

## COMPUTING THE NEAREST DOUBLY STOCHASTIC MATRIX WITH A PRESCRIBED ENTRY\*

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**Abstract.** In this paper a nearest doubly stochastic matrix problem is studied. This problem is to find the closest doubly stochastic matrix with the prescribed  $(1, 1)$  entry to a given matrix. According to the well-established dual theory in optimization, the dual of the underlying problem is an unconstrained differentiable, but not twice differentiable, convex optimization problem. A Newton-type method is used for solving the associated dual problem, and then the desired nearest doubly stochastic matrix is obtained. Under some mild assumptions, the quadratic convergence of the proposed Newton method is proved. The numerical performance of the method is also demonstrated by numerical examples.

**Key words.** doubly stochastic matrix, generalized Jacobian, Newton’s method, quadratic convergence

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**1. Introduction.** A matrix  $A \in \mathbb{R}^{n \times n}$  is called *doubly stochastic* if it is nonnegative and all its row and column sums are equal to one. Doubly stochastic matrices have found many important applications in probability and statistics, quantum mechanics, the study of hypergroups, economics and operation research, physical chemistry, communication theory and graph theory, etc.; see [15, 3, 17, 19, 23] and the references therein.

In this paper, we are interested in the best approximation problem related to doubly stochastic matrices: Given a matrix  $T \in \mathbb{R}^{n \times n}$ , find its nearest doubly stochastic matrix with the same  $(1, 1)$  entry as the given matrix  $T$ . This problem can be mathematically stated as follows:

$$(1) \quad \begin{cases} \min & \frac{1}{2} \|M - T\|_F^2 \\ \text{s.t.} & M\mathbf{e} = \mathbf{e}, \quad \mathbf{e}^T M = \mathbf{e}^T, \\ & \mathbf{e}_1^T M \mathbf{e}_1 = \mathbf{e}_1^T T \mathbf{e}_1, \\ & M \geq 0, \end{cases}$$

where

$$\mathbf{e} = (1, \dots, 1)^T \in \mathbb{R}^n, \quad \mathbf{e}_1 = (1, 0, \dots, 0)^T \in \mathbb{R}^n,$$

and  $M \geq 0$  means that  $M$  is nonnegative. Problem (1) was originally suggested by Professor Zhaojun Bai (Department of Computer Science, UC Davis). It arose from

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numerical simulation of large (semiconductor, electronic) circuit networks. Padé approximation technique using the Lanczos process is very powerful for computing a lower order approximation to the linear system matrix describing the large linear network [1, 9]. The matrix  $T$  produced by the Lanczos process is in general not a doubly stochastic matrix. Suppose that the original system matrix is doubly stochastic; then we need to find the nearest doubly stochastic matrix  $M$  to  $T$  and at the same time match the moments.

Problem (1) has been studied in [10] based on the alternating projection method [2]. In [10, 14], problem (1) is simplified by removing the requirements on the  $(1, 1)$  entry and the nonnegativity of the matrix  $M$ . In this case, the solution can be obtained explicitly. We will revisit problem (1). Based on the dual approach in optimization [16], we will first reformulate (1) as an unconstrained differentiable but not twice differentiable convex optimization problem, next apply Newton's method to solve this convex problem, and then obtain the desired nearest doubly stochastic matrix. Under some mild assumptions, we will show that the proposed Newton method is quadratically convergent. We will also demonstrate the numerical performance of the method by numerical examples.

Throughout this paper, the following notation will be used:

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$$T = \begin{bmatrix} t_{1,1} & \cdots & t_{1,n} \\ \vdots & \cdots & \vdots \\ t_{n,1} & \cdots & t_{n,n} \end{bmatrix}.$$

- $A \geq 0$  ( $A > 0$ ) means that  $A$  is nonnegative (positive).

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$$\mathcal{K} = \{A : A \in \mathbb{R}^{n \times n}, A \geq 0\}, \quad (z)_+ = \max\{0, z\}.$$

- $\Pi_{\mathcal{K}}(X)$  denotes the metric projection of  $X$  onto  $\mathcal{K}$ , i.e.,

$$\Pi_{\mathcal{K}}(X) = \begin{bmatrix} (x_{1,1})_+ & \cdots & (x_{1,n})_+ \\ \vdots & \cdots & \vdots \\ (x_{n,1})_+ & \cdots & (x_{n,n})_+ \end{bmatrix} \quad \forall X = \begin{bmatrix} x_{1,1} & \cdots & x_{1,n} \\ \vdots & \cdots & \vdots \\ x_{n,1} & \cdots & x_{n,n} \end{bmatrix} \in \mathbb{R}^{n \times n}.$$

**2. Newton's method.** In this section we consider a Newton-type method for computing the solution of problem (1).

Let

$$f(M) := \frac{1}{2} \|M - T\|_F^2, \quad \mathcal{A}(M) := \begin{bmatrix} M\mathbf{e} \\ [I_{n-1} \ 0] M^T \mathbf{e} \\ \mathbf{e}_1^T M \mathbf{e}_1 \end{bmatrix}, \quad b := \begin{bmatrix} \mathbf{e} \\ [I_{n-1} \ 0] \mathbf{e} \\ \mathbf{e}_1^T T \mathbf{e}_1 \end{bmatrix};$$

then problem (1) is equivalent to

$$(2) \quad \begin{cases} \min & f(M) \\ \text{s.t.} & \mathcal{A}(M) = b, \\ & M \in \mathcal{K}. \end{cases}$$

The dual problem [16] of (2) is

$$(3) \quad \begin{cases} \sup & -\theta(x) \\ \text{s.t.} & x \in \mathbb{R}^{2n}, \end{cases}$$

where

$$\theta(x) = \frac{1}{2} \|\Pi_{\mathcal{K}}(T + \mathcal{A}^*(x))\|_F^2 - x^T b - \frac{1}{2} \|T\|_F^2,$$

and  $\mathcal{A}^*$  is the adjoint of  $\mathcal{A}$  and is defined by

$$\begin{aligned} \mathcal{A}^*(x) &= [ I_n \quad 0 ] x \mathbf{e}^T + \mathbf{e} x^T \begin{bmatrix} 0_{n \times (n-1)} & 0 \\ I_{n-1} & 0 \\ 0 & 0 \end{bmatrix} + \mathbf{e}_1 [ 0 \quad 1 ] x \mathbf{e}_1^T \\ &= \begin{bmatrix} x_1 + x_{n+1} + x_{2n} & x_1 + x_{n+2} & \cdots & x_1 + x_{2n-1} & x_1 \\ x_2 + x_{n+1} & x_2 + x_{n+2} & \cdots & x_2 + x_{2n-1} & x_2 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ x_n + x_{n+1} & x_n + x_{n+2} & \cdots & x_n + x_{2n-1} & x_n \end{bmatrix} \\ \forall x &= \begin{bmatrix} x_1 \\ \vdots \\ x_{2n} \end{bmatrix} \in \mathbb{R}^{2n}. \end{aligned}$$

The relation between the values of (2) at its minimum and of the dual (3) at its maximum is stated in the following theorem.

**THEOREM 2.1.** *There exists a matrix  $M \in \mathbb{R}^{n \times n}$  in the topological interior of  $\mathcal{K}$  such that  $\mathcal{A}(M) = b$  if and only if*

$$(4) \quad 0 < \mathbf{e}_1^T T \mathbf{e}_1 < 1.$$

Under the condition (4),

- (i) *problem (2) has a unique solution, denoted by  $M^*$ ;*
- (ii) *the supremum of dual problem (3) is actually a maximum. Let this maximum be achieved at  $x^*$ . Then*

$$(5) \quad M^* = \Pi_{\mathcal{K}}(T + \mathcal{A}^*(x^*)).$$

*Proof.* If  $M$  is in the topological interior of  $\mathcal{K}$  and  $\mathcal{A}(M) = b$ , then (4) follows directly from the properties that

$$\mathbf{e}_1^T T \mathbf{e}_1 = \mathbf{e}_1^T M \mathbf{e}_1 > 0, \quad \mathbf{e}_1^T M \mathbf{e} = 1,$$

and all entries of  $\mathbf{e}_1^T M$  are positive. Conversely, if (4) holds, then it is clear that the matrix  $M$  defined by

$$(6) \quad M := \frac{1}{n-1} \begin{bmatrix} r_0 & r & \cdots & r & r \\ r & r_0 & \ddots & & r \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ r & & \ddots & \ddots & r \\ r & r & \cdots & r & r_0 \end{bmatrix},$$

$$\text{with } r_0 = (n-1) \mathbf{e}_1^T T \mathbf{e}_1 > 0, \quad r = 1 - \mathbf{e}_1^T T \mathbf{e}_1 > 0,$$

satisfies that  $M$  is in the topological interior of  $\mathcal{K}$  and  $\mathcal{A}(M) = b$ . Hence Theorem 2.1 follows.

Under the condition (4), parts (i) and (ii) of the theorem are now well known; see [12, 16, 21].  $\square$

*Remark 1.* In [12], the condition ensuring that there exists a matrix  $M \in \mathbb{R}^{n \times n}$  in the topological interior of  $\mathcal{K}$  such that  $\mathcal{A}(M) = b$  is called the *Slater condition* for (2). Hence, we can regard (4) as the Slater condition for (2).

According to Theorem 2.1, once we can compute an optimal solution  $x^*$  of the dual problem (3), then we can obtain the optimal solution  $M^*$  of problem (2) by using (5).

Define

$$(7) \quad F(x) := \mathcal{A}(\Pi_{\mathcal{K}}(T + \mathcal{A}^*(x))) - b$$

$$= \begin{bmatrix} (t_{1,1} + x_1 + x_{n+1} + x_{2n})_+ + \sum_{i=2}^{n-1} (t_{1,i} + x_1 + x_{n+i})_+ + (t_{1,n} + x_1)_+ \\ \sum_{i=1}^{n-1} (t_{2,i} + x_2 + x_{n+i})_+ + (t_{2,n} + x_2)_+ \\ \vdots \\ \sum_{i=1}^{n-1} (t_{n,i} + x_n + x_{n+i})_+ + (t_{n,n} + x_n)_+ \\ (t_{1,1} + x_1 + x_{n+1} + x_{2n})_+ + \sum_{j=2}^n (t_{j,1} + x_j + x_{n+1})_+ \\ \sum_{j=1}^n (t_{j,2} + x_j + x_{n+2})_+ \\ \vdots \\ \sum_{j=1}^n (t_{j,n-1} + x_j + x_{2n-1})_+ \\ (t_{1,1} + x_1 + x_{n+1} + x_{2n})_+ \end{bmatrix} - \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 1 \\ 1 \\ \vdots \\ 1 \\ t_{11} \end{bmatrix}$$

for any

$$x = \begin{bmatrix} x_1 \\ \vdots \\ x_{2n} \end{bmatrix} \in \mathbb{R}^{2n}.$$

It is easy to know that the function  $\theta(x)$  is continuously differentiable and that its gradient  $\nabla\theta(x) = F(x)$  is globally Lipschitz continuous. Thus, both gradient-type methods and quasi-Newton methods can be directly employed to solve (3). However, since  $\theta(x)$  is not twice continuously differentiable, the convergence rates of these methods are at most linear.

Since  $\theta(x)$  is convex and differentiable, at solution  $x^*$  of (3),

$$\nabla\theta(x^*) = 0; \quad \text{i.e., } F(x^*) = 0.$$

This indicates that we can obtain a solution of (3) by solving the equation  $F(x) = 0$ .  $F(x)$  is globally Lipschitz continuous. According to Rademacher’s theorem [22, Chapter 9.J],  $F(x)$  is Fréchet differentiable almost everywhere. Let  $\Omega_F$  be the set of points at which  $F$  is Fréchet differentiable. Denote the Jacobian of  $F(x)$  at  $x \in \Omega_F$  by  $F'(x)$ . The generalized Jacobian  $\partial F(x)$  of  $F$  at  $x \in \mathbb{R}^{2n}$  in the sense of Clarke [6] is defined by

$$\partial F(x) := \text{conv}\{\partial_B F(x)\},$$

where “conv” denotes the convex hull and

$$\partial_B F(x) := \left\{ V \in \mathbb{R}^{2n \times 2n} : V \text{ is an accumulation point of } F'(x^{(k)}), x^{(k)} \rightarrow x, x^{(k)} \in \Omega_F \right\}.$$

The nonsmooth Newton method for solving equation

$$(8) \quad F(x) = 0$$

is given by

$$(9) \quad x^{(k+1)} = x^{(k)} - V_k^{-1}F(x^{(k)}), \quad V_k \in \partial F(x^{(k)}).$$

The following result was established in [20].

**THEOREM 2.2** (see [20]). *Let  $x^*$  be a solution of the equation  $F(x) = 0$ . If all  $V \in \partial F(x^*)$  are nonsingular and  $F$  is semismooth at  $x^*$ , i.e.,  $F$  is directionally differentiable at  $x^*$  and for any  $V \in \partial F(x^* + \delta x)$  and  $\delta x \rightarrow 0$*

$$F(x^* + \delta x) - F(x^*) - V(\delta x) = o(\|\delta x\|_F),$$

*then every sequence generalized by (9) is superlinearly convergent to  $x^*$ , provided that the starting point  $x^{(0)}$  is sufficiently close to  $x^*$ . Moreover, if  $F$  is strongly semismooth at  $x^*$ , i.e.,  $F$  is semismooth at  $x^*$  and*

$$F(x^* + \delta x) - F(x^*) - V(\delta x) = o(\|\delta x\|_F^2) \quad \forall V \in \partial F(x^* + \delta x), \quad \delta x \rightarrow 0,$$

*then the convergence rate is quadratic.*

Motivated by Theorem 2.2, in the following we discuss the strong semismoothness of  $F$  and the nonsingularity of all  $V \in \partial F(x^*)$  at a solution  $x^*$  of  $F(x) = 0$ .

Since

$$x = \begin{bmatrix} x_1 \\ \vdots \\ x_{2n} \end{bmatrix} \in \Omega_F,$$

i.e.,  $F'(x)$  exists if and only if

$$\begin{cases} t_{11} + x_1 + x_{n+1} + x_{2n} \neq 0, \\ t_{1,j} + x_1 + x_{n+j} \neq 0, \quad j = 2, \dots, n-1, \\ t_{i,j} + x_i + x_{n+j} \neq 0, \quad i = 2, \dots, n, \quad j = 1, \dots, n-1, \\ t_{i,n} + x_i \neq 0, \quad i = 1, \dots, n, \end{cases}$$

in the case that the inequalities above hold,

$$\begin{aligned} a_{1,1} &:= \frac{\partial(t_{11} + x_1 + x_{n+1} + x_{2n})_+}{\partial x_1} = \frac{\partial(t_{11} + x_1 + x_{n+1} + x_{2n})_+}{\partial x_{n+1}} \\ &= \frac{\partial(t_{11} + x_1 + x_{n+1} + x_{2n})_+}{\partial x_{2n}} = \begin{cases} 1 & \text{if } t_{11} + x_1 + x_{n+1} + x_{2n} > 0, \\ 0 & \text{if } t_{11} + x_1 + x_{n+1} + x_{2n} < 0, \end{cases} \\ a_{1,j} &:= \frac{\partial(t_{1,j} + x_1 + x_{n+j})_+}{\partial x_1} = \frac{\partial(t_{1,j} + x_1 + x_{n+j})_+}{\partial x_{n+j}} \\ &= \begin{cases} 1 & \text{if } t_{1,j} + x_1 + x_{n+j} > 0, \\ 0 & \text{if } t_{1,j} + x_1 + x_{n+j} < 0, \end{cases} \quad j = 2, \dots, n-1, \\ a_{i,j} &:= \frac{\partial(t_{i,j} + x_i + x_{n+j})_+}{\partial x_i} = \frac{\partial(t_{i,j} + x_i + x_{n+j})_+}{\partial x_{n+j}} \\ &= \begin{cases} 1 & \text{if } t_{i,j} + x_i + x_{n+j} > 0, \quad i = 2, \dots, n, \\ 0 & \text{if } t_{i,j} + x_i + x_{n+j} < 0, \quad j = 1, \dots, n-1, \end{cases} \\ a_{i,n} &:= \frac{\partial(t_{i,n} + x_i)_+}{x_i} = \begin{cases} 1 & \text{if } t_{i,n} + x_i > 0, \\ 0 & \text{if } t_{i,n} + x_i < 0, \end{cases} \quad i = 1, \dots, n, \end{aligned}$$

and

$$F'(x) = \left[ \begin{array}{cccc|cccc} \sum_{i=1}^n a_{1,i} & & & & a_{1,1} & a_{1,2} & \cdots & a_{1,n-1} & a_{1,1} \\ & \sum_{i=1}^n a_{2,i} & & & a_{2,1} & a_{2,2} & \cdots & a_{2,n-1} & 0 \\ & & \ddots & & \vdots & \vdots & \cdots & \vdots & \vdots \\ & & & \sum_{i=1}^n a_{n,i} & a_{n,1} & a_{n,2} & \cdots & a_{n,n-1} & 0 \\ \hline a_{1,1} & a_{2,1} & \cdots & a_{n,1} & \sum_{i=1}^n a_{i,1} & & & & a_{1,1} \\ a_{1,2} & a_{2,2} & \cdots & a_{n,2} & & \sum_{i=1}^n a_{i,2} & & & 0 \\ \vdots & \vdots & \cdots & \vdots & & & \ddots & & \vdots \\ a_{1,n-1} & a_{2,n-1} & \cdots & a_{n,n-1} & & & & \sum_{i=1}^n a_{i,n-1} & 0 \\ \hline a_{1,1} & 0 & \cdots & 0 & a_{1,1} & 0 & \cdots & 0 & a_{1,1} \end{array} \right].$$

Thus, for any

$$x = \begin{bmatrix} x_1 \\ \vdots \\ x_{2n} \end{bmatrix} \in \mathbb{R}^{2n},$$

(10)

$$V \in \partial_B F(x) \Leftrightarrow V =$$

$$\left[ \begin{array}{cccc|cccc} \sum_{i=1}^n b_{1,i} & & & & b_{1,1} & b_{1,2} & \cdots & b_{1,n-1} & b_{1,1} \\ & \sum_{i=1}^n b_{2,i} & & & b_{2,1} & b_{2,2} & \cdots & b_{2,n-1} & 0 \\ & & \ddots & & \vdots & \vdots & \cdots & \vdots & \vdots \\ & & & \sum_{i=1}^n b_{n,i} & b_{n,1} & b_{n,2} & \cdots & b_{n,n-1} & 0 \\ \hline b_{1,1} & b_{2,1} & \cdots & b_{n,1} & \sum_{i=1}^n b_{i,1} & & & & b_{1,1} \\ b_{1,2} & b_{2,2} & \cdots & b_{n,2} & & \sum_{i=1}^n b_{i,2} & & & 0 \\ \vdots & \vdots & \cdots & \vdots & & & \ddots & & \vdots \\ b_{1,n-1} & b_{2,n-1} & \cdots & b_{n,n-1} & & & & \sum_{i=1}^n b_{i,n-1} & 0 \\ \hline b_{1,1} & 0 & \cdots & 0 & b_{1,1} & 0 & \cdots & 0 & b_{1,1} \end{array} \right],$$

where

$$(11) \quad \begin{cases} b_{1,1} = 1 & \text{if } t_{11} + x_1 + x_{n+1} + x_{2n} > 0, \\ b_{1,1} \in \{0, 1\} & \text{if } t_{11} + x_1 + x_{n+1} + x_{2n} = 0, \\ b_{1,1} = 0 & \text{if } t_{11} + x_1 + x_{n+1} + x_{2n} < 0, \\ \\ b_{1,j} = 1 & \text{if } t_{1,j} + x_1 + x_{n+j} > 0, \\ b_{1,j} \in \{0, 1\} & \text{if } t_{1,j} + x_1 + x_{n+j} = 0, \quad j = 2, \dots, n-1, \\ b_{1,j} = 0 & \text{if } t_{1,j} + x_1 + x_{n+j} < 0, \\ \\ b_{i,j} = 1 & \text{if } t_{i,j} + x_i + x_{n+j} > 0, \quad i = 2, \dots, n, \\ b_{i,j} \in \{0, 1\} & \text{if } t_{i,j} + x_i + x_{n+j} = 0, \quad j = 1, \dots, n-1, \\ b_{i,j} = 0 & \text{if } t_{i,j} + x_i + x_{n+j} < 0, \\ \\ b_{i,n} = 1 & \text{if } t_{i,n} + x_i > 0, \\ b_{i,n} \in \{0, 1\} & \text{if } t_{i,n} + x_i = 0, \quad i = 1, \dots, n, \\ b_{i,n} = 0 & \text{if } t_{i,n} + x_i < 0, \end{cases}$$

As a result, we obtain the following result.

THEOREM 2.3.  $V \in \partial F(x)$  if and only if  $V$  is of the form

$$(12) \quad V = \left[ \begin{array}{cccc|cccc} \sum_{i=1}^n v_{1,i} & & & & v_{1,1} & v_{1,2} & \cdots & v_{1,n-1} & v_{1,1} \\ & \sum_{i=1}^n v_{2,i} & & & v_{2,1} & v_{2,2} & \cdots & v_{2,n-1} & 0 \\ & & \ddots & & \vdots & \vdots & \cdots & \vdots & \vdots \\ & & & \sum_{i=1}^n v_{n,i} & v_{n,1} & v_{n,2} & \cdots & v_{n,n-1} & 0 \\ \hline v_{1,1} & v_{2,1} & \cdots & v_{n,1} & \sum_{i=1}^n v_{i,1} & & & & v_{1,1} \\ v_{1,2} & v_{2,2} & \cdots & v_{n,2} & & \sum_{i=1}^n v_{i,2} & & & 0 \\ \vdots & \vdots & \cdots & \vdots & & & \ddots & & \vdots \\ v_{1,n-1} & v_{2,n-1} & \cdots & v_{n,n-1} & & & & \sum_{i=1}^n v_{i,n-1} & 0 \\ \hline v_{1,1} & 0 & \cdots & 0 & v_{1,1} & 0 & \cdots & 0 & v_{1,1} \end{array} \right],$$

where

$$(13) \quad \begin{cases} v_{1,1} = 1 & \text{if } t_{11} + x_1 + x_{n+1} + x_{2n} > 0, \\ v_{1,1} \in [0, 1] & \text{if } t_{11} + x_1 + x_{n+1} + x_{2n} = 0, \\ v_{1,1} = 0 & \text{if } t_{11} + x_1 + x_{n+1} + x_{2n} < 0, \\ \\ v_{1,j} = 1 & \text{if } t_{1,j} + x_1 + x_{n+j} > 0, \\ v_{1,j} \in [0, 1] & \text{if } t_{1,j} + x_1 + x_{n+j} = 0, \quad j = 2, \dots, n-1, \\ v_{1,j} = 0 & \text{if } t_{1,j} + x_1 + x_{n+j} < 0, \\ \\ v_{i,j} = 1 & \text{if } t_{i,j} + x_i + x_{n+j} > 0, \quad i = 2, \dots, n, \\ v_{i,j} \in [0, 1] & \text{if } t_{i,j} + x_i + x_{n+j} = 0, \quad j = 1, \dots, n-1, \\ v_{i,j} = 0 & \text{if } t_{i,j} + x_i + x_{n+j} < 0, \\ \\ v_{i,n} = 1 & \text{if } t_{i,n} + x_i > 0, \\ v_{i,n} \in [0, 1] & \text{if } t_{i,n} + x_i = 0, \quad i = 1, \dots, n, \\ v_{i,n} = 0 & \text{if } t_{i,n} + x_i < 0, \end{cases}$$

We are now ready to present our results on the strong semismoothness of  $F$  and the nonsingularity of all  $V \in \partial F(x)$ .

THEOREM 2.4. At any point  $x \in \mathbb{R}^{2n}$ ,  $F(x)$  is directionally differentiable and

$$(14) \quad F(x + \delta x) - F(x) - V\delta x = 0 \quad \forall V \in \partial F(x + \delta x), \delta x \rightarrow 0.$$

Hence,  $F$  is strongly semismooth at any  $x \in \mathbb{R}^{2n}$ .

Proof. A simple calculation yields that

$$\lim_{t \rightarrow 0^+} \frac{F(x + th) - F(x)}{t}$$

exists for any  $x, h \in \mathbb{R}^{2n}$ , and so  $F(x)$  is directionally differentiable at any point  $x \in \mathbb{R}^{2n}$ . In addition, it can be verified using (10) and (11) that

$$F(x + \delta x) - F(x) - V\delta x = 0 \quad \forall V \in \partial_B F(x + \delta x), \delta x \rightarrow 0.$$

Since any  $V \in \partial F(x + \delta x)$  is just a convex combination of elements in  $\partial_B F(x + \delta x)$ , (14) holds.  $\square$

THEOREM 2.5. For any

$$x = \begin{bmatrix} x_1 \\ \vdots \\ x_{2n} \end{bmatrix} \in \mathbb{R}^{2n},$$

let

$$\begin{aligned}
 M &:= \begin{bmatrix} m_{1,1} & \cdots & m_{1,n} \\ \vdots & \dots & \vdots \\ m_{n,1} & \cdots & m_{n,n} \end{bmatrix} = \Pi_{\mathcal{K}}(T + \mathcal{A}^*(x)) \\
 &= \Pi_{\mathcal{K}} \left( \begin{bmatrix} t_{1,1} + x_1 + x_{n+1} + x_{2n} & t_{1,2} + x_1 + x_{n+2} & \cdots & t_{1,n-1} + x_1 + x_{2n-1} & t_{1,n} + x_1 \\ t_{2,1} + x_2 + x_{n+1} & t_{2,2} + x_2 + x_{n+2} & \cdots & t_{2,n-1} + x_2 + x_{2n-1} & t_{2,n} + x_2 \\ \vdots & \vdots & \dots & \vdots & \vdots \\ t_{n,1} + x_n + x_{n+1} & t_{n,2} + x_n + x_{n+2} & \cdots & t_{n,n-1} + x_n + x_{2n-1} & t_{n,n} + x_n \end{bmatrix} \right)
 \end{aligned}$$

and

$$N_M = \left[ \begin{array}{cccc|cccc|c}
 \sum_{i=1}^n m_{1,i} & & & & m_{1,1} & m_{1,2} & \cdots & m_{1,n-1} & m_{1,1} \\
 & \sum_{i=1}^n m_{2,i} & & & m_{2,1} & m_{2,2} & \cdots & m_{2,n-1} & 0 \\
 & & \ddots & & \vdots & \vdots & \dots & \vdots & \vdots \\
 & & & \sum_{i=1}^n m_{n,i} & m_{n,1} & m_{n,2} & \cdots & m_{n,n-1} & 0 \\
 \hline
 m_{1,1} & m_{2,1} & \cdots & m_{n,1} & \sum_{i=1}^n m_{i,1} & & & & m_{1,1} \\
 m_{1,2} & m_{2,2} & \cdots & m_{n,2} & & \sum_{i=1}^n m_{i,2} & & & 0 \\
 \vdots & \vdots & \dots & \vdots & & & \ddots & & \vdots \\
 m_{1,n-1} & m_{2,n-1} & \cdots & m_{n,n-1} & & & & \sum_{i=1}^n m_{i,n-1} & 0 \\
 \hline
 m_{1,1} & 0 & \cdots & 0 & m_{1,1} & 0 & \cdots & 0 & m_{1,1}
 \end{array} \right].$$

Then

- (i)  $N_M$  is symmetric and positive semidefinite.
- (ii) All  $V \in \partial F(x)$  are nonsingular if and only if  $N_M$  is positive definite.

*Proof.* (i) Since

$$m_{i,j} \geq 0, \quad i, j = 1, \dots, n,$$

for any

$$h = \begin{bmatrix} h_1 \\ \vdots \\ h_{2n} \end{bmatrix} \in \mathbb{R}^{2n}$$

we find

$$\begin{aligned}
 h^T N_M h &= m_{1,1} (h_1 + h_{n+1} + h_{2n})^2 + \sum_{i=2}^n m_{i,1} (h_i + h_{n+1})^2 \\
 &\quad + \sum_{j=2}^{n-1} \sum_{i=1}^n m_{i,j} (h_i + h_{n+j})^2 + \sum_{i=1}^n m_{i,n} h_i^2 \geq 0
 \end{aligned}$$

and  $N_M$  is symmetric, so  $N_M$  is symmetric and positive semidefinite.

- (ii) Among all  $V \in \partial F(x)$ , we consider the following one:

(15)  $V_{min} =$

$$\left[ \begin{array}{cccc|cccc} \Sigma_{i=1}^n v_{1,i}^{(min)} & & & & v_{1,1}^{(min)} & v_{1,2}^{(min)} & \dots & v_{1,n-1}^{(min)} & v_{1,1}^{(min)} \\ & \Sigma_{i=1}^n v_{2,i}^{(min)} & & & v_{2,1}^{(min)} & v_{2,2}^{(min)} & \dots & v_{2,n-1}^{(min)} & 0 \\ & & \ddots & & \vdots & \vdots & \dots & \vdots & \vdots \\ & & & \Sigma_{i=1}^n v_{n,i}^{(min)} & v_{n,1}^{(min)} & v_{n,2}^{(min)} & \dots & v_{n,n-1}^{(min)} & 0 \\ \hline v_{1,1}^{(min)} & v_{2,1}^{(min)} & \dots & v_{n,1}^{(min)} & \Sigma_{i=1}^n v_{i,1}^{(min)} & & & & v_{1,1}^{(min)} \\ v_{1,2}^{(min)} & v_{2,2}^{(min)} & \dots & v_{n,2}^{(min)} & & \Sigma_{i=1}^n v_{i,2}^{(min)} & & & 0 \\ \vdots & \vdots & \dots & \vdots & & & \ddots & & \vdots \\ v_{1,n-1}^{(min)} & v_{2,n-1}^{(min)} & \dots & v_{n,n-1}^{(min)} & & & & \Sigma_{i=1}^n v_{i,n-1}^{(min)} & 0 \\ \hline v_{1,1}^{(min)} & 0 & \dots & 0 & v_{1,1}^{(min)} & 0 & \dots & 0 & v_{1,1}^{(min)} \end{array} \right],$$

where

$$(16) \quad \begin{cases} v_{1,1}^{(min)} = 1 & \text{if } m_{1,1} = (t_{11} + x_1 + x_{n+1} + x_{2n})_+ > 0, \\ v_{1,1}^{(min)} = 0 & \text{if } m_{1,1} = (t_{11} + x_1 + x_{n+1} + x_{2n})_+ = 0, \\ \begin{cases} v_{1,j}^{(min)} = 1 & \text{if } m_{1,j} = (t_{1,j} + x_1 + x_{n+j})_+ > 0, \\ v_{1,j}^{(min)} = 0 & \text{if } m_{1,j} = (t_{1,j} + x_1 + x_{n+j})_+ = 0, \end{cases} & j = 2, \dots, n-1, \\ \begin{cases} v_{i,j}^{(min)} = 1 & \text{if } m_{i,j} = (t_{i,j} + x_i + x_{n+j})_+ > 0, \\ v_{i,j}^{(min)} = 0 & \text{if } m_{i,j} = (t_{i,j} + x_i + x_{n+j})_+ = 0, \end{cases} & i = 2, \dots, n, \\ & j = 1, \dots, n-1, \\ \begin{cases} v_{i,n}^{(min)} = 1 & \text{if } m_{i,n} = (t_{i,n} + x_i)_+ > 0, \\ v_{i,n}^{(min)} = 0 & \text{if } m_{i,n} = (t_{i,n} + x_i)_+ = 0, \end{cases} & i = 1, \dots, n, \end{cases}$$

$V_{min}$  and  $V - V_{min}$  are symmetric and positive semidefinite since all  $V \in \partial F(x)$  are given by (12) and (13),

$$v_{i,j}^{(min)} \geq 0, \quad v_{i,j} - v_{i,j}^{(min)} \geq 0,$$

and for any

$$h = \begin{bmatrix} h_1 \\ \vdots \\ h_{2n} \end{bmatrix} \in \mathbb{R}^{2n},$$

we find

$$\begin{aligned} h^T V_{min} h &= v_{1,1}^{(min)} (h_1 + h_{n+1} + h_{2n})^2 + \sum_{i=2}^n v_{i,1}^{(min)} (h_i + h_{n+1})^2 \\ &+ \sum_{j=2}^{n-1} \sum_{i=1}^n v_{i,j}^{(min)} (h_i + h_{n+j})^2 + \sum_{i=1}^n v_{i,n}^{(min)} h_i^2 \geq 0, \end{aligned}$$

$$\begin{aligned} h^T (V - V_{min}) h &= (v_{1,1} - v_{1,1}^{(min)}) (h_1 + h_{n+1} + h_{2n})^2 + \sum_{i=2}^n (v_{i,1} - v_{i,1}^{(min)}) (h_i + h_{n+1})^2 \\ &+ \sum_{j=2}^{n-1} \sum_{i=1}^n (v_{i,j} - v_{i,j}^{(min)}) (h_i + h_{n+j})^2 + \sum_{i=1}^n (v_{i,n} - v_{i,n}^{(min)}) h_i^2 \geq 0. \end{aligned}$$

Thus, all  $V \in \partial F(x)$  are nonsingular if and only if  $V_{min}$  is positive definite.

Recall that  $v_{i,j}^{(min)} > 0$  if and only if  $m_{i,j} > 0$ ,  $i, j = 1, \dots, n$ , and for any

$$h = \begin{bmatrix} h_1 \\ \vdots \\ h_{2n} \end{bmatrix} \in \mathbb{R}^{2n},$$

we have

$$\begin{aligned} h^T V_{min} h &= v_{1,1}^{(min)} (h_1 + h_{n+1} + h_{2n})^2 + \sum_{i=2}^n v_{i,1}^{(min)} (h_i + h_{n+1})^2 \\ &\quad + \sum_{j=2}^{n-1} \sum_{i=1}^n v_{i,j}^{(min)} (h_i + h_{n+j})^2 + \sum_{i=1}^n v_{i,n}^{(min)} h_i^2, \\ h^T N_M h &= m_{1,1} (h_1 + h_{n+1} + h_{2n})^2 + \sum_{i=2}^n m_{i,1} (h_i + h_{n+1})^2 \\ &\quad + \sum_{j=2}^{n-1} \sum_{i=1}^n m_{i,j} (h_i + h_{n+j})^2 + \sum_{i=1}^n m_{i,n} h_i^2, \end{aligned}$$

so that we get that  $h^T V_{min} h > 0$  if and only if  $h^T N_M h > 0$ . This implies that  $V_{min}$  is positive definite if and only if  $N_M$  is positive definite. Hence, part (ii) is proved.  $\square$

*Remark 2.* The positive semidefiniteness of  $N_M$  can be proved<sup>1</sup> alternatively as follows: Let

$$\mathcal{N}_1 = \left[ \begin{array}{cccc|cccc|c} \sum_{i=2}^n m_{1,i} & & & & 0 & m_{1,2} & \cdots & m_{1,n-1} & 0 \\ & \sum_{i=1}^n m_{2,i} & & & m_{2,1} & m_{2,2} & \cdots & m_{2,n-1} & 0 \\ & & \ddots & & \vdots & \vdots & \cdots & \vdots & \vdots \\ & & & \sum_{i=1}^n m_{n,i} & m_{n,1} & m_{n,2} & \cdots & m_{n,n-1} & 0 \\ \hline 0 & m_{2,1} & \cdots & m_{n,1} & \sum_{i=2}^n m_{i,1} & & & & 0 \\ m_{1,2} & m_{2,2} & \cdots & m_{n,2} & & \sum_{i=1}^n m_{i,2} & & & 0 \\ \vdots & \vdots & \cdots & \vdots & & & \ddots & & \vdots \\ m_{1,n-1} & m_{2,n-1} & \cdots & m_{n,n-1} & & & & \sum_{i=1}^n m_{i,n-1} & 0 \\ \hline 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 \end{array} \right]$$

and

$$\mathcal{N}_2 = \left[ \begin{array}{cccc|cccc|c} m_{1,1} & & & & m_{1,1} & 0 & \cdots & 0 & m_{1,1} \\ & 0 & & & 0 & 0 & \cdots & 0 & 0 \\ & & \ddots & & \vdots & \vdots & \cdots & \vdots & \vdots \\ & & & 0 & 0 & 0 & \cdots & 0 & 0 \\ \hline m_{1,1} & 0 & \cdots & 0 & m_{1,1} & & & & m_{1,1} \\ 0 & 0 & \cdots & 0 & & 0 & & & 0 \\ \vdots & \vdots & \cdots & \vdots & & & \ddots & & \vdots \\ 0 & 0 & \cdots & 0 & & & & 0 & 0 \\ \hline m_{1,1} & 0 & \cdots & 0 & m_{1,1} & 0 & \cdots & 0 & m_{1,1} \end{array} \right].$$

<sup>1</sup>This alternative proof was suggested by an anonymous referee.

Then

$$N_M = \mathcal{N}_1 + \mathcal{N}_2.$$

Obviously,  $\mathcal{N}_2$  is positive semidefinite. Furthermore,  $\mathcal{N}_1$  is nonnegative, symmetric, and weakly diagonally dominant, so the well-known Gershgorin theorem [13] gives that all eigenvalues of  $\mathcal{N}_1$  are nonnegative. Thus,  $\mathcal{N}_1$  is positive semidefinite. Hence,  $N_M = \mathcal{N}_1 + \mathcal{N}_2$  is also positive semidefinite.

If  $x = x^*$  with  $F(x^*) = 0$ , then Theorem 2.5(ii) can be simplified significantly, as shown in the next result.

**THEOREM 2.6.** *Let  $M^*$  be the (unique) solution of problem (2), and  $x^* \in \mathbb{R}^{2n}$  satisfy  $F(x^*) = 0$ . Denote*

$$(17) \quad M^* =: \begin{bmatrix} t_{1,1} & m_{1,2}^* & \cdots & m_{1,n-1}^* & m_{1,n}^* \\ m_{2,1}^* & m_{2,2}^* & \cdots & m_{2,n-1}^* & m_{2,n}^* \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ m_{n,1}^* & m_{n,2}^* & \cdots & m_{n,n-1}^* & m_{n,n}^* \end{bmatrix},$$

$$(18) \quad L^* := \begin{bmatrix} \frac{1}{\sqrt{1-t_{1,1}}} & & & & \\ & I & & & \\ & & & & \\ & & & & \\ & & & & \end{bmatrix} \begin{bmatrix} 0 & m_{1,2}^* & \cdots & m_{1,n-1}^* \\ m_{2,1}^* & m_{2,2}^* & \cdots & m_{2,n-1}^* \\ \vdots & \vdots & \cdots & \vdots \\ m_{n,1}^* & m_{n,2}^* & \cdots & m_{n,n-1}^* \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{1-t_{1,1}}} & & & & \\ & I & & & \\ & & & & \\ & & & & \\ & & & & \end{bmatrix}.$$

Then the following hold:

(i) It is true that

$$(19) \quad \|L^*\|_2 \leq 1.$$

(ii) All  $V \in \partial F(x^*)$  are nonsingular if and only if

$$(20) \quad \|L^*\|_2 < 1.$$

*Proof.* We have from Theorem 2.5(i) that  $N_{M^*}$  is symmetric and positive semidefinite. Now  $0 < t_{1,1} < 1$ , and  $M^*$  satisfies that

$$(21) \quad \begin{cases} 0 < m_{1,1}^* = t_{1,1} < 1, & \sum_{i=2}^n m_{1,i}^* = 1 - t_{1,1}, & \sum_{i=2}^n m_{i,1}^* = 1 - t_{1,1}, \\ \sum_{i=1}^n m_{j,i}^* = 1, & j = 2, \dots, n, \\ \sum_{i=1}^n m_{i,j}^* = 1, & j = 2, \dots, n-1, \end{cases}$$

and thus we obtain, by using the positive semidefiniteness of  $N_{M^*}$ , that the matrix

$$(22) \quad \mathcal{N}_{M^*} := \left[ \begin{array}{cccc|cccc} 1-t_{1,1} & & & & 0 & m_{1,2}^* & \cdots & m_{1,n-1}^* \\ & 1 & & & m_{2,1}^* & m_{2,2}^* & \cdots & m_{2,n-1}^* \\ & & \ddots & & \vdots & \vdots & \cdots & \vdots \\ & & & 1 & m_{n,1}^* & m_{n,2}^* & \cdots & m_{n,n-1}^* \\ \hline 0 & m_{2,1}^* & \cdots & m_{n,1}^* & 1-t_{1,1} & & & \\ m_{1,2}^* & m_{2,2}^* & \cdots & m_{n,2}^* & & 1 & & \\ \vdots & \vdots & \cdots & \vdots & & & \ddots & \\ m_{1,n-1}^* & m_{2,n-1}^* & \cdots & m_{n,n-1}^* & & & & 1 \end{array} \right]$$

is positive semidefinite. Equivalently, (19) holds.

(ii) By Theorem 2.5(ii) we know that all  $V \in \partial F(x^*)$  are nonsingular if and only if  $N_{M^*}$  is positive definite, which is equivalent to saying that the matrix  $\mathcal{N}_{M^*}$  defined by (22) is positive definite. Therefore, part (ii) follows directly from the property that  $\mathcal{N}_{M^*}$  is positive definite if and only if (20) holds.  $\square$

Theorem 2.6 is very pleasant because it indicates that for almost all  $T \in \mathbb{R}^{n \times n}$ , all  $V \in \partial F(x^*)$  are nonsingular for the solution  $x^*$  of the equation  $F(x) = 0$ .

The following corollary contains two important sufficient conditions ensuring that all  $V \in \partial F(x^*)$  are nonsingular for the solution  $x^*$  of the equation  $F(x) = 0$ .

**COROLLARY 2.7.** *With the notation in Theorem 2.6, if  $M^*e_i > 0$  for some  $1 \leq i \leq n$ , or  $e_j^T M^* > 0$  for some  $1 \leq j \leq n$ , then all  $V \in \partial F(x^*)$  are nonsingular. Here  $e_i$  and  $e_j$  are the  $i$ th and  $j$ th, respectively, columns of  $I_n$ .*

*Proof.* By Theorem 2.6 and its proof we need to show only that  $\mathcal{N}_{M^*}$  defined by (22) is positive definite, provided  $M^*e_i > 0$  for some  $1 \leq i \leq n$  (or  $e_j^T M^* > 0$  for some  $1 \leq j \leq n$ ).

In the following we assume only that  $M^*e_i > 0$  for some  $1 \leq i \leq n$  because the case that  $e_j^T M^* > 0$  for some  $1 \leq j \leq n$  can be discussed similarly.

First, we have

$$0 < t_{1,1} < 1, \quad 0 \leq m_{1,j}^* < 1, \quad 0 \leq m_{j,1}^* < 1, \quad j = 2, \dots, n,$$

and for any

$$h = \begin{bmatrix} h_1 \\ \vdots \\ h_{2n-1} \end{bmatrix} \in \mathbb{R}^{2n-1},$$

we find

$$(23) \quad h^T \mathcal{N}_{M^*} h = \sum_{i=2}^n m_{i,1}^* (h_i + h_{n+1})^2 + \sum_{j=2}^{n-1} \sum_{i=1}^n m_{i,j}^* (h_i + h_{n+j})^2 + \sum_{i=1}^n m_{i,n}^* h_i^2.$$

Next, we show by considering three different cases that  $h^T \mathcal{N}_{M^*} h = 0$  only if  $h = 0$ , as follows.

*Case 1:*  $m_{2,1}^* \neq 0, \dots, m_{n,1}^* \neq 0$ . In this case

$$\begin{aligned} & h^T \mathcal{N}_{M^*} h = 0 \\ \implies & \begin{cases} h_2 = \dots = h_n = -h_{n+1}, \\ h^T \mathcal{N}_{M^*} h = \sum_{j=2}^{n-1} (h_{n+1} - h_{n+j})^2 \sum_{i=2}^n m_{i,j}^* + h_{n+1}^2 \sum_{i=2}^n m_{i,n}^* \\ \quad + \sum_{j=2}^{n-1} m_{1,j}^* (h_1 + h_{n+j})^2 + m_{1,n}^* h_1^2 = 0 \end{cases} \\ \implies & \begin{cases} h_2 = \dots = h_n = -h_{n+1} = \dots = -h_{2n-1} = 0, \\ h^T \mathcal{N}_{M^*} h = h_1^2 \sum_{j=2}^n m_{1,j}^* = 0 \end{cases} \\ & \left( \text{since } 0 < \sum_{i=2}^n m_{i,j}^* = 1 - m_{1,j}^* \leq 1, \quad j = 2, \dots, n \right) \\ \implies & h_1 = \dots = h_{2n-1} = 0 \quad \left( \text{since } 0 < \sum_{j=2}^n m_{1,j}^* = 1 - t_{1,1} < 1 \right) \\ \implies & h = 0. \end{aligned}$$

Case 2:  $m_{1,k}^* \neq 0, \dots, m_{n,k}^* \neq 0$  for some  $k$  with  $2 \leq k \leq n - 1$ . In this case, we have

$$\begin{aligned} & h^T \mathcal{N}_{M^*} h = 0 \\ \implies & \begin{cases} h_1 = \dots = h_n = -h_{n+k}, \\ h^T \mathcal{N}_{M^*} h = (h_{n+k} - h_{n+1})^2 \sum_{i=2}^n m_{i,1}^* + \sum_{j=2}^{k-1} (h_{n+k} - h_{n+j})^2 \sum_{i=1}^n m_{i,j}^* \\ \quad + \sum_{j=k+1}^{n-1} (h_{n+k} - h_{n+j})^2 \sum_{i=1}^n m_{i,j}^* + h_{n+k}^2 \sum_{i=1}^n m_{i,n}^* \end{cases} \\ \implies & h_1 = \dots = h_{2n-1} = 0 \\ & \left( \text{since } 0 < \sum_{i=2}^n m_{i,1}^* = 1 - t_{1,1} \neq 0, \sum_{i=1}^n m_{i,n}^* = 1, \sum_{i=1}^n m_{i,j}^* = 1, \right. \\ & \quad \left. j = 2, \dots, k-1, k+1, \dots, n-1 \right) \\ \implies & h = 0. \end{aligned}$$

Case 3:  $m_{1,n}^* \neq 0, \dots, m_{n,n}^* \neq 0$ . In this case, we have

$$\begin{aligned} & h^T \mathcal{N}_{M^*} h = 0 \\ \implies & \begin{cases} h_1 = \dots = h_n = 0, \\ h^T \mathcal{N}_{M^*} h = h_{n+1}^2 \sum_{i=2}^n m_{i,1}^* + \sum_{j=2}^{n-1} h_{n+j}^2 \sum_{i=1}^n m_{i,j}^* \end{cases} \\ \implies & h_1 = \dots = h_n = 0, h_{n+1} = \dots = h_{2n-1} = 0 \\ & \left( \text{since } 0 < \sum_{i=2}^n m_{i,1}^* = 1 - t_{1,1} \neq 0, \sum_{i=1}^n m_{i,j}^* = 1, j = 2, \dots, n-1 \right) \\ \implies & h = 0. \end{aligned}$$

Now we have shown that  $h^T \mathcal{N}_{M^*} h = 0$  only if  $h = 0$ . This means that  $\mathcal{N}_{M^*}$  is positive definite.  $\square$

*Remark 3.* Corollary 2.7 can be proved<sup>2</sup> alternatively as follows: Consider non-negative matrix

$$Z = \begin{bmatrix} D & R \\ R^T & D \end{bmatrix},$$

where  $D = \begin{bmatrix} t_{1,1} & 0 \\ 0 & 0 \end{bmatrix} \in \mathbb{R}^{n \times n}$  and  $R$  is obtained from the matrix  $M^*$  by replacing its  $(1, 1)$  entry with 0. Then  $Z$  is symmetric doubly stochastic with the largest eigenvalue equal to 1. If  $M^*$  has a nonzero row or a nonzero column, then  $Z$  is irreducible. Thus, up to a multiple,

$$\begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} \in \mathbb{R}^{2n}$$

is its only eigenvector corresponding to the largest eigenvalue 1. Now, let us remove the last row and the last column of  $Z$  to get the matrix  $\tilde{Z} \in \mathbb{R}^{(2n-1) \times (2n-1)}$ ; then

<sup>2</sup>This alternative proof was also provided by an anonymous referee.

there is no positive vector  $v \in \mathbb{R}^{2n-1}$  such that  $\tilde{v} = v$ . In other words, the largest eigenvalue of  $\tilde{Z}$  is less than 1. Hence,  $I_{2n-1} - \tilde{Z}$  is positive definite, and so is

$$\mathcal{N}_{M^*} = (-I_n \oplus I_{n-1})(I_{2n-1} - \tilde{Z})(-I_n \oplus I_{n+1}).$$

An important consequence of Theorems 2.4 and 2.6 is on the convergence of Newton’s method (9).

**THEOREM 2.8.** *Let  $x^* \in \mathbb{R}^{2n}$  be the solution of  $F(x) = 0$ . If (20) holds, then Newton’s method (9) is quadratically convergent, provided that  $x^{(0)}$  is sufficiently close to  $x^*$ .*

**3. Numerical algorithm.** In our numerical implementation we use the following globalized version of Newton’s method for solving the dual problem (3). Recall that  $\nabla\theta(x) = F(x)$  for any  $x \in \mathbb{R}^{2n}$ .

ALGORITHM 1 (nonsmooth Newton’s method).

**Step 0.** *Given  $x^{(0)} \in \mathbb{R}^{2n}$ ,  $\eta \in (0, 1)$ ,  $\rho, \delta \in (0, 1/2)$ .  $k := 0$ .*

**Step 1** (Newton’s iteration). *Let  $V_{min}^{(k)}$  be defined by (15) and (16) with  $x$  being replaced by  $x^{(k)}$ , and apply the conjugate gradient (CG) method [11, Algorithm 10.2.1] to compute an approximate solution  $\Delta x^{(k)} \in \mathbb{R}^{2n}$  to*

$$(24) \quad F(x^{(k)}) + V_{min}^{(k)}\Delta x = 0$$

*such that*

$$(25) \quad \|F(x^{(k)}) + V_{min}^{(k)}\Delta x^{(k)}\|_F \leq \min\{\eta, \|F(x^{(k)})\|_F\}\|F(x^{(k)})\|_F$$

*if  $V_{min}^{(k)}$  is nonsingular. If (25) is not achieved, or if the condition*

$$(26) \quad (\Delta x^{(k)})^T F(x^{(k)}) \leq -\min\{\eta, \|F(x^{(k)})\|_F\}(\Delta x^{(k)})^T \Delta x^{(k)}$$

*is not satisfied, or if  $V_{min}^{(k)}$  is singular, let*

$$\Delta x^{(k)} = -F(x^{(k)}).$$

**Step 2** (line search in the descent direction  $\Delta x^{(k)}$  of  $\theta(x)$  at  $x^{(k)}$ ). *Let  $s_k$  be the smallest nonnegative integer  $s$  such that*

$$\theta(x^{(k)} + \rho^s \Delta x^{(k)}) - \theta(x^{(k)}) \leq \delta \rho^s (\Delta x^{(k)})^T F(x^{(k)}).$$

*Set*

$$x^{(k+1)} := x^{(k)} + \rho^{s_k} \Delta x^{(k)}.$$

**Step 3.** *Replace  $k$  by  $k + 1$  and go to Step 1.*

In Algorithm 1, we choose the starting point  $x^{(0)}$  as the solution of the following simplified version of (2):

$$(27) \quad \begin{aligned} \min \quad & \frac{1}{2} \|M - T\|_F^2 \\ \text{s.t.} \quad & \mathcal{A}(M) = b. \end{aligned}$$

This simplified problem has been studied in [10]. As in section 2, by the dual approach, we know that the unique solution  $M^0$  to problem (27) is given by

$$(28) \quad M^0 = T + \mathcal{A}^*(x^{(0)}),$$



In the rest of this section, we report our numerical results for solving (1) by Algorithm 1. All the tests are implemented in MATLAB 7.0.1 running on a P4 PC with a 2.40GHz CPU. We also compare the performance of our method with that of the alternating projection method proposed in [10].

In our experiments, we tested the following two classes of problems.

*Example 1.* Let  $M$  be given by (6). Set

$$T := M + \tau R,$$

where  $R$  is a random  $n \times n$  real matrix with entries in  $[-1.0, 1.0]$  and  $\tau \in \mathbb{R}$  is a perturbed parameter. Here, we set  $t_{1,1} = 0.5 < 1$  to ensure that (4) holds. We report our numerical results for  $n = 500, 1000, 1500, 2000, 2500, 3000, 3500, 4000, 4500, 5000$ , and  $\tau = 0.1, 1.0, 10.0$ .

*Example 2.* The matrix  $T$  is generated randomly with entries uniformly distributed between  $-10.0$  and  $10.0$ , but we set  $t_{1,1} = 0.5 < 1$ . We give our numerical results for  $n = 500, 1000, 1500, 2000, 2500, 3000, 3500, 4000, 4500, 5000$ .

To demonstrate the performance of Algorithm 1, the linear systems (24) and (30) are solved with provision for lower (inexact) and higher (approximately exact) accuracy requirements.<sup>3</sup> To do this, in our numerical experiments we set the parameters used in our algorithm as either

- (a)  $\text{To1} = 10^{-6}$ ,  $\eta = 10^{-6}$ ,  $\rho = 0.5$ , and  $\delta = 10^{-4}$ , or
- (b)  $\text{To1} = 10^{-10}$ ,  $\eta = 10^{-15}$ ,  $\rho = 0.5$ , and  $\delta = 10^{-4}$ .

Here,  $\text{To1}$  is the required tolerance used in the stopping criterion defined by

$$\|\nabla\theta(x^{(k)})\|_F = \|F(x^{(k)})\|_F \leq \text{To1}.$$

Our numerical results are given in Tables 1–4, where Time, Iter., Res0., Res\*, and Err\* stand for the CPU times required for convergence, the number of iterations, the residuals  $\|\nabla\theta(\cdot)\|_F$  at the starting point  $x^{(0)}$  and the final iterate of Algorithm 1, and the error

$$\left\| \begin{bmatrix} M\mathbf{e} \\ M^T\mathbf{e} \\ \mathbf{e}_1^T M\mathbf{e}_1 \end{bmatrix} - \begin{bmatrix} \mathbf{e} \\ \mathbf{e} \\ \mathbf{e}_1^T T\mathbf{e}_1 \end{bmatrix} \right\|_F$$

at the computed solution  $M^*$ , respectively.

In our experiments, the quadratic convergence of Algorithm 1 is observed. From Tables 1–4, we note that if we solve the linear system (24) with a lower accuracy, it needs less CPU time, but we can obtain a coarser solution. Conversely, if we solve the linear system (24) with a higher accuracy, we can obtain a relatively more precise solution, but it needs relatively more CPU time. Finally, in our experiments, the largest numerical examples contain 25,000,000 unknowns in the primal problem (1) and 10,000 unknowns in the dual problem (3). This shows that Algorithm 1 is very efficient for large scale problems.

Next, we compare the performance of our Algorithm 1 with that of the alternating projection method in [10]. For the purpose of comparison, we set the stopping tolerance for both algorithms at

$$\left\| \begin{bmatrix} M\mathbf{e} \\ M^T\mathbf{e} \\ \mathbf{e}_1^T M\mathbf{e}_1 \end{bmatrix} - \begin{bmatrix} \mathbf{e} \\ \mathbf{e} \\ \mathbf{e}_1^T T\mathbf{e}_1 \end{bmatrix} \right\|_F \leq \text{To1}.$$

<sup>3</sup>As an anonymous referee pointed out, the linear system (30) can also be solved in linear time by using the direct methods exploiting the structure of the coefficient matrix of (30) [4, 5, 8, 18].

TABLE 1  
*Numerical results of Example 1(a).*

Tol = $10^{-6}$ , $\eta = 10^{-6}$ , $\rho = 0.5$ , and $\delta = 10^{-4}$						
$\tau$	$n$	Time	Iter.	Res0.	Res*.	Err*.
0.1	500	5.6 s	6	$3.9 \times 10^2$	$7.8 \times 10^{-8}$	$7.8 \times 10^{-8}$
	1,000	26.2 s	7	$1.1 \times 10^3$	$7.2 \times 10^{-13}$	$7.2 \times 10^{-13}$
	1,500	1 m 01 s	7	$2.0 \times 10^3$	$4.6 \times 10^{-12}$	$4.6 \times 10^{-12}$
	2,000	1 m 55 s	7	$3.1 \times 10^3$	$1.1 \times 10^{-7}$	$1.1 \times 10^{-7}$
	2,500	3 m 34 s	8	$4.4 \times 10^3$	$1.3 \times 10^{-13}$	$1.3 \times 10^{-13}$
	3,000	5 m 15 s	8	$5.8 \times 10^3$	$2.8 \times 10^{-13}$	$2.8 \times 10^{-13}$
	3,500	7 m 20 s	8	$7.3 \times 10^3$	$6.4 \times 10^{-13}$	$6.4 \times 10^{-13}$
	4,000	10 m 07 s	8	$8.9 \times 10^3$	$2.0 \times 10^{-12}$	$2.0 \times 10^{-12}$
	4,500	13 m 18 s	8	$1.1 \times 10^4$	$3.8 \times 10^{-12}$	$3.8 \times 10^{-12}$
5,000	16 m 52 s	9	$1.2 \times 10^4$	$1.2 \times 10^{-8}$	$1.2 \times 10^{-8}$	
1.0	500	8.5 s	8	$3.9 \times 10^3$	$1.3 \times 10^{-11}$	$1.3 \times 10^{-11}$
	1,000	37.3 s	9	$1.1 \times 10^4$	$8.0 \times 10^{-12}$	$8.0 \times 10^{-12}$
	1,500	1 m 27 s	9	$2.1 \times 10^4$	$8.3 \times 10^{-13}$	$8.3 \times 10^{-13}$
	2,000	2 m 39 s	9	$3.2 \times 10^4$	$2.7 \times 10^{-11}$	$2.7 \times 10^{-11}$
	2,500	4 m 15 s	9	$4.4 \times 10^4$	$2.0 \times 10^{-11}$	$2.0 \times 10^{-11}$
	3,000	6 m 16 s	9	$5.8 \times 10^4$	$9.3 \times 10^{-11}$	$9.3 \times 10^{-11}$
	3,500	8 m 50 s	9	$7.3 \times 10^4$	$8.5 \times 10^{-11}$	$8.5 \times 10^{-11}$
	4,000	11 m 52 s	9	$8.9 \times 10^4$	$4.4 \times 10^{-7}$	$4.4 \times 10^{-7}$
	4,500	17 m 16 s	10	$1.1 \times 10^5$	$1.5 \times 10^{-12}$	$1.5 \times 10^{-12}$
5,000	23 m 34 s	10	$1.2 \times 10^5$	$6.2 \times 10^{-12}$	$6.2 \times 10^{-12}$	
10.0	500	12.5 s	10	$3.9 \times 10^4$	$1.6 \times 10^{-11}$	$1.6 \times 10^{-11}$
	1,000	46.4 s	10	$1.1 \times 10^5$	$1.2 \times 10^{-10}$	$1.2 \times 10^{-10}$
	1,500	1 m 44 s	10	$2.1 \times 10^5$	$5.0 \times 10^{-10}$	$5.0 \times 10^{-10}$
	2,000	3 m 11 s	10	$3.2 \times 10^5$	$2.1 \times 10^{-9}$	$2.3 \times 10^{-9}$
	2,500	5 m 38 s	11	$4.4 \times 10^5$	$2.4 \times 10^{-12}$	$2.4 \times 10^{-12}$
	3,000	8 m 11 s	11	$5.8 \times 10^5$	$1.7 \times 10^{-12}$	$1.7 \times 10^{-12}$
	3,500	11 m 23 s	11	$7.3 \times 10^5$	$3.7 \times 10^{-11}$	$3.7 \times 10^{-11}$
	4,000	15 m 24 s	11	$8.9 \times 10^5$	$2.6 \times 10^{-11}$	$2.6 \times 10^{-11}$
	4,500	19 m 46 s	11	$1.1 \times 10^6$	$1.3 \times 10^{-9}$	$1.3 \times 10^{-9}$
5,000	27 m 14 s	11	$1.2 \times 10^6$	$2.5 \times 10^{-10}$	$2.5 \times 10^{-10}$	

Here, we choose Tol to be different values, e.g., Tol =  $10^{-6}, 10^{-10}$ , etc. Consequently, in Algorithm 1 (24) is solved with varying accuracies; see  $\eta = 10^{-6}, 10^{-15}$ , etc. The values of the remaining parameters used in Algorithm 1 are set as above. Tables 5–6 list the numerical results for Example 1 with varying  $n$ , Tol, and  $\eta$ , where Dist is the distance between  $T$  and the computed closest matrix  $M$  in the Frobenius norm. Here, we report the numerical results only for  $\tau = 0.1$  and  $n = 500, 1000, 1500, 2000, 2500, 3000$ , and  $3500$ , as the other cases behave similarly.

From Tables 5–6 we observe that Algorithm 1 is much more efficient than the alternating projection method in [10].

**4. Conclusions.** In this paper we proposed to solve the dual problem (3) by Algorithm 1 in order to obtain the solution of the nearest doubly stochastic matrix problem (1). Under the mild assumptions (4) and (20), we have shown that Algorithm 1 is quadratically convergent. We have also demonstrated its numerical performance by some examples.

In problem (1), only the (1, 1) entry of the matrix  $M$  is fixed to be identical to the given matrix  $T$ . This is an assumption without loss of generality, since the framework we establish in this paper can be easily applied to the nearest doubly stochastic matrix problem with  $k$  prescribed entries. In fact, consider the following problem:



TABLE 3  
Numerical results of Example 2(a).

Tol = 10 <sup>-6</sup> , η = 10 <sup>-6</sup> , ρ = 0.5, and δ = 10 <sup>-4</sup>					
n	Time	Iter.	Res0.	Res*.	Err*.
500	13.0 s	10	3.9 × 10 <sup>4</sup>	4.4 × 10 <sup>-11</sup>	4.4 × 10 <sup>-11</sup>
1,000	46.7 s	10	1.1 × 10 <sup>5</sup>	7.4 × 10 <sup>-11</sup>	7.4 × 10 <sup>-11</sup>
1,500	1 m 48 s	10	2.1 × 10 <sup>5</sup>	4.5 × 10 <sup>-10</sup>	4.5 × 10 <sup>-10</sup>
2,000	3 m 19 s	10	3.2 × 10 <sup>5</sup>	7.1 × 10 <sup>-10</sup>	7.1 × 10 <sup>-10</sup>
2,500	5 m 20 s	10	4.4 × 10 <sup>5</sup>	2.2 × 10 <sup>-9</sup>	2.2 × 10 <sup>-9</sup>
3,000	8 m 39 s	10	5.8 × 10 <sup>5</sup>	2.1 × 10 <sup>-11</sup>	2.1 × 10 <sup>-11</sup>
3,500	12 m 06 s	11	7.3 × 10 <sup>5</sup>	3.9 × 10 <sup>-11</sup>	3.9 × 10 <sup>-11</sup>
4,000	15 m 54 s	11	8.9 × 10 <sup>5</sup>	8.0 × 10 <sup>-11</sup>	8.0 × 10 <sup>-11</sup>
4,500	21 m 15 s	11	1.1 × 10 <sup>6</sup>	5.0 × 10 <sup>-11</sup>	5.0 × 10 <sup>-11</sup>
5,000	27 m 12 s	11	1.2 × 10 <sup>6</sup>	1.1 × 10 <sup>-10</sup>	1.1 × 10 <sup>-10</sup>

TABLE 4  
Numerical results of Example 2(b).

Tol = 10 <sup>-10</sup> , η = 10 <sup>-15</sup> , ρ = 0.5, and δ = 10 <sup>-4</sup>					
n	Time	Iter.	Res0.	Res*.	Err*.
500	29.7 s	9	3.9 × 10 <sup>4</sup>	3.9 × 10 <sup>-12</sup>	3.9 × 10 <sup>-12</sup>
1,000	2 m 03 s	10	1.1 × 10 <sup>5</sup>	3.2 × 10 <sup>-13</sup>	3.2 × 10 <sup>-13</sup>
1,500	4 m 25 s	10	2.1 × 10 <sup>5</sup>	7.8 × 10 <sup>-13</sup>	7.8 × 10 <sup>-13</sup>
2,000	8 m 22 s	11	3.2 × 10 <sup>5</sup>	6.0 × 10 <sup>-13</sup>	6.0 × 10 <sup>-13</sup>
2,500	14 m 26 s	11	4.4 × 10 <sup>5</sup>	7.5 × 10 <sup>-13</sup>	7.5 × 10 <sup>-13</sup>
3,000	19 m 57 s	11	5.8 × 10 <sup>5</sup>	9.2 × 10 <sup>-13</sup>	9.2 × 10 <sup>-13</sup>
3,500	26 m 45 s	11	7.3 × 10 <sup>5</sup>	1.0 × 10 <sup>-12</sup>	1.0 × 10 <sup>-12</sup>
4,000	33 m 12 s	11	8.9 × 10 <sup>5</sup>	1.2 × 10 <sup>-12</sup>	1.2 × 10 <sup>-12</sup>
4,500	49 m 47 s	12	1.1 × 10 <sup>6</sup>	1.4 × 10 <sup>-12</sup>	1.4 × 10 <sup>-12</sup>
5,000	56 m 41 s	11	1.2 × 10 <sup>6</sup>	1.5 × 10 <sup>-12</sup>	1.5 × 10 <sup>-12</sup>

$$f(M) := \frac{1}{2} \|M - T\|_F^2, \quad \mathcal{B}(M) := \begin{bmatrix} Me \\ [I_{n-1} \ 0] M^T e \\ e_{i_1}^T M e_{j_1} \\ \vdots \\ e_{i_k}^T M e_{j_k} \end{bmatrix}, \quad c := \begin{bmatrix} e \\ [I_{n-1} \ 0] e \\ e_{i_1}^T T e_{j_1} \\ \vdots \\ e_{i_k}^T T e_{j_k} \end{bmatrix};$$

then problem (31) is equivalent to

$$(32) \quad \begin{cases} \min & f(M) \\ \text{s.t.} & \mathcal{B}(M) = c, \\ & M \in \mathcal{K}. \end{cases}$$

The dual problem of (32) is

$$(33) \quad \begin{cases} \sup & -\theta(x) \\ \text{s.t.} & x \in \mathbb{R}^{2n+k-1}, \end{cases}$$

where

$$\theta(x) = \frac{1}{2} \|\Pi_{\mathcal{K}}(T + \mathcal{B}^*(x))\|_F^2 - x^T c - \frac{1}{2} \|T\|_F^2,$$

and  $\mathcal{B}^*$  is the adjoint of  $\mathcal{B}$ . Hence, we can extend the results that we derived for problem (1) to problem (31) and apply a Newton-type method to solve the dual problem (33) and then obtain the desired solution of the problem (31).

TABLE 5  
*Numerical results of Example 1(a).*

Tol = $10^{-6}$				
	$n$	Time	Iter.	Dist
Algorithm 1	500	6.7 s	6	28.028746
	1,000	26.2 s	7	56.855379
	1,500	1 m 05 s	7	85.690588
	2,000	2 m 01 s	7	114.556635
	2,500	3 m 08 s	7	143.421146
	3,000	5 m 16 s	8	172.273970
	3,500	7 m 24 s	8	201.138311
Algorithm 1	500	7.0 s	6	28.028746
	1,000	31.7 s	7	56.855379
	1,500	1 m 17 s	7	85.690588
	2,000	2 m 25 s	7	114.556635
	2,500	3 m 42 s	7	143.421146
	3,000	6 m 21 s	8	172.273970
	3,500	8 m 40 s	8	201.138311
Algorithm 1	500	8.6 s	6	28.028746
	1,000	39.0 s	7	56.855379
	1,500	1 m 32 s	7	85.690588
	2,000	2 m 51 s	7	114.556635
	2,500	4 m 16 s	7	143.421146
	3,000	7 m 22 s	8	172.273970
	3,500	10 m 10 s	8	201.138311
Method in [10]	500	21.1 s	181	28.028746
	1,000	2 m 53 s	263	56.855379
	1,500	10 m 51 s	321	85.690588
	2,000	25 m 55 s	371	114.556635
	2,500	53 m 19 s	417	143.421146
	3,000	1 h 59 m 01 s	457	172.273970
	3,500	2 h 58 m 54 s	495	201.138311

TABLE 6  
*Numerical results of Example 1(b).*

Tol = $10^{-10}$				
	$n$	Time	Iter.	Dist
Algorithm 1	500	7.3 s	6	28.0045624140
	1,000	33.6 s	7	56.8449830344
	1,500	1 m 18 s	7	85.6644919002
	2,000	2 m 47 s	8	114.5446535050
	2,500	4 m 27 s	8	143.4251826139
	3,000	6 m 31 s	8	172.3135425545
	3,500	9 m 08 s	8	201.0862903056
Algorithm 1	500	9.0 s	6	28.0045624140
	1,000	40.9 s	7	56.8449830344
	1,500	1 m 35 s	7	85.6644919002
	2,000	3 m 17 s	8	114.5446535050
	2,500	5 m 13 s	8	143.4251826139
	3,000	7 m 32 s	8	172.3135425545
	3,500	10 m 16 s	8	201.0862903056
Method in [10]	500	35.1 s	294	28.0045624140
	1,000	4 m 36 s	413	56.8449830344
	1,500	16 m 10 s	503	85.6644919002
	2,000	40 m 01 s	581	114.5446535050
	2,500	1 h 30 m 24 s	643	143.4251826139
	3,000	2 h 47 m 51 s	709	172.3135425545
	3,500	4 h 20 m 10 s	770	201.0862903056

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