0.1 Variational methods

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Example 1 (Overdamped harmonic oscillator with variational methods)**:**

Consider a particle immersed in a harmonic potential $U(x) = m\omega^2 x^2/2$ and subject to thermal noise, moving in a viscous medium. In the **overdamped limit** $m/\gamma \to 0$ (where $\gamma = 6\pi\eta a$, with η the medium's viscosity and a the particle's radius), the equation of motion becomes:

$$\mathrm{d}x(t) = -kx(t)\,\mathrm{d}t + \sqrt{2D}\,\mathrm{d}B(t) \qquad k = \frac{m\omega^2}{\gamma}$$

A path $\{x(\tau)\}$ solving that equation has a *infinitesimal* probability given by:

$$\mathrm{d}P = \left(\prod_{\tau=0^+}^{t} \frac{\mathrm{d}x(\tau)}{\sqrt{4\pi D\,\mathrm{d}\tau}}\right) \exp\left(-\frac{1}{4D}\int_0^t (\dot{x} + kx)^2\,\mathrm{d}\tau\right)$$

as we already derived. We are now interested in computing the transition probabilities:

$$W(x, t|x_0, 0) = \int_{\mathbb{R}^T} \delta(x(t) - x)\,\mathrm{d}P$$

Following the variational method, we arrive to:

$$W(x, t|x_0, 0) = \Phi(t) \exp\left(-\frac{1}{4D} S[x_c(\tau)]\right) \tag{1}$$

where S is the *action functional* for the harmonic potential:

$$S[x(\tau)] = \int_0^t L(\dot{x}, x)\,\mathrm{d}\tau \qquad L(\dot{x}, x) = (\dot{x} + kx)^2$$

and $x_c(\tau)$ is the path that *stationarizes* $S[x(\tau)]$, meaning that $\delta S[x_c(\tau)] = 0$ and so it satisfies the Euler-Lagrange equation:

$$0 \overset{!}{=} \frac{\partial L}{\partial x}\Big|_{x_c} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}}\Big|_{x_c} = 2k(\dot{x}_c + kx_c) - 2(\ddot{x}_c + k\dot{x}_c) = 2(k^2 x_c - \ddot{x}_c)$$

as:

$$\frac{\partial L}{\partial x} = 2k(\dot{x} + kx)$$
$$\frac{\partial L}{\partial \dot{x}} = 2(\dot{x} + kx)$$

So, to find $x_c(\tau)$ we need to solve:

$$\begin{cases} \ddot{x}_c = k^2 x_c \\ x_c(0) = x_0 \\ x_c(t) = x \end{cases}$$

This is the second order ordinary differential equation for an *harmonic repulsor*, which has the following general integral:

$$x_c(\tau) = Ae^{k\tau} + Be^{-k\tau}$$

Imposing the boundary conditions leads to:

$$\begin{cases} x_0 \overset{!}{=} A + B \\ x \overset{!}{=} Ae^{kt} + Be^{-kt} \end{cases} \Rightarrow \begin{cases} B = x_0 - A \\ xe^{kt} = Ae^{2kt} + B \end{cases} \Rightarrow xe^{kt} - x_0 = A[e^{2kt} - 1]$$

$$\Rightarrow A = \frac{xe^{kt} - x_0}{e^{2kt} - 1}\frac{e^{-kt}}{e^{-kt}} = \frac{(xe^{kt} - x_0)e^{-kt}}{\frac{e^{kt} - e^{-kt}}{2} 2} = \frac{x - x_0 e^{-kt}}{2\sinh(kt)}$$

$$B = x_0 - A = -\frac{x - x_0 e^{kt}}{2\sinh(kt)} = 2$$

Then we evaluate the action at the stationary path $x_c(\tau)$:

$$S[x_c(\tau)] = \int_0^t (\dot{x} + kx)^2 \, \mathrm{d}\tau = \int_0^t [2kAe^{k\tau}]^2 \, \mathrm{d}\tau = 4k^2A^2 \frac{1}{2k} e^{2k\tau}\Big|_0^t =$$

$$= 4kA^2 \frac{e^{2kt} - 1}{2} \frac{e^{-kt}}{e^{-kt}} = 4kA^2 \sinh(kt) \, e^{kt} =$$

$$= \cancel{4}k \frac{(x - x_0 e^{-kt})^2}{\cancel{4}\sinh(kt)} e^{kt} = \frac{k(x - x_0 e^{-kt})^2}{e^{kt} - e^{-kt}} \frac{2}{e^{-kt}} = \frac{2k(x - x_0 e^{-kt})^2}{1 - e^{-2kt}}$$

Substituting back in (1):

$$W(x, t|x_0, 0) = \Phi(t) \exp\left(-\frac{k}{2D(1 - e^{-2kt})}[x - x_0 e^{-kt}]^2\right)$$

All that's left to find $\Phi(t)$ is to use the normalization condition:

$$1 \overset{!}{=} \int_{\mathbb{R}} \mathrm{d}x \, W(x, t|x_0, 0) = \Phi(t) \int_{\mathbb{R}} \mathrm{d}x \exp\left(-\overbrace{\frac{k}{2D(1 - e^{-2kt})}}^{\alpha}[x - x_0 e^{-kt}]^2\right) =$$

$$= \Phi(t)\sqrt{\frac{\pi}{\alpha}} = \Phi(t)\sqrt{\frac{2\pi D(1 - e^{-2kt})}{k}} \Rightarrow \Phi(t) = \sqrt{\frac{k}{2\pi D}} \frac{1}{\sqrt{1 - e^{-2kt}}}$$

And so the full solution is:

$$W(x, t|x_0, 0) = \sqrt{\frac{k}{2\pi D}} \frac{1}{\sqrt{1 - e^{-2kt}}} \exp\left(-\frac{k}{2D} \frac{(x - x_0 e^{-kt})^2}{(1 - e^{-2kt})}\right)$$

$$\xrightarrow[t \to \infty]{} \sqrt{\frac{k}{2\pi D}} \exp\left(-\frac{k}{2Dx^2}\right)$$

As before, we can compute the $t \to \infty$ with a Maxwell-Boltzmann distribution $e^{-\beta U(x)}$, obtaining:

$$\frac{1}{2}\beta m\omega^2 x^2 = \frac{k}{2D}x^2 \Rightarrow D = \frac{k}{\beta m\omega^2} = \frac{1}{\beta\gamma} = \frac{k_B T}{\gamma} \Rightarrow D\gamma = k_B T$$

as we previously derived.

If we do not consider the overdamped limit, however, the equation of motion is given by:

$$m\ddot{x} = -\gamma\dot{x} - m\omega^2 x + \sqrt{2D}\gamma\xi$$

This can be rewritten as a system of two first order (stochastic) differential equations:

$$\begin{cases} \mathrm{d}x\,(\tau) = v(\tau)\,\mathrm{d}\tau \\ \mathrm{d}v\,(\tau) = -\dfrac{\gamma}{m}v(\tau)\,\mathrm{d}\tau + \dfrac{\gamma\sqrt{2D}}{m}\,\mathrm{d}B \end{cases}$$

It is convenient to "symmetrize" the system, by adding a stochastic term also in the first equation:

$$\begin{cases} \mathrm{d}x\,(\tau) = v(\tau)\,\mathrm{d}\tau + 2\hat{D}\sqrt{\mathrm{d}\hat{B}} \\ \mathrm{d}v\,(\tau) = -\dfrac{\gamma}{m}v(\tau)\,\mathrm{d}\tau + \dfrac{\gamma\sqrt{2D}}{m}\,\mathrm{d}B \end{cases}$$

and then we'll consider the limit $\hat{D} \to 0$.
First, as usual, we discretize, with $\{t_i\}_{i=0,\dots,n}$ and $t_0 \equiv 0$, $t_n \equiv t$, arriving to:

$$\begin{cases} \Delta x_i = v_{i-1}\Delta t_i + \sqrt{2\hat{D}}\Delta\hat{B}_i \\ \Delta v_i = -\dfrac{\gamma}{m}v_{i-1}\Delta t_i + \dfrac{\gamma}{m}\sqrt{2D}\Delta B_i \end{cases}$$

Where the velocity is evaluated at t_{i-1} as per Ito's prescription. As ΔB_i and $\Delta\hat{B}_i$ are **independent** gaussian increments, their joint distribution is just a product:

$$\mathrm{d}P\left(\Delta B_1, \Delta\hat{B}_1, \dots, \Delta B_n, \Delta\hat{B}_n\right) = \left(\prod_{i=1}^{n} \frac{\mathrm{d}\Delta B_i}{\sqrt{2\pi\Delta t_i}} \frac{\mathrm{d}\Delta\hat{B}_i}{\sqrt{2\pi\Delta t_i}}\right) \exp\left(-\frac{1}{2}\sum_{i=1}^{n}\frac{\Delta B_i^2}{\Delta t_i} - \frac{1}{2}\sum_{i=1}^{n}\frac{\Delta\hat{B}_i^2}{\Delta t_i}\right)$$

As done previously (see 14/11 notes), to get the distribution for Δx_i and Δv_i we make a change of random variables:

$$\begin{aligned} \Delta\hat{B}_i &= \frac{\Delta x_i - v_{i-1}\Delta t_i}{\sqrt{2\hat{D}}} \\ \Delta B_i &= \left(\Delta v_i + \frac{\gamma}{m}v_{i-1}\Delta t_i\right)\frac{m}{\gamma\sqrt{2D}} \end{aligned}$$

with jacobian:

$$\det\left|\frac{\partial\{\Delta\hat{B}_i\}}{\partial\{\Delta x_i\}}\right| = (2\hat{D})^{-n/2}$$

$$\det\left|\frac{\partial\{\Delta B_i\}}{\partial\{\Delta x_i\}}\right| = \det\left|\frac{\partial\{\Delta x_i\}}{\partial\{\Delta B_i\}}\right|^{-1} = \left(\frac{\gamma}{m}\sqrt{2D}\right)^{-n} = \left(\frac{\gamma^2}{m^2}2D\right)^{-n/2}$$

leading to:

$$
\begin{aligned}
\mathrm{d}P\left(\{\Delta x_i\},\{\Delta v_i\}\right) = &\left(\prod_{i=1}^{n} \frac{\mathrm{d}\Delta x_i}{\sqrt{4\pi D\Delta t_i}} \frac{\mathrm{d}\Delta v_i}{\sqrt{4\pi D\Delta t_i \gamma^2/m^2}}\right)\cdot \\
&\cdot \exp\left(-\frac{1}{2}\sum_{i=1}^{n} \frac{m^2}{2\gamma^2 D}\left[\left(\frac{\Delta v_i + \gamma/m v_{i-1}\Delta t_i}{\Delta t_i}\right)^2 \Delta t_i\right]\right)\cdot \\
&\cdot \exp\left(-\frac{1}{2}\sum_{i=1}^{n} \frac{1}{2\hat{D}}\left[\left(\frac{\Delta x_i - v_{i-1}\Delta t_i}{\Delta t_i}\right)^2 \Delta t_i\right]\right) = \\
= &\left(\prod_{i=1}^{n} \frac{\mathrm{d}\Delta x_i}{\sqrt{4\pi D\Delta t_i}} \frac{\mathrm{d}\Delta v_i}{\sqrt{4\pi D\Delta t_i \gamma^2/m^2}}\right)\cdot \\
&\cdot \exp\left(-\frac{m^2}{4D\gamma^2}\sum_{i=1}^{n}\left[\left(\frac{\Delta v_i}{\Delta t_i} + \frac{\gamma}{m} v_{i-1}\right)^2 \Delta t_i\right]\right)\cdot \\
&\cdot \exp\left(-\frac{1}{4\hat{D}}\sum_{i=1}^{n}\left[\left(\frac{\Delta x_i}{\Delta t_i} - v_{i-1}\right)^2 \Delta t_i\right]\right)
\end{aligned} \tag{2}
$$

Taking the continuum limit $n \to \infty$ leads to:

$$
\begin{aligned}
\mathrm{d}P\left(\{x(\tau), v(\tau)\}\right) = &\left(\prod_{\tau=0^+}^{t} \frac{\mathrm{d}x(\tau)}{\sqrt{4\pi \hat{D}\,\mathrm{d}\tau}} \frac{\mathrm{d}v(\tau)}{\sqrt{4\pi D\,\mathrm{d}\tau\,\gamma^2/m^2}}\right)\cdot \\
&\cdot \exp\left(-\frac{m^2}{4D\gamma^2}\int_0^t \mathrm{d}\tau\left[\dot{v}(\tau) + \frac{\gamma}{m}v(\tau)\right]^2 - \frac{1}{4\hat{D}}\int_0^t \mathrm{d}\tau\,[\dot{x}(\tau) - v(\tau)]^2\right)
\end{aligned}
$$

In the limit $\hat{D} \to 0^+$, $1/(4\hat{D}) \to +\infty$, and so the gaussian pdf for the $\Delta\hat{B}_i$ becomes *infinitely thin*, and the only path with a non-vanishing probability will be the one where:

$$
\int_0^t \mathrm{d}\tau\,[\dot{x} - v(\tau)]^2 = 0
$$

As any > 0 value will lead to $\exp(-\infty) = 0$. In particular, the i-th factor of the discretization becomes:

$$
\begin{aligned}
&\frac{1}{\sqrt{4\pi\hat{D}\Delta t_i}} \exp\left[-\frac{1}{4\hat{D}}\left(\frac{\Delta x_i}{\Delta t_i} - v_0^2\right)\Delta t_i\right] = \\
&= \frac{1}{\sqrt{4\pi\hat{D}\Delta t_i}} \exp\left(-\frac{1}{4\hat{D}\Delta t_i}(\Delta x_i - v_{i-1}\Delta t_i)^2\right) \xrightarrow[\hat{D}\to 0]{} \delta(\Delta x_i - v_{i-1}\Delta t_i)
\end{aligned}
$$

where we used a limit definition for the δ:

$$
\lim_{\epsilon\to 0} \frac{1}{\sqrt{4\pi\epsilon}} \exp\left(-\frac{x^2}{4\epsilon}\right) = \delta(x)
$$

with $\epsilon = \hat{D}\Delta t_i$ and $x = \Delta x_i - v_{i-1}\Delta t_i$.

Substituting back in (2):

$$
\mathrm{d}P\left(\{\Delta x_i\},\{\Delta v_i\}\right)=\left(\prod_{i=1}^{n}\mathrm{d}\Delta x_i\,\delta(\Delta x_i-v_{i-1}\Delta t_i)\frac{\mathrm{d}\Delta v_i}{\sqrt{4\pi D\Delta t_i\gamma^2/m^2}}\right)\cdot
\\
\cdot\exp\left(-\frac{m^2}{4D\gamma^2}\sum_{i=1}^{n}\left[\left(\frac{\Delta v_i}{\Delta t_i}+\frac{\gamma}{m}v_{i-1}\right)^2\Delta t_i\right]\right)
$$

Now consider the discretized transition probability:

$$
\begin{aligned}
W(x_n,v_n,t_n|x_0,v_0,0)&=\int_{\mathbb{R}^n\times\mathbb{R}^n}\mathrm{d}P\left(\{x_i,v_i\}\right)\delta(x_n-x)\delta(v_n-x)= &(3)\\
&=\int_{\mathbb{R}^n\times\mathbb{R}^n}\left(\prod_{i=1}^{n}\mathrm{d}\Delta x_i\,\delta(\Delta x_i-v_{i-1}\Delta t_i)\frac{\mathrm{d}\Delta v_i}{\sqrt{4\pi D\Delta t_i\gamma^2/m^2}}\right)\cdot\\
&\quad\cdot\exp\left(-\frac{m^2}{4D\gamma^2}\sum_{i=1}^{n}\left[\left(\frac{\Delta v_i}{\Delta t_i}+\frac{\gamma}{m}v_{i-1}\right)^2\Delta t_i\right]\right)\delta(v_n-v)\delta(x_n-x)
\end{aligned}
$$

Let's focus on the integrations over x_i:

$$
\begin{aligned}
&\int_{\mathbb{R}^n}\left(\prod_{i=1}^{n}\mathrm{d}\Delta x_i\,\delta(\Delta x_i-v_{i-1}\Delta t_i)\right)\delta(x_n-x)=\\
&=\int_{\mathbb{R}^n}\mathrm{d}\Delta x_1\ldots\mathrm{d}\Delta x_n\,\delta(\Delta x_1-v_0\Delta t_1)\ldots\delta(\Delta x_n-v_{n-1}\Delta t_n)\delta(x_n-x)
\end{aligned}
$$

We then perform the change of variables $\Delta x_1=x_1-x_0$, with x_0 constant, so that $\mathrm{d}\Delta x_1=\mathrm{d}x_1$. Then we integrate over $\mathrm{d}x_1$, eliminating the first δ and setting $x_1=x_0-v_0\Delta t_1$:

$$
\int_{\mathbb{R}^n}\mathrm{d}x_1\,\mathrm{d}\Delta x_2\ldots\mathrm{d}\Delta x_n\,\delta(x_1-x_0-v_0\Delta t_1)\delta(\Delta x_2-v_1\Delta t_2)\ldots\delta(\Delta x_n-v_{n-1}\Delta t_n)\delta(x_n-x)=
\\
\int_{\mathbb{R}^{n-1}}\mathrm{d}\Delta x_2\ldots\mathrm{d}\Delta x_n\,\delta(x_2-x_0-v_0\Delta t_1-v_1\Delta t_2)\ldots\delta(\Delta x_n-v_{n-1}\Delta t_n)\delta(x_n-x)
$$

Repeating these steps for all the other variables except the last one, we arrive to:

$$
=\int_{\mathbb{R}}\mathrm{d}x_n\,\delta\left(x_n-x_0-\sum_{i=1}^{n}v_{i-1}\Delta t_i\right)\delta(x_n-x)=\delta\left(x-x_0-\sum_{i=1}^{n}v_{i-1}\Delta t_i\right)
$$

In the continuum limit, this becomes:

$$
\delta\left(x-x_0-\int_0^t v(\tau)\,\mathrm{d}\tau\right)
$$

Substituting back in (3) and finally taking the limit $n\to\infty$:

$$
W(x,v,t|x_0,v_0,0)=\int_{\mathbb{R}^T}\left(\prod_{\tau=0^+}^{t}\frac{\mathrm{d}v(\tau)}{\sqrt{4\pi D\,\mathrm{d}\tau\,\gamma/m^2}}\right)\exp\left(-\frac{m^2}{4D\gamma}\int_0^t\left(\dot v(\tau)+\frac{\gamma}{m}v(\tau)\right)^2\mathrm{d}\tau\right)
\\
\cdot\,\delta(v(t)-v)\delta\left(x-x_0-\int_0^t v(\tau)\,\mathrm{d}\tau\right)
$$

We can now use the variational method to compute that integral. So, let $v_c(\tau)$ be the path, starting at $v(0) = v_0$ that *stationarizes* the action functional:

$$S[v(\tau)] = \int_0^t \left(\dot{v}(\tau) + \frac{\gamma}{m} v(\tau)\right)^2 \mathrm{d}\tau$$

so that $\delta S[v_c(\tau)] = 0$, and also satisfies the constraints imposed by the δ:

$$v(t) \stackrel{!}{=} v \qquad x - x_0 \stackrel{!}{=} \int_0^t v(\tau)\,\mathrm{d}\tau$$

Then, the path integral is given by:

$$W(x, v, t|x_0, v_0, 0) = \Phi(t) \exp\left(-\frac{m^2}{4D\gamma} \int_0^t \left(\dot{v}_c(\tau) + \frac{\gamma}{m} v_c(\tau)\right)^2 \mathrm{d}\tau\right) \tag{4}$$

All that's left is to compute $v_c(\tau)$ and evaluate the integral. This is a problem of *constrained optimization*, for which we use the method of Lagrange multipliers.

Brief refresher of Lagrange multipliers. Suppose we have two functions $F, g\colon \mathbb{R}^2 \to \mathbb{R}$, with $F(x, y)$ being the function to maximize, and $g(x, y) = c \in \mathbb{R}$ a constraint. A stationary point (x_0, y_0) of F subject to the constraint $g(x, y) = c$ is such that if we move slightly from (x_0, y_0) along the contour $g(x, y) = c$, the value of $F(x, y)$ does not change (to first order). This happens if the contour of F passing through the stationary point $F(x, y) = F(x_0, y_0)$ is parallel at (x_0, y_0) to that of $g(x, y) = c$, meaning that at (x_0, y_0) the gradients of F and g are parallel:

$$\nabla_{x,y} F = \lambda \nabla_{x,y} g \qquad \lambda \in \mathbb{R}$$

(Here we assume that $\nabla_{x,y} g(x_0, y_0) \neq \mathbf{0}$). Rearranging:

$$\nabla_{x,y}(F(x, y) - \lambda g(x, y)) = \mathbf{0}$$

Together with the constraint equation $g(x, y) = c$, we have now 3 equations in 3 unknowns (x, y, λ) that can be solve to yield the desired stationary point (x_0, y_0).

In this case, we have *functionals* instead of functions, and *functionals derivatives* (i.e. variations) instead of derivatives. So, to find the stationary points of:

$$\int_0^t \left(\dot{v}(\tau) + \frac{\gamma}{m} v(\tau)\right)^2 \mathrm{d}\tau \qquad (a)$$

subject to the constraint:

$$\int_0^t v(\tau)\,\mathrm{d}\tau = x - x_0 \qquad (b)$$

we need to solve:

$$\delta \int_0^t \underbrace{\left[\left(\dot{v}(\tau) + \frac{\gamma}{m} v(\tau)\right)^2 - \lambda v(\tau)\right]}_{L(v, \dot{v})} \mathrm{d}\tau = 0$$

And applying the definition of first variation (the δ above) leads to solving the Euler-Lagrange equations:

$$\frac{\partial L}{\partial v} - \frac{\mathrm{d}}{\mathrm{d}\tau}\frac{\partial L}{\partial \dot{v}}\bigg|_{v=v_c} \stackrel{!}{=} 0$$

Expanding the computations:

$$2\left(\dot{v}_c + \frac{\gamma}{m}v_c\right)\frac{\gamma}{m} - \lambda - \frac{\mathrm{d}}{\mathrm{d}\tau}\left[2\left(\dot{v}_c + \frac{\gamma}{m}v_c\right)\right] = 0 \Rightarrow \ddot{v}_c(\tau) = v_c(\tau)\left(\frac{\gamma}{m}\right)^2 - \frac{\lambda}{2}$$

The homogeneous solution is again a combination of exponentials:

$$v_c(\tau) = A\exp\left(-\frac{\gamma}{m}\tau\right) + B\exp\left(\frac{\gamma}{m}\tau\right)$$

And for the inhomogeneous general integral we just need to add a particular solution, for example the one with constant velocity $\dot{v}(\tau) = \text{const} \Rightarrow \ddot{v}_c(\tau) = 0$, given by:

$$v_c(\tau) = \frac{\lambda}{2}\left(\frac{m}{\gamma}\right)^2$$

Then, we need to impose the boundary conditions:

$$v_c(0) = v_0 \qquad v_c(t) = v \qquad \int_0^t v(\tau)\,\mathrm{d}\tau = (x - x_0)$$

So we have 3 parameters (the two constants of integration A, B and λ) and 3 equations. After finding all of them, we just need to evaluate the integral (4) (computations omitted).