AM216 Stochastic Differential Equations

Lecture 15

List of topics in this lecture

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

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Review

Feynman-Kac formula

Stochastic differential equation (SDE)

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

$u(x, t, T)$ is defined using path integral

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

Paths, $X(s)$, are from the SDE, independent of function $\psi(x, s)$.

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

= reward at final time T per population at time t,

averaged over all paths starting at $X(t) = x$

(including the effects of fatality/growth in $[t, T]$)

Governing equation for $u(x, t, T)$

$$0 = u_t + b(x,t)u_x + \frac{1}{2}a(x,t)u_{xx} - \psi(x,t)u$$

This is the backward equation with a fatality/growth term

The end/final condition

$u(x, t, T)|_{t=T} = f(x)$

Key step in deriving the equation

Law of total probability

$$E_{\{X(s),t\le s\le T\}}\left(*\,\middle|\,X(t)=x\right)=E_{dX}\left(E_{\{X(s),t+\Delta t\le s\le T\}}\left(*\,\middle|\,X(t+dt)=x+dX\right)\right)$$

Remarks:

- If we know the PDE, we can solve the PDE for solution $u(x, t, T)$.
- If we don't know the PDE but we are given a set of sample paths, we can calculate $u(x, t, T)$ using Feynman-Kac formula, and use it to learn about the PDE.

End of review

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:

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

Definition 2: $\int h(x)u(x,t)dx=E\left(h(X(t))\exp\left(-\int_0^t \psi(X(s),s)ds\right)\right)$

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

We use the forward view for $u(x, t)$:

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

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

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

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

Taylor expansion of $h(X(t)+dX)$ and $\exp\left(-\int_t^{t+dt}\psi(X(s),s)ds\right)$

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

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

Using the law of total expectation to write the average over $\{X(s),\ 0 \le s \le t+dt\}$ as

$$= E_{\{X(s),0<s<t+dt\}}(\,*\,) = E_{\{X(s),0<s<t\}}\left(E_{dX(t)}\left(*\,\middle|\,X(t)\right)\right)$$

Using the moments of dX, $E_{dX(t)}\left(h'(X(t))dX\,\middle|\,X(t)\right)=h'(X(t))b(X(t),t)dt$, …

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

Note that definition #2 (method of test function) of $u(x, t)$ gives

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

Setting $g(x) = h'(x)b(x, t)$, $g(x) = h''(x)a(x, t)$, …, we write the RHS above as

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

Taylor expanding the LSH and integrating by parts the RHS yields

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

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

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

$$\text{LHS} = \int h(x) u_t \, dx$$

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

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 $u(x, t)$

Consider an ensemble of paths $\{X(s)\}$.

Based on definition #1 of $u(x, t)$,

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

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

= ensemble density at time t of paths surviving to reach time t.

= ensemble density at time t of the surviving ensemble.

Initial condition for $u(x, t)$

$u(x, 0) = f_0(x)$ = ensemble density of the starting ensemble.

$u(x, t)$ = ensemble density at time t of the surviving ensemble.

Remarks:

- Although we interpret $\psi(x, s)$ as the fatality rate, the Feynman-Kac formula is well defined for any function $\psi(x, s)$, not associated with any physical fatality.
- The Feynman-Kac formula provides a way of calculating $u(x, t)$ from a set of sample paths of the SDE. The SDE is not affected by the fatality function.

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

- Given a set of sample paths $\{X^{(j)}(t), \text{j} = 1, 2, \ldots, N\}$ of the SDE, we can calculate $u(x, t)$ as follows

$$u(x,t)=\frac{1}{N\cdot\Delta x}\sum_{x\le X^{(j)}(t)<x+\Delta x}\exp\left(-\int_0^t \psi(X^{(j)}(s),s)ds\right)$$

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

An application of Feynman-Kac formula

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:

a (large) set of sample paths $\{X^{(j)}(t), j = 1, 2, \ldots, N\}$

Goal:

to determine the potential $V(x)$ in the SDE

Method:

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

The forward equation (the Fokker-Planck equation)

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

The time evolution of density $\rho(x, t)$ 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

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

Equilibrium distribution

At equilibrium, the probability flux must be identically zero.

$J(x) \equiv 0$, for all all x

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

==> $\left(\exp(V(x))\rho(x)\right)' = 0$

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

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

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

Caution:

When $J(x, t) \equiv \text{const} \neq 0$, we still have $\rho_t = 0$.

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

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

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

Estimating potential from equilibrium measurements

Suppose we measure a set of sample paths $\{X^{(j)}(t)$, j = 1, 2, …, $N\}$ when the system is at equilibrium.

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

$$\rho^{(\text{eq})}(x) \approx \frac{1}{N \cdot \Delta x} \sum_{x \le X^{(j)}(t_k) < x+\Delta x} 1 \qquad \text{at a particular time level } t_k$$

where N is the number of sample paths.

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

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

where K_T is the number of time levels.

At equilibrium $\rho^{(\text{eq})}(x) \propto \exp(-V(x))$. We write the potential $V(x)$ as

$$V(x) = -\log \rho^{(\text{eq})}(x) + \underbrace{C}_{\substack{\text{additive constant} \\ \text{won't matter}}}$$

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 with high $V(x)$ value is visited only very infrequently.

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

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 $\rho^{(\text{eq})}(x)$ in a region with high $V(x)$ vale.

Remedy:

We need to perturb the system to non-equilibrium.

Non-equilibrium with an applied force

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

$$F(t) = \frac{L}{k_B T} F_{\text{phy}}(t)$$

In experiments, $F(t)$ is controlled.

For example, in AFM (Atomic Force Microscopy) experiments, the force is controlled by moving an actuator to stretch an elastic link.

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

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 the applied force $F(t)$, the 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 that has the same form as the Boltzmann distribution, with $V(x)$ replaced by $H(x, t)$ while the normalizing constant Z is kept unchanged. Consider $\rho^{(F)}(x, t)$ defined as

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

Remark:

We call $\rho^{(F)}(x, t)$ "hypothetical" density because it is not the density of some physical population. In particular, $\rho^{(F)}(x, t)$ is NOT the density of particle position in potential well $V(x)$, under applied force $F(t)$. In the procedure below for constructing potential $V(x)$, we interpret $\rho^{(F)}(x, t)$ as the density of a "hypothetical" population, whose 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 value in the static potential $V(x)$ can have a relatively low value in the tilted potential $H(x, t)$.

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

Goal: construct potential $V(x)$

Steps of working with $H(x, t)$ and $\rho^{(F)}(x, t)$ toward that goal:

1. Find the governing PDE for $\rho^{(F)}(x, t)$
2. Identify the "fatality" 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

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

The corresponding 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.

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

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

Now consider the "hypothetical" density $\rho^{(F)}(x, t)$.

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

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

$$\rho_t^{(F)} = L_{\{H\}}\left[\rho^{(F)}\right] + \underbrace{F'(t)x\cdot\rho^{(F)}}_{\substack{\text{We view this}\\ \text{as the fatality term}}}$$

<u>Step 2:</u> Identify the "fatality" term $\psi(x, s)$ in the PDE

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

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

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

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

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

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

Suppose we measure a set of sample paths $\{X^{(j)}(t)$, j = 1, 2, …, $N\}$ <u>when the system is driven by the applied force schedule $F(t)$.</u>

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

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

where N is the number of sample paths.

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

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

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

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

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

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 $\rho^{(eq)}(x)$.

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

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

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

where K_T is the number of time levels.

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

$$V(x)=-\log\rho^{(eq)}(x)+\underbrace{C}_{\substack{\text{additive constant}\\ \text{won't matter}}}$$

<u>Summary:</u>

- The stochastic evolution of $X(t)$ is independent of the fatality/growth rate $\psi(x, t)$.
- Mathematically, the surviving ensemble is obtained by evolving the starting ensemble according to the SDE and at each time step removing a path or adding a new path according to fatality/growth rate.

- We can use any function $\psi(x, t)$ in the Feynman-Kac formula. The resulting path integral is governed by the forward equation with the corresponding fatality/growth rate.
- The "hypothetical" density $\rho^{(F)}(x, t)$ satisfied the forward equation with fatality/growth rate $\psi(x, t) = -F'(t)x$ where $F(t)$ is the applied force schedule. This is a hypothetical fatality/growth rate that exists only in the mathematical imagination. It does not correspond to any physical fatality/growth.
- $\rho^{(F)}(x, t)$ is the ensemble density of the surviving ensemble determined according to the hypothetical fatality/growth rate $\psi(x, t) = -F'(t)x$.
- The path integral expression (Feynman-Kac formula) of $\rho^{(F)}(x, t)$ allows us to calculate $\rho^{(F)}(x, t)$ from measured data.
- The analytical expression of $\rho^{(F)}(x, t)$ in terms of potential $V(x)$ allows us to construct potential $V(x)$ once we obtain $\rho^{(F)}(x, t)$.