

Math 106 – Notes

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Time Reversal and Detailed Balance (3.8)

Let $\{X_t\}_{t \geq 0}$ be a Q -process on $\Omega = \{1, \dots, I\}$ initialized in a steady state π , and define the time-reversed process

$$\hat{X}_t = X_{T-t}, \quad (1)$$

where $T > 0$ is arbitrary (since X is initialized in a steady state). We seek to describe the process \hat{X}_t . Using Bayes' theorem, we can easily see that it is a Markov process whose transition matrix $\hat{P}_{i,j}(t)$ is given by

$$\hat{P}_{i,j}(t) = \mathbb{P}(X_{s-t} = j \mid X_s = i) = \mathbb{P}(X_s = i \mid X_{s-t} = j) \frac{\mathbb{P}(X_{s-t} = j)}{\mathbb{P}(X_s = i)} = P_{j,i}(t) \frac{\pi_j}{\pi_i}. \quad (2)$$

Generator of the time-reversed process

Let \hat{Q} denote the generator of \hat{X} . By the **backward equation**

$$\frac{d}{dt} \hat{P}_{i,j}(t) = \sum_{k=1}^I \hat{Q}_{i,k} \hat{P}_{k,j}(t) \quad (3)$$

On the other hand, using the **forward equation** for X ,

$$\frac{d}{dt} \hat{P}_{i,j}(t) = \frac{d}{dt} \left(P_{j,i}(t) \frac{\pi_j}{\pi_i} \right) = \sum_{k=1}^I P_{j,k}(t) Q_{k,i} \frac{\pi_j}{\pi_i} = \sum_{k=1}^I \left(P_{j,k}(t) \frac{\pi_j}{\pi_k} \right) \left(Q_{k,i} \frac{\pi_k}{\pi_i} \right) \quad (4)$$

$$= \sum_{k=1}^I \hat{Q}_{i,k} \hat{P}_{k,j}(t) \quad \text{with} \quad \hat{Q}_{i,j} = \frac{\pi_j}{\pi_i} Q_{j,i}. \quad (5)$$

Detailed balance and probability fluxes

The chain is said to satisfy *detailed balance* with respect to π if

$$\pi_i Q_{i,j} = \pi_j Q_{j,i}, \quad \text{for all } i \neq j. \quad (6)$$

Comparing with the formula for \hat{Q} , we see that detailed balance is equivalent to

$$\hat{Q}_{i,j} = Q_{i,j} \quad \text{for all } i, j. \quad (7)$$

Thus, a stationary Q -process is reversible if and only if it satisfies detailed balance; in that case the time-reversed process has the same generator as the forward process.

To interpret detailed balance, note that in stationarity the average rate at which the process makes transitions from state i to state j is

$$J_{i \rightarrow j} := \pi_i Q_{i,j}. \quad (8)$$

This quantity has the interpretation of a *probability flux* along the directed edge $i \rightarrow j$. The net flux along the undirected edge $\{i, j\}$ is

$$J_{i \leftrightarrow j}^{\text{net}} = J_{i \rightarrow j} - J_{j \rightarrow i} = \pi_i Q_{i,j} - \pi_j Q_{j,i}. \quad (9)$$

The detailed balance condition is precisely the requirement that

$$J_{i \leftrightarrow j}^{\text{net}} = 0 \quad \text{for every pair } i, j, \quad (10)$$

i.e. the flux from i to j is exactly balanced by the flux from j to i on each edge.

Mere stationarity of π only requires

$$\sum_{j=1}^I \pi_i Q_{i,j} = 0 \quad \text{for each } i, \quad (11)$$

which says that the total outgoing flux from each state i is balanced by the total incoming flux, but allows for nonzero *circulating currents* around cycles. Detailed balance rules out such circulating probability currents; at equilibrium the chain looks statistically the same when run forwards or backwards in time.

Hermitian structure

Assume that Q is reversible with respect to π , i.e. it satisfies detailed balance. Let D_π be the diagonal matrix

$$(D_\pi)_{i,i} = \pi_i, \quad (D_\pi)_{i,j} = 0 \text{ for } i \neq j. \quad (12)$$

Consider the similarity transform

$$S := D_\pi^{1/2} Q D_\pi^{-1/2}. \quad (13)$$

The (i, j) -entry of S is

$$S_{i,j} = (D_\pi^{1/2})_{i,i} Q_{i,j} (D_\pi^{-1/2})_{j,j} = \sqrt{\pi_i} Q_{i,j} \frac{1}{\sqrt{\pi_j}}. \quad (14)$$

Using detailed balance,

$$\pi_i Q_{i,j} = \pi_j Q_{j,i} \implies \sqrt{\pi_i} Q_{i,j} \frac{1}{\sqrt{\pi_j}} = \sqrt{\pi_j} Q_{j,i} \frac{1}{\sqrt{\pi_i}}, \quad (15)$$

so

$$S_{i,j} = S_{j,i}. \quad (16)$$

Hence S is real symmetric.

Because Q is similar to the symmetric matrix S , it follows that Q is diagonalizable with real eigenvalues. More precisely, there exists an invertible matrix S and a real diagonal matrix Λ such that

$$Q = S \Lambda S^{-1}, \quad \Lambda = \text{diag}(\lambda_1, \dots, \lambda_I), \quad \lambda_k \in \mathbb{R}. \quad (17)$$

For a finite, irreducible Q -process, 0 is a simple eigenvalue with eigenvector $\mathbf{1}$, and all other eigenvalues satisfy

$$\lambda_k < 0 \quad \text{for } k \geq 2. \quad (18)$$

The transition semigroup then has the spectral representation

$$P(t) = e^{tQ} = S e^{t\Lambda} S^{-1}, \quad (19)$$

so each nontrivial mode decays as a pure exponential $e^{\lambda_k t}$ with a real decay rate $\lambda_k < 0$. In particular, an equilibrium Q -process (one satisfying detailed balance) does not relax via oscillations: there are no complex-conjugate pairs of eigenvalues, and thus no oscillatory components in the relaxation dynamics; all deviations from equilibrium decay monotonically in time along real exponential modes.