Time reversible stochastic processes and the relevant Feynman-Kac formula

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LisMath Seminar,
24th of April 2015

Content

Continuous Stochastic Process

Definition

A *probability space* is a triple $(\Omega, \mathcal{A}, P)$ such that Ω is a given set, $\mathcal{A}$ is a σ-algebra and P a probability measure.

- $W^n = C([0,\infty); \mathbb{R}^n)$.
- $\mathcal{B}(W^n) = \sigma\{B \in W^n,\ B \textit{ cylinder set}\}$.

Definition

X is a *n-dimensional continuous process* on $(\Omega, \mathcal{A}, P)$ if is a W^n-valued random variable, i.e. $X : \Omega \to W^n$ is $\mathcal{A}/\mathcal{B}(W^n)$-measurable.

Definition

$X = (X_t)_{t\geq 0}$ is *measurable* if the mapping $X : [0,\infty) \times \Omega \to \mathbb{R}^n$ is $\mathcal{B}([0,\infty)) \times \mathcal{A}/\mathcal{B}(\mathbb{R}^n)$-measurable.

Filtration

Let $(\Omega, \mathcal{A}, P)$ be a probability space.

Definition

A *Filtration* $(\mathcal{A}_t)_{t\geq 0}$ is an increasing family of sub σ-fields of $\mathcal{A}$,

$$\mathcal{A}_t \subset \mathcal{A}_s \quad 0 \leq t \leq s$$

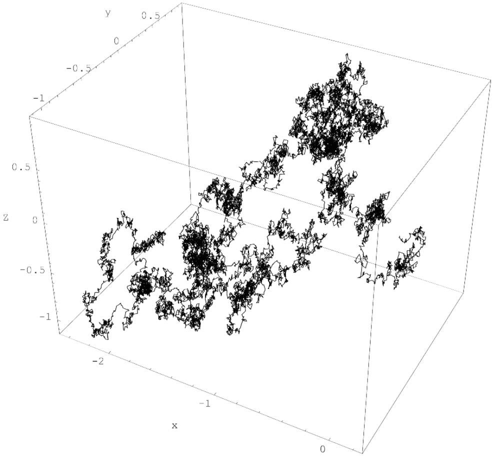
Definition

$X = (X_t)_{t\geq 0}$ is *adapted* to $(\mathcal{A}_t)_{t\geq 0}$ if X_t is $\mathcal{A}_t$-measurable for every t.

Next,

- $(\mathcal{P}_t)_{t\geq 0} := (\mathcal{A}_t)_{t\geq 0}$ will denote the increasing *Past filtration*.
- $(\mathcal{F}_t)_{t\geq 0}$ will denote the decreasing *Future filtration*.

Brownian Motion

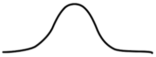


A single realization of a 3d Wiener process.
Wikipedia.

- 19th cent. Brown,
- 1906 Einstein,
- 1923 Wiener and 1940 Kolmogorov,
- 1948 Levy,
- 1950 Itô.

Brownian Motion

$$p(t,x) = \frac{1}{(2\pi t)^{n/2}} e^{\frac{|x|^2}{2t}}, \qquad t > 0,\ x \in \mathbb{R}^n$$



Definition

A n-dimensional process $(W_t)_{t\geq 0}$ such that for every $0 < t_1 < \ldots < t_m$ and $E_i \in \mathcal{B}(\mathbb{R}^n), i = 1, \ldots, m$

$$P\{W_{t_1} \in E_1, \ldots, W_{t_m} \in E_m\} = \int_{\mathbb{R}^n} \mu(dx) \int_{E_1} p(t_1, x_1 - x) dx_1$$
$$\int_{E_2} p(t_2 - t_1, x_2 - x_1) dx_2 \cdots \int_{E_m} p(t_m - t_{m-1}, x_m - x_{m-1}) dx_m$$

with μ a probability measure on $(\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n))$, is called a *n-dimensional Brownian motion with the initial distribution* μ

Remark

If $P\{W_0 = 0\} = 1$, $(W_t)_{t\geq 0}$ is a *"standard" Brownian motion*.

Properties of Brownian Motion

$(W_t)_{t\geq 0}$ is a $(\mathcal{P}_t)_{t\geq 0}$-*standard Brownian motion*.

- $W_t - W_s \sim N(0, t-s)$ for $t > s \geq 0$.
- $W_t - W_s \perp\!\!\!\perp \mathcal{P}_s$.
- Trajectories of Brownian motion are *not differentiable* a.e. with probability one.
- $(W_t)_{t\geq 0}$ is a *Markov process* i.e. for any bounded measurable f

$$E[f(W_t)|\mathcal{P}_s] = E[f(W_t)|W_s], \quad s \leq t$$

Definition

$(X_t)_{t\geq 0}$ is a *Bernstein process* if for any bounded measurable f and for all $u \leq t \leq v$

$$E[f(X_t)|\mathcal{P}_u \cup \mathcal{F}_v] = E[f(X_t)|X_u, X_v].$$

Probability $\leftrightsquigarrow$ PDE

$$u(x,t) := \int_{\mathbb{R}^n} \varphi(y) p(t, x-y) dy = E[\varphi(W_0) | W_t = x]$$

solves the heat equation

$$\frac{\partial}{\partial t} u(x,t) = \frac{1}{2} \Delta u(x,t) \text{ with } u(x,0) = \varphi(x).$$

Theorem (Feynman-Kac formula)

$$u(t,x) := E\left[\varphi(W_T) \exp\left\{ - \int_t^T V(W_s) ds \right\} | W_t = x\right]$$

solves the (backward) heat equation

$$-\frac{\partial}{\partial t} u(x,t) = \frac{1}{2} \Delta u(x,t) + V(x) u(x,t) \text{ with } u(x,T) = \varphi(x)$$

with V continuous and lower bounded.

Our framework

Ambient space, $L^2(\mathbb{R}^3)$. On $\mathbb{R}^3 \times [0, T]$ for $T > 0$ consider

$$-\hbar \frac{\partial}{\partial t} \hat{\eta}(x,t) = -\frac{\hbar^2}{2} \Delta \hat{\eta}(x,t) + V(x)\hat{\eta}(x,t),$$
$$\hat{\eta}(x,0) = \hat{\chi}(x)$$

and

$$\hbar \frac{\partial}{\partial t} \eta(x,t) = -\frac{\hbar^2}{2} \Delta \eta(x,t) + V(x)\eta(x,t),$$
$$\eta(x,T) = \chi(x) \qquad \leftarrow \text{final condition!}$$

- $V : \mathbb{R}^3 \to \mathbb{R}$ such that $H := -\frac{\hbar^2}{2}\Delta + V$ is a lower bounded self-adjoint operator on $L^2(\mathbb{R}^3)$.
- $\hat{\chi}, \chi \in \mathcal{D}(e^{TH})$ positive and bounded. $\exists$ (strong) solutions in $L^2(\mathbb{R}^3)$.

Let $h(t-s,x,y)$ be the integral kernel of $e^{-(t-s)H}$ in $L^2(\mathbb{R}^3)$

Is it possible to construct from h a probability density?

- $h(t-s,x,y)$ is jointly continuous in $x, y, t-s$, (V in Kato class).
- $h(t-s,x,y)$ is strictly positive, (V continuous and lower bounded).

Set

$$H(s,x;t,A;u,z) := \int_A \frac{h(s,x;t,y)h(t,y;u,z)}{h(s,x;u,z)} dy$$

for $s \le t \le u$, $A \in \mathcal{B}(\mathbb{R}^3)$.

Remark

$A \mapsto H(s,x;t,A;u,z)$ is a "reciprocal" probability measure, in the sense of S. Bernstein (1932).

Time reversible processes

Let $\sigma_I = \sigma\{X_t, t \in I\}$.

Theorem

Let $m(x, y)$ be a probability measure on $\mathcal{B}(\mathbb{R}^3) \times \mathcal{B}(\mathbb{R}^3)$. $\exists!\, P_m$ probability measure such that, Z_t, $t \in I = [0, T]$ is a Bernstein process w.r.t. $(\mathbb{R}^3, \sigma_I, P_m)$ and

- $P_m(Z_0 \in B_0, Z_T \in B_T) = m(B_0 \times B_T)$, $B_0, B_T \in \mathcal{B}(\mathbb{R}^3)$;
- $P_m(Z_0 \in B_0, Z_1 \in B_1, \dots, Z_n \in B_n, Z_T \in B_T) = \int_{B_0 \times B_T} dm(x, y)$ $\int_{B_1} H(0, x; t_1, x_1; T, y) dx_1 \cdots \int_{B_n} H(t_{n-1}, x_{n-1}; t_n, x_n; T, y) dx_n$

When is a Bernstein process also Markovian?

Theorem

$Z_t,\ t \in I = [0, T]$ is Markovian $\Leftrightarrow$ there exist two nonzero bounded function of the same sign $\hat{\varphi}_0, \varphi_T$ such that

$$m(B_0 \times B_T) = \int_{B_0 \times B_T} \hat{\varphi}_0(x) h(0, x; T, y) \varphi_T(y) dxdy,$$

$B_0, B_T \in \mathcal{B}(\mathbb{R}^3)$.

Remark

Marginal probability densities:

$$p_0(x)dx := \hat{\varphi}_0(x)dx \int_{\mathbb{R}^3} h(0, x; T, y)\varphi_T(y)dy,$$

$$p_T(y)dy := \varphi_T(y)dy \int_{\mathbb{R}^3} \hat{\varphi}_0(x)h(0, x; T, y)dx,$$

1. $\forall t \in I, z \in \mathbb{R}^3$, $\rho(z,t) := \hat{\varphi}_t(z)\varphi_t(z)dz$ is a probability density,

$$P\{Z(t) \in A\} = \int_A \hat{\varphi}_t(z)\varphi_t(z)dz, \quad t \in I$$

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2. (Forward) transition probability density

$$\hat{\varphi}_s(x)\varphi_s(x)dx \bullet \longrightarrow \ h(s,x;t,y)\frac{\varphi_t(y)}{\varphi_s(x)}dy$$

3. (Backward) transition probability density

$$\frac{\hat{\varphi}_s(x)}{\hat{\varphi}_t(y)}\hat{h}(t,y;s,x)dx \ \longleftarrow \bullet \ \hat{\varphi}_t(y)\varphi_t(y)dy$$

for $x, y \in \mathbb{R}^3$ and $s < t$.

Remark

Under our assumptions,

$$V \text{ potential} + \hat{\varphi}_0(x) = \hat{\eta}(x,0),\ \varphi_T(x) = \eta(x,T)$$
$$\downarrow$$
$$\text{Markovian Bernstein process!}$$

Corollary

If $\varphi_T, \hat{\varphi}_0$ are positive and C^2, the Markovian Bernstein process Z_t is a *diffusion* satisfying the following $\mathcal{P}_t, \mathcal{F}_t$ Itô's stochastic differential equations

$$dZ_t = \hbar^{1/2} dW_t + \hbar \nabla \ln \eta(Z_t) dt,$$
$$d^* Z_t = \hbar^{1/2} d^* \hat{W}_t - \hbar \nabla \ln \hat{\eta}(Z_t) dt$$

with $d^* f(t) = f(t) - f(t - dt),\ dt > 0$ and $\hat{W}_t$ a $\mathcal{F}_t$-Brownian motion.

Examples

- Brownian motion as a Bernstein.
- Brownian bridge.
- Ornstein-Uhlenbeck process.

Feynman-Kac formula for time reversible processes

Let $\varepsilon > 0$ and $V_1 : \mathbb{R}^3 \to \mathbb{R}$ measurable potential such that

$$-\hbar \frac{\partial}{\partial t}\hat{\eta}_1(x,t) = -\frac{\hbar^2}{2}\Delta\hat{\eta}_1(x,t) + V(x)\hat{\eta}_1(x,t) + \varepsilon V_1 \hat{\eta}_1(x,t),$$
$$\hat{\eta}_1(x,0) = \hat{\chi}(x),$$

has a sufficiently regular solution $\hat{\eta}_1$

$$\hat{\eta}_1(x,t) = \hat{\eta}(x,t) - \frac{\varepsilon}{\hbar}\int_0^t \int_{\mathbb{R}^3} h(t-t_n; x, x_n) V_1(x_n) \hat{\eta}_1(x_n, t_n) dx_n dt_n$$

Feynman-Kac formula for time reversible processes

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$$\hat{\eta}_1(x,t) = \hat{\eta}(x,t) - \frac{\varepsilon}{\hbar} \int_0^t \int_{\mathbb{R}^3} h(t-t_n; x, x_n) V_1(x_n) \hat{\eta}(x_n, t_n) dx_n dt_n +$$
$$... + \left(-\frac{\varepsilon}{\hbar}\right)^n \int_0^t \int_0^{t_n} ... \int_0^{t_2} \int_{\mathbb{R}^3} ... \int_{\mathbb{R}^3} h(t-t_n; x, x_n) V_1(x_n)$$
$$h(t_n - t_{n-1}; x_n, x_{n-1}) V_1(x_{n-1}) ... h(t_2 - t_1; x_2, x_1) V_1(x_1) \hat{\eta}_1(x_1, t_1)$$
$$dx_1 ... dx_n dt_1 ... dt_n.$$

Feynman-Kac formula for time reversible processes

Let $\varepsilon > 0$ and $V_1 : \mathbb{R}^3 \to \mathbb{R}$ measurable potential such that

$$-\hbar\frac{\partial}{\partial t}\hat{\eta}_1(x,t) = -\frac{\hbar^2}{2}\Delta\hat{\eta}_1(x,t) + V(x)\hat{\eta}_1(x,t) + \varepsilon V_1\hat{\eta}_1(x,t),$$
$$\hat{\eta}_1(x,0) = \hat{\chi}(x),$$

has a sufficiently regular solution $\hat{\eta}_1$

$$\frac{\hat{\eta}_1(x,t)}{\hat{\eta}(x,t)} = 1 - \frac{\varepsilon}{\hbar}\int_0^t p(t-t_n;x,x_n)V_1(x_n)dx_n dt_n +$$
$$\dots + \left(-\frac{\varepsilon}{\hbar}\right)^n \int_0^t \int_0^{t_n} \dots \int_0^{t_2} \int_{\mathbb{R}^3} \dots \int_{\mathbb{R}^3} p(t-t_n;x,x_n)V_1(x_n)$$
$$p(t_n - t_{n-1}; x_n, x_{n-1})V_1(x_{n-1}) \dots p(t_2 - t_1; x_2, x_1)V_1(x_1)\frac{\hat{\eta}_1(x_1,t_1)}{\hat{\eta}(x_1,t_1)}$$
$$dx_1 \dots dx_n dt_1 \dots dt_n$$

where p is the backward transition probability density of Z_t!

$$\frac{\hat{\eta}_1(x,t)}{\hat{\eta}(x,t)} = 1 - \frac{\varepsilon}{\hbar}\int_0^t p(t-t_n;x,x_n)V_1(x_n)dx_n dt_n +$$
$$... + \left(-\frac{\varepsilon}{\hbar}\right)^n \int_0^t \int_0^{t_n} ... \int_0^{t_2} \int_{\mathbb{R}^3} ... \int_{\mathbb{R}^3} p(t-t_n;x,x_n)V_1(x_n)$$
$$p(t_n - t_{n-1};x_n,x_{n-1})V_1(x_{n-1})...p(t_2-t_1;x_2,x_1)V_1(x_1)$$
$$dx_1...dx_n dt_1...dt_n + ...$$ well-defined probabilistic meaning

...

$$...\frac{\hat{\eta}_1(x,t)}{\hat{\eta}(x,t)} = \sum_{n=0}^{+\infty} \frac{(-1)^n}{n!}\left(\frac{\varepsilon}{\hbar}\right) E_{t,x}\left[\left(\int_0^t V_1(\hat{Z}_s)ds\right)^n\right]$$
$$= E_{t,x}\left[\exp\left\{-\frac{\varepsilon}{\hbar}\int_0^t V_1(Z_s)ds\right\}\right].$$

Under the hypothesis set before,

$$u(t,x) := \frac{\hat{\eta}_1(x,t)}{\hat{\eta}(x,t)} = E_{t,x}\left[\exp\left\{-\frac{\varepsilon}{\hbar}\int_0^t V_1(Z_s)ds\right\}\right]$$

where

$$d^* Z_t = \hbar^{1/2} d^* \hat{W}_t - \hbar \nabla \ln \hat{\eta}(Z_t) dt$$

Theorem ($\mathcal{F}_t$ Feynman-Kac formula for Bernstein)

$u(t,x)$ solves

$$D_* u(t,x) + \frac{\varepsilon}{\hbar} V_1(x) u(t,x) = 0$$

$$\lim_{t \to 0^+} u(t,x) = 1.$$

where $D_* := \frac{\partial}{\partial t} + B_* \nabla - \frac{\hbar}{2}\Delta$ and $B_*(t,x) = -\hbar \nabla \ln \hat{\eta}(t,x)$

Analogously

$$v(t,x) := \frac{\eta_1(x,t)}{\eta(x,t)} = E_{t,x}\left[\exp\left\{-\frac{\varepsilon}{\hbar}\int_t^T V_1(Z_s)ds\right\}\right]$$

where

$$dZ_t = \hbar^{1/2}dW_t + \hbar\nabla \ln \eta(Z_t)dt$$

Theorem ($\mathcal{P}_t$ Feynman-Kac formula for Bernstein)

$v(t,x)$ solves

$$Dv(t,x) - \frac{\varepsilon}{\hbar}V_1(x)v(t,x) = 0$$

$$\lim_{t\to T^-} v(t,x) = 1.$$

where $D := \frac{\partial}{\partial t} + B\nabla + \frac{\hbar}{2}\Delta$ and $B(t,x) = \hbar\nabla \ln \eta(t,x)$.

Examples

- Usual Feynman-Kac formula.
- Absolute continuity relations.
- Other relations between stochastic processes.

Richard Feynman, *The Principle of Least Action in Quantum Mechanics*

- Space-time visualization of quantum path.

Let $t \in [s, u]$ and $\Omega_x^z = \{\omega \in C([s, u]; \mathbb{R}^3) : \omega(s) = x, \omega(u) = z\}$

$$L(\omega, \dot{\omega}) = \frac{1}{2}|\dot{\omega}|^2 - V(\omega) \text{ and } S[\omega, u - s] = \int_s^u L(\omega(t), \dot{\omega}(t))dt$$

Feynman Path Integral:

$$< \psi_u|\varphi_u >= \int \int \int_{\Omega_x^z} \psi_s(x) e^{\frac{i}{\hbar} S[\omega, u-s]} \mathcal{D}\omega \bar{\varphi}_u(z) dxdz$$

with $\mathcal{D}\omega = \prod_{s \le \tau \le t} d\omega(t)$ and ψ_u, φ_u two states at time u.

Integration by parts formula:

$$< \delta F[\omega](\delta\omega) >_S = -\frac{i}{\hbar} < F\delta S[\omega](\delta\omega) >_S$$

- $\delta F[\omega](\delta\omega)$ the directional derivative of a regular funcional.
- $< \cdot >_S$ the expectation wrt the measure $e^{iS[w]/\hbar}\mathcal{D}\omega$ on $\Omega^y = \{\omega \in C^2([s,t];\mathbb{R}^3) : \omega(t) = y\}$.

Integration by parts formula implies:

- $$< \ddot{\omega} >_S = - < \nabla V(\omega) >_S$$

  (Ehrenfest theorem $\frac{d^2}{d\tau^2} < \psi|Q(\tau)\psi >_2 = - < \psi|\nabla V(Q(\tau))\psi >_2$).

- $< \omega_k(\tau)\frac{(\omega(\tau)-\omega(\tau-\Delta\tau))_j}{\Delta\tau} >_S - < \frac{(\omega(\tau+\Delta\tau)-\omega(\tau))_j}{\Delta\tau}\omega_k(\tau) >_S = i\hbar\delta_{k,j}$

  (Heisenberg commutation relations $Q_k P_j - P_j Q_k = i\hbar\delta_{k,j}$.)

with $Q, P, H = -\frac{\hbar^2}{2}\Delta + V$ the position, momentum and energy observables. $< \cdot >_2$ inner product of $L^2(\mathbb{R}^3)$.

Remark

- Feynman path integral approach inspired all existing Feynman-Kac and integration by parts formula in Stochastic Analysis.
- Probabilistic version of Feynman's path integral approach also motivated stochastic perturbation of Geometric Mechanics.
  - Classical Lagrangian evaluated on the stochastic process and its *mean derivative*,

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