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AN SVD APPROACH TO IDENTIFYING METASTABLE STATES OF MARKOV CHAINS*

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Abstract. Being one of the key tools in conformation dynamics, the identification of metastable states of Markov chains has been subject to extensive research in recent years, especially when the Markov chains represent energy states of biomolecules. Some previous work on this topic involved the computation of the eigenvalue cluster close to one, as well as the corresponding eigenvectors and the stationary probability distribution of the associated stochastic matrix. More recently, since the eigenvalue cluster algorithm may be nonrobust, an optimization approach was developed. As a possible less costly alternative, we present an SVD approach of identifying metastable states of a stochastic matrix, where we only need the singular vector associated with the second largest singular value. We also introduce a concept of block diagonal dominance on which our algorithm is based. We outline some theoretical background and discuss the advantages of this strategy. Some simulated and real numerical examples illustrate the effectiveness of the proposed algorithm.

Key words. Markov chain, stochastic matrix, conformation dynamics, metastable, eigenvalue cluster, singular value decomposition, block diagonal dominance

AMS subject classifications. 15A18, 15A51, 60J10, 60J20, 65F15

1. Introduction.

The research for this paper has been motivated by the work on conformation dynamics, or more specifically, on the identification of metastable conformations of biomolecules done by Deuflhard et al., see, e.g., [7], [8], and the references therein. This problem arises for instance in drug design, where it is important to study different conformations of the drug molecule in order to optimize its shape for best possible binding properties with respect to the target molecule [22]. Different conformations, also called aggregates or metastable states of a molecule are sets of states such that the transition within the set is very probable whereas the transition between these sets only rarely occurs.

We briefly describe this problem from a mathematical point of view. Given a stochastic matrix B representing some states of a biomolecule, but including some noise due to measurements, find a permutation P so that $P^TBP = A + E$, where A is stochastic and block diagonal, and E has small entries. The diagonal blocks of A correspond to the metastable states, and E consists of the noise and also of the small probabilities that the molecule might move from one aggregate to another. The number of blocks in A is of particular interest, and it is not known *a priori*.

The approach to identify metastable conformations of biomolecules presented in [7] involves the computation of the eigenvalue cluster of B close to one, the so-called Perron cluster, as well as the corresponding eigenvectors. The number of eigenvalues in the cluster, then, represents the number of different metastable states. The algorithm also uses a sign structure analysis of the corresponding eigenvectors to identify the different sets. Since this algorithm may be nonrobust, an optimization approach was developed in [8]. The main idea of the approach in [8] is to find a transformation of the computed perturbed eigenvectors such

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that the transformed eigenvectors are contained in a simplex with unit vectors as vertices. The number of vertices is taken to be the number of diagonal blocks, it may be smaller than the number of computed eigenvectors. In both approaches the Markov chain is assumed to be reversible in order to exploit the fact that the transition matrix is then symmetric with respect to an inner product, which in its definition requires the stationary distribution of the Markov chain.

The main drawbacks of these two approaches are firstly, that the identification of the Perron cluster may be difficult or even impossible if the transition matrix of the Markov chain has no significant spectral gaps; and secondly in the first method, the calculation of the stationary distribution, although usually well conditioned [11], [16], [20], [29], may be costly and badly conditioned if the Perron cluster contains many eigenvalues very close to 1; see, e.g., [25]. In this case, also the identification of the Perron cluster may be difficult or even impossible. We compare our new method to these two methods of [7] and [8], since they seem to be the state of the art methods used to identify conformations of biomolecules.

In this paper, we present a different approach to identifying metastable states of a Markov chain: we find a permutation of a given stochastic transition matrix of a Markov chain, such that the resulting matrix is block diagonally dominant. We also introduce a concept of block diagonal dominance different than that used in [7], [8]. In our method we do not need to know the number of metastable states in advance but instead it is calculated in the process. Hence, the functionality of the algorithm does not depend on a significant gap in the spectrum of the transition matrix of the Markov chain. Furthermore, instead of calculating many eigenvectors or employing costly optimization procedures, we calculate only two singular vectors that correspond to the two largest singular values. This allows us to use iterative procedures such as Lanczos or Arnoldi iteration for our computations [3]. Since we are dealing with singular vectors instead of eigenvectors, we do not need the reversibility assumption on the Markov chain. Under this assumption, the transition matrix is symmetric in a non-Euclidean scalar product defined using the stationary distribution. Symmetry on the other hand is needed for accuracy of calculations. In the case of singular vectors, we do not need this, since singular vectors form an orthogonal basis.

The basic idea of our algorithm is to calculate the singular vector that corresponds to the second largest singular value, sort its entries and apply the thus obtained permutation to the transition matrix. This idea is based on an observation due to I. Slapnicar [23]. Our strategy partly reflects well-studied ideas from the literature on computer science and discrete mathematics. In graph partitioning, the Fiedler vector, which is the eigenvector corresponding to the second smallest eigenvalue of a Laplacian matrix plays an important role, see, e.g., [12], [21] for the basics and [1], [24] for further reading. Ideas of using the singular value decomposition for graph clustering can be found, e.g., in [9], [30], or in the case of the seriation and the consecutive ones problem, e.g., in [2].

Our paper is organized as follows. In Section 2 we introduce the notation and some well-known definitions and theorems that we will use throughout the paper. In Section 3, we formulate some theoretical results for uncoupled Markov chains followed by Section 4, where we translate these results to the nearly uncoupled case. In Section 5, we describe our algorithm in detail. Finally, in Section 6, we present some constructed and some real numerical examples that illustrate the functionality of our new method.

2. Preliminaries.

We call a vector $v \in \mathbb{R}^n$, $v = [v_i]_{i=1,\ldots,n}$ *positive* and we write $v > 0$ if all its entries v_i are positive. A matrix $T \in \mathbb{R}^{n\times n}$, $T = [t_{ij}]_{i,j=1,\ldots,n}$ is called *positive (nonnegative)* and we write $T > 0$ ($T \geq 0$) if all entries t_{ij} are positive (nonnegative). The matrix T is called *reducible* if there exists a permutation matrix $P \in \mathbb{R}^{n\times n}$, such that

$PTP^T = \begin{bmatrix} T_{11} & 0 \\ T_{21} & T_{22} \end{bmatrix}$, where T_{11}, T_{22} are square. Otherwise it is called *irreducible*. We call the matrix T *(strictly) diagonally dominant* if $|t_{ii}| > \sum_{\substack{j=1 \\ j \neq i}}^{n} |t_{ij}|$ for all $i = 1, \ldots, n$. We denote by $\mathbb{1}$ the vector of all ones $[1, \ldots, 1]^T$. For $u, v \in \mathbb{R}^n$, we denote by $\langle u, v \rangle$ the Euclidean scalar product.

A scalar $\lambda \in \mathbb{R}$ is called an *eigenvalue* of the matrix $T \in \mathbb{R}^{n \times n}$ if a vector $v \in \mathbb{R}^n$, $v \neq 0$ exists, such that $Tv = \lambda v$. Such a vector v is called a *(right) eigenvector* of T associated with λ. A vector $w \in \mathbb{R}^n$, $w \neq 0$ with $w^T T = \lambda w^T$ is called a *(left) eigenvector* of T. Let $T \in \mathbb{R}^{n \times n}$ have the eigenvalues λ_i, $i = 1, \ldots, n$. We call $\rho(T) = \max_{1 \leq i \leq n} |\lambda_i|$ the *spectral radius of* T.

A process is called *finite homogeneous Markov chain* if it has n states $s_1, \ldots, s_n$ and the transition probability $P[s_i \rightsquigarrow s_j] =: t_{ij}$ is time-independent. The matrix $T = [t_{ij}]_{i,j=1,\ldots,n}$ satisfies $t_{ij} \geq 0$ and $\sum_{j=1}^{n} t_{ij} = 1$ for $i, j = 1, \ldots, n$, i.e., it is *(row) stochastic* and it is called the *transition matrix* of a Markov chain. We denote by $x^k = [x_i^k]_{i=1,\ldots,n}$ the *probability distribution vector*, where x_i^k is the probability that the system is in state s_i after k steps. We have, $x_i^k \geq 0$ and $\sum_{i=1}^{n} x_i^k = 1$ for each k. A distribution vector x is said to be *stationary* if $x^T T = x^T$. A matrix A is called *block stochastic* if A is block-diagonal, i.e..,

$$A = \operatorname{diag}(A_1, \ldots, A_m), \tag{2.1}$$

the matrices $A_i \in \mathbb{R}^{n_i \times n_i}$, $i = 1, \ldots, m$, are (row) stochastic matrices, and $\sum_{i=1}^{m} n_i = n$. For every block A_i, we define sets S_i of n_i indices corresponding to the block A_i. We have $\bigcup_{i=1}^{m} S_i = \{1, \ldots, n\}$ and $S_i \cap S_j = \emptyset$ for $i \neq j$. We define by $A_{ij} = A(S_i, S_j)$ the subblock of A that contains entries a_{kl}, where $k \in S_i, l \in S_j$.

The (adjacency) graph of a matrix $A = [a_{ij}]_{i,j=1,\ldots,n}$ is defined by letting the vertices represent the unknowns. There is an edge from node v_i to node v_j whenever $a_{ij} \neq 0$. We call a graph and, hence, the corresponding matrix *simply connected* if for all $i, j \in \{1, \ldots, n\}$ there exists a path from node i to node j or from node j to node i.

The well-known Perron-Frobenius Theorem (see, e.g., [4, p. 27]) guarantees the existence and uniqueness of a stationary distribution.

THEOREM 2.1 (Perron-Frobenius Theorem). *Let $T \geq 0$ be irreducible with spectral radius $\rho(T)$. Then $\rho(T)$ is a simple eigenvalue and T has a positive left and right eigenvector corresponding to $\rho(T)$. Any positive eigenvector x of a nonnegative matrix T corresponds to $\rho(T)$.*

In this paper we apply the singular value decomposition to identify metastable states of a Markov chain. The following well-known theorem (see, e.g., [14, p. 70]) states the existence of a singular value decomposition.

THEOREM 2.2 (SVD). *Let $A \in \mathbb{R}^{n \times n}$. Then, there exist orthogonal matrices $U = [u_1, \ldots, u_n] \in \mathbb{R}^{n \times n}$ and $V = [v_1, \ldots, v_n] \in \mathbb{R}^{n \times n}$, such that*

$$A = U \Sigma V^T, \tag{2.2}$$

where $\Sigma = \operatorname{diag}(\sigma_1, \ldots, \sigma_n)$ and $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n \geq 0$.

We call $\sigma_1, \ldots, \sigma_n$, *singular values*, $u_1, \ldots, u_n$, *left singular vectors* and $v_1, \ldots, v_n$, *right singular vectors* of A. Singular values with multiplicity one are called *simple*.

3. Uncoupled Markov chains and the SVD. In this section we formulate the theoretical basis for the sign structure approach that we use in our algorithm. In Theorem 3.1, following the lines of [7, Lemma 2.5], we show an important sign structure property for singular vectors. Subsequently, we explain how we use this property in our approach and state the advantages of this strategy.

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If a block stochastic matrix A is permuted to $B = PAP^T$ then clearly A and B have the same singular values. In the following we present an approach to obtain a permutation matrix $\tilde{P}$ that yields $\tilde{A} = \tilde{P}^T B \tilde{P}$ where $\tilde{A}$ is block-diagonal and reveals the hidden block-structure of B. We will determine such a $\tilde{P}$ by means of the singular value decomposition. One motivation for our approach is the fact that the singular vectors of B are obtained from those of A by the same permutation that permutes A to B.

THEOREM 3.1. *Let A be a block-stochastic matrix of the form (2.1) with m simply connected diagonal blocks of order $n_1, \dots, n_m$, denoted by $A_1, \dots, A_m$. Let S_i be the set of n_i indices corresponding to the block A_i, $i = 1, \dots, m$. Let*

$$A = \tilde{U} \Sigma \tilde{V}^T$$

be a singular value decomposition of A as in (2.2) and let $\tilde{u}_1, \dots, \tilde{u}_m$ be the m left singular vectors corresponding to the largest singular value of each of the blocks $A_1, \dots, A_m$, respectively. Associate with every state s_i its sign structure

$$\operatorname{sign}(s_i) := \left[\operatorname{sgn}(\tilde{u}_1)_i, \dots, \operatorname{sgn}(\tilde{u}_m)_i\right],$$

where

$$\begin{aligned} \operatorname{sgn} : \mathbb{R} &\longrightarrow \{-1, 0, 1\} \\ \alpha &\longmapsto \begin{cases} 1, & \alpha > 0 \\ 0, & \alpha = 0 \\ -1, & \alpha < 0 \end{cases} . \end{aligned}$$

Then,

- *i) states that belong to the same block of A exhibit the same sign structure, i.e., for any A_j and all $k, l \in S_j$, we have $\operatorname{sign}(s_k) = \operatorname{sign}(s_l)$;*
- *ii) states that belong to different blocks of A exhibit different sign structure, i.e., for any A_i, A_j with $i \neq j$ and all $k \in S_i, l \in S_j$ we have $\operatorname{sign}(s_k) \neq \operatorname{sign}(s_l)$.*

Proof. i) The left singular vectors of a matrix A are the eigenvectors of AA^T, since from (2.2) we get $AA^T = \tilde{U}\Sigma^2\tilde{U}^T$, see, e.g., [14]. Note that the singular values of A are the square roots of the eigenvalues of AA^T.

Since we have assumed A to have m simply connected blocks, the matrix product $A_i A_i^T$ is irreducible and we have $A_i A_i^T \geq 0$. Hence, by the Perron-Frobenius Theorem 2.1 we have that $\rho(A_i A_i^T)$ is a simple eigenvalue and the corresponding right eigenvector $\hat{u}_i$ is strictly positive. Thus, the vector

$$\tilde{u}_i = [0, \dots, 0, \hat{u}_i^T, 0, \dots, 0]^T \tag{3.1}$$

is an eigenvector of AA^T corresponding to the largest eigenvalue of the block $A_i A_i^T$, i.e., it is a left singular vector corresponding to the largest singular value of the block A_i. This implies that states that belong to the same block exhibit the same sign structure.

ii) Since by part i) all states that belong to the same block have the same sign structure, without loss of generality, we may assume that every block consists of only one state, i.e., $n = m$. Then, since $\tilde{U} = [\tilde{u}_1, \dots, \tilde{u}_m] \in \mathbb{R}^{m \times m}$ is orthogonal, the rows of $\tilde{U}$ are also orthogonal and, hence, no two vectors can have the same sign structure. $\square$

Note, that the same results can be obtained for the right singular vectors by considering the matrix $A^T A$ instead of AA^T.

To illustrate the sign structure property established in Theorem 3.1 we consider the following example.

EXAMPLE 3.2. Consider a block diagonal transition matrix of a Markov chain with three blocks of sizes 2, 3, 2. Then, the three singular vectors v_1, v_2, v_3 corresponding to the largest singular values of each of the blocks are linear combinations of the vectors $\tilde{u}_i$ in (3.1). We have that the vectors $\tilde{u}_i$

$$\begin{array}{cccc} & \tilde{u}_1 & \tilde{u}_2 & \tilde{u}_3 \\ \begin{array}{c} s_1 \\ s_2 \\ s_3 \\ s_4 \\ s_5 \\ s_6 \\ s_7 \end{array} & \begin{bmatrix} + \\ + \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} & \begin{bmatrix} 0 \\ 0 \\ + \\ + \\ + \\ 0 \\ 0 \end{bmatrix} & \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ + \\ + \end{bmatrix} \end{array}$$

are positive on the block they correspond to and zero elsewhere. A possible linear combination for the orthogonal vectors v_i could lead to the following sign structure.

$$\begin{array}{cccc} & v_1 & v_2 & v_3 \\ \begin{array}{c} s_1 \\ s_2 \\ s_3 \\ s_4 \\ s_5 \\ s_6 \\ s_7 \end{array} & \begin{bmatrix} + \\ + \\ + \\ + \\ + \\ + \\ + \end{bmatrix} & \begin{bmatrix} + \\ + \\ - \\ - \\ - \\ - \\ - \end{bmatrix} & \begin{bmatrix} - \\ - \\ - \\ - \\ - \\ + \\ + \end{bmatrix} \end{array}.$$

Here, the states s_1, s_2 belong to the first block and have the sign structure $(+, +, -)$, the states s_3, s_4, s_5 belong to the second block and have the sign structure $(+, -, -)$ and the states s_6, s_7 belong to the third block and have the sign structure $(+, -, +)$.

The idea to sort the singular vector corresponding to the second largest singular value and to apply the resulting permutation to the matrix is due to an observation by Slapnicar [23]. This method always works for matrices with only two blocks, see Section 5 for an example, and usually works for matrices with a few blocks. For larger matrices having more blocks, however, this simple approach is not sufficient to reveal the block structure.

By using the sign structure property established in Theorem 3.1 we modify this idea into a recursive bisectioning algorithm that is suitable for large matrices with any number of blocks. The main strategy is to identify two blocks in each step and apply the sorting procedure recursively to each of the blocks. The details of the algorithm are presented in Section 5.

The advantages of this approach in comparison to the eigenvalue approach presented in [7] are the following:

- we do not need to know the number of blocks in advance. Instead, we only set a tolerance threshold for the size of the entries in the off-diagonal blocks. The number of identified blocks then reflects the given tolerance, see Section 4;
- instead of computing all eigenvectors corresponding to the eigenvalue 1, we only calculate two singular vectors in each recursion step;
- it is less costly than an optimization approach in terms of runtime, since we need to calculate only two singular values and vectors per recursion, which can efficiently be done by Arnoldi-type iterative procedures [19];
- to compute eigenvectors accurately, it is usually assumed that the transition matrix is symmetric in a non-Euclidean inner product defined using the stationary distribu-

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tion; for the computation of singular vectors, we do not need this assumption, since singular vectors are by definition orthogonal;
- the approach makes use of combinatorial aspects of the problem.

4. Nearly uncoupled Markov chains. In the previous section we have considered uncoupled Markov chains. In applications, due to perturbations, noise and actual weak couplings between aggregates, the Markov chains are nearly uncoupled. Such a matrix B, consisting of m nearly uncoupled blocks, can be transformed by a permutation matrix P to

$$PBP^T = A + E = \begin{bmatrix} A_{11} & E_{12} & \dots & E_{1m} \\ E_{21} & A_{22} & \dots & E_{2m} \\ \vdots & \vdots & & \vdots \\ E_{m1} & E_{m2} & \vdots & A_{mm} \end{bmatrix}, \tag{4.1}$$

where the elements of each E_{ij} are small. In this case, we are looking for some permutation matrix $\tilde{P}$, possibly different from the matrix P in (4.1), that permutes B into a block diagonally-dominant matrix of the form (4.1). In order to define diagonal dominance for blocks, we need to introduce a measure for the smallness of the off-diagonal blocks or, equivalently, a measure for the largeness of the diagonal blocks.

For this purpose, in Definition 4.2 below, we first define a norm that is more general than that of [7, Definitions 2.3, 2.4]. The norm used in [7, Definitions 2.3, 2.4] and the $\mathbb{1}$-norm that we will use in the following, will then be special cases of the general norm in Definition 4.2.

Let $S_k, S_l \subseteq \{1, \dots, n\}$ be sets of indices. In the following, we denote by $B_{kl} = B(S_k, S_l)$ the subblock of B corresponding to the index sets S_k, S_l. For simplicity, for any k, we write B_k for the diagonal block B_{kk}.

DEFINITION 4.1 (Conditional transition probability). *Let $B = [b_{ij}] \in \mathbb{R}^{n\times n}$ be a stochastic matrix. Let $v = [v_1, \dots, v_n]^T$ be a positive vector with $\sum_{i=1}^n v_i = 1$. Let $S_k, S_l \subseteq \{1, \dots, n\}$ be sets of indices with $S_k \cap S_l = \emptyset$ and let $B_k = B(S_k, S_k), B_l = B(S_l, S_l)$ be the corresponding blocks.. Then, the conditional transition probability from B_k to B_l is given by*

$$\omega_v(B_k, B_l) = \frac{\sum_{i\in S_k, j\in S_l} v_i |b_{ij}|}{\sum_{i\in S_k} v_i}. \tag{4.2}$$

Note that in (4.2), in order to define a norm in the following Definition 4.2, we use absolute values of b_{ij}, although in our case these entries are all nonnegative.

DEFINITION 4.2 (v-Norm). *For any vector $v > 0$, we define the v-norm of a matrix (block) B_{kl} by*

$$||B_{kl}||_v := \omega_v(B_k, B_l). \tag{4.3}$$

DEFINITION 4.3 (Coupling matrix). *Let $S_1, \dots, S_m \subseteq \{1, \dots, n\}$ be sets of indices such that $\bigcup_{i=1}^n S_i = \{1, \dots, n\}$ and $S_i \cap S_j = \emptyset$, for all $i \neq j$. Let $B_k = B(S_k, S_k)$, $k = 1, \dots, m$, be the diagonal blocks of the corresponding block decomposition of B. The coupling matrix of the decomposition is given by the stochastic matrix W_v defined by*

$$(W_v)_{kl} = \omega_v(B_k, B_l),$$

for $k, l = 1, \dots, m$.

In [7] and [8] the vector v is taken to be the stationary distribution of the Markov chain, i.e., $v = \pi$, where $\pi^T B = \pi^T$ and $\pi^T \mathbb{1} = 1$. Hence, the norm used in [7] and [8] is called

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the π-norm. If we use $v = \mathbb{1}$ instead and recalling that n_k is the cardinality of S_k, then we obtain

$$\|B_{kl}\|_{\mathbb{1}} = \frac{1}{n_k} \sum_{i\in S_k, j\in S_l} |b_{ij}|, \tag{4.4}$$

and we call this norm the $\mathbb{1}$-norm. Note that the $\mathbb{1}$-norm is simply the average row sum of a matrix (block).

We discuss the difference of the $\mathbb{1}$-norm and the norm used in [7] and [8] in Section 6. The advantage of our choice is that we avoid calculating the stationary distribution of the Markov chain, which, although usually well conditioned [11], [16], [20], [29], may be costly and badly conditioned if the Perron cluster contains many eigenvalues very close to 1, see, e.g., [25]. We claim to obtain the same qualitative results with both norms, see Section 6. The following lemma gives the factors for the equivalence between the two norms (4.3) and (4.4) for a diagonal block.

LEMMA 4.4. *Let $B = [b_{ij}] \in \mathbb{R}^{n\times n}$ be a stochastic matrix. Let $S_k \subseteq \{1,\dots,n\}$ be a set of n_k indices and $B_k = B(S_k, S_k)$ the corresponding principal subblock. Furthermore, let $v = [v_1,\dots,v_n]^T$ be a positive vector and $v_{\min}$, $v_{\max}$ the minimum and maximum values of the entries in $v(S_k) = \{v_i \mid i \in S_k\}$. Then, we have*

$$\|B_k\|_v \le \frac{v_{\max}}{v_{\min}} \|B_k\|_{\mathbb{1}} \le \frac{v_{\max}^2}{v_{\min}^2} \|B_k\|_v.$$

Proof. We have

$$\|B_k\|_v = \frac{\sum_{i,j\in S_k} v_i |b_{ij}|}{\sum_{i\in S_k} v_i}, \quad \|B_k\|_{\mathbb{1}} = \frac{1}{n_k} \sum_{i,j\in S_k} |b_{ij}|.$$

Since $v_{\min} \le v_i \le v_{\max}$ for all $i \in S_k$, we have that

$$\|B_k\|_v \le \frac{\sum_{i,j\in S_k} v_{\max} |b_{ij}|}{\sum_{i\in S_k} v_{\min}} = \frac{v_{\max}}{v_{\min}} . \frac{1}{n_k} \sum_{i,j\in S_k} |b_{ij}| = \frac{v_{\max}}{v_{\min}} \|B_k\|_{\mathbb{1}}.$$

Similarly,

$$\|B_k\|_v \ge \frac{\sum_{i,j\in S_k} v_{\min} |b_{ij}|}{\sum_{i\in S_k} v_{\max}} = \frac{v_{\min}}{v_{\max}} \|B_k\|_{\mathbb{1}}. \qquad \square$$

Note, that if we take v to be the stationary distribution π of the Markov chain, then v_{min} can be arbitrarily close to zero.

In the numerical examples in Section 6, we can see that for the diagonal blocks the π-norm is usually larger than the $\mathbb{1}$-norm. Lemma 4.4 indicates that even if $\|B_k\|_v$ is larger than $\|B_k\|_{\mathbb{1}}$, the former cannot exceed the latter by more than a factor $v_{\max}/v_{\min}$. However $\|B_k\|_v$ is not always larger than $\|B_k\|_{\mathbb{1}}$ as the following example demonstrates.

EXAMPLE 4.5. Consider the stochastic matrix

$$B = \left[\begin{array}{cc|c} 0.1 & 0.9 & 0 \\ 0.1 & 0.8 & 0.1 \\ \hline 0.3 & 0.1 & 0.6 \end{array}\right].$$

The stationary distribution of B is given by $\pi^T = \begin{bmatrix} 0.1346 & 0.6923 & 0.1731 \end{bmatrix}$. For the first 2×2 block B_1 we have $\|B_1\|_\pi = 0.9163 < 0.95 = \|B_1\|_{\mathbb{1}}$.

We now use the $\mathbb{1}$-norm to introduce a measure of the largeness of diagonal blocks.

DEFINITION 4.6 (Nearly uncoupled). *We call two or more diagonal blocks of a stochastic matrix nearly uncoupled if the $\mathbb{1}$-norm of each of the blocks is larger than a given threshold* $\mathrm{thr} = 1 - \delta$ *for some small* $\delta > 0$. *We call a matrix* $\tilde{B}$ *with*

$$\tilde{B} = \begin{bmatrix} \boxed{B_1} & B_{12} & \dots & B_{1m} \\ B_{21} & \boxed{B_2} & & \\ \vdots & & \ddots & \vdots \\ B_{m1} & & \dots & \boxed{B_m} \end{bmatrix}$$

nearly uncoupled if its m *diagonal blocks are nearly uncoupled and the corresponding coupling matrix (see Definition 4.3) is diagonally dominant.*

Our algorithm is designed to determine the possibly maximal number of blocks such that the coupling matrix is diagonally dominant.

In the previous section we have shown that singular vectors that correspond to the largest singular values of each of the blocks have a specific sign structure. States that belong to the same block exhibit the same sign structure and states that belong to different blocks exhibit different sign structures. Since our identification algorithm is based on this sign structure, we need to show that under certain conditions the assertions of Theorem 3.1 are still true under perturbations.

4.1. Perturbation theory. In this section we consider componentwise perturbation theory of singular vectors (or equivalently eigenvectors of symmetric matrices) according to [17], since we are interested not only in the size of the componentwise deviation of the perturbed singular vector from the unperturbed but also in its sign. For the normwise perturbation theory for singular vectors see, e.g., [26]. A survey of componentwise perturbation theory in absolute values can be found in [15]. Perturbation theory in terms of canonical angles of singular subspaces is discussed, e.g., in [5], [10], [27].

Consider the perturbed stochastic matrix

$$B = \hat{A} + \epsilon R,$$

for some $\epsilon > 0$. Here both $\hat{A}$ and B are stochastic. For sufficiently small real ϵ, the matrix $T(\epsilon) = BB^T$ is a linear symmetric operator that can be written as

$$T(\epsilon) = T + \epsilon T^{(1)} + \mathcal{O}(\epsilon^2), \tag{4.5}$$

where $T(0) = T = \hat{A}\hat{A}^T$ is the unperturbed operator and $T^{(1)} = \hat{A}R^T + R\hat{A}^T$ is a Lyapunov perturbation operator; see [17, pp. 63, 120]. For all real $\epsilon > 0$, the matrix-valued function $T(\epsilon)$ is a product of a stochastic matrix with its transpose, that is symmetric and nonnegative. Note, that the perturbations here are also symmetric. According to [17, Section 6.2], for such a $T(\epsilon)$ there exists an orthonormal basis of eigenvectors $\varphi_k(\epsilon)$ that are analytic functions of ϵ. In particular, the eigenvectors $\varphi_k(\epsilon)$ depend smoothly on ϵ and admit a Taylor expansion

$$\varphi_k(\epsilon) = \varphi_k + \epsilon\varphi_k^{(1)} + \mathcal{O}(\epsilon^2), \tag{4.6}$$

where φ_k are the orthonormal eigenvectors of the unperturbed operator T, i.e., linear combinations of the vectors $\tilde{u}_i$ in (3.1), and $\varphi_k^{(1)}$ is the (vector) coefficient of the first order error

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that we will derive in the following; see also [17, Section 6.2] for details. The following is a generalization from eigenvectors to singular vectors of [7, Theorem 3.1] and [8, Lemma 2.1]. Note that in [8, Lemma 2.1] a term is missing.

THEOREM 4.7. *Let $T(\epsilon)$ as in (4.5) have the two largest eigenvalues $\lambda_1(\epsilon) \geq \lambda_2(\epsilon)$. Suppose that the unperturbed matrix $T = T(0)$ as in (4.5) can be permuted to $\tilde{T} = PTP^T$ such that $\tilde{T}$ has m uncoupled irreducible blocks. Let $\lambda_1 > \lambda_2 > \ldots > \lambda_m$ be the largest eigenvalues corresponding to each of the blocks. Then, the perturbed orthonormal eigenvector $\varphi_2(\epsilon)$ corresponding to the perturbed singular value $\lambda_2(\epsilon)$ is of the form*

$$\varphi_2(\epsilon) = \sum_{j=1}^{m}(\alpha_j + \epsilon\beta_j)\tilde{u}_j + \epsilon \sum_{j=m+1}^{n} \left\langle \varphi_j, \varphi_2^{(1)} \right\rangle \varphi_j + \mathcal{O}(\epsilon^2), \tag{4.7}$$

where $\tilde{u}_j$ are the eigenvectors in (3.1) and α_j, β_j are suitable coefficients.

Proof. Assume that $\tilde{T}$ has m uncoupled irreducible blocks and suppose that $\lambda_1, \ldots, \lambda_m$ are the largest eigenvalues corresponding to each of the blocks, i.e., the corresponding eigenvectors φ_k are linear combinations of the vectors in (3.1). For $k = 1, \ldots, m$, let P_k be the orthogonal projection onto the eigenspace of the eigenvalue λ_k. Then, by [17, Sec. II.2.1], the perturbed projection $P_k(\epsilon)$ is analytic in ϵ and admits a Taylor expansion

$$P_k(\epsilon) = P_k + \epsilon P_k^{(1)} + \mathcal{O}(\epsilon^2),\ k = 1, \ldots, m,$$

where $P_k^{(1)}$ is the coefficient of the first order error as defined in [17, Sec. II.2.1(2.14)], i.e.,

$$P_k^{(1)} = \sum_{\substack{j\in\{1,\ldots,n\}\\ j\neq k}} \frac{1}{\lambda_k - \lambda_j}(P_kT^{(1)}P_j + P_jT^{(1)}P_k),\ k = 1, \ldots, m.$$

Let $P_{1,\ldots,m}$ be the orthogonal projection onto the eigenspace corresponding to the distinct eigenvalues $\lambda_1, \ldots, \lambda_m$. Then,

$$\begin{aligned} P_{1,\ldots,m}(\epsilon) &= \sum_{i=1}^{m} P_i(\epsilon) = \\ &= \sum_{i=1}^{m} P_i + \epsilon \sum_{i=1}^{m} \sum_{\substack{j\in\{1,\ldots,n\}\\ j\neq i}} \frac{1}{\lambda_i - \lambda_j}(P_iT^{(1)}P_j + P_jT^{(1)}P_i) + \mathcal{O}(\epsilon^2) = \\ &= P_{1,\ldots,m} + \epsilon \sum_{i=1}^{m} \sum_{j=m+1}^{n} \frac{1}{\lambda_i - \lambda_j}(P_iT^{(1)}P_j + P_jT^{(1)}P_i) + \mathcal{O}(\epsilon^2), \end{aligned} \tag{4.8}$$

since the terms for $j \leq m$ cancel out. For the corresponding eigenvectors $\varphi_1(\epsilon), \ldots, \varphi_m(\epsilon)$, we have that

$$\varphi_k(\epsilon) = P_{1,\ldots,m}(\epsilon)\varphi_k(\epsilon),\ k = 1, \ldots, m. \tag{4.9}$$

By plugging (4.6) and (4.8) into the right hand side of (4.9), we obtain

$$\begin{aligned} \varphi_k(\epsilon) &= \varphi_k + \epsilon\varphi_k^{(1)} + \mathcal{O}(\epsilon^2) = \\ &= P_{1,\ldots,m}\varphi_k + \epsilon\Big(\sum_{j=m+1}^{n} \frac{1}{\lambda_k - \lambda_j} P_jT^{(1)}\varphi_k + P_{1,\ldots,m}\varphi_k^{(1)}\Big) + \mathcal{O}(\epsilon^2). \end{aligned}$$

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Comparing the coefficients corresponding to ϵ, we get

$$(I - P_{1,\dots,m})\varphi_k^{(1)} = \sum_{j=m+1}^{n} \frac{1}{\lambda_k - \lambda_j} P_j T^{(1)} \varphi_k.$$

Since $(I - P_{1,\dots,m})$ is the orthogonal projection complementary to $P_{1,\dots,m}$, which is the projection onto the eigenspace corresponding to the eigenvectors $\varphi_1 \dots, \varphi_m$, we obtain

$$\varphi_k^{(1)} = \sum_{j=1}^{m} \tilde{\beta}_{kj}\varphi_j + \sum_{j=m+1}^{n} \frac{1}{\lambda_k - \lambda_j} P_j T^{(1)} \varphi_k, \tag{4.10}$$

with some coefficients $\tilde{\beta}_{kj} \in \mathbb{R}$. By inserting (4.10) into (4.6), we obtain

$$\begin{aligned} \varphi_k(\epsilon) &= \varphi_k + \epsilon\varphi_k^{(1)} + \mathcal{O}(\epsilon^2) = \\ &= \sum_{j=1}^{m} (\alpha_{kj} + \epsilon\beta_{kj})\tilde{u}_j + \epsilon \sum_{j=m+1}^{n} \frac{1}{\lambda_k - \lambda_j} P_j T^{(1)} \varphi_k + \mathcal{O}(\epsilon^2), \end{aligned} \tag{4.11}$$

with some coefficients $\alpha_{kj}, \beta_{kj} \in \mathbb{R}$, since the eigenvectors φ_k are linear combinations of the vectors $\tilde{u}_j$ in (3.1).

Following the lines of the proof of [8, Lemma 2.1] we can rewrite the second summand in (4.11) as follows. First, for $k = 1, \dots, m$, we expand the perturbed eigenvalues

$$\lambda_k(\epsilon) = \lambda_k + \epsilon\lambda_k^{(1)} + \mathcal{O}(\epsilon^2),$$

and rewrite the second summand as a projection in terms of the Euclidean scalar product $\langle , \rangle$,

$$\sum_{j=m+1}^{n} \frac{1}{\lambda_k - \lambda_j} P_j T^{(1)} \varphi_k = \sum_{j=m+1}^{n} \frac{1}{\lambda_k - \lambda_j} \left\langle \varphi_j, T^{(1)}\varphi_k \right\rangle \varphi_j.$$

Now we need an expression for $T^{(1)}$. For $k = 1, \dots, m$ we have

$$T(\epsilon)\varphi_k(\epsilon) = \lambda_k(\epsilon)\varphi_k(\epsilon).$$

We insert all expansions and obtain

$$(T + \epsilon T^{(1)} + \mathcal{O}(\epsilon^2))(\varphi_k + \epsilon\varphi_k^{(1)} + \mathcal{O}(\epsilon^2)) = (\lambda_k + \epsilon\lambda_k^{(1)} + \mathcal{O}(\epsilon^2))(\varphi_k + \epsilon\varphi_k^{(1)} + \mathcal{O}(\epsilon^2)). \tag{4.12}$$

Comparing the coefficients for the zero order terms in (4.12) yields

$$T\varphi_k = \lambda_k\varphi_k.$$

For the first order terms in (4.12) we get

$$T\varphi_k^{(1)} + T^{(1)}\varphi_k = \lambda_k\varphi_k^{(1)} + \lambda_k^{(1)}\varphi_k,$$

which transforms to

$$T^{(1)}\varphi_k = (\lambda_k I - T)\varphi_k^{(1)} + \lambda_k^{(1)}\varphi_k.$$

Now, we can rewrite the scalar product expression

$$\begin{aligned}\left\langle \varphi_j, T^{(1)}\varphi_k \right\rangle &= \left\langle \varphi_j, (\lambda_k I - T))\varphi_k^{(1)} + \lambda_k^{(1)}\varphi_k \right\rangle = \\ &= \left\langle \varphi_j, (\lambda_k I - T)\varphi_k^{(1)} \right\rangle + \underbrace{\lambda_k^{(1)} \langle \varphi_j, \varphi_k \rangle}_{=0}.\end{aligned}$$

The last term vanishes due to the orthogonality of the unperturbed eigenvectors of a symmetric operator. For the first term, since T is symmetric, we obtain

$$\begin{aligned}\left\langle \varphi_j, (\lambda_k I - T)\varphi_k^{(1)} \right\rangle &= \left\langle (\lambda_k I - T)\varphi_j, \varphi_k^{(1)} \right\rangle = \\ &= (\lambda_k - \lambda_j) \left\langle \varphi_j, \varphi_k^{(1)} \right\rangle.\end{aligned}$$

Finally, we can write (4.11) as

$$\varphi_k(\epsilon) = \sum_{j=1}^{m} (\alpha_{kj} + \epsilon\beta_{kj})\tilde{u}_j + \epsilon \sum_{j=m+1}^{n} \left\langle \varphi_j, \varphi_k^{(1)} \right\rangle \varphi_j + \mathcal{O}(\epsilon^2),$$

which for $k = 2$ and setting $\alpha_j = \alpha_{2j}$ and $\beta_j = \beta_{2j}$, is the result (4.7). ☐

The first sum in (4.7) does not spoil the sign structure as long as α_j, β_j have the same sign or, in case of different sign, ϵ is small enough such that $|\alpha_j| > \epsilon|\beta_j|$ holds for $j = 1, \ldots, m$, respectively. The third term depends on the orthogonality of the first order perturbation of the second singular vector $\varphi_2^{(1)}$ with respect to the singular vectors $\varphi_{m+1}, \ldots, \varphi_n$. If it is close to orthogonal, this term will be close to zero. However, the largeness of the third term essentially depends on the gap between the second and the $(m+1)$-st unperturbed singular values. One can see this by considering $\varphi_2^{(1)}$, which on the subspace corresponding to the singular vectors $\varphi_{m+1}, \ldots, \varphi_n$ yields

$$(I - P_{1,\ldots,m})\varphi_2^{(1)} = \sum_{j=m+1}^{n} \frac{1}{\lambda_2 - \lambda_j} P_j T^{(1)} \varphi_2.$$

The smaller this gap, the smaller the perturbation of the operator has to be in order not to spoil the sign structure. However, in many practical examples this gap is larger than the gap between the first m eigenvalues and the rest of the spectrum, which intuitively explains the better performance of the proposed method over the existing methods based on the Perron cluster. In the worst case, if the second sum of (4.7) has a different sign than the first sum, then also

$$\epsilon < \frac{\left| \left[\sum_{j=1}^{m} (\alpha_j + \epsilon\beta_j)\tilde{u}_j \right]_i \right|}{\left| \left[\sum_{j=m+1}^{n} \left\langle \varphi_j, \varphi_2^{(1)} \right\rangle \varphi_j \right]_i \right|},$$

has to hold. In this case, up to first order error, the sign will not be spoiled.

5. The algorithm.

In this section we propose an algorithm to determine a permutation of a stochastic matrix that permutes it into block diagonally dominant form (4.1) by recursively identifying diagonally dominant blocks. We first present an identification procedure in the case of two blocks. Then, we imbed this procedure into a recursive method that works for any number of blocks. Note that everything that is stated for left singular vectors in this section applies to right singular vectors as well.

Consider the case of two nearly uncoupled blocks. Let $PBP^T = A + E$ be a matrix of the form (4.1) that consists of two blocks ($m = 2$), where P is not known. Since B is not uncoupled, BB^T is irreducible and from the Perron-Frobenius Theorem 2.1, we know that B has a simple largest singular value σ_1 and a corresponding positive left singular vector u_1. Consider now the second largest singular value σ_2 and the corresponding left singular vector u_2.

Since singular vectors are orthogonal (or by the Perron-Frobenius theorem), u_2 must have a change in sign, i.e., there exist two indeces i and j such that $(u_2)_i(u_2)_j < 0$. From Theorem 3.1 we assume that states that correspond to values of different sign in u_2 belong to different blocks. We sort the second singular vector, e.g., in increasing order and use this permutation to permute the matrix B. Then, we split the permuted matrix $\tilde{B} = \tilde{P}B\tilde{P}^T$ such that the first block $\tilde{B}_1$ is of size equal to the number of negative values in u_2 and the second block $\tilde{B}_2$ is of size equal to the number of positive values in u_2. We obtain a matrix $\tilde{B}$ that reveals the hidden block structure of B, i.e., $\tilde{B}$ has the same diagonal block structure as A up to a permutation of the blocks and of the entries within a block.

The following example illustrates the identification procedure in the case of two blocks.

EXAMPLE 5.1. Consider the row stochastic matrix

$$A = \begin{bmatrix} 0.2000 & 0.8000 & 0 & 0 & 0 \\ 0.4000 & 0.6000 & 0 & 0 & 0 \\ 0 & 0 & 0.3000 & 0.3000 & 0.4000 \\ 0 & 0 & 0.2000 & 0.2000 & 0.6000 \\ 0 & 0 & 0.1000 & 0.1000 & 0.8000 \end{bmatrix}.$$

The singular vectors of A are given by

$$U = \begin{bmatrix} 0 & -0.7555 & 0 & -0.6552 & 0 \\ 0 & -0.6552 & 0 & 0.7555 & 0 \\ -0.4590 & 0 & 0.7891 & 0 & 0.4082 \\ -0.5702 & 0 & 0.0908 & 0 & -0.8165 \\ -0.6813 & 0 & -0.6076 & 0 & 0.4082 \end{bmatrix}.$$

We can see that the singular vectors are only nonzero on the one block they correspond to.

Now consider the perturbed matrix $A + E$, where

$$E = \begin{bmatrix} -0.0345 & -0.1128 & 0.0887 & 0.0393 & 0.0192 \\ -0.0592 & -0.1041 & 0.0667 & 0.0421 & 0.0544 \\ 0.0428 & 0.0015 & -0.0473 & 0.0154 & -0.0125 \\ 0.0252 & 0.0636 & -0.0212 & -0.0112 & -0.0564 \\ 0.0720 & 0.0799 & 0.0252 & -0.0656 & -0.1116 \end{bmatrix},$$

is chosen such that the matrix

$$\tilde{A} = A + E = \left[\begin{array}{cc|ccc} 0.1655 & 0.6872 & 0.0887 & 0.0393 & 0.0192 \\ 0.3408 & 0.4959 & 0.0667 & 0.0421 & 0.0544 \\ \hline 0.0428 & 0.0015 & 0.2527 & 0.3154 & 0.3875 \\ 0.0252 & 0.0636 & 0.1788 & 0.1888 & 0.5436 \\ 0.0720 & 0.0799 & 0.1252 & 0.0344 & 0.6884 \end{array}\right],$$

is again row stochastic. Here, the error matrix E has been obtained as follows. We chose a random matrix R of same size as E, where the entries that correspond to the diagonal blocks are uniformly distributed in $(-1, 1)$ and the entries that correspond to the off-diagonal

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blocks are uniformly distributed in $(0,1)$. Then, we computed the matrix $A+\epsilon R$, with $\epsilon := 10^{-2}$, and this matrix is no longer stochastic. We then scale each row by dividing each of its elements by the row sum and obtain the stochastic matrix $\tilde{A}$. We have $E=\tilde{A}-A$ and E has zero row sums.

Furthermore, consider a permuted matrix $B=P\tilde{A}P^T$, where P is a random symmetric permutation matrix. We obtain

$$B=\begin{bmatrix}0.1655 & 0.0393 & 0.0887 & 0.0192 & 0.6872\\ 0.0252 & 0.1888 & 0.1788 & 0.5436 & 0.0636\\ 0.0428 & 0.3154 & 0.2527 & 0.3875 & 0.0015\\ 0.0720 & 0.0344 & 0.1252 & 0.6884 & 0.0799\\ 0.3408 & 0.0421 & 0.0667 & 0.0544 & 0.4959\end{bmatrix}.$$

The matrix B is of a form in which we usually would get these matrices from applications. The left singular vectors of B are given by

$$\begin{bmatrix}-0.3558 & 0.6822 & 0.0367 & -0.6258 & -0.1220\\ -0.5048 & -0.2770 & 0.0711 & -0.1661 & 0.7973\\ -0.4216 & -0.2631 & 0.7608 & 0.0775 & -0.4100\\ -0.5738 & -0.3030 & -0.6440 & 0.0368 & -0.4035\\ -0.3339 & 0.5448 & -0.0006 & 0.7572 & 0.1357\end{bmatrix}.$$

We now sort the second column, i.e., the left singular vector corresponding to the second singular value, and obtain the permutation $(4,2,3,5,1)$, which corresponds to the permutation matrix

$$\tilde{P}=\begin{bmatrix}0&0&0&1&0\\0&1&0&0&0\\0&0&1&0&0\\0&0&0&0&1\\1&0&0&0&0\end{bmatrix}.$$

We apply the permutation to the matrix B and obtain

$$\tilde{B}=\tilde{P}B\tilde{P}^T=\left[\begin{array}{ccc|cc}0.6884 & 0.0344 & 0.1252 & 0.0799 & 0.0720\\ 0.5436 & 0.1888 & 0.1788 & 0.0636 & 0.0252\\ 0.3875 & 0.3154 & 0.2527 & 0.0015 & 0.0428\\ \hline 0.0544 & 0.0421 & 0.0667 & 0.4959 & 0.3408\\ 0.0192 & 0.0393 & 0.0887 & 0.6872 & 0.1655\end{array}\right],$$

which exhibits the original block structure of $\tilde{A}$.

Once we know how to permute one large block that contains at least two subblocks into two blocks, we can employ this procedure recursively.

We compute a left singular vector corresponding to the second singular value, sort it in increasing order and apply the permutation. Then, we check if the $\mathbb{1}$-norm (average row sum) of the potential blocks is above a given threshold, see Definition 4.6. In this case, we have found two blocks and proceed recursively with each of the two blocks. Since we measure the size of the entries in the diagonal blocks and not in the off-diagonal blocks, the threshold can stay the same for all recursive calls. If the norm of the potential blocks is not above a given threshold, we cannot split the block any further and stop.

Note, that for the bisectioning procedure, we use only the second singular value and a corresponding singular vector; we do not compute other singular vectors. It would be natural

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Algorithm 1: Identification of nearly decoupled blocks

Input: Matrix B, threshold $thr(= 1 - \delta)$.
Output: Number m and sizes $n_i,\ i = 1, \dots, m$, of identified blocks in B, a permutation matrix P such that $PBP^T = A + E$.

1 Compute the second left singular vector u_2 of B.
2 Sort it in increasing order and use the resulting permutation P to permute the matrix B.
3 Identify two potential blocks B_1 and B_2 by using the change in sign in u_2.
4 The size of the first block is the number of negative values in u_2, the size of the second block is the number of positive values in u_2.
5 **if** *the norm of the diagonal blocks is larger than thr* **then**
6   We have found two blocks and separate them.
7   Proceed recursively with step 1. applied to each of the blocks.
8 **else**
9   The current block cannot be further reduced.
10   Increase the counter of blocks by one.

to consider not just the the second singular vector, but m singular vectors, if there were m diagonal blocks. We do not consider such an approach. One reason is that m, the number of blocks is not known in advance. Also, finding a singular vector corresponding just to the second singular value is less costly.

A problem may arise if the second and third (or even more) singular values are equal or not well separated within the perturbation range due to round-off errors. In this case it is not clear what the singular vector associated with the second singular value is and thus we cannot decide on the sign-structure. In this case, it may be necessary to carry out a refinement step, which considers linear combinations of the corresponding singular vectors in the decision process. Currently, we do not know how to handle this situation. However, in the examples that we have tested so far (see Section 6) the second and third singular values are well separated within the perturbation range due to round-off errors. We expect this to be generally the case for the discussed applications.

Another problem may arise if the the second largest eigenvalue in modulus of the transition matrix is negative.

EXAMPLE 5.2. Consider the following stochastic matrix

$$A = \left[\begin{array}{c|cc} 0.80 & 0.10 & 0.10 \\ \hline 0.05 & 0.05 & 0.90 \\ 0.10 & 0.80 & 0.10 \end{array}\right],$$

that obviously has two metastable blocks.

The eigenvalues of A are $\begin{bmatrix} 1.0000 & -0.7737 & 0.7237 \end{bmatrix}$, i.e., the second largest eigenvalue in modulus $\lambda = -0.7737$ is negative. If we calculate the singular value decomposition, we obtain

$$A = \begin{bmatrix} -0.51 & 0.49 & -0.71 \\ -0.69 & -0.72 & -0.00 \\ -0.51 & 0.49 & 0.71 \end{bmatrix} \begin{bmatrix} 1.01 & 0 & 0 \\ 0 & 0.79 & 0 \\ 0 & 0 & 0.70 \end{bmatrix} \begin{bmatrix} -0.49 & 0.51 & -0.71 \\ -0.49 & 0.51 & 0.71 \\ -0.72 & -0.69 & -0.00 \end{bmatrix}.$$

Here, the left and the right second singular vectors exhibit a sign structure that would break up the two by two block. This is due to the following fact. The two by two block consists of

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two states, where with a high probability the chain does not stay within the same state. With a high probability, it cycles between the two states. This means that one could actually view the two states as one.

In the real world examples that we have tested, this problem does not occur. However, we propose an algorithm that handles this possible situation. It is based on the Tarjan algorithm [28], that finds strongly connected components (cycles) of a graph that we construct from comparatively "large" entries of the transition matrix. For this we use the implementation by T. A. Davis [6]. The idea is to find states that are connected by "large" probabilities in a cyclic way, and consider them in a single block. At least for the application of our identification algorithm such cliques of states can be viewed as one state, since these states belong to one block.

Note that in the case of diagonally dominant matrices this problem does not occur. Therefore, before looking for potential cycles, we remove diagonally dominant states, i.e. states where the probability of staying is larger than the sum of probabilities for leaving the state. As a second step, we remove comparatively "small" entries in the matrix, since we are only interested in cycles with "large" weights. We merge the states within each found cycle by using the norms for matrix blocks defined in Section 4. We add the previously removed diagonally dominant states and run Algorithm 1 to find the metastable blocks. Finally, we redistribute the states within the cycles to recover the original number of states in B.

The main procedure is outlined in the following algorithm that forms an outer loop for Algorithm 1.

Algorithm 2: Identification of nearly decoupled blocks in the presence of cycles with "large" weights

---

Input: Matrix B, threshold $thr(= 1 - \delta)$.
Output: Number m and sizes $n_i,\ i = 1, \dots, m$, of identified blocks in B, a permutation matrix P such that $PBP^T = A + E$.

1 Find and temporarily remove diagonally dominant states in B.
2 Temporarily remove "small" entries in B.
3 **if** *the current matrix B has strongly connected components* **then**
4 Temporarily merge the states within every strongly connected component into one state.
5 Add the previously removed diagonally dominant states to B.
6 Run Algorithm 1 on the current matrix B and apply permutation.
7 Redistribute the states within every strongly connected component.

A nice side effect of this procedure is that the transition matrix to which Algorithm 1 is applied, is typically much smaller than the original matrix if many cycles have been merged. Note that the additional preprocessing in Algorithm 2 has complexity of $O(n + nnz)$, where n is the size of the transition matrix without the diagonally dominant states and nnz the number of "large" nonzero entries. Thus, it is comparatively cheap to perform, and would add very little computational complexity to Algorithm 1, where singular values and vectors of the whole transition matrix are calculated.

6. Numerical tests. In this section, we present three types of numerical examples. In Section 6.1 we discuss examples constructed in a manner similar to Example 5.1, with a fixed block structure, with random entries, random added noise, and permuted with a random permutation, resulting in matrices for which we know the hidden structure. We illustrate the

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ability of the algorithm to recover a hidden structure and discuss limitations of the algorithm in the presence of large perturbations.

In Section 6.2, we show results for the molecule n-pentane, that was also used as a test example in [7], and in this case we obtain the same results. In Section 6.3, we present two slightly more challenging examples, where the algorithms in [7] and [8] have difficulties identifying the metastable states.

For numerical tests, Algorithm 1, was implemented in MATLAB® Version 7.0 and run on a PC with an Intel(R) Pentium(R) 4 CPU 3.20GHz processor. The relative machine precision was $\texttt{eps} = 2.2204 \times 10^{-16}$. In all example figures, we denote by n the number of unknowns and by nz the number of nonzero elements in the matrix.

6.1. Constructed examples. The first example illustrates the ability of our method to recover a hidden block structure. It is constructed in the same manner as Example 5.1 in Section 5, is of size $n = 338$ and has $nz = 113906$ nonzero entries.

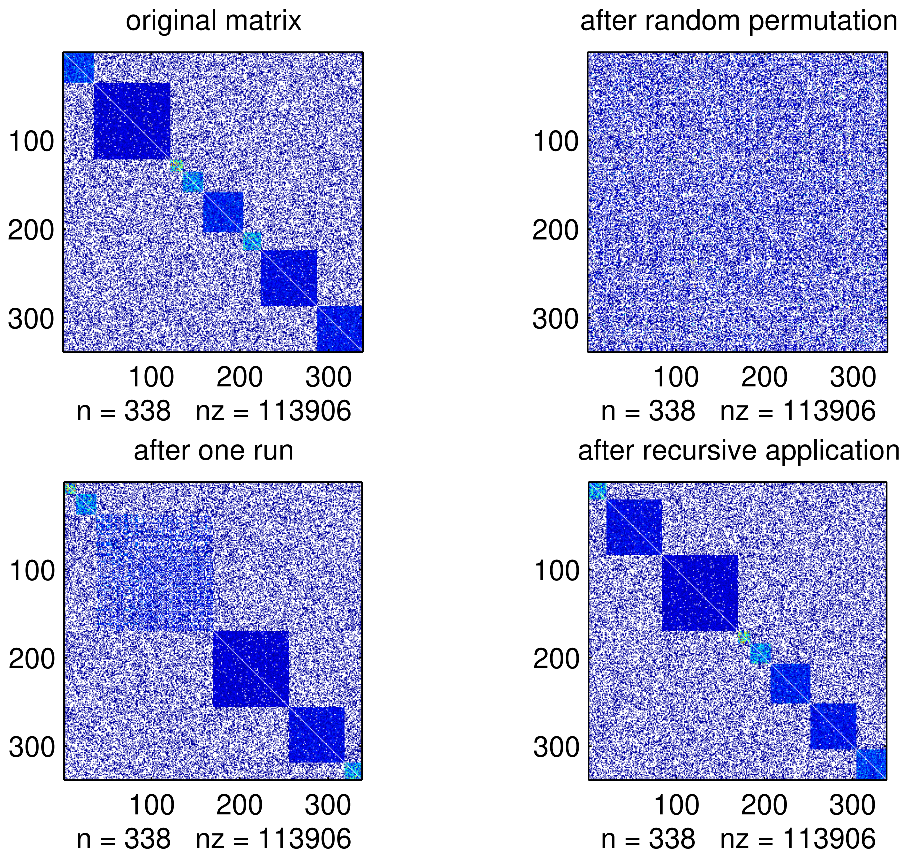

FIGURE 6.1. *Random example revealing 8 blocks*

In Figure 6.1, the upper left matrix is the original block diagonally dominant matrix, where we clearly can distinguish the diagonal blocks. The corresponding coupling matrix is diagonally dominant with values slightly larger than 0.5 on the diagonal. Hence, the perturbation here is quite large. The upper right matrix is a random symmetric permutation of the first matrix. Here, no structure can be seen. The lower left matrix depicts the recovered

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blocks after the calculation of one singular vector and the application of the corresponding permutation. One can see, that the block structure is to a large extent recovered but some parts are not fully restored yet. The lower right matrix now depicts the recovered structure after recursive application of the algorithm. We can see that we have obtained the same blocks as in the original matrix up to permutation of the blocks and the entries within a block.

For some examples with such a large perturbation as in the previous example, the algorithm may fail as we can see in the random example in Figure 6.2. Here, the structure cannot be recovered.

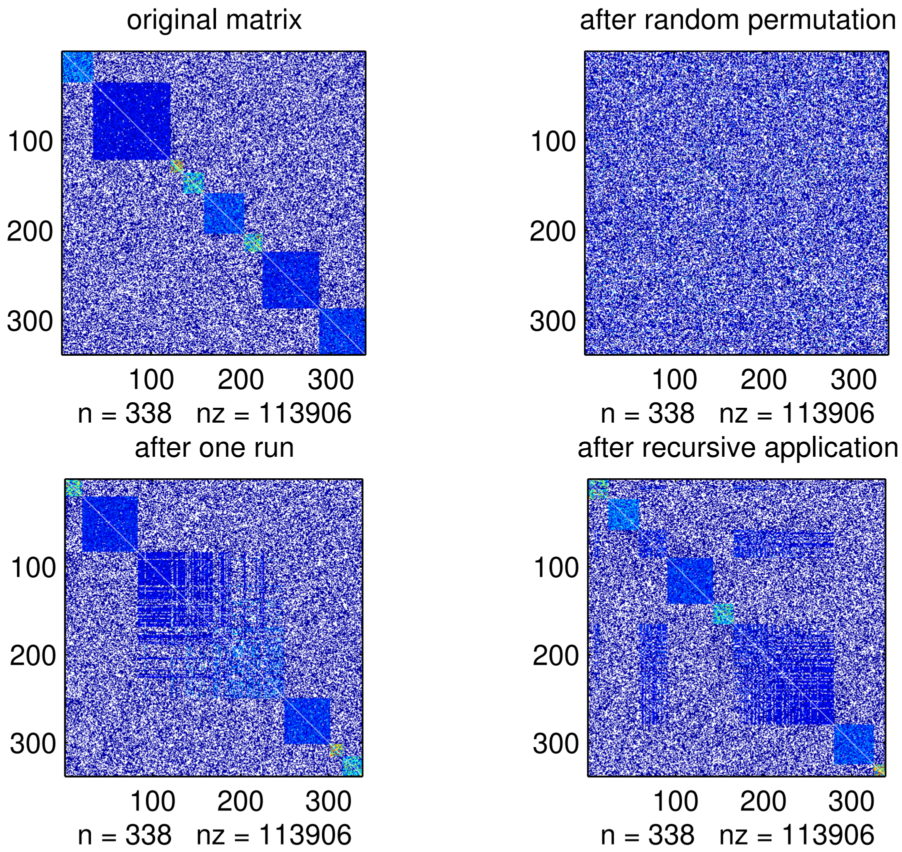

FIGURE 6.2. *Random example where the algorithm fails due to a very large error*

In general, one can say that the smaller the perturbation the better the algorithm recovers the hidden structure. We have tested 3 types of randomly generated examples. In the first type the diagonal entries of the coupling matrix are slightly larger than 0.5, in the second they are between 0.6 and 0.7, and in the third type the diagonal entries of the coupling matrix are about 0.9. We have run 1000 examples of each type. The structure could be recovered in the first case in 57,6%, in the second case in 85% and in the third case in 98,1% of all cases.

For comparison reasons, we have also run our algorithm using the right singular vectors instead of the left singular vectors. For the same 3 types of examples as in the previous paragraph, the optimal solution was found in the first case in 61,3%, in the second case in 84,9% and in the third case in 98,1% of all cases.

The performance could be slightly enhanced by running the algorithm a second time

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using the right (left) singular vectors in case that it failed to find the optimal solution in the first run using left (right) singular vectors. In this case we obtained the optimal solution in the first case in 65,2%, in the second case in 87,8% and in the third case in 99,5% of all cases.

From this we may already conclude that as for some other problems (see, e..g., [18] and the references therein) the choice of left versus right singular vector may be important; see further our experience with harder problems in sections 6.2 and 6.3. At this point it is not clear that left or right singular vector should be preferred since both produce good results. This issue still needs to be further studied. Unless specified otherwise we have used left singular vectors for our computations.

6.2. n-Pentane. The example of n-pentane was presented in [7, Section 5.2]. We will use this example to discuss the difference or the equivalence of the π-norm used in [7] and the $\mathbb{1}$-norm proposed in Section 4. This example is of size $n = 255$ and has $nz = 6464$ nonzero entries.

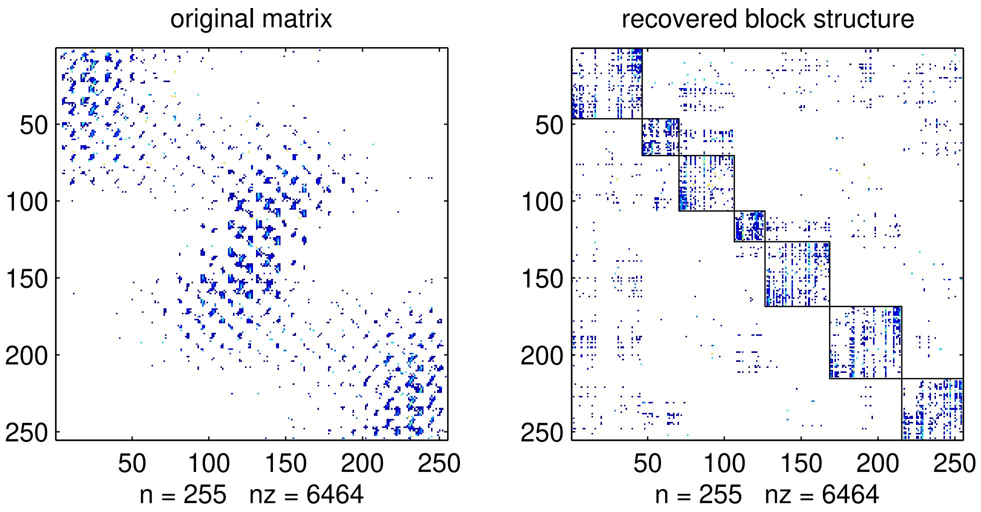

FIGURE 6.3. *Algorithm 1 using the $\mathbb{1}$-norm for n-Pentane (Ph300) revealing 7 blocks of sizes 46, 24, 36, 20, 42, 47, 40.*

In Figure 6.3 we illustrate the results of our algorithm using the $\mathbb{1}$-norm. We obtain 7 blocks of sizes 46, 24, 36, 20, 42, 47, 40. Both coupling matrices $W_{\mathbb{1}}$ and W_π are diagonally dominant; see [13] for the values of their entries.

To compare the norms, we now run our algorithm using the π-norm. The result that we obtain is depicted in Figure 6.4. We see that we obtain the same block structure up to permutation of the blocks. The coupling matrices $W_{\mathbb{1}}$ and W_π are the same as for Algorithm 1 run with the $\mathbb{1}$-norm. In this example it does not make any difference which norm we use for calculations except for the cost, as already discussed.

Our next example is the same molecule but in a different temperature setting. This example is of size $n = 307$ and has $nz = 19116$ nonzero entries. Again, we first run the algorithm using the $\mathbb{1}$-norm. In this case, we obtain only 5 blocks depicted in Figure 6.5. The corresponding coupling matrices $W_{\mathbb{1}}$ and W_π are both diagonally dominant; see [13] for details. If we also run the algorithm using the π-norm, then we obtain the six blocks, one more than with the $\mathbb{1}$-norm. The result is depicted in Figure 6.6.

We see that we have the same blocks except that the block of size 88 is subdivided into

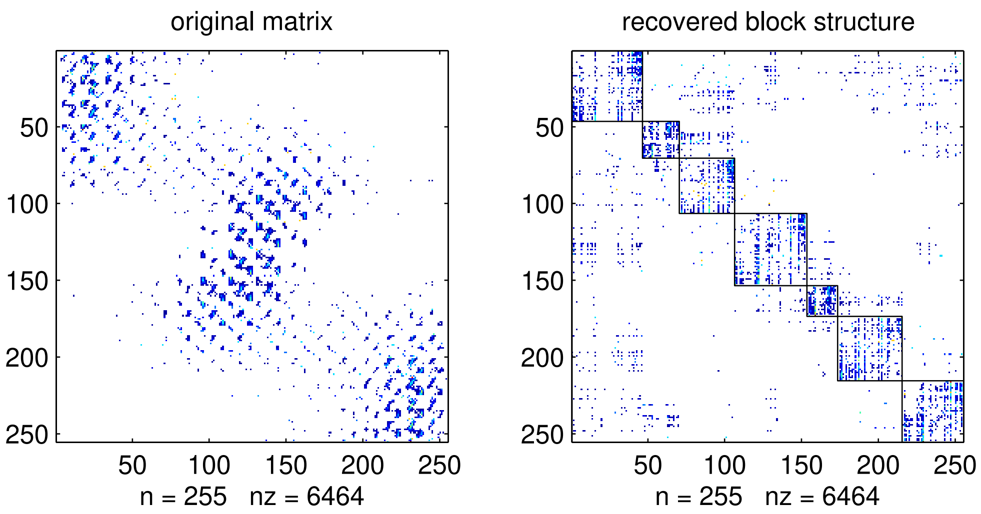

FIGURE 6.4. *Algorithm 1 using the π-norm for n-Pentane (Ph300) revealing 7 blocks of sizes 46, 24, 36, 47, 20, 42, 40.*

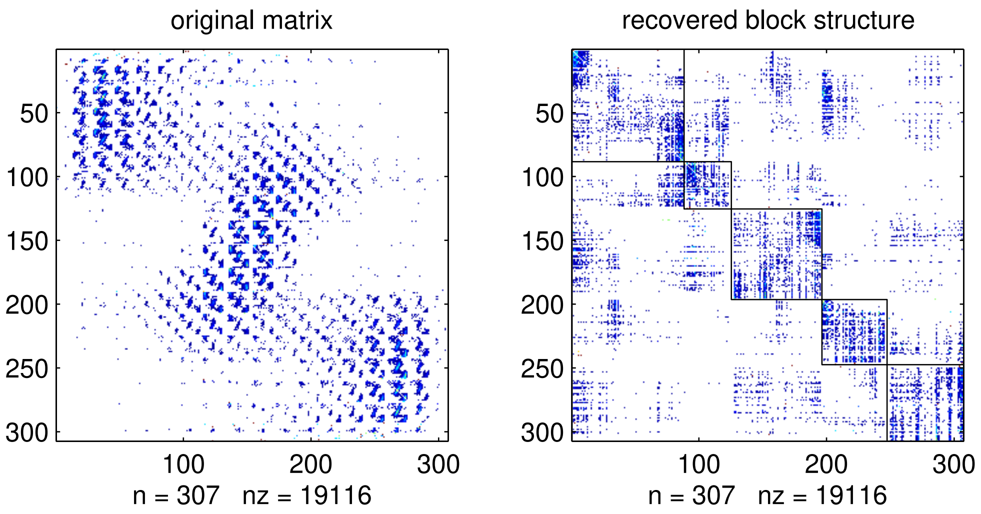

FIGURE 6.5. *Algorithm 1 using the $\mathbb{1}$-norm for n-Pentane (Ph500) revealing 5 blocks of sizes 88, 37, 71, 51, 60.*

two blocks of sizes 45 and 43. If we look at the coupling matrices, we can see the reason. The π-norm coupling matrix

$$W_\pi = \begin{bmatrix} 0.7642 & 0.0236 & 0.0036 & 0.0913 & 0.0808 & 0.0365 \\ 0.0628 & 0.7921 & 0.1123 & 0.0069 & 0.0079 & 0.0180 \\ 0.0240 & 0.2784 & 0.5842 & 0.1054 & 0.0058 & 0.0021 \\ 0.1516 & 0.0043 & 0.0265 & 0.7738 & 0.0274 & 0.0164 \\ 0.2107 & 0.0078 & 0.0023 & 0.0430 & 0.6977 & 0.0386 \\ 0.0787 & 0.0146 & 0.0007 & 0.0213 & 0.0320 & 0.8527 \end{bmatrix}$$

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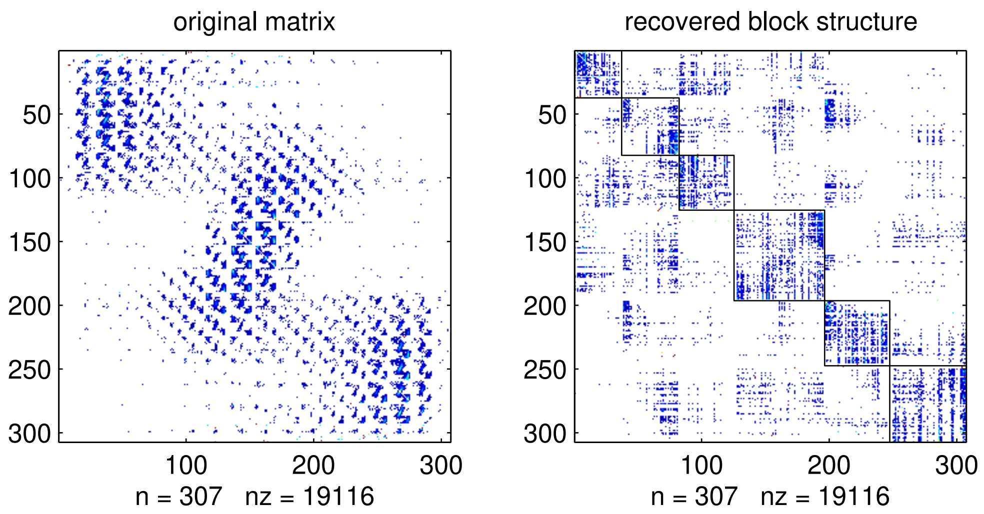

FIGURE 6.6. *Algorithm 1 using the π-norm for n-Pentane (Ph500) revealing 6 blocks of sizes 37, 45, 43, 71, 51, 60.*

is diagonally dominant. Yet, the $\mathbb{1}$-norm coupling matrix

$$W_{\mathbb{1}} = \begin{bmatrix} 0.4897 & 0.0765 & 0.0354 & 0.1191 & 0.2204 & 0.0589 \\ 0.1576 & 0.5290 & 0.1593 & 0.0213 & 0.0980 & 0.0348 \\ 0.0365 & 0.2507 & 0.5523 & 0.1336 & 0.0228 & 0.0042 \\ 0.1585 & 0.0244 & 0.1016 & 0.6150 & 0.0288 & 0.0718 \\ 0.1329 & 0.0123 & 0.0034 & 0.0348 & 0.6725 & 0.1440 \\ 0.1105 & 0.0206 & 0.0013 & 0.1411 & 0.0716 & 0.6549 \end{bmatrix}$$

has one value smaller than 0.5 on the diagonal. Hence, with both norms we obtain the same qualitative results, meaning that the additional block that we obtain using the π-norm is not diagonally dominant in the $\mathbb{1}$-norm.

Using right instead of left singular vectors for these examples leads to the same number of blocks in the first example, although of different size and, hence, with a different diagonally dominant coupling matrix. A slight improvement can be achieved with right singular vectors in the second example, where we obtain the six blocks depicted in Figure 6.7 with both coupling matrices being diagonally dominant, whereas with the left vectors we obtain 6 blocks with only W_π being diagonally dominant, see [13] for details.

6.3. Two more difficult cases. In this section we present two cases where the algorithms presented in [7] and [8] have difficulties identifying metastable conformations.

For the first matrix, that is of size $n = 158$ and has $nz = 24806$ nonzero entries, the difficulties are that the algorithms in [7] and [8] identify the number of blocks by looking at spectral gaps. In this example, the spectrum of the matrix does not have any gaps. Our algorithm, on the contrary, does not need to know the number of blocks in advance but it is calculated in the process. Using right singular vectors, which is the better choice here, we obtain 8 blocks depicted in Figure 6.8. Here, both coupling matrices $W_{\mathbb{1}}$ and W_π are diagonally dominant; see [13] for the values of their entries.

The second example which is of size $n = 1772$ and has $nz = 289432$ nonzero entries is problematic in a different way. Here, we have a very large cluster of eigenvalues very close

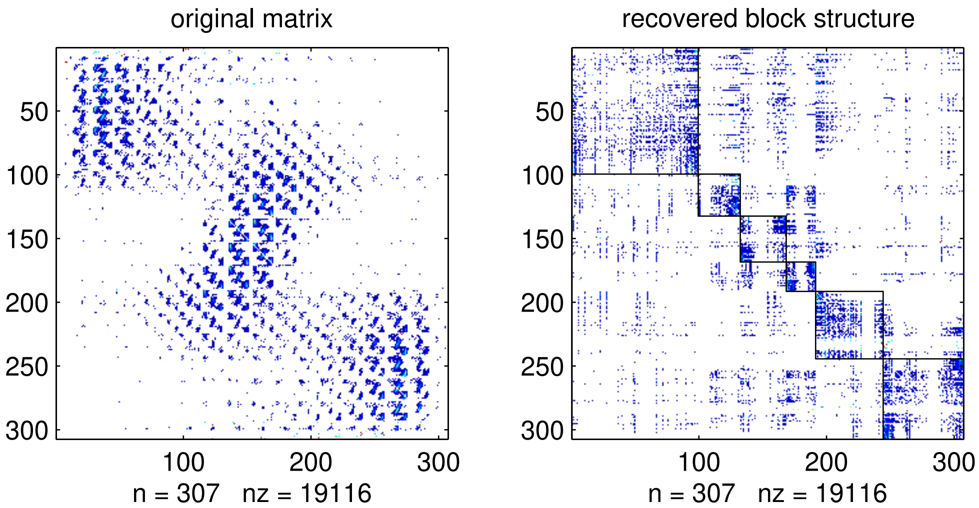

FIGURE 6.7. *Algorithm 1 run using right singular vectors for n-Pentane (Ph500) revealing 6 blocks of sizes 99, 33, 36, 23, 53, 63.*

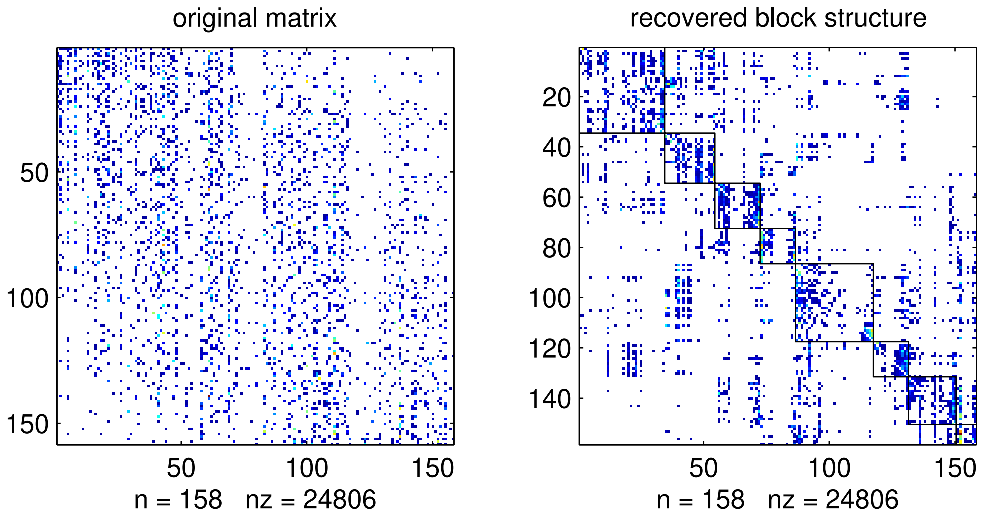

FIGURE 6.8. *Algorithm run using right singular vectors for a matrix without a spectral gap (Pmatrix2) revealing 8 blocks of sizes 34, 20, 18, 14, 31, 14, 19, 8.*

to 1. This makes the matrix very badly conditioned, especially as far as the calculation of the stationary distribution is concerned. Also, the algorithms in [7] and [8] have difficulties identifying the right number of blocks. In Figure 6.9, we depict the results calculated with the $\mathbb{1}$-norm and using left singular vectors. This is the maximum number of blocks that we can identify, such that the coupling matrix is diagonally dominant. Yet, blocks of very small sizes probably do not make a lot of sense from the chemical point of view. However, this is not a problem, since smaller blocks can always be merged into larger blocks. An alternative strategy could be to restrict the minimal block size in advance. In this case, we would only

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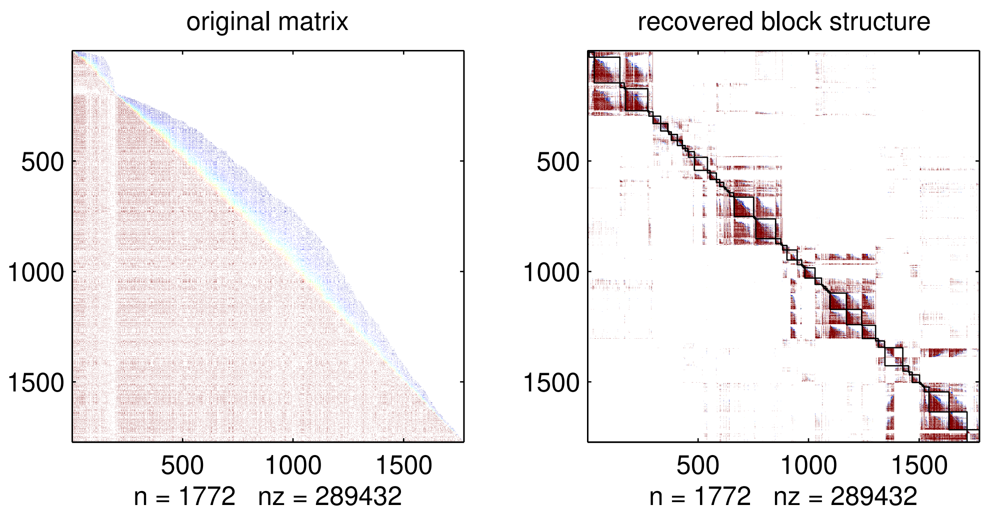

FIGURE 6.9. *Algorithm 1 using the $\mathbb{1}$-norm for a badly conditioned matrix with a large eigenvalue cluster very close to 1, revealing 77 blocks of sizes 2, 2, 2, 2, 3, 3, 3, 3, 3, 3, 3, 3, 3, 3, 3, 3, 4, 4, 4, 4, 4, 4, 5, 5, 5, 5, 5, 5, 5, 6, 6, 6, 6, 6, 7, 7, 9, 11, 12, 12, 12, 13, 20, 21, 21, 23, 23, 23, 25, 26, 27, 29, 29, 29, 33, 34, 34, 46, 46, 56, 59, 60, 69, 74, 81, 81, 88, 90, 91, 100, 116 sorted in ascending order.*

split up into blocks if they are of required size. Using right singular vectors in this case leads to only 55 blocks.

From the examples presented in this section we conclude that if the perturbation is not too large, a block diagonally dominant structure can be recovered or identified by the proposed algorithm. Both norms, the $\mathbb{1}$-norm and the π-norm can be used for calculations. Qualitatively, one obtains similar results. Since for the real examples the "correct" answer is not known, we cannot decide, which norm is the "better" one. However, it is much cheaper to use the $\mathbb{1}$-norm, and for a large eigenvalue cluster around 1, the calculation of the stationary distribution may be badly conditioned. Also, we may conclude from these examples that to optimize the results it makes sense to use left or right singular vectors depending on the problem. The question of whether to choose left or right singular vectors is an interesting issue that needs further investigation.

7. Conclusions. In this paper, we have presented a bisectioning algorithm for identifying metastable states of a Markov chain based on the calculation and sorting of a singular vector corresponding to the second largest singular value. The algorithm determines a number of blocks, such that the coupling matrix is diagonally dominant. Hence, we do not need to know the number of blocks in advance but it is calculated in the process. This is the main difference to most other methods that use the SVD or spectral analysis. Another advantage of our approach is that it does not depend on a significant spectral gap between the Perron cluster and the rest of the spectrum in the transition matrix of the Markov chain. Thus, matrices without a spectral gap or with a very large Perron cluster can be treated. A third advantage is that we calculate only two singular vectors instead of many eigenvectors. This allows to use iterative procedures such as Lanczos or Arnoldi iteration. We suggest to abstain from using the stationary distribution in the norm needed to determine the diagonally dominance, since its calculation may be costly and badly conditioned. We show that the same qualitative results can be achieved using an alternative norm. This is illustrated by numerical experiments.

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