The Kramers-Moyal Expansion

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Abstract

Monte-Carlo Markov Chain (MCMC) techniques allow us to sample from a probability distribution which is difficult to evaluate or difficult to sample from directly. Gibbs sampling is a particular MCMC technique which

1 The Kramers-Moyal Expansion

Given many instantiations of a stochastic variable V, we can construct a normalize histogram over all observations as a function of time $P(V,t)$. However, in order to systematically explore the relationship between the parameterization of the process and $P(V,t)$ we require an expression for $\dot{P}(V,t)$. If we make a fundamental assumption that the evolution of $P(V,t)$ follows a Markov process i.e. its evolution has the memoryless property, then we can write

$$P(V',t) = \int T(V',t|V,t-\tau)P(V,t-\tau)dV \tag{1}$$

which is known at the Chapman-Kolmogorov equation. The factor $T(V',t|V,t-\tau)$ is known as the *transition operator* in a Markov process and determines the evolution of $P(V,t)$ in time. We proceed by writing $T(V',t|V,t-\tau)$ in a form referred to as the Kramers-Moyal expansion

$$\begin{aligned} T(V',t|V,t-\tau) &= \int \delta(u-V')T(u,t|V,t-\tau)du \\ &= \int \delta(V+u-V'-V)T(u,t|V,t-\tau)du \end{aligned}$$

If we use the Taylor expansion of the δ-function

$$\delta(V+u-V'-V) = \sum_{n=0}^{\infty} \frac{(u-V)^n}{n!}\left(-\frac{\partial}{\partial V}\right)^n \delta(V-V')$$

Inserting this into the result from above, pulling out terms independent of u and swapping the order of the sum and integration gives

$$T(V', t|V, t-\tau) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{\partial}{\partial V}\right)^n \delta(V - V') \int (u - V)^n T(u, t|V, t-\tau) du \tag{2}$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{\partial}{\partial V}\right)^n \delta(V - V') M_n(V, t) \tag{3}$$

noticing that $M_n(V, t) = \int (u - V)^n T(u, t|V, t-\tau) du$ is just the nth moment of the transition operator T. Plugging (2.6) back in to (2.4) gives

$$P(V, t) = \int \left(1 + \sum_{n=1}^{\infty} \frac{1}{n!} \left(-\frac{\partial}{\partial V}\right)^n M_n(V, t)\right) \delta(V - V') P(V, t-\tau) dV \tag{4}$$

$$= P(V', t-\tau) + \sum_{n=1}^{\infty} \frac{1}{n!} \left(-\frac{\partial}{\partial V}\right)^n [M_n(V, t) P(V, t)] \tag{5}$$

Approximating the derivative as a finite difference and taking the limit $\tau \to 0$ gives

$$\dot{P}(V, t) = \lim_{\tau \to 0} \left(\frac{P(V, t) - P(V, t-\tau)}{\tau}\right) \tag{6}$$

$$= \sum_{n=1}^{\infty} \frac{1}{n!} \left(-\frac{\partial}{\partial V}\right)^n [M_n(V, t) P(V, t)] \tag{7}$$

which is formally known as the Kramers-Moyal (KM) expansion. The Fokker-Planck equation is a special case of (2.10) where we neglect terms $n > 2$ in the *diffusion approximation*.