Stochastic Systems: Master equation.

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The Master Equation

This is basically the continuous time version of Markov chains.

Derivation from the Chapman-Kolmogorov (CK) equation

The CK equation is

$$p(n, t+\Delta t|n_0, t_0) = \sum_{n'} p(n, t+\Delta t|n', t)p(n', t|n_0, t_0).$$

Now, we assume that

$$p(n, t+\Delta t|n', t) = \begin{cases} 1 - \kappa_n(t)\Delta t + \mathcal{O}(\Delta t)^2, & \text{if } n = n', \\ w_{nn'}(t)\Delta t + \mathcal{O}(\Delta t)^2, & \text{if } n \neq n'. \end{cases} \tag{1}$$

$w_{nn'}(t)$ is the *transition rate* and is only defined for $n \neq n'$

Now, by normalisation,

$$\begin{aligned} 1 &= \sum_n p(n, t+\Delta t|n', t) \\ &= 1 - \kappa_{n'}(t)\Delta t + \mathcal{O}(\Delta t)^2 + \sum_{n\neq n'} w_{nn'}(t)\Delta t + \mathcal{O}(\Delta t)^2 \end{aligned}$$

$$\Rightarrow \kappa_{n'}(t) = \sum_{n \neq n'} w_{nn'}(t).$$

Alternatively, switching the indices,

$$\kappa_n(t) = \sum_{n' \neq n} w_{n'n}(t). \tag{2}$$

Therefore, using (1), we see that the CK equation reads

$$\begin{aligned} p(n, t + \Delta t | n_0, t_0) &= (1 - \kappa_n(t)\Delta t + \ldots) p(n, t | n_0, t_0) \\ &+ \sum_{n' \neq n} w_{nn'}(t) p(n', t | n_0, t_0) \Delta t + \mathcal{O}(\Delta t)^2, \end{aligned}$$

$$\begin{aligned} &\Rightarrow \frac{p(n, t + \Delta t | n_0, t_0) - p(n, t | n_0, t_0)}{\Delta t} \\ &= -\kappa_n(t) p(n, t | n_0, t_0) + \sum_{n' \neq n} w_{nn'}(t) p(n', t | n_0, t_0) + \mathcal{O}(\Delta t). \end{aligned}$$

Now let $\Delta t \to 0$:

$$\frac{dp(n,t|n_0,t_0)}{dt} = -\kappa_n(t)p(n,t|n_0,t_0) + \sum_{n' \neq n} w_{nn'}(t)p(n',t|n_0,t_0).$$

Using (2), the middle term may be rewritten to find

$$\frac{dp(n,t|n_0,t_0)}{dt} = -\sum_{n' \neq n} w_{n'n}(t)p(n,t|n_0,t_0) + \sum_{n' \neq n} w_{nn'}(t)p(n',t|n_0,t_0).$$

If we had started, not from the CK equation, but from the first relation which defines Markov processes:

$$p(n,t+\Delta t) = \sum_{n'} p(n,t+\Delta t|n',t)p(n',t)$$

then exactly the same sequence of steps would lead to

$$\frac{dp(n,t)}{dt} = -\sum_{n' \neq n} w_{n'n}(t)p(n,t) + \sum_{n' \neq n} w_{nn'}(t)p(n',t).$$

This equation could also have been obtained by multiplying the equation for $p(n, t|n_0, t_0)$ by $p(n_0, t_0)$ and summing over all initial states, since

$$p(n, t) = \sum_{n_0} p(n, t|n_0, t_0)p(n_0, t_0).$$

Therefore both $p(n, t|n_0, t_0)$ and $p(n, t)$ satisfy the same equation. We will frequently write it for $p(n, t)$, with the understanding that this could also be thought of as the conditional probability.

The equation is the desired *master equation*,

$$\frac{dp(n, t)}{dt} = \sum_{n' \neq n} w_{nn'}(t)p(n', t) - \sum_{n' \neq n} w_{n'n}(t)p(n, t). \tag{3}$$

The interpretation of the master equation is straightforward. The first term is just the probability of going from $n' \to n$, and the second the probability of going from $n \to n'$.

In words, the rate of change of being in a state n is equal to the probability of making a transition into n, minus the probability of transitioning out of n.

In applications the $w_{nn'}$ are assumed to be given (this specifies the model) and we wish to determine the $p(n, t)$.

Comments:

• Notice that because of the Markov property, $w_{nn'}$ only depends on the current state of the system (n'), and does not depend on previous states (i.e. how the system got to n').

• In the derivation we have assumed that $w_{nn'}$ depends on time (which it does in general, just as for Markov chains), but usually we are only interested in situations where it is time-independent.

More informal derivations of the master equation

The master equation is essentially a balance equation; the rate of moving into the state n minus the rate of moving out of the same state is the rate of change of $p(n, t)$. That is, Rate of change of $p(n,t) =$

[Rate due to transitions into the state n from all the other states n'] -

[Rate due to transitions out of the state n into all other states n']

When expressed this way, and assuming the process is Markov, the master equation

$$\frac{dp(n,t)}{dt} = \sum_{n' \neq n} w_{nn'}(t) p(n',t) - \sum_{n' \neq n} w_{n'n}(t) p(n,t),$$

appears very reasonable.

Another derivation, which is also less rigorous than the original, starts from the system described as a Markov chain, and moves to continuous time by taking the duration of the time-step to zero:

So, let us start from

$$P_n(t+1) = \sum_{n'} Q_{nn'}(t) P_{n'}(t),$$

where the columns of the transition matrix add to unity:

$$\sum_{n'} Q_{n'n}(t) = 1.$$

So, if we write

$$P_n(t+1) - P_n(t) = \sum_{n'} Q_{nn'}(t) P_{n'}(t) - \sum_{n'} Q_{n'n}(t) P_n(t),$$

then the terms in the sums with $n' = n$ can be cancelled to give

$$P_n(t+1) - P_n(t) = \sum_{n' \neq n} Q_{nn'}(t) P_{n'}(t) - \sum_{n' \neq n} Q_{n'n}(t) P_n(t),$$

Now, we take the time step to be Δt, rather than unity, and divide through by the time step;

$$\frac{P_n(t+\Delta t) - P_n(t)}{\Delta t} = \sum_{n' \neq n} \frac{Q_{nn'}}{\Delta t} P_{n'}(t) - \sum_{n' \neq n} \frac{Q_{n'n}}{\Delta t} P_n(t).$$

Then, it is clear that taking the time step to zero, reduces the left-hand side to a differential of the probability, with respect to time. Furthermore instead of assuming that exactly one sampling event happens per time step, we assume that *on average* one event happens in the time step. To achieve this set

$$Q_{nn'}(t) = w_{nn'}(t)\Delta t + \mathcal{O}(\Delta t)^2, \quad n \neq n'.$$

So letting $\Delta t \to 0$ we obtain the master equation:

$$\frac{dP_n}{dt} = \sum_{n' \neq n} w_{nn'}(t) P_{n'}(t) - \sum_{n' \neq n} w_{n'n}(t) P_n(t).$$