TD 10: Harmonic analysis for stochastic dynamics - Solutions

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November 26, 2021

The autocorrelation function and the Wiener-Kinchin theorem. For stationary stochastic dynamics, the autocorrelation function is defined as $C_x(t,t') = \langle x(t)x(t')\rangle$, where $\langle\cdot\rangle$ denotes the ensemble average (average over the stationary distribution).

1. What property of C_x is ensured by stationarity? Write C_x as a function of $\tau = t' - t$.

2. Assuming ergodicity, show that the autocorrelation function is an even function.

3. *(Bonus)* Show that for any integrable function g,

$$\int_{-T/2}^{T/2} dt \int_{-T/2}^{T/2} ds g(s-t) = \int_{-T}^{T} g(\tau)(T - |\tau|) d\tau.$$

4. The power spectral density of a signal $x(t)$ is defined as

$$\hat{P}_x(\omega) = \lim_{T\to\infty} \frac{1}{T}\langle|\hat{x}_T(\omega)|^2\rangle,$$

where $\hat{x}_T(\omega) = \int_{-T/2}^{T/2} x(t)e^{i\omega t}dt$, the Fourier transform of $x(t)$ over the interval $t \in [-T/2, T/2]$. Show that the power spectral density is the Fourier transform of the autocorrelation function:

$$\hat{P}_x(\omega) = \mathcal{F}(C_x(\tau))$$

where $\mathcal{F}$ represent the Fourier transform.

5. How can we get the autocorrelation function from the power spectral density? These relations are known as the Wiener-Kinchin theorem.

Leveraging Fourier transforms to estimate the correlation function. We now leverage the Wiener-Kinchin theorem in example applications

6. Consider the following stochastic dynamics for the velocity of a damped particle,

$$m\dot{v} = -\gamma v + \sigma\eta,$$

where η is a Gaussian uncorrelated random variable $\langle\eta(t)\eta(t')\rangle = \delta(t-t')$, γ is a damping coefficient and σ is the magnitude of the noise. Write down the Fourier transform of the Langevin equation, and estimate the correlation function of v through the Wiener-Kinchin theorem.

7. What is the value of σ that keeps the particle at thermal equilibrium? Compare with the results of TD9.

8. Consider now the Langevin dynamics of a particle confined in a harmonic (quadratic) potential and in contact with a heat bath in equilibrium:

$$m\ddot{x} = -\gamma\dot{x} - kx + \eta(t),$$

Where $\eta(t)$ is Gaussian white noise. What is its equation of motion in phase space? What is the correlation function of the noise in equilibrium?

9. Compute the autocorrelation function of the particle's position using the Wiener-Kinchin theorem, and show that it obeys qualitatively different behaviors in the underdamped and overdamped regimes.

Correction

1. Stationarity ensures that $C_x(t+\tau,t)$ only depends on the time difference τ. Thus, we may write $C_x(\tau)$.

2. For ergodic dynamics, the ensemble average equals a long time average, and so the autocorrelation function can be written as,

$$C_x(\tau) = \lim_{T\to\infty} \frac{1}{T}\int_0^T x(t)x(t+\tau)dt.$$

A function is symmetric when $f(x) = f(-x)$, so we need to compute $C_x(-\tau)$,

$$\begin{aligned}
C_x(-\tau) &= \lim_{T\to\infty} \frac{1}{T}\int_0^T x(t)x(t-\tau)dt \\
&= \lim_{T\to\infty} \frac{1}{T}\int_{-\tau}^{T-\tau} x(t'+\tau)x(t')dt' \\
&= \lim_{T\to\infty} \frac{1}{T}\left[\int_{-\tau}^{0} x(t')x(t'+\tau)dt' + \int_0^T x(t')x(t'+\tau)dt' - \int_{T-\tau}^{T} x(t')x(t'+\tau)dt'\right] \\
&= \lim_{T\to\infty} \frac{1}{T}\int_0^T x(t)x(t+\tau)dt = C_x(\tau),
\end{aligned}$$

where we've performed a change of variables $t' = t-\tau$, $t' \in [-\tau, T-\tau]$, and then in the limit $T\to\infty$, only the middle integral contributes. Another way to derive this is to write down $C_x(-\tau) = \langle x(t)x(t-\tau)\rangle$, make the same change of variables to $\langle x(t'+\tau)x(t')\rangle$ and then realize that due to stationarity (time-translation invariance) we can change this back to $\langle x(t)x(t+\tau) = C_x(\tau)\rangle$.

3. Performing the change of variables $u = s-t$, $v = s+t$, we get,

$$\begin{aligned}
\int_{-T/2}^{T/2} dt \int_{-T/2}^{T/2} ds g(s-t) &= \int_{-T}^{T} du \int_{-T+|u|}^{T-|u|} dudv g(u)\det(J) && (1)\\
&= \frac{1}{2}\int_{-T}^{T} du g(u) \int_{-T+|u|}^{T-|u|} dv = \int_{-T}^{T} du g(u)(T-|u|) && (2)
\end{aligned}$$

4. From the expression of the power spectral density we get,

$$\begin{aligned}
\hat{P}_x(\omega) &= \lim_{T\to\infty} \frac{1}{T}\langle|\hat{x}_T(\omega)|^2\rangle \\
&= \lim_{T\to\infty} \frac{1}{T}\int_{-T/2}^{T/2} ds \int_{-T/2}^{T/2} dt \langle x(s)x(t)\rangle e^{i\omega(s-t)} \\
&= \lim_{T\to\infty} \frac{1}{T}\int_{-T/2}^{T/2} ds \int_{-T/2}^{T/2} dt C_x(s-t) e^{i\omega(s-t)} \\
&= \lim_{T\to\infty} \int_{-T}^{T} d\tau C_x(\tau) e^{i\omega\tau}\left(1-\frac{|\tau|}{T}\right) \\
&= \lim_{T\to\infty} \int_{-\infty}^{\infty} d\tau C_x(\tau) e^{i\omega\tau}\epsilon_T(\tau) \\
&= \int_{-\infty}^{\infty} d\tau C_x(\tau) e^{i\omega\tau} \\
&= \mathcal{F}(C_x(\tau)),
\end{aligned}$$

where we have used the previous result with $g(\tau) = C_x(\tau)e^{i\omega(\tau)}$ and set $\epsilon_T(\tau) = \left(1-\frac{|\tau|}{T}\right)\mathbb{1}_{|t|\le T}$ which converges to 1 at each point and is dominated by 1. Taken the limit $T\to\infty$, ϵ_T disappears thanks to the dominated convergence theorem.

5.

$$\hat{P}_x(\omega) = \mathcal{F}(C_x(\tau)) \Rightarrow C_x(\tau) = \mathcal{F}^{-1}(\hat{P}_x(\omega))$$

where $\mathcal{F}$ represent the Fourier transform and $\mathcal{F}^{-1}$ the inverse Fourier transform.

6. One can easily show that $\mathcal{F}(\dot{x}(t)) = -i\omega\hat{x}(\omega)$. Therefore, taking the Fourier transform of the Langevin equation, we get,

$$-i\omega m\hat{v}(\omega) = -\gamma\hat{v}(\omega) + \sigma\eta(\omega)$$

which is simple to solve in Fourier space, yielding,

$$\hat{v}(\omega) = \frac{\sigma\eta(\omega)}{\gamma - i\omega m}.$$

From this, we can directly estimate the power spectral density,

$$\begin{aligned}
\hat{P}_v(\omega) &\propto \langle\hat{v}(\omega)\hat{v}^*(\omega)\rangle \\
&= \frac{\sigma^2\langle\eta(\omega)\eta^*(\omega)\rangle}{m^2\left(\omega - i\frac{\gamma}{m}\right)\left(\omega + i\frac{\gamma}{m}\right)}.
\end{aligned}$$

The power spectral density of the noise can be obtained by taking the Fourier transform of the correlation function

$$\hat{P}_\eta(\omega) = \int_{-\infty}^{\infty} \langle \eta(t)\eta(0)\rangle e^{i\omega t} dt = \int_{-\infty}^{\infty} \delta(t-0) e^{i\omega t} dt = 1.$$

Thus,

$$\hat{P}_v(\omega) = \frac{\sigma^2}{m^2\left(\omega - i\frac{\gamma}{m}\right)\left(\omega + i\frac{\gamma}{m}\right)}.$$

To get the correlation function we need to compute the inverse Fourier transform of the power spectral density. Given the convention for the Fourier transform used in 4., the inverse Fourier transform is given by,

$$\mathcal{F}^{-1}(\hat{x}(\omega)) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, \hat{x}(\omega) e^{-i\omega t}.$$

The power spectral density of v is proportional to $\hat{P}_v(\omega) \propto \langle \hat{v}(\omega)\hat{v}^*(\omega)\rangle$, and so we get,

$$\begin{aligned} C_v(\tau) &= \mathcal{F}^{-1}\left(\frac{\sigma^2}{m^2\left(\omega - i\frac{\gamma}{m}\right)\left(\omega + i\frac{\gamma}{m}\right)}\right) \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega \frac{\sigma^2 e^{-i\omega\tau}}{m^2\left(\omega - i\frac{\gamma}{m}\right)\left(\omega + i\frac{\gamma}{m}\right)}, \end{aligned}$$

which we can solve through Cauchy's residue theorem. Since the exponent in in the negative half-plane, we integrate over a clockwise contour with a simple pole at $\omega = -i\frac{\gamma}{m}$. This yields,

$$\begin{aligned} C_v(\tau) &= \frac{1}{2\pi m^2}(-2\pi i)\frac{\sigma^2 e^{-i(-i\frac{\gamma}{m}\tau)}}{-2i\frac{\gamma}{m}} \\ C_v(\tau) &= \frac{\sigma^2}{2\gamma m} e^{-\frac{\gamma}{m}\tau} \end{aligned}$$

7. In order for the particle to be in thermal equilibrium, we must have $C_v(0) = \frac{k_B T}{m}$, therefore

$$\sigma^2 = 2\gamma k_B T.$$

So we recover the results of TD9, but γ is rescaled by the mass.

8. The harmonic potential has the form $V(x) = kx^2$, so the equation of motion for a particle in a harmonic potential connected to a heat bath is,

$$m\ddot{x} = -\gamma\dot{x} - kx + \eta(t),$$

which in phase space results in a system of equations for the position and velocity,

$$\begin{cases} \dot{x} = v \\ \dot{v} = -\frac{\gamma}{m}v - \frac{k}{m}x + \frac{1}{m}\eta(t). \end{cases} \tag{3}$$

In equilibrium, we have seen that the strength of the noise must obeys $\sigma^2 = 2\gamma k_B T$. Therefore, in equilibrium we must have,

$$\begin{aligned} \langle \eta(t)\rangle &= 0 \\ \langle \eta(t_1)\eta(t_2)\rangle &= 2\gamma k_B T m^2 \delta(t_1 - t_2). \end{aligned}$$

9. Leveraging the Wiener-Kinchin theorem, we can estimate the autocorrelation functions as,

$$C_x(\tau) = \langle x(t)x(t+\tau)\rangle = \mathcal{F}^{-1}\left(\hat{P}_x(\omega)\right)$$

where $\mathcal{F}^{-1}$ represent the inverse Fourier transform, and $\hat{P}_x(\omega)$ is the spectral density. Taking the Fourier transform of Eq. (3) we get,

$$\begin{aligned} -i\omega\hat{x}(\omega) &= \hat{v}(\omega) \\ -i\omega\hat{v}(\omega) &= -\frac{\gamma}{m}\hat{v}(\omega) - \omega_0^2\hat{x}(\omega) + \frac{1}{m}\hat{\eta}(\omega), \end{aligned}$$

where $\omega_0^2 = \frac{k}{m}$. Solving for $\hat{x}(\omega)$ we get,

$$\hat{x}(\omega) = \frac{1}{m}\frac{\hat{\eta}(\omega)}{\omega_0^2 - \omega^2 - i\omega\frac{\gamma}{m}}.$$

The power spectral density is then

$$\hat{P}_x(\omega) = \left\langle \frac{1}{m^2} \frac{\hat{P}_\eta(\omega)}{(\omega_0^2 - \omega^2 - i\omega\frac{\gamma}{m})(\omega_0^2 - \omega^2 + i\omega\frac{\gamma}{m})} \right\rangle$$
$$\hat{P}_x(\omega) = \frac{1}{m^2} \frac{2\gamma k_B T m^2}{(\omega_0^2 - \omega^2 - i\omega\frac{\gamma}{m})(\omega_0^2 - \omega^2 + i\omega\frac{\gamma}{m})},$$

where we leverage the Fourier transform of the correlation function of the noise. Leveraging the Wiener-Kinchin theorem, we can now obtain the correlation function of x as,

$$C_x(t) = \frac{2\gamma k_B T}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{(\omega_0^2 - w^2)^2 + \frac{\gamma^2}{m^2}\omega^2}.$$

We solve this integral with the residue theorem. Since the exponent is located in the negative half plane, we take a clockwise contour of the lower half plane resulting in,

$$C_x(t) = \frac{\gamma k_B T}{\pi}(-2\pi i) \sum \text{residues}$$

The roots of the denominator are located at

$$\omega = \pm\frac{i\gamma}{2m} \pm \sqrt{\omega_0^2 - \frac{\gamma^2}{4m^2}}.$$

When $\omega_0^2 - \frac{\gamma^2}{4m^2} > 0$, we are in the underdamped regime, in which the harmonic oscillations dominate over the damping, and so we have two poles in the negative half plane,

$$\omega = \pm\omega_1 - i\frac{\gamma}{2m},$$

resulting in,

$$\begin{aligned}
C_x(t) &= \gamma k_B T(-2i) \left[\frac{e^{-i(\omega_1 - i\frac{\gamma}{2m})t}}{(2\omega_1)(2\omega_1 - i\frac{\gamma}{m})(-i\frac{\gamma}{m})} + \frac{e^{-i(-\omega_1 - i\frac{\gamma}{2m})t}}{(-2\omega_1)(-2\omega_1 - i\frac{\gamma}{m})(-i\frac{\gamma}{m})} \right] \\
&= \gamma k_B T(-2i) \left[\frac{e^{-\omega_1 t} e^{-\frac{\gamma}{2m}t}(2\omega_1 + i\frac{\gamma}{m}) + e^{\omega_1 t} e^{-\frac{\gamma}{2m}t}(2\omega_1 - i\frac{\gamma}{m})}{(-2i)\frac{\gamma}{m}\omega_1 4\omega_0^2} \right] \\
&= \frac{k_B T m}{4\omega_0^2} \frac{e^{-\frac{\gamma}{2m}t}}{\omega_1} \left[2\omega_1 \left(e^{i\omega_1 t} + e^{-i\omega_1 t} \right) + i\frac{\gamma}{m} \left(e^{-i\omega_1 t} - e^{i\omega_1 t} \right) \right] \\
&= \frac{k_B T m}{\omega_0^2} e^{-\frac{\gamma}{2m}t} \left(\cos\omega_1 t + \frac{\gamma}{2m\omega_1} \sin\omega_1 t \right),
\end{aligned}$$

And so in the underdamped regime the autocorrelation function exhibits an oscillatory component. When $\omega_0^2 - \frac{\gamma^2}{4m^2} < 0$, we are in the overdamped regime, in which the damping dominates the dynamics and oscillations are no longer present. In this case we also have two poles in the negative half plane,

$$\omega = \pm i\hat{\omega}_1 - i\frac{\gamma}{2m},$$

where $\hat{\omega}_1^2 = \frac{\gamma^2}{4m} - \omega_0^2$, and thus $\frac{\gamma}{2m} > \sqrt{\frac{\gamma^2}{4m} - \omega_0^2}$. In this case, the correlation function becomes,

$$\begin{aligned}
C_x(t) &= \gamma k_B T(-2i) \left[\frac{e^{-i(i\hat{\omega}_1 - i\frac{\gamma}{2m})t}}{(2i\hat{\omega}_1)(2\hat{\omega}_1 - i\frac{\gamma}{m})(-i\frac{\gamma}{m})} + \frac{e^{-i(-i\hat{\omega}_1 - i\frac{\gamma}{2m})t}}{(-2i\hat{\omega}_1)(-2i\hat{\omega}_1 - i\frac{\gamma}{m})(-i\frac{\gamma}{m})} \right] \\
&= \gamma k_B T(-2i) \left[\frac{e^{\hat{\omega}_1 t} e^{-\frac{\gamma}{2m}t}(2\hat{\omega}_1 + \frac{\gamma}{m}) + e^{-\hat{\omega}_1 t} e^{-\frac{\gamma}{2m}t}(2\hat{\omega}_1 - \frac{\gamma}{m})}{(-2i)\frac{\gamma}{m}\hat{\omega}_1 4\omega_0^2} \right] \\
&= \frac{k_B T m}{4\omega_0^2} \frac{e^{-\frac{\gamma}{2m}t}}{\hat{\omega}_1} \left[2\hat{\omega}_1 \left(e^{\hat{\omega}_1 t} + e^{-\hat{\omega}_1 t} \right) + i\frac{\gamma}{m} \left(e^{\hat{\omega}_1 t} - e^{-\hat{\omega}_1 t} \right) \right] \\
&= \frac{k_B T m}{\omega_0^2} e^{-\frac{\gamma}{2m}t} \left(\cosh\hat{\omega}_1 t + \frac{\gamma}{2m\hat{\omega}_1} \sinh\hat{\omega}_1 t \right),
\end{aligned}$$

and so the oscillatory behavior of the correlation function vanishes accordingly.