System Size Expansion

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1 Introduction

This report contains notes on the system size expansion due to N.G. van Kampen. The general idea is to characterize the fluctuations of the deterministic limit of density dependent Markov chains.

2 Multi-Component MJPs

We consider an MJP X on $\mathcal{X} = \mathbb{N}_0^d$ that is characterized by a finite set of possible transitions $x \to x+v_i$ for $v_i \in \mathbb{Z}^d$ and $i = 1, \ldots, r$. Associated with the transition i is a state dependent transition rate $h_i(x)$. The probability of the process $p(x,t) := P(X(t) = x)$ is governed by a master equation of the form

$$\frac{d}{dt}p(x,t) = \sum_{i=1}^{r} h_i(x - v_i)p(x - v_i, t) - \sum_{i=1}^{r} h_i(x)p(x,t)\,. \tag{1}$$

By introducing the step operator E_i^l such that $E_i^l f(x) = f(x + le_i)$, the master equation can be conveniently written as

$$\frac{d}{dt}p(x,t) = \sum_{i=1}^{r} \left(\prod_{j=1}^{d} E_j^{-v_{ij}} - 1 \right) h_i(x)p(x,t)\,. \tag{2}$$

We also observe that the global transition function Q of the process takes the form

$$Q(x,y) = \begin{cases} h_i(x) & \text{for } y = x + v_i \\ 0 & \text{otherwise} \end{cases}. \tag{3}$$

No consider a function $f : \mathcal{X} \times [0,\infty) \to \mathbb{R}$ with finite expectation. We are interested in the time evolution of $\mathsf{E}[f(X(t),t)]$. Using the product rule of differentiation an the master equation (1) we obtain

$$\frac{d}{dt}\mathsf{E}[f(X(t),t)] = \sum_{i=1}^{r} \mathsf{E}\left[\left(f(X(t) + v_i) - f(X(t)) \right) h_i(X(t)) \right] + \mathsf{E}\left[\frac{\partial}{\partial t} f(X(t),t) \right] , \tag{4}$$

where the term within the right expectation refers to the partial derivative of f with respect to the second component evaluates at $X(t)$.

3 Deterministic Limit

It is well-known that systems described by an MJP on a microscopic scale give rise to deterministic behavior on a macroscopic scale. To see this, we have to perform a form of thermodynamic limit. Let Ω be the size of the system (e.g. total volume or number of entities) and consider the concentration variable $y^{\Omega}(t) = \frac{X(t)}{\Omega}$. We are interested in the dynamic behavior of y^{Ω} in the limit $\Omega \to \infty$.
Clearly, such a limit does not make sense for general processes. In order to observe non-trivial behavior, the rate functions have to scale in a certain way, namely

$$h_i^{\Omega}(x) = \Omega g_i\left(\frac{x}{\Omega}\right) \tag{5}$$

giving rise to the process family X^{Ω}.

4 Scaled Fluctuation Process

Sometimes it is not sufficient to know the macroscopic limit and we are also interested in the fluctuations. This gives rise to studying the rescalred stochastic process

$$Z^{\Omega}(t) = \frac{X(t) - \Omega\varphi(t)}{\sqrt{\Omega}} \tag{6}$$

Where φ is a deterministic function to be determined. As suggested by the notation, it will turn out that φ is the deterministic limit from the previous section. Our goal is to describe the time evolution of the fluctuation process Z^{Ω} in the limit of large Ω.
We observe that Z^{Ω} lives on a state space $\mathcal{Z}^{\Omega} \subset \mathbb{R}^d$ that depends the system size. Since $\mathcal{X}$ is countable, $\mathcal{Z}^{\Omega}$ is countable and consequently the limiting state space will also be countable. We may, however, hope that there exists a continuous process Z on a subset of $\mathbb{R}^d$ that is equal in distribution to the limiting process of Z^{Ω}. In order to do this, consider a twice differentiable function $f : \mathbb{R}^d \to \mathbb{R}$. Then we may write

$$\mathsf{E}\left[f(Z(t))\right] = \mathsf{E}\left[f\left(\frac{X(t) - \Omega\varphi(t)}{\sqrt{\Omega}}\right)\right]\,. \tag{7}$$

Since X is a jump process known to obey a master equation, we may exploit the general moment equation (4). Inserting the special form of the rate functions $h_i(x) = \Omega g_i\left(\frac{x}{\Omega}\right)$ we get

$$\begin{aligned}\frac{d}{dt}\mathsf{E}\left[f(Z(t))\right] = &\sum_{i=1}^{r}\mathsf{E}\left[\left(f\left(\frac{X(t) + v_i - \Omega\varphi(t)}{\sqrt{\Omega}}\right) - f\left(\frac{X(t) - \Omega\varphi(t)}{\sqrt{\Omega}}\right)\right)\Omega g_i\left(\frac{X(t)}{\Omega}\right)\right] \\ &- \sqrt{\Omega}\mathsf{E}\left[\nabla f\left(\frac{X(t) - \Omega\varphi(t)}{\sqrt{\Omega}}\right)\cdot\dot{\varphi}(t)\right]\,.\end{aligned} \tag{8}$$

The r.h.s. is now given in terms of expectations with respect to X. We proceed by replacing these such that we have a closed form expression in terms of Z. We get

$$\begin{aligned}\frac{d}{dt}\mathsf{E}\left[f(Z(t))\right] = &\sum_{i=1}^{r}\mathsf{E}\left[\left(f\left(Z(t) + \frac{v_i}{\sqrt{\Omega}}\right) - f\left(Z(t)\right)\right)\Omega g_i\left(\varphi(t) + \frac{Z(t)}{\sqrt{\Omega}}\right)\right] \\ &- \sqrt{\Omega}\mathsf{E}\left[\nabla f\left(Z(t)\right)\cdot\dot{\varphi}(t)\right]\,.\end{aligned} \tag{9}$$

Note that the above equation does not contain any approximation yet. For large Ω, the terms proportional to $\Omega^{-\frac{1}{2}}$ become small. Since f is twice continuously differentiable, we can exploit a Taylor expansion

$$f\left(Z(t) + \frac{v_i}{\sqrt{\Omega}}\right) = f(Z(t)) + \frac{v_i}{\sqrt{\Omega}}\cdot\nabla f(Z(t)) + \frac{1}{2\Omega}v_i^T\Delta f(Z(t))v_i + \mathcal{O}(\Omega^{-\frac{3}{2}})\,, \tag{10}$$

$$g_i\left(\varphi(t) + \frac{Z(t)}{\sqrt{\Omega}}\right) = g_i\left(\varphi(t)\right) + \frac{Z(t)}{\sqrt{\Omega}}\cdot\nabla g_i(\varphi(t)) + \mathcal{O}(\Omega)\,. \tag{11}$$

Inserting these equations into (9) and sorting by powers of Ω we get

$$\begin{aligned}\frac{d}{dt}\mathsf{E}\left[f(Z(t))\right] = &\sqrt{\Omega}\mathsf{E}\left[\left(\sum_{i=1}^{r}g_i(\varphi(t))v_i\right)\cdot\nabla f(Z(t))) - \dot{\varphi}(t)\cdot\nabla f(Z(t))\right] + \mathcal{O}(\Omega^{-\frac{1}{2}}) \\ &+ \sum_{i=1}^{r}\mathsf{E}\left[\left(v_i\cdot\nabla f(Z(t))\right)\left(Z(t)\cdot\nabla g_i(\varphi(t))\right))\right] + \sum_{i=1}^{r}\frac{g_i(\varphi(t))}{2}v_i^T\mathsf{E}[\Delta f(Z(t))]v_i\end{aligned} \tag{12}$$

Note that the first term is diverging as $\Omega \to \infty$. Fortunately, by choosing the function ϕ such that

$$\dot{\varphi}(t) = \sum_{i=1}^{r}g_i(\varphi(t))v_i\,, \tag{13}$$

the diverging tame can be made to vanish. Choosing this particular form of φ, only the second line of (12) survives in the limit. To obtain the final result, observe that

$$\sum_{i=1}^{r} \left(v_i \cdot \nabla f(Z(t))\right) \left(Z(t) \cdot \nabla g_i(\varphi(t))\right)) = \nabla f(Z(t)) \cdot (BZ(t)) \ , \qquad \text{with} \qquad B = \sum_{i=1}^{r} v_i \nabla g_i(\varphi(t))^T \tag{14}$$

and

$$\sum_{i=1}^{r} \frac{g_i(\varphi(t))}{2} v_i^T \mathsf{E}[\Delta f(Z(t))] v_i = \mathrm{Tr}(G\Delta f(Z(t))) \qquad \text{with} \qquad G = \sum_{i=1}^{r} g_i(\varphi(t)) v_i v_i^T \tag{15}$$

which leads to

$$\frac{d}{dt}\mathsf{E}\left[f(Z(t))\right] = \mathsf{E}\left[\nabla f(Z(t)) \cdot (BZ(t))\right] + \frac{1}{2}\mathrm{Tr}(G\mathsf{E}[\Delta f(Z(t))])\,. \tag{16}$$

(16) has the form of a backward equation of an Ito process. The corresponding Fokker-Planck equation for the probability density reads

$$\frac{d}{dt}p(z,t) = -\nabla \cdot ((Bz)p(z,t)) + \frac{1}{2}\mathrm{Tr}(\mathrm{G}\Delta \mathrm{p}(\mathrm{z},\mathrm{t}))\,. \tag{17}$$

Since (17) is linear, the solution is a Gaussian with time-dependent mean μ and covariance matrix Σ, i.e.

$$p(z,t) = (\det 2\pi\Sigma)^{-\frac{1}{2}} \exp\left[-\frac{1}{2}\left(x-\mu(t)\right)^T \Sigma(t)^{-1}\left(x-\mu(t)\right)\right] \ , \tag{18}$$

as long as the initial distribution is also Gaussian. From (16), we can obtain ODE's for μ and Σ directly by considering the special choices $f(z) = z_i$ and $f(z) = (z_i z_j$. This results in

$$\begin{aligned} \frac{d}{dt}\mu(t) &= B\mu(t)\,, \\ \frac{d}{dt}\Sigma(t) &= B\Sigma + \Sigma B^T + G\,. \end{aligned} \tag{19}$$

Finally, we conclude that we can obtain an approximation of the original process X for large but finite Ω by inverting the scaled fluctuation relation 6. Since the normal distribution is invariant under linear transformation, the result will again be Gaussian.

5 Examples

5.1 Predator Prey Dynamics

Consider the following model consisting of a prey species X_1 and a predator species X_2 that interact stochastically via a MJP with transition function Q whose non-zero elements are given by

$$\begin{aligned} Q(x, x+e_1) &= c_1 x_1, & Q(x, x-e_1) &= c_2 x_1 x_2, \\ Q(x, x+e_2) &= c_3 x_1 x_2, & Q(x, x-e_2) &= c_4 x_2. \end{aligned}$$

Formulated as above, there is no size parameter involved and we cannot obtain a scaling limit. To obtain the correct form of the intensity functions we set

$$\begin{aligned} c_1 &= k_1, & c_2 &= k_2\Omega^{-1}, \\ c_3 &= k_3\Omega^{-1}, & c_1 &= k_1\,. \end{aligned} \tag{20}$$

Intuitively, Ω can be understood as the size of the habitat. To obtain the form required for the expansion, we note that the change vectors and corresponding rate functions are given by

$$\begin{aligned}
v_1 &= e_1, & h_1(x) &= \Omega k_1 \frac{x_1}{\Omega}, \\
v_2 &= -e_1, & h_2(x) &= \Omega k_2 \frac{x_1}{\Omega}\frac{x_2}{\Omega}, \\
v_3 &= e_2, & h_3(x) &= \Omega k_3 \frac{x_1}{\Omega}\frac{x_2}{\Omega}, \\
v_4 &= -e_2, & h_4(x) &= \Omega k_4 \frac{x_2}{\Omega}.
\end{aligned} \tag{21}$$

This allows us to directly obtain the equation for the deterministic limit φ by exploiting (13)

$$\begin{aligned}
\dot{\varphi}_1(t) &= k_1\varphi_1(t) - k_2\varphi_1(t)\varphi_2(t) \\
\dot{\varphi}_2(t) &= k_3\varphi_1(t)\varphi_2(t) - k_4\varphi_2(t)\,,
\end{aligned} \tag{22}$$

which are the well-known ODE's from the classical Lotka-Volterra model. For the fluctuation process, observe that the matrix B is nothing but the Jacobian of r.h.s of (22), hence

$$B = \begin{pmatrix} k_1 - k_2\varphi_2 & -k_2\varphi_1 \\ k_3\varphi_2 & -k_4 \end{pmatrix}. \tag{23}$$

For the second matrix G we obtain

$$G = \begin{pmatrix} k_1\varphi_1 + k_2\varphi_1\varphi_2 & 0 \\ 0 & k_3\varphi_1\varphi_2 + k_4\varphi_2 \end{pmatrix}. \tag{24}$$

We are now able to state the equations for the fluctuations of the process

$$lkj; \tag{25}$$