Markov Chains and Algorithmic Applications: WEEK 6

1 Rate of convergence: proofs

1.1 Reminder

Let $(X_n,\, n \geq 0)$ be a Markov chain with state space S and transition matrix P, and consider the following assumptions:

- X is ergodic (irreducible, aperiodic and positive-recurrent), so there exists a stationary distribution π and it is a limiting distribution as well.
- The state space S is finite, $|S| = N$.
- Detailed balance holds ($\pi_i p_{ij} = \pi_j p_{ji} \quad \forall i, j \in S$).

Statement 1.1. Under these assumptions, we have seen that there exist numbers $\lambda_0 \geq \lambda_1 \geq \ldots \geq \lambda_{N-1}$ and vectors $\phi^{(0)}, \phi^{(1)}, \ldots, \phi^{(N-1)} \in \mathbb{R}^N$ such that

$$P\phi^{(k)} = \lambda_k \phi^{(k)}, \quad k = 0, \ldots, N-1$$

and $\phi_j^{(k)} = \frac{u_j^{(k)}}{\sqrt{\pi_j}}$, where $u^{(0)}, \ldots, u^{(N-1)}$ is an orthonormal basis of $\mathbb{R}^N$ ($u^{(k)}$ are the eigenvectors of the symmetric matrix Q, where $q_{ij} = \sqrt{\pi_i}\, p_{ij}\, \frac{1}{\sqrt{\pi_j}}$). Note that the $\phi^{(k)}$ do not usually form an orthonormal basis of $\mathbb{R}^N$.

Facts

1. $\phi_j^{(0)} = 1 \quad \forall j \in S, \quad \lambda_0 = 1 \quad$ and $\quad |\lambda_k| \leq 1 \quad \forall k \in \{0, \ldots, N-1\}$
2. $\lambda_1 < +1$ and $\lambda_{N-1} > -1$

Definition 1.2. Let us define $\lambda_* = \max_{k \in \{1,\ldots,N-1\}} |\lambda_k| = \max\{\lambda_1, -\lambda_{N-1}\}$. The spectral gap is defined as $\gamma = 1 - \lambda_*$.

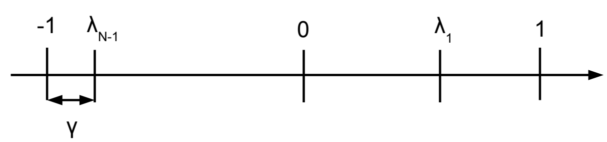


Figure 1: Spectral gap

Theorem 1.3. Under all the assumptions made above, we have

$$\|P_i^n - \pi\|_{\mathrm{TV}} = \frac{1}{2}\sum_{j \in S} |p_{ij}(n) - \pi_j| \leq \frac{1}{2\sqrt{\pi_i}}\, \lambda_*^n \leq \frac{1}{2\sqrt{\pi_i}}\, e^{-\gamma n}, \quad \forall i \in S,\, n \geq 1$$

1.2 Proof of Fact 1

Let us first prove that $\phi_j^{(0)} = 1 \quad \forall j \in S$ and $\lambda_0 = 1$.

Consider $\phi_j^{(0)} = 1 \quad \forall j \in S$; we will prove that $(P\phi^{(0)})_i = \phi_i^{(0)}$ (so $\lambda_0 = 1$):

$$(P\phi^{(0)})_i = \sum_{j \in S} p_{ij} \underbrace{\phi_j^{(0)}}_{=1} = \sum_{j \in S} p_{ij} = 1 = \phi_i^{(0)}$$

Also, we know that $\phi_i^{(0)} = \frac{u_i^{(0)}}{\sqrt{\pi_i}}$, so $u_i^{(0)} = \sqrt{\pi_i}\,\phi_i^{(0)} = \sqrt{\pi_i}$. The norm of $u^{(0)}$ is therefore equal to 1:

$$\|u^{(0)}\|^2 = \sum_{i \in S} (u_i^{(0)})^2 = \sum_{i \in S} \pi_i = 1$$

Let us then prove that $|\lambda_k| \leq 1 \quad \forall k \in \{0, \dots, N-1\}$.

Let $\phi^{(k)}$ be the eigenvector corresponding to λ_k. We define i to be such that $|\phi_i^{(k)}| \geq |\phi_j^{(k)}| \quad \forall j \in S$ ($|\phi_i^{(0)}| > 0$ because an eigenvector cannot be all-zero). We will use $P\phi^{(k)} = \lambda_k \phi^{(k)}$ in the following:

$$|\lambda_k \phi_i^{(k)}| = \left|(P\phi^{(k)})_i\right| = \left|\sum_{j \in S} p_{ij}\phi_j^{(k)}\right| \leq \sum_{j \in S} p_{ij} \underbrace{|\phi_j^{(k)}|}_{\leq |\phi_i^{(k)}|, \forall j \in S} \leq |\phi_i^{(k)}| \underbrace{\sum_{j \in S} p_{ij}}_{=1}$$

So we have $|\lambda_k||\phi_i^{(k)}| \leq |\phi_i^{(k)}|$, which implies that $|\lambda_k| \leq 1$, as $|\phi_i^{(k)}| > 0$. $\square$

1.3 Proof of Fact 2

We want to prove that $\lambda_1 < +1$ and $\lambda_{N-1} > -1$, which together imply that $\lambda_* < 1$.
By the assumptions made, we know that the chain is irreducible, aperiodic and finite, so $\exists n_0 > 1$ such that $p_{ij}(n) > 0$, $\forall i, j \in S, \forall n \geq n_0$.

$\boldsymbol{\lambda_1 < +1}$:

Assume ϕ is such that $P\phi = \phi$: we will prove that ϕ can only be a multiple of $\phi^{(0)}$, which implies that the eigenvalue $\lambda = 1$ has a unique eigenvector associated to it, so $\lambda_1 < 1$. Take i such that $|\phi_i| \geq |\phi_j|$, $\forall j \in S$, and let $n \geq n_0$.

$$\phi_i = (P\phi)_i = (P^n\phi)_i \overset{(*)}{=} \sum_{j \in S} p_{ij}(n)\,\phi_j$$

so

$$|\phi_i| = \left|\sum_{j \in S} p_{ij}(n)\,\phi_j\right| \leq \sum_{j \in S} p_{ij}(n) \underbrace{|\phi_j|}_{\leq |\phi_i|} \leq |\phi_i| \underbrace{\sum_{j \in S} p_{ij}(n)}_{1} = |\phi_i|$$

So we have $|\phi_i| \leq \sum_{j \in S} p_{ij}(n)|\phi_j| \leq |\phi_i|$. To have equality, we clearly need to have $|\phi_i| = |\phi_j|$, $\forall j \in S$ (because $p_{ij}(n) > 0$ for all i, j and $\sum_{j \in S} p_{ij}(n) = 1$ for all $i \in S$). Because $(*)$ is satisfied, we also have $\phi_i = \sum_{j \in S} p_{ij}(n)\phi_j$, which in turn implies that $\phi_j = \phi_i$ for all $j \in S$. So the vector ϕ is constant. $\square$

$\lambda_{\mathbf{N-1}} > \mathbf{-1}$:

Assume there exists $\phi \neq 0$ such that $P\phi = -\phi$: we will prove that this is impossible, showing therefore that no eigenvalue can take the value -1. Take i such that $|\phi_i| \geq |\phi_j|$, $\forall j \in S$ and let n odd be such that $n \geq n_0$.

Now, as $P^n\phi = P\phi = -\phi$, we have $-\phi_i \overset{(*)}{=} \sum_{j\in S} p_{ij}(n)\,\phi_j$ and $|\phi_i| \leq \sum_{j\in S} p_{ij}(n)\,|\phi_j| \leq |\phi_i|$. So, as above, we need to have $|\phi_j| = |\phi_i|$, for all $j \in S$ and then, thanks to $(*)$, $\phi_j = -\phi_i$, for all $j \in S$. This implies that $\phi_i = -\phi_i = 0$, and leads to $\phi_j = 0$ for all $j \in S$, which is impossible. $\square$

1.4 Proof of the theorem

We will first use the Cauchy-Schwarz inequality which states that

$$\left|\sum_{j\in S} a_j b_j\right| \leq \left(\sum_{j\in S} a_j^2\right)^{1/2} \left(\sum_{j\in S} b_j^2\right)^{1/2}$$

so as to obtain

$$\begin{aligned}
\|P_i^n - \pi\|_{\mathrm{TV}} &= \frac{1}{2}\sum_{j\in S} \underbrace{\left|\frac{p_{ij}(n) - \pi_j}{\sqrt{\pi_j}}\right|}_{a_j} \underbrace{\sqrt{\pi_j}}_{b_j} \leq \frac{1}{2}\left(\sum_{j\in S}\left(\frac{p_{ij}(n)}{\sqrt{\pi_j}} - \sqrt{\pi_j}\right)^2\right)^{1/2} \underbrace{\left(\sum_{j\in S}\pi_j\right)^{1/2}}_{1} \\
&= \frac{1}{2}\left(\sum_{j\in S}\left(\frac{p_{ij}(n)}{\sqrt{\pi_j}} - \sqrt{\pi_j}\right)^2\right)^{1/2}
\end{aligned}$$

Lemma 1.4.

$$\frac{p_{ij}(n)}{\sqrt{\pi_j}} - \sqrt{\pi_j} = \sqrt{\pi_j}\sum_{k=1}^{N-1} \lambda_k^n \phi_i^{(k)} \phi_j^{(k)}$$

Proof. Remember that $u^{(0)}, \ldots, u^{(N-1)}$ is an orthonormal basis of $\mathbb{R}^N$, so we can write for any $v \in \mathbb{R}^N$ $v = \sum_{k=0}^{N-1}(v^T u^{(k)})u^{(k)}$ i.e. $v_j = \sum_{k=0}^{N-1}(v^T u^{(k)})u_j^{(k)}$. For a fixed $i \in S$, take $v_j = \frac{p_{ij}(n)}{\sqrt{\pi_j}}$. We obtain

$$(v^T u^{(k)}) = \sum_{j\in S}\frac{p_{ij}(n)}{\sqrt{\pi_j}} u_j^{(k)} = \sum_{j\in S} p_{ij}(n)\phi_j^{(k)} = (P^n\phi^{(k)})_i = \lambda_k^n \phi_i^{(k)}$$

which in turn implies

$$v_j = \frac{p_{ij}(n)}{\sqrt{\pi_j}} = \sum_{k=0}^{N-1}\lambda_k^n\phi_i^{(k)}u_j^{(k)} = \sum_{k=0}^{N-1}\lambda_k^n\phi_i^{(k)}\phi_j^{(k)}\sqrt{\pi_j} = \underbrace{\lambda_0^n\phi_i^{(0)}\phi_j^{(0)}}_{1}\sqrt{\pi_j} + \sqrt{\pi_j}\sum_{k=1}^{N-1}\lambda_k^n\phi_i^{(k)}\phi_j^{(k)}$$

$\square$

Let us continue with the proof of the theorem using this lemma.

$$\begin{aligned}
\|P_i^n - \pi\|_{\mathrm{TV}} &\leq \frac{1}{2}\left(\sum_{j\in S}\left(\frac{p_{ij}(n)}{\sqrt{\pi_j}} - \sqrt{\pi_j}\right)^2\right)^{1/2} = \frac{1}{2}\left(\sum_{j\in S}\left(\sqrt{\pi_j}\sum_{k=1}^{N-1}\lambda_k^n \phi_i^{(k)}\phi_j^{(k)}\right)^2\right)^{1/2} \\
&= \frac{1}{2}\left(\sum_{j\in S}\pi_j\sum_{k,l=1}^{N-1}\lambda_k^n\phi_i^{(k)}\phi_j^{(k)}\lambda_l^n\phi_i^{(l)}\phi_j^{(l)}\right)^{1/2} = \frac{1}{2}\left(\sum_{k,l=1}^{N-1}\lambda_k^n\phi_i^{(k)}\lambda_l^n\phi_i^{(l)}\sum_{j\in S}\pi_j\phi_j^{(k)}\phi_j^{(l)}\right)^{1/2} \\
&= \frac{1}{2}\left(\sum_{k=1}^{N-1}\lambda_k^{2n}(\phi_i^{(k)})^2\right)^{1/2}
\end{aligned}$$

where we have used the fact that $\sum_{j\in S}\pi_j\phi_j^{(k)}\phi_j^{(l)} = \sum_{j\in S}u_j^{(k)}u_j^{(l)} = (u^{(k)})^T u^{(l)} = \delta_{kl}$. Remembering now that $|\lambda_k| \leq \lambda_*$ for every $1 \leq k \leq N-1$, we obtain

$$\|P_i^n - \pi\|_{\mathrm{TV}} \leq \frac{1}{2}\,\lambda_*^n\left(\sum_{k=1}^{N-1}(\phi_i^{(k)})^2\right)^{1/2}$$

In order to compute the term in parentheses, remember again that $v_j = \sum_{k=0}^{N-1}(v^T u^{(k)})\,u_j^{(k)}$ for every $v \in \mathbb{R}^N$, so by choosing $v = e_i$, i.e., $v_j = \delta_{ij} = \begin{cases}1 & \text{if } i = j\\ 0 & \text{otherwise}\end{cases}$, we obtain:

$$v^T u^{(k)} = u_i^{(k)} \quad \text{and} \quad \delta_{ij} = \sum_{k=0}^{N-1}u_i^{(k)}u_j^{(k)}$$

For $i = j$, we get $\delta_{ii} = 1 = \sum_{k=0}^{N-1}(u_i^{(k)})^2 = \sum_{k=0}^{N-1}\pi_i\,(\phi_i^{(k)})^2$, so

$$\sum_{k=1}^{N-1}(\phi_i^{(k)})^2 = \sum_{k=0}^{N-1}(\phi_i^{(k)})^2 - \underbrace{(\phi_i^{(0)})^2}_{1} = \frac{1}{\pi_i} - 1 \leq \frac{1}{\pi_i}$$

which finally leads to the inequality

$$\|P_i^n - \pi\|_{\mathrm{TV}} \leq \frac{\lambda_*^n}{2\sqrt{\pi_i}}$$

and therefore completes the proof. □

1.5 Lazy random walks

Adding self-loops to a Markov chain makes it a priori "lazy". Surprisingly perhaps, this might in some cases speed up the convergence to equilibrium!

Adding self-loops of weight $\alpha \in (0,1)$ to every state has the following impact on the transition matrix: assuming P is the transition matrix of the initial Markov chain, the new transition matrix $\widetilde{P}$ becomes

$$\widetilde{P} = \alpha\, I + (1-\alpha)\, P$$

As a consequence:

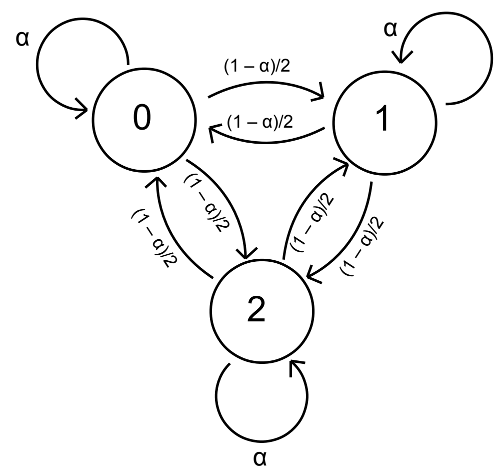
- The eigenvalues also change from λ_k to $\widetilde{\lambda}_k = \alpha + (1-\alpha)\lambda_k$, which sometimes reduces the value of $\lambda_* = \max_{1\leq k\leq N-1}|\lambda_k|$. The spectral gap being equal to $\gamma = 1 - \lambda_*$, we obtain that by reducing λ_*, we might increase the spectral gap as well as the convergence rate to equilibrium.

- Note that λ_0 stays the same: $\widetilde{\lambda}_0 = \alpha + (1-\alpha)\,\lambda_0 = 1$, as well as the stationary distribution π:

$$\pi\widetilde{P} = \pi\,(\alpha I + (1-\alpha)P) = \alpha\pi + (1-\alpha)\,\underbrace{\pi P}_{=\pi} = \pi$$

Example 1.5. Random walk on the circle with $N = 3$:

$$P = \begin{pmatrix} 0 & 1/2 & 1/2 \\ 1/2 & 0 & 1/2 \\ 1/2 & 1/2 & 0 \end{pmatrix} \xrightarrow{\text{add } \alpha} \widetilde{P} = \begin{pmatrix} \alpha & \frac{1-\alpha}{2} & \frac{1-\alpha}{2} \\ \frac{1-\alpha}{2} & \alpha & \frac{1-\alpha}{2} \\ \frac{1-\alpha}{2} & \frac{1-\alpha}{2} & \alpha \end{pmatrix}$$



Example 1.6 (PageRank)**.** The basic principle behind Google's search engine algorithm is as follows. One can represent the web as a graph with the hyperlinks being the edges and the webpages being the vertices. We define the transition probabilities of a random walk on this graph as

$$p_{ij} = \begin{cases} \frac{1}{d_i} & \forall j \text{ such that there is an outgoing edge from } i \to j, \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

where d_i is the *outgoing* degree of webpage i.

The principle is that the most popular pages are the webpages visited the most often. If π is the stationary distribution of the above random walk, then π_i is a good indicator of the popularity of page i.

To rank pages we therefore need to solve $\pi = \pi P$. In practice however, due to the size of the state space, solving this linear system takes too long in real time. Also the detailled balance condition is typically not satisfied here since the graph is directed (this can be seen explicitly when there is are pairs (i, j) with a directed link and no link in the reverse direction).

What PageRank does is to compute instead $\pi^{(0)}P^n$ for some initial distribution $\pi^{(0)}$ and a small value of n, which is meant to give a good approximation of the stationary distribution π. The quality of the approximation is of course directly linked to the rate of convergence to equilibrium. Adding self-loops of weight α to the graph seems to help also in this case: the practical value chosen for α is around 15%.