A gentle introduction to combinatorial stochastic processes VII

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Outline

The starting point

We shall illustrate the concept and problems of metastability with an example. Let us start with a reducible Markov chain with three states labelled by 1, 2 and 3 and transition probability matrix given by

$$P = \begin{pmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The perturbed matrix

Let us now perturb the previous transition probability with a small parameter $\delta \ll 1$ in this way

$$P = \begin{pmatrix} 1/2 & 1/2-\delta & \delta \\ 1/2-\delta & 1/2 & \delta \\ \delta & \delta & 1-2\delta \end{pmatrix}.$$

The probability of leaving the set of states $\{1,2\}$ is $2-\delta$, equal to the probability of leaving state 3. This is an irreducible and aperiodic Markov chain, it is reversible and symmetric and therefore the invariant distribution is uniform:

$$\pi = (1/3, 1/3.1/3).$$

A Monte Carlo simulation illustrates the meaning of *metastability* in this case.

Definition of mixing time

Consider two distributions on a finite set of values **p** and **q**. We can define the total variation distance as

$$d_{TV}(\mathbf{p}, \mathbf{q}) = \max_i |p_i - q_i| = \frac{1}{2} \sum_i |p_i - q_i|.$$

Let $\mathbf{p}(n)$ be the marginal probability distribution of an irreducible and aperiodic Markov chain with invariant distribution π at step n, let $d(n) = d_{TV}(\mathbf{p}(n), \pi)$. Then the mixing time $t_{\text{mix}}(\varepsilon)$ is defined as

$$t_{\text{mix}}(\varepsilon) = \min\{n : d(n) \leq \varepsilon\}.$$

Spectral gap and mixing times for reversible chains I

Let P be the transition probability matrix of an irreducible, aperiodic and reversible Markov chain with invariant distribution π. We have this decomposition theorem for the t step transition probabilities $P^t(x, y)$.

Theorem

There is an orthonormal basis of real-valued eigenfunctions f_j corresponding to real eigenvalues λ_j and the eigenfunction f_1 corresponding to $\lambda_1 = 1$ can be taken to be the constant vector $(1, \ldots, 1)$. Moreover, the transition matrix P^t can be decomposed as

$$\frac{P^t(x, y)}{\pi(x)} = 1 + \sum_{j \geq 2} f_i(x) f_j(y) \lambda_j^t.$$

Spectral gap and mixing times for reversible chains II

Let P the transition matrix of an irreducible, aperiodic and reversible chain matrix with state space $\mathcal{S}$. We order its eigenvalues

$$1 = \lambda_1 \geq \lambda_2 \ldots \geq \lambda_{|\mathcal{S}|} \geq -1.$$

We let $\lambda_* = \max\{|\lambda| : \lambda \text{ is an eigenvalue of } P, \lambda \neq 1\}$ and define $\gamma_* = 1 - \lambda_*$ to be the absolute spectral gap. The spectral gap is defined to be $\gamma = 1 - \lambda_2$.
The relaxation time for a reversible Markov chain is defined as

$$t_{\mathrm{rel}} = \frac{1}{\gamma_*}.$$

Spectral gap and mixing times for reversible chains III

For a reversible Markov chain there are upper and lower bounds for the mixing time:

$$(t_{\mathrm{rel}} - 1) \log \left(\frac{1}{2\varepsilon} \right) \leq t_{\mathrm{mix}}(\varepsilon) \leq t_{\mathrm{rel}} \log \left(\frac{1}{\varepsilon \pi_{\mathrm{min}}} \right),$$

where $\pi_{\mathrm{min}} = \min_{x \in \mathcal{S}} \pi(x)$.