On the Scaling of Multidimensional Matrices*

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Dedicated to Alan J. Hoffman on the occasion of his 65th birthday.

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ABSTRACT

Elementary proofs are given for theorems of Bapat and Raghavan on the scaling of nonnegative multidimensional matrices. Theorems of Sinkhorn and of Brualdi, Parter, and Schneider are derived as corollaries. For positive two-dimensional matrices, Hilbert's projective metric and a theorem of G. Birkhoff are used to prove that Sinkhorn's original iterative procedure converges geometrically; the ratio of convergence is estimated from the given data.

1. INTRODUCTION

R. Bapat [1] and independently T. E. S. Raghavan [15] have considered the problem of scaling multidimensional positive matrices to achieve specific one-dimensional marginals. Their proofs are quite different, one relying on Kronecker's topological index theorem, the other on the duality theorem of linear programming. Neither proof could handle the general case allowing zero entries.

Recently they combined the two methods to take care of the case with zero entries. They extend the scaling of matrices to a more general setting. In [2, Theorem 1], they extend a theorem of Darroch and Ratcliff [7] on

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loglinear models. Whereas Darroch and Ratcliff used a constructive iterative procedure, Bapat and Raghavan prove their extended theorem by ideas derived from Kronecker's index theorem and from the duality theorem of linear programming, with reference to generalized transportation matrices.

In the next section of this paper we prove the results of Bapat and Raghavan [2] using only calculus. All we use is Lagrange multipliers; we do not need the Kuhn-Tucker theorems or any result from linear programming or topology. As applications, we prove results of Sinkhorn [16] and of Brualdi, Parter, and Schneider [5].

In the last section we discuss the rate of convergence of Sinkhorn's original iterative procedure [18] for the scaling of two-dimensional positive matrices. We use Hilbert's projective metric together with a result of G. Birkhoff [4] on the contraction ratio of positive operators.

2. SCALING MULTIDIMENSIONAL MATRICES

First we will prove an elementary lemma. Then we will use the lemma to prove the three theorems of Bapat and Raghavan that appear in [2], extending their results that appear in [1] and [15].

NOTATION. $\mathbf{R}^n$ is the space of vectors x with n real components $x_1, \dots, x_n$. $\mathbf{P}^n$ is the subset with all $x_j \geqslant 0$. The inequality $x \geqslant 0$ means all $x_j \geqslant 0$; the inequality $x > 0$ means all $x_j > 0$.

LEMMA 1. *Let C be an $m \times n$ real matrix. Let b lie in $\mathbf{R}^m$. Assume $Cy = b$ for some $y > 0$. Assume $x > 0$, $x \in \mathbf{P}^n$. For all $u \in \mathbf{P}^n$ define*

$$\Phi(u) = \sum_{j=1}^{n} u_j \log \frac{u_j}{x_j}. \tag{2.1}$$

Then there exists a unique $u^0 \in \mathbf{P}^n$ satisfying

$$\Phi(u^0) = \min\{\Phi(u) : u \in \mathbf{P}^n, \ Cu = b\}. \tag{2.2}$$

Necessarily, $u^0 > 0$; and u^0 is the unique point such that $u > 0$, $Cu = b$, and

$$\frac{\partial}{\partial u_j}\left[\Phi(u) - q^T C u\right] = 0 \qquad (j = 1, \dots, n) \tag{2.3}$$

for some $q \in \mathbf{R}^m$. The Lagrange vector q is unique apart from increments w satisfying $w^TC = 0$.

NOTE. We do *not* need to assume that the feasible set $\{u : u \in \mathbf{P}^n, Cu = b\}$ is bounded. The key part of the lemma is that all components of u^0 are positive.

Proof. For $0 \leqslant u_j < \infty$ the function $u_j \log(u_j/x_j)$ varies continuously from $-e^{-1}x_j$ to ∞, attaining a finite minimum value at $u_j = e^{-1}x_j$. Therefore, the sum $\Phi(u)$ is continuous on $\mathbf{P}^n$; $\Phi(u)$ attains a finite minimum value, and $\Phi(u) \to \infty$ if any $u_j \to \infty$. Hence, for some finite $\omega > 0$ and for some fixed $y > 0$ with $Cy = b$,

$$\Phi(u) > \Phi(y) \qquad \text{if} \quad u \in \mathbf{P}^n \text{ and } \sum u_j > \omega. \tag{2.4}$$

Define the closed, bounded set

$$S = \left\{ u : \in \mathbf{P}^n, \sum u_j \leqslant \omega, Cu = b \right\}. \tag{2.5}$$

By (2.4), the fixed positive vector y lies in S, and the minimum of $\Phi(u)$ for $u \in \mathbf{P}^n$ and $Cu = b$ is attained at a point u^0 in the set S.

Positivity. To prove $u^0 > 0$, let $0 < \epsilon < 1$ and define the positive vector $u(\epsilon) = (1-\epsilon)u^0 + \epsilon y$. This vector is a competitor in the minimization (2.2). Define the sets of indices

$$J_0 = \left\{ j : u_j^0 = 0 \right\}, \qquad J_1 = \left\{ j : u_j^0 > 0 \right\}$$

Then, for $0 < \epsilon < 1$,

$$\frac{d}{d\epsilon}\Phi(u(\epsilon)) = \sum_{j=1}^{n} \left(y_j - u_j^0 \right) \left(1 + \log \frac{u_j(\epsilon)}{x_j} \right)$$

If J_0 is not empty, as $\epsilon \to +0$ this derivative satisfies

$$\frac{d}{d\epsilon}\Phi(u(\epsilon)) = \left(\sum_{J_0} y_j \right) \log \epsilon + O(1),$$

which would tend to $-\infty$. That would imply $\Phi(u(\epsilon)) < \Phi(u^0)$ for small $\epsilon > 0$, contradicting the minimizing property (2.2) of u^0. Therefore, J_0 is empty, i.e., $u^0 > 0$.

Uniqueness. Suppose u^1 also minimizes $\Phi(u)$ under the constraints $u \geqslant 0$, $Cu = b$. By the preceding argument, we must have $u^1 > 0$. To prove $u^1 = u^0$, define the competing vector

$$u(\theta) = (1-\theta)u^0 + \theta u^1 \qquad (0 \leqslant \theta \leqslant 1).$$

If $u^0 \neq u^1$, then

$$\frac{d^2}{d\theta^2}\Phi(u(\theta)) = \sum_{j=1}^{n} \frac{\left(u_j^0 - u_j^1\right)^2}{u_j(\theta)} > 0,$$

which would imply the absurdity $\Phi(u(\frac{1}{2})) < \min \Phi(u)$. Therefore, $u^1 = u^0$, i.e., the minimizing u is unique.

Lagrange multipliers. Since $u^0 > 0$, if z is fixed in $\mathbf{R}^n$, then $u^0 + \epsilon z > 0$ for all sufficiently small $|\epsilon|$. If $Cz = 0$, then $u^0 + \epsilon z$ competes in the minimization (2.2). Then

$$\frac{d}{d\epsilon}\Phi(u^0 + \epsilon z) = 0 \qquad \text{at} \quad \epsilon = 0,$$

which says that z is orthogonal to the gradient of $\Phi(u)$ at $u = u^0$. Since this must be true for all z in the null space of C, there must exist a vector $q \in \mathbf{R}^m$ such that

$$(\nabla \Phi(u))^T = q^T C \qquad \text{at} \quad u = u^0. \tag{2.6}$$

This proves the Lagrange equations (2.3). The vector q is uniquely defined by (2.6) apart from increments w satisfying $w^T C = 0$.

Finally, suppose $u^1 > 0$, $Cu^1 = b$, and

$$(\nabla \Phi(u))^T = q^T C \qquad \text{at} \quad u = u^1. \tag{2.7}$$

We must prove $u^1 = u^0$. Suppose $u^1 \neq u^0$. Then, by the uniqueness of u^0 in (2.2), $\Phi(u^1) > \Phi(u^0)$. The convexity of $\Phi(u)$ now implies

$$\frac{d}{d\epsilon}\Phi\big((1-\epsilon)u^1 + \epsilon u^0\big) < 0 \qquad \text{at} \quad \epsilon = 0,$$

which says

$$(\nabla\Phi(u))^T(u^0 - u^1) < 0 \qquad \text{at} \quad u = u^1.$$

Now the Lagrange equation (7) implies

$$q^T C(u^0 - u^1) < 0,$$

which is absurd, because $C(u^0 - u^1) = b - b = 0$. This completes the proof of the lemma. ∎

We now quote the main theorem of Bapat and Raghavan in [2]:

THEOREM 1. *Let $C = (c_{ij})$ be a real $m \times n$ matrix. Let b be any nonzero m-vector. Let $K = \{\pi : C\pi = b,\ \pi \geqslant 0\}$ be bounded. Let $x = (x_1, \dots, x_n)$, $y = (y_1, \dots, y_n)$ be two nonnegative vectors with the same zero pattern, that is, $x_j = 0 \Leftrightarrow y_j = 0$ for any coordinate j. If $y \in K$, then there exists a π in K where for some $z_1 > 0,\ z_2 > 0, \dots, z_m > 0$*

$$\pi_j = x_j \prod_{i=1}^{m} z_i^{c_{ij}}, \qquad j = 1, \dots, n. \tag{2.8}$$

Proof. We will prove this theorem using our elementary lemma. We will assume somewhat less and prove somewhat more: we will not assume that the feasible set K is bounded, and we will prove that the required vector π not only exists but is unique.

Let J be the set of indices j for which x_j and y_j are positive. Then we are given

$$\begin{gathered} \sum_{j \in J} c_{ij} y_j = b_i \qquad (i = 1, \dots, m), \\ y_j > 0 \qquad \forall j \in J. \end{gathered} \tag{2.9}$$

For all $j \in J$ we must show that there exist $\pi_j > 0$ satisfying

$$\pi_j = x_j \prod_{i=1}^{m} z_i^{c_{ij}} \quad \forall j \in J, \qquad \sum_{j \in J} c_{ij}\pi_j = b_i \quad (i = 1, \dots, m) \tag{2.10}$$

for some $z_1 > 0, \dots, z_m > 0$. For j not in J we have $x_j = 0$, and we simply set $\pi_j = 0$ to complete the solution of the equations (2.8).

Thus, with no loss of generality, we may assume that *all* components x_j and y_i are positive for $j = 1, \dots, n$. In this form Theorem 1 was proved by Darroch and Ratcliff [7]. Their proof is constructive, but the following proof is perhaps easier.

According to our lemma, there exists a unique point u^0 achieving

$$\min_u \left\{ \sum_{j=1}^{n} u_j \log \frac{u_j}{x_j} : u \geqslant 0, \ Cu = b \right\}.$$

Necessarily, $u^0 > 0$, $Cu^0 = b$, and

$$1 + \log \frac{u_j^0}{x_j} = \sum_{i=1}^{m} q_i c_{ij} \qquad (j = 1, \dots, n)$$

for some Lagrange multipliers q_i. Taking exponentials, we find

$$\pi_j = x_j \prod_{i=1}^{m} z_i^{c_{ij}} \qquad (j = 1, \dots, n),$$

where $\pi_j = eu_j^0$ and $z_i = \exp(q_i)$. ■

We now quote Theorems 2 and 3 in the report [2] by Bapat and Raghavan.

THEOREM 2. *Let $X = (x_{ij})$, $Y = (y_{ij})$ be two $r \times s$ matrices with nonnegative entries. Let $x_{ij} = 0 \Leftrightarrow y_{ij} = 0$ for any i, j. Let the row sums and column sums of Y be positive. Then there exist $u_1, u_2, \dots, u_r$, $v_1, v_2, \dots, v_s$, all positive, such that $(\pi_{ij}) = (x_{ij}u_i v_j)$ has the same row sums and column sums as Y.*

THEOREM 3. *Let $X = (x_{ijk})$, $Y = (y_{ijk})$ be two $r \times s \times t$ matrices with nonnegative entries and with the same zero pattern (i.e., $x_{ijk} = 0 \Leftrightarrow y_{ijk} = 0$).*

If the one-dimensional marginals $\Sigma_j\Sigma_k y_{ijk}$, $\Sigma_i\Sigma_k y_{ijk}$, $\Sigma_i\Sigma_j y_{ijk}$ *are all positive, then there exist positive scalars* $u_1, u_2, \dots, u_r$, $v_1, v_2, \dots, v_s$, $w_1, w_2, \dots, w_t$ *such that* $(\pi_{ijk}) = (x_{ijk}u_i v_j w_k)$ *has the same one-dimensional marginals as* Y.

Bapat and Raghavan derive these theorems from their Theorem 1. We will prove Theorem 3 directly from our elementary lemma. Theorem 2 could be proved in exactly the same way, as could the obvious extension to multidimensional matrices of arbitrary dimension $d > 3$.

Proof of Theorem 3. Assume $y_{ijk} > 0$ and $x_{ijk} > 0$ for $(i, j, k) = (i_\nu, j_\nu, k_\nu)$ $(\nu = 1, \dots, n)$. For all z in $\mathbf{P}^n$ we define

$$z_{i_\nu j_\nu k_\nu} = z_\nu \geqslant 0 \qquad (\nu = 1, \dots, n), \tag{2.11}$$

and we define $z_{ijk} = 0$ if $y_{ijk} = x_{ijk} = 0$.

The given marginal equations for Y can be expressed in the form $Cy = b$ where $y > 0$, $y \in \mathbf{P}^n$, and $b > 0$, $b \in \mathbf{P}^m$, with $m = r + s + t$. If q is any vector in $\mathbf{R}^m$, we may write

$$q^T = (\alpha_1, \dots, \alpha_r, \beta_1, \dots, \beta_s, \gamma_1, \dots, \gamma_t).$$

Then for all z in $\mathbf{P}^n$ we have the bilinear form

$$q^T C z = \sum_{i=1}^{r} \sum_{j=1}^{s} \sum_{k=1}^{t} (\alpha_i + \beta_j + \gamma_k) z_{ijk} \tag{2.12}$$

expressed as triple sum.

For all $z \in \mathbf{P}^n$ define the function

$$\Phi(z) = \sum_{\nu=1}^{n} z_\nu \log \frac{z_\nu}{x_\nu}, \tag{2.13}$$

where $\{x_1, \dots, x_n\} = \{x_{ijk} : x_{ijk} > 0\}$, according to (2.11). By our elementary lemma, there exists a unique z^0 in $\mathbf{P}^n$ such that

$$\Phi(z^0) = \min\{\Phi(z) : z \in \mathbf{P}^n,\ Cz = b\}. \tag{2.14}$$

Necessarily, $z^0 > 0$; and z^0 is the unique point z such that $z > 0$, $Cz = b$, and

$$\frac{\partial}{\partial z_j}\left[\Phi(z) - q^T Cz\right] = 0 \qquad (j = 1, \dots, n) \tag{2.15}$$

for some point $q \in \mathbf{R}^m$.

Using Equations (2.11), (2.12), and (2.13), we write the Lagrange equations (2.15) in the form

$$1 + \log\frac{z^0_{ijk}}{x_{ijk}} - (\alpha_i + \beta_j + \gamma_k) = 0$$

for all i, j, k such that x_{ijk} is positive. Taking exponentials, we find

$$ez^0_{ijk} = x_{ijk}e^{\alpha_i}e^{\beta_j}e^{\gamma_k} \tag{2.16}$$

for all $x_{ijk} > 0$. Naturally, these equations also hold for $x_{ijk} = z^0_{ijk} = 0$. If we now identify

$$\pi_{ijk} = ez^0_{ijk}, \qquad u_i = e^{\alpha_i}, \qquad v_j = e^{\beta_j}, \qquad w_k = e^{\gamma_k},$$

we obtain the theorem of Bapat and Raghavan. ■

We note that our lemma implies the uniqueness of the vector z^0 and hence the uniqueness of the three-dimensional matrix (π_{ijk}).

Of course, one can generalize Theorem 3 to multidimensional matrices of any dimension and to consistent marginals of any dimension.

EXAMPLE. Suppose $X = (x_{ijkl})$ and $Y = (y_{ijkl})$ are nonnegative four-dimensional matrices with the same zero pattern. Let Y have the three-dimensional marginals

$$y_{ijk\cdot} = \alpha_{ijk}, \qquad y_{ij\cdot l} = \beta_{ijl}, \qquad y_{i\cdot kl} = \gamma_{ikl}, \qquad y_{\cdot jkl} = \delta_{jkl}.$$

Then there is a unique four-dimensional array π_{ijkl} such that $\forall\, i, j, k, l$

$$\pi_{ijkl} = x_{ijkl}t_{ijk}u_{ijl}v_{ikl}w_{jkl}$$

for some positive three-dimensional arrays T, U, V, W, where (π_{ijkl}) has the same three-dimensional marginals as Y.

Here the Lagrange function has the form

$$\Phi(z) = \sum_{i,j,k,l:\, x_{ijkl}>0} \left(z_{ijkl} \log \frac{z_{ijkl}}{x_{ijkl}} - \left(\alpha'_{ijk} + \beta'_{ijl} + \gamma'_{ikl} + \delta'_{jkl} \right) z_{ijkl} \right).$$

The required result follows directly from our elementary lemma.

One of the first results on matrix scaling of this type was published by R. Sinkhorn in 1964. We quote from his paper [16]:

THEOREM. *To a given strictly positive $N \times N$ matrix A there corresponds exactly one doubly stochastic matrix T_A which can be expressed in the form $T_A = D_1 A D_2$ where D_1 and D_2 are diagonal matrices with positive diagonals. The matrices D_1 and D_2 are themselves unique up to a scalar factor.*

This result follows immediately from the result of Bapat and Raghavan for two-dimensional matrices. We define $x_{ij} = a_{ij} > 0$, $y_{ij} = N^{-1} > 0$ for all i, j. Then we find positive π_{ij}, u_i, v_j such that

$$\pi_{ij} = x_{ij} u_i v_j, \quad \pi_{i\cdot} = 1, \quad \pi_{\cdot j} = 1 \qquad (i, j = 1, \dots, N). \tag{2.17}$$

Setting $T_A = (\pi_{ij})$, $D_1 = \operatorname{diag}(u_i)$, $D_2 = \operatorname{diag}(v_j)$, we get Sinkhorn's theorem.

R. A. Brualdi, S. V. Parter, and Hans Schneider [5] published a generalization of Sinkhorn's theorem. They derived the same conclusion assuming only that the $N \times N$ matrix A is nonnegative and fully indecomposable. This generalization was discovered independently and proved differently by R. Sinkhorn and Paul Knopp [17]. We can easily prove this generalization if we use a result [14] of H. Perfect and L. Mirsky: for every fully indecomposable matrix A there exists a doubly stochastic matrix Y with the same zero pattern. The generalization now follows directly from Theorem 2. As in Sinkhorn's original theorem [16], the doubly stochastic matrix T_A is uniquely determined by A. Since A is fully indecomposable, the diagonal matrices D_1 and D_2 are uniquely determined up to scalar factors.

Sinkhorn proved his theorem by an iterative procedure, which we will discuss in the following section.

3. HILBERT'S PROJECTIVE METRIC AND SINKHORN'S ITERATION

Sinkhorn's Iteration

We are given a positive $m \times n$ matrix $A = (a_{ij})$ and positive vectors $p \in \mathbf{R}^m$, $q \in \mathbf{R}^n$ with

$$p_1 + \cdots + p_m = q_1 + \cdots + q_n.$$

The aim of Sinkhorn's iteration [18] is to find a positive matrix $\hat{B}$ of the form D_1AD_2, where D_1 and D_2 are diagonal matrices, which has row sums $p_1,\dots,p_m$ and column sums $q_1,\dots,q_n$. We denote by e the vector $e=(1,1,\dots,1)^T$ of dimension m or n. Starting with $A_0=A$, Sinkhorn defines the sequences A_k, A'_k of column and row normalized matrices by the following process.

(1) Let $r^{(k)}=A_ke$ denote the vector of row sums, and let

$$A'_k=S_kA_k,\qquad S_k=\operatorname{diag}\left(p_i/r_i^{(k)}\right)$$

denote the row normalized matrix.

(2) Let $c^{(k)}=A_k'^Te$ denote the vector of column sums, and let

$$A_{k+1}=A'_kT_k,\qquad T_k=\operatorname{diag}\left(q_j/c_j^{(k)}\right)$$

denote the column normalized matrix.

Then Sinkhorn shows convergence

$$A_k\to\hat{B},\quad A'_k\to\hat{B}\qquad\text{as}\quad k\to\infty,$$

where $\hat{B}=D_1AD_2$ is the unique matrix which is diagonally equivalent to A and has the prescribed row and column sums, i.e.,

$$\hat{B}e=p,\qquad\hat{B}^Te=q.$$

Hilbert's Projective Metric

We want to apply Hilbert's projective metric and a result of G. Birkhoff to study the Sinkhorn iteration. One obtains immediately a geometric rate of convergence, and the rate factor can be estimated *a priori*. As in similar applications of the contraction-mapping theorem, one can derive error bounds from computable quantities.

Let $\mathbf{R}^m_+$ denote the set of all vectors $x\in\mathbf{R}^m$ with $x_i>0$, $i=1,\dots,m$. Then

$$d(x,x')=\log\max_{i,k}\frac{x_ix'_k}{x'_ix_k}$$

defines a projective metric on $\mathbf{R}^m_+$; i.e., the following rules are valid for $x, x', x'' \in \mathbf{R}^m_+$:

$$d(x,x') = 0 \quad \Leftrightarrow \quad x = \alpha x' \qquad \text{for some scalar} \quad \alpha > 0; \tag{3.1}$$

$$d(x,x') = d(x',x); \tag{3.2}$$

$$d(x,x'') \leqslant d(x,x') + d(x',x''). \tag{3.3}$$

The function d is known as Hilbert's projective metric. (See Bushell [6] for a survey of applications and historical remarks; see Kohlberg [9] and Kohlberg and Pratt [10] for further applications and extensions.)

A positive $m \times n$ matrix $A = (a_{ij})$ maps $\mathbf{R}^n_+$ into $\mathbf{R}^m_+$. The number

$$\begin{aligned} \vartheta(A) &= \sup\{ d(Ay, Ay') : y, y' \in \mathbf{R}^+_n \} \\ &= \max_{i,j,k,l} \frac{a_{ik}a_{jl}}{a_{jk}a_{il}} \end{aligned} \tag{3.4}$$

measures the diameter of the image. The following result is essentially due to Birkhoff [4]; see also Bauer [3].

LEMMA 1. *Let*

$$\kappa(A) = \sup\left\{ \frac{d(Ay, Ay')}{d(y,y')} : y, y' \in \mathbf{R}^n_+ ,\ y \neq \alpha y' \right\}$$

denote the contraction ratio of A. *Then*

$$\kappa(A) = \frac{\vartheta(A)^{1/2} - 1}{\vartheta(A)^{1/2} + 1}. \tag{3.5}$$

Let us write $A \sim B$ if A and B are two positive $m \times n$ matrices that are diagonally equivalent, i.e., there are two diagonal matrices X, Y with positive diagonal entries such that $B = XAY$.

The formula (3.4) for $\vartheta(A)$ shows that

$$A \sim B \quad \text{implies} \quad \vartheta(A) = \vartheta(B). \tag{3.6}$$

Therefore, the contraction ratio $\kappa(A_k)$ does not change during the iteration. The rules

$$\vartheta(A)=\vartheta(A^T), \qquad \kappa(A)=\kappa(A^T), \tag{3.7}$$

$$\kappa(A_1A_2)\leqslant\kappa(A_1)\kappa(A_2) \tag{3.8}$$

follow from (3.4), (3.5), and the definition of κ.

NOTATION. For positive vectors x, x' let x/x' denote the vector with components x_i/x_i'.

It is easy to show that

$$d(x/x',e)=d(x,x').$$

The key observation which connects Sinkhorn's iteration with Hilbert's metric and Birkhoff's result is

LEMMA 2. *Let $A=A_0$ be column normalized, i.e., $A^Te=q$. Then*

$$d(r^{(1)},p)\leqslant\gamma d(r^{(0)},p),$$

$$d(c^{(1)},q)\leqslant\gamma d(c^{(0)},q)$$

where $\gamma=\kappa(A)^2$.

Proof. We write $A'=A_0'$. From $r^{(1)}=A_1e=A'T_0e=A'q/c^{(1)}$ and $A'e=p$ we find

$$\begin{aligned}d(r^{(1)},p)&=d\left(A'\frac{q}{c^{(1)}},A'e\right)\\&\leqslant\kappa(A)d\left(\frac{q}{c^{(1)}},e\right)\\&=\kappa(A)d(q,c^{(1)}).\end{aligned}$$

Furthermore,

$$c^{(1)} = A'^T e = A^T S_0 e = A^T \frac{p}{r^{(0)}}$$

and $A^T e = q$ imply

$$d(q, c^{(1)}) = d\left(A^T e, A^T \frac{p}{r^{(0)}} \right) \leqslant \kappa(A^T) d(r^{(0)}, p).$$

This gives the estimate for the row sums. The estimate for the column sums follows similarly.

By construction, all matrices A_k, $k \geqslant 1$, are column normalized. Hence, repeated application of the previous lemma yields

$$d(r^{(k)}, p) \leqslant \gamma^k d(r^{(0)}, p),$$

$$d(c^{(k)}, q) \leqslant \gamma^k d(c^{(0)}, q).$$

Main Result

For the given positive $m \times n$ matrix A let

$$E_A = \{ B: A \sim B, b_{ij} > 0 \}$$

denote the set of matrices diagonally equivalent to A. If

$$B, B' \in E_A, \qquad B = XB'Y, \quad X = \operatorname{diag}(x_i), \quad Y = \operatorname{diag}(y_j),$$

then we set

$$\Delta(B, B') = d(x, e) + d(y, e).$$

This defines a metric Δ on the set E_A. It is not difficult to show that (E_A, Δ) is a complete metric space. Our main result is

THEOREM 4. *Assume $A^T e = q$, and let A_k, A'_k denote the sequences of Sinkhorn's iteration. Let $\hat{B}$ denote the unique matrix with*

$$\hat{B}e = p, \qquad \hat{B}^T e = q, \qquad \hat{B} \sim A.$$

Then

$$\Delta(A_k, \hat{B}) \leqslant \frac{1}{1-\gamma}\{d(r^{(k)}, p) + d(c^{(k)}, q)\}$$

$$\leqslant \frac{\gamma^k}{1-\gamma}\{d(r^{(0)}, p) + d(c^{(0)}, q)\}.$$

Similarly,

$$\Delta(A'_k, \hat{B}) \leqslant \frac{1}{1-\gamma}\{d(r^{(k+1)}, p) + d(c^{(k)}, q)\}$$

$$\leqslant \frac{\gamma^k}{1-\gamma}\{d(r^{(1)}, p) + d(c^{(0)}, q)\},$$

where $\gamma = \kappa(A)^2$.

Proof. Recall $A_{k+1} = S_k A_k T_k$, where

$$S_k = \operatorname{diag}(s_i^{(k)}), \qquad s^{(k)} = \frac{p}{r^{(k)}},$$

$$T_k = \operatorname{diag}(t_j^{(k)}), \qquad t^{(k)} = \frac{q}{c^{(k)}}.$$

Thus we obtain

$$\Delta(A_k, A_{k+1}) = d\left(\frac{p}{r^{(k)}}, e\right) + d\left(\frac{q}{c^{(k)}}, e\right)$$

$$= d(r^{(k)}, p) + d(c^{(k)}, q)$$

$$\leqslant \gamma^k\{d(r^{(0)}, p) + d(c^{(0)}, q)\}.$$

By the triangle inequality,

$$\Delta(A_0, A_{l+1}) \leqslant (1 + \cdots + \gamma^l)\{d(r^{(0)}, p) + d(c^{(0)}, q)\},$$

and we obtain for $l \to \infty$

$$\Delta(A_0, \hat{B}) \leqslant \frac{1}{1-\gamma}\{d(r^{(0)}, p) + d(c^{(0)}, q)\}.$$

This proves the first estimate for $k = 0$. The result for general k and for A'_k follows in the same way. ■

NOTE. In our proof we used the convergence $A_l \to \hat{B}$ in (E_A, Δ), which follows from the convergence in the usual sense; the latter is proved in [18]. However, if we use the completeness of the metric space (E_A, Δ), then the existence of the limit $\hat{B}$ and the convergence $A_l \to \hat{B}$ in (E_A, Δ) also follow independently.

Error Bounds

Suppose a bound

$$\Delta(A_k, \hat{B}) \leqslant \epsilon$$

has been computed. Then an application of the following lemma gives the estimate

$$\exp(-\epsilon) \leqslant \frac{\hat{b}_{ij}}{a_{ij}^{(k)}} \leqslant \exp(\epsilon). \tag{3.9}$$

LEMMA 3. *Let $A \sim B$ and $A^Te = B^Te$. If $\Delta(A, B) \leqslant \epsilon$, then*

$$\exp(-\epsilon) \leqslant \frac{b_{ij}}{a_{ij}} \leqslant \exp(\epsilon)$$

for all i, j.

Proof. There exist diagonal matrices X, Y with $XAY = B$ and

$$d(x, e) \leqslant \epsilon, \qquad d(y, e) \leqslant \epsilon.$$

Here X has the positive diagonal entries x_i, etc. We can scale the minimum element of x to be one and have

$$1 \leqslant x_i \leqslant \exp(\epsilon), \qquad i = 1, \ldots, m. \tag{3.10}$$

From $YA^T = B^T X^{-1}$ and $A^T e =: q = B^T e$ it follows that

$$Yq = YA^T e = B^T X^{-1} e. \tag{3.11}$$

The following vector inequalities are understood componentwise. The estimate (3.10) gives

$$\exp(-\epsilon)\, e \leqslant X^{-1} e \leqslant e;$$

thus, if we multiply by B^T,

$$\exp(-\epsilon) q \leqslant B^T X^{-1} e \leqslant q.$$

Now (3.11) implies the inclusion

$$\exp(-\epsilon) \leqslant y_j \leqslant 1, \qquad j = 1, \dots, n.$$

Therefore the estimate

$$\exp(-\epsilon) \leqslant x_i y_j = b_{ij}/a_{ij} \leqslant \exp(\epsilon)$$

follows from (3.10). ∎

We finally give two simple examples to demonstrate the usefulness of Hilbert's metric and Birkhoff's theorem in the present context of diagonal equivalence of matrices. Theorem 4 and Equation (3.9) allow one to compute error bounds

$$\lambda_k^{-1} \leqslant \frac{\hat{b}_{ij}}{a_{ij}^{(k)}} \leqslant \lambda_k, \qquad \lambda_k = \exp(\epsilon),$$

$$\epsilon = \frac{1}{1-\gamma}\left\{ d(r^{(k)}, p) + d(c^{(k)}, q) \right\}. \tag{3.12}$$

In our examples we compute the actual limit $\hat{B}$ of the sequence A_k, and we compare the bounds (3.12) with the actual error $\hat{\lambda}_k$, defined as the *smallest* constant with

$$\hat{\lambda}_k^{-1} \leqslant \frac{\hat{b}_{ij}}{a_{ij}^{(k)}} \leqslant \hat{\lambda}_k \qquad \text{for all } i, j.$$

EXAMPLE 1.

$$p = q = \left(\tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}\right)^T,$$

$$A = A_0 = \frac{1}{30}\begin{bmatrix} 1 & 3 & 8 \\ 1 & 4 & 1 \\ 8 & 3 & 1 \end{bmatrix},$$

$$\hat{B} = \begin{pmatrix} 0.029629630 & 0.066666667 & 0.237037037 \\ 0.066666667 & 0.2 & 0.066666667 \\ 0.237037037 & 0.066666667 & 0.029629630 \end{pmatrix},$$

$$\vartheta(A) = 64, \qquad \kappa(A) = \tfrac{7}{9}, \qquad \gamma = \tfrac{49}{81}.$$

The results are shown in Table 1.

In the next example γ is much smaller.

TABLE 1

ACTUAL ERROR AND ERROR BOUND

k	$\hat{\lambda}_k$	λ_k
0	2.0	10.643722
1	1.1	1.418624
2	1.015094	1.057195
3	1.002393	1.008932
4	1.000382	1.001424
5	1.000061	1.000228

TABLE 2

ACTUAL ERROR AND ERROR BOUND

k	$\hat{\lambda}_k$	λ_k
0	1.165685425	1.344914461
1	1.001839973	1.002817612
2	1.000001594	1.000002439
3	1.000000001	1.000000002

EXAMPLE 2.

$$p = q = \left(\tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}\right)^T,$$

$$A = A_0 = \frac{1}{30}\begin{pmatrix} 3 & 4 & 4 \\ 3 & 3 & 3 \\ 4 & 3 & 4 \end{pmatrix},$$

$$\hat{B} = \begin{pmatrix} 0.093836321 & 0.125115095 & 0.114381917 \\ 0.114381917 & 0.114381917 & 0.104569950 \\ 0.125115095 & 0.093836321 & 0.114381917 \end{pmatrix},$$

$$\vartheta(A) = \tfrac{16}{9}, \qquad \kappa(A) = \tfrac{1}{7}, \qquad \gamma = \tfrac{1}{49}.$$

The results are shown in Table 2.

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