Lecture 5: Simulation by MCMC Methods

Instructor: Fei Tan

@econdojo @BusinessSchool101 Saint Louis University

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The Road Ahead

Big Picture of MCMC

Central equation

$$\int_A \int_{\mathbb{R}^d} p(x, y) f(x) dx dy = \int_A f(y) dy, \quad \forall A \in \mathcal{B}(\mathbb{R}^d)$$

- What is Markov chain theory doing? Know transition kernel $p(\cdot, \cdot)$, find invariant distribution $f(\cdot)$

$$\int_A \int_{\mathbb{R}^d} p(x, y) f^{(n-1)}(x) dx dy = \int_A f^{(n)}(y) dy \to \int_A f(y) dy$$

- Markov chain Monte Carlo (MCMC) is doing opposite: know $f(\cdot)$, find corresponding $p(\cdot, \cdot)$ such that

$$f(x)p(x, y) = f(y)p(y, x) \quad \text{(reversibility)}$$

- MCMC methods greatly broaden Bayesian scope though at cost of simulating *dependent* samples

Gibbs Algorithm

Algorithm 1

1. Choose $x^{(0)} = (x_1^{(0)}, \ldots, x_d^{(0)})$ and set $g = 0$
2. Sample $x_i^{(g+1)} \sim f(x_i | x_{-i}^{(g)})$ for $i = 1, \ldots, d$
3. Set $g = g + 1$ and go to step 2

- Represent joint $f(x)$ by sampling conditional $f(x_i | x_{-i})$
  - discard burn-in phase, $\{x^{(g)}\}_{g=1}^G$ approximate $f(x)$
  - Rao-Blackwellization: $\hat{f}(x_i) = \frac{1}{G} \sum_{g=1}^G f(x_i | x_{-i}^{(g)})$
  - rule of thumb: highly correlated x_i's in one block
  - what if some $f(x_i | x_{-i})$ cannot be sampled directly?
- Exercise: prove for $d = 2$ blocks, Gibbs kernel has invariant distribution $f(\cdot)$

$$p(x, y) = f(y_1 | x_2) f(y_2 | y_1), \quad x = (x_1, x_2), \quad y = (y_1, y_2)$$

Gibbs Algorithm (Cont'd)

- Consider Gaussian model
  - likelihood: $y_i \sim_{i.i.d.} \mathcal{N}(\mu, h^{-1})$, $i = 1, \ldots, n$
  - conditionally conjugate prior: $\mu \sim \mathcal{N}(\mu_0, h_0^{-1})$, $h \sim \mathcal{G}(\frac{\alpha_0}{2}, \frac{\delta_0}{2})$
  - conditional posteriors are of same family
- Gibbs algorithm
  - step 1: choose $\mu = \mu^{(0)}$, $h = h^{(0)}$, set $g = 0$
  - step 2: sample recursively

$$\mu^{(g+1)} \sim \mathcal{N}\left(\frac{h_0\mu_0 + h^{(g)}n\bar{y}}{h_0 + h^{(g)}n}, (h_0 + h^{(g)}n)^{-1}\right)$$

$$h^{(g+1)} \sim \mathcal{G}\left(\frac{\alpha_0 + n}{2}, \frac{\delta_0 + \sum_{i=1}^n (y_i - \mu^{(g+1)})^2}{2}\right)$$

  - step 3: set $g = g + 1$ and go to step 2

Python Code

```
def gibbs_sampler(data, n, m0, h0, a0, d0):
    sample = np.zeros((n, 2))
    sample[0, 0] = m0
    sample[0, 1] = a0 / d0

    for i in range(1, n):
        m1 = (h0 * m0 + sample[i - 1, 1] * sum(data)) / (h0 + sample[i - 1, 1] * len(data))
        h1 = h0 + sample[i - 1, 1] * len(data)
        sample[i, 0] = stats.norm.rvs(size=1, loc=mu1, scale=1 / np.sqrt(h1))
        a1 = a0 + len(data)
        d1 = d0 + sum((data - sample[i, 0])**2)
        sample[i, 1] = stats.gamma.rvs(a1 / 2, size=1, scale=2 / d1)
    return sample
```

Marginal Likelihood

Marginal likelihood identity

$$m(y) = \frac{f(y|\theta^*)\pi(\theta^*)}{\pi(\theta^*|y)}, \qquad \forall \theta^* \in \Theta$$

- Chib (1995) computes $\pi(\theta^*|y)$ at high-density point θ^* from Gibbs output, e.g.

$$\pi(\theta_1^*, \theta_2^*, \theta_3^*|y) = \pi(\theta_1^*|y)\pi(\theta_2^*|\theta_1^*, y)\pi(\theta_3^*|\theta_1^*, \theta_2^*, y)$$

  - full run: $\hat{\pi}(\theta_1^*|y) = \frac{1}{G}\sum_{g=1}^{G} \pi(\theta_1^*|\theta_2^{(g)}, \theta_3^{(g)}, y)$, where $\theta^{(g)} \sim \pi(\theta|y) \Rightarrow (\theta_2^{(g)}, \theta_3^{(g)}) \sim \pi(\theta_2, \theta_3|y)$
  - reduced run: $\hat{\pi}(\theta_2^*|\theta_1^*, y) = \frac{1}{G}\sum_{g=1}^{G} \pi(\theta_2^*|\theta_1^*, \theta_3^{(g)}, y)$, where $\theta_{-1}^{(g)} \sim \pi(\theta_{-1}|\theta_1^*, y) \Rightarrow \theta_2^{(g)} \sim \pi(\theta_2|\theta_1^*, y)$, $\theta_3^{(g)} \sim \pi(\theta_3|\theta_1^*, y)$
  - $\pi(\theta_3^*|\theta_1^*, \theta_2^*, y)$ can be evaluated directly

Python Code

```
def marg_lik(data, sample, m, h, m0, h0, a0, d0):
    m1 = (h0 * m0 + sample[:, 1] * sum(data)) / (h0 + sample[:, 1] * len(data))
    h1 = h0 + sample[:, 1] * len(data)
    log_post1 = np.log(np.mean(stats.norm.pdf(m, loc=m1, scale=1 / np.sqrt(h1))))

    a1 = a0 + len(data)
    d1 = d0 + sum((data - m)**2)
    log_post2 = stats.gamma.logpdf(h, a1 / 2, scale=2 / d1)

    log_lik = sum(stats.norm.logpdf(data, loc=m, scale=1 / np.sqrt(h)))
    log_prior = stats.norm.logpdf(m, loc=m0, scale=1 / np.sqrt(h0)) + stats.gamma.logpdf(h, a0 / 2, scale=2 / d0)
    return log_lik + log_prior - log_post1 - log_post2
```

Metropolis-Hastings Algorithm

Algorithm 2

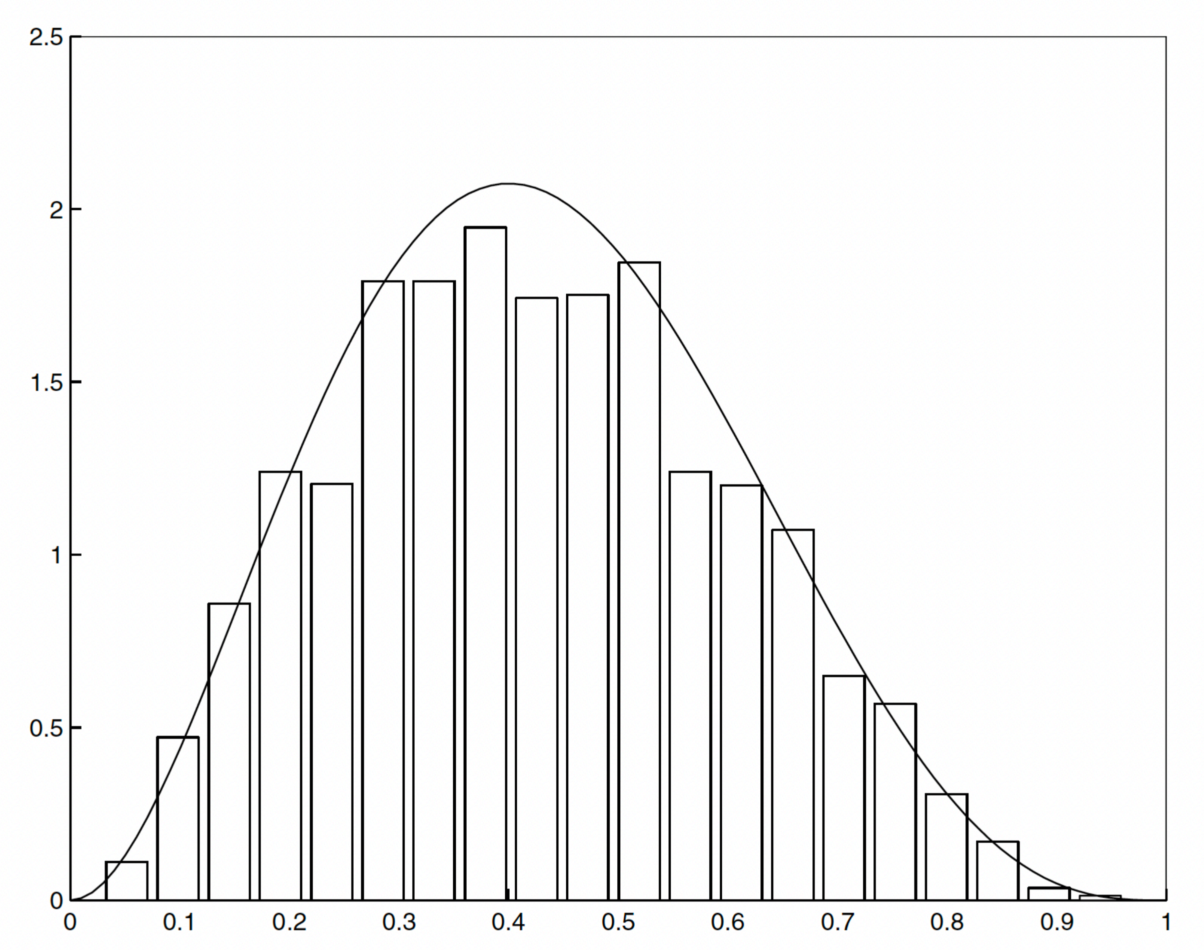
1. Choose $x^{(0)}$ and set $g = 0$
2. Sample proposal $y \sim q(x^{(g)}, y)$, $u \sim \mathcal{U}(0,1)$. If

$$u \leq \alpha(x^{(g)}, y) = \begin{cases} \min\left\{\frac{f(y)q(y, x^{(g)})}{f(x^{(g)})q(x^{(g)}, y)}, 1\right\}, & \text{if } f(x^{(g)})q(x^{(g)}, y) > 0 \\ 0, & \text{otherwise} \end{cases}$$

   set $x^{(g+1)} = y$; otherwise, set $x^{(g+1)} = x^{(g)}$
3. Set $g = g + 1$ and go to step 2

- Chib & Greenberg (1995): MH kernel $p(x, y) = \alpha(x, y)q(x, y)$ is reversible and has invariant distribution $f(\cdot)$
  - choice of proposal: random-walk/independence, but good mixing requires 'tailoring' proposal to target
  - more generally, MH-within-Gibbs algorithm

MH Algorithm (Cont'd)



- Target: $\mathcal{B}(3,4)$; proposal: $\mathcal{U}(0,1)$; $G = 5,000$ draws

Python Code

```
def mh_sampler(n):
    sample = np.zeros(n)
    sample[0] = 0.5
    rej = 0

    for i in range(1, n):
        x = np.random.rand(1)
        alpha = min(1, stats.beta.pdf(x, 3, 4) / stats.beta.pdf(sample[i - 1], 3, 4))
        if np.random.rand(1) > alpha:   # reject
            rej += 1
            sample[i] = sample[i - 1]
        else:   # accept
            sample[i] = x

    return sample, rej
```

Marginal Likelihood Revisited

Marginal likelihood identity

$$m(y) = \frac{f(y|\theta^*)\pi(\theta^*)}{\pi(\theta^*|y)}, \qquad \forall \theta^* \in \Theta$$

- Chib and Jeliazkov (2001) compute $\pi(\theta^*|y)$ at high-density point θ^* from MH output, e.g. for one-block case

  $$\alpha(\theta, \theta^*|y)q(\theta, \theta^*|y)\pi(\theta|y) = \alpha(\theta^*, \theta|y)q(\theta^*, \theta|y)\pi(\theta^*|y)$$

  from which

  $$\pi(\theta^*|y) = \frac{\int \alpha(\theta, \theta^*|y)q(\theta, \theta^*|y)\pi(\theta|y)d\theta}{\int \alpha(\theta^*, \theta|y)q(\theta^*, \theta|y)d\theta}$$

  - numerator: $\frac{1}{G}\sum_{g=1}^{G} \alpha(\theta^{(g)}, \theta^*|y)q(\theta^{(g)}, \theta^*|y)$, $\theta^{(g)} \sim \pi(\theta|y)$
  - denominator: $\frac{1}{G}\sum_{g=1}^{G} \alpha(\theta^*, \theta^{(g)}|y)$, $\theta^{(g)} \sim q(\theta^*, \theta|y)$

Python Code

```python
def post_ord(prop, sample, x):
    n = len(sample)
    num = np.zeros(n)
    den = np.zeros(n)

    for i in range(n):
        num[i] = min(1, stats.beta.pdf(x, 3, 4) / stats.beta.pdf(sample[i], 3, 4))
        den[i] = min(1, stats.beta.pdf(prop[i], 3, 4) / stats.beta.pdf(x, 3, 4))

    return np.log(np.mean(num)) - np.log(np.mean(den))
```

Convergence

- Measures of convergence
  - numerical standard error (n.s.e.)

$$\text{n.s.e.} = \frac{1}{b(b-1)} \sum_{i=1}^{b} (m_i - \bar{m})^2$$

    where m_i = batch i mean, $\bar{m}$ = overall mean

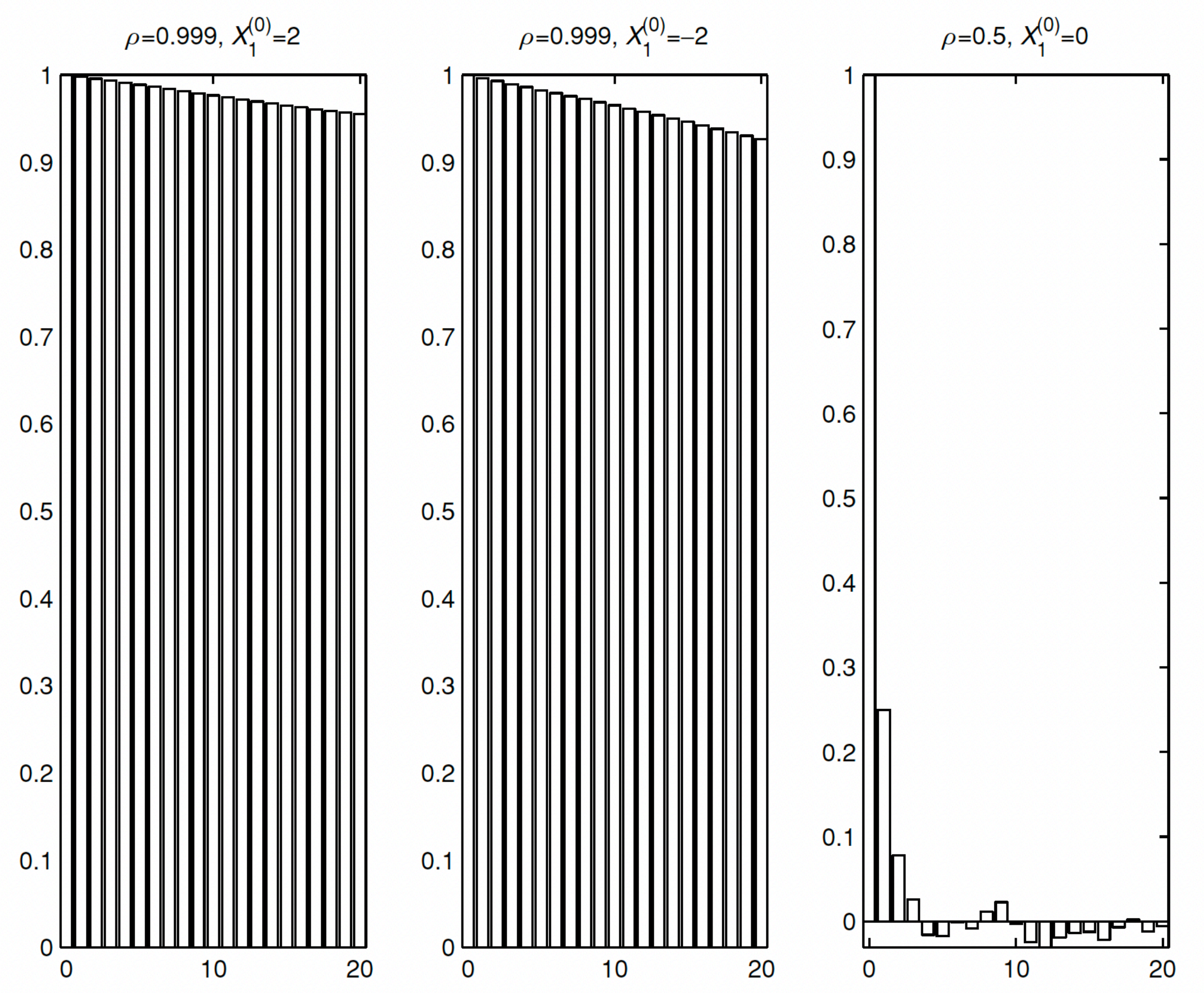
  - autocorrelation function $\rho(\cdot)$ and inefficiency factor

$$\frac{\text{numerical variance of MCMC draws}}{\text{numerical variance of i.i.d. draws}} \approx 1 + 2\sum_{j=1}^{K} w(j/K)\rho(j)$$

    $\rho(\cdot)$ is truncated by K and weighted by Parzen kernel $w(\cdot)$

- Judging convergence is as much art as science: 'low' serial correlation and inefficiency factor

Convergence (Cont'd)



- Gibbs sampler for $\mathcal{N}(0, \Sigma)$, $\Sigma = [1, \rho; \rho, 1]$

Readings

- Chib (1995), "Marginal Likelihood from the Gibbs Output," *Journal of the American Statistical Association*
- Chib & Greenberg (1995), "Understanding the Metropolis-Hastings Algorithm," *The American Statistician*
- Chib & Jeliazkov (2001), "Marginal Likelihood from the Metropolis-Hastings Output," *Journal of the American Statistical Association*