Lumping Complex Networks*

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Abstract

We clarify the mathematical setting of spectral coarse graining of complex networks as recently introduced in [1, 2]. We show that this concept is equivalent with lumping of a Markov chain and give exact dual eigenvector conditions for strong lumpability of a complex network. We apply this mathematical setting to the size reduction of oscillator networks preserving synchronizability.

Keywords. Lumpability, spectral segmentation, complex networks, random walks on graphs, synchronization of oscillator networks.

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1 Introduction

Large assemblies of interacting dynamical systems have received much attention in several fields of science (see Boccaletti et al. [3] for a recent review). The way to describe such systems is to model them as networks whose nodes represent the dynamical units, and whose links stand for the interactions between them.
This unifies structure and dynamics into complex dynamic networks and merges the discrete world of graph theory with the world of dynamical systems. The "in-between" gives rise to new questions involving robustness, spreading and synchronization. The crucial role played by the network topology for answering these questions is by now well

*In honor of Prof. Ludwig Streit on the occasion of his 70th birthday.

established. The notorious difficulties for a full analysis however remain, mainly because of the characteristics of the involved networks [4]. They have the following properties:

- **Large**: The size of the network typically ranges from hundreds of thousands to billions of vertices.
- **Sparse**: The number of edges is linear, i.e., within a small multiple of the number of vertices.
- **Small world**: They join two properties: small distances (two vertices are joined by a short path) and clustering (two vertices sharing a common neighbor are more likely to know each other)
- **Power law degree distribution**: The number k of adjacent vertices of a fixed vertex follows a power law distribution $p(k) \propto k^{-\beta}$.

In this paper, we deal with the first point and shall focus on reducing the complexity of large dynamical networks using the mathematical framework of "lumping a Markov chain"[5]. Our paper is motivated by the recent work of Gfeller and Los Rios [1, 2] wherein the authors reinvent the concept of "lumping" in order to achieve size reduction of large networks preserving on the same time spectral properties of the underlying graph. This is tantamount of preserving the large scale behaviour of the nearest neighbor random walk on the initial network if considered on the coarse grained network. We expose this idea within the language of "lumpability" and clarify how and why spectral properties of the network are conserved. As an example, we show how lumpability is used to select a topology in the coupling configuration that provides enhancement of the synchronization features.

The proposed size-reduction method is related to the problem of finding clusters in a network. These methods are capable of delivering impressive image segmentation results as demonstrated for example in [6, 7]. Intuitively, clusters are recognized as parts of the network where a random walker, once in one of the parts, tends to remain.

2 Coarse graining oscillator networks

In [2] Gfeller and Los Rios propose a coarse graining technique for large oscillator networks which preserves synchronizability. The authors consider a system of N identical oscillators with a coupling given by a connected graph $\Gamma = (V, E)$. Γ has vertex set V with $|V| = N$ and undirected edge set E containing whether loops nor multiple edges. The (combinatorial) Laplacian is $\mathbf{L} = \mathbf{D} - \mathbf{A}$ where $\mathbf{A}$ is the adjacency

matrix and $\mathbf{D}$ denotes the diagonal matrix with d_i equal the degree of vertex $i \in V$. The equations of motion of the system are

$$\dot{\mathbf{x}}_i = \mathbf{F}(\mathbf{x}_i) + \sigma \sum_{j=1}^{N} L_{ij}\mathbf{H}(\mathbf{x}_j), \quad i \in V \tag{1}$$

with $\mathbf{x}_i \in \mathbb{R}^d$ the state variables, $\mathbf{F} : \mathbb{R}^d \to \mathbb{R}^d$ a differentiable evolution function, σ the coupling strength and with $\mathbf{H} : \mathbb{R}^d \to \mathbb{R}^d$ a differentiable coupling function. In this model neither $\mathbf{F}$ nor $\mathbf{H}$ depend on the vertices and hence the information about the network topology is carried entirely in the Laplacian $\mathbf{L}$. For this reason the focus is on the eigenvalues and eigenvectors of the Laplacian when coarse graining the network Γ.
It is well known that the eigenvalues of $\mathbf{L}$ are all real and satisfy $0 = \lambda_1 < \lambda_2 \leq ... \leq \lambda_N$ (see [4] for background material). It is less well known that for a large class of functions $\mathbf{F}$ and $\mathbf{H}$, the network capability to give rise to synchronized dynamics is governed by the ratio λ_N/λ_2 between the largest and the second smallest eigenvalue of $\mathbf{L}$: "the more packed the eigenvalues of $\mathbf{L}$ are, the higher is the chance of having all Lyapunov exponents – associated to the dynamics (1) – within the stability range for some fixed σ" [8]. Therefore, the possibility of preserving some eigenvalues of $\mathbf{L}$ when coarse graining Γ is important.

In order to find a coarse graining procedure which preserves parts of the spectrum of $\mathbf{L}$ Gfeller and Los Rios observe that if two nodes, say 1 and 2, have exactly the same neighbors, they display exactly the same dynamical behavior, that is $\dot{\mathbf{x}}_1(t) = \dot{\mathbf{x}}_2(t)$. Hence these two nodes are safely merged together without loosing too much information. Proceeding along this idea they deduced a matrix formulation for the coarse graining scheme which gives the Laplacian $\widetilde{\mathbf{L}}$ of the reduced network in the form

$$\widetilde{\mathbf{L}} = \mathbf{KLR} \tag{2}$$

where $\mathbf{K}$ and $\mathbf{R}$ are rectangular matrices defined by

$$R_{i,C} = \delta_{C,i} \quad and \quad K_{C,i} = \frac{1}{|C|}\delta_{C,i}, \tag{3}$$

where $C = 1, ..., \tilde{N}$ stands for the label of the groups of merged nodes, $|C|$ the cardinality of the set C of merged nodes and $\delta_{C,i}$ equals 1 if $i \in C$ and zero otherwise. They note that if groups are formed such that the components of a right eigenvector $\mathbf{u}^\alpha$ are equal within

each group, the reduced vector $\mathbf{Ku}^\alpha$ is a right eigenvector of $\widetilde{\mathbf{L}}$ with eigenvalue λ^α since

$$\mathbf{RKu}^\alpha = \mathbf{u}^\alpha \tag{4}$$

The point is that the matrix condition (2) together with (4) is formally equivalent to what is called **lumping a random walk** (see proposition 1) and is a common aggregation method in the theory of Markov chains [5]. This gives immediate access to a number of results relevant for the spectral properties of the "lumped network". A few of them are exposed in the next section.

3 Lumping networks

Lumping a Markov chain addresses the fundamental question under what conditions does a function of a Markov process still join the Markov-property [9]. By definition, a (strongly) lumpable Markov chain allows for a state space reduction without loosing the Markov property [5]. Applied to networks, this concept will translate into size reduction without loosing too much of the spectral properties of the original network.
We first introduce the concept of lumping a network by recalling the existing definition for Markov chains. We then give an eigenvector condition useful for checking if a given partition of the state space leads to a lumped Markov chain (proposition 1) and a dual eigenvector condition in order to find potential lumpings (proposition 3). It is this dual condition which allows for controlled size reduction of complex networks preserving specific spectral properties.

Consider a homogeneous Markov chain $X = \{X_t\}_{t\in\mathbb{N}}$ with finite state space $S = \{1, ..., N\}$ and transition probability matrix $\mathbf{P}$ with entries $p_{ij} = \Pr(X_{t+1} = j \mid X_t = i)$.
Definition. The Markov chain X is strongly lumpable with respect to a given partition $\mathcal{L} = \{L_1, ..., L_M\}$ of the state space S, if for any pair of sets L and L' in $\mathcal{L}$ and any state i in L the probability of going from i to L' does not depend on i:

$$\Pr(X_{t+1} \in L' \mid X_t = i) = \sum_{j\in L'} p_{ij}, \quad \text{is independent of } \ i.$$

Remarks.

1. The transition probabilities

$$p_{LL'} = \Pr(X_{t+1} \in L' \mid X_t \in L) = \sum_{j\in L'} p_{ij}$$

define a Markov chain $\widehat{X}$, the lumped chain, with state space $\mathcal{L}$. The lumped chain just reports in which orbit the original chain is.

2. The definition goes back to what is commonly called Dynkins criteria: *the lumped chain is Markov if and only if* $\sum_{j\in L'} p_{ij}$ *doesn't depend on the choice of* i *in* L.

3. Besides strong lumpability, other forms of lumpability exist [10]. We will not make use of these variants.

Example (from [11]). Set $a = \frac{1}{5}$ and $b = \frac{1}{4}$. Consider a homogeneous Markov chain X with state space $S = \{1, ..., 8\}$ and transition probability matrix $\mathbf{P}$. We lump the state space according to the partition $\{\{1,2\},\{3,4\},\ \{5,6,7,8\}\}$ and find the transition probabilities $\widetilde{\mathbf{P}}$:

$$\mathbf{P} = \begin{array}{c|cccccccc} & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ \hline 1 & 0 & a & a & a & a & 0 & a & 0 \\ 2 & a & 0 & a & a & 0 & a & 0 & a \\ \hline 3 & a & a & 0 & a & 0 & a & a & 0 \\ 4 & a & a & a & 0 & a & 0 & 0 & a \\ \hline 5 & b & 0 & 0 & b & 0 & 0 & b & b \\ 6 & 0 & b & b & 0 & 0 & 0 & b & b \\ 7 & b & 0 & b & 0 & b & b & 0 & 0 \\ 8 & 0 & b & 0 & b & b & b & 0 & 0 \end{array} \qquad \widetilde{\mathbf{P}} = \begin{array}{c|ccc} & L_1 & L_2 & L_3 \\ \hline L_1 & a & 2a & 2a \\ L_2 & 2a & a & 2a \\ L_3 & b & b & 2b \end{array}$$

As it is clear from the definition, lumping a Markov chain corresponds to a kind of projection, one that reduces dimensionality from the number of states to the number of lumps. We have indeed the following lumpability criterion [12]:

Proposition 1. Given a partition $\{L_j\}_{j=1..M}$ of the state space $S = \{1, ..., N\}$ of a Markov chain X with transition matrix $\mathbf{P}$. Form the $N \times M$ matrix $\mathbf{R}$ whose columns are indicator variables for the elements of the partition: $r_{ij} = 1$ if state i belongs to set L_j, 0 otherwise. Let $\mathbf{K} = (\mathbf{R}^T\mathbf{R})^{-1}\mathbf{R}^T$. Then X is lumpable if and only if $\mathbf{RKPR} = \mathbf{PR}$ in which case the transition matrix of the lumped chain $\widetilde{X} = X\mathbf{R}$ is

$$\widetilde{\mathbf{P}} := \mathbf{KPR}. \tag{5}$$

Note that the relation between the Laplacians L and $\widetilde{L}$ in (5) is exactly the same as the one between $\widetilde{\mathbf{P}}$ and $\mathbf{P}$ expressed in (2). This motivates the following

Definition. Given a partition $\mathcal{L} = \{L_1, ..., L_M\}$ of the vertex set V of a connected undirected graph $\Gamma = (V, E)$. We say that Γ is strongly

lumpable with respect to $\mathcal{L}$ if the nearest neighbor random walk on Γ is lumpable.

Recall that for a connected undirected graph $\Gamma = (V, E)$ without loops nor multiple edges the nearest neighbor random walk on Γ is defined as follows. The random walker on V moves from i to a neighboring j with probability depending on the degree of i. This walk has transition matrix

$$p_{ij} = (D^{-1}A)_{ij} = \begin{cases} \frac{1}{d_i} & \text{if } i \text{ and } j \text{ are adjacent,} \\ 0 & \text{otherwise,} \end{cases}$$

where A is the adjacency matrix. The unique stationary distribution $\pi(i)$ is proportional to the number of edges that meet at i :

$$\pi(i) = \frac{d_i}{Vol(G)}, \quad \text{with} \quad Vol(G) = \sum_j d_j. \tag{6}$$

By inspection, the pair $\mathbf{P}$, π is seen to be reversible: $\pi(i)p_{ij} = \pi(j)p_{ji}$. We note that any reversible Markov chain can be represented as a random walk on an (edge weighted) graph.

Example. For the above example we have

$$\mathbf{R} = \begin{pmatrix} L_1 & L_2 & L_3 \\ \hline 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix} \quad \mathbf{K} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{pmatrix}$$

The columns of $\mathbf{R}$ are necessarily orthogonal. Because they are indicators for the lumps, we refer to their span $\langle \mathbf{R} \rangle$ as "lump space". The orthogonal projection onto lump space is given by the symmetric matrix $\mathbf{P}_\perp = \mathbf{RK}$ and reads for our example

$$\mathbf{P}_\perp = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ 0 & 0 & 0 & 0 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ 0 & 0 & 0 & 0 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ 0 & 0 & 0 & 0 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{pmatrix}.$$

With the projection $\mathbf{P}_\perp$, which is a transition matrix in its own right, the lumpability criterion proposition 1 can be restated as: $\mathbf{PR}$ *equals its projection onto lump space* $\mathbf{P}_\perp\mathbf{PR}$. Note that this is condition (4) as introduced by Gfeller and Los Rios.

Using proposition 1, one infers easily a necessary lumpability criterion involving left eigenvectors of the transition matrix $\mathbf{P}$ [12]:

Proposition 2. *The eigenvalues of* $\widetilde{\mathbf{P}}$ *(resp.* $\widetilde{\mathbf{L}}$*) are a subset of the eigenvalues of* $\mathbf{P}$ *(resp.* $\mathbf{L}$*).*

Hence, the spectral gap of $\widetilde{\mathbf{P}}$ is never smaller than that of $\mathbf{P}$ and the same is true for $\widetilde{\mathbf{L}}$. This makes lumping a possible strategy for accelerating convergence of a random walk towards stationary distribution.

Moreover, the ratio of the biggest and the second smallest eigenvalue of the lumped network is never smaller than that of the original network. This is what makes lumping a possible strategy for improving synchronizability.

Two questions rises: how likely is it that a given network is lumpable? and if a network is lumpable, how can we find a lumping in order to preserve a specific part of the spectrum of $\mathbf{L}$?

Unfortunately, the first question has a partial answer which is not very promising: We will indeed see in section 4 that a large graph "picked at random" will almost surely not be lumpable.

To answer the second question we take a closer lock to what is known for Markov chains. According to the result of Barr and Thomas [12] we have that if $\mathbf{vP} = \lambda\mathbf{v}$ than $\widetilde{\mathbf{v}}\widetilde{\mathbf{P}} = \lambda\widetilde{\mathbf{v}}$ with $\widetilde{\mathbf{v}} = \mathbf{vR}$. It follows that if λ is an eigenvalue of both $\mathbf{P}$ and $\widetilde{\mathbf{P}}$, then $\widetilde{\mathbf{v}}$ is an eigenvector of $\widetilde{\mathbf{P}}$, but if λ is not an eigenvalue of $\widetilde{\mathbf{P}}$ then $\widetilde{\mathbf{v}} = \mathbf{vR} = \mathbf{0}$ i.e, $\mathbf{v}$ is orthogonal to the lump space. Hence $\mathbf{R}$ eliminates left eigenvectors, the ones orthogonal to the lump space $\langle\mathbf{R}\rangle$.
This simple observation has recently been developed by M.N. Jacobi and O. Görnerup [13]. They note that a set of left eigenvectors $\{\mathbf{v}^\alpha\}_{\alpha\in J}$ satisfying the condition $\mathbf{v}^\alpha\mathbf{R} = \mathbf{0}$ is spanned by complementary right eigenvectors $\mathbf{u}^\alpha$. These right eigenvectors span the lump space $\langle\mathbf{R}\rangle$. The point is now that, requiring that $\mathbf{R}$ consists of zeros and ones correspond to a criterion of repeated elements within each complementary right eigenvector $\mathbf{u}^\alpha$. This yields possible lumpings by simply identifying repeated elements in the right eigenvectors. Their precise result is the following:

Proposition 3. Assume that $\mathbf{P}$ is a diagonalizable transition matrix with full rank[1] describing a homogeneous Markov process $X_{t+1} = X_t\mathbf{P}$

[1]The transition matrix $(1-\zeta)\mathbf{P} + \zeta 1, 0 \leq \zeta < 1$, allows exactly the same lumping as P

with state space $S = \{1, ..., N\}$. Consider a set $\{\mathbf{u}^\alpha\}_{\alpha \in I}$ of linearly independent right eigenvectors of $\mathbf{P}$ (i.e., $\mathbf{P}\mathbf{u}^\alpha = \lambda^\alpha \mathbf{u}^\alpha$) with $I \subset S$. Form state equivalence classes defined by states with identical elements in all eigenvectors $\mathbf{u}^\alpha$, i.e. $i \sim j$ iff $\mathbf{u}_i^\alpha = \mathbf{u}_j^\alpha$ for all $\alpha \in I$. The equivalence classes define a partitioning $\mathcal{L}$ of the state space. This partitioning is a lumping of the Markov chain if the number of partition elements equals the number of eigenvectors, i.e. $|\mathcal{L}| = |I|$. Conversely, if $\mathcal{L}$ is a lumping then there exist $|\mathcal{L}|$ linearly independent right eigenvectors that are invariant under permutations within the lumps.

Example (from [11] and [13]). Consider again the Markov chain of the first example with transition matrix $\mathbf{P}$. The associated right eigenvectors u^α have the following structure (columns sorted in order of decreasing $|\lambda|$):

$$(u^1, u^2, ..., u^8) = \begin{pmatrix} 1 & 0 & 0 & -1 & 0 & 1 & -1 & 1 \\ 1 & 0 & 0 & 1 & 0 & -1 & -1 & 1 \\ 1 & 0 & -1 & 0 & -1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 1 \\ 1 & -1 & -c_1 & c_1 & c_2 & c_2 & 0 & -\frac{5}{4} \\ 1 & -1 & c_1 & -c_1 & -c_2 & -c_2 & 0 & -\frac{5}{4} \\ 1 & 1 & c_1 & c_1 & -c_2 & c_2 & 0 & -\frac{5}{4} \\ 1 & 1 & -c_1 & -c_1 & c_2 & -c_2 & 0 & -\frac{5}{4} \end{pmatrix}$$

for some numerical constants c_1 and c_2. The eigenvalues are:

$$\lambda_1 = 1,\ \lambda_2 = -\frac{1}{2},\ \lambda_{3,4} = \frac{-1 - \sqrt{11}}{10},\ \lambda_{5,6} = \frac{-1 + \sqrt{11}}{10},\ \lambda_7 = -\frac{1}{5},\ \lambda_8 = \frac{1}{10}.$$

All possible lumpings of $\mathbf{P}$ and the corresponding subsets of right eigenvectors are given in table 1.

It is instructive to illustrate a partition by folding the graph associated with $\mathbf{P}$ (see figure 1).

The partition $\mathcal{L}_3$ for example can be obtained through folding the graph along the x and y axes passing through the center of the graph. Symmetries in the graph do indeed suggest lumpings. One way to find them is to use proposition 3. The equivalence relation between identical elements in the right eigenvectors implies invariance under a permutation symmetry. In the case of $\mathcal{L}_3$ the group of permutation symmetries $\mathcal{S}_{\mathcal{L}_3}$ can be identified with the Klein four-group

$$\mathcal{S}_{\mathcal{L}_3} = \mathcal{S}_2 \times \mathcal{S}_2$$

according to Theorem 1. The rank condition is therefore not a real restriction.

Lumping	Subset of eigenvectors
$\mathcal{L}_1 = \Big\{\{1,2,3,4,5,6,7,8\}\Big\}$	$\{u^1\}$
$\mathcal{L}_2 = \Big\{\{1,2,3,4\},\{5,6,7,8\}\Big\}$	$\{u^1, u^8\}$
$\mathcal{L}_3 = \Big\{\{1,2\},\{3,4\},\{5,6,7,8\}\Big\}$	$\{u^1, u^7, u^8\}$
$\mathcal{L}_4 = \Big\{\{1,2,3,4\},\{5,6\},\{7,8\}\Big\}$	$\{u^1, u^2, u^8\}$
$\mathcal{L}_5 = \Big\{\{1,2\},\{3,4\},\{5,6\},\{7,8\}\Big\}$	$\{u^1, u^2, u^7, u^8\}$
$\mathcal{L}_6 = \Big\{\{1,2\},\{3\},\{4\},\{5,8\},\{6,7\}\Big\}$	$\{u^1, u^3, u^5, u^7, u^8\}$
$\mathcal{L}_7 = \Big\{\{1\},\{2\},\{3,4\},\{5,7\},\{6,8\}\Big\}$	$\{u^1, u^4, u^6, u^7, u^8\}$
$\mathcal{L}_8 = \Big\{\{1,3\},\{2,4\},\{5,6\},\{7\},\{8\}\Big\}$	$\{u^1, u^2, u^3+u^4, u^5-u^6, u^8\}$
$\mathcal{L}_9 = \Big\{\{1,4\},\{2,3\},\{5\},\{6\},\{7,8\}\Big\}$	$\{u^1, u^2, u^3-u^4, u^5+u^6, u^8\}$
$\mathcal{L}_{10} = \Big\{\{1\},\{2\},...,\{7\},\{8\}\Big\}$	$\{u^1, u^2, ..., u^7, u^8\}$

Table 1: All possible lumpings of $\mathbf{P}$ and associated eigenvectors.

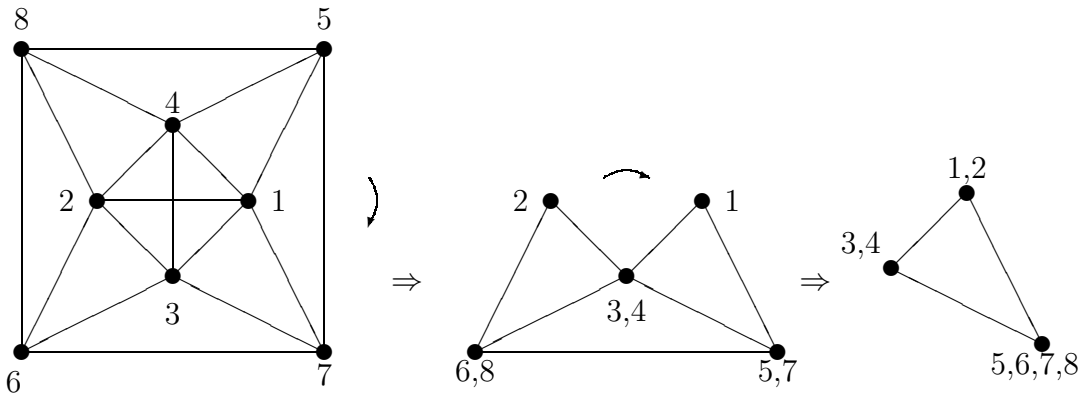


Figure 1: Folding a graph

where $\mathcal{S}_2$ is the symmetric group with two elements. The lumpings are orbits of the permutation group acting on the graph. This give rise to a promising connection with orbit and representation theory.

4 Orbit theory

[2]Let a connected graph $\Gamma = (V, E)$ have vertex set V and undirected edge set E. We allow loops but not multiple edges. Let $w(i, j)$ be positive weights on the edges (note that since the graph is undirected we have $w(i, j) = w(j, i)$ for $(i, j) \in E$ and that for unweighted graphs we have $w(i, j)$ equal to either 0 or 1 according to the entry of the adjacency matrix).
These ingredients define a random walk on V that moves from i to a neighboring j with probability proportional to $w(i, j)$. This walk has transition matrix

$$p_{ij} = \frac{w(i,j)}{W(i)}, \quad \text{where} \quad W(i) = \sum_j w(i,j). \tag{7}$$

The Markov chain with transition matrix $\mathbf{P} = (p_{ij})$ has unique stationary distribution $\pi(i)$ proportional to the sum of the edge weights that meet at i :

$$\pi(i) = \frac{W(i)}{W}, \quad \text{with} \quad W = \sum_j W(j). \tag{8}$$

Using the symmetry of $w(i, j)$, the pair $\mathbf{P}$, π is seen to be reversible: $\pi(i)p_{ij} = \pi(j)p_{ji}$. For a given reversible Markov chain $\mathbf{P}$ with stationary distribution π define $L^2(\pi) = \{f : V \to \mathbb{R}\}$ with inner product

$$\langle f_1, f_2 \rangle = \sum_i f_1(i) f_2(i) \pi(i).$$

The matrix $\mathbf{P} = (p_{ij})$ operates on L^2 by $\mathbf{P}f(i) = \sum_j p_{ij} f(j)$ and reversibility of the chain is equivalent to self-adjointness of $\mathbf{P}$.

Definition. An *automorphism* of a weighted graph is a permutation $g : V \to V$ respecting edges and weights i.e., such that if $(i, j) \in E$, then $(gi, gj) \in E$ and $w(i, j) = w(gi, gj)$. The set of automorphisms together with the composition roule forms the (full) automorphism group of the graph.

Example. The symmetry group of a square D_4 actes on the graph Γ given in figure 1. Every subgroup of D_4 is naturally an automorphism group of Γ.

[2]This section follows the excellent paper [14] by Boyd et al.

Let G be a group of automorphisms. We note the following elementary facts: G acts on $L^2(\pi)$ by

$$T_g f(i) = f(g^{-1}i).$$

We have the relation

$$T_g \mathbf{P} = \mathbf{P} T_g, \quad g \in G.$$

and the couple $(T, L^2(\pi))$ is a unitary representation of G. We have indeed

Proposition 4. For random walk on an edge weighted graph defined as in eq. (7), the stationary distribution π eq. (8) is invariant under all automorphisms G.

Proof.

$$T_g\pi(i) = \sum_j \frac{w(g^{-1}i, j)}{W} = \sum_k \frac{w(g^{-1}i, g^{-1}k)}{W} = \sum_k \frac{w(i,k)}{W} = \pi(i). \quad \square$$

Orbit theory is based on the following observation:

Proposition 5. Let H be a group of automorphisms acting on a connected graph $\Gamma = (V, E)$. The vertex set V partitions into orbits $O_i = \{hi \mid h \in H\}$. Then the nearest neighbor random walk on Γ is lumpable with respect to the partition induced by the orbits of Γ.

Proof. It is enough to proof that $p_{O_i,O_j} := p_{v,O_j} = \sum_{u \in O_j} p_{v,u}$ does not depend on the choice of v in O_i. Take $v' \in O_i$ with $v = h'v'$ for some $h' \in H$. Then,

$$\begin{aligned} \sum_{u \in O_j} p_{v,u} &= \frac{1}{W(v)} \sum_{u \in O_j} w(v,u) = \frac{1}{W(h'v')} \sum_{u \in O_j} w(v', h'^{-1}u) \\ &= \frac{1}{W(v')} \sum_{\tilde{u} \in h'O_j} w(v', \tilde{u}) = \sum_{u \in O_j} p_{v',u}. \end{aligned} \quad \square$$

The transition matrix of the orbit chain is denoted by $\mathbf{P}_H = (p_{O_i,O_j})$.

Example. The the orbits of the 10 subgroups of D_4 (trivial group S_1, the cyclic group C_2 (5 times), the Klein four-group D_2 twice, the cyclic group C_4 (once) and the full group D_4) generate all lumpings of 1 except $\mathcal{L}_1$, the trivial one (all states in one lump).

Propositions 2 and 3 find an elegant reformulation in this setting. We give passage conditions for spectral properties when going from the

orbit graph to the initial graph and vice-versa. In the following let $(\mathbf{P}, \pi)$ be a reversible Markov chain with automorphism group G. Let $H \subseteq G$ be a subgroup and define $\mathbf{P}_H$ as above:

Lifting.

1. If $\overline{f}$ is an eigenfunction of $\mathbf{P}_H$ with eigenvalue $\overline{\lambda}$, then $\overline{\lambda}$ is an eigenvalue of $\mathbf{P}$ with H-invariant eigenfunction f which is constant on orbits: $f(v) = \overline{f}(Ov)$.
2. Conversely, every H-invariant eigenfunction appears uniquely from this construction.

Projection.

1. Let f be an eigenfunction of $\mathbf{P}$ with eigenvalue λ and let $\overline{f}(j) = \sum_{h \in H} f(h^{-1}j)$. If $\overline{f}(j) \neq 0$, then $\overline{f}$ is an eigenfunction for $\mathbf{P}_H$ with eigenvalue λ.
2. Let f be an eigenfunction of $\mathbf{P}$ with eigenvalue λ. Then λ appears as an eigenvalue in $\mathbf{P}_H$ if H has a fixed point v^* with $f(v^*) \neq 0$.

In view of our applications of spectral coarse graining we may ask which orbit chains are needed to get all the eigenvalues of the original chain. The following theorem gives a simple answer [14].

Theorem. Let G be the automorphism group of the reversible Markov chain $(\mathbf{P}, \pi)$. Suppose that $V = O_1 \cup ... \cup O_k$ as a disjoint union of G-orbits. Choose vertices $o_i \in O_i$ for $i = 1...k$ and denote by H_i the isotropy groups associated to o_i i.e., $H_i = \{g \in G \mid go_i = o_i\}$. Then, all eigenvalues of $\mathbf{P}$ occur among the eigenvalues of $\{P_{H_i}\}_{i=1}^k$.

The drawback of orbit theory is that the automorphism group for large graphs are trivial. Erdös and Rényi showed [15].

Theorem. *Almost all graphs have no non-trivial automorphisms.*

That is, the proportion of graphs on n vertices which have a non trivial automorphism tends to zero as $n \to \infty$. We therefore have to relay on approximations in order to lump large networks. The basic idea of how to lump approximately a network comes from image segmentation [6] and is based on the observation that lifted eigenvectors are constant on orbits.

5 Approximated lumping

According to proposition 3 if $\mathcal{L} = \{L_1, ..., L_M\}$ is a lumping of a Markov chain $\mathbf{P}$ there exists $|\mathcal{L}|$ linearly independent right eigenvec-

tors $\{\mathbf{u}^\alpha\}_{\alpha\in I}$ which are constant on the lumps. Hence for these eigenvectors there exists constants c_i, depending on $\alpha \in I$, such that

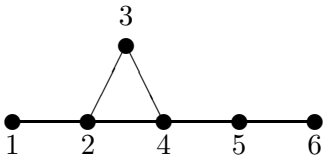
$$u_i^\alpha = \begin{cases} c_1 & \text{if } i \in L_1 \\ \vdots & \vdots \\ c_M & \text{if } i \in L_M \end{cases} \tag{9}$$

Following [6], we call a vector satisfying (9) a piecewise constant vector w.r.t. the partition $\mathcal{L}$ and define an abstract algorithm for lumping a network:

1. Compute $\mathbf{P}$ from $\mathbf{A}$ and its eigenvalues and eigenvectors
2. Select the eigenvalues $\{\lambda^\alpha\}_{\alpha\in I}$ which should be preserved (for example the second and the last one) and the corresponding right eigenvectors u^α.
3. construct an approximate lumping by finding the approximately equal elements in the selected eigenvectors.

This last step may be implemented by dividing the intervals – enclosed by the smallest and largest components of the selected eigenvalues – into a fixed number of pieces and then to collect elements falling within the same interval.

Example. We consider the random walk on the simplest graph (apart the trivial graph with one vertex) with trivial automorphism group.



$$\mathbf{P} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

The spectrum of P is $\text{spect}(P) = \{1, \pm\sqrt{2}/2, -\frac{1}{3} \pm \frac{\sqrt{10}}{6}, -\frac{1}{3}\}$. To form lumps we select $\lambda^2 = \sqrt{2}/2$, $\lambda^6 = -\frac{1}{3} - \frac{1}{6}\sqrt{10}$ and the corresponding right eigenvectors

$$\begin{aligned} p^2 &= (0.404, 0.286, 0.202, 0, -0.488, -0.690)^T \\ p^6 &= (0.192, -0.165, -0.096, 0.330, -0.590, 0.686)^T. \end{aligned}$$

We then divide the interval between the largest and smallest components of p^2 (resp. p^6) by the number of lumps we want (here 3), to get a threshold value ϵ_2 (resp. ϵ_6). Identifying components lying within

distance ϵ_2 (resp. ϵ_6) gives

$$\mathbf{V}_2 = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{resp.} \mathbf{V}_6 = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

Hence the suggested lumping V respecting both V_2 and V_6 together with the transition matrix for the lumped chain read as

$$\mathbf{V} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \widetilde{\mathbf{P}} = \begin{pmatrix} 0.7222 & 0.2778 & 0 & 0 \\ 0.6667 & 0 & 0.3333 & 0 \\ 0 & 0.5000 & 0 & 0.5000 \\ 0 & 0 & 1.0000 & 0 \end{pmatrix}.$$

The spectrum of $\widetilde{\mathbf{P}}$ is $\{1, 0.712, -0.156, -0.833\}$ and the ratio $\lambda_6/\lambda_2 = -1.217$ changes only slightly (less than 4%) for the lumped chain: $\widetilde{\lambda}_4/\widetilde{\lambda}_2 = -1.171$.

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