On Constructing Orthogonal Generalized Doubly Stochastic Matrices

Gianluca Oderda∗, Alicja Smoktunowicz† and Ryszard Kozera‡

September 21, 2018

Abstract

A real quadratic matrix is generalized doubly stochastic (g.d.s.) if all of its row sums and column sums equal one. We propose numerically stable methods for generating such matrices having possibly orthogonality property or/and satisfying Yang-Baxter equation (YBE). Additionally, an inverse eigenvalue problem for finding orthogonal generalized doubly stochastic matrices with prescribed eigenvalues is solved here. The tests performed in MATLAB illustrate our proposed algorithms and demonstrate their useful numerical properties.

AMS Subj. Classification: 15B10, 15B51, 65F25, 65F15.
Keywords: stochastic matrix, orthogonal matrix, Householder QR decomposition, eigenvalues, condition number.

1 Introduction

We propose efficient algorithms for constructing generalized doubly stochastic matrix $A \in \mathbb{R}^{n \times n}$. Recall that $A$ is a generalized doubly stochastic matrix (g.d.s.) if all of its row sums and column sums equal one. Let $I_n$ denote the

∗Ersel Asset Management SGR S.p.A., Piazza Solferino, 11, 10121 Torino, Italy, e-mail: Gianluca.Oderda@ersel.it
†Faculty of Mathematics and Information Science, Warsaw University of Technology, Koszykowa 75, 00-662 Warsaw, Poland, e-mail: A.Smoktunowicz@mini.pw.edu.pl
‡Faculty of Applied Informatics and Mathematics, Warsaw University of Life Sciences - SGGW, Nowoursynowska str. 159, 02-776 Warsaw, Poland and Department of Computer Science and Software Engineering, The University of Western Australia, 35 Stirling Highway, Crawley, WA 6009, Perth, Australia, e-mail: ryszard.kozera@gmail.com
$n \times n$ identity matrix and $e = (1, 1, \ldots, 1)^T = \sum_{i=1}^{n} e_i \in \mathbb{R}^n$, where $\{e_i\}_{i=1}^{n}$ forms a canonical basis in $\mathbb{R}^n$. The set

$$\mathcal{A}_n = \{ A \in \mathbb{R}^{n \times n} : Ae = e, \quad A^T e = e \}$$

of all such g.d.s. matrices is investigated in this paper. Noticeably, the class of g.d.s. matrices $\mathcal{A}_n$ includes a thinner subset of all doubly stochastic matrices (bistochastic) - see [5], pp. 526-529. However, in contrast to the latter, a generalized doubly stochastic matrix does not necessarily permit only non-negative entries.

Let $\mathcal{B}_n$ define the space of orthogonal generalized doubly stochastic matrices determined by the following condition:

$$\mathcal{B}_n = \{ Q \in \mathcal{A}_n : Q^T Q = I_n \}.$$

Some applications of doubly stochastic matrices or g.d.s. matrices are outlined in [1]-[3]. More specifically, in economy, the orthogonal generalized doubly stochastic matrices permit to map a space of original quantities (asset prices) into a space of transformed asset prices.

Recall that if $A \in \mathbb{R}^{n \times n}$ is bistochastic and orthogonal then $A$ is actually a permutation matrix (see e.g. [5]). The situation is different for orthogonal generalized doubly stochastic matrices. Indeed, as simple inspection reveals

$$A = \frac{1}{3} \begin{pmatrix} -1 & 2 & 2 \\ 2 & 2 & -1 \\ 2 & -1 & 2 \end{pmatrix}$$

forms an orthogonal generalized doubly stochastic matrix evidently not yielding a permutation matrix.

We address now the question of how to construct generalized doubly stochastic matrices and orthogonal g.d.s. matrices. Let us denote by $\mathcal{Q}_n$ the set of all orthogonal matrices of size $n$:

$$\mathcal{Q}_n = \{ Q \in \mathbb{R}^{n \times n} : Q^T Q = I_n \},$$

and define

$$\mathcal{U}_n = \{ Q \in \mathcal{Q}_n : q_1 = Qe_1 = \frac{1}{\sqrt{n}} e \}.$$

The following theorem will be suitable later for the construction of some herein proposed algorithms.
Theorem 1.1 Given any $Q \in \mathcal{U}_n$ and any $X \in \mathbb{R}^{(n-1)\times(n-1)}$. Define
\begin{equation}
B = \begin{pmatrix} 1 & 0^T \\ 0 & X \end{pmatrix}.
\end{equation}

Then $A = QBQ^T$ is a generalized doubly stochastic matrix.

On the other hand, if $A \in \mathbb{R}^{n\times n}$ is a g.d.s. matrix and $Q \in \mathcal{U}_n$ then for $B = Q^T AQ$ we have (1) for some $X \in \mathbb{R}^{(n-1)\times(n-1)}$.

Moreover, $A$ is orthogonal if and only if $X$ defined in (1) is orthogonal.

Proof. First, observe that from (1) it follows that $Be_1 = e_1$ and $B^T e_1 = e_1$. Since $Q \in \mathcal{U}_n$ we have $Q^T e = \sqrt{n}e_1$, and so

\[ Ae = QB(Q^T e) = \sqrt{n}Q(Be_1) = \sqrt{n}Qe_1 = e. \]

Similarly,

\[ A^T e = QB^T(Q^T e) = \sqrt{n}Q(B^T e_1) = \sqrt{n}Qe_1 = e. \]

The proof for $B = Q^T AQ$ may be handled analogously.

Clearly, $A = QBQ^T$ is orthogonal for any orthogonal matrix $B$. \(\square\)

Remark 1.1 Theorem 1.1 is a slight reformulation of the result established in [3], for $q_n = Qe_n$ instead of $q_1 = Qe_1$.

Note that if $A_1, A_2 \in \mathcal{A}_n$ then $(A_1 + A_2)/2 \in \mathcal{A}_n$ and $A_1 A_2 \in \mathcal{A}_n$. Clearly, if $A_1, A_2 \in \mathcal{B}_n$ then also $A_1 A_2 \in \mathcal{B}_n$. Visibly, the latter renders various possible schemes for the derivation of the orthogonal doubly stochastic matrices.

This paper focuses on constructing orthogonal generalized doubly stochastic matrices with additional special properties enforced. More specifically, in Section 2 some new algorithms for generating matrix $Q \in \mathcal{U}_n$ using the Householder QR decomposition (see e.g. [4]) are proposed. We also describe a method for constructing $A \in \mathcal{B}_n$ and propose the new algorithms for computing orthogonal generalized doubly stochastic matrices with prescribed eigenvalues. At the end of Section 2 a new scheme for constructing orthogonal generalized doubly stochastic matrices satisfying the Yang-Baxter equation (YBE) is also given. Section 3 includes numerical examples all implemented in MATLAB illustrating the new methods introduced in this work. Finally, the Appendix annotating this paper includes the respective codes in MATLAB for all algorithms in question.
2 Algorithms

The Algorithms 1—6 for constructing orthogonal generalized doubly stochastic matrices are proposed and discussed below. The respective MATLAB codes of implemented algorithms are attached in the Appendix.

2.1 Construction of a symmetric $A \in B_3$

The aim is now to find a symmetric matrix $A \in B_3$ in the following form:

$$A = \begin{pmatrix} x & y & z \\ y & z & x \\ z & x & y \end{pmatrix},$$ (2)

which also satisfies

$$x + y + z = 1,$$ (3)

and meets the orthogonality conditions:

$$x^2 + y^2 + z^2 = 1,$$ (4)

$$xy + yz + xz = 0.$$ (5)

Clearly, the equation (5) follows from (3)-(4) due to:

$$1 = (x + y + z)^2 = x^2 + y^2 + z^2 + 2(xy + yz + xz).$$

Furthermore by (3) we obtain:

$$x + y = 1 - z.$$ (6)

Hence

$$x^2 + y^2 + z^2 = (x + y)^2 - 2xy + z^2 = (1 - z)^2 - 2xy + z^2,$$

which together with (4) yields:

$$xy = z(z - 1).$$ (7)

For a given real number $z$ the solution $x$ of (6)-(7) should satisfy the quadratic equation $x^2 - x(1 - z) - z(1 - z) = 0$. Since $\Delta = (1 - z)(1 + 3z)$ we conclude that $x$ remains real if and only if $z \in [-1/3, 1] = I$. In this case we have two real solutions: $x_1 = (1 - z + \sqrt{\Delta})/2$ and $x_2 = (1 - z - \sqrt{\Delta})/2$. Consequently, for $i = 1, 2$ two pairs of real solutions $(x_i, y_i)$ satisfying (5) and (7) can be now found according to the procedures specified below (Algorithm 1 for $x = x_1$ and Algorithm 1a for $x = x_2$). However, the choice $x = x_2$ in Algorithm 1a leads to severe loss of accuracy of the computed result once $z$ gets very close to 0. Indeed, here two nearly equal numerator’s numbers $1 - z$ and $\sqrt{\Delta}$ are then subtracted yielding an undesirable effect.
of “nearly zero cancellation”. In contrast, for \( z \in I \) the Algorithm 1 does not bear such computational deficiency adding merely two positive numbers in its numerator, respectively. For more details see [6], Sec. 1.8. Solving a Quadratic equation, pp. 10-12. The comparison between two methods demonstrating the above mentioned cancellation pitfall is given later in Example 1.

**Algorithm 1.** *Construction of \( A \in B_3 \) of the form \((2)\).*

Choose first an arbitrary \( z \in [-1/3, 1] \). The algorithm consists of the following steps:

- If \( z = 1 \) then \( A = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \).

- If \(-1/3 \leq z < 1\) then compute
  
  \[
  \Delta = (1 - z)(1 + 3z),
  \]
  \[
  x_1 = (1 - z + \sqrt{\Delta})/2,
  \]
  \[
  y_1 = -z(1 - z)/x_1,
  \]
  \[
  A = \begin{pmatrix} x_1 & y_1 & z \\ y_1 & z & x_1 \\ z & x_1 & y_1 \end{pmatrix}.
  \]

**Algorithm 1a (unstable for \( z \approx 0 \)).** *Construction of \( A \in B_3 \).*

Choose first an arbitrary \( z \in [-1/3, 1] \). The algorithm consists of the following steps:

- If \( z = 1 \) then \( A = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \).

- If \( z = 0 \) then \( A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \).

- If \( z \neq 0 \) and \(-1/3 \leq z < 1\) then compute
  
  \[
  \Delta = (1 - z)(1 + 3z),
  \]
  \[
  x_2 = (1 - z - \sqrt{\Delta})/2,
  \]
\[- y_2 = -z(1 - z)/x_2, \]
\[- A = \begin{pmatrix} x_2 & y_2 & z \\ y_2 & z & x_2 \\ z & x_2 & y_2 \end{pmatrix}. \]

2.2 Construction of $Q \in U_n$ by Householder QR method

In this subsection, we resort to the Householder method for computing the QR factorization of a given matrix $X \in \mathbb{R}^{n \times n}$. Recall that in MATLAB, the statement $[Q, R] = qr(X)$ decomposes $X$ into an upper triangular matrix $R \in \mathbb{R}^{n \times n}$ and orthogonal matrix $Q \in \mathbb{R}^{n \times n}$ so that $X = QR$. This method uses a suitably chosen sequence of Householder transformations. The reason for selecting the Householder method instead of the others including e.g. Gram-Schmidt orthogonalization methods, is that the Householder QR decomposition is unconditionally stable (see, e.g. [6], Chapter 18).

Recall that a Householder transformation (Householder reflector) is a matrix of the form

$$H = I_n - \frac{2}{z^T z} z z^T, \quad 0 \neq z \in \mathbb{R}^n.$$ 

Note that $H$ is symmetric and orthogonal. Householder matrices are very useful while introducing zeros into vectors to transform matrices into simpler forms (e.g. triangular, bidiagonal etc.).

For example, if $z = e + \sqrt{n} e_1$ is taken then

$$H e = (I_n - \frac{2}{z^T z} z z^T)e = e - \frac{2}{z^T z} z (z^T e) = -\sqrt{n} e_1.$$

Similarly $H e_1 = -\frac{1}{\sqrt{n}} e$ and therefore $Q = -H \in U_n$.

In this paper a different algorithm (Algorithm 2) for computing $Q \in U_n$ based on Householder QR decomposition is proposed. It enables to generate a vast class of orthogonal matrices with the first column equal to $\frac{1}{\sqrt{n}} e$.

**Algorithm 2. Construction of $Q \in U_n$.**

Let $X = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^{n \times n}$ be an arbitrary quadratic matrix, with each $x_i \in \mathbb{R}^n$.

The subsequent steps read as:

- $q = \frac{1}{\sqrt{n}} e$,

- $\hat{X} = (q, x_2, \ldots, x_n)$,
• $\tilde{X} = \tilde{Q} \hat{R}$ (Householder QR factorization),
• $Q = -\hat{Q}$.

Remark 2.1 Note that if $Q \in U_n$ and $Z \in Q_n$ is an arbitrary orthogonal matrix such that $Ze_1 = e_1$ then $QZ \in U_n$, and therefore there are many other choices to create the matrix $Q \in U_n$.

2.3 General method for constructing $A \in B_n$

Note also that Theorem 1.1 permits to establish a general method for generating orthogonal g.d.s. matrix. Indeed the following scheme accomplishes such task:

Algorithm 3. Construction of $A \in B_n$.

Take first arbitrary $Q \in U_n$ and $W \in Q_{n-1}$.

The algorithm is determined now by two steps:

• $B = \begin{pmatrix} 1 & 0^T \\ 0 & W \end{pmatrix}$,
• $A = QBQ^T$.

At this point, we remark that at the preliminary step $Q$ can be generated by Algorithm 2 and $W$ can be determined upon applying Householder QR decomposition.

2.4 Orthogonal generalized doubly stochastic matrices with prescribed eigenvalues

This subsection focuses on constructing the orthogonal generalized doubly stochastic matrix with prescribed eigenvalues. In doing so, a real Schur decomposition of orthogonal matrices is applied. More specifically, recall a well-known result (Theorem 7.4.1 in [4]):

Theorem 2.1 (Real Schur Decomposition) If $A \in \mathbb{R}^{n \times n}$, then there exists an orthogonal $W \in \mathbb{R}^{n \times n}$ and $R \in \mathbb{R}^{n \times n}$ such that $A = WRW^T$, where

\[ R = \begin{pmatrix} R_{11} & R_{12} & \ldots & R_{1s} \\ 0 & R_{22} & \ldots & R_{2s} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & R_{ss} \end{pmatrix}, \tag{8} \]
and each $R_{kk}$ is either a 1-by-1 matrix or a 2-by-2 matrix having complex conjugate eigenvalues.

Lemma 2.1 If $A$ in Theorem 2.1 is additionally orthogonal then $R$ in (8) is also orthogonal and hence $R$ is a block diagonal matrix

$$R = \begin{pmatrix} R_{11} & 0 & \cdots & 0 \\ 0 & R_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & R_{ss} \end{pmatrix},$$

(9)

with each $R_{kk}$ forming either $\pm 1$ or a 2-by-2 real matrix having complex conjugate eigenvalues $z_k = c_k + is_k$ and $\bar{z}_k = c_k - is_k$, where $c_k^2 + s_k^2 = 1$.

We apply now Lemma 2.1 to generate a special form (9) of orthogonal g.d.s. matrices.

Algorithm 4. Construction of $A \in B_n$ with prescribed eigenvalues.

Input:

- $r$- the number of the eigenvalues of $A$ equal to 1, $r \geq 1$,
- $p$- the number of the eigenvalues of $A$ equal to $-1$, $p \geq 1$,
- given $z = (z_1, z_2, \ldots, z_m)^T \in \mathbb{C}^m$- the vector of the eigenvalues of $A$, $m \geq 1$,
- given arbitrary $Q \in U_n$, where $n = r + p + 2m$.

Output: $A \in B_n$ having the eigenvalues $\pm 1$, and $z_k, \bar{z}_k$ for $k = 1, \ldots, m$.

The subsequent steps of the algorithm obey the following pattern:

- Find $c_k$ and $s_k$ such that $z_k = c_k + is_k$ ($c_k$ is the real part and $s_k$ is the imaginary part of $z_k$), for $k = 1, \ldots, m$,
- compute the rotation matrices $M_k$, for $k = 1, 2, \ldots, m$

$$R_k = \begin{pmatrix} c_k & s_k \\ -s_k & c_k \end{pmatrix},$$

(10)

- create a block diagonal matrix $R(2m \times 2m)$

$$R = \begin{pmatrix} R_1 & 0 & \cdots & 0 \\ 0 & R_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & R_m \end{pmatrix},$$

(11)
• form the matrix $B$ according to:

\[
B = \begin{pmatrix}
I_r & 0 & 0 \\
0 & -I_p & 0 \\
0 & 0 & R
\end{pmatrix},
\]

• compute $A = QBQ^T$.

**Remark 2.2** Note that $R_k$ defined by (10) is an orthogonal matrix with the eigenvalues equal to $c_k + is_k$ and $c_k - is_k$. Clearly, one can extend Algorithm 4 to the special cases of $p = 0$ or $m = 0$. It is omitted here for the sake of brevity. Noticeably, the case of $r = 0$ in Algorithm 4 is excluded.

### 2.5 Construction of $A \in B_\mathcal{N}$ satisfying the Yang-Baxter equation

Recall that matrix $A \in \mathbb{R}^{n^2 \times n^2}$ satisfies the Yang-Baxter Equation (YBE) if

\[
(A \otimes I_n)(I_n \otimes A)(A \otimes I_n) = (I_n \otimes A)(A \otimes I_n)(I_n \otimes A),
\]

where $X \otimes Y$ is the Kronecker product (tensor product) of the matrices $X$ and $Y$: $X \otimes Y = (x_{i,j}Y)$. That is, the Kronecker product $X \otimes Y$ is a block matrix whose $(i, j)$ blocks are $x_{i,j}Y$.

The Yang-Baxter equation has been extensively studied due to its application in many fields of mathematics or quantum information science— for detailed applications see e.g. [7]. Solutions of the Yang-Baxter equation have many interesting properties. Of particular importance to this work is the following theorem (see [7]):

**Theorem 2.2** If $A \in \mathbb{R}^{n^2 \times n^2}$ satisfies the Yang-Baxter equation (12) and $P \in \mathbb{R}^{n \times n}$ is arbitrary non-singular matrix, then $\hat{X} = (P \otimes P)A(P \otimes P)^{-1}$ also satisfies the Yang-Baxter equation (12).

Based on the latter the efficient algorithm (see [7]), for generating special solutions of the Yang-Baxter equation (12) can be now formulated.

**Algorithm 5.** Construction of $A = A(d) \in \mathbb{R}^{n^2 \times n^2}$ satisfying the Yang-Baxter equation.

Select an arbitrary $d = (d_1, d_2, \ldots, d_{n^2})^T \in \mathbb{R}^{n^2}$.

The algorithm obeys the following pattern:
• Form $n^2$-by-$n^2$ matrix $S$:

$$S = \begin{pmatrix}
1 & 2 & 3 & \cdots & n-1 & n \\
n+1 & n+2 & n+3 & \cdots & 2n-1 & 2n \\
2n+1 & 2n+2 & 2n+3 & \cdots & 3n-1 & 3n \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
(n-1)n+1 & (n-1)n+2 & (n-1)n+3 & \cdots & n^2-1 & n^2
\end{pmatrix}$$

(13)

• take $p = (p_1, p_2, \ldots, p_{n^2}) = (s_1^T, s_2^T, \ldots, s_{n^2}^T)$, where $s_j$ denotes the $j$th column of $S$,

• set $A = (d_{p_1} e_{p_1}, d_{p_2} e_{p_2}, \ldots, d_{p_{n^2}} e_{p_{n^2}})$,

• then define $A = DP$, where $D = \text{diag}(d_1, d_2, \ldots, d_{n^2})$ and $P = (e_{p_1}, e_{p_2}, \ldots, e_{p_{n^2}})$ is a permutation matrix.

Remark 2.3 Note that the matrix $X$ generated by Algorithm 5 satisfies $X e_1 = d_1 e_1$ and $X^T e_1 = d_1 e_1$ for arbitrary $d = (d_1, d_2, \ldots, d_{n^2})^T \in \mathbb{R}^{n^2}$. In particular, upon taking $n = 2$ and $d = (d_1, d_2, d_3, d_4)^T$ we arrive at:

$$X = \begin{pmatrix}
d_1 & 0 & 0 & 0 \\
0 & d_2 & 0 & 0 \\
0 & d_3 & 0 & 0 \\
0 & 0 & 0 & d_4
\end{pmatrix}.$$  

More detailed information can be found in [7].

In order to generate the orthogonal solutions to the YBE we prove now the following:

Theorem 2.3 Let $P \in U_n$. Assume that $B \in \mathbb{R}^{n^2 \times n^2}$ is an orthogonal matrix satisfying the Yang-Baxter equation:

$$(B \otimes I_n)(I_n \otimes B)(B \otimes I_n) = (I_n \otimes B)(B \otimes I_n)(I_n \otimes B),$$

with the additional conditions $Be_1 = e_1$ and $B^T e_1 = e_1$.

Define $Q = P \otimes P$ and $A = QBQ^T$. Then $Q \in U_{n^2}$ and $A \in B_{n^2}$ is orthogonal and satisfies the Yang-Baxter equation (12).
Proof. Observe that $Q$ is orthogonal since

$$Q^TQ = (P^T \otimes P^T)(P \otimes P) = (P^TP) \otimes (P^TP) = I_n \otimes I_n = I_{n^2}.$$ 

We shall verify now that $Qe_1 = \frac{1}{\sqrt{n}}\bar{e}$, where $\bar{e} = (1, 1, \ldots, 1)^T \in \mathbb{R}^{n^2}$. Clearly, $\bar{e} = e \otimes e$, where $e = (1, 1, \ldots, 1)^T \in \mathbb{R}^n$.

Since $P \in U_n$, we have $P\hat{e}_1 = \frac{1}{\sqrt{n}}e$, where $\hat{e}_1 = (1, 0, \ldots, 0)^T \in \mathbb{R}^n$. Hence we obtain $P^Te = \sqrt{n}\hat{e}_1$.

Exploiting now the standard properties of the Kronecker product yields:

$$Q^T\bar{e} = (P^T \otimes P^T)(e \otimes e) = (P^Te) \otimes (P^Te) = n(\hat{e}_1) \otimes (\hat{e}_1) = ne_1,$$

and so finally $Qe_1 = \frac{1}{\sqrt{n^2}}\bar{e}$. The proof is complete.

Having established Theorem 2.3 we pass now to the formulation of the last algorithm.

**Algorithm 6.** Construction of orthogonal generalized doubly stochastic matrix $A \in \mathbb{R}^{n^2 \times n^2}$ satisfying the Yang-Baxter equation (12).

Let $P \in U_n$ and $B \in \mathbb{R}^{n^2 \times n^2}$ form an arbitrary matrix satisfying the assumptions of Theorem 2.3.

The algorithm splits into two steps:

- $Q = P \otimes P$,
- $A = QBQ^T$.

In order to initialize the above procedure, the matrix $P$ is obtainable from Algorithm 2, whereas $B$ is computable with the aid of Algorithm 5, where $d_1 = 1$ and $d_2, \ldots, d_{n^2}$ are arbitrary parameters satisfying $|d_i| = 1$, for all $i$.

### 3 Numerical Experiments

The final section of this paper reports on the results of the numerical experiments examining the computational properties of Algorithms 1-6. All tests are performed in MATLAB version 8.4.0.150421 (R2014b), with machine precision $\varepsilon_M \approx 2.2 \cdot 10^{-16}$.

We report on the following statistics for a given matrix $A$:

- $err_{orth} = \|I_n - A^T A\|_2$ (the orthogonality error),
- $err_{rows} = \|Ae - e\|_2$ (the error in the row sums),
• $err_{\text{columns}} = \| A^T e - e \|_2$ (the error in the column sums).

Here $\| \cdot \|_2$ denotes the standard spectral norm of a matrix or a vector.

The justification for the statistics used from above is given by the following theorem (for details see [3], pp. 132, 370-371):

**Theorem 3.1** Let $A \in \mathbb{R}^{n \times n}$ and $0 \leq \epsilon < 1$. Then

1. $\| I_n - A^T A \|_2 \leq \epsilon \iff$ There exists an orthogonal matrix $Q$ and $E$ such that $A = Q + E$, where $\| E \|_2 \leq \epsilon$. That is, the matrix $A$ is very close to the true orthogonal matrix.

2. $\| A e - e \|_2 \leq \epsilon \iff$ There exists $E_1$ such that $(A + E_1)e = e$, where $\| E_1 \|_2 \leq \frac{1}{\sqrt{n}} \epsilon$. That is, all of $A + E_1$ row sums equal one.

3. $\| A^T e - e \|_2 \leq \epsilon \iff$ There exists $E_2$ such that $(A + E_2)^T e = e$, where $\| E_2 \|_2 \leq \frac{1}{\sqrt{n}} \epsilon$. That is, all of $A + E_2$ column sums equal one.
Table 1: The results for Example 1 and the matrices $A(3 \times 3)$ computed by Algorithm 1.

| $z$ | $10^{-3}$ | $10^{-6}$ | $10^{-9}$ | $10^{-12}$ | $10^{-14}$ |
|-----|-----------|-----------|-----------|-----------|-----------|
| $\text{err}_{\text{orth}}$ | $9.12E-20$ | $2.22E-16$ | $5.65E-26$ | $4.84E-29$ | $6.03E-31$ |
| $\text{err}_{\text{rows}}$ | $1.11E-16$ | $2.71E-16$ | 0 | 0 | 0 |
| $\text{err}_{\text{columns}}$ | $1.11E-16$ | $2.71E-16$ | 0 | 0 | 0 |

Table 2: The results for Example 1 and the matrices $A(3 \times 3)$ computed by Algorithm 1a.

| $z$ | $10^{-3}$ | $10^{-6}$ | $10^{-9}$ | $10^{-12}$ | $10^{-14}$ |
|-----|-----------|-----------|-----------|-----------|-----------|
| $\text{err}_{\text{orth}}$ | $1.23E-13$ | $1.12E-11$ | $1.65E-07$ | $1.55E-04$ | $0.0016$ |
| $\text{err}_{\text{rows}}$ | $1.07E-13$ | $9.75E-12$ | $1.43E-07$ | $1.34E-04$ | $0.0014$ |
| $\text{err}_{\text{columns}}$ | $1.03E-13$ | $9.75E-12$ | $1.43E-07$ | $1.34E-04$ | $0.0014$ |

Several examples to test our algorithms are considered.

**Example 1** We present a comparison of Algorithm 1 and Algorithm 1a for $z$ very close to 0. Notice that the matrices $A$ generated by these two methods for the same value of $z$ may be completely different. We see that the catastrophic cancellation occurs in Algorithm 1a for $z \approx 0$, see Table 2. In contrast, Algorithm 1 gives perfectly accurate results, see Table 1.

**Example 2** We test Algorithm 2 on random matrices $X(n \times n)$ generated by the MATLAB code:

```matlab
randn('state',0);
X=randn(n);
Q=Algorithm2(X);
err_orth=norm(eye(n)-Q'*Q);
```

Random matrices of entries are from the normal distribution $\mathcal{N}(0,1)$. They are generated by the MATLAB function "randn". Before each call, the random number generator is reset to its initial state.
Table 3: The orthogonality error for Example 2 and the matrix $Q(n \times n)$ computed by Algorithm 2.

| $n$  | 10     | 50     | 100    | 500    | 1000   |
|------|--------|--------|--------|--------|--------|
| $err_{orth}$ | $1.34E-15$ | $2.21E-15$ | $2.30E-15$ | $3.40E-15$ | $6.34E-15$ |

Table 4: The results for Example 3 and the matrix $A(n \times n)$ computed by Algorithm 3.

| $n$  | 10     | 50     | 100    | 500    | 1000   |
|------|--------|--------|--------|--------|--------|
| $err_{orth}$ | $1.34E-15$ | $2.21E-15$ | $2.30E-15$ | $3.40E-15$ | $6.34E-15$ |
| $err_{rows}$  | $1.12E-15$ | $4.50E-15$ | $7.26E-15$ | $2.43E-14$ | $4.34E-14$ |
| $err_{columns}$ | $1.09E-15$ | $4.69E-15$ | $7.56E-15$ | $2.39E-14$ | $4.03E-14$ |

Visibly Algorithm 2 gives very satisfactory results (see Table 2). Theorem 3.1 guarantees that every computed matrix $Q$ is very close to the exactly orthogonal matrix.

**Example 3** In the next step we test Algorithm 3 on matrices $Q(n \times n)$ generated by Algorithm 2 as specified in Example 2 and on orthogonal matrices $W((n-1) \times (n-1))$ generated by Householder QR decomposition of random matrices.

The following MATLAB code is used:

```matlab
randn('state',0);  
X=randn(n); Q=Algorithm2(X);  
Y=randn(n-1); [W,R]=qr(Y);  
A=Algorithm3(Q,W);  
e=ones(n,1);
```

Again, as illustrated in Table 2, Algorithm 3 yields very good results.

**Example 4** We test now Algorithm 4 with the following MATLAB code:

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randn(’state’,0);
i=sqrt(-1); r=2;p=3;z=[0.6+0.8*i,-0.8+0.6*i];
n=r+p+4;
X=randn(n); Q=Algorithm2(X);
A=Algorithm4(r,p,z,Q);
eigA=eig(A) % The vector eigA contains the computed eigenvalues of A

The exact eigenvalues of $A$ are: 1,1,−1,−1,−1,0.6 ± 0.8i,−0.8 ± 0.6.

The corresponding eigenvalues of computed matrix $A$ generated by Algorithm 4 are:

eigA = 
6.000000000000000e-01 + 8.000000000000000e-01i 
6.000000000000000e-01 - 8.000000000000000e-01i 
-7.999999999999996e-01 + 5.999999999999996e-01i 
-7.999999999999996e-01 - 5.999999999999996e-01i 
1.000000000000000e+00 + 0.000000000000000e+00i 
1.000000000000000e+00 + 0.000000000000000e+00i 
-1.000000000000000e+00 + 0.000000000000000e+00i 
-1.000000000000000e+00 + 0.000000000000000e+00i 
-9.999999999999998e-01 + 0.000000000000000e+00i

Thus, upon comparing the latter, the statistics

er{orth} = 1.08E − 15,  er{rows} = 8.88E − 16,  er{columns} = 9.15E − 16,

renders all results almost perfect in floating-point arithmetic.

**Example 5** Finally, the performance of Algorithm 6 is tested. In doing so, the following MATLAB code is used:

n=2; m=n^2;d=[1,-1,1,1];
B=Algorithm5(n,d);
randn(’state’,0); X=randn(n); P=Algorithm2(X);
A=Algorithm6(B,P)
e=ones(m,1);
err_orth=norm(eye(m)-A’*A)
err_rows=norm(A*e-e)
err_columns=norm(A’*e-e)
The outcoming statistics read as:
\begin{align*}
\text{err}_{\text{orth}} &= 8.55E - 16, \\
\text{err}_{\text{rows}} &= 9.28E - 16, \\
\text{err}_{\text{columns}} &= 9.15E - 16.
\end{align*}

Clearly all results produces high accuracy in floating-point arithmetic’s.

Recall that in the first step of Algorithm 6, the Algorithm 5 is applied.

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4 Appendix - MATLAB Codes

For the sake of completeness, we enclose MATLAB codes to all discussed Algorithms in question.

function [A]=Algorithm1(z)
  % [A]=Algorithm1(z)
  % A(3x3) is orthogonal and symmetric generalized stochastic matrix.
  % Parameter z should be in the interval [-1/3,1].
  n=3; A=zeros(n);
  if z>1 || z<-1/3
    disp('z should be in the interval [-1/3,1]');
    return;
  end
  t=1-z;
  if t==0
    x=0; y=0;
    A=[0 0 1;0 1 0;1 0 0];
    return;
  end
  delta=t*(1+3*z);
  x=(t+sqrt(delta))/2;
  y=-z*t/x(1);
  A=[x y z;y z x;z x y];
end

function [A]=Algorithm1a(z)
  % [A]=Algorithm1a(z) (unstable for z close to 0)
  % A(3x3) is orthogonal and symmetric generalized stochastic matrix.
  % Parameter z should be in the interval [-1/3,1].
  n=3; A=zeros(n);
  if z>1 || z<-1/3
    disp('z should be in the interval [-1/3,1]');
    return;
  end
  t=1-z;
  if t==0
    A=[0 0 1;0 1 0;1 0 0];
    return;
  end
end
delta=t*(1+3*z);
if z==0
    A=[0 1 0; 1 0 0; 0 0 1];
    return;
end
x=(t-sqrt(delta))/2;
y=-z*t/x;
A=[x y z; y z x; z x y];
end

function [Q]=Algorithm2(X)
% [Q]=Algorithm2(X).
% Q(nxn) is orthogonal and g.d.s.
% The first column of Q is e/sqrt(n), where e=(1,1,...,1).
% Householder Q-R decomposition is used.
[m,n]=size(X);
Q=zeros(n);
if m~=n
    disp('X should be a square matrix.');
    return;
end
e=ones(n,1);
norm_e=sqrt(n);
X(:,1)=e/norm_e;
[Q,~]=qr(X);
Q=-Q;
end

function [A]=Algorithm3(Q,W)
% [A]=Algorithm3(Q,W)
% A(nxn) is orthogonal generalized doubly stochastic matrix.
% Q(nxn) is an orthogonal matrix with the first column e/sqrt(n).
% W(n-1)x(n-1) is an orthogonal matrix.
[m,n]=size(Q);
A=zeros(n);
if m~=n
    disp('X should be a square matrix.');
    return;
end
function A=Algorithm4(r,p,z,Q)
% [A]=Algorithm4(r,p,z,Q)
% A(nxn) is orthogonal generalized doubly stochastic.
% n=r+p+2m, where m is the length of a vector z,
% r is the number of 1’s, and p is the number of -1’s of A.
% Here |z(k)|=1 for k=1,..., m.
% Assume that r>=1, p>=1, and m>=1.
% Q(nx n) is an orthogonal matrix with the first column e/sqrt(n).
z=z(:);
m=length(z);
n=r+p+2*m;
A=eye(n);
c=real(z);s=imag(z);
R=zeros(2*m,2*m);
for k=1:m
    Rk=[c(k) s(k);-s(k) c(k)];
    R(2*k-1:2*k,2*k-1:2*k)=Rk;
end
B=[eye(r) zeros(r,p) zeros(r,2*m)
    zeros(p,r) -eye(p) zeros(p,2*m)
    zeros(2*m,r) zeros(2*m,p) R];
A=Q*B*Q';
end

[k,l]=size(W);
if k~=l
    disp('Y should be a square matrix.');
    return;
end
if k~=(n-1)
    disp('Size of Y should be equal to n-1');
    return;
end
z=zeros(n-1,1);
B=[1,z'; z,W];
A=Q*B*Q';
end
function [X] = Algorithm5(n,d)
% [X] = Algorithm5(n,d)
% X(mxm), m=n^2, X is a solution of the YBE
% d=(d(1),..., d(m)), where m=n^2.
% m=max(size(d));
if ~(m==n*n)
    disp('Wrong dimensions');
    return;
end
for j=1:n
    for i=1:n
        S(i,j)=(i-1)*n+j;
    end
end
p=[];
for i=1:n
    p=[p; S(:,i)];
end
p=p';
X=diag(d);
X=X(:,p);
end

function [A]=Algorithm6(B,P)
% [A]=Algorithm6(B,P)
% B(mxm), m=n^2, satisfies the Yang-Baxter equation.
% Be1=e1 and B'e1=e1, where e1=(1,0,...,0)^t.
% P(nxn) is orthogonal with the first column e/sqrt(n), where e=(1,1,...,1)^t.
% A(mxm) is orthogonal generalized doubly stochastic matrix satisfying the Yang-
% [m,m]=size(B);
% [n,n]=size(P);
A=eye(m);
if m~=n^2
    disp('Wrong dimensions!');
    return;
end
Q=kron(P,P);
A=Q*B*Q';
end