times 10^{-5} & 4.0 \times 10^{-5} & 1.4 \times 10^{-5} & 2.7 \times 10^{-6} & 5.2 \times 10^{-7} \\
\text{I: iteration } k & 156.3 & 160.2 & 160.0 & 161.3 & 160.4 \\
\text{II: eigenvalue distance} & 3.4 \times 10^{-5} & 4.3 \times 10^{-5} & 1.5 \times 10^{-5} & 2.4 \times 10^{-6} & 9.7 \times 10^{-7} \\
\text{II: iteration } k & 161.3 & 161.2 & 162.1 & 160.4 & 164.2 \\
\hline
\text{I: eigenvalue distance} & 1.2 \times 10^{-8} & 4.4 \times 10^{-10} & 1.3 \times 10^{-10} & 1.0 \times 10^{-11} \\
\text{I: iteration } k & 160.5 & 159.3 & 159.8 & 160.2 \\
\text{II: eigenvalue distance} & 7.8 \times 10^{-9} & 6.2 \times 10^{-10} & 7.4 \times 10^{-11} & 9.9 \times 10^{-12} \\
\text{II: iteration } k & 162.3 & 161.5 & 160.3 & 158.8 \\
\hline
\end{array}
\]
[7] Karpelevic FI. On the characteristic roots of matrices with nonnegative elements. Izv Ross Akad Nauk Ser Mat. 1951;15(4):361–383.

[8] Minc H. Nonnegative matrices. New York: John Wiley & Sons, Inc.; 1988. (Wiley-Intersci. Ser. Discrete Math. Optim.).

[9] Ito H. A new statement about the theorem determining the region of eigenvalues of stochastic matrices. Linear Algebra Appl. 1997;267:241–246.

[10] Johnson CR, Paparella P. A matricial view of the Karpelevič theorem. Linear Algebra Appl. 2017;520:1–15.

[11] Egleston PD, Lenker TD, Narayan SK. The nonnegative inverse eigenvalue problem. Linear Algebra Appl. 2004;379:475–490.

[12] Johnson CR, Marijuán C, Paparella P, et al. The NIEP. In: André C, Bastos M, Karlovich A, Silbermann B, Zaballa, I, editors. Operator theory, operator algebras, and matrix theory. Springer; 2018. p. 199–220.

[13] Xu S. An introduction to inverse algebraic eigenvalue problems. Peking: Peking University Press; 1998.

[14] Ciampolini L, Meignen S, Menut O, et al. Direct solution of the inverse stochastic problem through elementary Markov state disaggregation. Archive Ouvrert; 2014.

[15] Lin MM. An algorithm for constructing nonnegative matrices with prescribed real eigenvalues. Appl Math Comput. 2015;256:582–590.

[16] Orsi R. Numerical methods for solving inverse eigenvalue problems for nonnegative matrices. SIAM J Matrix Anal Appl. 2006;28(1):190–212.

[17] Chu MT, Driessel KR. Constructing symmetric nonnegative matrices with prescribed eigenvalues by differential equations. SIAM J Math Anal. 1991;22(5):1372–1387.

[18] Chu MT, Guo Q. A numerical method for the inverse stochastic spectrum problem. SIAM J Matrix Anal Appl. 1998;19(4):1027–1039.

[19] Zhao Z, Jin X-Q, Bai Z-J. A geometric nonlinear conjugate gradient method for stochastic inverse eigenvalue problems. SIAM J Numer Anal. 2016;54(4):2015–2035.

[20] Horn RA, Johnson CR. Matrix analysis. New York: Cambridge University Press; 2012.

[21] Loewy R, London D. A note on an inverse problem for nonnegative matrices. Linear Multilinear Algebra. 1978;6(1):83–90.

[22] Plonka G, Potts D, Steidl G, et al. Numerical Fourier analysis. Basel: Springer; 2018.

[23] Rossmann W. Lie groups: an introduction through linear groups. New York: Oxford University Press; 2006.

[24] Bertsekas D, Nedic A. Convex analysis and optimization. Belmont, MA: Athena Scientific; 2003.

[25] Wang Y, Zhao Z, Bai Z-J. Riemannian Newton-CG methods for constructing a positive doubly stochastic matrix from spectral data; 2020. Preprint arXiv:2006.13439.

[26] Bai Z, Demmel JW. On swapping diagonal blocks in real Schur form. Linear Algebra Appl. 1993;186:75–95.

[27] Brandts JH. Matlab code for sorting real Schur forms. Numer Linear Algebra Appl. 2002;9(3):249–261.

[28] Hager W, Zhang H. A survey of nonlinear conjugate gradient methods. Pacific J Optim. 2006;2(1):35–58.

[29] Daniel JW. The conjugate gradient method for linear and nonlinear operator equations. SIAM J Numer Anal. 1967;4(1):10–26.

[30] Zhang L, Zhou W, Li D-H. A descent modified Polak–Ribière–Polyak conjugate gradient method and its global convergence. IMA J Numer Anal. 2006;26(4):629–640.

[31] Smith ST. Optimization techniques on Riemannian manifolds. Fields Institute Commun. 1994;3(3):113–135.

[32] Absil P-A, Mahony R, Sepulchre R. Optimization algorithms on matrix manifolds. Princeton, NJ: Princeton University Press; 2009.

[33] Andrucho E, Larotonda G, Recht L, et al. The left invariant metric in the general linear group. J Geom Phys. 2014;86:241–257.
Algorithm 4. Further, let $x^{(k)} = (S^{(k)}, Q^{(k)}, V^{(k)}, a^{(k)}, b^{(k)}) \in \mathcal{M}_t$, $d^{(k)}$, $y^{(k)}$ be the iterates generated by Algorithm 3 with $\alpha^{(k)}$ as in Algorithm 4. Further, let

$$Z := \text{lev}_{F(x^{(0)})} F.$$ 

By Proposition 4.2, $Z \subset \mathcal{M}_t$ is compact and $x^{(k)} \in Z$ for all $k \in \mathbb{N}$. The proof is based on various auxiliary lemmas.

**Lemma A.1:** It holds

$$\lim_{k \to \infty} \alpha^{(k)} \|d^{(k)}\|_{x^{(k)}} = 0.$$ 

**Proof:** The linesearch in Algorithm 4 ensures that

$$\delta \sum_{k=0}^{\infty} \alpha^{(k)^2} \|d^{(k)}\|_{x^{(k)}}^2 \leq \sum_{k=0}^{\infty} (F(x^{(k)}) - F(x^{(k+1)})) = F(x^{(0)}) - \inf_{k \in \mathbb{N}} F(x^{(k)}) < \infty,$$

where the last inequality follows since $\inf_{x \in Z} F(x)$ is finite by Proposition 4.2. 

**Lemma A.2:** There exists a constant $C > 0$ such that for all $k$ sufficiently large,

$$\|y^{(k)}\|_{x^{(k+1)}} \leq C \alpha^{(k)} \|d^{(k)}\|_{x^{(k)}}.$$ 

**Proof:** By the applied vector transport (25) and since the projection is nonexpansive, we obtain

$$\|y^{(k)}\|_{x^{(k+1)}}^2 = \|g^{(k+1)} - T_{x^{(k)}} \alpha^{(k)} d^{(k)} g^{(k)}\|_{x^{(k+1)}}^2 = \|g^{(k+1)} - \Pi_{T_{x^{(k+1)}} \mathcal{M}_t} g^{(k)}\|_{x^{(k+1)}}^2 \\
\leq \|\nabla_{S,Q,V,b} F(x^{(k+1)}) - \nabla_{S,Q,V,b} F(x^{(k)})\|^2 + \|\nabla a F(x^{(k+1)}) - \nabla a F(x^{(k)})\|^2_{a^{(k+1)}} \\
\leq \|\nabla_{S,Q,V,b}^E F(x^{(k+1)}) - \nabla_{S,Q,V,b}^E F(x^{(k)})\|^2 + (a^{(k+1)})^{-2} \|\nabla a F(x^{(k+1)}) - \nabla a F(x^{(k)})\|^2,$$

where $\nabla_{S,Q,V,b}^E$ denotes the Euclidean gradient on $(\mathbb{R}^{n+m} \times \mathbb{R}').$ By Lemma 6.1, the gradients are continuously differentiable on $\mathcal{M}_t$ such that they are Lipschitz continuous on $Z$. Hence there exists $C > 0$ with

$$\|y^{(k)}\|_{x^{(k+1)}}^2 \leq C \text{dist}_{\mathcal{M}_t}^2 (x^{(k+1)}, x^{(k)}) = C \text{dist}_{\mathcal{M}_t}^2 (\mathcal{R}_{x^{(k)}} (\alpha^{(k)} d^{(k)}), x^{(k)}),$$

Since $Z$ is compact and by using Lemma A.1 together with [32, Proposition 7.4.5], we finally obtain

$$\|y^{(k)}\|_{x^{(k+1)}} \leq C \alpha^{(k)} \|d^{(k)}\|_{x^{(k)}}.$$ 

**Lemma A.3:** Suppose that there exists $\epsilon > 0$ such that

$$\|\nabla_{\mathcal{M}_t} F(x^{(k)})\|_{x^{(k)}} \geq \epsilon$$

for all $k \in \mathbb{N}$. Then there exists $C > 0$ such that for all $k \in \mathbb{N}$ it holds

$$\|d^{(k)}\|_{x^{(k)}} \leq C.$$
**Proof:** First, by compactness of $Z$ and continuity of $\nabla_{\mathcal{M}}F$ on $Z$, there exists $\gamma > 0$ such that

$$\|\nabla_{\mathcal{M}}F(x)\|_x \leq \gamma$$

(A1)

for all $x \in Z$. Since the $a$ component of $Z$ is uniformly bounded away from zero, it holds for $x \in Z$, $d \in T_x\mathcal{M}_t$, $\xi \in T_x\mathcal{M}_t$ and $z = R_x(d) \in Z$ that

$$\|T_xd\xi\|_z = \left\|\Pi_{T_x\mathcal{M}_t}(\xi)\right\|_z \leq \|\xi\|_z \leq C\|\xi\|_x, \quad C > 0,$$

(A2)

and we can estimate $|\theta^{(k)}|$ in Algorithm 3 as follows

$$|\theta^{(k)}| = \frac{\left|\langle \nabla_{\mathcal{M}}F(x^{(k+1)}), T_{x^{(k)}}d^{(k)}\rangle\right|}{\|\nabla_{\mathcal{M}}F(x^{(k)})\|_{x^{(k)}}} \leq C\|d^{(k)}\|_{x^{(k)}} \frac{\|\nabla_{\mathcal{M}}F(x^{(k+1)})\|_{x^{(k+1)}}}{\|\nabla_{\mathcal{M}}F(x^{(k)})\|_{x^{(k)}}}.$$  

(A3)

Similarly, we obtain for $\beta^{(k)}$ using Lemma A.2 that there exists an integer $k_1 > 0$ such that for all $k \geq k_1$ it holds

$$|\beta^{(k)}| \leq C\alpha^{(k)}\|d^{(k)}\|_{x^{(k)}} \frac{\|\nabla_{\mathcal{M}}F(x^{(k+1)})\|_{x^{(k+1)}}}{\|\nabla_{\mathcal{M}}F(x^{(k)})\|_{x^{(k)}}}.$$  

(A4)

Using the definition of $d^{(k+1)}$ together with (A1), (A2) and Lemma A.2, we get for all $k \geq k_1$ that

$$\|d^{(k+1)}\|_{x^{(k+1)}} \leq \gamma + C\|d^{(k)}\|_{x^{(k)}} (|\beta^{(k)}| + \alpha^{(k)}|\theta^{(k)}|).$$

Next, plugging in (A3) and (A4) gives

$$\|d^{(k+1)}\|_{x^{(k+1)}} \leq \gamma + 2C\alpha^{(k)}\|d^{(k)}\|_{x^{(k)}} \frac{\|\nabla_{\mathcal{M}}F(x^{(k+1)})\|_{x^{(k+1)}}}{\|\nabla_{\mathcal{M}}F(x^{(k)})\|_{x^{(k)}}} \leq \gamma + \frac{2C\gamma}{\epsilon^2}\frac{\|d^{(k)}\|_{x^{(k)}}}{\|d^{(k)}\|_{x^{(k)}}}.$$  

By Lemma A.1, there exist $r \in (0, 1)$ and $k_2 > 0$ such that for all $k \geq k_2$,

$$2C\frac{\gamma}{\epsilon^2}\frac{\|d^{(k)}\|_{x^{(k)}}}{\|d^{(k)}\|_{x^{(k)}}} \leq r.$$  

Then, we conclude for all $k \geq k_0 := \max(k_1, k_2)$ that

$$\|d^{(k+1)}\|_{x^{(k+1)}} \leq \gamma + r\|d^{(k)}\|_{x^{(k)}} \leq \gamma + \frac{r^k}{1 - r} \leq \frac{\gamma}{1 - r} + \|d^{(k_0)}\|_{x^{(k_0)}}.$$  

Finally, we estimate

$$\|d^{(k)}\|_{x^{(k)}} \leq \frac{\gamma}{1 - r} + \max_{1 \leq i \leq k_0} \|d^{(i)}\|_{x^{(k)}}.$$  

Now, we are able to prove Theorem 6.3.

**Proof of Theorem 6.3:** For the sake of contradiction, we assume that there exists a constant $\epsilon > 0$ such that $\|\nabla_{\mathcal{M}}F(x^{(k)})\|_{x^{(k)}} \geq \epsilon$ for all $k \in \mathbb{N}$. By construction of $d^{(k)}$ we get

$$\|\nabla_{\mathcal{M}}F(x^{(k)})\|_{x^{(k)}}^2 = -\langle d^{(k)}, \nabla_{\mathcal{M}}F(x^{(k)})\rangle_{x^{(k)}} \leq \|d^{(k)}\|_{x^{(k)}} \|\nabla_{\mathcal{M}}F(x^{(k)})\|_{x^{(k)}},$$

which implies $\|\nabla_{\mathcal{M}}F(x^{(k)})\|_{x^{(k)}} \leq \|d^{(k)}\|_{x^{(k)}}$. Combining this with Lemma A.1, we get

$$\lim_{k \to \infty} \alpha^{(k)}\|\nabla_{\mathcal{M}}F(x^{(k)})\|_{x^{(k)}} = 0$$

and consequently also $\lim_{k \to \infty} \alpha^{(k)} = 0$.  


It follows from the line search condition in Algorithm 4 that
\[
F \circ R_{x(k)}(\tau^{-1} \alpha^{(k)} d^{(k)}) - F(x^{(k)}) \geq -\delta \tau^{-2} \alpha^{(k)} d^{(k)}_2 |x^{(k)}_2|^2. \tag{A5}
\]
Next, we consider the so-called pullback function \( \hat{F} := F \circ R : TM_t \to \mathbb{R} \), which is \( C^\infty \) as concatenation of \( C^\infty \) functions and fulfills
\[
\nabla \hat{F}_x(0) = \nabla_{\mathcal{M}_t} F(x), \quad x \in \mathcal{M}_t,
\]
due to the properties of retractions. For \( x \in \mathcal{M}_t \), we denote the restriction of \( \hat{F} \) to \( T_x \mathcal{M}_t \) by \( \hat{F}_x \). Since \( \hat{F} \) is \( C^\infty \) and hence its gradient is Lipschitz on compact sets, there exists \( L > 0 \) such that
\[
\| \nabla \hat{F}_x(\eta) - \nabla \hat{F}_x(0) \| x \leq L \| \eta \| x \tag{A6}
\]
for all \( x \in \mathcal{Z} \) and \( \eta \in T_x \mathcal{M}_t \) with \( \| \eta \| x \leq 1 \).

By the mean-value theorem we obtain for some \( \omega^{(k)} \in (0, 1) \) that
\[
F \circ R_{x(k)}(\tau^{-1} \alpha^{(k)} d^{(k)}) - F(x^{(k)}) = \hat{F}_{x(k)}(\tau^{-1} \alpha^{(k)} d^{(k)}) - \hat{F}_{x(k)}(0)
\]
\[
= \tau^{-1} \alpha^{(k)} \langle \nabla \hat{F}_{x(k)}(0), d^{(k)} \rangle_{x(k)} + \omega^{(k)} \tau^{-2} \alpha^{(k)} |d^{(k)}|_x^2,
\]
and further by (A6) for \( \| \alpha^{(k)} d^{(k)} \|_{x^{(k)}} \leq \tau \) that
\[
F \circ R_{x(k)}(\tau^{-1} \alpha^{(k)} d^{(k)}) - F(x^{(k)})
\]
\[
= \tau^{-1} \alpha^{(k)} \langle \nabla \hat{F}_{x(k)}(0), d^{(k)} \rangle_{x(k)} + \omega^{(k)} \tau^{-2} \alpha^{(k)} |d^{(k)}|_x^2
\]
\[
\leq -\tau^{-1} \alpha^{(k)} \| \nabla_{\mathcal{M}_t} F(x^{(k)}) \|_{x^{(k)}}^2 + L \omega^{(k)} \tau^{-2} \alpha^{(k)} |d^{(k)}|_x^2
\]
Together with (A5) we conclude for sufficiently large \( k \) that
\[
\| \nabla_{\mathcal{M}_t} F(x^{(k)}) \|_{x^{(k)}}^2 \leq -\frac{\tau}{\alpha^{(k)}} (F \circ R_{x(k)}(\tau^{-1} \alpha^{(k)} d^{(k)}) - F(x^{(k)})) + L \tau^{-1} \alpha^{(k)} |d^{(k)}|_x^2
\]
\[
\leq (L + \delta) \tau^{-1} \alpha^{(k)} |d^{(k)}|_x^2.
\]
Since \( |d^{(k)}|_k \) is bounded by Lemma A.3 and \( \lim_{k \to \infty} \alpha^{(k)} = 0 \), we obtain the contradiction
\[
\lim_{k \to \infty} \| \nabla_{\mathcal{M}_t} F(x^{(k)}) \|_{x^{(k)}} = 0,
\]
which concludes the proof. \( \blacksquare \)