7 Numerical Integration

7.1 Elementary Algorithms

Let us suppose we are confronted with a function $f(x)$ tabulated at the points $x_1, x_2, x_3...x_n$, not necessarily equally spaced. We require the integral of $f(x)$ from x_1 to x_n. How do we proceed? The simplest algorithm we can use, valid both for equally and unequally spaced points, is the *trapezoidal rule*. The trapezoidal rule assumes that the function is linear between the tabulated points. With this assumption, it can be seen that the integral from x_1 to x_2 is given by

$$\int_{x_1}^{x_2} f(x)dx \approx \frac{1}{2}h(f_1 + f_2)$$

where $h = x_2 - x_1$.
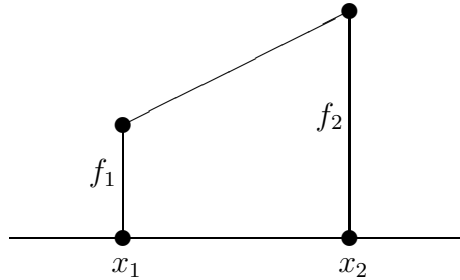
This equation can be extended to n points for equally spaced points

$$\int_{x_1}^{x_n} f(x)dx \approx h(\frac{1}{2}f_1 + f_2 + f_3 \ldots + \frac{1}{2}f_n) \tag{1}$$

and

$$\int_{x_1}^{x_n} f(x)dx \approx \frac{1}{2}(x_2-x_1)(f_1+f_2)+\frac{1}{2}(x_3-x_2)(f_2+f_3)\ldots+\frac{1}{2}(x_n-x_{n-1})(f_{n-1}+f_n)$$

for unevenly spaced points.

Exercise 7.1: Use the trapezoidal rule to evaluate the integral

$$\int_1^2 x \sin x \, dx$$

with 10 points. Double the number of points and re-evaluate the integral. The "exact" value of this integral is 1.440422. Rewrite your program to evaluate the integral at an arbitrary number of points input by the user. Are 1000 points better than 100 points?

Exercise 7.2: The heat capacity of many substances can be represented with the equation (for one mole)

$$C_P = a + bT - \frac{c}{T^2}$$

and the change in the entropy, S, of these substances as the temperature changes from T_i to T_f can be determined from the equation

$$\Delta S = \int_{T_i}^{T_f} \frac{C_P}{T} dT$$

For graphite, $a = 16.86 \text{K/J}$, $b = 4.77 \times 10^{-3} \text{J/K}^2$, and $c = 8.54 \times 10^5 \text{J·K}$. Calculate the change in the entropy of one mole of graphite that is heated from 298K to 500K. Use 20 points for your integral. The correct answer, obtained analytically, is 6.59 J/K.

For equally spaced points the trapezoidal rule has an error $O(h^3)$, which means that the error for each interval in the rule is proportional to the cube of the spacing. This means, of course, that if the interval size is reduced, the error decreases. In terms of the total number of points (N) used, the total error for the trapezoidal rule can be expressed as $O(1/N^2)$ – i.e. if we double the number of points, the error goes down by a factor of 4. Eventually, however, we run into the law of diminishing returns – either we hit the limit of machine accuracy, or the cumulative error involved in using many tiny intervals begins to build and becomes unacceptably high. In addition, if we use very small intervals, we pay dearly in computer time for the many function evaluations. If the function is complex and thus expensive to compute, this can become prohibitive.

Despite these disadvantages, the trapezoidal rule is adequate for most applications, and it is the only choice if your function is tabulated at unequally spaced points. For those applications which require more accuracy than the trapezoidal rule permits, or which are attempting to integrate very complex

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functions, "higher order" integration schemes are available. The most popular is *Simpson's rule* which is based on parabolic interpolation. The formula for Simpson's rule, a three-point formula, is:

$$\int_{x_1}^{x_3} f(x)dx \approx h\left[\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{1}{3}f_3\right] + O(h^5) \tag{2}$$

The "extended" version of this formula over N steps (note that N must be *odd*) is:

$$\int_{x_1}^{x_N} f(x)dx \approx \frac{h}{3}\left[f_1 + 4f_2 + 2f_3 + 4f_4 + ... + 2f_{N-2} + 4f_{N-1} + f_N\right] + O\left(\frac{1}{N^4}\right)$$

Exercise 7.3: Calculate the integral of **Exercise 7.1** with Simpson's rule using 9 points in the interval (1,2), and then repeat the exercise with 19 points. Compare with the results from **Exercise 7.1** for 10 and 20 points respectively.

Exercise 7.4: Re-do the problem of **Exercise 7.2** with Simpson's rule using 19 points. Compare your answer to the one you got with the Trapezoidal rule.

Note that if you have a tabulated function with an *even* number of points, you can still use Simpson's rule. Simply evaluate the integral over the first interval using the trapezoidal rule and then use Simpson's rule for the remaining odd number of points.

Even higher-order formulae can be used to carry out numerical integration, but, in practice, these are hardly ever used. There are advanced techniques, which we will not go into, which can extract virtually any desired precision from the trapezoidal rule and Simpson's rule, and thus it is hardly ever necessary to utilize higher-order formulae.

Exercise 7.5: To explore one of these "advanced techniques", go back to the program you wrote for **Exercise 7.1** and rewrite it to calculate the value of the integral with $N = 30$ and 80 points. Setting $x = 1/N^2$ and

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y = the value of the integral for each value of N defines two points. The program should find the equation of the line between these two points. The y-intercept of this equation should be a very accurate approximation to the integral. Why? Since $x = 1/N^2$ †, the y-intercept (where $x = 0$) corresponds to $N = \infty$. The program should print out the value of the integral and its deviation from the "exact" value 1.440422 for $N = 30, 80$, and "∞" points.

Exercise 7.6: (Graduate Students) Numerical estimation of the Stefan-Boltzmann constant. The total power output of a blackbody radiator, integrated over the entire electromagnetic spectrum is given by $A\sigma T^4$, where $\sigma = 5.6697 \times 10^{-8}$ W/m^{2}K^4 and A is the radiating area of the blackbody radiator. σ is not a fundamental constant – it can be expressed in terms of a number of other fundamental constants, but it can be derived numerically as follows: For a blackbody radiator of unit area, the power output is given by the integral

$$P = 2\pi h c^2 \int_0^\infty \frac{d\lambda}{\lambda^5(e^{hc/\lambda kT} - 1)} = \sigma T^4$$

where $h = 6.62606957 \times 10^{-34}$m^2 kg/s, $c = 2.99792458 \times 10^8$m/s, and $k = 1.3806488 \times 10^{-23}$m^{2}kg/s^{2}K. Wavelength λ is in meters. Note that you will have to deal with the infinite interval in the integral. That cannot be done numerically, so you will have to integrate over a finite interval. As an example, if you use $T = 3000$K, it will probably be adequate to integrate from $\lambda = 1 \times 10^{-9}$m to 1×10^{-4}m. Try different step sizes, and experiment with the limits to get the best result. Use Simpson's rule.

7.2 Gaussian Integration

In the previous section, we found that we could obtain significantly higher accuracy in numerical integration using the same number of points in a given interval by changing the *weighting* used for the points. For instance, in trapezoidal integration, each point, except for the end points, enter into the formula (equation 1) with equal weights. In Simpson's rule (equation 2) the points are not given equal weights. Note that the odd *abscissas* are given weights of 2/3, whereas the even abscissas are given weights of 4/3.

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†Why do we set $x = 1/N^2$? Because the error in the trapezoidal method goes as $O(1/N^2)$, and thus the error in the determination of the integral should scale linearly with $1/N^2$.

It turns out that if we relax the restriction that the abscissas should be evenly spaced in the interval, we can then choose abscissas and corresponding weights that yield very high accuracies. This is the basis of *Gaussian integration.* We do not have the time to go into this method in great detail, but it is important that you are at least acquainted with this method of integration, as it is commonly and widely used.

Gaussian integration is based on integrals of the form:

$$\int_a^b W(x)f(x)dx$$

which can be approximated by the sum

$$\sum_{i=1}^{N} w_i f(x_i)$$

The weights (w_i) and the abscissas (x_i) can be chosen, for a given $W(x)$, to make the approximation *exact* if $f(x)$ is a polynomial. If $f(x)$ can be "well approximated" by a polynomial, then the integration formula above yields very high accuracy. Different $W(x)$'s, of course, lead to different choices for the abscissas and weights. $W(x) = 1$, for instance, leads to "Gauss-Legendre" integration, $W(x) = (1 - x^2)^{-1/2}$ leads to Gauss-Chebyshev integration, etc. We will concentrate here on the simplest and the most useful case, Gauss-Legendre integration.

For a given number of abscissas, it is possible to compute the x_i's and the w_i's for Gauss-Legendre integration. We won't go into how this is actually done; details can be found in *Numerical Recipes.* Below, find a table listing the abscissas and weights for a number of different values of N. These abscissas are based on the interval [-1,1]:

Gauss-Legendre Integration

N	x_i	w_i
2	± 0.57735	1.000000
3	0	0.888889
	± 0.774597	0.555556
4	± 0.339981	0.652145
	± 0.861136	0.347855
5	0	0.568889
	± 0.538469	0.478629
	± 0.90618	0.236927

If your integration is not over the limits [-1,1], then the abscissas must be transformed accordingly. For instance, if the interval is [a,b] instead of [-1,1], then the new abscissas t_i are given by:

$$t_i = \frac{a+b}{2} + \frac{b-a}{2}x_i$$

and note that

$$dt = \frac{b-a}{2}dx$$

hence

$$\int_a^b f(t)dt = \int_{-1}^1 f(\frac{a+b}{2} + \frac{b-a}{2}x)\frac{b-a}{2}dx$$

thus:

$$\int_a^b f(t)dt \approx \frac{b-a}{2}\sum_{i=1}^N w_i f(\frac{a+b}{2} + \frac{b-a}{2}x_i)$$

where the weights and abscissas are as displayed in the table above, and we are assuming that $W(x) = 1$.

Exercise 7.7: Repeat exercise 7.1 using Gauss-Legendre integration with 5 abscissas. Compare the accuracy with your results from exercises 7.1 and 7.3.

Exercise 7.8: Repeat exercise 7.2 using Gauss-Legendre integration with 5 abscissas. Compare the accuracy with your results from exercises 7.2 and 7.4.

7.3 Multidimensional Integrals

Numerical integrations of functions of several variables over regions with dimensions greater than one are very difficult to carry out. First, to get sufficient precision, the numerical integration may involve literally tens of thousands of function evaluations. Second, if the boundary of the integration region is complex, this can greatly complicate the procedure. Thus, if possible, before resorting to multidimensional techniques, try to reduce the dimension of your integral. Sometimes this may be done by exploiting the symmetries of the integrand. For instance, if you are integrating a spherically symmetric function over a spherical region, switch to spherical coordinates. The integral will reduce to a one-dimensional integral! If this does not work, and the function is otherwise fairly well behaved (for instance, is not strongly peaked in a certain region), and you don't require great accuracy, explore *Monte Carlo* techniques (see next section). Otherwise, a multidimensional integral can be attacked using one-dimensional techniques in the following way:

Let us suppose we have the following integral:

$$I = \int_{x_1}^{x_2} dx \int_{y_1(x)}^{y_2(x)} dy \int_{z_1(x,y)}^{z_2(x,y)} f(x,y,z)dz$$

where the limits on the integrals define the region of integration in the usual way. If we let

$$G(x,y) = \int_{z_1(x,y)}^{z_2(x,y)} f(x,y,z)dz$$

and

$$H(x) = \int_{y_1(x)}^{y_2(x)} G(x,y)dy$$

then

$$I = \int_{x_1}^{x_2} H(x)dx$$

The third integral for I can be evaluated using one of the one-dimensional techniques discussed in §7.1. However, in this procedure $H(x)$ will have to be evaluated at a number of values of x, and this must be done by integrating $G(x,y)$, again using a one-dimensional technique for each of those values of x. $G(x,y)$, however, can only be evaluated by carrying out the first integral for each value of x and y encountered in the evaluation of the second and third integrals. Thus, while the third integral is evaluated only once, the

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second integral is evaluated many times and the third integral many, many times leading to a great number of function evaluations.

Example: Evaluate the integral

$$\int_{-1}^{1} dx \int_{-\sqrt{(1-x^2)}}^{\sqrt{(1-x^2)}} (x^2 + y^2) dy$$

using two applications of the trapezoidal method. *Note - this integral can be reduced to a single integral in polar coordinates. The exact value of this integral is $\pi/2 = 1.570796$. Here is some code that will do the job:*

```
/*
Functions employed:

trap: carries out 1-D trapezoidal integration
integrand: evaluates the integrand
l1, l2: the limits
twoDtrap: implements 2-D trapezoidal integration
H: Carries out integration of the integrand for a given value of x
x: to make things easy, x is declared as an external variable, so that
we don't have to pass it to each function


*/
#include <stdio.h>
#include <math.h>

double trap(double a, double b, double (*func)(double), int N);
double integrand(double y);
double l1();
double l2();
double twoDtrap(double a, double b,int N);
double H(double y1, double y2);
double x;
int N;
```

```
int main()
{
  double a = -1.0;
  double b = 1.0;
  double result;

  printf("\nEnter number of points for both x and y > ");
  scanf("%d",&N);

  result = twoDtrap(a,b,N);

  printf("\nIntegral = %e\n",result);

  return(0);
}

/* twoDtrap  carries out trapezoidal integration on H between the limits
   y1 = l1(x), y2 = l2(x) and x = a and x = b */

double twoDtrap(double a, double b, int N)
{
  double h,integral;
  int i;

  h = (b-a)/(double)(N-1);

  integral = 0.0;
  x = a;
  integral += 0.5*H(l1(),l2());
  x = b;
  integral += 0.5*H(l1(),l2());
  x = a+h;
  for(i=2;i<N;i++) {
    integral += H(l1(),l2());
    x += h;
  }
  integral *= h;
```

```c
  return(integral);
}

double H(double y1, double y2)
{
  return(trap(y1,y2,integrand,N));
}

/* Remember that x is external, so it need not be passed to l1 and l2 */
double l1()
{
  return(-sqrt(1-x*x));
}

double l2()
{
  return(sqrt(1-x*x));
}

/* Only y is passed to integrand, as x is external */

double integrand(double y)
{
  return(x*x + y*y);
}

/* Note that trap is written generally, so that any function (func) can
   be passed to it.  Study carefully how a function is passed to another
   function, and how the passed function is referred to inside the second
   function.  Note that in this case, only one variable can be passed to
   func in this case y.   */

double trap(double a, double b, double (*func)(double), int N)
{
  double h,integral,x;
  int i;

  if(a == b) return(0.0);
```

```
  h = (b-a)/(double)(N-1);

  integral = 0.0;
  integral += 0.5*((*func)(a) + (*func)(b));
  x = a+h;
  for(i=2;i<N;i++) {
    integral += (*func)(x);
    x += h;
  }
  integral *= h;
  return(integral);
}
```

Exercise 7.9: Evaluate the integral

$$\int_{-1}^{1} dx \int_{-\pi/2}^{\pi/2} x^2 \cos y \, dy$$

using two applications of the trapezoidal method. The exact value of this integral is $4/3$.

Exercise 7.10: The gravitational potential at a point (X, Y) due to an infinitessimal mass (dm) at position (x, y) is given by

$$dV = -G\frac{dm}{r}$$

where r is the distance between (x, y) and (X, Y). Calculate the gravitational potential, V, for the square mass shown in the figure below at the point (X, Y), which is in the plane of the square and lies outside of the square, by integrating the above expression for dV over the mass. Note that the surface density σ of the square is a function of position: $\sigma = (x^2 + y^2)$ kg/m^2, and that $dm = \sigma dx dy$. The square has dimensions 2m $\times$ 2m and is centered on the origin. Prompt the user for the (X, Y) coordinates, and reprompt if (X, Y) lies inside the square.

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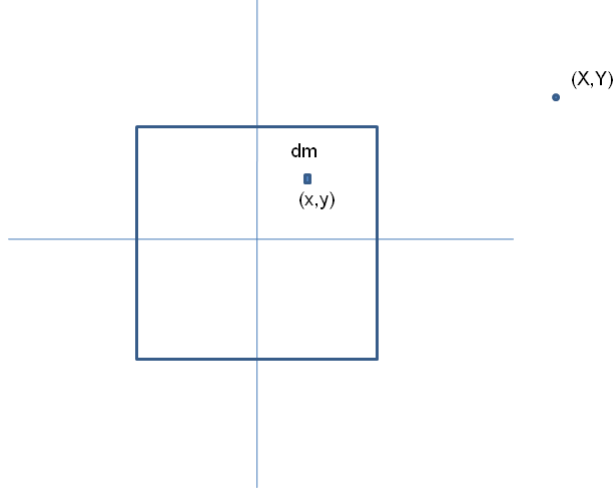
7.4 Monte Carlo Integration

This technique of numerical integration is named after the famous casino in Monte Carlo not because it is risky or chancy, but because it uses random numbers to carry out an integration. How does this work? Suppose we have an integral of a function f over a given volume V and we choose N random points in that volume. Then,

$$\int \int \int_V f \, dV \approx V \langle f \rangle \pm V \left(\frac{\langle f^2 \rangle - \langle f \rangle^2}{N} \right)^{\frac{1}{2}} \tag{3}$$

where $\langle f \rangle$ is the arithmetic mean of f over the N random points:

$$\langle f \rangle = \frac{1}{N} \sum_{i=1}^{N} f(x_i)$$

and

$$\langle f^2 \rangle = \frac{1}{N} \sum_{i=1}^{N} f^2(x_i)$$

Note that the error term in equation (1) is proportional to $\sqrt{1/N}$, which is one of the great disadvantages of the Monte Carlo method of numerical integration; the error reduces very slowly with increasing N, and thus many

random points are needed for high accuracy. Nonetheless, Monte Carlo integration is sometimes "the only way to go", especially if the region of integration is complicated.

Before we proceed any further with Monte Carlo integration, we should discuss in a bit more detail the generation of random numbers by a computer. All "C" compilers come with a pair of library routines

```
void srand(unsigned seed);
int rand(void);
```

The `rand` function is the actual random number generator, but the random number generator must be initialized by `srand` by supplying `srand` with an arbitrary unsigned integer, the "seed". Note that the same initializing value of `seed` will always return the same random number sequence. The function `rand` returns, upon each call, a random number in the range 0 to the largest positive value the computer can produce for variables of type `int`; this number is available in `stdlib.h` as `RAND_MAX`. Thus, if we want a random floating point number in the range $0.0 - 1.0$ we can use the code fragment:

```
x = (float)rand()/(RAND_MAX+1.0);
```

Unfortunately, `rand` is not a good enough random number generator, even for government work. It does not give truly random sequences, and this can be fatal for Monte Carlo integrations. It is much better to use the function `float ran1(long *idum)` (see *Numerical Recipies* for details). This function is available in `comphys.c` and defined in `comphys.h` and, as we saw in Chapter 2, should be initialized by setting `idum` to a negative number thus:

```
  long idum;
  float rn;

  /* Initialize ran1 */
  idum = -1;
  rn = ran1(&idum);

  /* Use ran1 */
  rn = ran1(&idum);
```

The function `ran1`, which returns a random floating point number between 0.0 and 1.0 *is* good enough for government work and is much superior to `rand`. Note, however, that if you use the same negative number seed `idum` each time, you will get the same sequence of random numbers. It is thus better to use the scheme outlined in Chapter 2 to set `idum = -1*now`, where `now` is a time variable.

Now, back to Monte Carlo integration. Suppose we want to integrate a function g over an irregular region W that is difficult to sample randomly. What do we do? We find a region V that contains W and which *is* easy to sample randomly - say, for instance, a rectangle or a cube. We then define $f = g$ at points inside of W but $f = 0$ at points inside of V but outside of W. It is in our own interest to make V fit around W as snugly as possible, as the zero values of f will increase the factor $\langle f^2 \rangle - \langle f \rangle^2$ in the error term of equation (1) and will reduce the effective value of N.

For an example, let us take the integral in the example in § 7.3. The region of interest W is a circle with radius 1 and center at (0,0). We take the region V to be a square with the same center (see below – 100 random points are also plotted in region V). The Monte Carlo integration is carried out by the following code:

```c
#include <stdio.h>
#include <stdlib.h>
#include <time.h>
#include "comphys.h"
#include "comphys.c"
#define N 100

int main()
{
  float x,y,rn,r2,f,integral,V,sum,av,sum2,av2;
  float error;
  long i;
  long idum = -1;
  time_t now;

  /* Use the time function to supply a different seed to the
     random number generator every time the program is run */
```

```c
    now = time(NULL);

    idum = -1*now;

    /* Initialize random number generator */

    rn = ran1(&idum);

    /* Our region V that encloses W, a circle of unit radius,
       is a square with sides of length 2.  Thus, the area of
       this square is 4 */

    V = 4.0;
    sum = 0.0;
    sum2 = 0.0;
    for(i=0;i<N;i++) {
      /* Following gives x and y between -1.0 and 1.0 */
      x = 2.0*ran1(&idum) - 1.0;
      y = 2.0*ran1(&idum) - 1.0;
      r2 = x*x + y*y;

      /* Is the point in the region W? */
      if(r2 <= 1.0) f = r2;
      else f = 0.0;

      /* Evaluate sums */
      sum += f;
      sum2 += f*f;
    }
    /* Calculate Integral and error */
    av = sum/(float)N;
    av2 = sum2/(float)N;
    integral = av*V;
    error = V*sqrt((av2-av*av)/(float)N);

    printf("\nIntegral = %f +/- %f\n",integral,error);
    return(0);
}
```
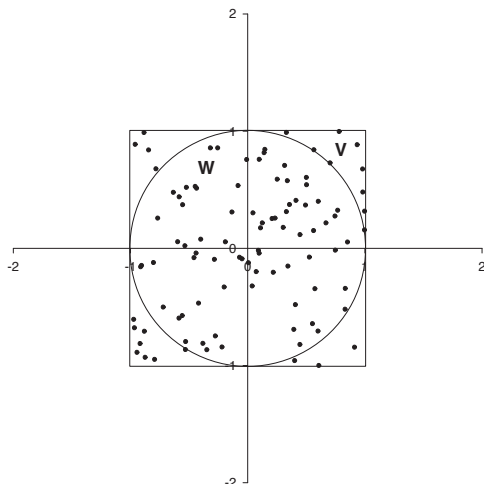
The result of the first 10 runs of this program (your numbers will be different) with $N = 100$ are: 1.825, 1.640, 1.414, 1.700, 1.532, 1.571, 1.413, 1.600, 1.519, 1.745 each with a calculated error of about ± 0.130. The mean of these determinations is 1.596 ± 0.043 (where the error is the standard error of the mean). If we increase N to 1000, we get the following run: 1.593, 1.574, 1.614, 1.589, 1.545, 1.531, 1.592, 1.570, 1.627, 1.579 each with a calculated error of about ± 0.042. The mean of these determinations is 1.581 ± 0.009. Notice that increasing N by a factor of 10 decreased the error by a factor of only about 3. A single run with $N = 100000$ gives 1.575 ± 0.004. Recall that the exact value of this integral is $\pi/2 = 1.571$.

The moral of the story is – run your Monte Carlo program many times as the individual results are scattered around the true value.

Exercise 7.11: Use Monte Carlo integration to evaluate the integral in Exercise 7.9. The program should prompt the user for N, the number of random points used in the integration.

Exercise 7.12: Using Monte Carlo integration, find the center of mass of

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a 2-D right triangle with base of length 1 and height of length 2. With the right angle positioned at (0,0), the density varies as $\rho = y \sin x^2 + 2$. Recall that the center of mass of a planar object is given by

$$X = \frac{1}{M} \int \int x \rho dS$$

$$Y = \frac{1}{M} \int \int y \rho dS$$

where

$$M = \int \int \rho dS$$

Exercise 7.13: Repeat the problem of **Exercise 7.10** using Monte Carlo integration.

Exercise 7.14 The Ising Model: Monte Carlo methods may be used in applications other than integration. Consider the following from atomic physics. An Ising chain is a 1-D array made of N particles with spin. The spin (s) of an individual particle can be either up (+1) or down (-1), and the total energy of the chain is given by

$$E = -J \sum_{i=1}^{N-1} s_i s_{i+1}$$

The energy is a minimum when all the spins are the same. Consider an event that randomly flips the spin of one of the particles in the array. Thermodynamically, if that change results in a lower energy, it is highly probable. If the change results in a higher energy, it will have a probability given by the Boltzmann distribution

$$R = \exp(-\Delta E / kT)$$

Write a program that will implement the following algorithm:
1) Generate a trial spin configuration consisting of N particles with random spins s_i.
2) Pick a particle j randomly, flip its spin, and calculate the resulting new energy E_{new}.
3) Accept the new configuration if $E_{new} \leq E_{old}$. If $E_{new} > E_{old}$, then assign

a relative probability R given by the above equation. Generate a random number $0 < r < 1$. If $R > r$ accept the new configuration. If not, restore the old configuration as the accepted configuration and go back to step 2.

The above steps $2 \to 3$ should be incorporated into a `for` loop which will run from `l=1` to 5000. Print out `l` and the energy resulting from the configuration decided upon in step 3 for each passage through the loop. Take the following values for the constants: $N = 50$, $J = 2.0$, $k = 0.001$. Use Gnuplot to plot out l versus E. Note that for low temperatures $(T < 1000)$, the system rapidly declines in energy and reaches equilibrium within the 5000 iterations. For high temperatures, the energy simply fluctuates and does not reach equilibrium. The Ising model can be used to simulate many quantum physical systems. One example is magnetism. In a ferromagnetic material, individual atoms have a net magnetic moment. Magnetization will occur when those magnetic moments line up, and this represents the minimum energy configuration. In the presence of an external magnetic field, a macroscopic sample of the material can be magnetized, but as the temperature increases, the alignment of the magnetic moments becomes more chaotic. At sufficiently high temperatures, no magnetization will occur.