MCMC I

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Agenda

- Like Ordinary Monte Carlo (OMC), but better?
- SLLN and Markov chain CLT
- Variance estimation
- AR(1) example
- Metropolis-Hastings algorithm (with an exercise)

Markov chain Monte Carlo

- A Markov chain is a dependent sequence of random variables $X_1, X_2, \ldots$ or random vectors $X_1, X_2, \ldots$ having the property that the future is independent of the past given the present
- Conditional distribution of X_{n+1} given $X_1, \ldots, X_n$ depends only on X_n
- Markov chain has **stationary transition probabilities** if the conditional distribution of X_{n+1} given X_n is the same for all n
  - Every Markov chain used in MCMC has this property
- The joint distribution of $X_1, \ldots, X_n$ is determined by the initial distribution of the Markov chain and the transition probabilities
  - Marginal distribution of X_1
  - Conditional distribution of X_{n+1} given X_n

Markov chain Monte Carlo

- A scalar functional of a Markov chain is a time series, but not necessarily a Markov chain
- A Markov chain is **stationary** if its initial distribution is stationary
  - Different from having stationary transition probabilities
  - All chains used in MCMC have stationary transition probabilities, but none are exactly stationary

Markov chain Monte Carlo

- To be (exactly) stationary, must start the chain with simulation from the equilibrium (invariant, stationary) distribution
- If chain is stationary, then every iterate X_i has the same marginal distribution, which is the equilibrium distribution
- If chain is not stationary but has a unique equilibrium distribution, which includes chains used in MCMC, then the marginal distribution X_i converges to the equilibrium distribution as $i \to \infty$

Markov chain Monte Carlo

- Let π be a probability distribution having support $\mathcal{X} \subseteq \mathbb{R}^d$, $d \geq 1$ we want to explore
- When i.i.d. observations are unavailable, a Markov chain with stationary distribution π can be utilized
- Summarize π with expectations, quantiles, density plots ...

Markov chain Monte Carlo

- Suppose $X_1, \ldots, X_n$ are simulation from a Markov chain having a unique equilibrium distribution (say π), and suppose we want to know an expectation

$$\mu_g = E[g(X_i)] = \int_{\mathcal{X}} g(x)\, \pi(dx)$$

  where the expectation is with respect to unique equilibrium distribution π
- If $E_\pi |g(X_i)| < \infty$, then

$$\hat{\mu}_n = \frac{1}{n} \sum_{i=1}^{n} g(X_i) \overset{a.s.}{\to} \mu_g \quad \text{as } n \to \infty \ (SLLN).$$

Markov chain Monte Carlo

- The central limit theorem (CLT) for Markov chains says

$$\sqrt{n}(\hat{\mu}_n - E_\pi g(X_i)) \to \mathrm{N}(0, \sigma^2) \ ,$$

where

$$\sigma^2 = \mathrm{Var} g(X_i) + 2 \sum_{k=1}^{\infty} \mathrm{Cov}\left[g(X_i), g(X_{i+k})\right]$$

- CLT holds if $E_\pi |g(X_i)|^{2+\epsilon} < \infty$ and the Markov chain is geometrically ergodic
- Can estimate σ^2 in various ways
- Verifying such a mixing condition is generally very challenging
- Nevertheless, we expect the CLT to hold in practice when using a **smart** sampler

Batch means

- In order to make MCMC practical, need a method to estimate the variance σ^2 in the CLT, then can proceed just like in OMC
- If $\hat{\sigma}^2$ is a consistent estimate of σ^2, then an asymptotic 95% confidence interval for μ_g is

$$\hat{\mu}_n \pm 1.96 \frac{\hat{\sigma}}{\sqrt{n}}$$

- The method of batch means estimates the asymptotic variance for a stationary time series

Batch means

- Markov chain CLT says

$$\hat{\mu}_n \approx \mathrm{N}\left(\mu_g, \frac{\sigma^2}{n}\right)$$

- Suppose b evenly divides n and we have the means

$$\hat{\mu}_{b,k} = \frac{1}{b} \sum_{i=bk+1}^{bk+b} g(X_i)$$

for $k = 1, \ldots, a = n/b$
- Then each of these **batch means** satisfies (if b is sufficiently large)

$$\hat{\mu}_{b,k} \approx \mathrm{N}\left(\mu_g, \frac{\sigma^2}{b}\right)$$

Batch means

- Thus empirical variance of the sequence of batch means

$$\frac{1}{a}\sum_{k=1}^{a}(\hat{\mu}_{b,k}-\hat{\mu}_n)^2$$

  estimates σ^2/b
- And b/n times this estimates σ^2/n, the asymptotic variance of $\hat{\mu}_n$
- Batch means can produce a strongly consistent estimator of σ^2 if $b \to \infty$ and $a \to \infty$ as $n \to \infty$

Stopping rules

- Suppose $\epsilon > 0$, then a **fixed-width stopping rule** terminates the simulation the first time half-width (or width) of a confidence interval is sufficiently small
- That is, simulate until

$$1.96 \frac{\hat{\sigma}}{\sqrt{n}} < \epsilon.$$

Example: AR(1)

- Consider the Markov chain such that

$$X_i = \rho X_{i-1} + \epsilon_i$$

where $\epsilon_i \overset{iid}{\sim} N(0,1)$

  - Consider $X_1 = 0$, $\rho = .95$, and estimating $E_\pi X = 0$
  - Run until

$$w_n = 2z_{.975}\frac{\hat{\sigma}}{\sqrt{n}} \leq 0.2$$

where $\hat{\sigma}$ is calculated using batch means

Example: AR(1)

The following will provide an observation from the MC 1 step ahead

```
ar1 <- function(m, rho, tau) {
rho*m + rnorm(1, 0, tau)
}
```

Next, we add to this function so that we can give it a Markov chain and the result will be p observations from the Markov chain

```
ar1.gen <- function(mc, p, rho, tau, q=1) {
loc <- length(mc)
junk <- double(p)
mc <- append(mc, junk)

for(i in 1:p){
j <- i+loc-1
mc[(j+1)] <- ar1(mc[j], rho, tau)
}
return(mc)
}
```

Example: AR(1)

```r
set.seed(20)
library(mcmcse)
```

```
## Warning: package 'mcmcse' was built under R version 4.0.2

## mcmcse: Monte Carlo Standard Errors for MCMC
## Version 1.4-1 created on 2020-01-29.
## copyright (c) 2012, James M. Flegal, University of California, Riverside
##                     John Hughes, University of Colorado, Denver
##                     Dootika Vats, University of Warwick
##                     Ning Dai, University of Minnesota
##  For citation information, type citation("mcmcse").
##  Type help("mcmcse-package") to get started.
```

```r
tau <- 1
rho <- .95
out <- 0
eps <- 0.1
start <- 1000
r <- 1000
```

Example: AR(1)

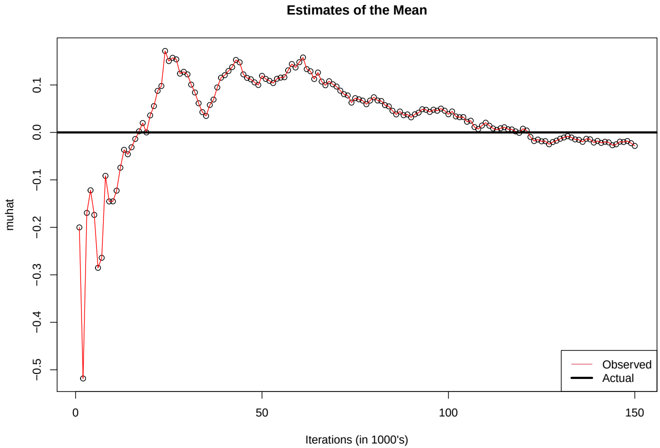
```
out <- ar1.gen(out, start, rho, tau)
MCSE <- mcse(out)$se
N <- length(out)
t <- qt(.975, (floor(sqrt(N) - 1)))
muhat <- mean(out)
check <- MCSE * t

while(eps < check) {
out <- ar1.gen(out, r, rho, tau)
MCSE <- append(MCSE, mcse(out)$se)
N <- length(out)
t <- qt(.975, (floor(sqrt(N) - 1)))
muhat <- append(muhat, mean(out))
check <- MCSE[length(MCSE)] * t
}

N <- seq(start, length(out), r)
t <- qt(.975, (floor(sqrt(N) - 1)))
half <- MCSE * t
sigmahat <- MCSE*sqrt(N)
N <- seq(start, length(out), r) / 1000
```

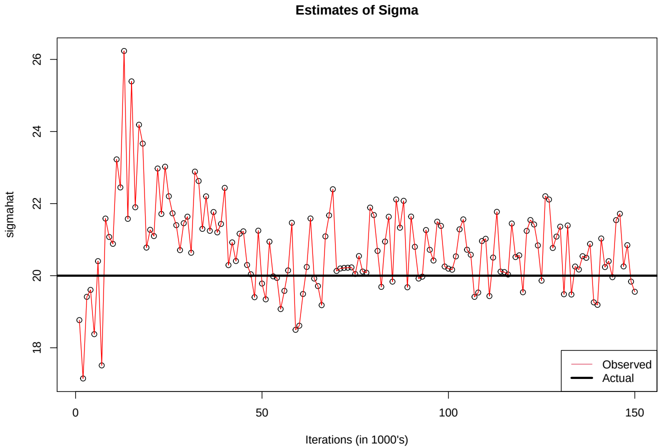
Example: AR(1)

```
plot(N, muhat, main="Estimates of the Mean", xlab="Iterations (in 1000's)")
points(N, muhat, type="l", col="red") ; abline(h=0, lwd=3)
legend("bottomright", legend=c("Observed", "Actual"), lty=c(1,1), col=c(2,1), lwd=c(1,3))
```



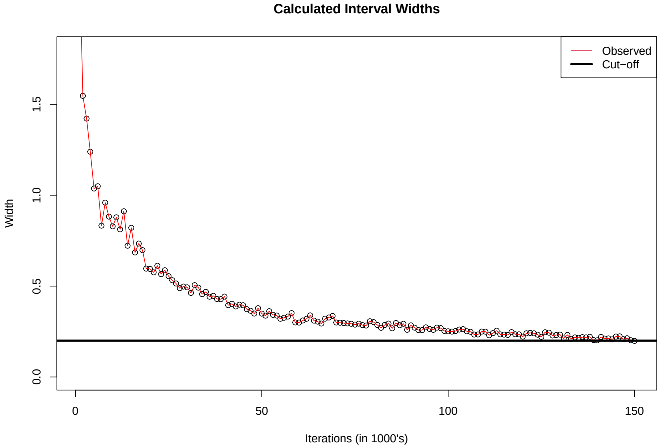
Example: AR(1)

```
plot(N, sigmahat, main="Estimates of Sigma", xlab="Iterations (in 1000's)")
points(N, sigmahat, type="l", col="red"); abline(h=20, lwd=3)
legend("bottomright", legend=c("Observed", "Actual"), lty=c(1,1), col=c(2,1), lwd=c(1,3))
```



Example: AR(1)

```r
plot(N, 2*half, main="Calculated Interval Widths", xlab="Iterations (in 1000's)",
     ylab="Width", ylim=c(0, 1.8))
points(N, 2*half, type="l", col="red"); abline(h=0.2, lwd=3)
legend("topright", legend=c("Observed", "Cut-off"), lty=c(1,1), col=c(2,1), lwd=c(1,3))
```



Markov chain Monte Carlo

- MCMC methods are used most often in Bayesian inference where the equilibrium (invariant, stationary) distribution is a posterior distribution
- Challenge lies in construction of a suitable Markov chain with f as its stationary distribution
- A key problem is we only get to observe t observations from $\{X_t\}$, which are serially **dependent**
- Other questions to consider
  - How good are my MCMC estimators?
  - How long to run my Markov chain simulation?
  - How to compare MCMC samplers?
  - What to do in high-dimensional settings?
  - ...

Metropolis-Hastings algorithm

Setting $X_0 = x_0$ (somehow), the Metropolis-Hastings algorithm generates X_{t+1} given $X_t = x_t$ as follows:

1. Sample a candidate value $X^* \sim g(\cdot|x_t)$ where g is the proposal distribution
2. Compute the MH ratio $R(x_t, X^*)$, where

$$R(x_t, X^*) = \frac{f(x^*)g(x_t|x^*)}{f(x_t)g(x^*|x_t)}$$

3. Set

$$X_{t+1} = \begin{cases} x^* \text{ w.p. } \min\{R(x_t, X^*), 1\} \\ x_t \text{ otherwise} \end{cases}$$

Metropolis-Hastings algorithm

- Irreducibility and aperiodicity depend on the choice of g, these must be checked
- Performance (finite sample) depends on the choice of g also, be careful

Independence chains

- Suppose $g(x^*|x_t) = g(x^*)$, this yields an **independence** chain since the proposal does not depend on the current state
- In this case, the MH ratio is

$$R(x_t, X^*) = \frac{f(x^*)g(x_t)}{f(x_t)g(x^*)},$$

  and the resulting Markov chain will be irreducible and aperiodic if $g > 0$ where $f > 0$
- A good envelope function g should resemble f, but should cover f in the tails

Random walk chains

- Generate X^* such that $\epsilon \sim h(\cdot)$ and set $X^* = X_t + \epsilon$, then $g(x^*|x_t) = h(x^* - x_t)$
- Common choices of $h(\cdot)$ are symmetric zero mean random variables with a scale parameter, e.g. a Uniform$(-a, a)$, Normal$(0, \sigma^2)$, $c * T_\nu, \ldots$
- For symmetric zero mean random variables, the MH ratio is

$$R(x_t, X^*) = \frac{f(x^*)}{f(x_t)}$$

- If the support of f is connected and h is positive in a neighborhood of 0, then the chain is irreducible and aperiodic.

Example: Markov chain basics

Exercise: Suppose $f \sim Exp(1)$

1. Write an independence MH sampler with $g \sim Exp(\theta)$
2. Show $R(x_t, X^*) = \exp\{(x_t - x^*)(1 - \theta)\}$
3. Generate 1000 draws from f with $\theta \in \{1/2, 1, 2\}$
4. Write a random walk MH sampler with $h \sim N(0, \sigma^2)$
5. Show $R(x_t, X^*) = \exp\{x_t - x^*\} I(x^* > 0)$
6. Generate 1000 draws from f with $\sigma \in \{.2, 1, 5\}$
7. In general, do you prefer an independence chain or a random walk MH sampler? Why?
8. Implement the fixed-width stopping rule for you preferred chain

Example: Markov chain basics

Independence Metropolis sampler with Exp(θ) proposal

```
ind.chain <- function(x, n, theta = 1) {
  ## if theta = 1, then this is an iid sampler
  m <- length(x)
  x <- append(x, double(n))
  for(i in (m+1):length(x)){
    x.prime <- rexp(1, rate=theta)
    u <- exp((x[(i-1)]-x.prime)*(1-theta))
    if(runif(1) < u)
      x[i] <- x.prime
    else
      x[i] <- x[(i-1)]
  }
  return(x)
}
```

Example: Markov chain basics

Random Walk Metropolis sampler with $N(0, \sigma)$ proposal

```
rw.chain <- function(x, n, sigma = 1) {
  m <- length(x)
  x <- append(x, double(n))
  for(i in (m+1):length(x)){
    x.prime <- x[(i-1)] + rnorm(1, sd = sigma)
    u <- exp((x[(i-1)]-x.prime))
    u
    if(runif(1) < u && x.prime > 0)
      x[i] <- x.prime
    else
      x[i] <- x[(i-1)]
  }
  return(x)
}
```

Example: Markov chain basics

```r
trial0 <- ind.chain(1, 500, 1)
trial1 <- ind.chain(1, 500, 2)
trial2 <- ind.chain(1, 500, 1/2)
rw1 <- rw.chain(1, 500, .2)
rw2 <- rw.chain(1, 500, 1)
rw3 <- rw.chain(1, 500, 5)
```

Example: Markov chain basics