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 on a set of real world sparse matrices and random matrices.

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1. Introduction

Let $\mathbf{A} = [a_{ij}] \in \mathbb{R}^{n\times n}$. The matrix $\mathbf{A}$ is said to be doubly stochastic if $a_{ij} \geq 0$ 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 scalars $\alpha_1, \alpha_2, \ldots, \alpha_k$ 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* [1] states that $k \leq n^2 - 2n + 2$ for dense matrices; Brualdi and Gibson [2] and Brualdi [3] show that for a fully indecomposable sparse matrix with τ nonzeros $k \leq \tau - 2n + 2$.

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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 [3, 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). We also propose a heuristic (Section 3) for obtaining a BvN decomposition with a small number of permutation matrices. We investigate some of the properties of the 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 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 [4], if for each permutation matrix $\mathbf{P} \subseteq \mathbf{A}$, $p_{kl} = 1$ for at most one pair $(k, l) \in U$.

Lemma 1 (Brualdi [3])**.** *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 $\mathbf{A}$. Brualdi [3] shows that for any integer t with $1 \leq t \leq \lceil n/2 \rceil \lceil (n+1)/2 \rceil$, there exists an $n \times n$ doubly stochastic matrix $\mathbf{A}$ such that $\gamma(\mathbf{A}) = t$.

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 $i = 2, \ldots, n$:

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

We state and prove an obvious lemma to be used later in the paper.

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 $\{\frac{c_i}{\sum c_j} : \text{for } i = 1, \ldots, n\}$.*

Proof. Since the first row of $\mathbf{C}'$ has all nonzero entries and only n permutation matrices are permitted, the multi-set of coefficients must be the entries in the first row. □

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 $j = 1$.

Note that the lemma is not concerned by the uniqueness of the BvN decomposition which would need a unique set of permutation matrices as well. If all c_is were distinct, this would have been true, where the set of $\mathbf{D}_j$s 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 will correspond to the entries in a strongly stable set of cardinality k.

2.2. The computational complexity of MinBvNDec

Here, we prove that the MinBvNDec problem is NP-complete in the strong sense, i.e., it remains NP-complete when the instance is represented in unary. It suffices to do a reduction from a strongly NP-complete problem to prove the strong NP-completeness [5, Section 6.6].

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 a given matrix.

To establish NP-completeness, we demonstrate a reduction from the well-known 3-PARTITION problem 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 a $3m \times 3m$ circulant matrix whose first row is $a_1, \ldots, a_{3m}$. It is easy to see that $\mathbf{M}$ is doubly stochastic. A solution of $\mathcal{I}_2$ is a BvN decomposition of $\mathbf{M}$ with $k = 3m$ permutations. 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 decomposition 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 coefficients used in the BvN decomposition of $\frac{1}{mB}\mathbf{C}$. Note that these three indices i, j, k defining the three coefficients used for one entry of $\mathbf{E}_m$ cannot be used for another entry in the same row. 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 solution to $\mathcal{I}_1$, concluding the proof. $\square$

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 decompositions 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 [3]. 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 in $G^{(j-1)}$ find one whose minimum element is the maximum. That is, find a perfect matching M in $G^{(j-1)}$ where $\min\{\mathbf{P}_M \odot \mathbf{A}^{(j-1)}\}$ is the maximum. This "bottleneck" matching problem is polynomial time solvable, with for example MC64 [7]. 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 $\min\{\mathbf{P}_\ell \odot \mathbf{A}^{(j-1)}\} \geq \alpha_\ell$. $\square$

4. Experiments

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, preprocessed to be doubly stochastic. The second set contains a few 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 (UFL) Collection [8]: 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

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 sparse matrices from the UFL Collection. 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 $\max\{\|\mathbf{A1} - \mathbf{1}\|_\infty, \|\mathbf{1}^\mathbf{T}\mathbf{A} - \mathbf{1}^\mathbf{T}\|_\infty\}$ reported to six significant digits. The two heuristics are run to obtain at most 2000 permutation matrices, or until they accumulated a sum 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 $\max\{\|\mathbf{A}\mathbf{1}-\mathbf{1}\|_\infty, \|\mathbf{1}^\mathbf{T}\mathbf{A}-\mathbf{1}^\mathbf{T}\|_\infty\}$ was always less than 10^{-6}. For each n, the results are the averages of five different instances.

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. [9] 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 sum of at least 0.9999 with the coefficients. The accumulated sum of 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 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. [9] 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 in Table 2. In this table again, we see that the greedy heuristic obtains much smaller k than Birkhoff's heuristic.

The experimental observation that the greedy heuristic performs better than the Birkhoff heuristic is not surprising. This is for two reasons. First, as stated before, the original Birkhoff heuristic is not concerned with the number of permutation matrices. Second, the greedy heuristic is an adaptation of the Birkhoff heuristic to have large reductions at each step.

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 sparse and dense matrices, the greedy heuristic obtained 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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