The Feynman-Kac formula

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1 The Wiener process (Brownian motion)

Consider the Hilbert space $L^2(\mathbf{R}^d)$ and the self-adjoint operator

$$H_0 = -\frac{\sigma^2}{2}\Delta, \tag{1}$$

where Δ is the Laplace operator. Here $\sigma^2 > 0$ is a constant (the *diffusion constant*). It has dimensions of distance squared over time, so H_0 has dimensions of inverse time. The operator $\exp(-tH_0)$ for $t > 0$ is an self-adjoint integral operator, which gives the solution of the heat or diffusion equation. Here t is the time parameter. It is easy to solve for this operator by Fourier transforms. Since the Fourier transform of H_0 is the operator of multiplication by $(\sigma^2/2)k^2$, the Fourier transform of $\exp(-tH_0)$ is multiplication by $\hat{g}_t(k) = \exp(-t(\sigma^2/2)k^2)$. Therefore the operator $\exp(-tH_0)$ itself is convolution by the inverse Fourier transform. This is a Gaussian with mean zero and variance $\sigma^2 t$ in each component, that is,

$$g_t(x) = \left(\frac{1}{\sqrt{2\pi\sigma^2 t}}\right)^d \exp(-\frac{x^2}{2\sigma^2 t}). \tag{2}$$

In other words,

$$(\exp(-tH_0)f)(x) = \int g_t(x-y)f(y)\,dy. \tag{3}$$

This is interpreted in terms of a diffusing particle that starts at position x at time 0. At time t the probability density as a function of y is $g_t(x-y)$.

The idea of the Wiener process (or Brownian motion process) is to describe this diffusion in more detail, at more than one instant of time. Let C_x be the space of all continuous functions ω from $[0,+\infty)$ to $\mathbf{R}^d$ with $\omega(0) = x$. Each element of C_x is interpreted as a possible path of a diffusing particle starting at x. The Wiener process is a probability measure defined on measurable subsets of C_x. It defines an expectation E_x defined on bounded measurable functions defined on C_x. One kind of measurable function F on C_x is defined as follows. Let $0 < t_1 < t_2 < \ldots < t_n$ be time instants. Let f be a bounded measurable function on $\mathbf{R}^n$. Then $F(\omega) = f(\omega(t_1), \ldots, \omega(t_n))$ defines a function on C_x.

Theorem 1 (Existence of Wiener process) *There exists a unique probability measure on C_x such that its expectation satisfies*

$$E_x[F(\omega)] = \int \cdots \int g_{t_1}(x-y_1) g_{t_2-t_1}(y_1-y_2) \cdots g_{t_n-t_{n-1}}(y_{n-1}-y_n) f(y_1, \ldots, y_n)\, dy_1 \cdots dy_n. \tag{4}$$

This probability measure defines the Wiener process. It is not hard to see that the random variables $\omega(t)$ are Gaussian random variables with value in $\mathbf{R}^d$ with mean vector $E_x[\omega(t)] = x$ and covariance matrix $E_x[(\omega(t_1) - x)(\omega(t_2) - x)'] = \sigma^2 I t_1$ for $t_1 \leq t_2$.

2 The Feynman-Kac formula

This section presents the Feynman-Kac formula. Feynman invented this in the context of quantum mechanics; Kac gave a diffusion version. Here we mainly stay in the Kac framework.

Let V be a real function on $\mathbf{R}^d$, say continuous and bounded below. This has the dimensions of inverse time. Then V defines an operator V defined by multiplication: $(Vf)(x) = V(x)f(x)$. Then

$$H = H_0 + V \tag{5}$$

is a self-adjoint operator. Therefore for $t > 0$ the operator $\exp(-tH)$ is a self-adjoint operator. Computing this operator is a major challenge.

When $V \geq 0$ this operator has a diffusion interpretation. The quantity $V(y)$ represents the rate of killing at the point y. That is, when the diffusing particle reaches y, then it has some chance of vanishing, and this is determined by the killing rate at y. So if we write

$$(\exp(-tH)f)(x) = \int g_t^V(x, y) f(y)\, dy \tag{6}$$

then $g_t^V(x, y)$ represents the defective probability density as a function of y for a particle that has started at x and time 0 and diffused to y without vanishing. The integral of this defective density is less than or equal to one.

Theorem 2 (Feynman-Kac) *If $H = H_0 + V$, where V is the operator corresponding to multiplication by a continuous function that is bounded below, then*

$$(\exp(-tH)f)(x) = E_x[\exp(-\int_0^t V(\omega(s))\, ds) f(\omega(t))]. \tag{7}$$

This is the Feynman-Kac formula. One proof uses the Trotter product formula and the dominated convergence theorem. The Trotter product formula is a general theorem of operator theory. It says that

$$\exp(-tH)f = \lim_{n\to\infty} (\exp(-tH_0/n)\exp(-tV/n))^n f. \tag{8}$$

We can write this explicitly using the Wiener process. It says that

$$(\exp(-tH)f)(x) = \lim_{n\to\infty} E_x[\exp(-\sum_{j=1}^{n} V(\omega(j\frac{t}{n}))\frac{t}{n})f(\omega(t))]. \tag{9}$$

By the dominated convergence theorem this becomes the Feynman-Kac formula.

The interpretation of the Feynman-Kac formula is that to find out the defective probability density one can follow along each possible possible path of the diffusing particle and take the exponential of the integrated rate of killing along that path. Then an average over paths gives the result. Notice that when $\beta > 0$ is large the effect of the starting point x is less, and the largest contribution to the final defective density comes from the places y where $V(y)$ is smallest.

The Feynman path integral formula of quantum mechanics is the analogous formula for $(\exp(-itH)f)(x)$. This requires a Wiener process with a pure imaginary variance parameter $i\sigma^2$. Unfortunately, it is hard to make rigorous. The Trotter product formula part of the proof continues to work. However the passage to the limit via the dominated convergence theorem no longer works.

3 The Brownian bridge

The Brownian bridge is a Wiener process (or Brownian motion) conditioned to return to the starting point at a certain time.

Let $\beta > 0$ be a fixed time. The Brownian bridge is the image of the Wiener measure under the map that sends ω into ω_B, where $0 \le t \le \beta$ and

$$\omega_B(t) = \omega(t) - \frac{t}{\beta}(\omega(\beta) - x). \tag{10}$$

Thus the Brownian bridge is the measure whose expectation is

$$E^{\beta}_{xx}[F(\omega)] = E_x[F(\omega_B)]. \tag{11}$$

It is not hard to see that with respect to the Brownian bridge the random variables $\omega(t)$ are Gaussian random variables with value in $\mathbf{R}^d$ with mean vector $E^{\beta}_{xx}[\omega(t)] = x$ and covariance matrix $E^{\beta}_{xx}[(\omega(t_1) - x)(\omega(t_2) - x)'] = \sigma^2 I t_1(\beta - t_2)/\beta$ for $t_1 \le t_2$. In particular, the variance of $\omega(t)$ is

$$E^{\beta}_{xx}[(\omega(t) - x)(\omega - x)'] = \sigma^2 I \frac{t(\beta - t)}{\beta} = \sigma^2 I \frac{1}{\frac{1}{t} + \frac{1}{\beta - t}}. \tag{12}$$

In other words, one take the harmonic mean of the variances of the Wiener process at times t and $\beta - t$.

Next we prove the identity that says that the Wiener process conditioned on $\omega(\beta) = x$ gives the same results as the Brownian bridge. In other words,

$$E^{\beta}_{xx}[F(\omega)] = \frac{E_x[F(\omega)\delta(\omega(\beta) - x)]}{E_x[\delta(\omega(\beta) - x)]}. \tag{13}$$

Notice, by the way, that the denominator

$$E_x[\delta(\omega(\beta) - x)] = g_\beta(0). \tag{14}$$

The Wiener measure covariance of $\omega_B(t)$ with $\omega(\beta)$ is zero, so these variables are independent. When $\omega(\beta) = x$ we have $\omega = \omega_B$. So

$$\frac{E_x[F(\omega)\delta(\omega(\beta - x)]}{E_x[\delta(\omega(\beta) - x)]} = \frac{E_x[F(\omega_B)\delta(\omega(\beta - x)]}{E_x[\delta(\omega(\beta - x)]} = E_x[F(\omega_B)] = E^\beta_{xx}[F(\omega)]. \tag{15}$$

Here is a calculation that illustrates these ideas. By writing the Brownian bridge as a conditional Wiener measure we get

$$E^\beta_{xx}[f(\omega_B(t))] = \frac{1}{g_\beta(0)} \int g_t(x-y) f(y) g_{\beta-t}(y-x)\, dy. \tag{16}$$

However it is easy to compute that $g_t(x-y)g_{\beta-t}(x-y)/g_\beta(0) = g_\tau(x-y)$, where $\tau = t(\beta - t)/\beta$, as in the formula for the variance of the Brownian bridge at t. So this is also

$$E^\beta_{xx}[f(\omega_B(t))] = \int g_\tau(x-y) f(y)\, dy. \tag{17}$$

4 The trace

It is particularly important in quantum statistical mechanics to compute

$$\mathrm{tr}(\exp(-\beta H)) = \int g^V_\beta(x,x)\, dx. \tag{18}$$

We only expect this trace to exist in a case when H has a discrete spectrum, which may happen when $V(x)$ goes to $+\infty$ as $|x| \to \infty$.

This is done using the Feynman-Kac formula

$$g^V_\beta(x,y) = E_x[\exp(-\int_0^\beta V(\omega(t))\, dt)\delta(\omega(\beta) - y)]. \tag{19}$$

Hence

$$\mathrm{tr}(\exp(-\beta H)) = \int E_x[\exp(-\int_0^\beta V(\omega(t))\, dt)\delta(\omega(\beta) - x)]\, dx. \tag{20}$$

For large time β the dominant contribution should come from the places where the least killing has taken place, which is where $V(y)$ is small.

Theorem 3 *The trace is expressed in terms of the Brownian bridge as*

$$\mathrm{tr}(\exp(-\beta H)) = g_\beta(0) \int E^\beta_{xx}[\exp(-\int_0^\beta V(\omega(t))\, dt)]\, dx. \tag{21}$$

It says that the trace is the product of a term that does not depend on the function V times a perfectly reasonable expectation with respect to the Brownian bridge.

Theorem 4 *The quantum trace is bounded above by the classical trace. That is, we have*

$$\mathrm{tr}(\exp(-\beta H)) \leq \int \int \exp(-\beta[\frac{\sigma^2}{2}k^2 + V(y)]) \frac{dk\,dy}{(2\pi)^d}. \tag{22}$$

The proof is obtained by applying Jensen's inequality to the time integral in the exponent. This gives

$$\exp(-\frac{1}{\beta}\int_0^\beta \beta V(\omega(t))\,dt) \leq \frac{1}{\beta}\int_0^\beta \exp(-\beta V(\omega(t)))\,dt. \tag{23}$$

This gives

$$\mathrm{tr}(\exp(-\beta H)) \leq g_\beta(0)\frac{1}{\beta}\int_0^\beta E_{00}^\beta[\int \exp(-\beta V(x+\omega(t))\,dx]\,dt. \tag{24}$$

By the translation invariance of Lebesgue measure this gives

$$\mathrm{tr}(\exp(-\beta H)) \leq g_\beta(0)\frac{1}{\beta}\int_0^\beta E_{00}^\beta[\int \exp(-\beta V(x))\,dx]\,dt. \tag{25}$$

The integrand no longer depends on ω or on t. So the corresponding expectations can be performed, and the result is

$$\mathrm{tr}(\exp(-\beta H)) \leq g_\beta(0)\int \exp(-\beta V(y))\,dy. \tag{26}$$

This is equivalent to the result in the statement of the theorem.

Thus the quantum mechanical trace is bounded above by a classical trace. In particular, if $V(y)$ grows as $|y| \to \infty$ in such a way that the classical integral converges, then so does the quantum trace.

5 The Poisson summation formula

Theorem 5 (Poisson summation formula) *Let $\hat{g}(k)$ be the usual Fourier transform given as an integral over $\mathbf{R}^d$. Then*

$$\sum_a g(x+a) = \sum_k \exp(ikx)\hat{g}(k)(1/L)^d. \tag{27}$$

Here a is summed over $(L\mathbf{Z})^d$ and k is summed over $(\frac{2\pi}{L}\mathbf{Z})^d$.

The proof of the Poisson summation formula just uses Fourier series on the torus. Let $T^d = (\mathbf{R}/(L\mathbf{Z}))^d$ be the torus of side L. The Fourier coefficients of a function f on the compact group T^d are defined on the discrete group $(\frac{2\pi}{L}\mathbf{Z})^d$. These coefficients $\hat{f}(k)$ are defined like the Fourier transform, except that the integral is over the torus instead of the line. Thus

$$\hat{f}(k) = \int_{T^d} \exp(-iky) f(y)\, dy. \tag{28}$$

The inversion formula is then the Fourier series representation

$$f(x) = \sum_k \exp(ikx)\hat{f}(k)\frac{1}{L^d}. \tag{29}$$

The proof of the Poisson summation formula is based on the simple fact that if g is a function on $\mathbf{R}^d$ and we define $\bar{g}$ on T^d by

$$\bar{g}(x) = \sum_a g(x+a), \tag{30}$$

where the sum is over a in $(L\mathbf{Z})^d$, then the Fourier coefficients of $\bar{g}$ consist of the restriction of the Fourier transform of g to the discrete group $(\frac{2\pi}{L}\mathbf{Z})^d$. Thus the Fourier series representation of $\bar{g}$ is the Poisson summation formula.

6 The Wiener process on the torus

Sometimes it is convenient to deal instead with the Wiener process on the torus. Then H_0 acts in $L^2(T^d)$. In this case $\mathrm{tr}(\exp(-tH_0))$ exists and may be calculated explicitly. This is related to the fact that the spectrum is discrete in this case.

Apply the Poisson summation formula. The Fourier coefficient representation of H_0 is multiplication by $(\sigma^2/2)k^2$ for k in $(2\pi/L)^d\mathbf{Z}^d$. The Fourier coefficient representation of $\exp(-tH_0)$ is thus multiplication by $\exp(-t(\sigma^2/2)k^2)$. It follows that $\exp(-tH_0)$ is convolution on the torus by

$$\bar{g}_t(x) = \sum_a g_t(x+a). \tag{31}$$

Explicitly we have

$$(\exp(-tH_0)f)(x) = \sum_a \int_{T^d} g_t(x-y+a) f(y)\, dy. \tag{32}$$

Thus to diffuse from x on the torus to y on the torus is the same as diffusing from $x-a$ in the Euclidean space to y, for some a. This a corresponds to how many times the path winds around the torus.

Now we can compute $\mathrm{tr}(\exp(-\beta H_0))$ in the periodic case. We get

$$\mathrm{tr}(\exp(-\beta H_0)) = \sum_k \exp(-\beta(\sigma^2/2)k^2) = L^d \bar{g}_\beta(0) = L^d \sum_a g_\beta(a). \tag{33}$$

When we take V to be a function on the torus, we can define the operator $H = H_0 + V$. The Feynman-Kac formula and the trace formula are much as before. Thus for instance

$$\operatorname{tr}(\exp(-\beta H)) = \int_{T^d} \bar{E}_x[\exp(-\int_0^\beta V(\omega(t))\,dt)\delta(\omega(\beta)-x)]\,dx. \qquad (34)$$

Here $\bar{E}_x$ is the expectation for the Wiener process on the torus. In this case there should be no problem with the convergence of the x integral, since it is only over a torus. However notice that the Wiener process on the torus is no longer a Gaussian process.

The Brownian bridge on the torus is defined by conditioning the Wiener process to return to the starting point. Of course it can wrap around the torus any number of times in doing this. The trace formula in terms of the Brownian bridge on the torus is

$$\operatorname{tr}(\exp(-\beta H)) = \bar{g}_\beta(0) \int_{T^d} \bar{E}^\beta_{xx}[\exp(-\int_0^\beta V(\omega(t))\,dt)]\,dx. \qquad (35)$$

7 Example: An absorbing box

For simplicity consider the case of dimension $d = 1$. The idea is to consider a particle in a box (in the case the interval from 0 to L). The boundary condition is that the potential is infinite outside the box. This corresponds to Dirichlet boundary conditions. In the probability language it says that a particle that leaves the box is killed.

Let

$$G(x) = \sum_{m=-\infty}^{\infty} \exp(-2\frac{(x-mL)^2}{\sigma^2\beta}). \qquad (36)$$

Theorem 6 *Let x be in $[0, L]$ and consider the Brownian bridge ω starting at x. The probability that it never leaves the interval is*

$$P^\beta_{xx}[\omega([0,\beta]) \subset (0, L)] = G(0) - G(x). \qquad (37)$$

A direct proof may be found in R. M. Dudley, Real Analysis and Probability. It is a clever use of the reflection principle. The following proof uses the spectral representation and the Poisson summation formula.

First, note that H_0 with Dirichlet boundary conditions has eigenvalues $(\sigma^2/2)(n\pi/L)^2$ with eigenfunctions $\sin(\pi n/L)$ with norm squared $L/2$. This together with the expression of the Brownian bridge in terms of conditional probability gives

$$P^\beta_{xx}[\omega_\beta([0,\beta]) \subset (0,L)] = \frac{1}{g_\beta(0)}\frac{2}{L}\sum_{n=1}^{\infty} \exp(-\frac{1}{2}\beta\sigma^2\left(\frac{\pi n}{L}\right)^2)\sin^2(\frac{\pi n}{L}x) \qquad (38)$$

This probability may also be expressed as a frequency sum

$$P^\beta_{xx}[\omega_\beta([0,\beta]) \subset (0,L)] = \frac{1}{g_\beta(0)}\frac{1}{2L}\sum_{n=-\infty}^{\infty} \hat{g}_\beta(\frac{\pi n}{L})(1-\exp(i\frac{\pi n}{L}2x)). \qquad (39)$$

This is a sum of Fourier transforms of Gaussians over frequencies with spacing π/L. The Poisson summation formula then expresses this as a sum over Gaussians with spacing $2L$. This is

$$P^{\beta}_{xx}[\omega_{\beta}([0,\beta]) \subset (0,L)] = \frac{1}{g_{\beta}(0)} \sum_{m=-\infty}^{\infty} (g_{\beta}(2mL) - g_{\beta}(2x+2mL)) = G(0) - G(x). \tag{40}$$

Corollary 1 *The trace of* $\exp(-tH_0^{[0,L]})$ *confined to the box* $[0,L]$ *is*

$$\operatorname{tr}(\exp(-\beta H_0^{[0,L]})) = \sum_{n=1}^{\infty} \exp(-\frac{1}{2}\beta\sigma^2 \left(\frac{\pi n}{L}\right)^2) = Lg_{\beta}(0)G(0) - \frac{1}{2}. \tag{41}$$

8 Quantum terminology

In quantum mechanics the diffusion constant is $\sigma^2 = \hbar/m$. The replacements $H_0 \leftarrow H_0/\hbar$ and $V \leftarrow V/\hbar$ occur, so that $H = H_0 + V$ is the sum of kinetic and potential energies.

Also, the replacement $\beta \leftarrow \hbar\beta$ occurs, so that β has the units of inverse energy. It represents an inverse energy corresponding to inverse temperature. So at low temperature the dominant contribution in the Feynman-Kac formula comes from the the places q where the energy $V(q)$ is small.

Momentum is related to wave number by $p = \hbar k$. So the result that the quantum trace is bounded above by the classical trace takes the form

$$\operatorname{tr}(\exp(-\beta H)) \le \int\int \exp(-\beta[\frac{1}{2m}p^2 + V(q)]) \frac{dp\,dq}{(2\pi\hbar)^d}. \tag{42}$$

The right hand side is the integral of $\exp(-\beta h(p,q))$ over phase space, where $h(p,q) = p^2/(2m) + V(q)$ is the classical energy. The only place the quantum Planck constant $\hbar$ enters on the right hand side is in the normalization of the measure on phase space.