Detailed Balance

C.W. Seitz

July 12, 2022

1 Detailed Balance

This note will discuss the notion of *detailed balance* for Markov processes. Detailed balance is a property of a time-dependent probability density for which the net probability current is zero and in thus has a form that is independent of time. Under such conditions, we say that the density is stationary or at *equilibrium*. This concept has many important applications, for example in Markov Chain Monte Carlo (MCMC) algorithms, we design a Markov chain whose stationary distribution is a target distribution which we cannot sample from directly. Other examples come from thermodynamics and statistical mechanics, where detailed balance is synonymous with *reversibility* of a thermodynamic system.

We will start with a toy example where the phase space Ω of our system is discrete which implies that the density $P(\Omega)$ has finite support. In the following section we will generalize these concepts to the continuous setting. Consider a stochastic process represented by a series of values $(\omega_1, \omega_2, ..., \omega_t)$ which can be thought of as a path through the phase space Ω. Say we are in a state ω_i at time t, and we have a probability T_{ij} of transitioning to the arbitrary state ω_j where $i, j \in \Omega$ and we can have $i = j$. Formally, we have a conditional probability density over states j conditioned on the fact that we are currently in the state i, denoted $P(\omega_j|\omega_i)$.

Generally, we must express this for all possible ω_i and thus we have to write down $|\Omega|$ conditional distributions. Furthermore, it is not necessarily the case that $P(\omega_j|\omega_i)$ and $P(\omega_i|\omega_j)$ are equivalent, giving us $2|\Omega|$ distributions to work with. For a discrete system, these distributions are organized as a *transition matrix* sometimes called a stochastic matrix. When $|\Omega| = 3$ the transition matrix reads

$$T_{ij} = \begin{bmatrix} T_{11} & T_{21} & T_{31} \\ T_{12} & T_{22} & T_{32} \\ T_{13} & T_{23} & T_{33} \end{bmatrix} \qquad \sum_j T_{ij} = 1 \qquad \sum_i T_{ij} = 1$$

which has the property that rows and columns both sum to unity as they represent probability densities over Ω. Say that we start in state ω_1 and then let the system evolve over a time τ (where T_{ij} can be taken to have units of transition probability per unit time). The associated probability distribution is $P(\Omega, 0) = \langle 1, 0, 0 \rangle$.

$$P(\Omega, \tau) = P(\Omega, 0) + T_{ij} P(\Omega, 0) \cdot \tau$$

Taking the limit $\tau \to 0$ gives a so-called *master equation*

$$\frac{dP}{dt} = \lim_{\tau \to 0} \frac{P(\Omega, t + \tau) - P(\Omega, t)}{\tau} = T_{ij} P(\Omega, t)$$

The phenomenon of detailed balance occurs when there is zero net probability flow into any particular state ω, leaving the distribution invariant. In other words, the probability from $i \to j$ cancels the flow from $j \to i$ and $dP/dt = 0$. This suggests that there exists a distribution $\pi(\Omega)$ such that

$$T_{ij} \pi(\Omega) = \pi^T(\Omega) T_{ij}$$