which different mRNAs are translated into proteins; and other RNAs have other as yet unknown functions. So a change of one base, e.g. from A to C, might alter a protein or change the expression of a gene or be silent.

Sexual reproduction makes bigger random changes in genomes. In meiosis, the paternal and maternal versions of each of our 23 chromosomes are duplicated, and the four versions swap segments of DNA in a process called genetic recombination or crossing-over. The cell then divides twice producing four haploid germ cells each with a single paternal, maternal, or mixed version of each chromosome. This second kind of Metropolis step makes evolution more ergodic, which is why most complex modern organisms use sexual reproduction.

Other genomic changes occur when a virus inserts its DNA into that of a cell and when transposable elements (transposons) of DNA move to different sites in a genome.

In evolution, the rest of the Metropolis step is done by the new individual: if he or she survives and multiplies, then the change is accepted; if he or she dies without progeny, then the change is rejected. Evolution is slow, but it has succeeded in turning a soup of simple molecules into humans with brains of 100 billion neurons, each with 1000 connections to other neurons.

John Holland and others have incorporated analogs of these Metropolis steps into Monte Carlo techniques called genetic algorithms for solving wide classes of problems (Holland, 1975; Vose, 1999; Schmitt, 2001).

Evolution also occurs at the cellular level when a cell mutates enough to escape the control imposed on its proliferation by its neighbors and transforms into a cancer cell.

Further Reading

The classic Quarks, Gluons, and Lattices (Creutz, 1983) is a marvelous introduction to the subject; his website (latticeguy.net/lattice.html) is an extraordinary resource.

Exercises

14.1 Go to Michael Creutz’s website (latticeguy.net/lattice.html) and get his C-code for $Z_2$ lattice gauge theory. Compile and run it, and make a graph that exhibits strong hysteresis as you raise and lower $\beta = kT$.

Solution: Use a browser to go to the website latticeguy.net/lattice and click on link “Even simpler example for $Z_2$ gauge fields.” Download the C code z2.c and the file Makefile to some directory on a computer
Monte Carlo Methods

Figure 14.2 The strong hysteresis loop is evidence for a first-order phase transition. The steps in $\beta$ are $d\beta = 0.001$ or 10 times smaller than in Creutz’s code.

that has the C compiler gcc, which is freely available. In that directory, and on a computer running Unix, Linux, or MacOS, type “make z2.” If you type “z2,” then the program will run and type out values of $\beta$ and of the energy at that value of $\beta$ for values of $\beta$ running from 1 to 0 and then from 0 to 1. The two curves are different and exhibit strong hysteresis. The command “z2 > out” will save the output in the file out. The file out will contain numbers that you can use to graph strong hysteresis as $\beta = 1/kT$ is run from 1 to 0 and from 0 to 1. You should get something like what is plotted in Fig. 14.2. This plot exhibits strong hysteresis which is evidence of a first-order phase transition, that is, a discontinuity in the energy (or euclidian action) as the temperature is varied.

14.2 Modify his code and produce a graph showing the coexistence of two phases at the critical coupling $\beta_t = 0.5 \ln(1 + \sqrt{2}) = 0.440687$. Hint:
Do a cold start and then 100 updates at $\beta_t$, then do a random start and do 100 updates at $\beta_t$. Plot the values of the energy against the update number 1, 2, 3, \ldots 100.

**Solution:** After modifying his code and running it, one should get evidence for the existence of two phases at the critical inverse temperature $\beta_t = 0.5 \ln(1 + \sqrt{2})$, like what is plotted in Fig. 14.3. The modified part of his code is, for example:

```c
int main()
{
    double action, bt;
    int count, dcount;
    srand48(1234L); /* initialize random number generator */
    /* demonstrate two phases */
    bt=0.5*(log(1.0+sqrt(2)));
    dcount=1;
    coldstart();
    /* after a cold start */
    for (count = 1; count<101; count+=dcount){
        action=update(bt);
        printf("%d\t%g\n",count,action);
    }
    printf("\n\n");
    bt=0.5*(log(1.0+sqrt(2)));
    coldstart(); update(0.0);
    /* after a hot start */
    for (count = 1; count<101; count+=dcount){
        action=update(bt);
        printf("%d\t%g\n",count,action);
    }
    printf("\n\n");
    exit(0);
}
```

14.3 Modify Creutz’s C code for $Z_2$ lattice gauge theory so as to be able to vary the dimension $d$ of space-time. Show that for $d = 2$, there’s no hysteresis loop (there’s no phase transition). For $d = 3$, show that any hysteresis loop is minimal (there’s a second-order phase transition at $\beta = 0.7613$).

**Solution:** We first modify Creutz’s code so as to run on a $d = 3$ lattice of size $6^3$. The resulting Fig. 14.4, shows weak hysteresis.
Two phases at $\beta = \ln(1 + \sqrt{2})/2$ in $Z_2$ gauge theory

Figure 14.3 The existence of two phases at the critical (inverse) temperature $\beta = \ln(1 + \sqrt{2})/2$ is further evidence for a first-order phase transition at that temperature.

To check whether this weak hysteresis is due to a first-order phase transition, we change Creutz’s code to run on the much bigger $30^3$ lattice and we change the step size $d\beta$ from 0.01 to 0.00001. The resulting Fig. 14.5, shows little or no hysteresis because the phase transition at $\beta_t = 0.7613$ is of second order (the energy is continuous) as a function of the temperature.

To check even more carefully on a $6^3$ lattice, we do a cold start with 200 updates at $\beta_t = 0.7613$ and then do a hot start with 200 updates at $\beta_t$. Fig. 14.6 reveals that the energy sequence after a hot start (red) quickly overlaps the energy sequence after a cold start (blue) $Z_2$ lattice gauge theory in three dimensions. The phase transition at $\beta_t = 0.7613$ is of second order (the energy is continuous as a function of the temperature).
Weak hysteresis in $d = 3$ $Z_2$ gauge theory

Figure 14.4 In three dimensions, $Z_2$ lattice gauge theory exhibits weak hysteresis on a $6^3$ lattice in a thermal cycle of heating (red) and cooling (blue). The phase transition at $\beta = 0.7613$ is of second order (the energy is continuous as a function of the temperature).

Finally, after modifying Creutz’s code to run on a $6^2$ lattice, we see no hysteresis in Fig. 14.7 because there’s no phase transition in $Z_2$ gauge theory in two dimensions.

14.4 What happens when $d = 5$?

**Solution:** If we modify Creutz’s code so it runs on a $6^5$ lattice, then we find that the mean energy upon heating (red) lies below the mean energy upon cooling (blue) for $0.2 \lesssim \beta \leq 1$ as shown in Fig. 14.8. On a $20^5$ lattice with steps of $d\beta = 0.001$, we see in Fig. 14.9 strong hysteresis suggestive of a first-order phase transition near $\beta_t \approx 0.38$. 

No hysteresis in $d = 3$ $Z_2$ gauge theory

Figure 14.5 In three dimensions, $Z_2$ lattice gauge theory exhibits little or no hysteresis because the phase transition at $\beta = 0.7613$ is of second order (the energy is continuous) as a function of the temperature. The steps in $\beta$ are $d\beta = 0.0001$, and the lattice is $30^3$.

14.5 Use example 14.3 to compute the ten-dimensional integral

$$I = \int \exp \left[ - (x^2 + (x^2)^2) \right] d^{10}x \quad (14.27)$$

over $\mathbb{R}^{10}$ where $x^2 = x_1^2 + \cdots + x_{10}^2$.

**Solution:** We apply the Kalos-Whitlock trick (14.24)

$$I = \int f(x) \, d^n x \approx I[g] \int \frac{f(x)}{g(x)} \frac{g(x)}{I[g]} \, d^n x = I[g] \int \frac{f(x)}{g(x)} \, P(x) \, d^n x. \quad (14.28)$$

with $f(x) = \exp \left[ - (x^2 + (x^2)^2) \right]$ and $g(x) = \exp(-x^2)$. The known
Two phases at $\beta = 0.7613$ in $d = 3$ $Z_2$ gauge theory

Figure 14.6 The energy sequence at $\beta_t = 0.7613$ after a hot start (red) quickly overlaps the energy sequence at $\beta_t$ after a cold start (blue) $Z_2$ lattice gauge theory in three dimensions. The phase transition at $\beta_t = 0.7613$ is of second order (the energy is continuous as a function of the temperature).

The integral is

$$I[g] = \int \exp(-x^2) \, d^{10}x$$

$$= \frac{2\pi^5}{\Gamma(5)} \int_0^{\infty} r^9 e^{-r^2} \, dr$$

in which the prefactor is the area of a unit sphere in 10 dimensions. The integral over $r$ is almost exactly 12, and $\Gamma(5) = 4! = 24$, and so the known integral is

$$I[g] = \pi^5 = 306.02.$$  \hspace{1cm} (14.30)

The following fortran program gave the integral $\mathcal{I}$ as

$$\mathcal{I} = 2.1045 \pm 0.002.$$  \hspace{1cm} (14.31)
No hysteresis in \( d = 2 \) \( Z_2 \) gauge theory

Figure 14.7 On a \( 6^2 \) lattice, there is no hysteresis because there's no phase transition in \( Z_2 \) gauge theory in two dimensions.

Mathematica gives the exact value as

\[
\mathcal{I} = \frac{\pi^5}{12} \text{NIntegrate}[x^5 \cdot \text{Exp}[-x^2 - x^4], \{x, 0, \text{Infinity}\}]
\]

\[
= \frac{\pi^5}{12} \cdot 0.0825323 = 2.1047094.
\]

(14.32)

program kaloswhitlock

! Monte Carlo integration of \( f(x) \) guided by
! the known integral \( \mathcal{I}(g) \) of the similar function \( g(x) \):  

\[
\int f(x) \, dx = \int \left[ \frac{f(x)}{g(x)} \right] g(x) \, dx \\
= \mathcal{I}(g) \int \left[ \frac{f(x)}{g(x)} \right] \frac{g(x)}{\mathcal{I}(g)} \, dx \\
= \frac{1}{N} \sum_i \left[ \frac{f(x_i)}{g(x_i)} \right] \frac{g(x_i)}{\mathcal{I}(g)} \\
= \left( \frac{\mathcal{I}(g)}{N} \right) \sum_i \left[ \frac{f(x_i)}{g(x_i)} \right]
\]

! in which the \( \sum_i \) is guided by the probability distribution
! \( g(x)/\mathcal{I}(g) \).
Figure 14.8 On a $6^5$ lattice, the energy upon heating (red) lies below the energy upon cooling (blue) for $0.2 \lesssim \beta \leq 1$.

! Volume of sphere in $\mathbb{R}^n$ is $V_n = \pi^{n/2}/\Gamma(n/2+1)$
! = $\pi^{n/2}/\Gamma((n+2)/2))$
! Area of sphere in $\mathbb{R}^n$ is $A_{n-1} = 2 \pi^{n/2}/\Gamma(n/2)$
! In fortran95, gamma(x) is the Gamma function.
! NIntegrate[x^9*Exp[-x^2], {x, 0, Infinity}] = 12.00000000000040
! NIntegrate[x^9*Exp[-x^2 - x^4], {x, 0, Infinity}] = 0.08253231309769363
! What an amazing difference!
implicit none
integer::i,run
integer,parameter::ni=110000000,nrun=10
doubleprecision::sum(nrun),int,sigma,count,knownintegral
doubleprecision::naccept,nreject,oldE,newE,A9,actualintegral
doubleprecision::rdn1
doubleprecision,dimension(10)::x,oldx,rdn
doubleprecision,parameter::dx=1.0d0
Figure 14.9 On a $20^5$ lattice $Z_2$ gauge theory shows strong hysteresis which suggests that there is a first-order phase transition near $\beta_t \approx 0.38$.

doubleprecision,parameter::zero = 0.0d0, one = 1.0d0, two = 2.0d0
doubleprecision,parameter::half = 0.5d0, ten = 10.0d0
doubleprecision,parameter::pi = 4.0d0*atan(1.0d0)
doubleprecision,parameter::knownintegral0=12.00000000000040d0
doubleprecision,parameter::actualintegral0=0.08253231309769363d0
call init_random_seed() ! set new seed
A9 = two*pi**5/Gamma(5.0d0)
knownintegral = knownintegral0*A9
actualintegral = actualintegral0*A9
int = zero; sum = zero
naccept = zero; nreject = zero
do run = 1, nrun
   x = one; count = zero
   do i = 1, ni
      call random_number(rdn)
oldx = x; oldE = dot_product(x,x)
x = x + dx*(rdn-half); newE = dot_product(x,x)
if ( newE <= oldE ) then
    naccept = naccept + one
else
    call random_number(rdn1)
    if ( exp(-(newE - oldE)) >= rdn1 ) then
        naccept = naccept + one
    else
        nreject = nreject + one
    x = oldx
end if
end if
if ( i >= ni/10 ) then
    sum(run) = sum(run) + exp( - dot_product(x,x)**2 )
    count = count + one
end if
end do
sum(run) = knownintegral*sum(run)/count
int = int + sum(run)
write(6,*)'run =',run,' sum =', sum(run)
end do
int = int/dble(nrun)
write(6,*) 'int =', int
write(6,* ) 'actual integral =', actualintegral
sigma = zero
do run = 1, nrun
    sigma = sigma + (sum(run) - int)**2
end do
sigma = sigma/dble(nrun*(nrun-1))
sigma = sqrt(sigma)
write(6,*)'sigma =',sigma
write(6,* )'fraction accepted =', naccept/(naccept+nreject)
contains
subroutine init_random_seed()
    implicit none
    integer ir, nr, clock
    integer, dimension(:), allocatable :: seed
    call random_seed(size = nr) ! find size of seed
    allocate(seed(nr))

call system_clock(count=clock) ! get time of processor clock
seed = clock + 37 * (/ (ir-1, ir=1, nr) /) ! make seed
call random_seed(put=seed) ! set seed
deallocate(seed)
end subroutine init_random_seed
end program kaloswhitlock

! results
!Kevins-MacBook-Pro:canon kevincahill$ multiwhitlock
! run = 1 sum = 2.1073239692943817
! run = 2 sum = 2.1076973988367369
! run = 3 sum = 2.0964532399723028
! run = 4 sum = 2.0976698535854097
! run = 5 sum = 2.1138983925909400
! run = 6 sum = 2.1127625472638982
! run = 7 sum = 2.1084585638976745
! run = 8 sum = 2.1052440601425744
! run = 9 sum = 2.0986197353127372
! run = 10 sum = 2.0967198397662448
! int = 2.1044847600662897
! actual integral = 2.1047093698963630
! sigma = 2.10166287758995840E-003
! fraction accepted = 0.5247776509090909