STAT 535

MARKOV CHAIN MONTE CARLO

MCMC!

Motivation

MCMC is primarily motivated as a way to do Bayesian calculations (the target distribution is a posterior distribution). There are (many) other applications though.

Have (high-dimensional) *target distribution*, i.e., can evaluate unnormalized density $\pi(z)$, but may not have any further knowledge. Can't do integral to normalize and determine $\pi^*(z)$.

Want to learn about $\pi^*()$ by simulating a (large) Monte Carlo sample $Z^{(1)}, \ldots, Z^{(m)}$.

IID sampling from $\pi(z)$? TOO HARD!

Serially dependent sampling from $\pi(z)$? TOO HARD!

Serially dependent sampling with $dist(Z^{(i)})$ *converging* to $\pi^*()$ as $i \to \infty$?

NOW WE'RE TALKING!

How?

Set up a Markov Chain with $\pi^*()$ as the stationary distribution.

How?

(Homogeneous) Markov Chain Review

Distribution of $Z^{(i+1)}|Z^{(0)}, \ldots, Z^{(i)}$ depends only on $Z^{(i)}$.

Transition 'matrix' T(a,b) such that
$Pr(Z^{(i+1)} = b|Z^{(i)} = a) = T(a, b)$ for all i.

Given an initial distribution for $Z^{(0)}$ and a transition matrix $T()$ we can simulate a chain.

Recall a distribution π^* is 'the' stationary distribution of the chain if $Z^{(i)} \sim \pi^* \Rightarrow Z^{(i+1)} \sim \pi^*$.

Or mathematically, $\pi^* = \pi^*T$. That is, $(\pi^*, 1)$ is an *eigenpair* of T.

'THEOREM': Under weak conditions, for any $dist(Z^{(0)})$, $dist(Z^{(i)})$ converges 'quickly' to the stationary distribution associated with T as i increases.

'PROOF': Hand-waving linear algebra argument.

How to use this to advantage?

Have target (unnormalized) density $\pi()$. Need to construct a transition matrix T having $\pi^*()$ as its stationary distribution.

Then we could simulate the chain and discard some 'burn-in' (pre-convergence) iterations. The remaining values could be viewed as a serially dependent sample from $\pi^*()$.

Metropolis-Hastings Algorithm

Start with *any* transition matrix $Q(a, b)$. Don't know/care about its stationary distribution.

Define $T(a, b)$ as

- Have $Z^{(i)}$
- Generate $Z^* \sim Q(Z^{(i)}, \cdot)$
- Compute $p = \min\left\{\frac{\pi(Z^*)Q(Z^*, Z^{(i)})}{\pi(Z^{(i)})Q(Z^{(i)}, Z^{(*)})}, 1\right\}$.
- Set (using randomization)

$$Z^{(i+1)} \leftarrow \begin{cases} Z^{(*)} & \text{with probability } p, \\ Z^{(i)} & \text{with probability } 1-p. \end{cases}$$

Not so hard to check that $\pi T = \pi$, as desired.

Toy Example

$$\pi(z) = \begin{cases} \exp\{-(0.5)z^2\} & \text{if } z \le 0, \\ 1 & \text{if } 0 < z \le 1, \\ z^{-3} & \text{if } z > 1. \end{cases}$$

```
z <- 20
for (i in 1:10000) {
  zstr <- z + rnorm(1, sd=3)
  if (log(runif(1)) < (logtarg(zstr)-logtarg(z))) {
    z <- zstr }
  opt[i] <- z }
```

Note this is a common choice of $Q(a, b)$ - no special knowledge about $\pi()$ needed. So-called *random-walk* MH. Tuning???