Variational Methods and Fermat's Principle

We are accustomed in Physics class to seeing the laws of Physics stated in terms of forces, fields, and differential equations. As we have seen, such a formulation of a problem can provide a powerful means of obtaining the solution.

However, all of the familiar equations of elementary physics–Newton's laws, Hamilton's equations, Maxwell's equations, and Schrödinger's, to name a few—can equivalently be expressed in *variational* form—that is, as a statement that the state of the system (or the trajectory of a particle) is the one that minimizes some global property, usually expressed as an integral. For example,

- Hamilton's principle states that the motion $x(t)$ of a particle from time t_1 to time t_2 is the one that minimizes the *action* $\int_{t_1}^{t_2} L\,dt$, where $L = T - V$ is the Lagrangian of the system. It is easily shown that this principle is equivalent to the Lagrangian formulation of classical mechanics.

- The quantum-mechanical wave function ψ of a system with Hamiltonian H is the one that minimizes the quantity $\langle\psi|H\psi\rangle = \int dx\,\psi^* H\psi$ subject to the constraint that $\langle\psi|\psi\rangle$ is constant. This is equivalent to Schrödinger's equation.

There are many more examples. Often, a variational formulation is the most convenient or direct way of expressing the problem. The *calculus of variations* was developed precisely to handle such problems. Here we will adopt a Monte-Carlo approach to their solution. We will focus on two examples: Fermat's principle (described below) and energy minimization (next). In each case, we are seeking the configuration of a system that *minimizes* some integral property of the system.

Fermat's principle has to do with the path taken by a ray of light through a (possibly inhomogeneous) medium. It states that the path from point A to point B is the one that minimizes the light travel time between those two points. In the case of a homogeneous medium, that translates into the shortest distance between the two points—a straight line—but in general it means that, if the refractive index of the medium is $n(x, y)$ (in two dimensions, for simplicity) then the path $y(x)$ taken by the ray is the one that minimizes

$$\begin{aligned} t &= \int_A^B dt \\ &= \int_B^B \frac{ds}{v} \\ &= \frac{1}{c}\int_A^B n(x, y(x))\sqrt{1+\left(\frac{dy}{dx}\right)^2}\,dx\,, \end{aligned}$$

where $ds^2 = dx^2 + dy^2$. You may have seen this prolem solved analytically as an introductory example in variational calculus.

In the Monte-Carlo approach to this problem, we represent the path $y(x)$ as a series of $N+1$ discrete points (x_i, y_i), and choose a set of x_i values uniformly between $x_0 = x_A$ and $x_N = x_B$ (it is not actually necessary to choose the x_i uniformly, as we will see later). We then choose the corresponding y_i randomly, except that $y_0 = y_A$ and $y_N = y_B$. The procedure is simple:

1. Evaluate the quantity t for the current configuration, as

$$t = \sum_{i=0}^{N-1} n(x_i, y_i)\sqrt{dx_i^2 + dy_i^2}$$

   where $dx_i = x_{i+1} - x_i$ and similarly for dy_i.

2. Randomly choose one of the interior points i, with $1 \le i < N$.

3. Randomly change y_i by some amount in the range $[-dy, dy]$, where dy is some characteristic resolution scale of the problem.

4. Re-evaluate the quantity t. If the random change has reduced it from the previous value, accept the change. Otherwise, reject it and restore the previous value of y_i.

5. Go back to step (1), and repeat until some large number of trials fails to reduce t.

The procedure will work for and choice of $n(x, y)$ and any initial choice of y_i—and, in fact for any problem that can be cast in variational form!