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A Riemannian inexact Newton-CG method for stochastic inverse singular value problems

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Summary

In this article, we consider the stochastic inverse singular value problem (ISVP) of constructing a stochastic matrix from the prescribed realizable singular values. We propose a Riemannian inexact Newton-CG method with various choices of forcing terms for solving the stochastic ISVP. We show the proposed method converges linearly or superlinearly for different forcing terms under some assumptions. We also extend the proposed method to the case of prescribed entries. Finally, we report some numerical results to demonstrate the effectiveness of the proposed method.

KEYWORDS

forcing term, inverse singular value problem, Newton's method, Riemannian manifold

MOS SUBJECT CLASSIFICATION

65F18; 65F15; 15A18; 65K05; 90C26; 90C48

1 | INTRODUCTION

An inverse singular value problem (ISVP) aims to reconstruct a structured matrix from the prescribed singular values. The ISVP arises in many applications such as structural health monitoring, code division multiple access system, quadratic group, transient circuit simulation.[1-4] There are different structured ISVPs including the affine ISVP and the ISVP for Toeplitz-related matrices, nonnegative, positive, and antibisymmetric matrices.[5-11]

As in Reference 12, a list of nonnegative scalars, which are the singular values of some matrix, is called to be *realizable*. In this article, we consider the stochastic ISVP of constructing a stochastic matrix from the given singular values and/or the prescribed entries defined as follows.

StISVP. *Given a realizable list of n nonnegative scalars* $\{\sigma_1, \sigma_2, \ldots, \sigma_n\}$, *find an n-by-n stochastic matrix C such that it has the singular values* $\sigma_1, \sigma_2, \ldots, \sigma_n$.

StISVP-PE. *Given a realizable list of n nonnegative scalars* $\{\sigma_1, \sigma_2, \ldots, \sigma_n\}$ *and the prescribed nonnegative numbers* $\{g_{ij} : (i,j) \in \mathcal{L}\}$, *where* $\mathcal{L}$ *is an index subset of* $\mathcal{N} := \{(i,j) \mid i,j = 1, \ldots, n\}$, *find an n-by-n stochastic matrix* $C = (c_{ij})$ *such that it has the singular values* $\sigma_1, \sigma_2, \ldots, \sigma_n$ *and*

$$c_{ij} = g_{ij}, \quad \forall (i,j) \in \mathcal{L}.$$

An ISVP with prescribed entries for a general real matrix was also proposed in [13, pp. 115–116]. There exist some numerical methods for solving special ISVPs. In particular, some constructive methods were given for the ISVP for Toeplitz-related matrices, nonnegative, positive, and antibisymmetric matrices.[6,9-11] Several Newton-type methods and Ulm-like methods were proposed for the affine ISVP.[7,14-18] In Reference 2, a Newton-type method was given for solving the ISVP in some quadratic group. In Reference 19, an alternating projection method was proposed for solving the ISVP for nonnegative matrices with prescribed structure.

In this article, we propose a Riemannian inexact Newton-CG method with various choices of forcing terms for solving the StISVP. This is sparked by Zhao et al..[20] In Reference 20, a Riemannian inexact Newton-CG method was proposed for the nonnegative inverse eigenvalue problem with prescribed realizable spectrum. As the classical inexact Newton method,[21-25] we choose different forcing terms for solving the normal equations (i.e., (9) below) by using the conjugate gradient (CG) method.[26] Under some assumptions, we show that the proposed Riemannian inexact Newton-CG method converges globally and linear or superlinearly for different forcing terms. We also extend the proposed method to the solution of the StISVP-PE. The advantage of our method lies in that it is specially designed for solving the StISVP and different choices of forcing terms are such that our method is more flexible for practical problems. Finally, some numerical tests including a practical application in the hidden Markov model (HMM) are reported to illustrate the effectiveness of our method for solving the StISVP and StISVP-PE.

Throughout the article, we use the following notation. Let I_n be the identity matrix of order n. Let $\mathbb{R}^{m\times n}$ be the set of all m-by-n real matrices. Denote by $\|\cdot\|_F$ the Frobenius matrix norm. For a matrix $A \in \mathbb{R}^{n\times n}$, let $\boldsymbol{\sigma}(A) = (\sigma_1(A), \sigma_2(A), \ldots, \sigma_n(A))^T$, where $\sigma_i(A)$ denotes the ith largest singular value of A. The symbol A^T denotes the transpose of a matrix A. Let $A \odot B$ be the Hadamard product of two m-by-n matrices A and B. For a matrix $A \in \mathbb{R}^{n\times n}$, let $\mathrm{diag}(A)$ and $\mathrm{tr}(A)$ denote the diagonal matrix with the same diagonal entries as A and the trace of A, respectively. For a vector $\mathbf{x} \in \mathbb{R}^n$, $\mathrm{Diag}(\mathbf{x})$ is a diagonal matrix with $\mathbf{x}$ on its diagonal. Let $\mathcal{X}$ and $\mathcal{Y}$ be two finite-dimensional vector spaces equipped with a scalar inner product $\langle\cdot,\cdot\rangle$ and its induced norm $\|\cdot\|$. Let $\mathcal{A} : \mathcal{X} \to \mathcal{Y}$ be a linear operator such that $\mathcal{A}[x] \in \mathcal{Y}$ for all $x \in \mathcal{X}$ and the adjoint of $\mathcal{A}$ is denoted by $\mathcal{A}^*$. Define the operator norm of $\mathcal{A}$ by $|||\mathcal{A}||| := \sup\{\|\mathcal{A}[x]\| \mid x \in \mathcal{X} \text{ with } \|x\| = 1\}$.

The rest of this article is organized as follows. In Section 2, we present our Riemannian inexact Newton-CG method with various forcing terms for solving the StISVP. In Section 3, we derive the global and local linear or superlinear convergence of the proposed method under some assumptions. In Section 4, we extend the proposed method to the solution of the StISVP-PE. In Section 5, we report some numerical tests to indicate the effectiveness of our method. Finally, some concluding remarks are given in Section 6.

2 | RIEMANNIAN INEXACT NEWTON-CG METHOD

In this section, we turn the StISVP into a nonlinear matrix equation over a product matrix manifold. Then we provide a Riemannian inexact Newton-CG method with several choices of forcing terms for solving the manifold-constrained nonlinear matrix equation.

2.1 | Reformulation

For the given singular values $\sigma_1, \sigma_2, \ldots, \sigma_n$, without loss of generality, we assume that

$$\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n \geq 0.$$

Let

$$\Sigma := \mathrm{Diag}(\boldsymbol{\sigma}), \quad \boldsymbol{\sigma} := (\sigma_1, \ldots, \sigma_n)^T.$$

Define the set of all n-by-n orthogonal matrices by

$$\mathcal{O}(n) := \{Q \in \mathbb{R}^{n\times n} \mid Q^TQ = I_n\}.$$

As in Reference 27, define the set of all n-by-n stochastic matrices by

$$\mathcal{S} := \{S \odot S \mid S \in \mathbb{R}^{n\times n}, \operatorname{diag}(SS^T) = I_n\}.$$

The set of all n-by-n real matrices with the singular values $\sigma_1, \sigma_2, \ldots, \sigma_n$ can be defined by

$$\mathcal{M}(\Sigma) := \{U\Sigma V^T \mid U, V \in \mathcal{O}(n)\},$$

which is a matrix manifold. Then the StISVP has a solution if and only if $\mathcal{S} \cap \mathcal{M}(\Sigma) \neq \emptyset$.

Define a product matrix manifold $\mathcal{Z}$ by

$$\mathcal{Z} := \mathcal{OB} \times \mathcal{O}(n) \times \mathcal{O}(n), \tag{1}$$

where $\mathcal{OB}$ is the oblique manifold defined by Absil et al.[28]

$$\mathcal{OB} := \{S \in \mathbb{R}^{n\times n} \mid \operatorname{diag}(SS^T) = I_n\}. \tag{2}$$

By hypothesis, the list of n nonnegative numbers $\{\sigma_1, \sigma_2, \ldots, \sigma_n\}$ is realizable. Thus, the StISVP has at least one solution. To solve the StISVP, one may find a solution $(S, U, V) \in \mathcal{Z}$ to the following nonlinear matrix equation:

$$H(S, U, V) := S \odot S - U\Sigma V^T = \mathbf{0}_{n\times n}, \tag{3}$$

where $\mathbf{0}_{n\times n}$ is the zero matrix of order n and H is a nonlinear mapping from the product matrix manifold $\mathcal{Z}$ to the Euclidean space $\mathbb{R}^{n\times n}$. If $(\overline{S}, \overline{U}, \overline{V}) \in \mathcal{Z}$ is a solution to (3), then $\overline{S} \odot \overline{S}$ is a solution to the StISVP. We also see that the dimension of $\mathcal{Z}$ is given by Absil et al.[28]

$$\dim \mathcal{Z} = n(n-1) + \frac{1}{2}n(n-1) + \frac{1}{2}n(n-1) > \dim \mathbb{R}^{n\times n}, \quad n \geq 3.$$

Hence the manifold-constrained nonlinear equation $H(S, U, V) = \mathbf{0}_{n\times n}$ is underdetermined for all $n \geq 3$.

2.2 | Riemannian inexact Newton-CG method

Sparked by Zhao et al.,[20] we propose several Riemannian inexact Newton-CG methods for solving the StISVP (3). We first note that $\mathcal{Z}$ is an embedded submanifold of $\mathbb{R}^{n\times n} \times \mathbb{R}^{n\times n} \times \mathbb{R}^{n\times n}$. This induces a Riemannian metric on $\mathcal{Z}$ as follows:

$$g_{(S,U,V)}((\xi_1, \zeta_1, \eta_1), (\xi_2, \zeta_2, \eta_2)) := \operatorname{tr}(\xi_1^T \xi_2) + \operatorname{tr}(\zeta_1^T \zeta_2) + \operatorname{tr}(\eta_1^T \eta_2), \tag{4}$$

for all $(S, U, V) \in \mathcal{Z}$ and

$$(\xi_1, \zeta_1, \eta_1), (\xi_2, \zeta_2, \eta_2) \in T_{(S,U,V)}\mathcal{Z},$$

where $T_{(S,U,V)}\mathcal{Z}$ is characterized as in Appendix. For simplicity, in what follows, let $\langle \cdot, \cdot \rangle$ and $\| \cdot \|$ be the Riemannian metric and its induced norm on $\mathcal{Z}$, respectively.

As noted in References 20,29, the Riemannian Newton method for solving (3) can be described as follows: Given $X^k := (S^k, U^k, V^k) \in \mathcal{Z}$, define $X^{k+1} := R_{X^k}(\Delta X^k)$, where $\Delta X^k := (\Delta S^k, \Delta U^k, \Delta V^k) \in T_{X^k}\mathcal{Z}$ is determined by

$$\mathrm{D}H(X^k)[\Delta X^k] = -H(X^k). \tag{5}$$

Here, the differential $\mathrm{D}H(X^k)$ of H at X^k, its adjoint $(\mathrm{D}H\ (X^k))^*$, and the retraction R on $\mathcal{Z}$ are characterized in Appendix (A1).

We note that the Newton equation (5) is underdetermined, which is solvable if and only if

$$\mathrm{D}H(X^k) \circ (\mathrm{D}H(X^k))^{\dagger}[H(X^k)] = H(X^k), \tag{6}$$

where $(\mathrm{D}H\ (X^k))^{\dagger}$ means the pseudoinverse of the linear operator $\mathrm{D}H(X^k)$ [30, p. 163]. Especially, if $\mathrm{D}H(X^k)$ is surjective, that is, $\mathrm{D}H(X^k) \circ (\mathrm{D}H\ (X^k))^*$ is positive definite, then the minimum norm solution to (5) is given by $\Delta X^k = (\mathrm{D}H(X^k))^*[\Delta Z^k]$, where $\Delta Z^k \in T_{H(X^k)}\mathbb{R}^{n\times n}$ is determined by

$$\mathrm{D}H(X^k) \circ (\mathrm{D}H(X^k))^*[\Delta Z^k] = -H(X^k). \tag{7}$$

On the positive definiteness of $\mathrm{D}H(\cdot) \circ (\mathrm{D}H\ (\cdot))^*$, we have the following result, whose proof is given in Appendix.

Theorem 1. *Let $X = (S, U, V) \in \mathcal{Z}$ be arbitrary with $U = [\mathbf{u}_1, \ldots, \mathbf{u}_n]$ and $V = [\mathbf{v}_1, \ldots, \mathbf{v}_n]$. If the given singular values $\sigma_1, \sigma_2, \ldots, \sigma_n$ are all distinct and the matrix*

$$\begin{aligned} P := [&\mathrm{vec}(S \odot (\mathbf{u}_1\mathbf{v}_1^T) - \mathrm{diag}(S(S \odot (\mathbf{u}_1\mathbf{v}_1^T))^T)S), \ldots, \\ &\mathrm{vec}(S \odot (\mathbf{u}_n\mathbf{v}_n^T) - \mathrm{diag}(S(S \odot (\mathbf{u}_n\mathbf{v}_n^T))^T)S)] \in \mathbb{R}^{n^2\times n} \end{aligned} \tag{8}$$

is full column rank, then $(\mathrm{D}H(X) \circ (\mathrm{D}H\ (X))^*$ is positive definite, that is,

$$\langle \Delta Z, \mathrm{D}H(X) \circ (\mathrm{D}H(X))^*[\Delta Z]\rangle > 0, \quad \forall \Delta Z \in T_{H(X)}\mathbb{R}^{n\times n} \setminus \{\mathbf{0}_{n\times n}\}.$$

Suppose the given singular values $\sigma_1, \sigma_2, \ldots, \sigma_n$ are all distinct. We see from Theorem 1 that if $X = (S, U, V) \in \mathcal{Z}$ is such that there exist n rows are independent in the $n^2 \times n$ matrix P defined by (8), then the positive definiteness of $\mathrm{D}H(\cdot) \circ (\mathrm{D}H\ (\cdot))^*$ is guaranteed. Moreover, the positive definiteness conditions in Theorem 1 may be unnecessary in practice. This motivates us to propose the following Riemannian inexact Newton-CG algorithm for solving the StISVP (3).

Algorithm 1 *(* A Riemannian Inexact Newton-CG Algorithm)

Step 0. Choose an initial point $X^0 \in \mathcal{Z}$, $\bar{\epsilon} > 0$, $0 < \bar{\eta}_{\max} < 1$, $0 < t < 1$, $0 < \theta_{\min} < \theta_{\max} < 1$. Let $k := 0$.

Step 1. If $\|H(X^k)\|_F < \bar{\epsilon}$, stop.

Step 2. Apply the CG method to find an approximate solution $\Delta Z^k \in T_{H(X^k)}\mathbb{R}^{n\times n}$ to

$$\mathrm{D}H(X^k) \circ (\mathrm{D}H(X^k))^*[\Delta Z^k] = -H(X^k), \tag{9}$$

such that

$$\|\mathrm{D}H(X^k) \circ (\mathrm{D}H(X^k))^*[\Delta Z^k] + H(X^k)\|_F \le \bar{\eta}_k\|H(X^k)\|_F, \tag{10}$$

and

$$\|\mathrm{D}H(X^k) \circ (\mathrm{D}H(X^k))^*[\Delta Z^k] + H(X^k)\|_F < \|H(X^k)\|_F, \tag{11}$$

where $\bar{\eta}_k$ is a forcing term. Let

$$\widehat{\Delta X}^k := (\mathrm{D}H(X^k))^*[\Delta Z^k] \quad \text{and} \quad \hat{\eta}_k := \frac{\|\mathrm{D}H(X^k)[\widehat{\Delta X}^k] + H(X^k)\|_F}{\|H(X^k)\|_F}. \tag{12}$$

Step 3. Evaluate $H(R_{X^k}(\widehat{\Delta X}^k))$. Set $\eta_k = \hat{\eta}_k$ and $\Delta X^k = \widehat{\Delta X}^k$.

Repeat until $\|H(R_{X^k}(\Delta X^k))\|_F \le (1 - t(1 - \eta_k))\|H(X^k)\|_F$.

Choose $\theta \in [\theta_{\min}, \theta_{\max}]$.

Replace ΔX^k by $\theta\Delta X^k$ and η_k by $1 - \theta(1 - \eta_k)$.

end (Repeat)

Set

$$X^{k+1} := R_{X^k}(\Delta X^k).$$

Step 4. Replace k by $k+1$ and go to Step 1.

We observe that, in Step 3 of Algorithm 1, we need to choose a forcing term $\overline{\eta}_k$, which is critical to the efficiency and robustness of the proposed algorithm. As the classical inexact Newton method,[21-25] we choose different forcing terms as follows: a) $\overline{\eta}_k \le \overline{\eta}_{\max} < 1$; b) $\overline{\eta}_k = 1/(k+2)$; c) $\overline{\eta}_k = 1/2^{k+1}$; d) $\overline{\eta}_k = \min\{\overline{\eta}_{\max}, \|H(X^k)\|_F\}$; e) $\overline{\eta}_k = \min\{1/(k+2), \|H(X^k)\|_F\}$. Finally, one may choose the scaling factor θ for Step 3 of Algorithm 1 as in References 20,31, that is,

$$\theta = \min\left\{\max\left\{\theta_{\min}, \frac{-u'(0)}{2(u(1)-u(0)-u'(0))}\right\}, \theta_{\max}\right\},$$

where $u(0) = \|H(X^k)\|_F^2$, $u(1) = \|H(R_{X^k}(\Delta X^k))\|_F^2$, and $u'(0) = 2\langle \mathrm{D}H(X^k)[\Delta X^k], H(X^k)\rangle$.

3 | CONVERGENCE ANALYSIS

In this section, we establish the global and local linear or superlinear convergence of Algorithm 1. It is easy to see that $\mathcal{OB}$ and $\mathcal{O}(n)$ are two compact manifolds. For the retraction R on $\mathcal{Z}$ defined in (A1), there exist two scalars $\nu > 0$ and $\mu_\nu > 0$ such that [28, p. 149]

$$\nu\|\Delta X\| \ge \mathrm{dist}(X, R_X(\Delta X)), \tag{13}$$

for all $X := (S, U, V) \in \mathcal{Z}$ and

$$\Delta X := (\Delta S, \Delta U, \Delta V) \in T_X\mathcal{Z} \quad \text{with} \quad \|\Delta X\| \le \mu_\nu, \tag{14}$$

where "dist" means the Riemannian distance on $\mathcal{Z}$. The pullback $\hat{H}$ of H is a smooth mapping from the tangent bundle $T\mathcal{Z}$ of $\mathcal{Z}$ to $\mathbb{R}^{n\times n}$ defined by

$$\hat{H}(\xi) := H(R(\xi)), \quad \forall \xi \in T\mathcal{Z}. \tag{15}$$

For any $X \in \mathcal{Z}$, the restriction of $\hat{H}$ on $T_X\mathcal{Z}$ is defined by

$$\hat{H}_X(\xi_X) = H(R_X(\xi_X)), \quad \forall \xi_X \in T_X\mathcal{Z}. \tag{16}$$

Thus,

$$\mathrm{D}H(X) = \mathrm{D}\hat{H}_X(0_X), \quad \forall X \in \mathcal{Z}, \tag{17}$$

where 0_X is the origin of $T_X\mathcal{Z}$. As in References 20,32, a point $X \in \mathcal{Z}$ is called *a stationary point* of $\|H\|_F$ if

$$\|H(X)\|_F \le \|H(X) + \mathrm{D}H(X)[\Delta X]\|_F, \quad \forall \Delta X \in T_X\mathcal{Z}.$$

As noted in Reference 20, to derive the global and local linear or superlinear convergence of Algorithm 1, we need the following assumption.

Assumption 1. Suppose Algorithm 1 does not break down, $\sum_{k=0}^{\infty}(1-\eta_k)$ is divergent, and $\mathrm{D}H(\cdot)\circ(\mathrm{D}H(\cdot))^*$ is positive definite at an accumulation point of the sequence $\{X^k\}$ generated by Algorithm 1.

3.1 | Global convergence

For the iterate $\widehat{\Delta X}^k$ generated by Algorithm 1, we have the following estimate.

Lemma 1. *Let X^k be the current iterate generated by Algorithm 1. If X^k is not a stationary point of $\|H\|_F$, then*

$$\|\widehat{\Delta X}^k\| \le (1+\overline{\eta}_k)|||(\mathrm{D}H(X^k))^\dagger||| \cdot \|H(X^k)\|_F.$$

Proof. By hypothesis, X^k is not a stationary point of $\|H\|_F$. We can solve (9) such that conditions (10) and (11) are satisfied. By using (12), $\widehat{\Delta X}^k = (\mathrm{D}H(X^k))^*[\Delta Z^k]$ and thus $\widehat{\Delta X}^k \perp \mathrm{null}(\mathrm{D}H(X^k))$. Using Lemma 4 in page 17 of Reference 31, we have

$$\|\widehat{\Delta X}^k\| = \|(\mathrm{D}H(X^k))^\dagger \circ \mathrm{D}H(X^k)[\widehat{\Delta X}^k]\|. \tag{18}$$

It follows from (10), (12), and (18) that

$$\begin{aligned}
\|\widehat{\Delta X}^k\| &= \|(\mathrm{D}H(X^k))^\dagger \circ \mathrm{D}H(X^k)[\widehat{\Delta X}^k]\| \\
&= \|(\mathrm{D}H(X^k))^\dagger \circ \mathrm{D}H(X^k) \circ (\mathrm{D}H(X^k))^*[\Delta Z^k]\| \\
&\le |||(\mathrm{D}H(X^k))^\dagger||| \cdot \|\mathrm{D}H(X^k) \circ (\mathrm{D}H(X^k))^*[\Delta Z^k]\|_F \\
&\le |||(\mathrm{D}H(X^k))^\dagger||| \cdot (\|\mathrm{D}H(X^k) \circ (\mathrm{D}H(X^k))^*[\Delta Z^k] + H(X^k)\|_F + \|H(X^k)\|_F) \\
&= (1+\overline{\eta}_k)|||(\mathrm{D}H(X^k))^\dagger||| \cdot \|H(X^k)\|_F.
\end{aligned}$$

■

Using (10) and (12) we can easily get the upper bound of the iterate $\hat{\eta}_k$ generated by Algorithm 1.

Lemma 2. *Let X^k be the current iterate generated by Algorithm 1. If X^k is not a stationary point of $\|H\|_F$, then*

$$\hat{\eta}_k \le \overline{\eta}_k.$$

By following the similar proof of [20, lemma 4], we have the following result on the repeat-loop in Algorithm 1.

Lemma 3. *Let X^k be the current iterate generated by Algorithm 1. If X^k is not a stationary point of $\|H\|_F$, then the repeat-loop terminates in finite steps with ΔX^k and η_k satisfying*

$$\begin{cases} \|H(X^k) + \mathrm{D}H(X^k)[\Delta X^k]\|_F \le \eta_k \|H(X^k)\|_F, \\ \|H(X^{k+1})\|_F \le (1 - t(1-\eta_k))\|H(X^k)\|_F. \end{cases}$$

Then, we have the following result on the global convergence of Algorithm 1, whose proof follows from [20, theorem 2].

Theorem 2. *Let $\overline{X}$ be an accumulation point of the sequence $\{X^k\}$ generated by Algorithm 1. Suppose Assumption 1 is satisfied. Then the sequence $\{X^k\}$ converges to $\overline{X}$ and $H(\overline{X}) = 0_{n\times n}$.*

3.2 | Local convergence rate

We show the linear or superlinear convergence of Algorithm 1 with different choices of forcing term $\overline{\eta}_k$. We first have the following result on the backtracking line search procedure. This follows from the similar proof of [20, lemmas 4–5].

Lemma 4. *Let $\overline{X}$ be an accumulation point of the sequence $\{X^k\}$ generated by Algorithm 1. Suppose Assumption 1 is satisfied. Then $\eta_k = \hat{\eta}_k$ and $\Delta X^k = \widehat{\Delta X}^k$ for all k sufficiently large.*

In the rest of this section, we show the local linear or superlinear convergence of Algorithm 1 for different choices of $\overline{\eta}_k$.

Theorem 3. *Let $\overline{X}$ be an accumulation point of the sequence $\{X^k\}$ generated by Algorithm 1. Suppose Assumption 1 is satisfied. Then there exists a constant η with $\overline{\eta}_k \le \overline{\eta}_{\max} < \eta < 1$ such that the sequence $\{X^k\}$ converges to $\overline{X}$ linearly.*

Proof. It follows from Theorem 2 and Lemma 4 that the sequence $\{X^k\}$ converges to $\overline{X}$ with $H(\overline{X}) = 0$ and $\eta_k = \hat{\eta}_k$ and $\Delta X^k = \widehat{\Delta X}^k$ for all k sufficiently large with $\|\Delta X^k\| = \|\widehat{\Delta X}^k\| \to 0$ as $k \to \infty$. By hypothesis, $\mathrm{D}H(\overline{X})$ is surjective. Thus, for all k sufficiently large, $\mathrm{D}H(X^k)$ is surjective and

$$|||(\mathrm{D}H(X^k))^\dagger||| \le 2|||(\mathrm{D}H(\overline{X}))^\dagger|||. \tag{19}$$

Using Lemma 1, we have for all k sufficiently large,

$$\begin{aligned}\|\widehat{\Delta X}^k\| &\le (1+\overline{\eta}_k)|||(\mathrm{D}H(X^k))^\dagger||| \cdot \|H(X^k)\|_F \\ &\le 2(1+\overline{\eta}_k)|||(\mathrm{D}H(\overline{X}))^\dagger||| \cdot \|H(X^k)\|_F.\end{aligned} \tag{20}$$

Moreover, there exist two constants $L_1, L_2 > 0$ such that for all k sufficiently large,

$$\begin{cases}\|H(X^k) - H(\overline{X})\|_F \le L_1 \mathrm{dist}(X^k, \overline{X}), \\ \|\hat{H}_{X^k}(\Delta X^k) - \hat{H}_{X^k}(0_{X^k}) - \mathrm{D}\hat{H}_{X^k}(0_{X^k})[\Delta X^k]\|_F \le L_2\|\Delta X^k\|^2, \\ \mathrm{dist}(X^k, R_{X^k}(\Delta X^k)) \le \nu\|\Delta X^k\|,\end{cases} \tag{21}$$

where ν is the constant given in (13).

Let

$$\eta = \max\left\{\overline{\eta}_{\max}, \frac{1}{1+2c_2}\right\} < 1, \tag{22}$$

where $c_2 := L_1(2\nu(1+\overline{\eta}_{\max})|||(\mathrm{D}H(\overline{X}))^\dagger|||)/(t(1-\overline{\eta}_{\max}))$. Using (10) and (12) we have for all k sufficiently large,

$$\hat{\eta}_k \le \overline{\eta}_k \le \overline{\eta}_{\max} \le \eta < 1. \tag{23}$$

From (12) and (19) to (23) we have for all k sufficiently large,

$$\begin{aligned}\|H(X^{k+1})\|_F &= \|H(X^{k+1}) - H(X^k) - \mathrm{D}H(X^k)[\Delta X^k] + H(X^k) + \mathrm{D}H(X^k)[\Delta X^k]\|_F \\ &\le \|\hat{H}_{X^k}(\Delta X^k) - \hat{H}_{X^k}(0_{X^k}) - \mathrm{D}\hat{H}_{X^k}(0_{X^k})[\Delta X^k]\|_F \\ &\quad + \|\hat{H}_{X^k}(0_{X^k}) + \mathrm{D}\hat{H}_{X^k}(0_{X^k})[\Delta X^k]\|_F \\ &\le L_2\|\Delta X^k\|^2 + \hat{\eta}_k\|H(X^k)\|_F \\ &\le L_2(2(1+\overline{\eta}_k)|||(\mathrm{D}H(\overline{X}))^\dagger|||)^2\|H(X^k)\|_F^2 + \overline{\eta}_k\|H(X^k)\|_F \qquad (24) \\ &\le L_1L_2(2(1+\overline{\eta}_{\max})|||(\mathrm{D}H(\overline{X}))^\dagger|||)^2\|H(X^k)\|_F\mathrm{dist}(X^k, \overline{X}) + \overline{\eta}_k L_1 \mathrm{dist}(X^k, \overline{X}) \\ &\le L_1(c_1\|H(X^k)\|_F + \overline{\eta}_k)\mathrm{dist}(X^k, \overline{X}), \qquad (25)\end{aligned}$$

where $c_1 := L_2(2(1+\overline{\eta}_{\max})|||(\mathrm{D}H(\overline{X}))^\dagger|||)^2$. From (19), (21), (22), and (25) it follows that for all k sufficiently large,

$$\begin{aligned}\mathrm{dist}(X^{k+1}, \overline{X}) &\le \sum_{j=k+1}^{\infty}\mathrm{dist}(X^j, X^{j+1}) = \sum_{j=k+1}^{\infty}\mathrm{dist}(X^j, R_{X^j}(\Delta X^j)) \\ &\le \sum_{j=k+1}^{\infty}\nu\|\Delta X^j\| \le \sum_{j=k+1}^{\infty}2\nu(1+\overline{\eta}_{\max})|||(\mathrm{D}H(\overline{X}))^\dagger||| \cdot \|H(X^j)\|_F \\ &\le 2\nu(1+\overline{\eta}_{\max})|||(\mathrm{D}H(\overline{X}))^\dagger|||\sum_{j=0}^{\infty}(1-t(1-\hat{\eta}_k))^j\|H(X^{k+1})\|_F\end{aligned}$$

$$\leq 2\nu(1+\overline{\eta}_{\max})|||(\mathrm{D}H(\overline{X}))^{\dagger}|||\sum_{j=0}^{\infty}(1-t(1-\overline{\eta}_{\max}))^{j}\|H(X^{k+1})\|_F$$

$$= \frac{2\nu(1+\overline{\eta}_{\max})|||(\mathrm{D}H(\overline{X}))^{\dagger}|||}{t(1-\overline{\eta}_{\max})}\|H(X^{k+1})\|_F \tag{26}$$

$$\leq \frac{2\nu(1+\overline{\eta}_{\max})|||(\mathrm{D}H(\overline{X}))^{\dagger}|||}{t(1-\overline{\eta}_{\max})}L_1(c_1\|H(X^k)\|_F+\overline{\eta}_k)\mathrm{dist}(X^k,\overline{X})$$

$$= c_2(c_1\|H(X^k)\|_F+\overline{\eta}_k)\mathrm{dist}(X^k,\overline{X}) \tag{27}$$

$$\leq c_2\left(\frac{1}{1+2c_2}+\eta\right)\mathrm{dist}(X^k,\overline{X})$$

$$\leq \frac{2c_2}{1+2c_2}\mathrm{dist}(X^k,\overline{X}).$$

The proof is complete. ∎

Theorem 4. *Let $\overline{X}$ be an accumulation point of the sequence $\{X^k\}$ generated by Algorithm 1. Suppose Assumption 1 is satisfied. If $\overline{\eta}_k \leq 1/(k+2)$ or $\overline{\eta}_k \leq 1/2^{k+2}$, then the sequence $\{X^k\}$ converges to $\overline{X}$ superlinearly.*

Proof. By using Theorem 2 and the continuity of H we find that $\|H(X^k)\|_F \to 0$ as $k \to \infty$. By hypothesis, $\overline{\eta}_k = 1/(k+2) \to 0$ or $\overline{\eta}_k \leq 1/2^{k+2} \to 0$ as $k \to \infty$. Thus, it follows from (27) that

$$\mathrm{dist}(X^{k+1},\overline{X}) = o(\mathrm{dist}(X^k,\overline{X})) \quad \text{as } k \to \infty,$$

which completes the proof. ∎

By using the similar arguments of Theorem 3, which is similar to the proof of [20, theorem 3], we can easily establish the following theorem.

Theorem 5. *Let $\overline{X}$ be an accumulation point of the sequence $\{X^k\}$ generated by Algorithm 1. Suppose Assumption 1 is satisfied. If $\overline{\eta}_k = \min\{\overline{\eta}_{\max}, \|H(X^k)\|_F\}$ or $\overline{\eta}_k = \min\{1/(k+2), \|H(X^k)\|_F\}$, then the sequence $\{X^k\}$ converges to $\overline{X}$ quadratically.*

4 | EXTENSION

In this section, we extend the proposed Riemannian inexact Newton-CG method to the solution of the StISVP-PE. Let $G, \hat{W} \in \mathbb{R}^{n\times n}$ be defined by

$$G_{ij} := \begin{cases} g_{ij}, & \text{if } (i,j) \in \mathcal{L}, \\ 0, & \text{otherwise} \end{cases} \quad \text{and} \quad \hat{W}_{ij} := \begin{cases} 1, & \text{if } (i,j) \in \mathcal{L}, \\ 0, & \text{otherwise.} \end{cases}$$

Define a diagonal matrix $\hat{I}_n := I_n - \mathrm{Diag}(G\mathbf{e})$, where $\mathbf{e} = (1, \ldots, 1)^T \in \mathbb{R}^n$. Suppose the given index subset $\mathcal{L}$ is such that $\sum_{j=1}^{n} G_{ij} < 1$ for $i = 1, \ldots, n$. Then $\hat{I}_n$ is nonsingular. In addition, let

$$\hat{\mathcal{Z}} := \widehat{\mathcal{OB}} \times \mathcal{O}(n) \times \mathcal{O}(n),$$

where the manifold $\widehat{\mathcal{OB}}$ is defined by

$$\widehat{\mathcal{OB}} := \{S \in \mathbb{R}^{n\times n} \mid \mathrm{diag}(SS^T) = \hat{I}_n,\ \hat{W} \odot S = \mathbf{0}_{n\times n}\}.$$

Then StISVP-PE is to solve the following nonlinear equation

$$\Phi(S,U,V) := G + S \odot S - U\Sigma V^T = \mathbf{0}_{n\times n} \tag{28}$$

for $(S, U, V) \in \mathcal{Z}$, where Φ is a smooth mapping from the product manifold $\hat{\mathcal{Z}}$ to the Euclidean space $\mathbb{R}^{n\times n}$. We also remark that, if $(\overline{S}, \overline{U}, \overline{V}) \in \hat{\mathcal{Z}}$ is a solution to $\Phi(S, U, V) = \mathbf{0}_{n\times n}$, then $\overline{C} := G + \overline{S} \odot \overline{S}$ is a solution to StISVP-PE. Finally, we note that the dimension of the product manifold $\hat{\mathcal{Z}}$ is given by

$$\dim(\hat{\mathcal{Z}}) = n(n-1) - |\mathcal{L}| + \frac{n(n-1)}{2} + |\mathcal{J}|.$$

We see that the nonlinear equation $\Phi(S, U, V) = \mathbf{0}_{n\times n}$ is underdetermined if n is large and the number $|\mathcal{L}|$ of prescribed entries is small.

One may apply Algorithm 1 to solving (28). Under some assumptions as Assumption 1, the global and local linear or superlinear convergence can be established in a similar way as in Section 3.

5 | NUMERICAL TESTS

We report the numerical performance of Algorithm 1 for solving the StISVP and the StISVP-PE. We also use Algorithm 1 in an example for the parameter estimation in the HMM.[33] All numerical tests are carried out by using `MATLAB` on a Linux server having 8 cores with 4 Intel Xeon Gold 6134 processors at 3.2 GHz and 64 GB RAM.

For Algorithm 1, the starting point is generated randomly by the built-in functions `rand` and `svd`. In particular, for the StISVP, we choose (S^0, U^0, V^0) such that $S^0 = (\mathrm{diag}(\hat{S}\hat{S}^T))^{-\frac{1}{2}}\hat{S} \in \mathcal{OB}$ and $[U^0, \Sigma^0, V^0] =$ `svd` $(S^0 \odot S^0)$, where $\hat{S} \odot \hat{S} =$ `rand` (n, n). For the StISVP-PE, we choose (S^0, U^0, V^0) such that $S^0 = (\hat{I}_n)^{\frac{1}{2}}(\mathrm{diag}(((E - \hat{W}) \odot \hat{S})((E - \hat{W}) \odot \hat{S})^T))^{-\frac{1}{2}}((E - \hat{W}) \odot \hat{S}) \in \widehat{\mathcal{OB}}$, and $[U^0, \Sigma^0, V^0] =$ `svd`$(G + S^0 \odot S^0)$, where $\hat{S} \odot \hat{S} =$ `rand` (n, n) and $E \in \mathbb{R}^{n\times n}$ is a matrix of ones.

For comparison purposes, the stopping criteria for Algorithm 1 for solving the StISVP and the StISVP-PE are, respectively, set to be

$$\|H(X^k)\|_F < 10^{-10} \quad \text{and} \quad \|\Phi(X^k)\|_F < 10^{-10}$$

and we set $\overline{\eta}_{\max} = 0.1$, $\theta_{\min} = 0.1$, $\theta_{\max} = 0.9$, and $t = 10^{-4}$. The largest number of outer iterations in Algorithm 1 is set to be 100 and the largest number of iterations in the CG method is set to be n^2.

In our numerical tests, "`CT.`," "`IT.`," "`NF.`," "`NCG.`," "`Res.`," and "`Err-SV.`" mean the total computing time in seconds, the number of iterations, the number of function evaluations, the number of inner CG iterations, the residual $\|H(X^k)\|_F$ or $\|\Phi(X^k)\|_F$, and the relative error $\|\boldsymbol{\sigma}(S^k \odot S^k) - \boldsymbol{\sigma}_*\|/\|\boldsymbol{\sigma}_*\|$ at the final iterates of the corresponding algorithms accordingly.

We consider the following three examples with different problem size n.

Example 1. We consider the StISVP with varying n. Let $\tilde{C}$ be a random $n \times n$ nonnegative matrix with each entry generated from the uniform distribution on the interval $[0, 1]$. Let $\hat{C}$ be a random stochastic matrix given by

$$\hat{C} := \tilde{S} \odot \tilde{S}, \quad \tilde{S} = (\mathrm{diag}(\tilde{C}\tilde{C}^T))^{-\frac{1}{2}}\tilde{C}.$$

We choose the singular values of $\hat{C}$ as prescribed spectrum.

Example 2. We consider the StISVP-PE with prescribed diagonal entries. Let $\hat{C}$ be a random stochastic matrix generated as in Example 1. We choose the singular values of $\hat{C}$ as prescribed spectrum. In addition, we choose the index subset $\mathcal{L} := \{(i, i) \mid i = 1, \ldots, n\}$. This StISVP-PE can be seen as a special case of the ISVP in [13, p. 116], where the relationship between the prescribed diagonal entries and the prescribed singular values is established as in the Sing–Thompson theorem (see, for instance, References 34,35 and [13, theorem 4.26]). The prescribed nonnegative matrix $G \in \mathbb{R}^{n\times n}$ is defined by $(G)_{ij} = (\hat{C})_{ij}$, if $(i, j) \in \mathcal{L}$ and $(G)_{ij} = 0$, if $(i, j) \notin \mathcal{L}$. We report our numerical results for different n.

Example 3. We consider the StISVP-PE with prescribed entries at arbitrary locations. Let $\hat{C}$ be a random stochastic matrix generated as in Example 1. We choose the singular values of $\hat{C}$ as prescribed spectrum. In addition, we choose the index subset $\mathcal{L} := \{(i, j) \mid 3/(5n) < (\hat{C})_{ij} < 4/(5n), i, j = 1, \ldots, n\}$. The prescribed nonnegative matrix $G \in \mathbb{R}^{n\times n}$ is defined by $(G)_{ij} = (\hat{C})_{ij}$, if $(i, j) \in \mathcal{L}$ and $(G)_{ij} = 0$, if $(i, j) \notin \mathcal{L}$. We report our numerical results for various n.

TABLE 1 Numerical results for Example 1

$\overline{\eta}_k = 0.1$						
n	CT.	IT.	NF.	NCG.	Res.	Err-SV.
200	0.4194 s	8	9	35	7.96×10^{-12}	5.73×10^{-13}
500	3.0997 s	7	8	43	4.28×10^{-11}	1.62×10^{-12}
1000	16.84 s	7	8	46	3.14×10^{-11}	1.97×10^{-12}
2000	01 m 59 s	7	8	49	1.81×10^{-11}	8.37×10^{-13}
5000	17 m 34 s	6	7	46	8.92×10^{-11}	1.10×10^{-11}
$\overline{\eta}_k = 1/(k+2)$						
n	CT.	IT.	NF.	NCG.	Res.	Err-SV.
200	0.4225 s	9	10	30	4.19×10^{-11}	4.78×10^{-12}
500	3.1816 s	9	10	34	3.72×10^{-11}	2.45×10^{-12}
1000	17.34 s	9	10	36	3.21×10^{-11}	3.09×10^{-12}
2000	02 m 02 s	9	10	39	9.73×10^{-12}	7.46×10^{-13}
5000	18 m 16 s	8	9	36	7.83×10^{-11}	2.90×10^{-12}
$\overline{\eta}_k = 1/2^{k+1}$						
n	CT.	IT.	NF.	NCG.	Res.	Err-SV.
200	0.4086 s	6	7	45	1.59×10^{-11}	1.85×10^{-12}
500	3.1594 s	6	7	53	4.11×10^{-12}	2.12×10^{-13}
1000	17.59 s	6	7	57	2.88×10^{-12}	1.01×10^{-13}
2000	01 m 58 s	6	7	59	2.74×10^{-12}	1.29×10^{-13}
5000	17 m 18 s	5	6	56	5.87×10^{-11}	1.59×10^{-12}
$\overline{\eta}_k = \min\{0.1, \|H(X^k)\|_F\}$						
n	CT.	IT.	NF.	NCG.	Res.	Err-SV.
200	0.5294 s	3	4	128	1.39×10^{-15}	2.90×10^{-16}
500	4.1564 s	3	4	149	5.15×10^{-15}	2.73×10^{-15}
1000	25.18 s	3	4	171	2.04×10^{-15}	5.49×10^{-16}
2000	01 m 45 s	2	3	151	2.66×10^{-11}	1.50×10^{-11}
5000	21 m 02 s	2	3	172	2.10×10^{-13}	1.10×10^{-13}
$\overline{\eta}_k = \min\{1/(k+2), \|H(X^k)\|_F\}$						
n	CT.	IT.	NF.	NCG.	Res.	Err-SV.
200	0.4772 s	3	4	128	1.39×10^{-15}	2.90×10^{-16}
500	4.2615 s	3	4	148	5.15×10^{-15}	2.73×10^{-15}
1000	25.24 s	3	4	172	2.04×10^{-15}	5.49×10^{-16}
2000	01 m 41 s	2	3	151	2.66×10^{-11}	1.50×10^{-11}
5000	20 m 47 s	2	3	151	2.10×10^{-13}	1.10×10^{-13}

For demonstration purpose, in Tables 1-3, we report the numerical results for Examples 1-3. We see from Tables 1 to 3 that Algorithm 1 is very efficient for solving large-scale problems. We also observe that Algorithm 1 with the forcing terms $\overline{\eta}_k \le \overline{\eta}_{\max} < 1$, $\overline{\eta}_k = 1/(k+2)$, or $\overline{\eta}_k = 1/2^{k+1}$ works more efficiently in terms of the number of inner iterations, while for Examples 1 and 3, Algorithm 1 with the forcing terms $\overline{\eta}_k \le \overline{\eta}_{\max} < 1$, $\overline{\eta}_k = 1/(k+2)$, or $\overline{\eta}_k = 1/2^{k+1}$ works is slightly effective over the other forcing terms in terms of the computing time.

To further illustrate the effectiveness of our method, we consider the parameter estimation in the HMM.[33]

TABLE 2 Numerical results for Example 2

$\bar{\eta}_k = 0.1$							
n	$\lvert\mathcal{L}\rvert$	CT.	IT.	NF.	NCG.	Res.	Err-SV.
200	200	0.4171 s	8	9	37	8.59×10^{-12}	1.48×10^{-12}
500	500	3.15 s	7	8	44	3.89×10^{-11}	9.99×10^{-12}
1000	1000	17.92 s	7	8	46	4.56×10^{-11}	2.14×10^{-12}
2000	2000	02 m 04 s	7	8	50	2.14×10^{-11}	7.28×10^{-13}
5000	5000	19 m 14 s	7	8	43	9.48×10^{-12}	2.85×10^{-12}
$\bar{\eta}_k = 1/(k+2)$							
n	$\lvert\mathcal{L}\rvert$	CT.	IT.	NF.	NCG.	Res.	Err-SV.
200	200	0.4730 s	9	10	31	3.03×10^{-11}	1.94×10^{-12}
500	500	3.21 s	9	10	34	5.85×10^{-11}	4.32×10^{-12}
1000	1000	18.37 s	9	10	36	1.52×10^{-11}	6.30×10^{-13}
2000	2000	02 m 08 s	9	10	40	7.72×10^{-12}	2.69×10^{-13}
5000	5000	18 m 49 s	8	9	36	3.65×10^{-11}	1.55×10^{-12}
$\bar{\eta}_k = 1/2^{k+1}$							
n	$\lvert\mathcal{L}\rvert$	CT.	IT.	NF.	NCG.	Res.	Err-SV.
200	200	0.3783 s	6	7	40	1.50×10^{-11}	2.34×10^{-12}
500	500	3.29 s	6	7	54	2.86×10^{-12}	2.23×10^{-13}
1000	1000	18.79 s	6	7	57	1.91×10^{-12}	1.67×10^{-13}
2000	2000	02 m 04 s	6	7	62	1.82×10^{-12}	5.41×10^{-14}
5000	5000	24 m 13 s	6	7	65	5.59×10^{-13}	2.22×10^{-14}
$\bar{\eta}_k = \min\{0.1, \lVert\Phi(X^k)\rVert_F\}$							
n	$\lvert\mathcal{L}\rvert$	CT.	IT.	NF.	NCG.	Res.	Err-SV.
200	200	0.4707 s	3	4	107	2.60×10^{-12}	1.51×10^{-12}
500	500	4.43 s	3	4	150	1.02×10^{-14}	5.78×10^{-15}
1000	1000	27.04 s	3	4	171	2.08×10^{-15}	4.98×10^{-16}
2000	2000	01 m 43 s	2	3	152	1.17×10^{-11}	4.24×10^{-12}
5000	5000	20 m 40 s	2	3	172	3.07×10^{-12}	1.80×10^{-12}
$\bar{\eta}_k = \min\{1/(k+2), \lVert\Phi(X^k)\rVert_F\}$							
n	$\lvert\mathcal{L}\rvert$	CT.	IT.	NF.	NCG.	Res.	Err-SV.
200	200	0.4360 s	3	4	107	2.60×10^{-12}	1.51×10^{-12}
500	500	4.36 s	3	4	150	1.02×10^{-14}	5.78×10^{-15}
1000	1000	27.11 s	3	4	171	2.08×10^{-15}	4.98×10^{-16}
2000	2000	01 m 39 s	2	3	152	1.17×10^{-11}	4.24×10^{-12}
5000	5000	20 m 40 s	2	3	172	3.07×10^{-12}	1.80×10^{-12}

Example 4. We discuss the process of choosing a dice of four faces (1, 2, 3, and 4) and recording the number of dots by throwing the dice. Let A and B be two dies, where Dice A is fair and Dice B is biased. The probability distributions of the dots obtained by throwing die A and B are given in Table 4. Suppose each time a dice is chosen, if previously k ($k = 1, 2, 3, 4$) dots was obtained in the last throw, then with probability β_k, Dice A will be chosen, and with probability $(1 - \beta_k)$, Dice B will be chosen. This process is a HMM, which can be described by a Markov chain process with the transition probability

TABLE 3 Numerical results for Example 3

$\bar{\eta}_k = 0.1$							
n	$\lvert\mathcal{L}\rvert$	CT.	IT.	NF.	NCG.	Res.	Err-SV.
200	3979	0.5788 s	8	9	51	1.63×10^{-11}	5.26×10^{-15}
500	24,992	4.53 s	8	9	57	1.48×10^{-11}	7.21×10^{-13}
1000	99,918	19.43 s	7	8	54	9.38×10^{-11}	1.09×10^{-15}
2000	400,178	02 m 51 s	7	8	71	6.84×10^{-11}	8.28×10^{-12}
5000	2,499,962	28 m 45 s	8	9	57	9.37×10^{-12}	2.01×10^{-13}
$\bar{\eta}_k = 1/(k+2)$							
n	$\lvert\mathcal{L}\rvert$	CT.	IT.	NF.	NCG.	Res.	Err-SV.
200	3979	0.5912 s	9	10	43	5.25×10^{-11}	3.05×10^{-12}
500	24,992	4.50 s	9	10	50	2.44×10^{-11}	1.63×10^{-12}
1000	99,918	20.63 s	9	10	43	2.35×10^{-11}	1.25×10^{-12}
2000	400,178	02 m 28 s	9	10	47	3.69×10^{-11}	1.34×10^{-11}
5000	2,499,962	28 m 11 s	9	10	49	1.91×10^{-11}	1.09×10^{-12}
$\bar{\eta}_k = 1/2^{k+1}$							
n	$\lvert\mathcal{L}\rvert$	CT.	IT.	NF.	NCG.	Res.	Err-SV.
200	3979	0.5579 s	6	7	67	1.84×10^{-11}	3.24×10^{-12}
500	24,992	4.47 s	6	7	76	5.91×10^{-12}	3.93×10^{-13}
1000	99,918	20.33 s	6	7	67	8.26×10^{-12}	3.84×10^{-13}
2000	400,178	02 m 55 s	6	7	88	3.25×10^{-12}	7.80×10^{-14}
5000	2,499,962	28 m 28 s	6	7	76	4.78×10^{-12}	5.30×10^{-13}
$\bar{\eta}_k = \min\{0.1, \lVert\Phi(X^k)\rVert_F\}$							
n	$\lvert\mathcal{L}\rvert$	CT.	IT.	NF.	NCG.	Res.	Err-SV.
200	3979	0.6660 s	3	4	173	3.43×10^{-14}	5.26×10^{-15}
500	24,992	5.82 s	3	4	208	1.64×10^{-15}	3.84×10^{-16}
1000	99,918	29.79 s	3	4	200	2.82×10^{-15}	1.09×10^{-15}
2000	400,178	04 m 07 s	3	4	250	2.39×10^{-15}	6.93×10^{-16}
5000	2,499,962	41 m 11 s	3	4	225	3.90×10^{-15}	1.21×10^{-15}
$\bar{\eta}_k = \min\{1/(k+2), \lVert\Phi(X^k)\rVert_F\}$							
n	$\lvert\mathcal{L}\rvert$	CT.	IT.	NF.	NCG.	Res.	Err-SV.
200	3979	0.6650 s	3	4	173	3.43×10^{-14}	5.26×10^{-15}
500	24,992	5.72 s	3	4	208	1.64×10^{-15}	3.84×10^{-16}
1000	99,918	29.22 s	3	4	200	2.82×10^{-15}	1.09×10^{-15}
2000	400,178	03 m 56 s	3	4	250	2.39×10^{-15}	6.93×10^{-16}
5000	2,499,962	40 m 24 s	3	4	225	3.90×10^{-15}	1.21×10^{-15}

TABLE 4 The probability distributions

Dice	1	2	3	4
A	1/4	1/4	1/4	1/4
B	1/6	1/6	1/3	1/3

matrix being given by

$$P = \begin{array}{c} \\ A \\ B \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccccc} \text{State} & A & B & 1 & 2 & 3 & 4 \end{array} \\ \begin{bmatrix} 0 & 0 & 1/4 & 1/4 & 1/4 & 1/4 \\ 0 & 0 & 1/6 & 1/6 & 1/3 & 1/3 \\ \beta_1 & 1-\beta_1 & 0 & 0 & 0 & 0 \\ \beta_2 & 1-\beta_2 & 0 & 0 & 0 & 0 \\ \beta_3 & 1-\beta_3 & 0 & 0 & 0 & 0 \\ \beta_4 & 1-\beta_4 & 0 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

The problem is how to estimate β_k from an observed data sequence.

In Reference 33, a simple estimation method was proposed for estimating β_k. This method first computed the two-step transition probability matrix

$$P^2 = \begin{bmatrix} \frac{\beta_1+\beta_2+\beta_3+\beta_4}{4} & 1-\frac{\beta_1+\beta_2+\beta_3+\beta_4}{4} & 0 & 0 & 0 & 0 \\ \frac{\beta_1+\beta_2}{6}+\frac{\beta_3+\beta_4}{3} & 1-\frac{\beta_1+\beta_2}{6}-\frac{\beta_3+\beta_4}{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{6}+\frac{\beta_1}{12} & \frac{1}{6}+\frac{\beta_1}{12} & \frac{1}{3}-\frac{\beta_1}{12} & \frac{1}{3}-\frac{\beta_1}{12} \\ 0 & 0 & \frac{1}{6}+\frac{\beta_2}{12} & \frac{1}{6}+\frac{\beta_2}{12} & \frac{1}{3}-\frac{\beta_2}{12} & \frac{1}{3}-\frac{\beta_2}{12} \\ 0 & 0 & \frac{1}{6}+\frac{\beta_3}{12} & \frac{1}{6}+\frac{\beta_3}{12} & \frac{1}{3}-\frac{\beta_3}{12} & \frac{1}{3}-\frac{\beta_3}{12} \\ 0 & 0 & \frac{1}{6}+\frac{\beta_4}{12} & \frac{1}{6}+\frac{\beta_4}{12} & \frac{1}{3}-\frac{\beta_4}{12} & \frac{1}{3}-\frac{\beta_4}{12} \end{bmatrix}.$$

Then the following transition probability matrix was extracted

$$\hat{P} = \begin{bmatrix} \frac{1}{6}+\frac{\beta_1}{12} & \frac{1}{6}+\frac{\beta_1}{12} & \frac{1}{3}-\frac{\beta_1}{12} & \frac{1}{3}-\frac{\beta_1}{12} \\ \frac{1}{6}+\frac{\beta_2}{12} & \frac{1}{6}+\frac{\beta_2}{12} & \frac{1}{3}-\frac{\beta_2}{12} & \frac{1}{3}-\frac{\beta_2}{12} \\ \frac{1}{6}+\frac{\beta_3}{12} & \frac{1}{6}+\frac{\beta_3}{12} & \frac{1}{3}-\frac{\beta_3}{12} & \frac{1}{3}-\frac{\beta_3}{12} \\ \frac{1}{6}+\frac{\beta_4}{12} & \frac{1}{6}+\frac{\beta_4}{12} & \frac{1}{3}-\frac{\beta_4}{12} & \frac{1}{3}-\frac{\beta_4}{12} \end{bmatrix}. \tag{29}$$

To estimate β_k, the one-step transition probability matrix can be estimated from the observed sequence. Suppose a sequence of number dots is observed as follows Reference 33:

$$1, 2, 1, 2, 1, 2, 2, 4, 1, 2, 2, 1, 3, 3, 4, 1.$$

Then the estimated transition probability matrix was given by

$$\tilde{P} = \begin{bmatrix} 0 & \frac{4}{5} & \frac{1}{5} & 0 \\ \frac{1}{2} & \frac{1}{3} & 0 & \frac{1}{6} \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 1 & 0 & 0 & 0 \end{bmatrix}, \tag{30}$$

whose singular values are 1.1466, 0.8809, 0.6758, 0.1465. Then the expected β_k were obtained by solving the following minimizing problem:

$$\min_{\beta_k} \|\hat{P} - \tilde{P}\|_F^2 \quad \text{s.t.} \quad 0 \le \beta_k \le 1, \quad k = 1, 2, 3, 4.$$

The obtained optimal β_k was given by

$$\beta_1^* = 1, \quad \beta_2^* = 1, \quad \beta_3^* = 0, \quad \beta_4^* = 1$$

and the computed transition probability matrix was given by

$$\hat{P}^* = \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{6} & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{bmatrix}, \tag{31}$$

whose singular values are 1.0035, 0.1438, 0.0000, 0.0000.

In the following, we propose another possible method for estimating β_k. We observe that the extracted transition probability matrix $\hat{P}$ in (29) is linearly dependent on the parameters β_k, that is,

$$\hat{P} = P_0 + \beta_1 P_1 + \beta_2 P_2 + \beta_3 P_3 + \beta_4 P_4, \tag{32}$$

where

$$P_0 = \begin{bmatrix} \frac{1}{6} & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{6} & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{6} & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{6} & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} \end{bmatrix}, \quad P_1 = \begin{bmatrix} \frac{1}{12} & \frac{1}{12} & -\frac{1}{12} & -\frac{1}{12} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad P_2 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ \frac{1}{12} & \frac{1}{12} & -\frac{1}{12} & -\frac{1}{12} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

$$P_3 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{12} & \frac{1}{12} & -\frac{1}{12} & -\frac{1}{12} \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad P_4 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{12} & \frac{1}{12} & -\frac{1}{12} & -\frac{1}{12} \end{bmatrix},$$

and also is of low rank since

$$\hat{P} = \begin{bmatrix} \beta_1 & 1-\beta_1 \\ \beta_2 & 1-\beta_2 \\ \beta_3 & 1-\beta_3 \\ \beta_4 & 1-\beta_4 \end{bmatrix} \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{6} & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} \end{bmatrix}.$$

This shows that the desired parameters β_k is such that the expected transition probability matrix $\hat{P}$ is linearly dependent on the parameters β_k as in (32) and also is of rank 2. Thus, we first construct a rank-2 transition probability matrix $\overline{P}$ from the prescribed singular values 1.1466, 0.8809, 0, 0, where 1.1466 and 0.8809 are the dominated singular values of estimated transition probability matrix $\tilde{P}$ in (30). This is a StISVP, which can be solved by using Algorithm 1. Here, the initial guess (S^0, U^0, V^0) is such that $S^0 = (\mathrm{diag}(\hat{S}\hat{S}^T))^{-\frac{1}{2}}\hat{S} \in \mathcal{OB}$ and $[U^0, \Sigma^0, V^0] = \mathtt{svd}\,(S^0 \odot S^0)$, where

$$\hat{S} = \begin{bmatrix} 0.9 & 0.9 & 0.1 & 0.5 \\ 0.1 & 0.1 & 0.5 & 0.9 \\ 0.8 & 0.8 & 0.6 & 0.4 \\ 0.8 & 0.8 & 0.2 & 0.6 \end{bmatrix}$$

and the other parameters are set as above. Then, the expected β_k can be obtained by solving the following minimizing problem:

$$\min_{\beta_k} \|\hat{P} - \overline{P}\|_F^2 \quad \text{s.t.} \quad 0 \le \beta_k \le 1, \quad k = 1, 2, 3, 4.$$

TABLE 5 Numerical results for Example 4

$\overline{P}$	$\sigma(\overline{P})$	β^*
our method with $\overline{\eta}_k = 0.1$		
$\begin{pmatrix} 0.4492 & 0.0018 \\ 0.0185 & 0.0259 \\ 0.4525 & 0.0016 \\ 0.4220 & 0.0033 \end{pmatrix}$	$\begin{pmatrix} 1.1466 \\ 0.8809 \\ 0.0000 \\ 0.0000 \end{pmatrix}$	$\begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \end{pmatrix}$
our method with $\overline{\eta}_k = 1/(k+2)$		
$\begin{pmatrix} 0.4615 & 0.0000 \\ 0.0182 & 0.0317 \\ 0.4466 & 0.0011 \\ 0.4212 & 0.0029 \end{pmatrix}$	$\begin{pmatrix} 1.1466 \\ 0.8809 \\ 0.0000 \\ 0.0000 \end{pmatrix}$	$\begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \end{pmatrix}$
our method with $\overline{\eta}_k = 1/2^{k+1}$		
$\begin{pmatrix} 0.4570 & 0.0003 \\ 0.0179 & 0.0286 \\ 0.4513 & 0.0007 \\ 0.4148 & 0.0030 \end{pmatrix}$	$\begin{pmatrix} 1.1466 \\ 0.8809 \\ 0.0000 \\ 0.0000 \end{pmatrix}$	$\begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \end{pmatrix}$
our method with $\overline{\eta}_k = \min\{0.1, \|H(X^k)\|\}$		
$\begin{pmatrix} 0.4492 & 0.0018 \\ 0.0186 & 0.0258 \\ 0.4525 & 0.0016 \\ 0.4219 & 0.0033 \end{pmatrix}$	$\begin{pmatrix} 1.1466 \\ 0.8809 \\ 0.0000 \\ 0.0000 \end{pmatrix}$	$\begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \end{pmatrix}$
our method with $\overline{\eta}_k = \min\{1/(k+2), \|H(X^k)\|\}$		
$\begin{pmatrix} 0.4570 & 0.0003 \\ 0.0179 & 0.0286 \\ 0.4513 & 0.0007 \\ 0.4148 & 0.0030 \end{pmatrix}$	$\begin{pmatrix} 1.1466 \\ 0.8809 \\ 0.0000 \\ 0.0000 \end{pmatrix}$	$\begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \end{pmatrix}$

The numerical results for Example 4 are listed in Table 5. We see from Table 5 that the obtained optimal β_k are all the same (i.e., $\boldsymbol{\beta}^* = (\beta_1^*, \beta_2^*, \beta_3^*, \beta_4^*)^T = (1, 0, 1, 1)^T$), though the computed rank-2 transition probability matrix $\overline{P}$ is different for different forcing terms. The computed transition probability matrix is given by

$$\hat{P}^* = \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{6} & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{bmatrix},$$

which is comparable with the transition probability matrix $\hat{P}^*$ in (31) obtained by the method in Reference 33.

6 | CONCLUDING REMARKS

In this article, we present a Riemannian inexact Newton-CG method for solving the stochastic ISVP of constructing a stochastic matrix from the prescribed realizable singular values. Under some assumptions, the proposed method is showed to be globally and linearly or superlinearly convergent for different forcing terms. The proposed method is also

applied to solve the case of prescribed entries. Numerical results demonstrate that our method is very effective. We also use our method in the parameter estimation in the HMM. We point out that most of the computing time is spent on the CG method for solving the normal equation (9). To improve the efficiency of our method, it is better to find a good preconditioner for (9). In addition, the desired solution obtained by our method is dependent on the initial guess. These questions need further study.

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APPENDIX

In this appendix, we first give some preliminary results related to the product manifold $\mathcal{Z}$ defined in (1). Then we derive the differential of H defined in (3). We note that the tangent space of $\mathcal{Z}$ at $(S, U, V) \in \mathcal{Z}$ is given by

$$T_{(S,U,V)}\mathcal{Z} = T_S\mathcal{OB} \times T_U\mathcal{O}(n) \times T_V\mathcal{O}(n),$$

where $T_S\mathcal{OB}$, $T_U\mathcal{O}(n)$, and $T_V\mathcal{O}(n)$ are the tangent spaces of $\mathcal{OB}$ at $S \in \mathcal{OB}$, $U \in \mathcal{O}(n)$, and $V \in \mathcal{O}(n)$ accordingly, which are given by Absil et al.:[28]

$$\begin{cases} T_S\mathcal{OB} = \{T \in \mathbb{R}^{n\times n} \mid \operatorname{diag}(ST^T) = \mathbf{0}_{n\times n}\}, \\ T_U\mathcal{O}(n) = \{UZ \mid Z^T = -Z, Z \in \mathbb{R}^{n\times n}\}, \\ T_V\mathcal{O}(n) = \{VW \mid W^T = -W, W \in \mathbb{R}^{n\times n}\}. \end{cases}$$

A retraction R on $\mathcal{Z}$ is given by

$$R_{(S,U,V)}(\xi_S, \zeta_U, \eta_V) = (R_S(\xi_S), R_U(\zeta_U), R_V(\eta_V)) \tag{A1}$$

for all $(S, U, V) \in \mathcal{Z}$ and $(\xi_S, \eta_U, \eta_V) \in T_{(S,U,V)}\mathcal{Z}$, where R_S, R_U, and R_V denote the retractions on $\mathcal{OB}$, $\mathcal{O}(n)$ and $\mathcal{O}(n)$ accordingly, which may take the form of

$$\begin{cases} R_S(\xi_S) = (\operatorname{diag}((S+\xi_S)(S+\xi_S)^T))^{-1/2}(S+\xi_S), & \text{for } \xi_S \in T_S\mathcal{OB}, \\ R_U(\zeta_U) = \operatorname{qf}(U+\zeta_U), & \text{for } \zeta_U \in T_U\mathcal{O}(n), \\ R_V(\eta_V) = \operatorname{qf}(V+\eta_V), & \text{for } \eta_V \in T_V\mathcal{O}(n). \end{cases}$$

Here, $\operatorname{qf}(A)$ means the Q factor of the QR decomposition of a nonsingular matrix $A \in \mathbb{R}^{n\times n}$ in the form of $A = Q\tilde{R}$ with $Q \in \mathcal{O}(n)$ and $\tilde{R}$ being an upper triangular matrix with strictly positive diagonal entries. For other choices of retractions on $\mathcal{O}(n)$, one may refer to [28, pp. 58–59].

The differential $\mathrm{D}H(S, U, V)$: $T_{(S,U,V)}\mathcal{Z} \to T_{H(S,U,V)}\mathbb{R}^{n\times n} \simeq \mathbb{R}^{n\times n}$ of H defined in (3) at a point $(S, U, V) \in \mathcal{Z}$ is determined by

$$\mathrm{D}H(S, U, V)[(\Delta S, \Delta U, \Delta V)] = 2S \odot \Delta S - \Delta U\Sigma V^T - U\Sigma\Delta V^T \tag{A2}$$

for all $(\Delta S, \Delta U, \Delta V) \in T_{(S,U,V)}\mathcal{Z}$, where "$\simeq$" means the identification of two sets.

With respect to the Riemannian metric g as defined by (4), the adjoint $(\mathrm{D}H(S, U, V))^* : T_{H(S,U,V)}\mathbb{R}^{n\times n} \to T_{(S,U,V)}\mathcal{Z}$ of $\mathrm{D}H(S, U, V)$ is determined by

$$(\mathrm{D}H(S, U, V))^*[\Delta Z] = ((\mathrm{D}H_1(S, U, V))^*[\Delta Z], (\mathrm{D}H_2(S, U, V))^*[\Delta Z], (\mathrm{D}H_3(S, U, V))^*[\Delta Z]), \tag{A3}$$

for all $\Delta Z \in T_{H(S,U,V)}\mathbb{R}^{n\times n}$, where for any $\Delta Z \in T_{H(S,U,V)}\mathbb{R}^{n\times n}$,

$$\begin{cases} (\mathrm{D}H_1(S,U,V))^*[\Delta Z] = 2S\odot\Delta Z - 2\mathrm{diag}(S(S\odot\Delta Z)^T)S, \\ (\mathrm{D}H_2(S,U,V))^*[\Delta Z] = \frac{1}{2}(U\Sigma V^T\Delta Z^T - \Delta ZV\Sigma U^T)U, \\ (\mathrm{D}H_3(S,U,V))^*[\Delta Z] = \frac{1}{2}(V\Sigma U^T\Delta Z - \Delta Z^TU\Sigma V^T)V. \end{cases} \tag{A4}$$

Proof of Theorem 1. From (A3) to (A4) we have

$$\begin{aligned} &\langle \Delta Z, \mathrm{D}H(X)\circ(\mathrm{D}H(X))^*[\Delta Z]\rangle = \langle (\mathrm{D}H(X))^*[\Delta Z], (\mathrm{D}H(X))^*[\Delta Z]\rangle \\ &= 4\|S\odot\Delta Z - \mathrm{diag}(S(S\odot\Delta Z)^T)S\|^2 + \frac{1}{2}\|(U\Sigma V^T\Delta Z^T - \Delta ZV\Sigma U^T)U\|^2 \\ &\quad + \frac{1}{2}\|(V\Sigma U^T\Delta Z - \Delta Z^TU\Sigma V^T)V\|^2 \\ &= 4\|S\odot\Delta Z - \mathrm{diag}(S(S\odot\Delta Z)^T)S\|^2 + \frac{1}{4}\|U^T\Delta ZV\Sigma - \Sigma V^T\Delta Z^TU\|^2 \\ &\quad + \frac{1}{4}\|\Sigma U^T\Delta ZV - V^T\Delta Z^TU\Sigma\|^2, \end{aligned} \tag{A5}$$

for all $\Delta Z \in \mathbb{R}^{n\times n}$. For any $\Delta Z \in \mathbb{R}^{n\times n}$, let $\hat{\Delta Z} := U^T\Delta ZV$. It follows from (A5) that $\mathrm{D}H(X)\circ(\mathrm{D}H(X))^*$ is positive definite if and only if

$$\begin{aligned} &4\|S\odot(U\widehat{\Delta Z}V^T) - \mathrm{diag}(S(S\odot(U\widehat{\Delta Z}V^T))^T)S\|^2 + \frac{1}{4}\|\widehat{\Delta Z}\Sigma - \Sigma\widehat{\Delta Z}^T\|^2 \\ &+ \frac{1}{4}\|\Sigma\widehat{\Delta Z} - \widehat{\Delta Z}^T\Sigma\|^2 > 0, \quad \forall\widehat{\Delta Z}\in\mathbb{R}^{n\times n}\setminus\{\mathbf{0}_{n\times n}\}, \end{aligned} \tag{A6}$$

which holds if and only if the following system of equations

$$\begin{cases} S\odot(U\widehat{\Delta Z}V^T) - \mathrm{diag}(S(S\odot(U\widehat{\Delta Z}V^T))^T)S = \mathbf{0}_{n\times n}, \\ \widehat{\Delta Z}\Sigma - \Sigma\widehat{\Delta Z}^T = \mathbf{0}_{n\times n}, \\ \Sigma\widehat{\Delta Z} - \widehat{\Delta Z}^T\Sigma = \mathbf{0}_{n\times n} \end{cases} \tag{A7}$$

has a unique solution $\widehat{\Delta Z} = \mathbf{0}_{n\times n}$. The second and third equations of (A7) imply that

$$\begin{cases} \sigma_j\widehat{\Delta Z}_{ij} - \sigma_i\widehat{\Delta Z}_{ji} = 0, \\ \sigma_i\widehat{\Delta Z}_{ij} - \sigma_j\widehat{\Delta Z}_{ji} = 0, \end{cases} \tag{A8}$$

for all $1\le i<j\le n$. By using the distinctness of the given singular values $\sigma_1,\sigma_2,\ \dots\ ,\sigma_n$ and (A8) we obtain

$$\widehat{\Delta Z}_{ij} = \widehat{\Delta Z}_{ji} = 0, \quad \forall 1\le i<j\le n.$$

This, together with the first equation of (A7), yields

$$\sum_{i=1}^{n}(S\odot(\mathbf{u}_i\mathbf{v}_i^T) - \mathrm{diag}(S(S\odot(\mathbf{u}_i\mathbf{v}_i^T))^T)S)\widehat{\Delta Z}_{ii} = \mathbf{0}_{n\times n}.$$

Hence, if the given singular values $\sigma_1,\sigma_2,\ \dots\ ,\sigma_n$ are all distinct and the matrix is full column rank, then (A7) has a unique solution $\widehat{\Delta Z} = \mathbf{0}_{n\times n}$. The proof is complete. ∎