MARKOV CHAIN MONTE CARLO EXAMPLES

Hastings-Metropolis for Integration Problems:

$$E[h(\mathbf{X})] = \int_D h(\mathbf{x})p(\mathbf{x})d\mathbf{x} \approx \frac{1}{N}\sum_{i=1}^{N} h(\mathbf{X}_i).$$

H-M algorithms often sample from "neighboring" elements of states $\mathbf{X}$. Then the transition $q(\mathbf{X}, \mathbf{Y})$ is a distribution on the set of "neighbors" of $\mathbf{X}$,

for example,

a) Uniform for some box near $\mathbf{X}$ or

b) Normal near $\mathbf{X}$; then

$q(\mathbf{X}, \mathbf{Y}) = q(\mathbf{Y}, \mathbf{X})$, so $\alpha(\mathbf{X}, \mathbf{Y}) = min(\frac{p(\mathbf{Y})}{p(\mathbf{X})}, 1)$.

Basic H-M steps: choose $\mathbf{X} \in D$

for $n = 1$ to N

a) generate $\mathbf{Y}$ from neighborhood of $\mathbf{X}$;

b) compute $p(\mathbf{Y})$;

c) if $U < p(\mathbf{Y})/p(\mathbf{X})$, accept new $\mathbf{X} = \mathbf{Y}$;

d) save $V_n = h(\mathbf{X})$;

end.

MCMC EXAMPLES CONT.

Example Integration Problem using H-M to estimate

$$V = \int_0^1 \int_0^1 \int_0^1 xyz \ln(x+2y+3z) \sin(x+y+z) dxdydz \approx .138401.$$

For setup, first choose $p(x,y,z) = \sin(x+y+z)/C$ with

$$C = \int_0^1 \int_0^1 \int_0^1 \sin(x+y+z) dxdydz \quad = \cos(3) - 3\cos(2) + 3\cos(1) - 1,$$

then

$$V = C \int_0^1 \int_0^1 \int_0^1 xyz \ln(x+2y+3z) p(x,y,z) dxdydz.$$

If neighborhood of $\mathbf{X}$ is set of points within 1/4 of each component,
then $\mathbf{Y} = \mathbf{X} + (\mathbf{U}/2 - 1/4)$ for uniform $\mathbf{U}$;
$\mathbf{Y}$ is accepted if $\mathbf{Y} \in [0,1]^3$ and $U < p(\mathbf{Y})/p(\mathbf{X})$.
Steps are: initialize $\mathbf{X} = (1/2, 1/2, 1/2)$;
for $n = 1$ to N
a) $\mathbf{Y} = \mathbf{X} + \mathbf{U}/2 - 1/4$
b) if $\mathbf{Y} \in [0,1]^3$ and $U < p(\mathbf{Y})/p(\mathbf{X})$, set $\mathbf{X} = \mathbf{Y}$
c) $V(n) = CX_1X_2X_3 \ln(X_1 + 2X_2 + 3X_3)$;
end.

MCMC EXAMPLES CONT.

Example Matlab results:

```
N = 10000; C = cos(3)-3*cos(2)+3*cos(1)-1; X = ones(3,1)/2;
for n = 1 : N; Y = X + rand(3,1)/2-1/4;
  if min(Y) > 0 && max(Y) < 1 && ...
       rand < sin(sum(Y))/sin(sum(X)), X = Y;
  end, V(n) = C*prod(X)*log([1 2 3]*X);
end, disp([mean(V) 2*std(V)/sqrt(N)])
      0.13927    0.0036877
% Simpler Uniform Neighborhood:
for n = 1:N,  Y=rand(3,1);
   if rand < sin(sum(Y))/sin(sum(X)), X = Y; end,
   V(n) = C*prod(X)*log([1 2 3]*X);
end, disp([mean(V) 2*std(V)/sqrt(N)])
      0.13852    0.0035582
```

Try $p(x, y, z) = xyz\sin(x + y + z)$, but new unknown C must be estimated.
Some Matlab results with simpler $q(x, y)$

```
p = @(x)prod(x).*sin(sum(x)); X = ones(3,1)/2; N = 10000;
for n = 1 : N, Y = rand(3,1);
  if rand < p(Y)/p(X), X = Y; end, V(n)=log([1 2 3]*X); E(n) = p(Y);
end, V = V*mean(E); disp( [mean(V) 2*std(V)/sqrt(N)] )
     0.13896   0.00049663
```

MCMC EXAMPLES CONT.

Continuing with

$$V = \int_0^1 \int_0^1 \int_0^1 xyz \ln(x + 2y + 3z) \sin(x + y + z) dxdydz \approx .138401.$$

Alternately, could try $p(x, y, z) = \ln(x + 2y + 3z) \sin(x + y + z)$?,
but then new C is unknown, and must be estimated.

Some Matlab results with simpler $q(x, y)$

```
p = @(x)log([1:3]*x).*sin(sum(x));
X = ones(3,1)/2; N = 10000;
for n = 1 : N, Y = rand(3,1);
  if rand < p(Y)/p(X), X = Y; end, V(n)=prod(X); E(n) = p(Y);
end, V = V*mean(E); disp( [mean(V) 2*std(V)/sqrt(N)] )
     0.14026    0.0026653
X = ones(3,1)/2; N = 1000000;
for n = 1 : N, Y = rand(3,1);
  if rand < p(Y)/p(X), X = Y; end, V(n)=prod(X); E(n) = p(Y);
end, V = V*mean(E); disp( [mean(V) 2*std(V)/sqrt(N)] )
     0.13806    0.0002627
```

But there are problems with this calculation:
$\ln(x + 2y + 3z) < 0$ whenever $z + 2y + 3z < 1$ and those states are rejected, so some of the domain cannot be sampled.

MCMC EXAMPLES CONT.

Expected Value Problem $E[x] = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} x \, \frac{e^{-(x^2y^2+x^2+y^2-8x-8y)/2}}{C} \, dxdy$,
with $C \approx 20216.336$, but not needed; $E[x] \approx 1.85997$.
If neighbors of $\mathbf{X}$ are $\mathbf{Y} = \mathbf{X} + 2\mathbf{Z}$ with $Z_i \sim Normal(0,1)$,
then accept $\mathbf{Y}$ if $U < p(\mathbf{Y})/p(\mathbf{X})$, with $p(x,y) = e^{-(x^2y^2+x^2+y^2-8x-8y)/2}$.
Steps are: initialize $\mathbf{X} = (0,0)$;
for $n = 1$ to N
a) $\mathbf{Y} = \mathbf{X} + 2\mathbf{Z}$, with $Z_i \sim Normal(0,1)$,
b) if $U < p(\mathbf{Y})/p(\mathbf{X})$, set $\mathbf{X} = \mathbf{Y}$
c) $E(n) = X_1$;
end.
Example Matlab results:

```
pe = @(X)exp(-( prod(X)^2 + sum(X.^2) - 8*sum(X) )/2);
N = 100000; X = [0;0];
for n = 1:N, Y = X+2*randn(1,2);
  if rand < pe(Y)/pe(X), X = Y; end, E(n) = X(1);
end, disp([mean(E) 2*std(E)/sqrt(N)])
      1.8561     0.010621
      1.8235     0.010497  % Comparison from Gibbs Sampling
```

MCMC EXAMPLES CONT.

More MCMC Examples

- Sampling from large combinatorial sets,
  e.g. all permutations of $(x_1, x_2, \ldots, x_n)$.
  If H-M algorithm samples from "neighboring" states of $\mathbf{X}$, then the transition $q(\mathbf{X}, \mathbf{Y}) = \frac{1}{|N(\mathbf{X})|}$, where $|N(\mathbf{X})|$ is the number of $\mathbf{Y} \in N(\mathbf{X})$, the "neighbors" of $\mathbf{X}$, and $\alpha(\mathbf{X}, \mathbf{Y})$ depends on the problem.
  Basic H-M algorithm steps:
  a) generate $\mathbf{Y}$ uniformly from neighbors of $\mathbf{X}$;
  b) if $U < \alpha(\mathbf{X}, \mathbf{Y})$, accept new $\mathbf{X} = \mathbf{Y}$.

MCMC EXAMPLES CONT.

Traveling Salesperson Problem (TSP)
has cities $1, \ldots, n$ with distance c_{ij} between city i and j.
The problem is to choose a path $\mathbf{x} = (x_1, \ldots, x_n)$,
(some permutation of $(1, \ldots, n)$) to minimize $S(\mathbf{x}) = \sum_{i=1}^{n-1} c_{x_i, x_{i+1}} + c_{x_n, x_1}$.
Simulated annealing optimization uses the "Boltzmann" pdf
$p(\mathbf{x}) = ce^{-S(\mathbf{x})/T}$ with H-M algorithm.
Basic H-M algorithm chooses $\mathbf{X} = (1, \ldots, n)$, $T = T_0$ and
repeats

a) generate $\mathbf{Y}$ uniformly from neighbors of $\mathbf{X}$;
b) if $U < e^{-(S(\mathbf{Y})-S(\mathbf{X}))/T}$, accept new $\mathbf{X} = \mathbf{Y}$;
c) set $T = .99T$;

until convergence.
Step a) details: choose i uniformly from $\{1, \ldots, n\}$ and
choose j uniformly from $\{1, \ldots, n\}$, then
interchange x_i and x_j in $\mathbf{X}$ to get $\mathbf{Y}$.

MCMC EXAMPLES CONT.

Matlab test for TSP:

```
function [X SX] = trvlsp( N, n, C )
% Traveling Salesperson, N steps
T = 10; X = randperm(n); SX = distc( n, X, C );
 for k = 1 : N, Y = X;
   i = ceil(n*rand); j = ceil(n*rand);
   Y([i j]) = X([j i]); SY = distc( n, Y, C );
   if rand < exp((SX-SY)/T), X = Y; SX = SY; end
   T = .99*T; % disp([SX X]);
  end
% end trvlsp
function S = distc(n,x,C), S = C(x(n),x(1));
  for i = 1 : n-1, S = S + C(x(i),x(i+1)); end
% end distc
n = 20; C = round(20*rand(n)); C = C+C'; % random test network
[X SX] = trvlsp(1000,n,C); disp([SX X])
183 6 12 7 13 18 19 8 9 15 5 11 4 17 16 3 10 20 1 14 2
[X SX] = trvlsp(1000,n,C); disp([SX X])
182 12 17 18 13 9 8 19 20 10 3 7 14 11 4 5 15 16 2 1 6
```

MCMC EXAMPLES CONT.

Component Failure Problem: if there are 10 components, with component i functional with probability $p_i = .5 + i/40$, and F is the number of functional components, use simulation to estimate $P\{F = i | F \leq 4\}, i = 0, 1, 2, 3, 4$.

Let $\mathbf{x} = (x_1, x_2, \ldots, x_n)$, $x_i = 0$ or 1 indicating nonfunctional or functional component i.

For Gibbs sampling, given $\mathbf{X}$, pick one random component i, and set to 1 if $U < p_i$ and accept this new $\mathbf{Y}$ if $F(\mathbf{Y}) < 5$.

Example Matlab results:

```
N = 100000; P = zeros(N,5); p = .5 + [1:10]/40; X = zeros(10,1);
for n = 1:N,  i = ceil(10*rand);
 while 1, T = rand < p(i);
   if sum(X)-X(i)+T < 5, X(i)=T; break; end
 end, P(n,sum(X)+1)=1;
end, disp([mean(P); std(P)/sqrt(N)])
  0.00018  0.00494  0.04571 0.22681  0.72236
  0.00008  0.00044  0.00132 0.00265  0.00283
```

This is equivalent to Hastings-Metropolis if the neighborhood of $\mathbf{X}$ is the set of $\mathbf{Y}$s with one component different.