AM216 Stochastic Differential Equations

Lecture 15
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List of topics in this lecture

- Feynman-Kac formula for the forward equation, path integral $u(x, t)$, interpretation of path integral as mass density of the surviving cell population at time t, governing equation of $u(x, t)$
- An application of Feynman-Kac formula: reconstructing potential $V(x)$ from a set of sample paths of particle position; exploring non-equilibrium with an applied force; modeling the effect of applied force as a fatality/growth rate

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Recap

Feynman-Kac formula for the backward equation

We are back to the time-dependent SDE

$$dX = b(X,t)dt + \sqrt{a(X,t)}\,dW$$

$u(x, t, T)$ is defined by the Feynman-Kac path integral formula

$$u(x,t,T) = E\left(\exp\left(-\int_t^T \psi(X(s),s)ds \right) f(X(T)) \,\middle|\, X(t) = x \right)$$

Meaning of $u(x, t, T)$

$\psi(x, s)$ = fatality/growth rate of a cell at time s with $X(s) = x$.

$f(x)$ = reward for a cell surviving to time T with $X(T) = x$.

$u(x, t, T)$ = expected reward at final time T per unit population at time t

Each cell of the population gets its own reward. The growth increases the population size and increases the reward for the population.

Governing equation for $u(x, t, T)$ and the FVP

$$\begin{cases} 0 = u_t + b(x,t)u_x + \dfrac{1}{2}a(x,t)u_{xx} - \psi(x,t)u \\ u(x,t,T)\big|_{t=T} = f_0(x) \end{cases}$$

The solution of the FVP is given by the Feynman-Kac path integral formula.

Feynman-Kac formula for the forward equation (continued)

$$u(x,t)=E\left(\delta\left(X(t)-x\right)\exp\left(-\int_0^t\psi(X(s),s)ds\right)\right)$$

Items of the discussion:

1) We need to explain the δ function in the average.
2) We need to derive the governing equation for $u(x, t)$.
3) We need to explain the meaning of $u(x, t)$ and discuss the distribution of $X(0)$.

Item #1: Explaining the δ function in the average

View 1: $$u(x,t)=\lim_{\Delta x\to 0}\frac{1}{\Delta x}E\left(I_{[x,x+\Delta x]}(X(t))\exp\left(-\int_0^t\psi(X(s),s)ds\right)\right)$$

View 2: $$\int h(x)u(x,t)dx=E\left(h(X(t))\exp\left(-\int_0^t\psi(X(s),s)ds\right)\right)\qquad\text{for any } h(x)$$

(We use this view to derive the equation for $u(x, t)$).

Item #2: Derivation of the governing equation for $u(x, t)$

We start with View #2 at $(t+\Delta t)$. We apply the forward view on $[0 \to t+\Delta t]$.

$[0 \to t+\Delta t]$ is divided into $[0 \to t]$ and $[t \to t+\Delta t]$.

$$\underbrace{\int h(x)u(x,t+dt)dx}_{\text{LHS}}=\underbrace{E\left(h(X(t)+dX)\exp\left(-\int_0^{t+dt}\psi(X(s),s)ds\right)\right)}_{\text{RHS}}$$

$$=E\left(h(X(t)+dX)\exp\left(-\int_t^{t+dt}\psi(X(s),s)ds\right)\times\exp\left(-\int_0^t\psi(X(s),s)ds\right)\right)$$

In the RHS, we expand $h(X(t)+dX)$ and $\exp\left(-\int_t^{t+dt}\psi(X(s),s)ds\right)$

$$\text{RHS}=E\left(\left[h(X(t))+h'(X(t))dX+\frac{1}{2}h''(X(t))(dX)^2\right]\left(1-\psi(X(t),t)dt\right)\times\exp\left(-\int_0^t\psi\left(X(s),s\right)ds\right)\right)$$

$$=E\left(\left[h(X(t))+h'(X(t))dX+\frac{1}{2}h''(X(t))(dX)^2-h(X(t))\psi(X(t),t)dt\right]\times\underbrace{\exp\left(-\int_0^t\psi\left(X(s),s\right)ds\right)}_{\text{independent of } dX}\right)$$

In the RHS, the average is over $\{X(s), 0 \le s \le t+\Delta t\}$. We use the law of total expectation to rewrite is as averaging over $(dX(t) \mid X(t))$ and then over $\{X(s), 0 \le s \le t\}$.

$$E_{\{X(s),0\le s\le t+dt\}}(Q) = E_{\{X(s),0\le s\le t\}}\Big(E_{dX(t)}(Q\big|X(t))\Big)$$

We use the moments of $(dX(t) \mid X(t))$:

$$E_{dX(t)}(\,h'(X(t))dX\big|X(t)) = h'(X(t))b(X(t),t)dt$$

$$E_{dX(t)}(\,h''(X(t))(dX)^2\big|X(t)) = h''(X(t))a(X(t),t)dt$$

$$\text{RHS} = E\Bigg(\bigg[h(X(t)) + h'(X(t))b(X(t),t)dt + \frac{1}{2}h''(X(t))a(X(t),t)dt - h(X(t))\psi(X(t),t)dt\bigg] \times\exp\Big(-\int_0^t \psi(X(s),s)ds\Big)\Bigg)$$

View #2 (method of test function) of $u(x, t)$ gives

$$E\Big(g(X(t))\exp\Big(-\int_0^t \psi(X(s),s)ds\Big)\Big) = \int g(x)u(x,t)dx \qquad \text{for any } g(x).$$

In the RHS, we set respectively $g(x) = h(x)$ for term 1, $g(x) = h'(x)b(x, t)$ for term 2, …,

$$\text{RHS} = \int\Big(h(x) + h'(x)b(x,t)dt + \frac{1}{2}h''(x)a(x,t)dt - h(x)\psi(x,t)dt\Big)u(x,t)dx$$

In the RHS, we integrate by parts; in the LHS, we expand $u(x, t+dt)$.

$$\text{RHS} = \int h(x)\Big(u(x,t) - \big(b(x,t)u\big)_x dt + \frac{1}{2}\big(a(x,t)u\big)_{xx} dt - \psi(x,t)u\,dt\Big)dx$$

$$\text{LHS} = \int h(x)u(x,t+dt)dx = \int h(x)\big(u(x,t) + u_t dt\big)dx$$

Subtracting $\int h(x)\, u(x, t)dx$, dividing by dt, and taking the limit as $dt \to 0$, we obtain

$$\underbrace{\int h(x)u_t\,dx}_{\text{LHS}} = \underbrace{\int h(x)\Big(-\big(b(x,t)u\big)_x + \frac{1}{2}\big(a(x,t)u\big)_{xx} - \psi(x,t)u\Big)dx}_{\text{RHS}}$$

Since LHS = RHS for arbitrary test function $h(x)$, we arrive at

$$u_t = -\big(b(x,t)u\big)_x + \frac{1}{2}\big(a(x,t)u\big)_{xx} - \psi(x,t)u$$

This is the governing PDE for $u(x, t)$.

It is the forward equation with a fatality/growth term.

Item #3: Meaning of $u(x, t)$

View #1 of $u(x, t)$ gives

$$u(x,t)=\lim_{\Delta x\to 0}\frac{1}{\Delta x}E_{\omega}\left(I_{[x,x+\Delta x]}(X(t,\omega))\exp\left(-\int_0^t \psi(X(s,\omega),s)ds\right)\right)$$

The average is based on an ensemble $\{X(s, \omega), \omega \in \Omega\}$. It is worthwhile to emphasize that the evolution of $X(s)$ is governed solely by the SDE

$$dX=b(X,t)dt+\sqrt{a(X,t)}\,dW, \qquad \text{independent of } \psi(x, s)$$

In particular, $X(s)$ does not die or split. In $u(x, t)$, the fatality/growth effect of $\psi(x, s)$ is reflected in the factor $\exp\left(-\int_0^t \psi(X_j(s),s)ds\right)$.

To interpret $u(x, t)$, we consider the "cell" population associated with $X(s)$. The cell population includes the fatality/growth effect of $\psi(x, s)$, in the form of termination/addition of cells.

For a cell at time s with $X(s) = z$, the outcome of the cell in $[s, s+\Delta s]$ is

(Outcome in $[s, s+\Delta s]$ | having survived to s with $X(s) = z$)

$$=\begin{cases} \text{fatality with prob } =\psi(z,s)\Delta s & \text{if } \psi(z,s)>0 \\ \text{split into two with prob } =\big(-\psi(z,s)\big)\Delta s & \text{if } \psi(z,s)<0 \end{cases}$$

We write $u(x, t)$ in terms of the cell population and associated $X(s)$.

$$u(x,t)=\lim_{\Delta x\to 0}\frac{1}{\Delta x}E_{\omega}\big(\text{\# of cells surviving to time } t \text{ with } X(t,\omega)\in[x,x+dx]\big)$$

= mass density in x of the surviving cell population at time t.

The size of surviving population is different from the size of starting population.

Initial condition for $u(x, t)$

$u(x, 0) = f_0(x)$ = mass density in x of the starting cell population.

Remarks on the Feynman-Kac formula for the forward equation

- The evolution of $X(s)$ is governed solely by the SDE, independent of $\psi(x, s)$. $X(s)$ does not die or split.
- In the Feynman-Kac formula, the average is over an ensemble of $X(s)$. The fatality/growth effect of $\psi(x, s)$ is reflected in the factor $\exp\left(-\int_0^t \psi(X_j(s),s)ds\right)$.

  The Feynman-Kac formula is good for calculating $u(x, t)$ from an ensemble of $X(s)$.
- Given a LARGE set of sample paths of $\{X_j(s), j = 1, 2, \ldots, N\}$, we have

$$u(x,t)\approx\frac{1}{N\cdot\Delta x}\sum_{X_j(t)\in[x,x+\Delta x]}\exp\left(-\int_0^t\psi(X_j(s),s)ds\right)$$

The calculation does not directly involve the cell population.

- To interpret $u(x, t)$ defined in the Feynman-Kac formula, we follow the surviving cell population associated with $X(s)$, which includes the effect of fatality/growth.
- Although we interpret $\psi(x, s)$ as the fatality/growth rate, the Feynman-Kac formula is well defined for any $\psi(x, s)$, not associated with any physical fatality/growth.
- When $\psi(x, s)$ is not associated with any physical fatality/growth, the cell population exists only in our mathematical imagination (see the application below).

An application of Feynman-Kac formula

The big picture: When $b(x, t)$ in the SDE is unknown but a LARGE set of sample paths is available, we can use the Feynman-Kac formula to calculate the unknown $b(x, t)$.

Consider a particle diffusing in a potential well.

$X(t)$: position of particle at time t

$V(x)$: static potential well

The stochastic motion is governed by the over-damped Langevin equation.

$$dX=-\frac{D}{k_B T}V'(X)dt+\sqrt{2D}\,dW$$

After non-dimensionalization, we have

$$dX=-V'(X)dt+\sqrt{2}\,dW$$

What we can measure (data)

A large set of sample paths $\{X_j(t), j = 1, 2, ..., N\}$

Goal:

To reconstruct potential $V(x)$ from the data

Method:

We use Feymann-Kac formula to reconstruct potential $V(x)$.

Items of the discussion

A. Forward equation and equilibrium of probability density

B. Estimating potential from equilibrium measurements

C. A practical issue with equilibrium data

D. Exploring non-equilibrium with an applied force

E. Steps in constructing potential $V(x)$

Item A:

Forward equation (Fokker-Planck equation) of $dX = -V'(X)dt + \sqrt{2}\,dW$

Let $\rho(x, t)$ = probability density of X at time t.

Note: probability density = mass density of a population of one path.

The time evolution of $\rho(x, t)$ is governed by the forward equation

$$\rho_t = -\big(b(x)\rho\big)_x + \frac{1}{2}\big(a(x)\rho\big)_{xx}\,, \qquad a(x) = 2, \quad b(x) = -V'(x)$$

$$\Longrightarrow \quad \rho_t = \big(V'(x)\rho\big)_x + \rho_{xx}$$

We write the forward equation in conservation form

$$\rho_t = -\frac{\partial}{\partial x}J(x,t)\,, \qquad J(x,t) \equiv -\big(V'(x)\rho + \rho_x\big)$$

where $J(x, t)$ is the probability flux.

Equilibrium distribution

At equilibrium, the probability flux must be identically zero.

$$J(x) = 0, \qquad \text{for all } x$$

$$\Longrightarrow \quad V'(x)\rho + \rho_x = 0$$

$$\Longrightarrow \quad \big(\exp(V(x))\rho(x)\big)' = 0$$

$$\Longrightarrow \quad \exp(V(x))\rho(x) = \text{const}$$

$$\Longrightarrow \quad \rho^{(\text{eq})}(x) \propto \exp(-V(x))$$

As expected, the equilibrium is the Maxwell-Boltzmann distribution.

Caution: A steady state is different from equilibrium.

When $J(x)$ = const ≠ 0 for all x, we still have $\rho = \rho(x)$, independent of t.

It is called a steady state, which is different from equilibrium.

At equilibrium, we must have $J(x) = 0$ for all x.

In the terminology of deterministic dynamical systems, “steady state” and “equilibrium” are usually not distinguished.

Item B:

Estimating potential from equilibrium measurements

Suppose the system is at equilibrium and we measure a large set of sample paths $\{X_j(t),\ j = 1, 2, \ldots, N\}$.

The equilibrium density $\rho^{(eq)}(x)$ can be calculated as

$$\rho^{(eq)}(x) \approx \frac{1}{N \cdot \Delta x} \sum_{X_j(t_k) \in [x, x+\Delta x]} 1 \qquad \text{at a particular time level } t_k$$

where N is the number of sample paths.

To fully utilize the data set, we average $\rho^{(eq)}(x)$ over all t_k's

$$\rho^{(eq)}(x) \approx \frac{1}{K_T} \sum_{k=1}^{K_T} \left[\rho^{(eq)}(x) \text{ estimated at } t_k \right]$$

where K_T is the number of time levels.

Recall that $\rho^{(eq)}(x) \propto \exp(-V(x))$. We write potential $V(x)$ as

$$V(x) = -\log \rho^{(eq)}(x) + \underbrace{C}_{\text{additive constant}}$$

Item C:

A practical issue with equilibrium data

Unfortunately, the approach of using only equilibrium measurements does not work well. It requires an impractically large amount of data.

At equilibrium, a region of high $V(x)$ value is visited only very infrequently.

$$\rho^{(eq)}(x) \propto \exp(-V(x))$$

Consider a set of discrete sites (intervals of x). For a site with probability 10^{-8}, we need to sample 10^9 times to get 10 visits to that particular site. It is practically impossible to accurately estimate $\rho^{(eq)}(x)$ in a region of high $V(x)$ value.

Remedy: We need to perturb the system to non-equilibrium.

Item D:

Exploring non-equilibrium with an applied force

Let $F(t)$ be the applied force (non-dimensionalized).

In experiments, $F(t)$ is controlled. In AFM (Atomic Force Microscopy) experiments, the force is controlled by moving an actuator to stretch an elastic link.

$$F^{(AFM)}(t) = k\int_0^t u(s)ds$$

where k = spring constant; $u(s)$ velocity of actuator at time s.

Stochastic differential equation in the presence of an applied force

The applied force tilts the static potential. At time t, the tilted potential is

$$H(x,t) = V(x) - \underbrace{F(t)\cdot x}_{\substack{\text{Effect of}\\ \text{applied force}}}$$

Replacing $V'(x)$ with $H_x(x, t)$, we get the new SDE.

$$dX = -H_x(X,t)dt + \sqrt{2}\,dW$$

In the presence of an applied force, potential $H(x, t)$ changes with time. As a result, the system is not at equilibrium and the Boltzmann distribution does not apply.

Nevertheless we consider a "hypothetical" density, $\rho^{(F)}(x, t)$, defined as

$$\rho^{(F)}(x,t) \equiv \frac{1}{Z}\exp\left(-H(x,t)\right) = \frac{1}{Z}\exp\left(-V(x) + F(t)\cdot x\right)$$

$$\text{where} \quad Z = \int \exp\left(-V(x)\right)dx$$

Remark:

- We call $\rho^{(F)}(x, t)$ "hypothetical" density because it is not the mass density of any physical population. In particular, $\rho^{(F)}(x, t)$ is NOT the probability density of particle position. In the discussion below, we interpret $\rho^{(F)}(x, t)$ as the mass density of a "hypothetical" cell population, whose existence/fatality/growth is only in our mathematical imagination.

Advantage of working with $H(x, t)$ and $\rho^{(F)}(x, t)$

With a properly designed force schedule $F(t)$, a region of relatively high $V(x)$ value becomes a region of relatively low $H(x, t)$ value in the tilted potential.

In this way, different regions of $V(x)$ can be very well explored/sampled at different time t with a time-dependent force schedule $F(t)$.

Item E:

Steps in constructing potential $V(x)$

1. Find the governing PDE for $\rho^{(F)}(x, t)$
2. Identify the "fatality/growth" term $\psi(x, s)$ in the PDE
3. Express $\rho^{(F)}(x, t)$ in the Feynman-Kac formula

4. Use the Feynman-Kac formula to calculate $\rho^{(F)}(x, t)$ from a set of sample paths.
5. Determine potential $V(x)$ from $\rho^{(F)}(x, t)$.

Step 1: Find the governing PDE for $\rho^{(F)}(x, t)$

Let $\rho(x, t)$ be the density of particle position in the presence of applied force $F(t)$.

$\rho(x, t)$ is NOT the same as $\rho^{(F)}(x, t)$.

$$\rho(x, t) \neq \rho^{(F)}(x, t)$$

Stochastic motion of particle is governed by

$$dX = -H_x(X,t)dt + \sqrt{2}\,dW\,, \qquad H(x,t) \equiv V(x) - F(t)\cdot x$$

The forward equation (Fokker-Planck equation) for $\rho(x, t)$ is

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}\left(H_x(x,t)\rho + \frac{\partial}{\partial x}\rho \right)$$

We write the Fokker-Planck equation in terms of a differential operator.

$$\rho_t = L_{\{H\}}[\rho] \qquad \text{(FP\_forced)}$$

$$\text{where} \qquad L_{\{H\}}[\bullet] = \frac{\partial}{\partial x}\left(H_x(x,t)\bullet + \frac{\partial}{\partial x}\bullet \right)$$

We find the governing equation for the “hypothetical” density $\rho^{(F)}(x, t)$.

$$\rho^{(F)}(x,t) \equiv \frac{1}{Z}\exp\big(-H(x,t)\big) = \frac{1}{Z}\exp\big(-V(x) + F(t)\cdot x\big), \qquad Z = \int \exp\big(-V(x)\big)dx$$

Substitute $\rho^{(F)}(x, t)$ into operator $L_{\{H\}}[\,\cdot\,]$ and into operator $\partial/\partial t$

$$L_{\{H\}}\left[\rho^{(F)}(x,t)\right] = \frac{\partial}{\partial x}\left(H_x(x,t)\rho^{(F)}(x,t) + \frac{\partial}{\partial x}\rho^{(F)}(x,t) \right) = 0$$

$$\rho_t^{(F)}(x,t) = F'(t)x\cdot\rho^{(F)}(x,t)$$

It follows that $\rho^{(F)}(x, t)$ satisfies

$$\rho_t^{(F)} = L_{\{H\}}\left[\rho^{(F)}\right] + \underbrace{F'(t)x\cdot\rho^{(F)}}_{\text{fatality/growth}}$$

Step 2: Identify the “fatality/growth” term $\psi(x, s)$ in the PDE

$\rho^{(F)}(x, t)$ satisfies the forward equation with a fatality/growth term

$$\rho_t^{(F)} = L_{\{H\}}\left[\rho^{(F)}\right] - \psi(x,t)\cdot\rho^{(F)}\,, \qquad \psi(x,t) = -F'(t)x$$

Step 3: Express $\rho^{(F)}(x, t)$ using the Feynman-Kac formula

$$\rho^{(F)}(x,t)=E\left(\delta(X(t)-x)\exp\left(-\int_0^t \psi(X(s),s)ds\right)\right),\quad \psi(x,s)=-F'(s)x$$

$$\Longrightarrow\quad \rho^{(F)}(x,t)=E\left(\delta(X(t)-x)\exp\left(\int_0^t F'(s)X(s)ds\right)\right)$$

Remark: The ensemble of $X(s)$ is good for calculating $\rho^{(F)}(x, t)$. For that calculation, we don't need the hypothetical cell population that includes the stochastic addition/termination of cells.

Step 4: Calculate $\rho^{(F)}(x, t)$ from a set of sample paths.

Suppose we apply force $F(t)$ and measure a set of sample paths $\{X_j(s), j = 1, 2, \ldots, N\}$.

At each time level t_k, $\rho^{(F)}(x, t_k)$ can be calculated using the Feynman-Kac formula.

$$\rho^{(F)}(x,t_k)\approx\frac{1}{N\cdot\Delta x}\sum_{X_j(t_k)\in[x,\le x+\Delta x]}\exp\left(\int_0^{t_k}F'(s)X_j(s)ds\right)\qquad \text{at each time level } t_k$$

where N is the number of sample paths.

Step 5: Determine potential $V(x)$ from $\rho^{(F)}(x, t)$

Note that $\rho^{(F)}(x, t)$ and $\rho^{(eq)}(x)$ are related by

$$\rho^{(eq)}(x)=\frac{1}{Z}\exp\left(-V(x)\right)$$

$$\rho^{(F)}(x,t)=\frac{1}{Z}\exp\left(-V(x)+F(t)x\right)$$

$$\Longrightarrow\quad \rho^{(eq)}(x)=\rho^{(F)}(x,t)\exp\left(-F(t)x\right)$$

Once $\rho^{(F)}(x, t_k)$ is obtained at a time level t_k, we use it to calculate a sample version of equilibrium density $\rho^{(eq)}(x)$.

$$\rho^{(\mathrm{eq})}(x)=\rho^{(F)}(x,t_k)\exp\left(-F(t_k)x\right)\qquad \text{at each time level } t_k$$

Then we average the sample versions of $\rho^{(eq)}(x)$ over all t_k's.

$$\rho^{(\mathrm{eq})}(x)\approx\frac{1}{K_T}\sum_{k=1}^{K_T}\rho^{(F)}(x,t_k)\exp\left(-F(t_k)x\right)$$

where K_T is the number of time levels.

Once $\rho^{(eq)}(x)$ is accurately estimated, we write potential $V(x)$ as

$$V(x)=-\log\rho^{(\mathrm{eq})}(x)+\underbrace{C}_{\text{additive constant}}$$

<u>Remarks</u> on constructing potential $V(x)$

1. The "hypothetical" density $\rho^{(F)}(x, t)$ contains potential $V(x)$ and applied force $F(t)$, which allows us to extract potential $V(x)$ from $\rho^{(F)}(x, t)$ once $\rho^{(F)}(x, t)$ is obtained.
2. $\rho^{(F)}(x, t)$ satisfied the forward equation with a fatality/growth term $\psi(x, t) = -F'(t)x$. This hypothetical fatality/growth term exists only in our mathematical imagination. It does not correspond to the fatality/growth of any physical process.
3. The path integral expression (Feynman-Kac formula) of $\rho^{(F)}(x, t)$ allows us to calculate $\rho^{(F)}(x, t)$ from sample paths $\{X_j(s), j = 1, 2, \ldots, N\}$ and applied force $F(t)$.
4. Once $\rho^{(F)}(x, t)$ is obtained, we extract potential $V(x)$ from $\rho^{(F)}(x, t)$.