where $p(x)$ is an arbitrary function that need not be normalized. In Chapter 15 we will discuss the application of the Metropolis algorithm to problems in statistical mechanics.

For simplicity, we introduce the Metropolis algorithm in the context of estimating one-dimensional definite integrals. Suppose that we wish to use importance sampling to generate random variables according to $p(x)$. The Metropolis algorithm produces a random walk of points $\{x_i\}$ whose asymptotic probability distribution approaches $p(x)$ after a large number of steps. The random walk is defined by specifying a *transition probability* $T(x_i \to x_j)$ from one value x_i to another value x_j such that the distribution of points $x_0, x_1, x_2, \ldots$ converges to $p(x)$. It can be shown that it is sufficient (but not necessary) to satisfy the *detailed balance* condition

$$p(x_i)T(x_i \to x_j) = p(x_j)T(x_j \to x_i). \tag{11.53}$$

The relation (11.53) does not specify $T(x_i \to x_j)$ uniquely. A simple choice of $T(x_i \to x_j)$ that is consistent with (11.53) is

$$T(x_i \to x_j) = \min\left[1, \frac{p(x_j)}{p(x_i)}\right]. \tag{11.54}$$

If the "walker" is at position x_i and we wish to generate x_{i+1}, we can implement this choice of $T(x_i \to x_{i+1})$ by the following steps:

1. Choose a trial position $x_{\text{trial}} = x_i + \delta_i$, where δ_i is a uniform random number in the interval $[-\delta, \delta]$.
2. Calculate $w = p(x_{\text{trial}})/p(x_i)$.
3. If $w \geq 1$, accept the change and let $x_{i+1} = x_{\text{trial}}$.
4. If $w < 1$, generate a random number r.
5. If $r \leq w$, accept the change and let $x_{i+1} = x_{\text{trial}}$.
6. If the trial change is not accepted, then let $x_{i+1} = x_i$.

It is necessary to sample many points of the random walk before the asymptotic probability distribution $p(x)$ is attained. How do we choose the maximum step size δ? If δ is too large, only a small percentage of trial steps will be accepted, and the sampling of $p(x)$ will be inefficient. On the other hand, if δ is too small, a large percentage of trial steps will be accepted, but again the sampling of $p(x)$ will be inefficient. A rough criterion for the magnitude of δ is that approximately one third to one half of the trial steps should be accepted. We also wish to choose the value of x_0 such that the distribution $\{x_i\}$ will approach the asymptotic distribution as quickly as possible. An obvious choice is to begin the random walk at a value of x at which $p(x)$ is a maximum. A code fragment that implements the Metropolis algorithm is given below.

```
double xtrial = x + (2*rnd.nextDouble() - 1.0)*delta;
double w = p(xtrial)/p(x);
if (w > 1 || w > rnd.nextDouble()) {
   x = xtrial;
   naccept++;          // number of acceptances
}
```


Problem 11.17 Generating the Gaussian distribution

(a) Use the Metropolis algorithm to generate the Gaussian distribution $p(x) = Ae^{-x^2/2}$. Is the value of the normalization constant A relevant? Determine the qualitative dependence of the acceptance ratio and the equilibration time on the maximum step size δ. One possible criterion for equilibrium is that $\langle x^2 \rangle \approx 1$. What is a reasonable choice for δ? How many trials are needed to reach equilibrium for your choice of δ?

(b) Modify your program so that it plots the asymptotic probability distribution generated by the Metropolis algorithm.

*(c) Calculate the autocorrelation function $C(j)$ defined by (see Problem 7.31)

$$C(j) = \frac{\langle x_{i+j}x_i \rangle - \langle x_i \rangle^2}{\langle x_i^2 \rangle - \langle x_i \rangle^2}, \tag{11.55}$$

where $\langle \ldots \rangle$ indicates an average over the random walk. What is the value of $C(j = 0)$? What would be the value of $C(j \neq 0)$ if x_i were completely random? Calculate $C(j)$ for different values of j and determine the value of j for which $C(j)$ is close to zero. ■

Problem 11.18 Application of the Metropolis algorithm

(a) Although the Metropolis algorithm is not the most efficient method in this case, write a program to estimate the average

$$\langle x \rangle = \frac{\int_0^\infty xe^{-x}\,dx}{\int_0^\infty e^{-x}\,dx}, \tag{11.56}$$

with $p(x) = Ae^{-x}$ for $x \geq 0$ and $p(x) = 0$ for $x < 0$. Compute the histogram $H(x)$ showing the number of points in the random walk in the region x to $x + \Delta x$ with $\Delta x = 0.2$. Begin with $n \geq 1000$ and maximum step size $\delta = 1$. Allow the system to equilibrate for at least 200 steps before computing averages. Is the integrand sampled uniformly? If not, what is the approximate region of x where the integrand is sampled more often?

(b) Calculate analytically the exact value of $\langle x \rangle$ in (11.56). How do your Monte Carlo results compare with the exact value for $n = 100$ and $n = 1000$ with $\delta = 0.1$, 1, and 10? Estimate the standard error of the mean. Does this error give a reasonable estimate of the error?

(c) In part (b) you should have found that the estimated error is much smaller than the actual error. The reason is that the $\{x_i\}$ are not statistically independent. The Metropolis algorithm produces a random walk whose points are correlated with each other over short times (measured by the number of steps of the random walker). The correlation of the points decays exponentially with time. If τ is the characteristic time for this decay, then only points separated by approximately 2 to 3τ can be considered statistically independent. Compute $C(j)$ as defined in (11.55) and make a rough estimate of τ. Rerun your program with the data grouped into 20 sets of 50