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On uniqueness, analyticity, and first- and second-order derivatives of Sinkhorn-type DAD scalings

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ABSTRACT

We call a real square matrix A scalable if there is a diagonal matrix D with positive diagonal entries such that all row sums of DAD are equal to 1. In this case, D is called a scaling for A. For an entrywise nonnegative A, this means that DAD is a stochastic matrix. We prove that such a nonnegative A has a unique scaling if and only if it has a scaling D such that -1 is not an eigenvalue of DAD. If, on the contrary, a nonnegative A has multiple scalings, then we show that it already has infinitely many scalings. Furthermore, we prove that the function which maps a uniquely scalable, nonnegative matrix A to the diagonal vector $x = x(A)$ of its scaling, which we call the Sinkhorn vector of A, is a real analytic function. Finally, we give explicit, index-free formulas for the Jacobian and Hessian matrices of x with respect to the entries of A. In particular, we prove that $\frac{\partial x_i}{\partial A_{i,j}} \leq -\frac{1}{2}x_i^2 x_j < 0$ for all $i, j \in \{1, \ldots, n\}$ where n is the order of A.

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1. Introduction

In 1966, Sinkhorn [11] constructively proved that for every entrywise positive square matrix A there is a unique diagonal matrix D with positive diagonal such that DAD is stochastic, i.e., all row-sums of DAD are equal to 1. Also in 1966, Brualdi, Parter, and Schneider [1] proved the same for an even larger class of entrywise nonnegative square matrices. From these articles, a rich amount of research on diagonal scalings originated. We refer to the research article [7] of Johnson and Reams and the survey article [9] of Idel for more background information on this topic. Recently, Sinkhorn's DAD scaling also emerged in physical chemistry and chemical engineering applications, appearing in the so-called self-consistency equation in conductor-like screening models (COSMO), see [2] and the references therein. These applications caused this research.

For $m, n \in \mathbb{N} := \{1, 2, \dots\}$, the sets of real, entrywise nonnegative, and entrywise positive m-by-n matrices are denoted by $\mathbb{R}^{m\times n}$, $\mathbb{R}^{m\times n}_{\geq 0}$, and $\mathbb{R}^{m\times n}_{>0}$, respectively. If $n = 1$, then $\mathbb{R}^m$, $\mathbb{R}^m_{\geq 0}$, and $\mathbb{R}^m_{>0}$ denote the corresponding sets of column vectors of length m. The n-by-n identity matrix is denoted by I_n or just I if the dimension n is clear from the context. A matrix $A \in \mathbb{R}^{n\times n}$ is called *scalable* if there is a diagonal matrix $D = \operatorname{diag}(x)$ with entrywise positive diagonal vector $x \in \mathbb{R}^n_{>0}$ such that all row sums of DAD are equal to 1. In this case, D is called a *scaling* for A. For entrywise nonnegative A, this means that DAD is stochastic. Denoting the all-ones column vector of length n by $\mathbf{1} = \mathbf{1}_n$, we have $DAD\mathbf{1} = \mathbf{1}$. Another equivalent formulation is $Ax = x^{-1}$ whereby $x^{-1} := (x_1^{-1}, \dots, x_n^{-1})^\top$ is the entrywise inverse of x. It is convenient to identify the diagonal matrix D with its diagonal vector x, wherefore we also say that x is a scaling for A. For a better distinction, we also call x a *Sinkhorn vector* of A. The set of all Sinkhorn vectors of A is denoted by $\mathfrak{X}(A)$. Furthermore, we say that $A \in \mathbb{R}^{n\times n}$ is *uniquely scalable* if A has exactly one Sinkhorn vector. For column vectors $u \in \mathbb{R}^m$ and $v \in \mathbb{R}^n$, their stacking is denoted by $[u; v] := (u^\top, v^\top)^\top \in \mathbb{R}^{m+n}$. For $a, b, c, d \in \mathbb{N}$, $X \in \mathbb{R}^{a\times b}$, and $Y \in \mathbb{R}^{c\times d}$, the Kronecker product of X and Y is as usual defined by $X \otimes Y = (X_{i,j}Y) \in \mathbb{R}^{(ac)\times(bd)}$. If $a = c$ and $b = d$, then the Hadamard (or entrywise) product of X and Y is defined by $X \circ Y = (X_{i,j}Y_{i,j}) \in \mathbb{R}^{a\times b}$, and, if all entries of Y are nonzero, then $X/Y := (X_{i,j}/Y_{i,j}) \in \mathbb{R}^{a\times b}$ denotes the entrywise quotient of X and Y. Our main results are:

Theorem 1. *Suppose $A \in \mathbb{R}^{n\times n}$ has a scaling $D = \operatorname{diag}(x)$ such that -1 is not an eigenvalue of DAD. Then, there are open neighborhoods $\mathscr{U}$ of A and $\mathscr{V} \subseteq \mathbb{R}^n_{>0}$ of x, and a unique real analytic function $\xi : \mathscr{U} \to \mathscr{V}$ such that:*

(a) *$\xi(B)$ is a Sinkhorn vector of B for all $B \in \mathscr{U}$.*
(b) *If $y \in \mathscr{V}$ is a Sinkhorn vector of some $B \in \mathscr{U}$, then $y = \xi(B)$.*
(c) *For all $B \in \mathscr{U}$, $y := \xi(B)$, and $E := \operatorname{diag}(y)$, the matrix $I + EBE$ is regular, and the Jacobian matrix of ξ at B can be written as $J_\xi(B) = -E(I + EBE)^{-1}(E \otimes y^\top)$.*

Theorem 2. *Let $\mathscr{S}$ be the set of uniquely scalable nonnegative n-by-n matrices and let $A \in \mathbb{R}^{n\times n}_{\geq 0}$ be scalable.*

(a) *$s(A) := \dim\ker(I + DAD)$ is independent of a chosen scaling D for A and called Sinkhorn index of A. If $s(A) > 0$, then it is the geometric as well as the algebraic multiplicity of the eigenvalue -1 of DAD.*
(b) *$A \in \mathscr{S}$ if and only if $s(A) = 0$.*
(c) *$\mathscr{S}$ is relatively open in $\mathbb{R}^{n\times n}_{\geq 0}$.*
(d) *The function $x : \mathscr{S} \to \mathbb{R}^n_{>0}$ mapping $A \in \mathscr{S}$ to its unique Sinkhorn vector $x = x(A)$ is real analytic. In particular, the Jacobian matrix of x at A can be written as $J_x(A) = -D(I + DAD)^{-1}(D \otimes x(A)^\top)$ with $D := \operatorname{diag}(x(A))$. Moreover, it holds that $\frac{\partial x_i}{\partial A_{i,j}} \leq -\frac{1}{2}x_i^2 x_j < 0$ for all $i, j \in \{1, \ldots, n\}$.*

Theorem 3. *Let $\mathscr{N}$ be the set of multiply scalable nonnegative n-by-n matrices and let $A \in \mathbb{R}^{n\times n}_{\geq 0}$ be scalable.*

(a) *$A \in \mathscr{N}$ if and only if $s(A) > 0$.*
(b) *If $A \in \mathscr{N}$, then $s := s(A) > 0$ is maximum subject to existence of a permutation matrix P such that*

$$P^\top AP = \begin{pmatrix} \begin{smallmatrix} 0 & B_1 \\ C_1 & 0 \end{smallmatrix} & & & \\ & \ddots & & \\ & & \begin{smallmatrix} 0 & B_s \\ C_s & 0 \end{smallmatrix} & \\ * \quad * & * & * \quad * & Z \end{pmatrix} \tag{1}$$

where $B_i \in \mathbb{R}^{m_i\times n_i}_{\geq 0}$, $C_i \in \mathbb{R}^{n_i\times m_i}_{\geq 0}$, $\left(\begin{smallmatrix} 0 & B_i \\ C_i & 0 \end{smallmatrix}\right)$ is nonempty and irreducible for $i = 1, \ldots, s$, and $Z \in \mathbb{R}^{\ell\times\ell}_{\geq 0}$, $\ell \geq 0$.

For every such representation (1) and every scaling $D = \operatorname{diag}(x)$ for A, there are open neighborhoods $\mathscr{U} \subseteq \mathbb{R}^s_{>0}$ of $\mathbf{1}_s$ and $\mathscr{V} \subseteq \mathbb{R}^n_{>0}$ of x such that

$$\gamma : \mathscr{U} \to \mathscr{V}, \quad t = (t_1, \ldots, t_s) \mapsto DP\left[t_1\mathbf{1}_{m_1}; t_1^{-1}\mathbf{1}_{n_1}; \ldots; t_s\mathbf{1}_{m_s}; t_s^{-1}\mathbf{1}_{n_s}; \zeta(t)\right] \tag{2}$$

is an injective, real analytic parametrization of $\mathfrak{X}(A) \cap \mathscr{V} = \gamma(\mathscr{U})$ with $\gamma(\mathbf{1}_s) = x$. If $\ell = 0$, $\zeta(t)$ in (2) vanishes and we can take $\mathscr{U} = \mathbb{R}^s_{>0}$ and $\mathscr{V} = \mathbb{R}^n_{>0}$ so that $\mathfrak{X}(A) = \gamma(\mathbb{R}^s_{>0})$. Otherwise, $\zeta : \mathscr{U} \to \mathscr{W}$ is a uniquely determined real analytic function with $\zeta(\mathbf{1}_s) = \mathbf{1}_\ell$ where $\mathscr{W} \subseteq \mathbb{R}^\ell_{>0}$ is an open neighborhood of $\mathbf{1}_\ell$.
(c) *If $A \in \mathscr{N}$, then A has infinitely many scalings.*
(d) *If $A \in \mathscr{N}$ and if Z in (1) is empty, then $DAD = \widetilde{D}A\widetilde{D}$ for all scalings D and $\widetilde{D}$ for A.*

Before we proceed, some remarks are in order. First, Theorem 1 is proved by using the analytic implicit function theorem. Theorem 1 says that for a scalable matrix A and one of its possibly many scalings x, all matrices B close to A are scalable as well and have scalings $\xi(B)$ close to x, provided that $I + DAD$ is regular where $D = \operatorname{diag}(x)$. Moreover, this correspondence $B \mapsto \xi(B)$ is, in the vicinity of A, a uniquely determined real analytic function w.r.t. the entries of B. In this spirit, the derivatives of ξ at A can be considered as the derivatives of the specific Sinkhorn vector x of A. Determining the greatest possible domain $\mathscr{U}$ of ξ seems to be a difficult task beyond reach. However, using a recent general result by Jindal, Chatterjee, and Banavar [6] on estimating the size of the domain of an implicitly given function, a radius of a ball in $\mathscr{U}$ centered at A can be quantified, see Remark 4.

Second, Theorem 2 and Theorem 3 restrict to nonnegative scalable matrices. In particular, it turns out that such matrices are either uniquely scalable or possess infinitely many scalings. Thus, there are no nonnegative matrices having multiple but only finitely many scalings. For arbitrary scalable matrices, this does not hold true. For example, Johnson and Reams [7, pp. 129-130] construct symmetric 3-by-3 matrices with some negative entries which have multiple but finitely many scalings.

Third, the distinction between unique and nonunique scalability of nonnegative matrices is decided by whether or not $I + DAD$ is regular for some scaling D for A. In the regular case, D is indeed the only scaling for A. The difficult parts of Theorem 2 are (a) and (b). Items (c) and (d) mainly follow from Theorem 1. However, some caution in the interpretation of analyticity in boundary points of the domain $\mathscr{S}$ of the function x in (d) is necessary. These boundary points are exactly those $A \in \mathscr{S}$ which have some zero entries. By (c), there is an open neighborhood $\mathscr{U}$ of A such that $\mathscr{U} \cap \mathbb{R}^{n\times n}_{\geq 0} \subseteq \mathscr{S}$. In the first place, x is only defined on this relatively open neighborhood of A. But, by Theorem 1, $\mathscr{U}$ can be chosen such that x uniquely extends to a real analytic function ξ on all of $\mathscr{U}$. Analyticity of x in boundary points is meant this way.

Fourth, the final assertion $\frac{\partial x_i}{\partial A_{i,j}} < 0$ in Theorem 2 (d) means that the ith component x_i of the Sinkhorn vector x of A is a decreasing function w.r.t. each entry $A_{i,j}$.

Fifth, in Theorem 3 (b) the representation (1) is unique up to permutation of the irreducible blocks $\left(\begin{smallmatrix} 0 & B_i \\ C_i & 0 \end{smallmatrix}\right)$, permutation within these blocks, and permutation within the lower right diagonal block Z. This follows from basic facts on the normal form of reducible matrices, see [4], Ch. XIII, § 4.

Sixth, without going into details, Theorem 3 (b) can be phrased such that the set $\mathfrak{X}(A)$ of all Sinkhorn vectors of $A \in \mathscr{N}$ is an s-dimensional analytic submanifold of $\mathbb{R}^n_{>0}$ where s is the Sinkhorn index of A, i.e., the dimension of the eigenspace corresponding to the eigenvalue -1 of DAD for an arbitrary scaling D for A. The inverse of the parameterization γ defined in (2), namely $\gamma^{-1} : \mathfrak{X}(A) \cap \mathscr{V} \to \mathscr{U}$, can be taken as a chart at a point $x \in \mathfrak{X}(A)$.

The article is organized as follows. The next and main section contains the proofs of the theorems. In this regard, several additional results are stated which may be of particular interest on their own. In Section 3 we derive, in addition to the formula for the Jacobian matrix $J_x(A)$ in Theorem 2 (d), a compact, index-free formula for the Hessian matrix $H_x(A)$ of the Sinkhorn vector x w.r.t. the matrix entries of A. A short

MATLAB program computing $J_x(A)$ and $H_x(A)$ efficiently is provided in Listing 1. This is finally used in Listing 2 to calculate a second-order Taylor expansion of the Sinkhorn vector x around A.

2. Proofs

Let $g : \mathbb{R}^{n\times n} \to \mathbb{R}^n,\ M \mapsto (g_1(M),\ldots,g_n(M))^\top$ be a continuously differentiable function. Then, for $A \in \mathbb{R}^{n\times n}$, the Jacobian matrix of g evaluated at A is denoted by

$$\frac{\partial g}{\partial M}(A) := \left(\frac{\partial g_i}{\partial M_{k,\ell}}(A)\right)_{1\le i,k,\ell\le n} \in \mathbb{R}^{n\times n^2}\ .$$

To avoid three-dimensional tensors, $\frac{\partial g}{\partial M}(A)$ is regarded as an n-by-n^2 matrix. This is done by flattening pair indices (k,ℓ) to singleton indices $j := (k-1)n+\ell$:

$$\left(\frac{\partial g}{\partial M}\right)_{i,(k-1)n+\ell} := \frac{\partial g_i}{\partial M_{k,\ell}}\ . \tag{3}$$

Proof of Theorem 1. The function

$$f : \mathbb{R}^{n\times n}\times\mathbb{R}^n \to \mathbb{R}^n,\ (M,v)\mapsto v\circ(Mv)-\mathbf{1} = \left(v_i\sum_{j=1}^n M_{i,j}v_j - 1\right)_{1\le i\le n}$$

is real analytic, hence infinitely often differentiable. For $i,k,\ell\in\{1,\ldots,n\}$, we have

$$\frac{\partial f_i}{\partial M_{k,\ell}}(N,w) = \delta_{i,k}w_i w_\ell \qquad \text{and} \qquad \frac{\partial f_i}{\partial v_k}(N,w) = \delta_{i,k}(Nw)_i + w_i N_{i,k}$$

whereby δ is the Kronecker delta function on $\mathbb{N}$, i.e., $\delta_{i,j}=1$ if $i=j$ and $\delta_{i,j}=0$ if $i\ne j$ for $i,j\in\mathbb{N}$. Hence, the Jacobian matrices $\frac{\partial f}{\partial M}$ and $\frac{\partial f}{\partial v}$ of f w.r.t. M and v evaluated at (N,w) read

$$\frac{\partial f}{\partial M}(N,w) := \left(\frac{\partial f_i}{\partial M_{k,\ell}}(N,w)\right)_{1\le i,k,\ell\le n} = \operatorname{diag}(w)\otimes w^\top \tag{4}$$

$$\frac{\partial f}{\partial v}(N,w) := \left(\frac{\partial f_i}{\partial v_k}(N,w)\right)_{1\le i,k\le n} = \operatorname{diag}(Nw)+\operatorname{diag}(w)N. \tag{5}$$

Here, the flattening (3) is used in (4). For $N := A$ and $w := x$, using $Ax = x^{-1}$, equation (5) becomes

$$\frac{\partial f}{\partial v}(A,x) = D^{-1}+DA = (I+DAD)D^{-1}\ . \tag{6}$$

By assumption, -1 is not an eigenvalue of DAD. Thus, $I + DAD$ is invertible and $\frac{\partial f}{\partial v}(A, x)$ is invertible too. Hence, as f is analytic, the analytic implicit function theorem [3, Sec. X.2] supplies open neighborhoods $\mathscr{U}$ of A, $\mathscr{V} \subseteq \mathbb{R}^n_{>0}$ of $x \in \mathbb{R}^n_{>0}$, and a uniquely determined real analytic function $\xi : \mathscr{U} \to \mathscr{V}$ such that $\xi(A) = x$ and $f(B, \xi(B)) = 0$ for all $B \in \mathscr{U}$. Moreover, if $B \in \mathscr{U}$ and $y \in \mathscr{V}$ fulfill $f(B, y) = 0$, then $y = \xi(B)$. Note that $0 = f(B, \xi(B)) = \xi(B) \circ (B\xi(B)) - \mathbf{1}$ and $\xi(B) \in \mathscr{V} \subseteq \mathbb{R}^n_{>0}$ for $B \in \mathscr{U}$ imply $B\xi(B) = [\xi(B)]^{-1}$ so that $\xi(B)$ is a Sinkhorn vector of B. Furthermore, for $y := \xi(B)$ and $E := \operatorname{diag}(y)$, the implicit function theorem also supplies that the Jacobian of ξ at B reads

$$J_\xi(B) := \frac{\partial \xi}{\partial M}(B) = -\left[\frac{\partial f}{\partial v}(B, y)\right]^{-1} \frac{\partial f}{\partial M}(B, y) = -E(I + EBE)^{-1}(E \otimes y^\top) \ .$$

In particular, $I + EBE$ is regular. $\square$

As stated in the introduction, we will now apply a general result by Jindal, Chatterjee, and Banavar [6, Th. 3.3] on the size of the domain of an implicitly given function in order to quantify a radius of a ball centered at A that is contained in the domain $\mathscr{U}$ of the function ξ in Theorem 1. Although this finding will not be used later on, we considered such a quantitative statement as possibly helpful in view of applications. Recall the *maximum norm* $\|x\|_\infty := \max_{1 \le i \le n} |x_i|$ of a vector $x \in \mathbb{R}^n$ and its induced matrix norm $\|X\|_\infty := \max_{1 \le i \le m} \sum_{j=1}^n |X_{i,j}|$ of a matrix $X \in \mathbb{R}^{m \times n}$. We choose the maximum norm for ease of presentation. Other vector norms and induced matrix norms can be considered likewise. For $r > 0$, let $\mathscr{B}(x, r) := \{y \in \mathbb{R}^n \mid \|x - y\|_\infty < r\}$ and $\mathscr{B}(X, r) := \{Y \in \mathbb{R}^{m \times n} \mid \|X - Y\|_\infty < r\}$ denote the open balls around x and A with radius r w.r.t. the maximum norm.

Remark 4. Using the notation of Theorem 1, for given $R_1, R_2 > 0$, define the constants $\kappa_1 := 2(\|x\|_\infty + R_2)$, $\kappa_2 := 2(\|A\|_\infty + R_1)$, $\lambda_1 := \|x\|_\infty^2$, and $\lambda_2 := \|D(I + DAD)^{-1}\|_\infty$. Then, for all $0 < r_1 < R_1$ and $0 < r_2 < R_2$ satisfying

$$\kappa_1 r_1 r_2 + \frac{1}{2}\kappa_2 r_2^2 < \frac{r_2}{\lambda_2} - r_1 \lambda_1 \quad \text{and} \quad \kappa_1 r_1 + \kappa_2 r_2 < \frac{1}{\lambda_2} \ , \tag{7}$$

the sets $\mathscr{U}$ and $\mathscr{V}$ in Theorem 1 can be chosen such that

$$\mathscr{B}(A, r_1) \subseteq \mathscr{U} \quad \text{and} \quad \xi(\mathscr{B}(A, r_1)) \subseteq \mathscr{B}(x, r_2) \cap \mathbb{R}^n_{>0} \subseteq \mathscr{V} \ .$$

Proof. By (4), we have $\frac{\partial f}{\partial M}(N, w)(\tilde{N}) = \operatorname{diag}(w)\tilde{N}w$ for $\tilde{N} \in \mathbb{R}^{n \times n}$ and hence

$$\begin{aligned} L_1 := \left\|\frac{\partial f}{\partial M}(A, x)\right\|_\infty &= \sup\left\{\left\|\operatorname{diag}(x)\tilde{N}x\right\|_\infty \mid \tilde{N} \in \mathbb{R}^{n \times n}, \|\tilde{N}\|_\infty = 1\right\} \\ &\le \|\operatorname{diag}(x)\|_\infty \|x\|_\infty = \|x\|_\infty^2 = \lambda_1 \ . \end{aligned} \tag{8}$$

By (6), we also have

$$L_2 := \left\| \left[\frac{\partial f}{\partial v}(A, x) \right]^{-1} \right\|_\infty = \|D(I + DAD)^{-1}\|_\infty = \lambda_2 \ . \tag{9}$$

Differentiating (4) and (5) yields the second-order derivatives

$$\frac{\partial^2 f}{\partial M^2} \equiv 0 \ , \quad \frac{\partial^2 f}{\partial M \partial v}(N, w)(\tilde{N}, \tilde{w}) = (\mathrm{diag}(\tilde{N} w) + \mathrm{diag}(w)\tilde{N})\tilde{w} \ ,$$
$$\frac{\partial^2 f}{\partial v^2}(N, w)(\tilde{w}, \hat{w}) = (\mathrm{diag}(N\tilde{w}) + \mathrm{diag}(\tilde{w})N)\hat{w}$$

with $\tilde{w}, \hat{w} \in \mathbb{R}^n$. This implies the following bounds on the corresponding operator norms:

$$\begin{aligned} K_{1,1} &:= \sup \left\{ \left\| \frac{\partial^2 f}{\partial M^2}(N, w) \right\|_\infty \mid (N, w) \in \mathscr{B}(A, R_1) \times \mathscr{B}(x, R_2) \right\} = 0 \\ K_{1,2} &:= \sup \left\{ \left\| \frac{\partial^2 f}{\partial M \partial v}(N, w) \right\|_\infty \mid (N, w) \in \mathscr{B}(A, R_1) \times \mathscr{B}(x, R_2) \right\} \\ &\leq 2\|w\|_\infty \leq 2(\|x\|_\infty + R_2) = \kappa_1 \qquad (10) \\ K_{2,2} &:= \sup \left\{ \left\| \frac{\partial^2 f}{\partial v^2}(N, w) \right\|_\infty \mid (N, w) \in \mathscr{B}(A, R_1) \times \mathscr{B}(x, R_2) \right\} \\ &\leq 2\|N\|_\infty \leq 2(\|A\|_\infty + R_1) = \kappa_2 \ . \qquad (11) \end{aligned}$$

Inserting (8), (9), (10), (11) into both inequalities in (7) implies

$$\frac{1}{2} K_{1,1} r_1^2 + K_{1,2} r_1 r_2 + \frac{1}{2} K_{2,2} r_2^2 < \frac{r_2}{L_2} - r_1 L_1 \quad \text{and} \quad K_{1,2} r_1 + K_{2,2} r_2 < \frac{1}{L_2} \ .$$

These are inequalities (3.1a) and (3.1b) in Theorem 3.3 of [6], yielding the assertion. □

The following lemmas prepare Theorem 2 and Theorem 3. Recall that an n-by-n matrix A is *reducible* if there is a permutation matrix P such that $P^\top A P = \begin{pmatrix} * & 0_{r,n-r} \\ * & * \end{pmatrix}$ for some $r \in \{1, \ldots, n-1\}$. If A is not reducible, then A is called *irreducible*. In particular, all 1-by-1 matrices are irreducible.

Lemma 5. *Let $A \in \mathbb{R}^{n \times n}_{\geq 0}$ be irreducible and suppose $\|A\|_\infty$ is an eigenvalue of A, then $A\mathbf{1} = \|A\|_\infty \mathbf{1}$, i.e., all row sums of A are equal and the all-ones vector is the Perron vector of A with Perron root $\|A\|_\infty$.*

Proof. By Gershgorin's theorem [5, Th. 6.1.1], $\|A\|_\infty$ is contained in some Gershgorin disc of A. Clearly, $\|A\|_\infty$ cannot lie in the interior of any such disc wherefore it must necessarily lie on the boundary of the union of all Gershgorin discs. Since A is irreducible, Tausky's theorem [5, Th. 6.2.26] yields that $\|A\|_\infty$ lies on the boundary of every Gershgorin disc. Hence, $\sum_{j=1}^n A_{i,j} = \|A\|_\infty$ for $i = 1, \ldots, n$, i.e., $A\mathbf{1} = \|A\|_\infty \mathbf{1}$. □

Matrices $X, Y \in \mathbb{R}^{n\times n}$ are called *permutationally similar* if $Y = P^\top XP$ for some permutation matrix P.

Lemma 6. *Let $A \in \mathbb{R}^{n\times n}_{\geq 0}$ with $\|A\|_\infty \leq 1$.*

(a) *If A is stochastic and permutationally similar to*

$$\tilde{A} := \begin{pmatrix} 0 & B \\ C & 0 \end{pmatrix} \tag{12}$$

where the diagonal blocks are square and nonempty, then A has an eigenvalue -1.

(b) *If A is irreducible and has an eigenvalue -1, then A is stochastic and permutationally similar to an $\tilde{A}$ as in (12) and -1 is an algebraically simple eigenvalue.*

(c) *If A is irreducible, then -1 is an eigenvalue of A if and only if A is stochastic and permutationally similar to a matrix $\tilde{A}$ as in (12). In this case, -1 is an algebraically simple eigenvalue.*

(d) *If A is irreducible, stochastic, and has form (12), then $\mathfrak{X}(A) = \{[t\mathbf{1}_m; t^{-1}\mathbf{1}_\ell] \mid t > 0\}$ where m and ℓ are the orders of the zero diagonal blocks of A. In particular, we have $DAD = \widetilde{D}A\widetilde{D}$ for all scalings $D, \widetilde{D}$ for A.*

Proof. The assertion is trivial for $n = 1$. Thus, we can assume $n \geq 2$.
(a). Suppose that A is stochastic and permutationally similar to a matrix $\tilde{A}$ as in (12). Let $m \in \{1, \dots, n-1\}$ such that B is an m-by-$(n-m)$ and C an $(n-m)$-by-m block. Since all row sums of B and C are equal to 1, the column vector $x := [\mathbf{1}_m; -\mathbf{1}_{n-m}]$ fulfills $\tilde{A}x = [-B\mathbf{1}_{n-m}; C\mathbf{1}_m] = [-\mathbf{1}_m; \mathbf{1}_{n-m}] = -x$ so that -1 is an eigenvalue of $\tilde{A}$ and hence of A.
(b). Suppose that A is irreducible and has an eigenvalue -1. Since the spectral radius $\rho(A)$ fulfills $\rho(A) \leq \|A\|_\infty$ for any square matrix A, we have $1 \leq \rho(A) \leq \|A\|_\infty \leq 1$ so that $\rho(A) = \|A\|_\infty = 1$. Hence, $\|A\|_\infty$ is the Perron root of A and Lemma 5 yields $A\mathbf{1} = \mathbf{1}$, i.e., A is stochastic. Frobenius' theorem [5, Cor. 8.4.6] says that if A has k distinct eigenvalues of maximum modulus $\rho(A) = 1$, then these are the kth roots of unity $e^{2\pi\sqrt{-1}\, j/k}$, $j = 0, \dots, k-1$, and all these eigenvalues are algebraically simple. The number k is the *index of imprimitivity* of A. Since -1 is one of those eigenvalues, k must be even. By [10, Th. 1], A is permutationally similar to a matrix as in (12).
(c). This follows from (a) and (b).
(d). For $t > 0$, set $x_t := [t\mathbf{1}_m; t^{-1}\mathbf{1}_\ell]$ and $D_t := \operatorname{diag}(x_t)$. Then,

$$D_tAD_t = \begin{pmatrix} 0 & tBt^{-1} \\ t^{-1}Ct & 0 \end{pmatrix} = A.$$

Since A is stochastic, D_t is a scaling for A so that $x_t \in \mathfrak{X}(A)$. For the converse inclusion, let $x \in \mathfrak{X}(A)$. We must show that $x = x_t$ for some $t > 0$. This follows along the lines of the proof of [1, Lem. 8.1] which we adapt to our needs. Set $u := (x_1, \dots, x_m)^\top$ and

$v := (x_{m+1}, \dots, x_n)^\top$ so that $x = [u; v]$. Since x is a Sinkhorn vector of A, it holds that $\mathbf{1}_n = x \circ Ax = [u; v] \circ [Bv; Cu] = [u \circ Bv; v \circ Cu]$. Hence, $u \circ Bv = \mathbf{1}_m$ and $v \circ Cu = \mathbf{1}_\ell$. Set $\alpha := \max\{u_1, \dots, u_m\}$, $\beta := \min\{v_1, \dots, v_\ell\}$, $\mathscr{M} := \{i \in \{1, \dots, m\} \mid u_i = \alpha\}$, $\mathscr{L} := \{j \in \{1, \dots, \ell\} \mid v_j = \beta\}$, $a := |\mathscr{M}|$, and $b := |\mathscr{L}|$. Then, for $i \in \mathscr{M}$ and $j \in \mathscr{L}$, we have

$$1 = (u \circ Bv)_i = u_i \sum_{k=1}^{\ell} B_{i,k} v_k = \alpha \sum_{k=1}^{\ell} B_{i,k} v_k \geq \alpha\beta \sum_{k=1}^{\ell} B_{i,k} = \alpha\beta, \tag{13}$$

$$1 = (v \circ Cu)_j = v_j \sum_{k=1}^{m} C_{j,k} u_k = \beta \sum_{k=1}^{m} C_{j,k} u_k \leq \beta\alpha \sum_{k=1}^{m} C_{j,k} = \beta\alpha. \tag{14}$$

Thus, $\alpha\beta = 1$ and equality holds in (13) and (14). Therefore,

$$B_{i,k} = 0 \quad \text{for all } (i,k) \in \mathscr{M} \times (\{1, \dots, \ell\} \setminus \mathscr{L}), \tag{15}$$

$$C_{j,k} = 0 \quad \text{for all} (j,k) \in \mathscr{L} \times (\{1, \dots, m\} \setminus \mathscr{M}). \tag{16}$$

Take a permutation matrix P of order m that moves the indices of $\mathscr{M}$ to the front of $(1, \dots, m)$, and likewise take a permutation matrix Q of order ℓ that moves the entries of $\mathscr{L}$ to the front of $(1, \dots, \ell)$. For example, choose P and Q such that the entries of Pu are descending and the entries of Qv are ascending. By (15) and (16), it follows that

$$PBQ^\top = \begin{pmatrix} E & 0 \\ * & * \end{pmatrix} \qquad \text{for an } |\mathscr{M}|\text{-by-}|\mathscr{L}| \text{ matrix } E,$$

$$QCP^\top = \begin{pmatrix} G & 0 \\ * & * \end{pmatrix} \qquad \text{for an } |\mathscr{L}|\text{-by-}|\mathscr{M}| \text{ matrix } G.$$

Hence,

$$PBCP^\top = (PBQ^\top)(QCP^\top) = \begin{pmatrix} EG & 0 \\ * & * \end{pmatrix} \quad \text{and}$$

$$QCBQ^\top = (QCP^\top)(PBQ^\top) = \begin{pmatrix} GE & 0 \\ * & * \end{pmatrix} .$$

By [10, Th. 2 and its corollary], irreducibility of A implies irreducibility of BC and CB. Hence, $PBCP^\top = EG$ and $QCBQ^\top = GE$ so that $|\mathscr{M}| = m$ and $|\mathscr{L}| = \ell$. This means $u = \alpha\mathbf{1}_m$ and $v = \beta\mathbf{1}_\ell$ so that $x = x_t$ for $t := \alpha = \beta^{-1}$. □

Brualdi, Parter, and Schneider [1, Lem. 8.1] proved[1]:

[1] Note that in [1] the notation $S > 0$ means $S \geq 0$ and $S \neq 0$.

Lemma 7 *(Brualdi, Parter, Schneider). Let $S \in \mathbb{R}^{n\times n}_{\geq 0}$ be stochastic. Suppose there is a diagonal matrix $D \neq I$ with positive diagonal entries for which DSD is again stochastic. Then S is permutationally similar to a matrix of the form $\begin{pmatrix} 0 & B & 0 \\ C & 0 & 0 \\ * & * & Z \end{pmatrix}$ where the diagonal blocks are square and the first and second diagonal block are nonempty.*

The next Lemma 8, (a) ⇔ (b), shows that Lemma 7 is indeed an equivalence. The essential new contribution of Lemma 8 is part (d). There, not just the structure of the upper left block $\left(\begin{smallmatrix} 0 & B \\ C & 0 \end{smallmatrix}\right)$ is refined but, what is more crucial, existence of infinitely many distinct scalings $D \neq I$ is proven and a one-to-one parameterization of all these scalings in a neighborhood of the identity is given. The tool of choice for proving that is again the implicit function theorem.

Lemma 8. *Let $S \in \mathbb{R}^{n\times n}_{\geq 0}$ be stochastic and $s := \dim\ker(I+S)$. The following statements are equivalent.*

(a) *S has a scaling $D \neq I$.*
(b) *S is permutationally similar to a matrix of the form $\widetilde{S} := \begin{pmatrix} 0 & B & 0 \\ C & 0 & 0 \\ * & * & Z \end{pmatrix}$ where the diagonal blocks are square and the first and second zero diagonal block are nonempty.*
(c) *S has an eigenvalue -1, i.e., $s > 0$.*
(d) *$s > 0$ and there is a permutation matrix P such that*

$$P^\top SP = \begin{pmatrix} \begin{smallmatrix} 0 & B_1 \\ C_1 & 0 \end{smallmatrix} & & & \\ & \ddots & & \\ & & \begin{smallmatrix} 0 & B_s \\ C_s & 0 \end{smallmatrix} & \\ * \quad * & * & * \quad * & Z \end{pmatrix} \tag{17}$$

where $B_i \in \mathbb{R}^{m_i\times n_i}_{\geq 0}$, $C_i \in \mathbb{R}^{n_i\times m_i}_{\geq 0}$, $\left(\begin{smallmatrix} 0 & B_i \\ C_i & 0 \end{smallmatrix}\right)$ is nonempty and irreducible for $i = 1,\dots,s$, and $Z \in \mathbb{R}^{\ell\times\ell}_{\geq 0}$ is either empty or does not have an eigenvalue -1.

For every such representation (17) the following holds true. If Z is empty, then $\mathfrak{X}(S) = \{Px_t \mid t \in \mathbb{R}^s_{>0}\}$ where

$$x_t := [t_1\mathbf{1}_{m_1}; t_1^{-1}\mathbf{1}_{n_1}; \dots; t_s\mathbf{1}_{m_s}; t_s^{-1}\mathbf{1}_{n_s}]. \tag{18}$$

Otherwise, there are open neighborhoods $\mathscr{U} \subseteq \mathbb{R}^s_{>0}$ of $\mathbf{1}_s$, $\mathscr{E} \subseteq \mathbb{R}^n_{>0}$ of $\mathbf{1}_n$, $\mathscr{W} \subseteq \mathbb{R}^\ell_{>0}$ of $\mathbf{1}_\ell$, and a uniquely determined real analytic function $\zeta : \mathscr{U} \to \mathscr{W}$ with $\zeta(\mathbf{1}_s) = \mathbf{1}_\ell$ such that $\mathfrak{X}(S) \cap \mathscr{E} = \{P[x_t; \zeta(t)] \mid t \in \mathscr{U}\}$.

(e) *S has infinitely many scalings D and, for all of them, -1 is an eigenvalue of DSD with algebraic and geometric multiplicity $s > 0$.*

Proof. (a) ⇒ (b) is Brualdi, Parter, and Schneider's Lemma 7.

(b) ⇒ (c). Lemma 6 (a) applied to the upper left block $\left(\begin{smallmatrix} 0 & B \\ C & 0 \end{smallmatrix}\right)$ of $\widetilde{S}$ yields that -1 is an eigenvalue of $\widetilde{S}$ and hence of S.
(c) ⇒ (d). Suppose S has an eigenvalue -1. Choose a permutation matrix P such that

$$P^\top SP = \begin{pmatrix} S_1 & 0 & 0 \\ * & \ddots & 0 \\ * & * & S_r \end{pmatrix} \tag{19}$$

where the diagonal blocks $S_1, \dots, S_r$, $r \in \mathbb{N}$, are square, nonempty, and irreducible. Since S is stochastic, we have $\|S_i\|_\infty \le 1$ for all $i \in \{1, \dots, r\}$. By assumption, at least one block S_i has an eigenvalue -1. Let $\hat{s} \in \{1, \dots, r\}$ be the number of such blocks. By Lemma 6 (c), all these blocks have -1 as a simple eigenvalue, are stochastic, and are permutationally similar to $\left(\begin{smallmatrix} 0 & B_i \\ C_i & 0 \end{smallmatrix}\right)$ for some $B_i \in \mathbb{R}^{m_i \times n_i}_{\ge 0}$ and $C_i \in \mathbb{R}^{n_i \times m_i}_{\ge 0}$. In particular, all star entries in (19) to the left of these S_i are zero. Therefore, P can be chosen such that $P^\top SP$ has the form (17) with $\hat{s}$ instead of s. But then $\hat{s}$ is necessarily the algebraic as well as the geometric multiplicity of $P^\top SP$ and hence of S so that $\hat{s} = s$.

Now, suppose that a representation (17) is given and set $\hat{S} := P^\top SP$. If Z is empty, then Lemma 6 (d) implies that $\mathfrak{X}(\hat{S}) = \{x_t \mid t \in \mathbb{R}^s_{>0}\}$ with x_t as in (18). Thus, $\mathfrak{X}(S) = P\mathfrak{X}(\hat{S}) = \{Px_t \mid t \in \mathbb{R}^s_{>0}\}$. If Z is not empty, then it does not have -1 as an eigenvalue. Set $m := n - \ell$ and write (17) as $\hat{S} = \left(\begin{smallmatrix} X & 0 \\ Y & Z \end{smallmatrix}\right)$ with $X \in \mathbb{R}^{m \times m}_{\ge 0}$ and $Y \in \mathbb{R}^{\ell \times m}_{\ge 0}$. Similar but slightly different to the proof of Theorem 1, we will now exploit the implicit function theorem. Consider the function

$$f : \mathbb{R}^m \times \mathbb{R}^\ell \to \mathbb{R}^\ell, \quad (u, v) \mapsto v \circ (Yu + Zv) - \mathbf{1}_\ell \ .$$

Since $\hat{S}$ is stochastic, all row sums of $(Y, Z) \in \mathbb{R}^{\ell \times n}_{\ge 0}$ are equal to 1 so that $f(\mathbf{1}_m, \mathbf{1}_\ell) = 0$. Clearly, f is real analytic. Its derivative w.r.t. the second variable v evaluated at $(\mathbf{1}_m, \mathbf{1}_\ell)$ readily computes as

$$\frac{\partial f}{\partial v}(\mathbf{1}_m, \mathbf{1}_\ell) = I_\ell + Z \ .$$

By assumption, $I_\ell + Z$ is regular as -1 is not an eigenvalue of Z. The analytic implicit function theorem [3, Sec. X.2] supplies an open neighborhood $\mathscr{M} \subseteq \mathbb{R}^m_{>0}$ of $\mathbf{1}_m$, an open neighborhood $\mathscr{W} \subseteq \mathbb{R}^\ell_{>0}$ of $\mathbf{1}_\ell$, and a uniquely determined real analytic function $g : \mathscr{M} \to \mathscr{W}$ such that $g(\mathbf{1}_m) = \mathbf{1}_\ell$ and for all $(x, z) \in \mathscr{M} \times \mathscr{W}$ it holds that

$$0 = f(x, z) = z \circ (Yx + Zz) - \mathbf{1}_\ell \quad \Leftrightarrow \quad z = g(x). \tag{20}$$

The function $\chi : \mathbb{R}^s_{>0} \to \mathbb{R}^m_{>0}$, $t \mapsto x_t$ with x_t as defined in (18) is real analytic and in particular continuous. Therefore and since $\chi(\mathbf{1}_s) = \mathbf{1}_m$, the preimage $\mathscr{U} := \chi^{-1}(\mathscr{M})$ is an open neighborhood of $\mathbf{1}_s$ in $\mathbb{R}^s_{>0}$. Thus, the concatenation of g and χ, namely $\zeta : \mathscr{U} \to \mathscr{W}$, $t \mapsto g(\chi(t))$, is a well-defined, real analytic function and fulfills $\zeta(\mathbf{1}_s) = \mathbf{1}_\ell$.

Now, $f(x_t, \zeta(t)) = f(x_t, g(x_t)) = 0$ means $Yx_t + Z\zeta(t) = \zeta(t)^{-1}$. By Lemma 6 (d), also $Xx_t = x_t^{-1}$ holds so that

$$\hat{S}[x_t; \zeta(t)] = [Xx_t; Yx_t + Z\zeta(t)] = [x_t^{-1}; \zeta(t)^{-1}] = [x_t; \zeta(t)]^{-1} \quad \text{for all } t \in \mathscr{U}.$$

Thus, $[x_t; \zeta(t)] \in \mathfrak{X}(\hat{S}) \cap \hat{\mathscr{E}}$ for all $t \in \mathscr{U}$ where $\hat{\mathscr{E}} := \{[x; z] \mid (x, z) \in \mathscr{M} \times \mathscr{W}\} \subseteq \mathbb{R}^n_{>0}$ is an open neighborhood of $\mathbf{1}_n$. On the other hand, if $[x; z] \in \mathfrak{X}(\hat{S}) \cap \hat{\mathscr{E}}$ with $x \in \mathscr{M}$ and $z \in \mathscr{W}$, then $[Xx; Yx + Zz] = \hat{S}[x; z] = [x; z]^{-1} = [x^{-1}; z^{-1}]$ yields $Xx = x^{-1}$ and $Yx + Zz = z^{-1}$. Hence, $0 = z \circ (Yx + Zz) - \mathbf{1}_\ell = f(x, z)$ and (20) imply $z = g(x)$. Lemma 6 (d) gives $x = x_t$ for some $t \in \mathbb{R}^s_{>0}$ wherefore $t \in \chi^{-1}(\mathscr{M}) = \mathscr{U}$. Thus, $z = \zeta(t)$ and $[x; z] \in \{[x_t; \zeta(t)] \mid t \in \mathscr{U}\}$. We conclude $\mathfrak{X}(\hat{S}) \cap \hat{\mathscr{E}} = \{[x_t; \zeta(t)] \mid t \in \mathscr{U}\}$. Since $P\mathbf{1}_n = \mathbf{1}_n$, $\mathscr{E} := P\hat{\mathscr{E}} \subseteq \mathbb{R}^n_{>0}$ remains an open neighborhood of $\mathbf{1}_n$ and

$$\mathfrak{X}(S) \cap \mathscr{E} = P(\mathfrak{X}(\hat{S}) \cap \hat{\mathscr{E}}) = \{P[x_t; \zeta(t)] \mid t \in \mathscr{U}\}.$$

(d) $\Rightarrow$ (e). Since $x_t \neq x_{t'}$ for $t \neq t'$, see (18), it follows by (d) that $\mathfrak{X}(S)$ is infinite in any case, i.e., S has infinitely many scalings. This proves the first part of (e). For the second part, let P be a permutation matrix such that (17) holds true. By Lemma 6 (c), all diagonal blocks $\left(\begin{smallmatrix} 0 & B_i \\ C_i & 0 \end{smallmatrix}\right)$ in (17) have a simple eigenvalue -1. Since the lower right diagonal block Z in (17) is either empty or does not have -1 as an eigenvalue, the algebraic multiplicity of -1 as an eigenvalue of S equals its geometric multiplicity s. Now, let D be a scaling for S and set $\hat{S} := P^\top SP$ and $\hat{D} := P^\top DP$. Then, $\bar{S} := P^\top DSDP = \hat{D}\hat{S}\hat{D}$ and $\hat{D}$ is a scaling for $\hat{S}$. Therefore, Lemma 6 (d) implies

$$\bar{S} = \begin{pmatrix} \begin{smallmatrix} 0 & B_1 \\ C_1 & 0 \end{smallmatrix} & & & \\ & \ddots & & \\ & & \begin{smallmatrix} 0 & B_s \\ C_s & 0 \end{smallmatrix} & \\ * \quad * & * & * \quad * & \bar{Z} \end{pmatrix} \quad \text{for some } \bar{Z} \in \mathbb{R}^{\ell \times \ell}_{\geq 0}.$$

Hence, -1 is an eigenvalue of $\bar{S}$ and $\bar{s} := \dim\ker(I + \bar{S}) = \dim\ker(I + DSD) \geq s > 0$. Now, applying (c) $\Rightarrow$ (d) to DSD instead of S and interchanging the roles of DSD and S yields that $\bar{s}$ is also the algebraic multiplicity of -1 as an eigenvalue of DSD and $s \geq \bar{s}$ so that $s = \bar{s}$, finishing the proof of (e). Finally, (e) $\Rightarrow$ (a) is clear. $\square$

Proof of Theorem 2. (a). If A has two distinct scalings $D, \hat{D}$, then $\widetilde{D} := \hat{D}D^{-1} \neq I$ is a scaling for $S := DAD$ and Lemma 8 (a) $\Rightarrow$ (e) implies

$$\dim\ker(I + DAD) = \dim\ker(I + S) = \dim\ker(I + \widetilde{D}S\widetilde{D}) = \dim\ker(I + \hat{D}A\hat{D}).$$

Thus, $s(A) := \dim\ker(I + DAD)$ is independent of a chosen scaling D for A. If $s(A) > 0$, then -1 is an eigenvalue of $S = DAD$ and Lemma 8 (c) $\Rightarrow$ (e) implies that $s(A)$ is its geometric and algebraic multiplicity.

(b) is a reformulation of Lemma 8 $\neg$ (a) $\Leftrightarrow$ $\neg$ (c) with $S := DAD$, D a scaling for A, where $\neg$ means logical negation.

(c) and (d). Let $A \in \mathscr{S}$ and let D be its scaling. By (b), $I + DAD$ is regular. By Theorem 1, there is an open neighborhood $\mathscr{U}$ of A such that all $B \in \mathscr{U}$ are scalable as well and posses a scaling E such that $I + EBE$ is regular. Thus, if $B \in \mathscr{U} \cap \mathbb{R}^{n\times n}_{\geq 0}$, then (b) yields that B is uniquely scalable, i.e., $B \in \mathscr{S}$. Hence, $\mathscr{U} \cap \mathbb{R}^{n\times n}_{\geq 0} \subseteq \mathscr{S}$ which shows that $\mathscr{S}$ is relatively open in $\mathbb{R}^{n\times n}_{\geq 0}$. This proves (c). The function x in (d) coincides on $\mathscr{U} \cap \mathbb{R}^{n\times n}_{\geq 0}$ with the uniquely determined real analytic function ξ of Theorem 1. This proves the first part of (d) except for the final sentence. For that, consider the matrix $S := \frac{1}{2}(I + DAD)$ which is stochastic and regular. Since DAD is stochastic, S is also row diagonally dominant which means that $S_{i,i} \geq \sum_{j\neq i} S_{i,j}$ for all $i \in \{1, \ldots, n\}$. Now, by [8, Corollary 6], it holds that $\left[S^{-1}\right]_{i,i} \geq 1$ for all i. Thus, we conclude

$$\begin{aligned}\frac{\partial x_i}{\partial A_{i,j}} &= [J_x(A)]_{i,(i-1)n+j} = -\left[D(I + DAD)^{-1}(D \otimes x^\top)\right]_{i,(i-1)n+j} \\ &= -\frac{1}{2}\left[DS^{-1}(D \otimes x^\top)\right]_{i,(i-1)n+j} = -\frac{1}{2}x_i\left[S^{-1}\right]_{i,i}x_i x_j \leq -\frac{1}{2}x_i^2 x_j\ . \quad \square\end{aligned}$$

Proof of Theorem 3. (a) is clear by Theorem 2 (b).

(b). Suppose $A \in \mathscr{N}$. Then, $s := s(A) > 0$ by (a). Let $r \in \mathbb{N}_0 := \mathbb{N} \cup \{0\}$ be maximum subject to existence of a permutation matrix P such that (1) holds true with r instead of s. Furthermore, let $D = \operatorname{diag}(x)$ be a scaling for A and set $S := DAD$. Write $P^\top DP = \operatorname{diag}(E_1, F_1, \ldots, E_r, F_r, G)$ for diagonal matrices E_i of order m_i, F_i of order n_i, $i = 1, \ldots, r$, and G of order ℓ. Then,

$$P^\top SP = (P^\top DP)(P^\top AP)(P^\top DP) = \begin{pmatrix} \begin{smallmatrix} 0 & \hat{B}_1 \\ \hat{C}_1 & 0 \end{smallmatrix} & & & \\ & \ddots & & \\ & & \begin{smallmatrix} 0 & \hat{B}_r \\ \hat{C}_r & 0 \end{smallmatrix} & \\ * \quad * & * & * \quad * & \hat{Z} \end{pmatrix} \tag{21}$$

where $\hat{B}_i := E_i B_i F_i$, $\hat{C}_i := F_i C_i E_i$, $\left(\begin{smallmatrix} 0 & \hat{B}_i \\ \hat{C}_i & 0 \end{smallmatrix}\right)$ is nonempty and still irreducible for $i = 1, \ldots, r$, and $\hat{Z} := GZG$. If $\hat{Z}$ is nonempty, then it cannot have an eigenvalue -1 because otherwise Lemma 6 (c) would imply that $\hat{Z}$ is permutationally similar to a matrix of the form $\left(\begin{smallmatrix} 0 & \hat{B}_{r+1} & 0 \\ \hat{C}_{r+1} & 0 & 0 \\ * & * & * \end{smallmatrix}\right)$ whereby the upper left block $\left(\begin{smallmatrix} 0 & \hat{B}_{r+1} \\ \hat{C}_{r+1} & 0 \end{smallmatrix}\right)$ is square, nonempty, stochastic, and irreducible. The star entries in (21) to the left of the rows of this irreducible stochastic block are necessarily zero as $P^\top SP$ is stochastic. Transforming back, this would contradict the maximality of r. Using Lemma 6 (c) again, we derive $r = s$ so that (21) is a representation as stated in (17). We can now use the notation from Lemma 8 (d) and extend it by setting $\mathscr{E} := \mathbb{R}^n_{>0}$ and $\mathscr{U} := \mathbb{R}^s_{>0}$ if $\ell = 0$. Then, $\mathscr{V} := D\mathscr{E} \subseteq \mathbb{R}^n_{>0}$ is an open neighborhood of x whether $\ell = 0$ or not and, since

$\mathfrak{X}(A) = D\mathfrak{X}(S)$, we conclude $\mathfrak{X}(A) \cap \mathscr{V} = D(\mathfrak{X}(S) \cap \mathscr{E}) = \{DP[x_t; \zeta(t)] \mid t \in \mathscr{U}\}$ whereby $\zeta(t)$ disappears if $l = 0$. Then, the function $\gamma(t) = DP[x_t; \zeta(t)]$ defined in (2) has the stated properties.
(c). If $A \in \mathscr{N}$, then (b) implies that $\mathfrak{X}(A) \cap \mathscr{V} = \gamma(\mathscr{U})$ is infinite because $\mathscr{U}$ is infinite and γ is injective.
(d). If $A \in \mathscr{N}$ has empty Z in (1) and scalings $D, \widetilde{D}$, then $\hat{D} := P^\top \widetilde{D} D^{-1} P$ with P from (1) is a scaling for $S := P^\top DADP$ which has the form (17) with empty Z. By Lemma 6 (d), we have $S = \hat{D} S \hat{D}$ which implies $DAD = \widetilde{D} A \widetilde{D}$. □

We close this section by comparing Theorem 3 (a) to Theorem 2 of Johnson and Reams in [7] which reads:

Theorem 9 *(Johnson and Reams). Let $A \in \mathbb{R}^{n\times n}$. If A has two or more distinct scalings then A is positively diagonally congruent to a matrix that has both 1 and -1 as eigenvalues.*

Theorem 9 says that for multiply scalable, real A there is a diagonal matrix D with positive diagonal entries such that ± 1 are eigenvalues of DAD. The proof is a short matrix vector calculation. It takes two distinct scalings X and Y for A and shows that $D := (XY)^{1/2}$ fulfills the assertion. Note that D is in general not a scaling for A. For nonnegative, multiply scalable A, more can be said. By Theorem 3 (a), ± 1 are already eigenvalues of $\widetilde{D} A \widetilde{D}$ for every scaling $\widetilde{D}$ for A, and, by definition of scalings, the all-ones vector $\mathbf{1}$ is an eigenvector corresponding to the eigenvalue 1. Thus, both of the above scalings X, Y already fulfill the assertion of Theorem 9 so that the stated construction of D is not necessary. Theorem 9 is solely used to prove Corollary 3 in [7] which reads:

Corollary 10 *(Johnson and Reams). If $A \in \mathbb{R}^{n\times n}$ is*

(a) *positive definite, or*
(b) *positive semidefinite and scalable, or*
(c) *A is primitive (this includes the case of A having all positive entries), or*
(d) *A has nonnegative entries, is scalable, irreducible, and has the property that there does not exist a permutation matrix P so that*

$$PAP^\top = \begin{pmatrix} 0 & B \\ B^\top & 0 \end{pmatrix}, \tag{22}$$

then A has a unique scaling.

We are mainly interested in the nonnegative case (d). It seems that A is tacitly assumed to be symmetric in (d) because otherwise there would be counterexamples. Assuming that, the fact that the set of matrices $\mathscr{R}$ described by (d) is indeed a subset of $\mathscr{S}$ already follows as a special case from Bruladi, Parter, and Schneider's Lemma 7.

This is seen as follows. In order to derive a contradiction, suppose that there is an $A \in \mathscr{R}$ which has two distinct scalings E, F. Set $S := EAE$ and $D := E^{-1}F$. Then, S and D fulfill the assumptions of Lemma 7. Thus, there is a permutation matrix P such that $PSP^\top = \left(\begin{smallmatrix} 0 & B & 0 \\ C & 0 & 0 \\ * & * & * \end{smallmatrix}\right)$ where the diagonal blocks are square and the first and second zero diagonal block are nonempty. Since A is irreducible, so is S wherefore the star entries disappear. Hence, $PSP^\top = \left(\begin{smallmatrix} 0 & B \\ C & 0 \end{smallmatrix}\right)$. Since A and S are symmetric, we have $C = B^\top$ and

$$PAP^\top = (PEP^\top)^{-1} \begin{pmatrix} 0 & B \\ B^\top & 0 \end{pmatrix} (PEP^\top)^{-1} = \begin{pmatrix} 0 & X \\ X^\top & 0 \end{pmatrix}$$

for an according X. This contradicts (22).

3. Second-order derivatives of the Sinkhorn vector

Let $A = (a_{i,j}) \in \mathbb{R}^{n\times n}$ be scalable and let $D = \operatorname{diag}(x)$ be a scaling for A. We assume that $I + DAD$ is regular. Then, by Theorem 1, the correspondence between matrices in a neighborhood of A and their Sinkhorn vectors in a neighborhood of x is a well-defined analytic function w.r.t. matrix entries and we have already computed its Jacobian matrix. In what follows, we will also provide a compact index-free formula for the Hessian matrix. This is done by implicit differentiation. Abbreviate

$$J := \left(\frac{\partial x_i}{\partial a_{k,\ell}}\right)_{1\le i,k,\ell\le n} \in \mathbb{R}^{n\times n^2} \quad \text{and} \quad H := \left(\frac{\partial^2 x_i}{\partial a_{k,\ell}\partial a_{r,s}}\right)_{1\le i,k,\ell,r,s\le n} \in \mathbb{R}^{n\times n^4}.$$

The Jacobian J is regarded as an n-by-n^2 and the Hessian H as an n-by-n^4 matrix. As in (3), this is done by flattening pairs (k,ℓ) to singletons $j := (k-1)n+\ell$, and quadruples (k,ℓ,r,s) to $j := (r-1)n^3 + (s-1)n^2 + (k-1)n + \ell$:

$$J_{i,(k-1)n+\ell} := \frac{\partial x}{\partial a_{k,\ell}} \quad \text{and} \quad H_{i,(r-1)n^3+(s-1)n^2+(k-1)n+\ell} := \frac{\partial^2 x_i}{\partial a_{k,\ell}\partial a_{r,s}} \;.$$

Since $(x \circ Ax)_i = \sum_{j=1}^{n} a_{i,j}x_i x_j = 1$ for $i = 1,\dots,n$, implicit differentiation w.r.t. $a_{k,\ell}$ gives

$$\frac{\partial}{\partial a_{k,\ell}} \sum_{j=1}^{n} a_{i,j}x_i x_j = \frac{\partial x_i}{\partial a_{k,\ell}} \sum_{j=1}^{n} a_{i,j}x_j + x_i \sum_{j=1}^{n} a_{i,j}\frac{\partial x_j}{\partial a_{k,\ell}} + \delta_{i,k}x_k x_\ell = 0 \;. \tag{23}$$

In matrix notation, using $Ax = x^{-1}$, this becomes

$$(D^{-1} + DA)J = -D \otimes x^\top =: C \;. \tag{24}$$

The matrix

$$B := D^{-1} + DA = (I + DAD)D^{-1} \tag{25}$$

is invertible as $I + DAD$ is so that we obtain once again the formula for the Jacobian matrix $J = B^{-1}C$ stated in Theorem 2 (d). An inversion of B is not carried out in practice but, for instance, LU or QR factorization is used instead to solve such a matrix equation. The function `deriv` in Listing 1 uses MATLAB's fast built-in function `linsolve` for that. Differentiating (23) a second time w.r.t. $a_{r,s}$ gives

$$\begin{aligned}\frac{\partial^2}{\partial a_{r,s}\partial a_{k,\ell}}\sum_{j=1}^{n} a_{i,j}x_i x_j = {}& \frac{\partial^2 x_i}{\partial a_{r,s}\partial a_{k,\ell}}\sum_{j=1}^{n} a_{i,j}x_j + \frac{\partial x_i}{\partial a_{k,\ell}}\sum_{j=1}^{n} a_{i,j}\frac{\partial x_j}{\partial a_{r,s}} \\ &+ \frac{\partial x_i}{\partial a_{r,s}}\sum_{j=1}^{n} a_{i,j}\frac{\partial x_j}{\partial a_{k,\ell}} + x_i\sum_{j=1}^{n} a_{i,j}\frac{\partial^2 x_j}{\partial a_{r,s}\partial a_{k,\ell}} \\ &+ \delta_{i,k}\left(\frac{\partial x_k}{\partial a_{r,s}}x_\ell + \frac{\partial x_\ell}{\partial a_{r,s}}x_k\right) \\ &+ \delta_{i,r}\left(\frac{\partial x_r}{\partial a_{k,\ell}}x_s + \frac{\partial x_s}{\partial a_{k,\ell}}x_r\right) = 0\ .\end{aligned} \tag{26}$$

For $p, q \in \mathbb{N}$ and $X \in \mathbb{R}^{p\times q}$, the row- and columnwise flattenings of X to column vectors of length pq are denoted by

$$\begin{aligned}\operatorname{rvec}(X) &:= (X_{1,1},\dots,X_{1,q},\dots,X_{p,1},\dots,X_{p,q})^\top \\ \operatorname{cvec}(X) &:= (X_{1,1},\dots,X_{p,1},\dots,X_{1,q},\dots,X_{p,q})^\top\ .\end{aligned}$$

With this notation, (26) can be expressed in index-free form by

$$\begin{aligned}(D^{-1} + DA)H = -\Big\{&(\mathbf{1}_{n^2}^\top \otimes J)\circ(AJ\otimes \mathbf{1}_{n^2}^\top) \\ &+ (J\otimes \mathbf{1}_{n^2}^\top)\circ(\mathbf{1}_{n^2}^\top\otimes AJ) + (\mathbf{1}_{n^2}^\top\otimes I_n\otimes x^\top)\circ(J\otimes \mathbf{1}_{n^2}^\top) \\ &+ (\mathbf{1}_{n^2}^\top\otimes D\otimes \mathbf{1}_n^\top)\operatorname{diag}(\operatorname{cvec}(\mathbf{1}_n\otimes J)) + (I_n\otimes x^\top\otimes \mathbf{1}_{n^2}^\top)\circ(\mathbf{1}_{n^2}^\top\otimes J) \\ &+ (D\otimes \mathbf{1}_{n^3}^\top)\operatorname{diag}(\operatorname{cvec}(\mathbf{1}_n^\top\otimes J^\top))\Big\} =: Z\ .\end{aligned} \tag{27}$$

This linear system is uniquely solvable for H, namely $H = B^{-1}Z$ with B as in (25). The function `deriv` in Listing 1 computes the Jacobian J and the Hessian H of the Sinkhorn vector x w.r.t. the matrix entries of A according to equations (24) and (27). Input arguments are the matrix A and the Sinkhorn vector x which must be computed a priori. Output arguments are J and H. Let us remark that we checked J and H for safety also numerically against results obtained by finite difference quotients.

```
function [J,H] = deriv(A,x)
n = size(A,1); D = diag(x); D_inv = diag(1./x); B = D_inv + D*A;
C = -kron(D,x'); J = linsolve(B,C); % solve matrix equation BX = C
I = eye(n); e = ones(1,n); ee = ones(1,n^2); eee = ones(1,n^3); Y = A*J;
Z1 = kron(ee,J).*kron(Y,ee); Z2 = kron(J,ee).*kron(ee,Y);
Z3 = kron(ee,kron(I,x')).*kron(J,ee);
Z4 = kron(ee,kron(D,e)).*reshape(kron(e',J),1,[]);
Z5 = kron(kron(I,x'),ee).*kron(ee,J);
Z6 = kron(D,eee).*reshape(kron(e,J'),1,[]); Z = -(Z1+Z2+Z3+Z4+Z5+Z6);
H = linsolve(B,Z); % solve matrix equation BX = Z
```

Listing 1: First- and second-order derivatives of the Sinkhorn vector w.r.t. matrix entries.

For $A \in \mathscr{S}$ with Sinkhorn vector $x(A)$ and Jacobian and Hessian matrices J, H computed by the function `deriv`, a second-order Taylor expansion of x around A reads

$$x(A+E) \approx x(A) + Jf + \frac{1}{2}H(f \otimes f) \tag{28}$$

where $E \in \mathbb{R}^{n \times n}$ is a small perturbation and $f := \mathrm{rvec}(E)$ is its rowwise flattening.

Alternatively, we can evaluate (28) as follows without computing the matrices J and H explicitly, which is more efficient for large dimensions and small numbers of evaluation points. For a diagonal matrix $D \in \mathbb{R}^{n\times n}$, $x \in \mathbb{R}^n$, $U, V \in \mathbb{R}^{n\times n}$, $Y, Z \in \mathbb{R}^{n \times n^2}$, $u := \mathrm{rvec}(U)$, and $v := \mathrm{rvec}(V)$, it holds that

$$(D \otimes x^T)u = DUx \tag{29}$$

$$\left[(Y \otimes \mathbf{1}_{n^2}^\top) \circ (\mathbf{1}_{n^2}^\top \otimes Z)\right](u \otimes v) = Yu \circ Zv \tag{30}$$

$$\left[(\mathbf{1}_{n^2}^\top \otimes D \otimes \mathbf{1}_n^\top)\mathrm{diag}(\mathrm{cvec}(\mathbf{1}_n \otimes Y))\right](u \otimes v) = DVYu \tag{31}$$

$$\left[(D \otimes \mathbf{1}_{n^3}^\top)\mathrm{diag}(\mathrm{cvec}(\mathbf{1}_n^\top \otimes Y^\top))\right](u \otimes v) = DUYv\ . \tag{32}$$

Taking $x := x(A)$ and $D := \mathrm{diag}(x)$, it follows from (24) and (29) that

$$Ju = -D(I + DAD)^{-1}DUx\ . \tag{33}$$

Thus, for $U := E$ and $u := f$, the first-order deviation in (28) can be computed as

$$Jf = -D(I + DAD)^{-1}DEx\ . \tag{34}$$

Also, (27), (30), (31), (32) imply that the Hessian $H : \mathbb{R}^{n^2 \times n^2} \to \mathbb{R}^n, (U, V) \mapsto H(u \otimes v)$, interpreted as a bilinear map, can be evaluated as

$$H(U,V) = -D(I + DAD)^{-1}[(AJu + Ux) \circ Jv + (AJv + Vx) \circ Ju + DVJu + DUJv]$$

with Ju and Jv evaluated according to (33). Hence, for $U = V := E$, $u = v := f$, and Jf from (34), the second-order deviation in (28) can be calculated as

$$\frac{1}{2}H(f \otimes f) = -D(I + DAD)^{-1}[(AJf + Ex) \circ Jf + DEJf]\ . \tag{35}$$

```
 1 n = 5;                    % dimension, matrix order
 2 A = 10*rand(n);           % create a random positive n-by-n test matrix A
 3 E = (1e-2)*rand(n);       % create a random, small perturbution matrix E
 4 x = sinkhorn(A);          % compute Sinkhorn vector x of A
 5 y = sinkhorn(A+E);        % compute Sinkhorn vector y of A+E
 6 [J,H] = deriv(A,x);       % compute Jacobian J and Hessian H of x at A
 7 f = E'; f = f(:);         % rowwise flattening of E
 8 g = kron(f,f);
 9 p = x + J*f;              % first-order Taylor expansion of x around A
10 q = p + 0.5*H*g;          % second-order Taylor expansion of x around A
11 remainder_1st_order_expansion = norm(y-p,'inf')
12                           % approximation error first-order Taylor expansion
13 remainder_2nd_order_expansion = norm(y-q,'inf')
14                           % approximation error second-order Taylor expansion
15
16 % alternative computation
17 M = eye(n)+x.*A.*x';
18 Jf = -x.*linsolve(M,x.*E*x);
19 Hg = -2*x.*linsolve(M,(A*Jf+E*x).*Jf+x.*E*Jf);
20 p_ = x + Jf;
21 q_ = p_ + 0.5*Hg;
22 remainder_1st_order_expansion_2 = norm(y-p_,'inf')
23                           % approximation error first-order Taylor expansion
24 remainder_2nd_order_expansion_2 = norm(y-q_,'inf')
25                           % approximation error second-order Taylor expansion
26
27 function [x,k] = sinkhorn(A)
28 maxiter = 1000; % maximum number of iterations
29 tol = 1e-15;    % tolarence, termination condition
30 n = size(A,1);  % dimension, matrix order
31 x = ones(n,1);  % initialize x-values with all-ones vector
32 y = (A*x).^-1;  % initialize y-values
33 k = 0;          % initialize iteration counter
34 t = tol + 1;
35 while t > tol && k < maxiter
36   x_ = (A*y).^-1;                % new x-values
37   y_ = (A*x_).^-1;               % new y-values
38   tx = norm((x-x_)./x,'inf');    % max norm of relative x-iterate deviation
39   ty = norm((y-y_)./y,'inf');    % max norm of relative y-iterate deviation
40   t = max(tx,ty);                % overall max norm
41   x = x_;                        % update old x-values for next loop
42   y = y_;                        % update old y-values for next loop
43   k = k+1;                       % increment iteration counter
44 end
45 x = sqrt(y(1)/x(1))*x; % final result
46 end
```

Listing 2: Second-order Taylor expansion of the Sinkhorn vector.

For practitioners, Listing 2 states an executable, ready-to-use MATLAB script which exemplary computes a second-order Taylor expansion.

For $n = 5$, it creates a random positive A and a positive perturbation E. Then, the Sinkhorn vectors x of A and y of $A + E$ are computed in lines 4 and 5 using a simple iteration proposed by Sinkhorn [11], which is implemented in the function `sinkhorn` in lines 27 to 46. Afterwards, first- and second-order Taylor expansions p and q of x around A are computed according to (28) in lines 9 and 10. Finally, the maximum norm of the first- and second-order approximation errors $y - p$ and $y - q$ are displayed, see lines 11 and 13. The alternative computation of the Taylor expansion according to (34) and (35) is given in lines 17 to 24.

4. Conclusions

We considered Sinkhorn-type positive diagonal congruence DAD of a real n-by-n matrix A by a diagonal matrix $D = \mathrm{diag}(x)$ having an entrywise positive diagonal vector x such that all row sums of DAD are equal to 1. For entrywise nonnegative A, this means that DAD is a stochastic matrix. If, for given A, such a D exists, then A is called scalable and D a scaling for A. We investigated uniqueness and differentiable dependence of D with respect to A.

On the one hand, we proved that a scalable entrywise nonnegative A has a unique scaling D if and only if it has a scaling D such that -1 is not an eigenvalue of DAD, see Theorem 2 (a), (b). On the other hand, we proved that A has more than one scaling if and only if it has infinitely many scalings, see Theorem 3 (c). Thus, there are no entrywise nonnegative matrices having multiple but only finitely many scalings. This result essentially relies on the nonnegativity of A. For arbitrary matrices, this does not hold true. More precisely, Theorem 3 (b) even shows that each scaling D for A possesses infinitely many other scalings $\widetilde{D}$ for A in its neighborhood, and a parameterization of these scalings is stated in (2).

Furthermore, if an arbitrary real square matrix A has a scaling D such that -1 is not an eigenvalue of DAD, then, in a neighborhood of the pair (A, D), the correspondence between matrices and scalings is a well-defined real analytic function, see Theorem 1.

In particular, we stated compact, index-free formulas for the first- and second-order derivatives of the diagonal vector x of D, which we call a Sinkhorn vector of A, with respect to the entries of A. Based on that, a second-order Taylor expansion of the Sinkhorn vector can conveniently be computed, see Section 3.

Declaration of competing interest

There is no competing interest.

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Data availability

No data was used for the research described in the article.

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