Stochastic Differential Equations

Continuous Evolving Variables

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Outline

- Review of salient facts about Gaussian distributions (Gardiner p36-37)
  - Multivariate Gaussian: if $\mathbf{x}$ is a vector of n Gaussian r.v.s, then

$$P(\mathbf{x}) = [2\pi \det(\sigma)]^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{x}-\bar{\mathbf{x}})^T \sigma^{-1} (\mathbf{x}-\bar{\mathbf{x}})\right)$$

    where $\bar{\mathbf{x}}$ is the mean and σ is the (symmetric) covariance matrix.
  - Characteristic function

$$\phi(\mathbf{s}) = \langle \exp(i\mathbf{s}^T\mathbf{x}) \rangle = \exp(i\mathbf{s}^T\bar{\mathbf{x}} - \frac{1}{2}\mathbf{s}^T\sigma\mathbf{s})$$

  - General formulae for moments when $\bar{\mathbf{x}} = 0$: odd moments are zero, higher moments satisfy

$$\langle x_i x_j x_k \ldots \rangle = \frac{2N!}{N! 2^N} \{\sigma_{ij}\sigma_{kl}\sigma_{mn}\ldots\}_{\text{sym}}$$

- Definition of a Gaussian process (van Kampen p63-64)
  - "Hierarchy of Distribution Functions" (van Kampen p61+). Consider timepoints $t_1 < t_2 < t_3 \dots t_n$. Define

    $$P_n(x_1, t_1; x_2, t_2; \dots; x_n, t_n) \equiv P(x(t_1) = x_1, x(t_2) = x_2, \dots, x(t_n) = x_n$$
  - If P_n is an n-dimensional Gaussian $\forall n, \{t_1 \dots t_n\}$, then $x(t)$ is a *Gaussian process*
  - The covariance matrix is $\sigma_{ij} = \langle x(t_i)x(t_j)\rangle$
  - Marginals of a multivariate Gaussian are themselves multivariate Gaussians. The full distribution $P(x(t))$ can be thought of as an infinite-dimensional Gaussian, P_∞
  - A Gaussian process is effectively a prior over functions, that can be fully specified by the covariance function
- The *characteristic functional*, $G([k])$, plays a role analogous to the characteristic function for discrete processes. Define an arbitray auxiliary test function, $k(t)$

- Inference, prediction, clustering with GPs (MacKay chapter 45, p535-548; MacKay 1998, "Introduction to Gaussian Processes")
  - Suppose we have N datapoints, $\{\mathbf{x}^{(n)}, t_n\}_{n=1}^{N}$. The input variables $\mathbf{x}^{(n)}$ are I-dimensional vectors. The target variables t_n will be assumed real scalars (corresponding to interpolation or regression problems).
  - Goal: fit some (nonlinear) function $y(\mathbf{x})$. Posterior probability of $y(\mathbf{x})$ is

$$P(y(\mathbf{x})|\mathbf{t}_N, \mathbf{X}_N) = \frac{P(\mathbf{t}_N|y(\mathbf{x}), \mathbf{X}_N)P(y(\mathbf{x}))}{P(\mathbf{t}_N|\mathbf{X}_N)}$$

    (Typically $P(\mathbf{t}_N|y(\mathbf{x}), \mathbf{X}_N)$ is assumed to be separable Gaussian noise.) In parametric approaches, $y(\mathbf{x}) \equiv y(\mathbf{x}; \mathbf{w})$ where $\mathbf{w}$ is a set of parameters over which we place some prior. In nonparametric approaches (e.g. Gaussian

- Kramers-Moyal expansion (treatment follows van Kampen p197-198; see also Gillespie p74+)
  - The most general form of the *master equation* for a continuous-time stochastic process can be written

$$\frac{\partial}{\partial t}p(x,t) = \int W(x-r;r)p(x-r,t)dr - p(x,t)\int W(x;r)dr$$

    where $W(x;r)$ is the rate from x to $x+r$. In the notation we used for discrete state spaces, $W(x;r) \equiv R_{x,x+r}$
  - Assuming that $W(x;r)$ varies smoothly in x and is sharply peaked in r, we can write the term $W(x-r;r)p(x-r,t)$ in the first integral as a Taylor expansion in x:

$$\frac{\partial}{\partial t}p(x,t) = \sum_{n=0}^{\infty}\int \frac{(-r)^n}{n!}\frac{\partial^n}{\partial x^n}\left\{W(x;r)p(x,t)\right\} dr - p(x,t)\int W(x;r$$

    (Note that we're only allowed to expand $W(x;r)$ in x, not in

The Wiener process (undamped Brownian motion, diffusive drift, limit of random walk...)

- Derivation of Fick's equations for one-dimensional diffusion (Berg, "Random Walks in Biology", p18-20)
  - Discrete random walk: $x(n) = \sum_{i=1}^{n} d_i$ where $P(d_i = +\delta) = P(d_i = -\delta) = 1/2$
    - Implies that $\langle x(n) \rangle = 0$ and $\langle x(n)^2 \rangle = n\delta^2$
    - If each step takes time τ then $n = t/\tau$, so $\langle x(n)^2 \rangle = \frac{\delta^2}{\tau} t = 2Dt$ where $D = \delta^2/2\tau$ is the diffusion constant
    - Let $r(x,t) = P(x(t) = x)$. In time τ, a particle at x has probability $1/2$ of drifting to $x+\delta$, and a particle at $x+\delta$ has probability $1/2$ of drifting to x. The net flux of probability mass from x to $x+\delta$ is

$$J(x) = \frac{1}{\tau}\left(\frac{r(x,t)}{2} - \frac{r(x+\delta,t)}{2}\right) = D\frac{1}{\delta}\left(\frac{r(x,t)}{\delta} - \frac{r(x+\delta,t)}{\delta}\right)$$

The Ornstein-Uhlenbeck process: Brownian motion with exponential decay (van Kampen p83-85)

- Originally constructed to describe the *velocity* of a Brownian particle (van Kampen p84)
- Fokker-Planck equation (Gardiner p74-77)

$$\frac{\partial}{\partial t}p(x,t) = \frac{\partial}{\partial x}(kxp(x,t)) + \frac{1}{2}D\frac{\partial^2}{\partial x^2}p(x,t)$$

  Boundary condition is $p(x,0) = \delta(x - x_0)$.
- Characteristic equation for $\phi(s,t) = \langle \exp(\imath sx) \rangle$

$$\frac{\partial}{\partial t}\phi(s,t) + ks\frac{\partial}{\partial s}\phi(s,t) = -\frac{1}{2}Ds^2\phi(s,t) \qquad (2)$$

  Boundary condition is $\phi(s,0) = \exp(\imath sx_0)$.
  (Here we have used $\int \exp(\imath sx)\frac{\partial}{\partial x}(xp)dx =$

- Case study of an Ornstein-Uhlenbeck process in stochastic systems biology: the enzyme futile cycle
    - Samoilov M, Plyasunov S, Arkin AP. Stochastic amplification and signaling in enzymatic futile cycles through noise-induced bistability with oscillations. Proc Natl Acad Sci U S A. 2005 Feb 15;102(7):2310-5.
- Multivariate Ornstein-Uhlenbeck process (Gardiner p109-112)
- Case study of inference using a multivariate OU process: relationship between CD4 and beta-2-microglobulin in AIDS patients
    - Sy JP, Taylor JM, Cumberland WG. A stochastic model for the analysis of bivariate longitudinal AIDS data. Biometrics. 1997 Jun;53(2):542-55.

- Felsenstein, chapter 23 (p391-414)
- Consider tree ($.x_1.$ ($.x_2.$ $.x_4.$ $.x_5.$) ($.x_3.$ $.x_6.$ $.x_7.$)) where x_n are Brownian variables.
- For a (parent,child) pair (p, c) let t_c be distance from p to c and let $d_c = x_c - x_p$. We have $\langle d_c \rangle = 0$ and $\langle d_c^2 \rangle = Dt_c$.
- Covariance matrix
- Pruning algorithm

Summary

- SCFGs