AM216 Stochastic Differential Equations

Lecture 07

List of topics in this lecture

- Wiener process is continuous in probability
- Ornstein-Uhlenbeck process (OU), Stokes law, thermal excitations
- Solution of particle velocity in OU, colored noise, convergence to a white noise
- Fluctuation-dissipation theorem, Maxwell-Boltzmann distribution
- Solution of particle position in OU

Recap

Energy spectrum density (ESD), power spectrum density (PSD)

Stationary stochastic process, auto-correlation function (ACF)

Wiener-Khinchin theorem: PSD is Fourier transform of ACF

Definition of white noise: PSD is constant in frequency domain

Calculating ACF and PSD of $Z(t) \equiv dW/dt$

Constrained Wiener process (Bayes theorem)

$$\rho\left(W(a+\frac{h}{2}) = x \middle| W(a) = y_a \text{ and } W(a+h) = y_b \right) \sim N\left(\frac{y_a + y_b}{2}, \frac{h}{4} \right)$$

This is very useful in refining a discrete sample path of $W(t)$.

<u>The Wiener process is continuous in probability</u>

Recall the continuity of a <u>regular function</u>. $f(t)$ is continuous at t if for any $\varepsilon > 0$,

$\left| f(t+h) - f(t) \right| \geq \varepsilon$ is <u>impossible</u> when h is small enough.

<u>Definition</u> (continuity of $F(t, \omega)$ in probability)

<u>Intuitively</u>, $F(t, \omega)$ is continuous in probability if for any $\varepsilon > 0$,

$\left|F(t+h,\omega)-F(t,\omega)\right|\geq\varepsilon$ is almost impossible when h is small enough.

More precisely, $F(t,\omega)$ is continuous in probability if for any $\varepsilon>0$,

$$\lim_{h\to 0}\Pr\left(\left|F(t+h,\omega)-F(t,\omega)\right|\geq\varepsilon\right)=0$$

Theorem: $W(t)$ is continuous in probability.

Proof: To prove the theorem, we need

Chebyshev-Markov inequality:

Let X be a random variable X. For $\alpha > 0$, we write $E(|X|^\alpha)$ as

$$E\left(|X|^\alpha\right)=\int |x|^\alpha \rho(x)dx \geq \int_{|x|\geq\varepsilon} |x|^\alpha \rho(x)dx \geq$$

$$\geq \varepsilon^\alpha \int_{|x|\geq\varepsilon} \rho(x)dx=\varepsilon^\alpha \Pr\left(|X|\geq\varepsilon\right)$$

==> $\boxed{\Pr\left(|X|\geq\varepsilon\right)\leq\frac{1}{\varepsilon^\alpha}E\left(|X|^\alpha\right)}$ This is valid for any $\alpha > 0$.

This is called the Chebyshev-Markov inequality.

We apply the Chebyshev-Markov inequality to $X = W(t+h)-W(t)$ with $\alpha = 2$.

$$\Pr\left(|W(t+h)-W(t)|\geq\varepsilon\right)\leq\frac{E\left(|W(t+h)-W(t)|^2\right)}{\varepsilon^2}$$

$$=\frac{h}{\varepsilon^2}\to 0 \quad \text{as } h\to 0$$

Thus, the Wiener process $W(t)$ is continuous in probability.

Similar to the continuity of $F(t,\omega)$ in probability, we can define the convergence of sequence $\{X_n(\omega)\}$ in probability.

Definition (convergence of $\{X_n(\omega)\}$ in probability)

As $n\to+\infty$, $\{X_n(\omega)\}$ converges to q in probability if for any $\varepsilon>0$,

$$\lim_{n\to+\infty}\Pr\left(\left|X_n(\omega)-q\right|\geq\varepsilon\right)=0$$

Theorem (a sufficient condition for convergence in probability)

Suppose $\lim_{n\to 0}E\left(X_n(\omega)\right)=q$ and $\lim_{n\to 0}\mathrm{var}\left(X_n(\omega)\right)=0$.

Then $\{X_n(\omega)\}$ converges to q in probability as $n\to+\infty$.

Proof: (homework problem)

Ornstein-Uhlenbeck Process

Consider the stochastic motion of a small particle in water (as Robert Brown observed the motion of pollen particles in water under a microscope).

For simplicity, we discuss the one-dimensional motion. Let

X = position of the particle

Y = velocity of the particle

m = mass of the particle

Newton's second law

$$m\frac{dY}{dt} = \text{viscous drag} + \text{Brownian force}$$

We discuss these two forces.

Stokes law (for the viscous drag)

viscous drag = $-b\,Y$

where b is the drag coefficient. For a spherical particle, the drag coefficient is

$b = 6\pi\,\eta\,a$

a = radius of the particle

η = viscosity of the fluid media

A short digression: Pollution particles suspended in air

When an object is dropped in mid-air, it first accelerates downward, driven by the gravity. Then it reaches a steady velocity when the drag force balances the gravitational force. This steady velocity is called the terminal velocity for large objects (such as a spacecraft returning to Earth) or the settling velocity for small particles. Here we focus on small particles. The settling velocity satisfies

$$\underbrace{(6\pi\eta a)V_{\text{settling}}}_{\text{Drag force}} = \underbrace{\left(\frac{4}{3}\pi a^3\rho_{\text{mass}}\right)g}_{\text{Gravity}}$$

$$\Longrightarrow \quad V_{\text{settling}} = \left(\frac{2\rho_{\text{mass}}g}{9\eta}\right)a^2 \propto a^2$$

where the air viscosity is $\eta = 1.8\times10^{-4}\ \text{g(cm)}^{-1}\text{s}^{-1}$.

Consider BUD (budesonide), a drug used in treating asthma. It has $\rho_{\text{mass}} = 1.26\ \text{g/cm}^3$.

For a BUD particle of 0.1 mm in diameter

a = 50 μm ==> V_{settling} = 38 cm/s

For a particle of 10 μm in diameter (PM_{10} particles)

a = 5 μm ==> V_{settling} = 0.38 cm/s

For a particle of 2.5 μm in diameter ($PM_{2.5}$ particles)

a = 1.25 μm ==> V_{settling} = 0.0238 cm/s

With this tiny settling velocity, it takes more than 1 hour for a 2.5 μm particle to descend 1 meter with respect to the surrounding air.

$$T_{1\text{ meter}} = \frac{1\text{ meter}}{V_{\text{settling}}} = \frac{100\text{ cm}}{0.0238\text{ cm/s}} = 4200\text{ seconds} = 1.17\text{ hours}$$

Remark:

Small pollution particles are more dangerous for two reasons:

- They stay in air much longer (virtually forever)
- They can pass the filtration system of human body and enter the circulatory system (blood circulation).

End of digression

Back to the discussion of forces.

Thermal excitations (Brownian force)

We model the Brownian force as a white noise.

$$\text{Brownian force} = q\frac{dW}{dt}$$

where the coefficient q is to be determined in the fluctuation-dissipation relation.

The governing equation of the particle

$$mdY = \underbrace{-bY\,dt}_{\text{dissipation}} + \underbrace{q\,dW}_{\text{fluctuation}}$$

$$dX = Y\,dt$$

This is called the Ornstein-Uhlenbeck process.

Remark:

Both the viscous drag and the Brownian force on the particle are results from the particle colliding with surrounding fluid molecules: the viscous drag is the mean and the Brownian force is the fluctuations of the random colliding force. As a result, the fluctuation coefficient (q) and the dissipation coefficient (b) are related by the fluctuation-dissipation theorem, which we will discuss later.

Four goals in the discussion of the Ornstein-Uhlenbeck process

1) Solve for $Y(t)$
2) Show that
   A) $Y(t)$ is a colored noise and
   B) $Y(t)$ converges to a white noise as "m converges to zero".
3) Relate q to b (fluctuation-dissipation theorem)
4) Study the behavior of $X(t)$

Goal #1: We solve for $Y(t)$.

For mathematical convenience, we divide the equation by m

$$m\,dY = -bY\,dt + q\,dW$$

$$\Longrightarrow \quad dY = -\beta Y\,dt + \gamma\,dW\,, \qquad \beta = \frac{b}{m}\,, \quad \gamma = \frac{q}{m}$$

We use the method of integrating factor. Multiply by $e^{\beta t}$, we get

$$e^{\beta t}dY + \beta e^{\beta t}Y\,dt = \gamma e^{\beta t}dW$$

$$\Longrightarrow \quad d\left(e^{\beta t}Y(t)\right) = \gamma e^{\beta t}dW$$

Note:

$$\Delta\left(e^{\beta t}Y(t)\right) = e^{\beta(t+\Delta t)}Y(t+\Delta t) - e^{\beta t}Y(t) = e^{\beta t}\left(1+\beta\Delta t + o(\Delta t)\right)\left(Y(t)+\Delta Y\right) - e^{\beta t}Y(t)$$

$$= e^{\beta t}\Delta Y + \beta e^{\beta t}\,Y(t)\Delta t + o(\Delta t)$$

Therefore, $d\left(e^{\beta t}Y(t)\right) = e^{\beta t}dY + \beta e^{\beta t}Y\,dt$ is justified.

Summing over all time intervals gives us

$$e^{\beta t}Y(t) - Y(0) = \int_0^t \gamma e^{\beta s}\,dW(s) \equiv G(t)$$

where the integral of dW is defined as the limit of a Riemann sum.

$$G(t) \equiv \int_0^t \gamma e^{\beta s}\,dW(s) \equiv \lim_{N\to\infty}\sum_{j=0}^{N-1}\gamma e^{\beta s_j}\Delta W_j$$

where $\qquad \Delta s = \frac{t}{N}\,, \qquad s_j = j\Delta s\,, \qquad \Delta W_j = W(s_{j+1}) - W(s_j)\,.$

Recall that the sum of independent normal RVs is a normal RV.

$\{\Delta W_j,\ \ j = 0, 1, \ldots, N-1\}$ are independent normal RVs.

==> $G(t) \equiv \lim_{N\to\infty} \sum_{j=0}^{N-1} \gamma e^{\beta s_j} \Delta W_j$ is a normal RV.

The mean and variance of $G(t)$ are

$$E\big(G(t)\big) = \lim_{N\to\infty} \sum_j \gamma e^{\beta s_j} E(\Delta W_j) = 0$$

$$\mathrm{var}\big(G(t)\big) = \lim_{N\to\infty} \sum_j (\gamma e^{\beta s_j})^2 \,\mathrm{var}(\Delta W_j) = \lim_{N\to\infty} \sum_j (\gamma e^{\beta s_j})^2 \Delta s$$

$$= \int_0^t (\gamma e^{\beta s})^2 ds = \gamma^2 \int_0^t e^{2\beta s} ds = \frac{\gamma^2}{2\beta}(e^{2\beta t} - 1)$$

Caution:

For $t > 0$, $\int_0^t \gamma e^{\beta s} dW(s)$ is a sum of independent normal RVs.

For $t < 0$, increments $\{\Delta W_j,\ \ j = 0, 1, \ldots, N-1\}$ are backwards in time and are no longer independent. For now, we only consider $t > 0$.

Summary (distribution of $G(t)$)

$$G(t) \equiv \int_0^t \gamma e^{\beta s} dW(s) \sim N\left(0,\ \frac{\gamma^2}{2\beta}(e^{2\beta t} - 1)\right) \qquad \text{for } t > 0$$

In the above, we just derived a theorem.

Theorem:

$$\int_0^L f(t) dW(t) \sim N\left(0,\ \int_0^L f(t)^2 dt\right)$$

We continue solving for $Y(t)$

$$e^{\beta t} Y(t) - Y(0) = G(t), \qquad G(t) \sim N\left(0,\ \frac{\gamma^2}{2\beta}(e^{2\beta t} - 1)\right) \qquad \text{for } t > 0$$

==> $Y(t) = e^{-\beta t} Y(0) + e^{-\beta t} G(t) \qquad \text{for } t > 0$

==> $\big(Y(t) \big| Y(0) = y_0\big) \sim N\left(e^{-\beta t} y_0,\ \frac{\gamma^2}{2\beta}(1 - e^{-2\beta t})\right) \qquad \text{for } t > 0$

Summary (solution of $Y(t)$)

$$\big(Y(t_0 + t) \big| Y(t_0) = y_0\big) \sim N\left(e^{-\beta t} y_0,\ \frac{\gamma^2}{2\beta}(1 - e^{-2\beta t})\right) \qquad \text{for } t > 0$$

Equilibrium state:

For large t, $Y(t)$ reaches an equilibrium normal distribution.

$$\left(Y(t)\middle|Y(0)=y_0\right) \sim N\left(0, \frac{\gamma^2}{2\beta}\right) \quad \text{for large } t>0, \text{ independent of } y_0.$$

Goal #2: we show that

A) $Y(t)$ is a colored noise and

B) $Y(t)$ converges to a white noise as "m converges to zero".

We assume that the equilibrium has been reached long time ago and $Y(t)$ is already a stationary process. Under this assumption, $Y(t)$ has the equilibrium distribution.

$$Y(t) \sim N\left(0, \frac{\gamma^2}{2\beta}\right) \quad \text{for all } t$$

Goal #2A: We show that $Y(t)$ is a colored noise.

We calculate the autocorrelation function.

$$R(t) \equiv E\big(Y(t)Y(0)\big)$$

We use the law of total expectation.

$$E(Z_1) = E\big(E(Z_1|Z_2)\big)$$

We select $Z_1 = Y(t)\,Y(0)$ and $Z_2 = Y(0)$. We consider the case of $t > 0$.

$$R(t) \equiv E\big(Y(t)Y(0)\big) = E\Big(E\big(Y(t)Y(0)\big|Y(0)\big)\Big) = E\Big(Y(0)\cdot E\big(Y(t)\big|Y(0)\big)\Big)$$

Using $E\big(Y(t)\big|Y(0)\big) = e^{-\beta t}Y(0)$ for $t > 0$ and $Y(t) \sim N\left(0, \frac{\gamma^2}{2\beta}\right)$ for all t, we write

$$R(t) = E\big(Y(0)\cdot e^{-\beta t}Y(0)\big) = e^{-\beta t}E\big(Y(0)^2\big) = \frac{\gamma^2}{2\beta}e^{-\beta t} \quad \text{for } t>0$$

From the definition of auto-correlation function, $R(t)$ is an even function of t:

$$R(-t) \equiv E\big(Y(s-t)Y(s)\big) \quad \text{for all } s$$

$$\xrightarrow{\text{select } s=t} \; = E\big(Y(0)Y(t)\big) = R(t)$$

Therefore, we obtain

$$R(t) = \frac{\gamma^2}{2\beta}\exp(-\beta|t|) \quad \text{for } t \in (-\infty, +\infty)$$

The corresponding power spectrum density (PSD) is

$$s(\xi)=\frac{\gamma^2}{2\beta}F\left[\exp(-\beta|t|)\right]=\frac{\gamma^2}{2\beta}\cdot\frac{2\beta}{\beta^2+4\pi^2\xi^2}=\frac{\gamma^2}{\beta^2+4\pi^2\xi^2}$$

(Homework problem)

<u>In conclusion</u>, $Y(t)$ is a colored noise.

<u>Goal #2B:</u> We show that $Y(t)$ converges to a white noise as "$m \to 0$"

<u>A simplified story:</u> $m \to 0$ (while b and q stay unchanged)

This corresponds to the situation where the mass density of the particle goes to zero while the particle size is fixed.

Recall that $\beta=\frac{b}{m}$, $\gamma=\frac{q}{m}$.

$$R(t)=\frac{\gamma^2}{2\beta}\exp(-\beta|t|)==\frac{q^2}{b^2}\cdot\underbrace{\frac{b}{m}}_{1/h}\cdot\underbrace{\frac{1}{2}\exp\left(-\frac{b}{m}|t|\right)}_{f(t/h)},\qquad h\equiv\frac{m}{b}$$

We write it as a scaled probability density function.

$$R(t)=\frac{q^2}{b^2}\cdot\frac{1}{h}f\left(\frac{t}{h}\right),\qquad h\equiv\frac{m}{b},\qquad f(u)\equiv\frac{1}{2}\exp\left(-|u|\right)$$

$f(u)$ given above is a probability density function (satisfying $\int f(u)du = 1$).

It follows that

$$\lim_{h\to 0}\frac{1}{h}f\left(\frac{t}{h}\right)=\delta(t)\qquad\text{and}\qquad\lim_{m\to 0}R(t)=\frac{q^2}{b^2}\cdot\delta\left(t\right)$$

Therefore, $\lim\limits_{m\to 0}Y(t)$ is a white noise.

<u>The real story:</u>

Mathematically, the limit above is rigorous. The assumption of mass density converging to zero, however, is not a realistic one in physics.

The mass of a spherical particle is

$$m=\frac{4\pi}{3}\rho_{\text{mass}}a^3$$

where ρ_{mass} is the mass density and a the radius of particle.

In physics, we are interested in the situation where radius $a \to 0$ while ρ_{mass} is fixed.

We need to consider the effect of radius a on coefficients m, b and q.

$$m = \frac{4\pi}{3}\rho_{\text{mass}}\, a^3 = O(a^3) \to 0$$

$$b = 6\pi\eta a = O(a) \to 0$$

$$h \equiv \frac{m}{b} = O(a^2) \to 0$$

$$q = \sqrt{2k_B T b} = O(\sqrt{a}) \to 0$$ (we will derive q shortly)

$$\frac{q^2}{b^2} = O(a^{-1}) \to \infty$$

$$a\frac{q^2}{b^2} = O(1)$$ independent of a.

Consider $\sqrt{a}\,Y(t)$. We have

$$R_{\sqrt{a}Y}(t) = E\left(\sqrt{a}\,Y(s+t)\sqrt{a}\,Y(s)\right) = aE\left(Y(s+t)Y(s)\right) = aR_Y(t) = a\frac{q^2}{b^2}\cdot\frac{1}{h}f\left(\frac{t}{h}\right)$$

$$\lim_{a\to 0} R_{\sqrt{a}Y}(t) = \lim_{a\to 0} a\frac{q^2}{b^2}\cdot\frac{1}{h}f\left(\frac{t}{h}\right) = \left(a\frac{q^2}{b^2}\right)\cdot\delta(t) \quad \text{where} \quad \left(a\frac{q^2}{b^2}\right) = O(1)$$

Therefore, $\lim_{a\to 0}\sqrt{a}\,Y(t)$ is a white noise.

<u>In physics</u>, as radius $a \to 0$, $Y(t)$ converges to a white noise of magnitude $O\left(\frac{1}{\sqrt{a}}\right)$.

<u>Goal #3</u>: We relate the fluctuation coefficient q to the drag coefficient b.

To connect b and q, we need the Maxwell-Boltzmann distribution

<u>Maxwell-Boltzmann distribution</u>

For a system in equilibrium with a thermal bath, we have

$$\rho(Y = y) \propto \exp\left(\frac{-\text{Energy}(Y = y)}{k_B T}\right)$$

where k_B is the Boltzmann constant and

T is the absolute temperature of the thermal bath.

Maxwell-Boltzmann distribution is a universal law applicable to all thermodynamic systems. In our system, Y = velocity and

$$\text{Energy}(Y=y) = \frac{1}{2} m y^2$$

The Maxwell-Boltzmann distribution gives us

$$\rho(Y=y) \propto \exp\left(\frac{-\text{Energy}}{k_B T}\right) = \exp\left(\frac{-\frac{1}{2} m y^2}{k_B T}\right)$$

We write it into the form of a normal density $\exp\left(\frac{-y^2}{2\sigma^2}\right)$

$$\rho(Y=y) \propto \exp\left(\frac{-y^2}{2(k_B T/m)}\right) = \rho_{N(0,\,(k_B T/m))}(y)$$

We have two expressions for the equilibrium of $Y(t)$:

- The equilibrium described by the <u>Maxwell-Boltzmann distribution</u>:

$$Y(t) \sim N\left(0,\, \frac{k_B T}{m}\right)$$

- The equilibrium mathematically derived from the <u>OU process</u>:

$$Y(t) \sim N\left(0,\, \frac{\gamma^2}{2\beta}\right)$$

The OU process is a model. To make it consistent with the Maxwell-Boltzmann distribution, we equate these two equilibrium distributions.

$$\frac{\gamma^2}{2\beta} = \frac{k_B T}{m}, \qquad \beta = \frac{b}{m}, \quad \gamma = \frac{q}{m}$$

==> $\quad \frac{q^2}{m^2} \cdot \frac{m}{2b} = \frac{k_B T}{m}$

==> $\quad q^2 = 2 k_B T b$

Therefore, we arrive at the fluctuation dissipation theorem.

<u>Theorem</u> (fluctuation dissipation relation):

The fluctuation coefficient q and the drag coefficient b are related by

$$\boxed{q = \sqrt{2 k_B T b}}$$

With the fluctuation dissipation relation, the OU process becomes.

$$m\,dY = \underbrace{-bY\,dt}_{\text{dissipation}} + \underbrace{\sqrt{2k_B T b}\,dW}_{\text{fluctuation}}$$

Remark: Now all coefficients in the governing equation are specified.

Goal #4: we study the behavior of $X(t)$.

First, we solve for $X(t)$.

$$Y(t)=e^{-\beta t}Y(0)+e^{-\beta t}G(t) \qquad \text{for } t>0\,, \qquad G(t)\equiv\int_0^t \gamma e^{\beta s}\,dW(s)$$

$$X(t)-X(0)=\int_0^t Y(\tau)d\tau=\int_0^t\left(e^{-\beta\tau}Y(0)+e^{-\beta\tau}\int_0^\tau \gamma e^{\beta s}\,dW(s)\right)d\tau$$

$$=\frac{1}{\beta}(1-e^{-\beta t})Y(0)+\gamma\int_0^t\int_0^\tau e^{-\beta\tau}e^{\beta s}\,dW(s)d\tau$$

Change the order of integration

$$=\frac{1}{\beta}(1-e^{-\beta t})Y(0)+\gamma\int_0^t\left(\int_s^t e^{-\beta\tau}\,d\tau\right)e^{\beta s}\,dW(s)$$

$$=\frac{1}{\beta}(1-e^{-\beta t})Y(0)+\frac{\gamma}{\beta}\cdot\underbrace{\int_0^t(1-e^{-\beta(t-s)})dW(s)}_{G_2(t)}$$

$G_2(t)\equiv\int_0^t(1-e^{-\beta(t-s)})dW(s)$ is a sum of independent normal RVs.

==> $G_2(t)$ is a normal RV.

Therefore, $(X(t) - X(0))$ is a normal RV. We will look into it in more detail.