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CMMSE Algorithms for constructing Doubly Stochastic Matrices with the Relative Gain Array (Combined matrix) $A \circ A^{-T}$

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Abstract The Combined matrix of a nonsingular matrix A is defined by $\phi(A) = A \circ \left(A^{-1}\right)^T$ where $\circ$ means the Hadamard (entrywise) product. If the matrix A describes the relation between inputs and outputs in a multivariable process control, $\phi(A)$ describes the "relative gain array" (RGA) of the process and it defines the Bristol method [1] often used for Chemical processes [13, 15, 16]and [11, 8]. The combined matrix has been studied in several works such as [3], [6] and [10]. Since $\phi(A) = (c_{ij})$ has the property of $\sum_k c_{ik} = \sum_k c_{kj} = 1, \forall i, j$, when $\phi(A) \geq 0$, $\phi(A)$ is a doubly stochastic matrix. In certain chemical engineering applications a diagonal of the RGA in wchich the entries are near 1 is used to determine the pairing of inputs and outputs for further design analysis. Applications of these matrices can be found in Communication Theory, related with the satellite-switched time division multiple-access systems, and about a doubly stochastic automorphism of a graph. In this paper we present new algorithms to generate doubly stochastic matrices with the Combined matrix using Hessenberg matrices in section 3 and orthogonal/unitary matrices in section 4. In addition, we discuss what kind of doubly stochastic matrices are obtained with our algorithms and the possibility of generating a particular doubly stochastic matrix by the map ϕ.

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1 Introduction

Miroslav Fiedler ([5]) studied matrices of the form $A \circ A^{-1}$ and $A \circ A^{-T}$, where A is a nonsingular matrix and $\circ$ means the Hadamard product. Furthermore, the combined matrix $\phi(A) = A \circ A^{-T}$ gives the relation between eigenvalues and diagonal entries of a diagonalizable matrix ([9]). Results for the combined matrix of a nonsingular matrix have been obtained, for instance in [6] and [10]. It is well known ([9]) that the row and column sums of a combined matrix are always equal to one. Then, if $\phi(A)$ is a nonnegative matrix, it has interesting properties and applications since it is a doubly stochastic matrix. For instance, in [2], there are two applications, the first one concerning a topic in communication theory called satellite-switched and the second concerning a recent notion of doubly stochastic automorphism of a graph. In [14], some implications on nonnegative matrices and doubly stochastic matrices on graph theory, namely Graph spectra and Graph energy, are presented. In [3], conditions to obtain a nonnegative $\phi(A)$ are obtained.

Not long after, Edgard H. Bristol [1] gives a method based on the Hadamard product $A \circ A^{-T}$ of the state matrix of a multivariable control process. In this context, this product represents the "relative gain array" and is known as RGA for some authors. There are many works where the Bristol method has been used mainly in chemical information processing (see [13, 15, 16],[11]) for example in the extractive distillation control, Hodvd et al ([17]) applied (RGA) as a loop pairing criterion. Specifically the extractive distilation process for the separation of an ethyl formate-ethanol-water mixture with ethylene glycol as the extractive solvent was investigated with an Effective Relative Gain Array is used in ([18]). By other hand, in the study of chemical information processing, Golender et al.([8]) introduced another important matrix: doubly stochastic graph matrix associated with a graph, which may be used to describe some properties of the topological structure of chemical molecules.

In the next sections, we present new algorithms for constructing doubly stochastic matrices with (RGA) using Hessenberg matrices in section 3 and orthogonal/unitary matrices in section 4. The algorithms we show here are been implemented in Scilab.

2 Notation and previous results

For any $n \times n$ matrix A, we denote the submatrix lying in rows α and columns β, in which $\alpha, \beta \subseteq N = \{1, ..., n\}$, by $A[\alpha|\beta]$, and the principal submatrix $A[\alpha|\alpha]$ is abbreviated to $A[\alpha]$. Similarly, $A(\alpha|\beta)$ denotes the submatrix obtained from A by deleting rows α and columns β and $A(i|j)$ is abbreviated A_{ij}.

We recall that a matrix A is P-matrix (P_0-matrix) if all its principal minors of any order are positive (nonnegative). That is, if for every subsets $\alpha \subseteq N$: $\det(A[\alpha]) > 0(\geq 0)$.

Remember that the Hadamard (or entry–wise) product of two $n \times n$ matrices $A = [a_{ij}]$ and $B = [b_{ij}]$ is the matrix $A \circ B = [a_{ij} b_{ij}]$.

Definition 1 The combined matrix of a nonsingular real matrix A is defined as $\phi(A) = A \circ (A^{-1})^T$. Then, if $A = [a_{ij}]$,

$$A^{-1} = \left[\frac{1}{\det(A)} (-1)^{i+j} A_{ji} \right]$$

and

$$\phi(A) = \left[\frac{1}{\det(A)} (-1)^{i+j} a_{ij} A_{ij} \right].$$

It is clear that the combined matrix has the following properties: (i) $\phi(A)$= $\phi(A^T) = \phi(A^{-1})$ and (ii) $\phi(A)$ is doubly stochastic if $\phi(A)$ is nonnegative.

3 An algorithm for constructing doubly stochastic matrices with upper Hessenberg matrices

We will present an algorithm constructing doubly stochastic matrices from a special kind of upper Hessenberg matrices.

Recall that a Hessenberg matrix is a square matrix almost triangular. More precisely, A is called *upper Hessenberg* if it has zero entries below the first subdiagonal, i.e. if $a_{ij} = 0$ when $i > j+1$, and it is called *lower Hessenberg* if A^T is an upper Hessenberg matrix.

We can prove, by an inductive argument, that, if A is an upper Hessenberg matrix with nonnegative entries above the diagonal, positive diagonal entries, and nonpositive entries in the first sub-diagonal, namely, a matrix with this signpattern:

$$A = \begin{bmatrix} + & \cdots & \cdots & \cdots & + \\ - & \ddots & \cdots & \cdots & + \\ 0 & \ddots & \ddots & \cdots & + \\ \vdots & \ddots & \ddots & \ddots & + \\ 0 & \cdots & 0 & - & + \end{bmatrix}$$

then, $\phi(A)$ is a doubly stochastic matrix.

We need the following technical lemmas in order to get the main result of this section.

Lemma 1 *If $H = [h_{ij}]$ is an $n \times n$ matrix satisfying*

$$\begin{aligned} h_{i+1,i} &\leq 0 \\ h_{ij} &\geq 0, \quad \text{if } i \leq j \\ h_{ij} &= 0, \quad \text{otherwise} \end{aligned} \tag{1}$$

then

(i) *The matrix H is a P_0-matrix.*
(ii) *If $h_{ii} > 0$, $1 \leq i \leq n$, then, matrix H is a P-matrix.*

Proof The proof is by induction on n. To simplify notation we suppose $a_{ij} \geq 0$, $i, j = 1, 2, \ldots, n$, to show the sign of H entries.

Note that for $n = 1$ and 2 (and principal minors of these orders) the Hessenberg structure is not complete but the result is trivial. For $n = 3$ matrix H has the form

$$H = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ -a_{21} & a_{22} & a_{23} \\ 0 & -a_{23} & a_{33} \end{bmatrix}$$

then $\det H = a_{23} \det H_{23} + a_{33} \det H_{33} \geq 0$.

Suppose that the result holds for $(n-1) \times (n-1)$ matrices. In order to proof it for an $n \times n$ matrix H, we only need to prove that $\det H \geq 0$ (and $\det H > 0$ when $a_{ii} > 0$):

$$\begin{aligned} \det H =& \det \begin{bmatrix} a_{11} & a_{12} & & a_{1n-1} & a_{1n} \\ -a_{21} & a_{22} & & a_{2n-1} & a_{2n} \\ 0 & -a_{32} & \ddots & a_{3n-1} & a_{3n} \\ \vdots & \vdots & \ddots\ \ddots & \vdots & \vdots \\ 0 & 0 & \ddots & a_{n-1n-1} & a_{n-1n} \\ 0 & 0 & & -a_{nn-1} & a_{nn} \end{bmatrix} \\ =& a_{11} \det \begin{bmatrix} a_{22} & a_{23} & & a_{2n-1} & a_{2n} \\ -a_{32} & a_{33} & & a_{3n-1} & a_{3n} \\ 0 & -a_{32} & \ddots & a_{3n-1} & a_{3n} \\ \vdots & \vdots & \ddots\ \ddots & \vdots & \vdots \\ 0 & 0 & \ddots & a_{n-1n-1} & a_{n-1n} \\ 0 & 0 & & -a_{nn-1} & a_{nn} \end{bmatrix} \\ &+ a_{21} \det \begin{bmatrix} a_{12} & a_{13} & & a_{1n-1} & a_{1n} \\ -a_{32} & a_{33} & & a_{3n-1} & a_{3n} \\ 0 & -a_{32} & \ddots & a_{3n-1} & a_{3n} \\ \vdots & \vdots & \ddots\ \ddots & \vdots & \vdots \\ 0 & 0 & \ddots & a_{n-1n-1} & a_{n-1n} \\ 0 & 0 & & -a_{nn-1} & a_{nn} \end{bmatrix} \\ =& a_{11} \det H_{11} + a_{21} \det H_{21} \geq 0 \end{aligned}$$

Moreover, if $a_{ii} > 0$, then $\det H > 0$, because $a_{11} > 0$ and $\det H_{11} > 0$. $\square$

Lemma 2 *Let H be a square matrix satisfying* (1)*, then*

(i) $\det H_{i+1,i} \geq 0, \quad 1 \leq i \leq n-1$
(ii) $(-1)^{i+j} \det H_{ij} \geq 0, \quad 1 \leq i \leq j \leq n$

where $\det H_{ij} = \det(H(i|j)$ is the complementary minor of a_{ij}.

Proof

(i) By using $a_{ij} \geq 0$, for all i, j, $H_{i+1,i}$ has the form

$$H_{i+1,i} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1,i-1} & a_{1,i+1} & \cdots\cdots & a_{1,n-1} & a_{1n} \\ -a_{21} & a_{22} & \cdots & a_{2,i-1} & a_{2,i+1} & \cdots\cdots & a_{2,n-1} & a_{2n} \\ 0 & -a_{32} & \cdots & a_{3,i-1} & a_{3,i+1} & & a_{3,n-1} & a_{3n} \\ \vdots & \vdots & \ddots & & & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & -a_{i,i-1} & a_{i,i+1} & & a_{i,n-1} & a_{in} \\ 0 & 0 & \cdots & 0 & -a_{i+2,i+1} & \ddots & a_{i+2,n-1} & a_{i+2,n} \\ \vdots & \vdots & \ddots & & & \ddots\;\ddots & \vdots & \vdots \\ 0 & 0 & & \ddots & & \ddots & a_{n-1,n-1} & a_{n-1,n} \\ 0 & 0 & & & & & -a_{n,n-1} & a_{nn} \end{bmatrix}$$

So, applyng lemma 1, $\det H_{i+1,i} \geq 0$.

(ii)

$$H_{ij} = \left[\begin{array}{ccccc|ccc|cccc} a_{11} & a_{12} & \cdots & a_{1,i-2} & a_{1,i-1} & a_{1i} & \cdots & a_{1,j-1} & a_{1,j+1} & \cdots & \cdots & a_{1n} \\ -a_{21} & a_{22} & \cdots & a_{2,i-2} & a_{2,i-1} & a_{2i} & \cdots & a_{2,j-1} & a_{2,j+1} & \cdots & \cdots & a_{2n} \\ 0 & \ddots & \ddots & \ldots & \vdots & & & & & & & \\ \vdots & & & & & & & & & & & \\ 0 & 0 & \cdots & -a_{i-1,i-2} & a_{i-1,i-1} & a_{i-1,i} & \cdots & a_{i-1,j-1} & a_{i-1,j+1} & \cdots & \cdots & a_{i-1,n} \\ \hline 0 & & \cdots & & 0 & -a_{i+1,i} & \cdots & a_{i+1,j-1} & a_{i+1,j+1} & \cdots & \cdots & a_{i+1,n} \\ \vdots & & & & \vdots & 0 & \ddots & \vdots & \vdots & & & \vdots \\ 0 & & \cdots & & 0 & 0 & \cdots & -a_{j,j-1} & a_{j,j+1}\cdots & \cdots & \cdots & a_{jn} \\ \hline \vdots & & & & \vdots & 0 & \cdots & 0 & a_{j+1,j+1} & \cdots & a_{j+1,n-1} & a_{j+1,n} \\ 0 & & \cdots & & 0 & 0 & \cdots & 0 & -a_{j+2,j+1} & \cdots & a_{j+2,n-1} & a_{j+2,n} \\ & & & & & & & & 0 & \ddots & \ddots & \vdots \\ 0 & & \cdots & & 0 & 0 & \cdots & 0 & 0 & \cdots & -a_{n,n-1} & a_{nn} \end{array}\right]$$

If we denote by B_i, $1 \leq i \leq 3$ the diagonal blocks of the previous block triangular expression of H_{ij} then

$$\det H_{ij} = \det B_1 \det B_2 \det B_3 = (-1)^{j-i} \det B_1 \left(\prod_{k=i+1}^{j} a_{k,k-1} \right) \det B_3.$$

By using the hypothesis of induction and (1),

$$(-1)^{i+j} \det H_{ij} = \det B_1 \left(\prod_{k=i+1}^{j} a_{k,k-1} \right) \det B_3 \geq 0 \square$$

The next result is an immediate consequence of these lemmas.

Theorem 1 *If H is a square matrix satisfying conditions* (1) *then $\phi(H)$ and $\phi\left(H^T\right) = \phi(H)^T$ are doubly stochastic matrices.*

Using this result we can obtain several doubly stochastic matrices.

Algorithm 1 (This algorithm builds an $n \times n$ doubly stochastic matrix from $(n^2 + 3n - 2)/2$ real numbers)

Given an arbitrary set of real numbers $T = \{t_{i,j} : 1 \leq i \leq n, i-1 \leq j \leq n\}$ with $t_{i,i} \neq 0$, $1 \leq i \leq n$,

- Define the $H = [h_{ij}]$ matrix as $h_{ij} = \begin{cases} |t_{i,j}| & \text{if } i \leq j \\ -|t_{i+1,i}| & \\ 0 & \text{otherwise} \end{cases}$
- Compute $A = H \circ H^{-T}$

Example 1 Applying algorithm 1, for $T = \{1, 2, \ldots, 13\}$, we obtain an upper Hessenberg matrix, H, and the doubly stochastic matrix, A:

$$H = \begin{bmatrix} 1 & 2 & 3 & 4 \\ -5 & 6 & 7 & 8 \\ 0 & -9 & 10 & 11 \\ 0 & 0 & -12 & 13 \end{bmatrix} \qquad A = \phi(H) = \begin{bmatrix} 0.332 & 0.268 & 0.179 & 0.221 \\ 0.668 & 0.161 & 0.084 & 0.088 \\ 0. & 0.572 & 0.212 & 0.216 \\ 0. & 0. & 0.525 & 0.475 \end{bmatrix}$$

Note that, since $\phi(D_1 A D_2) = \phi(A)$ when D_1, D_2 are nonsingular diagonal matrices, it is of no interest to study another signpattern. Moreover, since $\phi(P_1 A P_2) = P_1 \phi(A) P_2$ where P_1 and P_2 are permutation matrices, we conclude the following statement

Corollary 1 *If A is an $n \times n$ upper Hessenberg matrix with the signpattern of theorem 1 and P_1 and P_2 are $n \times n$ permutation matrices, $\phi(P_1 A P_2)$ and $\phi(P_1 A^T P_2)$ are doubly stochastic matrices.*

4 An algorithm for constructing doubly stochastic matrices from orthogonal (or unitary) matrices

If Q is an orthogonal matrix then, $\phi(Q)$ is a doubly stochastic matrix, because $Q \circ Q^{-T} = Q \circ Q$ is obviously a nonnegative matrix. So, an algorithm that provides an orthogonal matrix defines a double stochastic matrix.

In the literature, we find several algorithms to construct orthogonal matrices, especially orthogonal matrices with rational entries. For example, Cremona in [4] shows how to generate all 3×3 orthogonal matrices with rational elements, working with the real algebra of quaternions. More generally, [7, p. 289] shows a one-to-one correspondence between skew-symmetric matrices and those orthogonal matrices that not have -1 as an eigenvalue: S is a skew-symmetric matrix if and only if $Q = (I - S)(I + S)^{-1}$ is an orthogonal matrix (and -1 is not a spectral value of Q). He also shows analogous bijections between skew-symmetric matrices and orthogonal matrices not having 1 as an eigenvalue (and, more generally, between skew-hermitian and unitary matrices). Liebeck and Osborne [12] shows that all orthogonal matrices are of the form DQ where D is a diagonal matrix of only ± 1 values in the diagonal and $Q = (I-S)(I+S)^{-1}$, being S a skew-symmetric matrix. Since $\phi(Q) = \phi(DQ)$ for any diagonal matrix D, we can avoid this product.

Using this result the following algorithm gives us a doubly stochastic matrix:

Algorithm 2 (This algorithm builds an $n \times n$ doubly stochastic matrix from an arbitrary set of $(n-1)n/2$ real numbers)

Given an arbitrary set of real numbers $T = \{a_{i,j} : 1 \le i \le n, i < j \le n\}$

- Define the $S = [s_{ij}]$ matrix as $s_{ij} = \begin{cases} a_{i,j} & \text{if } i < j \\ 0 & \text{if } i = j \\ -a_{j,i} & \text{otherwise} \end{cases}$
- Compute $Q = (I-S)(I+S)^{-1}$
- Compute $A = Q \circ Q$

Example 2 Applying algorithm 2, for $T = \{1,2,3,4,5,6\}$, We obtain these skew-symmetric, orthogonal and stochastic matrices:

$$S = \begin{bmatrix} 0 & 1 & 2 & 3 \\ -1 & 0 & 4 & 5 \\ -2 & -4 & 0 & 6 \\ -3 & -5 & -6 & 0 \end{bmatrix} \quad Q = \begin{bmatrix} 0. & -0.923 & 0.308 & -0.231 \\ 0.333 & -0.359 & -0.769 & 0.410 \\ -0.667 & -0.051 & -0.538 & -0.513 \\ 0.667 & 0.128 & -0.154 & -0.718 \end{bmatrix} \quad A = \begin{bmatrix} 0. & 0.852 & 0.095 & 0.053 \\ 0.111 & 0.129 & 0.592 & 0.168 \\ 0.444 & 0.003 & 0.290 & 0.263 \\ 0.444 & 0.016 & 0.024 & 0.515 \end{bmatrix}$$

Algorithm 2 can be generalised to the complex case, because if S is a skew-hermitian matrix then, $Q = (I-S)(I+S)^{-1}$ is a unitary matrix and, then, $A = \phi(Q) = Q \circ \overline{Q}$ is also a doubly stochastic matrix.

Algorithm 3 (This algorithm builds an $n \times n$ doubly stochastic matrix from an arbitrary set of $n(n+1)/2$ complex numbers)

Given an arbitrary set of complex numbers $T = \{a_{i,j} : 1 \le i \le n, i \le j \le n\}$

- Define the $S = [s_{ij}]$ matrix as $s_{ij} = \begin{cases} a_{i,j} & \text{if } i < j \\ (a_{i,i} - \overline{a_{i,i}})/2 & \text{if } i = j \\ -\overline{a_{j,i}} & \text{otherwise} \end{cases}$
- Compute $Q = (I-S)(I+S)^{-1}$
- Compute $A = Q \circ \overline{Q}$

Example 3 Applying algorithm 2, for $T = \{-2\mathrm{i}, 1+\mathrm{i}, -2\mathrm{i}, 0, 1-\mathrm{i}, 6\mathrm{i}\}$, we obtain the doubly stochastic matrix

$$A = \begin{bmatrix} 0.632 & 0.298 & 0.07 \\ 0.298 & 0.405 & 0.298 \\ 0.07 & 0.298 & 0.632 \end{bmatrix} \quad \square$$

Another well known method to generate orthogonal matrices is based on Householder transformations: if $\mathbf{u}$ is a unitary vector (an $n \times 1$ matrix such that $\mathbf{u}^T\mathbf{u} = 1$), then the Householder matrix $Q = I - 2\mathbf{u}\mathbf{u}^T$ is an orthogonal matrix. Then, $Q \circ Q$ is a doubly stochastic matrix. Here, you can substitute Q by a product of Householder matrices.

5 Conclusions and future work

In the present work we have developed different algorithms in order to obtain doubly stochastic matrices. Recognize what kind of doubly stochastic matrices are obtained with each algorithm and if, with these or similar algorithms, we can obtain any such matrix is the work that remains to be performed.

Johnson and Shapiro say in [10] that a basic question about the map ϕ is to determine its range, both for the case where the domain consist of real nonsingular matrices, and for the domain of complex nonsingular matrices, and conclude that $\phi(A) = \frac{1}{3}J_3$ has no real solution, where J_n denotes the $n \times n$ all-one matrix.

Moreover, Horn and Johnson in [9] gave an exemple ($B = \frac{1}{2}(J_3 - I)$) to show that not every doubly stochastic matrix is orthostochastic (the combined matrix of a unitary/orthogonal matrix). Thus, matrix B cannot be obtained from algorithm 2. We have another examples illustrating this result, also in the complex case. However, one can observe that $B = \phi(A)$ when

$$A = \begin{bmatrix} 0 & a & b \\ a & 0 & c \\ b & c & 0 \end{bmatrix} \qquad abc \neq 0$$

In the case of algorithm 1, it can be thought that there is greater freedom to obtain different matrices, however, the obtained matrices are always permutations of Hessenberg matrices.

By other hand, the next example is a doubly stochastic graph matrix

$$A = \begin{bmatrix} 0.3784 & 0.1622 & 0.1081 & 0.1622 & 0.1892 \\ 0.1622 & 0.4505 & 0.1892 & 0.1171 & 0.0811 \\ 0.1081 & 0.1892 & 0.4595 & 0.1892 & 0.0541 \\ 0.1622 & 0.1171 & 0.1892 & 0.4505 & 0.0811 \\ 0.1892 & 0.0811 & 0.0541 & 0.0811 & 0.5946 \end{bmatrix}$$

that was introduced in the study of chemical information processing, by Golender et al. [8] .

We ask two questions: Is there a nice characterization of those doubly stochastic matrices which are generated with our algorithms? When a doubly stochastic matrix is generated by the map ϕ?

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