Monte Carlo Methods

Anne Greenbaum *

January 20, 1998

1 Examples of Monte Carlo Computations

- Compute $\frac{\pi}{4}$.

- Buffon needle problem: Suppose a sheet of paper has lines a distance d apart. Drop a needle of length $L < d$ onto the paper. What is the probability that the needle intersects a line? The answer is now known analytically; it is $\frac{2L}{\pi d}$. It is reported that Buffon conjectured this value and actually did the experiment many times to confirm it before devising a proof.

*Math/AMath 381, Winter quarter, 1998. Ref. *Monte Carlo Methods*, by Kalos and Whitlock, Wiley, 1986.

- Multidimensional integration:

$$\int_0^1 \int_0^1 \dots \int_0^1 f(x_1, \dots, x_m)\, dx_1\, dx_2 \dots dx_m$$

A standard quadrature rule would approximate this integral using a formula of the form

$$(\Delta x)^m \sum_{i_1=1}^{n} \sum_{i_2=1}^{n} \dots \sum_{i_m=1}^{n} f(x_{1_{i_1}}, x_{2_{i_2}}, \dots, x_{m_{i_m}}),$$

and the work required would be $O(n^m)$. This is infeasible, say, for $n = 10$ and $m = 30$.

In a Monte Carlo computation, we choose many independent samples from $[0,1] \times [0,1] \times \dots \times [0,1]$ and approximate the integral by

$$\frac{1}{N} \sum_{k=1}^{N} f(\vec{x}_k).$$

The error is proportional to $N^{-1/2}$. This is rather slow convergence; we must increase the number of points by a factor of 4 in order to obtain a factor of 2 reduction in the error. But for m large, it is the only feasible method. Most Monte Carlo calculations can be interpreted as evaluating a multidimensional integral.

The Monte Carlo computation of π can be thought of as a 2-dimensional integral: Evaluate the integral over the square $[-1,1] \times [-1,1]$ of a function $f(x,y)$ that is equal to 1 if $x^2 + y^2 \leq 1$ and 0 otherwise.

Areas and volumes of more complicated regions are easily computed provided only that we can enclose the region in a box or other object of known volume and then determine whether a point lies inside or outside the region. For example, suppose we wish to find the weight and center of mass of a region that is the intersection of a torus with the edge of a large box. [Ref. *Numerical Recipes* by Press, et.al., Cambridge University Press, 1992.] Let the region be defined by the three simultaneous equations

$$z^2 + \left(\sqrt{x^2 + y^2} - 3\right)^2 \leq 1, \quad x \geq 1, \quad y \geq -3,$$

and assume that it has constant density γ.

We want to estimate the following integrals over the the complicated region:

$$\int \gamma \, dx \, dy \, dz, \quad \int x\gamma \, dx \, dy \, dz, \quad \int y\gamma \, dx \, dy \, dz, \quad \int z\gamma \, dx \, dy \, dz.$$

The coordinates of the center of mass will be the ratio of the latter three integrals to the first one (the weight).

The following piece of MATLAB code will provide such estimates:

```
w = 0;                  %Initialize weight and other integrals to zero.
wx = 0; wy = 0; wz = 0;

for i=1:n,
  x = 1 + 3*rand;       %Generate random points uniformly distributed
  y = -3 + 7*rand;      %in the enclosing box [1,4] X [-3,4] X [-1,1].
  z = -1 + 2*rand;
  if z^2 + ( sqrt(x^2+y^2) - 3 )^2 <= 1,  % Is point in the torus?
    w = w + gamma;                        % If so, add to various integrals.
    wx = wx + x*gamma;
    wy = wy + y*gamma;
    wz = wz + z*gamma;
  end;
end;

boxvol = 3*7*2;          %Volume of enclosing box.
weight = boxvol*w/n,     %Integrals are volume of box times fraction
xmoment = boxvol*wx/n,   %inside region.
ymoment = boxvol*wy/n,
zmoment = boxvol*wz/n,
```

This is fine, but the computed estimates of `weight`, etc. are not so useful unless we have some indication of how accurate they are. Here we use the central limit theorem: For n sufficiently large, the random variables `weight`, etc. produced by this code are normally distributed with means equal to the actual desired integral values and standard deviations given by $\sigma/\sqrt{n}$, where σ is the standard deviation of the individual distributions. Since the variance of a random variable X is $E(X^2) - (E(X))^2$, these standard deviations can be approximated, along with the integrals. For example, to compute `weight` and also provide an error estimate the following code could be used:

```
w = 0;                      %Initialize weight to zero.
varw = 0;                   %Initialize variance estimate to zero.

for i=1:n,
  x = 1 + 3*rand;           %Generate random points uniformly distributed
  y = -3 + 7*rand;          %in the enclosing box [1,4] X [-3,4] X [-1,1].
  z = -1 + 2*rand;
  if z^2 + ( sqrt(x^2+y^2) - 3 )^2 <= 1,  % Is point in the torus?
    w = w + gamma;                        % If so, add to w.
    varw = varw + gamma^2;                % Add to estimates of E(w^2).
  end;
end;

boxvol = 3*7*2;              %Volume of enclosing box.
weight = boxvol*w/n,         %Integral is volume of box times fraction
                             %inside region.
sigw = boxvol*sqrt((varw/n - (w/n)^2)/n), %Standard deviation for weight
```

Can you see how to compute similar error estimates for the other integrals? If the above code were run many, many times, how often would you expect the computed value of `weight` to lie within `sigw` of the actual weight?

2 Application: Radiation Transport

Assumptions:

1. Particles move in straight lines between collisions (true for neutral radiation — light, X-rays, neutrons; not for electrons and protons).

2. Collisions result in absorption or scattering, with some loss of energy.

3. Neglect effect of radiation on the medium.

4. Ignore effects of polarization on scattering.

5. Neglect crystal effects.

Example: Model X-ray photons in a dental X-ray. Determine dose of radiation received at a particular position; determine fraction of radiation that passes through a slab of matter of known thickness.

Independent variables: position (x, y, z), direction $(\Omega_x, \Omega_y, \Omega_z)$, energy (E), and time of production (t) of photons. Each independent variable is random and may be described by a pdf.

Once in matter, a photon may interact with an individual atom. Whether this interaction takes place and with which atom is random. The interaction usually involves the photon exchanging energy with an electron, effectively being scattered with reduced energy and changed direction. The photon may also give up all its energy to the electron, in which case it is considered to be absorbed and the history terminates. We must posit pdf's for each stochastic event, based on theoretical and measured properties of X-rays. Scattered photons are subject to the same processes as the original ones with the same energy. The life history of a photon is followed until it is absorbed or too low in energy or too far away to have an appreciable effect on the required answer.

2.1 Characterization of the Source

Assume a point source (x_0, y_0, z_0) and assume that each photon produced initially has energy E_0. (This is not quite right but close enough.) X-rays are produced by turning on an electron beam at time t_1 and turning it off at time t_2. Assume a uniform distribution of production times between t_1 and t_2. Take the intensity of the X-rays to be uniform in all directions. The initial state of a photon can be computed as follows:

```
x = x0;  y = y0;  z = z0;  E = E0;
t = t1 + (t2-t1)*rand;
phi = 2*pi*rand;
omegaz = 1 - 2*rand;
omegax = sqrt(1 - omegaz^2)*cos(phi); omegay = omegax*tan(phi);
```

2.2 Tracing a Path

Since X-rays travel in straight lines between collisions:

```
xnew = x + omegax * d;
ynew = y + omegay * d;
znew = z + omegaz * d;
tnew = t + d/v;
```

where v is the radiation velocity and d is the distance to the next interaction with an atom. The probability per unit pathlength of having an interaction, Σ_T, is a property of the material and does not change with the distance the photon has traveled. Consequently, the distribution of distances d is exponential in homogeneous materials:

$$F(d) = \exp(-\Sigma_T d) \equiv \xi \Rightarrow d = -\log(\xi)/\Sigma_T.$$

In MATLAB notation, insert the line:

```
d = -log(rand)/sigmat;
```

2.3 Modeling a Collision

There are two possibilities — absorption or scattering. If $\xi <$ Prob(absorption), absorption occurs; otherwise scattering.

Both neutrons and photons tend to scatter preferentially in the forward direction; the azimuth is uniformly distributed.

Example:

$$\rho(\cos\theta)\, d\cos\theta = \begin{cases} 2\cos\theta\, d\cos\theta, & 1 > \cos\theta > 0 \\ 0, & \cos\theta < 0 \end{cases}$$

$$\phi = 2\pi\xi.$$