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**Eigenvalues of non-reversible Markov
chains – A case study**

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Abstract

Finite reversible Markov chains are characterized by a transition matrix P that has real eigenvalues and π -orthogonal eigenvectors, where π is the stationary distribution of P . This means, that a transition matrix with complex eigenvalues corresponds to a non-reversible Markov chain. This observation leads to the question, whether the imaginary part of that eigendecomposition corresponds to or indicates the “pattern” of the non-reversibility. This article shows that the direct relation between imaginary parts of eigendecompositions and the non-reversibility of a transition matrix \tilde{P} is not given. It is proposed to apply the Schur decomposition of \tilde{P} instead of the eigendecomposition in order to characterize its non-reversibility. The Schur decomposition also allows to find the difference matrix ΔP which turns a non-reversible Markov chain \tilde{P} into a reversible one $P = \tilde{P} + \Delta P$, such that P and \tilde{P} have the same stationary distribution and the same metastabilities. P and \tilde{P} even have the same eigenvalues, if \tilde{P} is diagonalizable in \mathbb{R} .

Eigenvalues of non-reversible Markov chains – A case study

Marcus Weber

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1 Introduction

Markov chains on finite sets of n states are defined by a transition matrix $P \in \mathbb{R}^{n \times n}$. This matrix P is denoted as *stochastic*, i.e., its row-sums are 1 and its entries are non-negative. The Markov chain can be reversible or non-reversible. Reversibility means, that the matrix DP is symmetric. The entries of the diagonal matrix $D \in \mathbb{R}^{n \times n}$ are given by the stationary distribution $\pi \in \mathbb{R}^n$ of P , i.e., π is a vector which meets $\pi^T P = \pi^T$. Transition matrices of reversible Markov chains have real eigenvalues. Thus, it is also true that complex eigenvalues imply non-reversibility of P . However, this article will show that the magnitude of the imaginary part of the eigenvalues does not provide any information of the “magnitude” of the non-reversibility. In general, the eigenvalue analysis of P is used to decompose the matrix according to the equation $PX = X\Lambda$. In this equation the matrix $X \in \mathbb{R}^{n \times n}$ includes the eigenvectors as columns, whereas $\Lambda \in \mathbb{R}^{n \times n}$ is a diagonal matrix with the eigenvalues on its diagonal. There are many articles in literature (e.g., [3, 4, 6, 8, 5, 9, 10]) which discuss the cases where X and Λ are real valued versus the situation in which the entries become complex valued. To our knowledge it is rarely discussed that the transition matrix P can be non-diagonalizable. Even very simple examples lead to transition matrices which are non-diagonalizable. Here is an example for a doubly-stochastic matrix P , which can not be spectrally decomposed:

$$P = \begin{pmatrix} 5/12 & 5/12 & 1/6 \\ 1/4 & 1/4 & 1/2 \\ 1/3 & 1/3 & 1/3 \end{pmatrix}. \quad (1)$$

In this example, the geometric and algebraic multiplicity of the eigenvalue $\lambda = 0$ does not coincide. The situation of a problematic eigenvalue at $\lambda = 0$ is not the only case that can happen. In (11) below, we will construct a doubly-stochastic matrix, which has an eigenvalue $\lambda = 0.99$ that is algebraically double but geometrically simple. Thus, that matrix is another example for a non-diagonalizable case (with regard to the dominant part of its spectrum). The eigendecomposition may fail. However, the Schur decomposition is always possible [16] (but not unique). There is the common opinion, that non-reversibility of a Markov chain is connected to complex eigenvalues (see [12, 11, 15] for a very good analysis of this case). Recent investigations show [5], however, that the non-reversibility is not only connected to complex eigenvalues, but -more

general- it is connected to the non-symmetry of the real Schur decomposition. The real Schur decomposition of a matrix P is also given by an equation of the type $PX = X\Lambda$, but in this case X includes the real Schur vectors, whereas the matrix Λ (Schur-value-matrix) is an upper triangular matrix with (additional) 2×2 -blocks on its diagonal for every complex eigenvalue of P . We will use X_s, Λ_s for the Schur and X_e, Λ_e for the eigen decomposition in the following. For our case studies we will construct transition matrices $P = X_s \Lambda_s X_s^{-1}$ which have a Schur-value-matrix of the following form:

$$\Lambda_s = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0.99 & \epsilon & 0 & 0 \\ 0 & -\gamma & 0.98 + \delta & 0 & 0 \\ 0 & 0 & 0 & 0.005 & 0 \\ 0 & 0 & 0 & 0 & 0.001 \end{pmatrix}. \quad (2)$$

If and only if the non-negative numbers γ and ϵ are zero, then the Schur-value-matrix is symmetric. Only in this case, the transition matrix P will be reversible. If $\delta = 0.01$, then the transition matrix P has one (algebraically) multiple eigenvalue. This type of construction will show, that non-reversibility is not connected to the occurrence of complex eigenvalues. It is connected to the non-symmetry of the Schur-value-matrix Λ_s .

For the construction of P according to $P = X_s \Lambda_s X_s^{-1}$, the Schur vectors X_s are needed. In the case of a reversible Markov chain the matrix P is diagonalizable and the eigenvectors are orthogonal with regard to the stationary distribution of P . This means, that the eigenvector matrix X_e satisfies $X_e^T D X_e = I$, where I is the unit matrix. In order to account for this orthogonality condition in the Schur context, we will construct the Schur vector matrix X_s in such a way that $X_s^T D X_s = I$ for a pre-defined vector π . It is important to note that by the orthogonality construction of X_s via $X_s^T D X_s = I$ and by $P = X_s \Lambda_s X_s^{-1}$ it is assured, that π is the stationary distribution of P . This is because

$$\begin{aligned} \pi^T P &= (\pi^T) X_s \Lambda_s X_s^{-1} = (X_s(:, 1)^T D) X_s \Lambda_s X_s^{-1} = (X_s(:, 1)^T D X_s) \Lambda_s X_s^{-1} \\ &= (1, 0, \dots, 0) \Lambda_s X_s^{-1} = (1, 0, \dots, 0) X_s^{-1} = \pi^T, \end{aligned}$$

where $X_s(:, 1)$ denotes the first column of X_s which is the constant 1-vector.

In the case studies, the transition matrix P is constructed in such a way, that there exist three metastable subsets of states of the Markov chain. In order to meet this condition, the vectors corresponding to the three leading Schur values must span the space of the characteristic vectors χ of these subsets, i.e., there must exist a 3×3 -matrix \mathcal{A} , such that the leading three Schur vectors can be transformed into (see also references about PCCA+[7, 17, 14] and GenPCCA[13, 5]):

$$\chi = X_s(:, 1 : 3) \mathcal{A} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix}, \quad (3)$$

where the expression $X_s(:, 1 : 3)$ means, that we take all rows but only the first three columns of X_s . Since the leading eigenvector as well as the leading Schur vector of P is constant, the construction of X_s can be based on the following

full-rank matrix

$$\hat{X} = \begin{pmatrix} 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \end{pmatrix}, \quad (4)$$

such that the columns of X_s are stemming from a linear combination of the columns of \hat{X} by applying a Gram-Schmidt orthogonalisation with regard to the orthogonality condition $X_s^T D X_s = I$. The previous considerations lead to the following MATLAB®-Code for constructing different transition matrices P for the case studies in Sec. 2:

```
clear
eps=0.000;          % non-reversibility (0.004)
delta=0.00;        % 0.01 leads to missing or multiple eigenvalues
gamma=0.000;       % 1E-15 leads to complex eigenvalues
pi=[3,1,1,2,2];    % stationary distribution (doubly stoch [1,1,1,1,1])

% Construction of the Schur Decomposition
pi=pi/sum(pi); D=diag(pi);
X=[[1 0 0 1 1];[1 1 0 1 0];[1 1 0 0 1];[1 0 1 1 0];[1 0 1 0 0]];
L=diag([1 0.99 0.98+delta 0.005 0.001]);
L(2,3)=eps;
L(3,2)=-gamma;

% Orthogonalization with regard to stat. distr.
for i=1:5
    v=X(:,i);
    for j=1:(i-1)
        X(:,i)=X(:,i)-((X(:,j)')*D*v)*X(:,j));
    end
    X(:,i)=X(:,i)/sqrt(X(:,i)')*D*X(:,i));
end

% Construction of P
P=X*L*inv(X)
```

At the beginning of this code the entries of the Schur-value-matrix Λ_s in (2) can be determined and also the stationary distribution π of P . The Schur vectors X_s are pre-defined by applying an orthogonalization to \hat{X} in (4) with regard to the pre-defined stationary distribution π . The orthogonalization is generated using the Gram-Schmidt algorithm. At the end of the code, the transition matrix P is given by $P = X_s \Lambda_s X_s^{-1}$.

2 Cases to be studied

With the aid of the algorithm shown in Sec. 1 and with assigning different values to δ, ϵ, π , and γ we show different cases of reversible and non-reversible transition matrices and their Schur as well as their eigen decomposition.

2.1 Orthogonalization of \hat{X} ($\pi^T = (3, 1, 1, 2, 2)$)

The matrix \hat{X} is used to construct a transition matrix P such that there are three metastable subsets of states of the Markov chain. This is done by choosing the Schur vectors of the three highest Schur values to be a basis of the subspace of the characteristic functions shown in (3). Furthermore, the matrix P should have a certain stationary distribution $\pi^T = \frac{1}{9}(3, 1, 1, 2, 2)$, which can be satisfied by applying the Gram-Schmidt orthogonalization algorithm to the matrix \hat{X} such that:

$$X_s = \begin{pmatrix} 1.0000 & -0.5345 & -1.3093 & 0.0000 & 0.0000 \\ 1.0000 & 1.8708 & 0.0000 & 1.2247 & 1.7321 \\ 1.0000 & 1.8708 & 0.0000 & -1.2247 & -1.7321 \\ 1.0000 & -0.5345 & 0.9820 & 1.2247 & -0.8660 \\ 1.0000 & -0.5345 & 0.9820 & -1.2247 & 0.8660 \end{pmatrix}. \quad (5)$$

With the aid of this matrix X_s and with the special choice of Λ_s , the transition matrices are constructed. This approach to build P has an important consequence: In the following case studies the Schur decompositions (with the adjusted orthogonality condition $X_s^T D X_s = I$) of the P matrices are always given by $P X_s = X_s \Lambda_s$, where X_s is identical to (5) and Λ_s is given by (2). The eigen decompositions of the discussed matrices P are, however, very different for every case study and will be explained later. This difference between Schur and eigen decomposition in our opinion shows that the Schur decomposition is a better analytical tool to investigate transition matrices than using spectral decompositions.

2.2 P is reversible ($\epsilon = \delta = \gamma = 0$)

In the first case study we construct a reversible transition matrix P . For this purpose we set $\epsilon = \delta = \gamma = 0$ in (2) and use X_s from (5). The result is:

$$P_1 = X_s \Lambda_s X_s^{-1} = \begin{pmatrix} 0.9876 & 0.0011 & 0.0011 & 0.0051 & 0.0051 \\ 0.0033 & 0.4973 & 0.4949 & 0.0036 & 0.0009 \\ 0.0033 & 0.4949 & 0.4973 & 0.0009 & 0.0036 \\ 0.0076 & 0.0018 & 0.0004 & 0.4969 & 0.4932 \\ 0.0076 & 0.0004 & 0.0018 & 0.4932 & 0.4969 \end{pmatrix} \quad (6)$$

If we analyse the eigenvalues and eigenvectors of P_1 , then the result is that the eigenvalues are identical to the Schur values, i.e., $\Lambda_e = \Lambda_s$ and that the Schur vectors are also eigenvectors of P_1 , i.e., $X_e = X_s$. In order to get the correct scaling of the eigenvectors, the MATLAB®-Code should not simply use the eig-function. This would lead to orthogonal eigenvectors (with regard to D), but not to π -normalized eigenvectors. Thus, for computing the eigenvectors and eigenvalues we used a symmetrization of the reversible matrix P_1 and a sorting routine:

```
%Compute eigenvalues of the symmetrized matrix
[Xe, Le]=eig(sqrt(D)*P*inv(sqrt(D)));
```

```
% Sort them
```

```

[val, ind]=sort(-abs(diag(Le)));
Xe=sqrt(inv(D))*Xe(:,ind)
Le=Le(ind,ind)

```

Also for the computation of the Schur vectors and values this symmetrization trick is useful. Since the ordering of the Schur values is not unique, we apply the SRSchur-algorithm[2] to account for the correct order of the Schur values shown in (2):

```

% Compute Schur decomposition for the symmetrized matrix
[Xs,Ls]=schur(sqrt(D)*P*inv(sqrt(D)));

% Sort the Schur values
[Xs, Ls]=SRSchur(Xs, Ls, 1, 0);
Xs = sqrt(inv(D))*Xs

```

By these two practical approaches we always assure that the decomposition is correct, i.e., for a general matrix P we get $P = X_e \Lambda_e X_e^{-1} = X_s \Lambda_s X_s^{-1}$ and that the π -orthogonality holds. In the reversible case, there is no difference between Schur decomposition and eigendecomposition.

2.3 P is non-reversible with real eigenvalues ($\epsilon = 0.004$)

If we now set $\epsilon = 0.004$ and $\gamma = \delta = 0$ in the above example, then there will be a discrepancy between the Schur decomposition and the eigendecomposition of P . The constructed transition matrix which is result of the algorithm in Sec. 1 is:

$$P_2 = \begin{pmatrix} 0.9886 & 0.0011 & 0.0011 & 0.0046 & 0.0046 \\ 0.0001 & 0.4973 & 0.4949 & 0.0052 & 0.0025 \\ 0.0001 & 0.4949 & 0.4973 & 0.0025 & 0.0052 \\ 0.0086 & 0.0018 & 0.0004 & 0.4964 & 0.4928 \\ 0.0086 & 0.0004 & 0.0018 & 0.4928 & 0.4964 \end{pmatrix} \quad (7)$$

This matrix defines a non-reversible Markov chain, i.e., the matrix DP_2 is not symmetric, which implies that $D^{0.5}P_2D^{-0.5}$ is not symmetric. How can we see the non-reversibility in the eigendecomposition of P_2 ? The eigenvalues of P_2 are real $\{1, 0.99, 0.98, 0.005, 0.001\}$. The eigenvectors are real, too. The non-reversibility is given by the fact, that the eigenvectors are not pairwise π -orthogonal anymore. In contrast to that kind of decomposition, the Schur decomposition still leads to π -orthogonal Schur vectors X_s given by (5). The non-reversibility of P_2 is indicated by the non-symmetry of the Schur-value-matrix Λ_s in (2) which has one off-diagonal entry ϵ . The difference between the reversible matrix P_1 and P_2 is given by the dyadic product $\epsilon X_s(:, 3)X_s(:, 2)^T D = P_2 - P_1$, where $X_s(:, i)$ is the i -th column of X_s . Note that $X_s^T D = X_s^{-1}$. The deviation of P_2 from a reversible transition matrix is directly encoded in the off-diagonal entry of the matrix Λ_s , and the difference of P_2 to a reversible matrix can be computed by a weighted dyadic product of the two corresponding Schur vectors.

2.4 P is non-diagonalizable ($\epsilon = 0.004$, $\delta = 0.01$)

The next case study will turn the transition matrix P into a non-diagonalizable matrix. If we set $\epsilon = 0.004$, $\delta = 0.01$, and $\gamma = 0$, then there is an “incomplete” 2×2 -block on the diagonal of Λ_s in (2). The incompleteness is due to $\gamma = 0$. The corresponding matrix is:

$$P_3 = \begin{pmatrix} 0.9943 & 0.0011 & 0.0011 & 0.0018 & 0.0018 \\ 0.0001 & 0.4973 & 0.4949 & 0.0052 & 0.0025 \\ 0.0001 & 0.4949 & 0.4973 & 0.0025 & 0.0052 \\ 0.0043 & 0.0018 & 0.0004 & 0.4986 & 0.4949 \\ 0.0043 & 0.0004 & 0.0018 & 0.4949 & 0.4986 \end{pmatrix}. \quad (8)$$

This matrix has an eigenvalue 0.99 which is algebraically double but geometrically simple. P_3 does not have an eigendecomposition, it is not diagonalizable. Note, that reversible matrices are always diagonalizable. In this case, however, the non-diagonalizability implies the non-reversibility of P_3 . In contrast to the eigendecomposition, the Schur decomposition still exists. The Schur vectors are again given by the matrix X_s in (5) and the Schur-value-matrix Λ_s is given by (2). P_3 is non-reversible like the matrix P_2 . Again, the difference between P_3 and a reversible Markov chain is given by the dyadic product $\epsilon X_s(:, 3)X_s(:, 2)^T D$. The non-symmetry of Λ_s represents the non-reversibility of P_3 .

2.5 P is non-reversible with complex eigenvalues ($\epsilon = 0.004$, $\delta = 0.01$, $\gamma > 0$)

If the 2×2 -block is complete in the case of the matrix Λ_s in (2), then the corresponding transition matrix P has complex eigenvalues. If we set $\epsilon = 0.004$, $\delta = 0.01$, and $\gamma = 10^{-15}$, then the matrix looks like P_3 (for the shown digits). The difference is now, that this matrix is diagonalizable and the non-reversibility is implied by the complex valued spectrum of P . The complex eigenvalues are $\lambda_2 = 0.99 + 2.3 \cdot 10^{-9}i$ and $\lambda_3 = 0.99 - 2.3 \cdot 10^{-9}i$. The size of the imaginary part of those eigenvalues does not correspond to the “magnitude” of the non-reversibility of the transition matrix. We will give a further example: Instead of a very small value γ , we set $\gamma = 0.001$ and get the following transition matrix:

$$P_4 = \begin{pmatrix} 0.9940 & 0.0014 & 0.0014 & 0.0016 & 0.0016 \\ 0.0001 & 0.4973 & 0.4949 & 0.0052 & 0.0025 \\ 0.0001 & 0.4949 & 0.4973 & 0.0025 & 0.0052 \\ 0.0044 & 0.0016 & 0.0002 & 0.4987 & 0.4950 \\ 0.0044 & 0.0002 & 0.0016 & 0.4950 & 0.4987 \end{pmatrix}. \quad (9)$$

This matrix has two complex eigenvalues $\lambda_2 = 0.99 + 0.002i$ and $\lambda_3 = 0.99 - 0.002i$. The non-reversibility is again implied by the fact that there are complex eigenvalues. In case of the Schur decomposition, we still have the same real Schur vectors X_s like in all cases before. These Schur vectors are useful for identifying the metastable subsets of states via $\chi = X_s(:, 1 : 3)\mathcal{A}$. There is no special need for handling complex values. The non-reversibility of P_4 is indicated by the non-symmetry of the Schur-value-matrix Λ_s . Every off-diagonal entry of Λ_s leads to one additional dyadic product that indicates the deviation of P_4 from a reversible transition matrix, i.e., the matrix

$$P_4 - 0.004 \cdot X_s(:, 3)X_s(:, 2)^T D + 0.001 \cdot X_s(:, 2)X_s(:, 3)^T D$$

is reversible.

2.6 P is doubly stochastic ($\pi^T = (1, 1, 1, 1, 1)$)

The last example should show that the construction of transition matrices via the algorithm given in Sec. 1 is also able to provide doubly-stochastic matrices. The advantage of doubly-stochastic matrices (row sums and columns sums are 1) is, that a doubly-stochastic matrix is reversible if and only if it is symmetric. Thus, reversibility can easily be checked by checking symmetry. For doubly stochastic matrices, the Gram-Schmidt algorithm is based on the stationary distribution $\pi = \frac{1}{5}(1, 1, 1, 1, 1)$. This leads via \hat{X} to the following matrix of Schur vectors:

$$X_s = \begin{pmatrix} 1.0000 & -0.8165 & -1.8257 & 0.0000 & 0.0000 \\ 1.0000 & 1.2247 & -0.0000 & -1.1180 & 1.1180 \\ 1.0000 & 1.2247 & -0.0000 & 1.1180 & -1.1180 \\ 1.0000 & -0.8165 & 0.9129 & -1.1180 & -1.1180 \\ 1.0000 & -0.8165 & 0.9129 & 1.1180 & 1.1180 \end{pmatrix}. \quad (10)$$

In this last example, we want to analyse a doubly-stochastic transition matrix which is non-diagonalizable, i.e., we set $\epsilon = 0.004$, $\delta = 0.01$, and $\gamma = 0$, and end up with

$$P_5 = \begin{pmatrix} 0.9932 & 0.0020 & 0.0020 & 0.0014 & 0.0014 \\ 0.0002 & 0.4985 & 0.4955 & 0.0039 & 0.0019 \\ 0.0002 & 0.4955 & 0.4985 & 0.0019 & 0.0039 \\ 0.0032 & 0.0030 & 0.0010 & 0.4979 & 0.4949 \\ 0.0032 & 0.0010 & 0.0030 & 0.4949 & 0.4979 \end{pmatrix}. \quad (11)$$

The Schur decomposition of this matrix leads to similar results as provided for the matrix P_3 in Sec. 2.4. For doubly-stochastic matrices, however, there is an additional way to decompose them. This decomposition is denoted as Birkhoff-von Neumann decomposition[1]. A doubly-stochastic matrix can be represented as a weighted sum of permutation matrices. More precisely, it is a non-unique convex combination of permutation matrices. In our case the leading weights of such a decomposition are

$$P_5 = 0.4979 \cdot \Pi_{12345} + 0.4949 \cdot \Pi_{13254} + 0.002 \cdot \Pi_{34521} + 0.0019 \cdot \Pi_{25413} + \dots$$

In this decomposition, there are two main permutations: The matrix Π_{12345} represents the identity matrix, whereas, the matrix Π_{13254} represents the permutation within the metastable subsets of states (not in between these sets). A Birkhoff-von Neumann decomposition exists for every doubly-stochastic matrix P , also in the case that P does not have an eigendecomposition. The dominant permutation matrices in this Birkhoff-von Neumann decomposition represent “typical” transition pattern of the doubly-stochastic transition matrix. A permutation matrix is also an example for a transition matrix with (complex) eigenvalues on the unit circle. If and only if the doubly-stochastic matrix P is reversible, then the summed matrix taken over the permutation matrices, which have the same weight factor in the Birkhoff-von Neumann decomposition, is always symmetric. In the case of P_5 , the matrices Π_{12345} and Π_{13254} are symmetric. Symmetric permutation matrices have eigenvalues in $\{-1, 1\}$. The

non-symmetric permutation matrix Π_{34521} has the weight factor 0.002. It includes one 3-cycle of the form $1 \rightarrow 3 \rightarrow 5 \rightarrow 1$ and one 2-cycle $2 \rightarrow 4 \rightarrow 2$. Thus, Π_{34521} has the complex 3rd unit roots and -1 as its eigenvalues. 1 is geometrically and algebraically double. The multiplicity of the eigenvalue 1 corresponds to the number of different cycles that are included in the permutation matrix. The permutation matrix Π_{34521} can be seen as one typical transition pattern of P_5 which is non-reversible, i.e, P_5 includes at least one 3-cycle of weight 0.002.

3 Conclusion

This article shows that the Schur decomposition $P = X_s \Lambda_s X_s^{-1}$ is a useful mathematical tool to analyze transition matrices. In this Schur decomposition the matrix X_s encodes metastable subsets of states and X_s^{-1} provides the stationary distribution of the system. It is the first row of that inverse matrix. The matrix Λ_s encodes the non-reversibility of the Markov chain.

- If Λ_s is a diagonal matrix, then P is reversible.
- If Λ_s has different diagonal elements and additional off-diagonal elements in the upper right triangle only, then P is non-reversible with real eigenvalues.
- If Λ_s has multiple equal entries on the diagonal and “incomplete” 2×2 -blocks on the diagonal (in our example: $\epsilon > 0, \gamma = 0, \delta = 0.01$), then P is non-reversible and non-diagonalizable.
- If Λ_s has complete 2×2 -blocks on the diagonal, then P is non-reversible with complex eigenvalues.

In all cases, the deviation of P from a reversible matrix is always given by the sum of dyadic products of columns of X_s weighted with the corresponding off-diagonal elements of Λ_s and weighted with D .

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