

Markov Chain Monte Carlo II

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Lecture plan

- ▶ MCMC Convergence
- ▶ Simulated Annealing
- ▶ Gibbs sampler

Convergence diagnostics

- ▶ Autocorrelation sequence (x_1, \dots, x_n) k -th order autocorrelation

$$\rho_k = \frac{\sum_{t=1}^{n-k} (x_t - \bar{x})(x_{t+k} - \bar{x})}{\sum_{t=1}^{n-k} (x_t - \bar{x})^2}, \quad \bar{x} = \frac{1}{n} \sum_{t=1}^n x_t$$

- ▶ Partial k -th autocorrelation as a function of lag
- ▶ Geweke z-score test
- ▶ split sample first 10%, last 50%
- ▶ at stationary means are equal, z-test. $z_{score} > 2$ still drifting

$$Z_{score} = \frac{\mu_1 - \mu_2}{\sigma}$$

Simulated annealing

- ▶ "Hill climbing" optimization algorithm
- ▶ accepts probability of downhill move
- ▶ probability decreases with time (process)
- ▶ Metropolis sampling

$$\alpha(x_n, x^*) = \min \left[1, \left(\frac{p(x^*)}{p(x_n)} \right)^{1/T(t)} \right]$$

- ▶ "Cooling" schedule

$$T(t) = T_0 \left(\frac{T_f}{T_0} \right)^{t/n}$$

- ▶ T_f - final "temperature"

The Gibbs sampler

- ▶ joint multivariate density $p(\mathbf{x}) = p(x_1, \dots, x_n)$
- ▶ compute samples $\mathbf{X}_1, \dots, \mathbf{X}_k$
- ▶ compute marginal $p(x_1) = \int \dots \int p(x_1 \dots x_n) dx_1 \dots dx_n$
- ▶ can compute univariate $p(x_1 | x_2 \dots x_n)$
- ▶ generate sequence of univariate conditionals

Bivariate case

- ▶ distribution

$$p(x, y)$$

- ▶ marginal distribution

$$p(x) = \int p(x, y) dy$$

$$p(y) = \int p(x, y) dx$$

- ▶ conditional probability

$$p(x|y) = p(x, y)/p(y)$$

$$p(y|x) = p(x, y)/p(x)$$

- ▶ marginal from conditional distribution

$$p(x) = \int p(x|y)p(y) dy = E_{p(y)}[p(x|y)]$$

$$p(y) = \int p(y|x)p(x) dx = E_{p(x)}[p(y|x)]$$

Gibbs sampler: bivariate case

- ▶ Given: $p(x|y)$, $p(y|x)$
- ▶ Choose y_0 , $t = 0$
- ▶ do "sampler scan"
 - $x_t \sim p(x|y = y_t)$
 - $y_{t+1} \sim p(y|x = x_t)$
- ▶ repeat k -times, Gibbs sequence $(x_0, y_0), (x_1, y_1) \dots (x_k, y_k)$

Gibbs sampler

- ▶ $p(x_1, \dots, x_n)$
- ▶ single iteration:
 $x_1^{t+1} = p(x_1 | x_2^t, \dots, x_n^t)$
 $x_2^{t+1} = p(x_2 | x_1^{t+1}, x_3^t, \dots, x_n^t)$
 $x_j^{t+1} = p(x_j | x_1^{t+1}, \dots, x_{j-1}^{t+1}, x_{j+1}^t, \dots, x_n^t)$
- ▶ samples
 $\mathbf{X}^1 \dots \mathbf{X}^k, \mathbf{X} = (x_1, \dots, x_n)$

MCMC connection

- ▶ Metropolis-Hastings

$$\alpha(x, x^*) = \frac{p(x^*)Q(x^*, x)}{p(x)Q(x, x^*)} = \frac{p(x^*)Q(x|x^*)}{p(x)Q(x^*|x)}$$

- ▶ use conditional $p(x|x^*)$ as a candidate density $Q(x|x^*)$
 $(x^t, y^t) \rightarrow (x^{t+1}, y^t)$

$$\alpha = \frac{p(x^{t+1}, y^t)p(x^t|y^t)}{p(x^t, y^t)p(x^{t+1}|y^t)} = \frac{p(x^{t+1}, y^t)}{p(x^t, y^t)} \frac{p(x^t, y^t)}{p(y^t)} \frac{p(y^t)}{p(x^{t+1}, y^t)} = 1$$

- ▶ MCMC algorithm with acceptance probability 1