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Notes on Birkhoff-von Neumann decomposition of doubly stochastic matrices

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Abstract: Birkhoff-von Neumann (BvN) decomposition of doubly stochastic matrices expresses a double stochastic matrix as a convex combination of a number of permutation matrices. There are known upper and lower bounds for the number of permutation matrices that take part in the BvN decomposition of a given doubly stochastic matrix. We investigate the problem of computing a decomposition with the minimum number of permutation matrices and show that the associated decision problem is strongly NP-complete. We propose a heuristic and investigate it theoretically and experimentally.

Key-words: doubly stochastic matrix, Birkhoff-von Neumann decomposition

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Sur la décomposition de Birkhoff-von Neumann des matrices bistochastiques

Résumé : La décomposition de Birkhoff-von Neumann (BvN) des matrices bistochastiques exprime une telle matrice en tant qu'une combinaison convexe d'un nombre de matrices de permutations. On connaît des bornes supérieure et inférieure pour le nombre de matrices de permutations dans une décomposition BvN d'une matrice bistochastique. Nous étudions le problème de calcul d'une décomposition BvN avec le nombre minimum de matrices de permutations et nous montrons que le problème de décision associé est fortement NP-complet. Nous proposons une heuristique et l'étudions théoriquement et expérimentalement.

Mots-clés : matrices bistochastiques, décomposition de Birkhoff-von Neumann

1 Introduction

Let $\mathbf{A} = [a_{ij}] \in \mathbb{R}^{n\times n}$ be a doubly stochastic matrix: $a_{ij} \geq 0$ for all i, j and $\mathbf{A}e = \mathbf{A}^T e = e$, where e is the vector of all ones. By Birkhoff's Theorem, there exist $\alpha_1, \alpha_2, \ldots, \alpha_k \in (0, 1)$ with $\sum_{i=1}^{k} \alpha_i = 1$ and permutation matrices $\mathbf{P}_1, \mathbf{P}_2, \ldots, \mathbf{P}_k$ such that

$$\mathbf{A} = \alpha_1\mathbf{P}_1 + \alpha_2\mathbf{P}_2 + \cdots + \alpha_k\mathbf{P}_k\,. \tag{1}$$

This representation is also called Birkhoff-von Neumann (BvN) decomposition. We refer to the numbers $\alpha_1, \alpha_2, \ldots, \alpha_k$ as the coefficients of the decomposition. Such a representation of $\mathbf{A}$ as a convex combination of permutation matrices is not unique in general. For any such representation the *Marcus–Ree Theorem* [8] states that $k \leq n^2 - 2n + 2$ for dense matrices; Brualdi and Gibson [3] and Brualdi [2] show that for a fully indecomposable sparse matrix with τ nonzeros $k \leq \tau - 2n + 2$.

We are interested in the problem of finding the minimum number k of permutation matrices in the representation (1). More formally we investigate the MinBvNDec problem defined as follows:

> Input: A doubly stochastic matrix $\mathbf{A}$.
>
> Output: A Birkhoff-von Neumann decomposition of $\mathbf{A}$ as $\mathbf{A} = \alpha_1\mathbf{P}_1 + \alpha_2\mathbf{P}_2 + \cdots + \alpha_k\mathbf{P}_k$.
>
> Measure: The number k of permutation matrices in the decomposition.

Brualdi [2, p.197] investigates the same problem and concludes that this is a difficult problem. We continue along this line and show that the MinBvNDec problem is NP-hard (Section 2.2). We also propose a heuristic (Section 3) for obtaining a BvN decomposition with a small number of permutation matrices. We investigate the proposed heuristic theoretically and experimentally (Section 4).

2 The minimum number of permutation matrices

We show in this section that the decision version of the problem is NP-complete. We first give some definitions and preliminary results.

2.1 Preliminaries

A multi-set can contain duplicate members. Two multi-sets are equivalent if they have the same set of members with the same number of repetitions.

Let $\mathbf{A}$ and $\mathbf{B}$ be two $n\times n$ matrices. We write $\mathbf{A} \subseteq \mathbf{B}$ to denote that for each nonzero entry of $\mathbf{A}$, the corresponding entry of $\mathbf{B}$ is nonzero. In particular, if $\mathbf{P}$ is an $n \times n$ permutation matrix and $\mathbf{A}$ is a nonnegative $n \times n$ matrix, $\mathbf{P} \subseteq \mathbf{A}$ denotes that the entries of $\mathbf{A}$ at the positions corresponding to the nonzero entries of $\mathbf{P}$ are positive. We use $\mathbf{P} \odot \mathbf{A}$ to denote the entrywise product of $\mathbf{P}$ and $\mathbf{A}$, which selects the the entries of $\mathbf{A}$ at the positions corresponding to the nonzero entries of $\mathbf{P}$. We also use $\min\{\mathbf{P} \odot \mathbf{A}\}$ to denote the minimum entry of $\mathbf{A}$ at the nonzero positions of $\mathbf{P}$.

Let U be a set of positions of the nonzeros of $\mathbf{A}$. Then U is called strongly stable [1], if for each permutation matrix $\mathbf{P} \subseteq \mathbf{A}$, $p_{kl} = 1$ for at most one $(k, l) \in U$.

Lemma 1 (Brualdi [2]). *Let* $\mathbf{A}$ *be a doubly stochastic matrix. Then, in a BvN decomposition of* $\mathbf{A}$*, there are at least* $\gamma(\mathbf{A})$ *permutation matrices, where* $\gamma(\mathbf{A})$ *is the maximum cardinality of a strongly stable set of positions of* $\mathbf{A}$*.*

Note that $\gamma(\mathbf{A})$ is no smaller than the maximum number of nonzeros in a row or a column of $\mathbf{A}$ for any matrix $\mathbf{A}$.

An $n \times n$ circulant matrix $\mathbf{C}$ is defined as follows. The first row of $\mathbf{C}$ is specified as $c_1, \ldots, c_n$, and the ith row is obtained from the $(i-1)$th one by a cyclic rotation to the right, for $i = 2, \ldots, n$:

$$\mathbf{C} = \begin{bmatrix} c_1 & c_2 & \cdots & c_n \\ c_n & c_1 & \cdots & c_{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ c_2 & c_3 & \cdots & c_1 \end{bmatrix} .$$

Lemma 2. *Let* $\mathbf{C}$ *be an* $n \times n$ *positive circulant matrix whose first row is* $c_1, \ldots, c_n$*. The matrix* $\mathbf{C}' = \frac{1}{\sum c_j}\mathbf{C}$ *is doubly stochastic, and all BvN decompositions with* n *permutation matrices have the same multi-set of coefficients* $\{\frac{c_i}{\sum c_j} : \textit{for } i = 1, \ldots, n\}$*.*

Proof. That $\mathbf{C}' = \frac{1}{\sum c_j}\mathbf{C}$ is doubly stochastic is easily seen. Since there are n nonzero entries in a row of $\mathbf{C}'$, we need at least n permutation matrices in a BvN decomposition by Lemma 1.

Since we have n permutation matrices, the jth permutation matrix with its α_j should zero out exactly one entry per row and column; otherwise we would need more than n permutation matrices. Furthermore, all these permutation matrices should be disjoint (they do not have a common nonzero), otherwise we would need more than n permutation matrices to zero out n^2 entries of $\mathbf{C}'$. Therefore, for $j = 1, \ldots, n$, α_j should be equal to all n nonzero entries of $\mathbf{C}' - \sum_{i=1, i\neq j}^{n} \alpha_i \mathbf{P}_i$ which are at positions $\mathbf{P}_j$. Since these positions are not touched by any $\mathbf{P}_i$ for $i \neq j$, they have the same value; which is one of c_k/c coming from the original matrix. By looking at a single row of $\mathbf{C}'$ we identify c_1/c as one of the α_j's, c_2/c as another and so on so forth. □

In the lemma, if $c_i = c_j$ for some $i \neq j$, we will have the same value c_i/c for two different permutation matrices. As a sample BvN decomposition, let $c = \sum c_i$ and consider $\frac{1}{c}\mathbf{C} = \sum \frac{c_j}{c}\mathbf{D}_j$, where $\mathbf{D}_j$ is the permutation matrix corresponding to the $(j-1)$th diagonal: for $j = 1, \ldots, n$, the matrix $\mathbf{D}_j$ has 1s at the positions $(i, i+j-1)$ for $i = 1, \ldots, n-j+1$ and at the positions $(n-j+1+k, k)$ for $k = 1, \ldots, j-1$, where we assumed that the second set is void for $j = 1$.

We note that the lemma is not concerned by the uniqueness of BvN which would need a unique set of permutation matrices as well. If all the c_i were distinct, this would have been true, where the $\mathbf{D}_j$ described above would define the unique permutation matrices. Also, a more general variant of the lemma concerns the decompositions whose cardinality k is equal to the maximum cardinality of a strongly stable set. In this case too, the coefficients in the decomposition would correspond to the entries in a strongly stable set of cardinality k.

2.2 The computational complexity of MinBvNDec

Here we give the the proof of the NP completeness of the problem MinBvNDec.

Theorem 1. *The problem of deciding whether there is a Birkhoff-von Neumann decomposition of a given doubly stochastic matrix with* k *permutation matrices is strongly NP-complete.*

Proof. It is clear that the problem belongs to NP, as it is easy to check in polynomial time that a given decomposition is equal to the given matrix.

To establish NP-completeness, we demonstrate a reduction from 3-PARTITION which is NP-complete in the strong sense [6, p. 96]. Consider an instance of 3-PARTITION: given an array A of $3m$ positive integers, a positive integer B such that $\sum_{i=1}^{3m} a_i = mB$ and $B/4 < a_i < B/2$, does there exist a partition of A into m disjoint arrays $S_1, \ldots, S_m$ such that each S_i has three elements whose sum is B. Let $\mathcal{I}_1$ denote an instance of 3-PARTITION.

We build the following instance $\mathcal{I}_2$ of MinBvNDec corresponding to $\mathcal{I}_1$ given above. Let

$$\mathbf{M} = \begin{bmatrix} \frac{1}{m}\mathbf{E}_m & O \\ O & \frac{1}{mB}\mathbf{C} \end{bmatrix}$$

where $\mathbf{E}_m$ is an $m \times m$ matrix whose entries are 1, and $\mathbf{C}$ is an $3m \times 3m$ circulant matrix whose first row is $a_1, \ldots, a_{3m}$. It is easy to see that $\mathbf{M}$ is doubly stochastic. We ask whether $\mathcal{I}_2$ has a solution with $k = 3m$. We will show that $\mathcal{I}_1$ has a solution if and only if $\mathcal{I}_2$ has a solution.

Assume that $\mathcal{I}_1$ has a solution with $S_1, \ldots, S_m$. Let $S_i = \{a_{i,1}, a_{i,2}, a_{i,3}\}$ and observe that $\frac{1}{mB}(a_{i,1} + a_{i,2} + a_{i,3}) = 1/m$. We identify three permutation matrices $\mathbf{P}_{i,d}$ for $d = 1, 2, 3$ in $\mathbf{C}$ which contain $a_{i,1}$, $a_{i,2}$ and $a_{i,3}$, respectively. We can write $\frac{1}{m}\mathbf{E}_m = \sum_{i=1}^{m} \frac{1}{m}\mathbf{D}_i$ where $\mathbf{D}_i$ is the permutation matrix corresponding to the $(i-1)$th diagonal (described after the proof of Lemma 2). We prepend $\mathbf{D}_i$ to the three permutation matrices $\mathbf{P}_{i,d}$ for $d = 1, 2, 3$ and obtain three permutation matrices for $\mathbf{M}$. We associate these three permutation matrices with $\alpha_{i,d} = \frac{a_{i,d}}{mB}$. Therefore, we can write

$$\mathbf{M} = \sum_{i=1}^{m} \sum_{d=1}^{3} \alpha_{i,d} \begin{bmatrix} \mathbf{D}_i & \\ & \mathbf{P}_{i,d} \end{bmatrix},$$

and obtain a BvN decomposition of $\mathbf{M}$ with $3m$ permutation matrices.

Assume that $\mathcal{I}_2$ has a BvN with $3m$ permutation matrices. This also defines two BvN decompositions with $3m$ permutation matrices for $\frac{1}{m}\mathbf{E}_m$ and $\frac{1}{mB}\mathbf{C}$. We now establish a correspondence between these two BvN's to finish the proof. Since $\frac{1}{mB}\mathbf{C}$ is a circulant matrix with $3m$ nonzeros in a row, any BvN decomposition of it with $3m$ permutation matrices has the coefficients $\frac{a_i}{mB}$ for $i = 1, \ldots, 3m$ by Lemma 2. Since $a_i + a_j < B$, we have $\frac{a_i + a_j}{mB} < 1/m$. Therefore, each entry in $\frac{1}{m}\mathbf{E}_m$ needs to be included in at least three permutation matrices. A total of $3m$ permutation matrices covers any row of $\frac{1}{m}\mathbf{E}_m$, say the first one. Therefore, for each entry in this row we have $\frac{1}{m} = \alpha_i + \alpha_j + \alpha_k$, for $i \neq j \neq k$ corresponding to three disjoint permutation matrices used in the BvN of $\frac{1}{mB}\mathbf{C}$. Since the permutation matrices are all disjoint in $\mathbf{C}$, this correspondence defines a partition of the $3m$ numbers α_i for $i = 1, \ldots, 3m$ into m groups with three elements each, where each group has a sum of $1/m$. The corresponding three a_i's in a group therefore sums up to B, and we have a "yes" answer to $\mathcal{I}_1$. □

3 Two heuristics

Here we discuss two heuristics for obtaining a BvN decomposition of a given matrix $\mathbf{A}$, one from the literature and a greedy one that we propose. Both follow the same approach (as in the proof of the theorem that BvN decomposition exist). They proceed step by step. Let $\mathbf{A}^{(0)} = \mathbf{A}$. At every step $j \geq 1$, they find a permutation matrix $\mathbf{P}_j \subseteq \mathbf{A}^{(j-1)}$, use the minimum element of $\mathbf{A}^{(j-1)}$ at the nonzero positions of $\mathbf{P}_j$, i.e., $\min\{\mathbf{P}_j \odot \mathbf{A}^{(j-1)}\}$ as α_j, and update $\mathbf{A}^{(j)} = \mathbf{A}^{(j-1)} - \alpha_j \mathbf{P}_j$.

Given an $n \times n$ matrix $\mathbf{A}$, we can associate a bipartite graph $G_{\mathbf{A}} = (R \cup C, E)$ to it. The rows of $\mathbf{A}$ correspond to the vertices in the set R, and the columns of $\mathbf{A}$ correspond to the vertices in the set C so that $(r_i, c_j) \in E$ iff $a_{ij} \neq 0$. A perfect matching in $G_{\mathbf{A}}$, or G in short, is a set of n edges no two sharing a row or a column vertex. Therefore a perfect matching M in G defines a unique permutation matrix $\mathbf{P}_M \subseteq \mathbf{A}$.

Birkhoff's heuristic: This is the original heuristic used in proving that a doubly stochastic matrix has a BvN decomposition, described for example by Brualdi [2]. Let a be the smallest nonzero of $\mathbf{A}^{(j-1)}$ and $G^{(j-1)}$ be the bipartite graph associated with $\mathbf{A}^{(j-1)}$. Find a perfect matching M in $G^{(j-1)}$ containing a, set $\alpha_j \leftarrow a$ and $\mathbf{P}_j \leftarrow \mathbf{P}_M$.

A greedy heuristic: At every step j, among all perfect matchings find a perfect matching M in $G^{(j-1)}$ whose minimum element $\min\{\mathbf{P}_M \odot \mathbf{A}^{(j-1)}\}$ is the maximum. This "bottleneck" matching problem is polynomial time solvable, with for example MC64 [5]. In this greedy approach, α_j is the largest amount we can subtract from a row and a column of $\mathbf{A}^{(j-1)}$, and we hope to obtain a small k.

Lemma 3. *The greedy heuristic obtains $\alpha_1, \ldots, \alpha_k$ in a non-increasing order $\alpha_1 \geq \cdots \geq \alpha_k$, where α_j is obtained at the jth step.*

Proof. Observe that if $\alpha_1, \ldots, \alpha_k$ is obtained, at step $j \geq 1$ any permutation $\mathbf{P}_\ell$ for $\ell > j$ was available to the heuristic. If $\alpha_\ell > \alpha_i$, then $\mathbf{P}_\ell$ would have been chosen instead of $\mathbf{P}_j$, where $\min\{\mathbf{P}_\ell \odot \mathbf{A}^{(j-1)}\} \geq \alpha_\ell$. □

4 Experiments

Here we present results with the two heuristics. We note that the original Birkhoff heuristic was not concerned with the minimality of the number of permutation matrices. Therefore the presented results are not for comparing the two heuristics, but for giving results with what is available. We give results on two different set of matrices. The first set contains real world, sparse matrices. The second set contains a set of randomly created, dense, doubly stochastic matrices.

The first set of matrices was created as follows. We have selected all matrices with the following properties from the University of Florida Sparse Matrix Collection [4]: square, has at least 5000 and at most 10000 rows, fully indecomposable, and there are at most 50 and at least 2 nonzeros per row. This gave a set of 66 matrices. These 66 matrices are from 30 different group of problems; we have chosen at most two per group to remove any bias that might be arising from the group. This resulted in 32 matrices which we preprocessed as follows to obtain a set of doubly stochastic matrices. We first took the absolute values of the entries to make the matrices nonnegative. Then, we scaled them to be doubly stochastic using the algorithm of Knight et al. [7] with a tolerance of 10^{-6} with at most 1000 iterations. With this setting, the scaling algorithm tries to get the maximum deviation of a row/column sum from 1 to be less than 10^{-6} within 1000 iterations. In 7 matrices, the deviation was larger than 10^{-4}. We deemed this too big a deviation from a doubly stochastic matrix and discarded those matrices. At the end, we had 25 matrices given in Table 1.

We run the two heuristics for the BvN decomposition to obtain at most 2000 permutation matrices or until they accumulated a total of at least 0.9999 with the coefficients. The accumulated total coefficients $\sum_{i=1}^{k} \alpha_i$ and the number of permutation matrices k for the Birkhoff and greedy heuristics are given in Table 1. As seen in this table, the greedy heuristic obtains much smaller number of permutation matrices than Birkhoff's heuristic, except the matrix `n3c6-b7`. This is

matrix	n	τ	$d_{\max}$	dev.	Birkhoff $\sum_{i=1}^{k}\alpha_i$	Birkhoff k	greedy $\sum_{i=1}^{k}\alpha_i$	greedy k
aft01	8205	125567	21	0.0e+00	0.160	2000	1.000	120
aft02	8184	127762	82	1.0e-06	0.000	1434	1.000	234
barth	6691	46187	13	0.0e+00	0.160	2000	1.000	71
barth4	6019	40965	13	0.0e+00	0.140	2000	1.000	61
bcspwr10	5300	21842	14	1.0e-06	0.380	2000	1.000	63
bcsstk38	8032	355460	614	0.0e+00	0.000	2000	1.000	592$*$
benzene	8219	242669	37	0.0e+00	0.000	2000	1.000	113
c-29	5033	43731	481	1.0e-06	0.000	2000	1.000	870
EX5	6545	295680	48	0.0e+00	0.020	2000	1.000	229
EX6	6545	295680	48	1.0e-06	0.030	2000	1.000	226
flowmeter0	9669	67391	11	0.0e+00	0.510	2000	1.000	58
fv1	9604	85264	9	0.0e+00	0.620	2000	1.000	50
fv2	9801	87025	9	0.0e+00	0.620	2000	1.000	52
fxm3_6	5026	94026	129	1.0e-06	0.130	2000	1.000	383
g3rmt3m3	5357	207695	48	1.0e-06	0.050	2000	1.000	223
Kuu	7102	340200	98	0.0e+00	0.000	2000	1.000	330
mplate	5962	142190	36	0.0e+00	0.030	2000	1.000	153
n3c6-b7	6435	51480	8	0.0e+00	1.000	8	1.000	8
nemeth02	9506	394808	52	0.0e+00	0.000	2000	1.000	109
nemeth03	9506	394808	52	0.0e+00	0.000	2000	1.000	115
olm5000	5000	19996	6	1.0e-06	0.750	283	1.000	14
s1rmq4m1	5489	262411	54	0.0e+00	0.000	2000	1.000	211
s2rmq4m1	5489	263351	54	0.0e+00	0.000	2000	1.000	208
SiH4	5041	171903	205	0.0e+00	0.000	2000	1.000	574
t2d_q4	9801	87025	9	2.0e-06	0.500	2000	1.000	54

Table 1: Birkhoff's heuristic and the greedy heuristic on real world matrices. The column τ contains the number of nonzeros in a matrix. The column $d_{\max}$ contains the maximum number of nonzeros in a row or a column, setting up a lower bound for the number k of permutation matrices in a BvN decomposition. The column "dev." contains the maximum deviation of a row/column sum of a matrix $\mathbf{A}$ from 1, in other words the value $\max\{\|\mathbf{A1}-\mathbf{1}\|_\infty, \|\mathbf{1^TA}-\mathbf{1^T}\|_\infty\}$ reported to six significant digits. The two heuristics are run to obtain at most 2000 permutation matrices or until they accumulated a total of at least 0.9999 with the coefficients. In one matrix (marked with $*$), the greedy heuristic obtained this number in less than $d_{\max}$ permutation matrices—increasing the limit to 0.999999 made it return with 908 permutation matrices.

	Birkhoff		greedy	
n	$\sum_{i=1}^{k} \alpha_i$	k	$\sum_{i=1}^{k} \alpha_i$	k
100	0.99	9644	1.00	388
200	0.99	39208	1.00	717
300	1.00	88759	1.00	1042

Table 2: Birkhoff's heuristic and the greedy heuristic on random dense matrices. The maximum deviation of a row/column sum of a matrix $\mathbf{A}$ from 1, that is $\max\{\|\mathbf{A1}-\mathbf{1}\|_\infty, \|\mathbf{1^T A}-\mathbf{1^T}\|_\infty\}$ was always less than 10^{-6}.

a special matrix, with eight nonzeros in each row and column and all nonzeros are 1/8. Both heuristics find the same (minimum) number of permutation matrices. We note that the geometric mean of the ratios $k/d_{\max}$ is 3.4 for the greedy heuristic.

The second set of matrices was created as follows. For $n \in \{100, 200, 300\}$, we created five matrices of size $n \times n$ whose entries are randomly chosen integers between 1 and 100 (we performed tests with integers between 1 and 20 and the results were close to what we present here). We then scaled them to be doubly stochastic using the algorithm of Knight et al. [7] with a tolerance of 10^{-6} with at most 1000 iterations. We run the two heuristics for the BvN decomposition such that at most $n^2 - 2n + 2$ permutation matrices are found, or the total value of the coefficients was larger than 0.9999. We then took the average of the five instances with the same n. The results are shown in Table 2. In this table again we see that the greedy heuristic obtains much smaller k than Birkhoff's heuristic.

5 Conclusion

We investigated the problem of obtaining a Birkhoff-von Neumann decomposition of a given doubly stochastic matrix with the smallest number of permutation matrices. We showed that the problem is NP-hard. We proposed a natural greedy heuristic and presented experimental results with it along with results obtained by a known heuristic from the literature. On a set of real world matrices, we saw that the greedy heuristic obtains results that are not too far from a trivial lower bound. This calls for a better investigation of the heuristic to see if it has an approximation guarantee.

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