

## PS 4 Solutions

1. Use  $\int_a^b dx f(x) = \int_a^b dx w(x) \frac{f(x)}{w(x)} = \left\langle \frac{f}{w} \right\rangle_w$

with  $w(x) > 0$  and  $\int_a^b dx w(x) = 1 \iff w(x)$  is a pdf

Here,  $e^{-10x}$  is the rapidly varying part of  $f(x)$  so choose

$w(x) \propto e^{-10x}$   $\xrightarrow{\text{normalize}}$   $w(x) = 10 e^{-10x} + \mathcal{O}(e^{-10})$   $\swarrow$  neglect

The cdf of  $w$  is  $C(x) = \int_0^x dx' w(x') = 1 - e^{-10x}$

so choose random points  $y_i$  in  $(0,1)$  + let  $x_i = \frac{-1}{10} \log(1-y_i)$

Then  $\left\langle \frac{f}{w} \right\rangle_w = \frac{1}{N} \sum_{i=1}^N \frac{1}{1+x_i} \approx 0.0693$

```
program mc_int
```

```
  iseed=-829374781
```

```
  do i=1,1000
```

```
    x=ran2(iseed)
```

```
  enddo
```

```
  do
```

```
    print*, 'enter number of cycles'
```

```
    read*, ncy
```

```
    if(ncy.lt.0) exit
```

```
    xint=0.
```

```
    do i=1,ncy
```

```
      x=ran2(iseed)
```

```
      y=-0.1*(1-exp(-x))
```

```
      xint=xint+1./(1.+x)
```

```
    enddo
```

```
    xint=0.1*xint/float(ncy)
```

```
    print*, xint
```

```
  enddo
```

```
  stop
```

```
end
```

```

program mc_ising1
c
c Metroplis Monte Carlo for the 1-d Ising model
c
parameter (m=100)
dimension n(m)
c
c read parameters - temperature in units of epsilon/k_B
c
print*, 'enter temperature'
read*, t
beta=1./t
print*, 'enter random number seed (big negative integer)'
read*, idum
c
c warm up the random number generator
c
do i=1,1000
    x=ran2(idum)
enddo
c
c random initial configuration
c
do i=1,m
    n(i)=-1
    if(ran2(idum).gt.0.5) n(i)=+1
enddo
c
c initial values
c
ntot=0
ie=0.
do i=1,m-1
    ntot=ntot+n(i)
    ie=ie-n(i)*n(i+1)
enddo
ie=ie-n(m)*n(1)
ntot=ntot+n(m)
print*, 'initial total spin and energy/beta:',ntot,ie
c
c mc cycle loop
c
do
c
print*, 'enter number of cycles'
read*, ncy
if(ncy.lt.0) exit
c
ebar=0.
nch=0
nbar=0
c
c loop over cycles through the system
c

```

```

do icy=1,ncy
c
c loop over sites on each cycle
c
do itry=1,m
c
c choose a random site
c
i=100.*ran2(idum)+1.
nn=-n(i)
im1=i-1
if(i.eq.1) im1=m
ip1=i+1
if(i.eq.m) ip1=1
idelta_e = -2*nn*(n(im1)+n(ip1))
c
c Metropolis test
c
if(ran2(idum).lt.exp(-beta*idelta_e)) then
ntot=ntot+2*nn
n(i)=nn
ie=ie+idelta_e
nch=nch+1
endif
ebar=ebar+ie
nbar=nbar+ntot
enddo

enddo

rnorm=1./float(ncy*m)
print*, 'total spin and energy:',nbar*rnorm,beta*ebar*rnorm
print*, 'average number of flips/trial:',nch*rnorm

enddo

stop
end

FUNCTION ran2(idum)
INTEGER idum,IM1,IM2,IMM1,IA1,IA2,IQ1,IQ2,IR1,IR2,NTAB,NDIV
REAL ran2,AM,EPS,RNMX
PARAMETER (IM1=2147483563,IM2=2147483399,AM=1./IM1,IMM1=IM1-1,
*IA1=40014,IA2=40692,IQ1=53668,IQ2=52774,IR1=12211,IR2=3791,
*NTAB=32,NDIV=1+IMM1/NTAB,EPS=1.2e-7,RNMX=1.-EPS)
INTEGER idum2,j,k,iv(NTAB),iy
SAVE iv,iy,idum2
DATA idum2/123456789/, iv/NTAB*0/, iy/0/
if (idum.le.0) then
idum=max(-idum,1)
idum2=idum
do 11 j=NTAB+8,1,-1
...

```

```
mac_mc_ising1
enter temperature
2.
enter random number seed (big negative integer)
-193824921
initial total spin and energy/beta: 0 8
enter number of cycles
1000
total spin and energy: 1.12096000000000 -23.1063400000000
average number of flips/trial: 0.533690000000000
enter number of cycles
10000
total spin and energy: 0.234950000000000 -23.1921260000000
average number of flips/trial: 0.536792000000000
enter number of cycles
100000
total spin and energy: -8.55800000000000E-002 -23.1256038000000
average number of flips/trial: 0.537857600000000
enter number of cycles
1000000
total spin and energy: -5.56624600000000E-002 -23.1083481800000
average number of flips/trial: 0.537843660000000
```

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```
mac_mc_ising1
enter temperature
0.5
enter random number seed (big negative integer)
-193824921
initial total spin and energy/beta: 0 8
enter number of cycles
1000
total spin and energy: -4.33822000000000 -188.653600000000
average number of flips/trial: 5.57700000000000E-002
enter number of cycles
10000
total spin and energy: -18.7298020000000 -191.912888000000
average number of flips/trial: 4.02670000000000E-002
enter number of cycles
1000000
total spin and energy: 1.82687652000000 -193.104763680000
average number of flips/trial: 3.44799100000000E-002
enter number of cycles
10000000
total spin and energy: 1.83652817600000 -193.214329256000
average number of flips/trial: 3.39309530000000E-002
```