

Problem Set 1 Solutions

1. Volume of an n-sphere

MC code:

```

program vol
data iseed/-93847271/

do i=1,1000
    z=ran2(iseed)
enddo

write(6,*) 'enter dimension'
read(5,*) n

do
write(6,*) 'enter number of tries'
read(5,*) m
if(m.lt.1) exit

ma=0
do i=1,m
r2=0
do j=1,n
    z=ran2(iseed)
    x=2.*z-1.
    r2=r2+x*x
enddo
if(r2.lt.1.) ma=ma+1
enddo

vol1=ma*(2**n)/float(m)
write(6,*) 'n-volume =',vol1

enddo

stop
end
    
```

Analytic result:

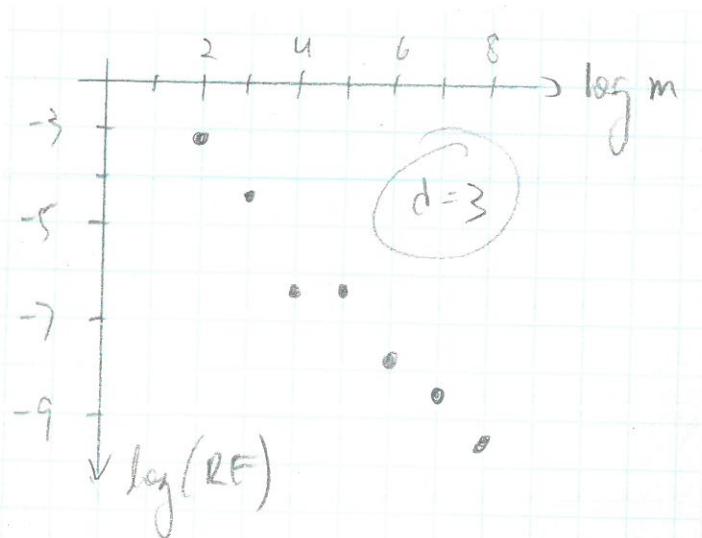
$$V_n = \frac{\pi^{n/2}}{\Gamma(\frac{n}{2}+1)}$$

π	$d=2$
$4\pi/3$	\geq
$\pi^2/2$	4
$8\pi^2/15$	5

Run for three dimensions:

```

%_ vol
enter dimension
3
enter number of tries
1000
n-volume = 4.136000000000000
enter number of tries
10000
n-volume = 4.180800000000000
enter number of tries
100000
n-volume = 4.180240000000000
enter number of tries
1000000
n-volume = 4.191232000000000
enter number of tries
10000000
n-volume = 4.187873600000000
enter number of tries
100000000
n-volume = 4.188469120
    
```



$$1b) \text{ Use } \int dx f(x) = \int dx \frac{f(x)}{p(x)} \cdot \underbrace{\frac{p(x)}{\int dx p(x)}}_{= P(x)} = \left\langle \frac{f}{p} \right\rangle_P \cdot \int dx p(x)$$

Here $f(x) = \frac{e^{-10x}}{1+x}$ so choose $p(x) = e^{-10x}$ = rapidly-varying part of f

$$\int_0^1 dx p(x) = \frac{1}{10} (1 - e^{-10}) \approx \frac{1}{10} \rightarrow P(x) \approx 10e^{-10x}$$

To generate points with pdf $P(x)$, find its cdf

$$C(x) = \int_0^x dx' P(x') = 1 - e^{-10x}$$

then take points y_i uniformly distributed in $(0,1)$ & let $x_i = C^{-1}(y_i) = \frac{1}{10} \log(1 - y_i)$ & then

$$\int dx f(x) \approx \underbrace{\frac{1}{N} \sum_{i=1}^N \frac{1}{1+x_i}}_{\left\langle \frac{f}{p} \right\rangle_P} \cdot \underbrace{\frac{1}{10}}_{\int dx p(x)} \approx 0.0916$$

```

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 (negative integer)'
read*, idum
c
c warm up the random number generator
c
do i=1,1000
    x=ran1(idum)
enddo
c
c random initial configuration
c
do i=1,m
    n(i)=-1
    if(ran1(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.*ran1(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(idelta_e.le.0.) then
ntot=ntot+2*nn
n(i)=nn
ie=ie+idelta_e
nch=nch+1
else if(ran1(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 ran1(idum)
INTEGER idum,IA,IM,IQ,IR,NTAB,NDIV
REAL ran1,AM,EPS,RNMX
PARAMETER (IA=16807,IM=2147483647,AM=1./IM,IQ=127773,IR=2836,
*NTAB=32,NDIV=1+(IM-1)/NTAB,EPS=1.2e-7,RNMX=1.-EPS)
INTEGER j,k,iv(NTAB),iy
SAVE iv,iy
DATA iv /NTAB*0/, iy /0/
if (idum.le.0.or.iy.eq.0) then
idum=max(-idum,1)
...

```

```
mac_mc_ising1
enter temperature
3
enter random number seed (negative integer)
-2945782387
initial total spin and energy/beta: -2 0
enter number of cycles
10000
total spin and energy: -0.365310000000000 -10.7141626666667
average number of flips/trial: 0.678135000000000
enter number of cycles
10000
total spin and energy: 1.134800000000000E-002 -10.7750613333333
average number of flips/trial: 0.677944000000000
enter number of cycles
10000
total spin and energy: -0.187926000000000 -10.7249786666667
average number of flips/trial: 0.679180000000000
enter number of cycles
100000
total spin and energy: 2.204360000000000E-002 -10.7083857333333
average number of flips/trial: 0.678573000000000
enter number of cycles
-1
```

```
mac_mc_ising1
enter temperature
1
enter random number seed (negative integer)
-493847276
initial total spin and energy/beta: -2 -4
enter number of cycles
10000
total spin and energy: 2.178100000000000 -76.1607160000000
average number of flips/trial: 0.238374000000000
enter number of cycles
10000
total spin and energy: 0.342462000000000 -76.3596680000000
average number of flips/trial: 0.236344000000000
enter number of cycles
10000
total spin and energy: 2.455544000000000 -76.3575000000000
average number of flips/trial: 0.236169000000000
enter number of cycles
100000
total spin and energy: -0.994435800000000 -76.2247252000000
```

average number of flips/trial: 0.238001300000000
enter number of cycles
100000
total spin and energy: -0.125363400000000 -76.1953408000000
average number of flips/trial: 0.238447100000000
enter number of cycles
-1

mac_mc_ising1

enter temperature
0.3
enter random number seed (negative integer)
-47483821
initial total spin and energy/beta: 4 -4
enter number of cycles
10000
total spin and energy: -97.1925440000000 -332.501373333333
average number of flips/trial: 2.52200000000000E-003
enter number of cycles
10000
total spin and energy: -100.000000000000 -333.333333333333
average number of flips/trial: 0.000000000000000
enter number of cycles
10000
total spin and energy: -99.9994220000000 -333.329786666667
average number of flips/trial: 6.00000000000000E-006
enter number of cycles
100000
total spin and energy: 26.2291804000000 -333.233637333333
average number of flips/trial: 2.95000000000000E-004
enter number of cycles
100000
total spin and energy: 99.7742274000000 -333.245633333333
average number of flips/trial: 2.64000000000000E-004
enter number of cycles
100000
total spin and energy: 99.9963710000000 -333.327490666667
average number of flips/trial: 1.70000000000000E-005
enter number of cycles
-1