Discrete Markov Chains - Eigenvectors and PCCA+

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In this lecture, it is our goal to understand the dynamical behaviour of a finite Markov chain based on its eigenvalues. To this end, we have to briefly discuss one more property of Markov chains which ensures that the eigenvalue decomposition has the shape that we would like it to have: Aperiodicity.

The Period of a Chain

Definition 1. Let i be a state of a finite Markov chain $\mathbf{T}$. Consider the set of all possible return times

$$\mathcal{T}(i) \quad = \quad \left\{k \geq 1 : \mathbf{T}_{ii}^k > 0\right\}.$$

Then we define the **period** of state i as the greatest common divisor of $\mathcal{T}(i)$:

$$p(i) \quad = \quad \gcd \mathcal{T}(i).$$

If $p(i) > 1$, the state is called **periodic**, and **aperiodic** otherwise.

Lemma 2. *If $\mathbf{T}$ is irreducible, then the period is the same for all states, i.e $p(i) = p$ for all i. For this case, we simply call the chain **periodic** or **aperiodic.***

Proof. Can be found in [3, Ch. 1.3]. □

Example 3. Consider two examples:

$$\mathbf{T}_1 \quad = \quad \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\mathbf{T}_2 \quad = \quad \begin{bmatrix} 0.5 & 0.5 & 0 \\ 0.1 & 0 & 0.9 \\ 0 & 0.01 & 0.99 \end{bmatrix}$$

Clearly, $\mathbf{T}_1$ is periodic with period 2, while $\mathbf{T}_2$ is aperiodic.

From our perspective, periodic chains do not make sense, by a simple argument. We will always discretize time- and space-continuous dynamical systems. There should be at least one state i which has positive return probability $\mathbf{T}_{ii} > 0$. This, together with irreducibility, implies aperiodicity.

Eigenvalue Decomposition

The first statement we need is a version of the very general and famous **Perron-Frobenius-Theorem**:

Theorem 4. *Let* $\mathbf{T}$ *be the transition matrix of an irreducible and aperiodic Markov chain. Then:*
(i) There is a non-degenerate largest eigenvalue $\lambda_1 = 1$*, with strictly positive left and right eigenvectors associated to it.*
(ii) Every other eigenvalue λ *satisfies* $|\lambda| < 1$*.*

Proof. Can be found, for instance, in [5, Ch.1,4]. □

Reversible transition matrices allow for a very powerful decomposition in terms of their eigenvalues.

Theorem 5. *Let* $\mathbf{T}$ *be a reversible and irreducible transition matrix with stationary vector* π*. Then, there is a set of right eigenvectors* $\mathbf{r}_m$*,* $m = 1, \ldots, n$ *of* $\mathbf{T}$*, corresponding to real eigenvalues* $\lambda_1, \lambda_2, \ldots, \lambda_n$*, that forms an orthonormal basis of* $\mathbb{R}^n$ *w.r.t. the weighted inner product*

$$\langle \mathbf{v}, \mathbf{w} \rangle_\pi = \sum_{i=1}^{n} v_i w_i \pi_i,$$

i.e.

$$\begin{aligned} \mathbf{T}\mathbf{r}_m &= \lambda_m \mathbf{r}_m, \\ \langle \mathbf{r}_m, \mathbf{r}_{m'} \rangle_\pi &= \delta_{m,m'}. \end{aligned}$$

The right eigenvectors $\mathbf{r}_m$ *can be converted into left eigenvectors* $\mathbf{l}_m$ *by pointwise multiplication with* π*, i.e.* $\mathbf{l}_m = \mathbf{\Pi}\mathbf{r}_m$*. Moreover,* $\mathbf{T}$ *can be decomposed as*

$$\begin{aligned} \mathbf{T}(i,j) &= \sum_{m=1}^{n} \lambda_m \mathbf{r}_m(i) \pi(j) \mathbf{r}_m(j) \\ &= \sum_{m=1}^{n} \lambda_m \mathbf{r}_m(i) \mathbf{l}_m(j). \\ \mathbf{T} &= \sum_{m=1}^{n} \lambda_m \mathbf{r}_m \mathbf{l}_m^T. \end{aligned}$$

Proof. Consider the matrix

$$\begin{aligned} \mathbf{S} &= \mathbf{\Pi}^{1/2} \mathbf{T} \mathbf{\Pi}^{-1/2}, \\ \mathbf{S}(i,j) &= \pi(i)^{1/2} \pi(j)^{-1/2} \mathbf{T}(i,j). \end{aligned}$$

This matrix is symmetric because of the detailed balance condition. Therefore, we can find n eigenvectors $\mathbf{v}_m$, $m = 1, \ldots, n$ of $\mathbf{S}$, corresponding to real eigenvalues λ_m, which are orthonormal w.r.t. the standard Euclidean inner product. It follows that $\mathbf{r}_m := \mathbf{\Pi}^{-1/2}\mathbf{v}_m$ is an eigenvector of $\mathbf{T}$ with the same eigenvalue:

$$\begin{aligned}
\mathbf{T}\mathbf{r}_m &= \mathbf{T}\boldsymbol{\Pi}^{-1/2}\mathbf{v}_m \\
&= \boldsymbol{\Pi}^{-1/2}\left(\boldsymbol{\Pi}^{1/2}\mathbf{T}\boldsymbol{\Pi}^{-1/2}\right)\mathbf{v}_m \\
&= \lambda_m\boldsymbol{\Pi}^{-1/2}\mathbf{v}_m \\
&= \lambda_m\mathbf{r}_m.
\end{aligned}$$

The statement about left eigenvectors follows similarly, and it can be checked that $\langle \mathbf{r}_m, \mathbf{r}_{m'}\rangle_\pi = \delta_{m,m'}$ because of the orthogonality of the $\mathbf{v}_m$. The final statement follows from the fact that $\mathbf{T}(i,j)$ is the i-th entry of the application of $\mathbf{T}$ to the unit vector $\mathbf{e}_j$ and the orthonormal basis property of the $\mathbf{r}_m$:

$$\begin{aligned}
\mathbf{T}(i,j) &= \left[\mathbf{T}\mathbf{e}_j\right](i) \\
&= \left[\mathbf{T}\left(\sum_{m=1}^{n}\langle \mathbf{e}_j, \mathbf{r}_m\rangle_\pi \mathbf{r}_m\right)\right](i) \\
&= \sum_{m=1}^{n}\langle \mathbf{e}_j, \mathbf{r}_m\rangle_\pi \mathbf{T}\mathbf{r}_m(i) \\
&= \sum_{m=1}^{n}\mathbf{r}_m(j)\pi(j)\lambda_m\mathbf{r}_m(i).
\end{aligned}$$

□

Consequently, the type of transition matrices we are going to focus on from now are irreducible, aperiodic, and reversible. We can now easily show the following convergence result:

Lemma 6. *Let* $\mathbf{T}$ *be the transition matrix of an irreducible, aperiodic and reversible Markov chain. Then, for any initial distribution* $\mathbf{p}_0$*, we have:*

$$\lim_{k\to\infty}\mathbf{p}_k = \pi.$$

Proof. The eigenvalue decomposition of $\mathbf{T}$ yields:

$$\begin{aligned}
\mathbf{p}_k^T &= \mathbf{p}_0^T\mathbf{T}^k \\
&= \mathbf{p}_0^T\left[\sum_{m=1}^{n}\lambda_m^k\mathbf{r}_m\mathbf{l}_m^T\right] \\
&= \sum_{m=1}^{n}\lambda_m^k\langle \mathbf{p}_0, \mathbf{r}_m\rangle\mathbf{l}_m^T \\
&= \pi + \sum_{m=2}^{n}\lambda_m^k\langle \mathbf{p}_0, \mathbf{r}_m\rangle\mathbf{l}_m^T. \qquad (1)
\end{aligned}$$

The statement follows if we go to the limit and the fact that $\lambda_m < 1$ for all $m \geq 2$. □

With this decomposition, we are able to understand the dynamical behaviour of the chain in detail. The decomposition tells us that the time evolution of any probability density is a superposition of relaxation processes. Moreover, there is a finite time we need to wait until the system has entirely forgotten about its initial state. If we run the chain for much longer than the **second implied timescale**

$$t_2 \quad = \quad -\frac{1}{\log(\lambda_2)},$$

all terms in Eq. (1) have vanished except the first. But we can do even better than this. Consider the example shown in Figure 1: Here, we study a discrete Markov chain on $n = 100$ states, where the states correspond to fine bins of an interval of the real line. The transition matrix (panel B) is set up to mimic the stochastic dynamics of a particle in the potential energy landscape shown in panel A. This particle will remain for long times in one of the four minima of the energy landscape, and it will only rarely transition between them. This is reflected in the transition probabilities and the stationary vector, also shown in panel A. Looking at the eigenvalues in panel D, we see that there are three eigenvalues λ_2, λ_3, λ_4, which are close to the Perron eigenvalue $\lambda_1 = 1$, whereas all remaining eigenvalues are clearly separated from 1. Moreover, the first three non-constant eigenvectors are nearly constant across the main minima, but they exchange their signs in between them: The second eigenvector $\mathbf{r}_2$ exchanges its sign across the largest barrier in the center, the next two are doing the same across the smaller barriers on the left and on the right. In this way, the eigenvectors corresponding to eigenvalues close to 1 seem to encode the slow structural transitions in the chain, and thus the essential dynamical information.

This is not a coincidence. Long-lived groups of states (or **macrostates** or **clusters**) that only allow for rare transitions to other states are called **metastable**. The existence of metastable macrostates is connected to eigenvalues close to the Perron eigenvalue λ_1, because their longevity implies slow convergence in Eq. (1). Moreover, metastable macrostates are related to eigenvectors that are nearly constant on the macrostates, as we will see below. This is exactly the pattern we are looking for when we try to model the dynamics of biological molecules, as metastable clusters are a typical feature of these systems. Frequently, they are associated to biological function or malfunction of a molecule.

Eigenvectors of Nearly Uncoupled Markov Chains

Let us give a more precise meaning to the observed sign pattern of the eigenvectors. First, consider an **uncoupled** Markov chain, which can be decomposed into $n_c < n$ separated clusters. The transition matrix can be assumed to possess a block-diagonal structure

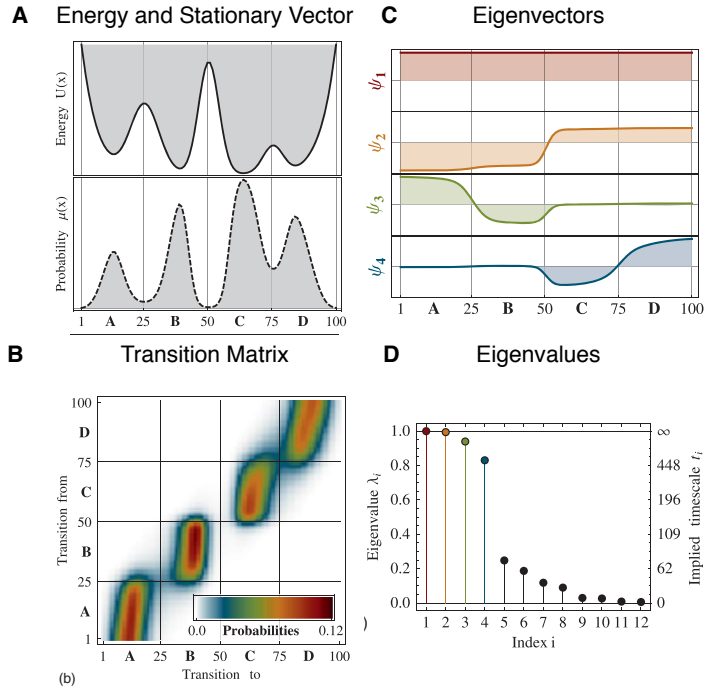

Figure 1: Illustration of eigenvalue decomposition for a metastable system.

$$\mathbf{T}_U \quad = \quad \begin{bmatrix} T_1 & 0 & \cdots & 0 \\ 0 & T_2 & 0 & \vdots \\ \vdots & & \ddots & \\ 0 & \cdots & & T_{n_c} \end{bmatrix}.$$

Due to the existence of the irreducible sub-chains, $\mathbf{T}_U$ has an n_c-fold eigenvalue $\lambda = 1$, and the space of right eigenvectors with eigenvalue 1 is n_c-dimensional. It follows that the right eigenvectors must be constant on the individual clusters. Denote the matrix of the first n_c right eigenvectors by $\mathbf{X}$. Introducing the characteristic vectors $\chi_j \in \mathbb{R}^n$, $j = 1, \ldots, n_c$:

$$\chi_j(i) \quad = \quad \begin{cases} 1 & \text{if } i\text{is in cluster } j \\ 0 & \text{otherwise} \end{cases},$$

and assembling them into a matrix $\chi \in \mathbb{R}^{n \times n_c}$, we find that there must be a regular transformation matrix $\mathbf{A} \in \mathbb{R}^{n_c \times n_c}$, s.t.

$$\chi \quad = \quad \mathbf{XA}.$$

We can now formulate the observation made above in a precise manner:

Theorem 7. *Let* $\mathbf{T}$ *be the transition matrix of a reversible, irreducible and aperiodic Markov chain which is nearly uncoupled, i.e.* $\mathbf{T}$ *is of nearly block-diagonal form:*

$$\mathbf{T} \quad = \quad \begin{bmatrix} T_1 & E_{12} & \cdots & E_{1n_c} \\ E_{21} & T_2 & \cdots & E_{2n_c} \\ \vdots & & \ddots & \vdots \\ E_{n_c1} & \cdots & & T_{n_c} \end{bmatrix},$$

where $\|E_{ij}\| \leq \epsilon$ *for all* i, j*. Then, apart from the unique Perron eigenvalue* $\lambda_1 = 1$ *and the constant eigenvector* $\mathbf{r}_1$ *corresponding to it, there are* $n_c - 1$ *eigenvalues close to* 1*. The matrix* $\mathbf{X}$ *of the first* n_c *eigenvectors satisfies*

$$\chi \quad = \quad \mathbf{XA} + \mathcal{O}(\epsilon)$$

for a regular transformation $\mathbf{A} \in \mathbb{R}^{n_c \times n_c}$*.*

Proof. Can be found in [1, Thm 3.1]. □

Coarse Graining by PCCA+

We know by now that the dominant eigenvectors of a metastable Markov chain can be expected to look as described above. How can we automatically detect the metastable states and thus coarse grain the chain down to its relevant features? Examination of the sign-structure of the eigenvectors turned out to

be difficult in practice for two reasons: Firstly, the number of possible sign-structures grows exponentially. Moreover, it is unclear how to treat transition states, i.e. states like those on top of the barriers of the potential in Figure 1. It does not make sense to assign these states to either of the metastable states. Consequently, the idea brought forward by [2, 4] under the name of **Perron Cluster Cluster Analysis (PCCA+)** is to compute a regular transformation $\mathbf{A}$ and a membership matrix χ where the strict assignment of each state i to a macrostate j is replaced by a soft assignment. Now, a microstate i belongs to each macrostate j with a certain probability $\chi_j(i)$. Thus, χ is replaced by a matrix satisfying the conditions:

$$\begin{aligned} \chi_j(i) &\geq 0 \,(\text{Positivity}) \\ \sum_{j=1}^{n_c} \chi_j(i) &= 1 \,(\text{Partition of Unity}). \end{aligned}$$

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