Math 106 – Notes
Week 3: January 20, 2026

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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

$$\hat{X}_t = X_{T-t}, \tag{1}$$

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

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

Generator of the time-reversed process

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

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

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

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

$$= \sum_{k=1}^{I}\left(P_{j,k}(t)\frac{\pi_j}{\pi_k}\right)\left(Q_{k,i}\frac{\pi_k}{\pi_i}\right) = \sum_{k=1}^{I}\hat{Q}_{i,k}\hat{P}_{k,j}(t), \tag{5}$$

with

$$\hat{Q}_{i,j} = \frac{\pi_j}{\pi_i}Q_{j,i}. \tag{6}$$

Detailed balance and probability fluxes

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

$$\pi_i Q_{i,j} = \pi_j Q_{j,i}, \qquad \text{for all } i \neq j. \tag{7}$$

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

$$\hat{Q}_{i,j} = Q_{i,j} \quad \text{for all } i, j. \tag{8}$$

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

$$J_{i\to j} := \pi_i Q_{i,j}. \tag{9}$$

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

$$J^{\text{net}}_{i\leftrightarrow j} = J_{i\to j} - J_{j\to i} = \pi_i Q_{i,j} - \pi_j Q_{j,i}. \tag{10}$$

The detailed balance condition is precisely the requirement that

$$J^{\text{net}}_{i\leftrightarrow j} = 0 \quad \text{for every pair } i, j, \tag{11}$$

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

$$\sum_{j=1}^{I} \pi_i Q_{i,j} = 0 \quad \text{for each } i, \tag{12}$$

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

$$(D_\pi)_{i,i} = \pi_i, \qquad (D_\pi)_{i,j} = 0 \text{ for } i \neq j. \tag{13}$$

Consider the similarity transform

$$S := D_\pi^{1/2}\, Q\, D_\pi^{-1/2}. \tag{14}$$

The (i, j)-entry of S is

$$S_{i,j} = \sqrt{\pi_i}\, Q_{i,j}\, \frac{1}{\sqrt{\pi_j}}. \tag{15}$$

Using detailed balance,

$$\pi_i Q_{i,j} = \pi_j Q_{j,i} \quad \Longrightarrow \quad \sqrt{\pi_i}\, Q_{i,j}\, \frac{1}{\sqrt{\pi_j}} = \sqrt{\pi_j}\, Q_{j,i}\, \frac{1}{\sqrt{\pi_i}}, \tag{16}$$

so

$$S_{i,j} = S_{j,i}. \tag{17}$$

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, since

$$S = D_\pi^{1/2} Q D_\pi^{-1/2}$$

is symmetric, there exists an orthogonal matrix O and a real diagonal matrix Λ such that

$$S = O \Lambda O^\top. \tag{18}$$

Setting

$$U := D_\pi^{-1/2} O, \tag{19}$$

we obtain the diagonalization

$$Q = U \Lambda U^{-1}, \qquad \Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_I), \quad \lambda_k \in \mathbb{R}. \tag{20}$$

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

$$\lambda_k < 0 \quad \text{for } k \geq 2. \tag{21}$$

The transition semigroup then has the spectral representation

$$P(t) = e^{tQ} = U\, e^{t\Lambda}\, U^{-1}, \tag{22}$$

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.