Advanced Statistical Computing

Fall 2012
Lecture 2

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Markov Chain Monte Carlo

- The goal is to generates sequence of random samples from an arbitrary probability density function (usually high dimensional),
- The sequence of random samples form a Markov chain,
- The purpose is simulation (Monte Carlo).

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Motivation

- Generate *iid* r.v. from high-dimensional arbitrary distributions is extremely difficult.
- Drop the "*independent*" requirement.
- How about the "*identically distributed*" requirement?

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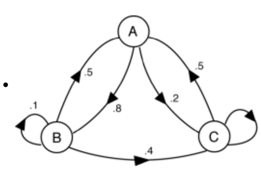
Markov chain

- Assume a finite state, discrete Markov chain with N different states.
- Random process X_n, $n = 0,1,2,\ldots$

  $x_n \in S = \{1,2,\ldots,N\}$



Markov graph of transiton probabilites between states A, B and C

- Markov property,

$$P(X_{n+1} = x \mid X_1 = x_1, X_2 = x_2, \ldots, X_n = x_n) = P(X_{n+1} = x \mid X_n = x_n)$$

- Time-homogeneous
- Order
  - Future state depends on the past m states.

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Key parameters

- Transition matrix

$$P(X_n = j \mid X_{n-1} = i) = p(i, j),$$
$$P = \{p(i, j)\}.$$

- Initial probability distribution $\pi^{(0)}$

$$\pi^{(n)}(i) = P(x_n = i).$$

- Stationary distribution (invariant/equilibrium)

$$\pi = \pi P.$$

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Reducibility

- A state *j* is accessible from state *i* (written $i \rightarrow j$) if $P(X_n = j \mid X_0 = i) = p_{ij}^{(n)} > 0.$
- A Markov chain is *irreducible* if it is possible to get to any state from any state.

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Recurrence

- A state i is *transient* if given that we start in state i, there is a non-zero probability that we will never return to i. State i is *recurrent* if it is not transient.

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Ergodicity

- A state i is *ergodic* if it is aperiodic and positive recurrent. If all states in an irreducible Markov chain are ergodic, the chain is *ergodic*.

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Reversible Markov chains

- Consider an ergodic Markov chain that converges to an invariant distribution π. A Markov chain is *reversible* if for all $x, y \in S$,

$$\pi(x)\,p(x,y) = \pi(y)\,p(y,x).$$

  which is known as the detailed balance equation.
- An ergodic chain in equilibrium and satisfying the detailed balance condition has π as its unique stationary distribution.

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Markov Chain Monte Carlo

- The goal is to generates sequence of random samples from an arbitrary probability density function (usually high dimensional),
- The sequence of random samples form a Markov chain,

  in Markov chain, $P \rightarrow \pi$

  in MCMC, $\pi \rightarrow P$.

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History

- Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N., Teller, A. H. and Teller, E. (1953).

  Equation of state calculations by fast computing machines. *Journal of Chemical Physics*, **21**, 1087–1092.

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Metropolis algorithm

- Direct sampling from the target distribution is impossible,
- Generating candidate draws from a proposal distribution,
- These draws then “corrected” so that asymptotically, they can be viewed as random samples from the desired target distribution.

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Pseudo code

- Initialize X_0,
- Repeat
  - Sample $Y \sim q(x,.)$,
  - Sample $U \sim Uniform\ (0,1)$,
  - If $U \leq \alpha\ (X,Y)$, set $X_i = y$,
  - Otherwise $X_i = x$.

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An informal derivation

- Find $\alpha\ (X,Y)$:
- Joint density of current Markov chain state and the proposal is $g(x,y) = q(x,y)\pi(x)$
- Suppose q satisfies detail balance

  $q(x,y)\ \pi(x) = q(y,x)\pi(y)$
- If $q(x,y)\ \pi(x) > q(y,x)\pi(y)$, introduce

  $\alpha(x,y) < 1$ and $\alpha(y,x) = 1$

  hence $\alpha(x,y) = \dfrac{\pi(y)q(y,x)}{\pi(x)q(x,y)}.$
- If $q(x,y)\ \pi(x) > q(y,x)\pi(y)$, …
- The probability of acceptance is $\alpha(x,y) = \min\left(1, \dfrac{\pi(y)q(y,x)}{\pi(x)q(x,y)}\right).$

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Metropolis-Hastings Algorithm

- Start with any $X^{(0)}=x_0$, and a "*proposal chain*" $T(x,y)$
- Suppose $X^{(t)}=x_t$. At time t+1,
  - Draw y~$T(x_t, y)$ (i.e., propose a move for the next step)
  - Compute ***"goodness ratio"***

$$r = \frac{\pi(y)T(y,x_t)}{\pi(x_t)T(x_t,y)}$$

  - **Acceptance/Rejection decision:** Let

$$X^{(t+1)} = \begin{cases} y, & \text{with } p = \min\{1, r\} \\ x_t, & \text{with } 1-p \end{cases}$$

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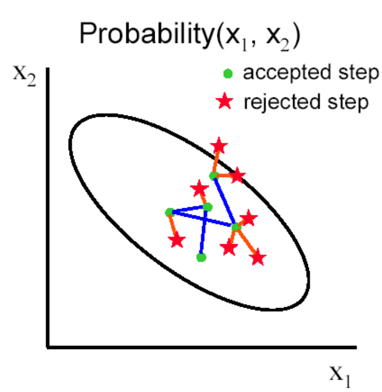
Remarks

- Relies only on calculation of target pdf up to a normalizing constant.



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Remarks

- How to choose a good proposal function is crucial.
- Sometimes tuning is needed.
  - Rule of thumb: 30% acceptance rate
- Convergence is slow for high dimensional cases.

Illustration of Metropolis-Hastings

- Suppose we try to sample from a bi-variate normal distributions. $N\left(\begin{pmatrix}0\\0\end{pmatrix},\begin{pmatrix}1 & \rho\\ \rho & 1\end{pmatrix}\right)$
- Start from (0, 0)
- Proposed move at each step is a two dimensional random walk

$$\begin{aligned} &x_{t+1} = x_t + s\cos\theta \\ &y_{t+1} = y_t + s\sin\theta \\ &\textit{with} \\ &s \sim U(0,1) \\ &\theta \sim U(0,2\pi) \end{aligned}$$

Illustration of Metropolis-Hastings

- At each step, calculate $r = \dfrac{\pi(x_{t+1}, y_{t+1})}{\pi(x_t, y_t)}$

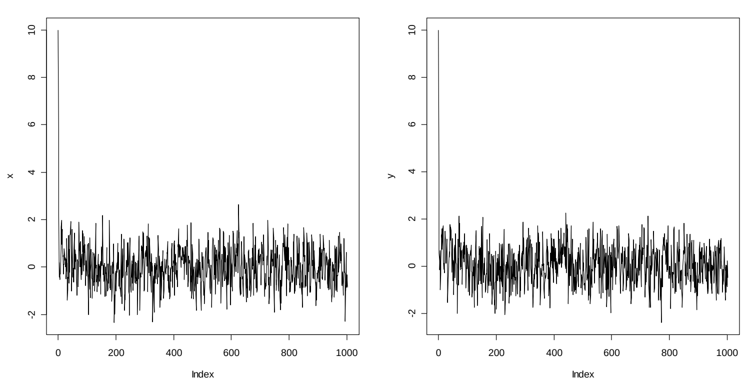
  since $T((x_t, y_t),(x_{t+1}, y_{t+1})) = T((x_{t+1}, y_{t+1}),(x_t, y_t)) = 1/\pi^2$

$$r = \frac{\frac{1}{2\pi\sqrt{1-\rho^2}}\exp\left(-\frac{1}{2(1-\rho^2)}\left(x_{t+1}^2 - 2\rho x_{t+1}y_{t+1} + y_{t+1}^2\right)\right)}{\frac{1}{2\pi\sqrt{1-\rho^2}}\exp\left(-\frac{1}{2(1-\rho^2)}\left(x_t^2 - 2\rho x_t y_t + y_t^2\right)\right)}$$

$$= \exp\left(-\frac{1}{2(1-\rho^2)}\left(\left(x_{t+1}^2 - 2\rho x_{t+1}y_{t+1} + y_{t+1}^2\right) - \left(x_t^2 - 2\rho x_t y_t + y_t^2\right)\right)\right)$$

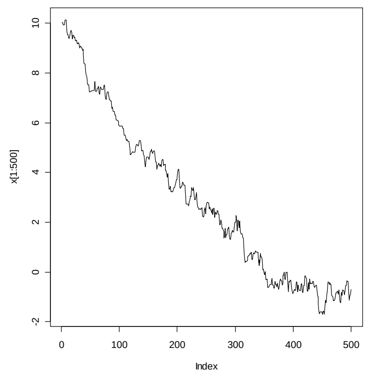
Convergence

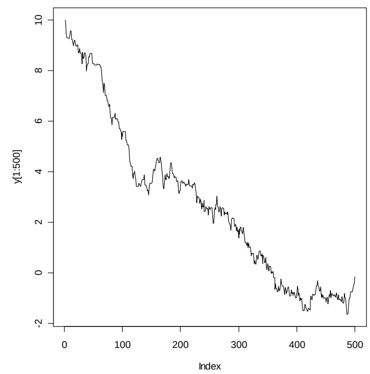
- Trace plot Good



Convergence

- Trace plot Bad





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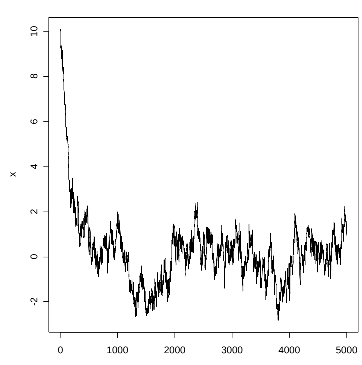
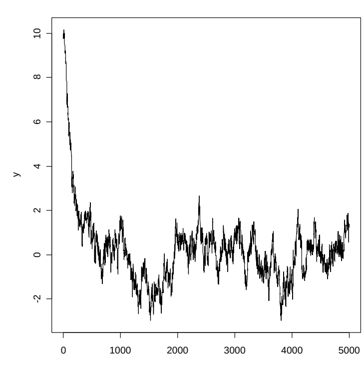
Convergence

- Trace plot





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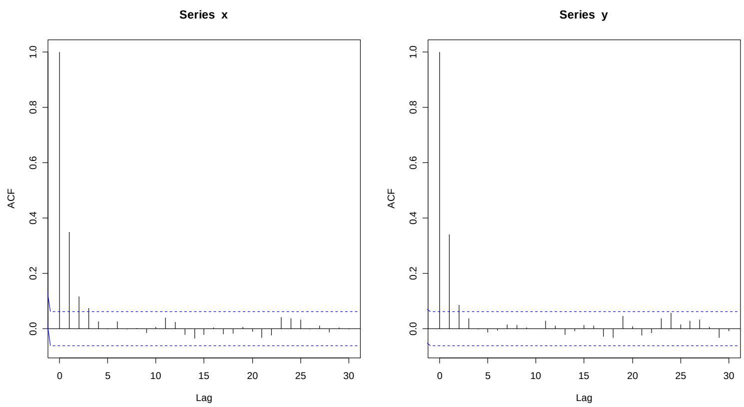
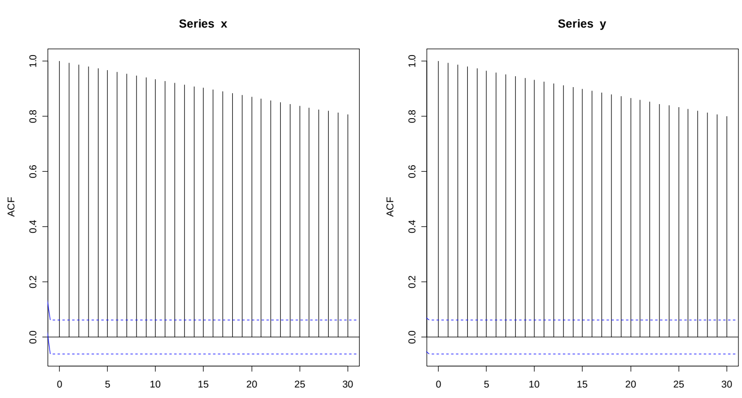
Convergence

- Autocorrelation plot   Good



Convergence

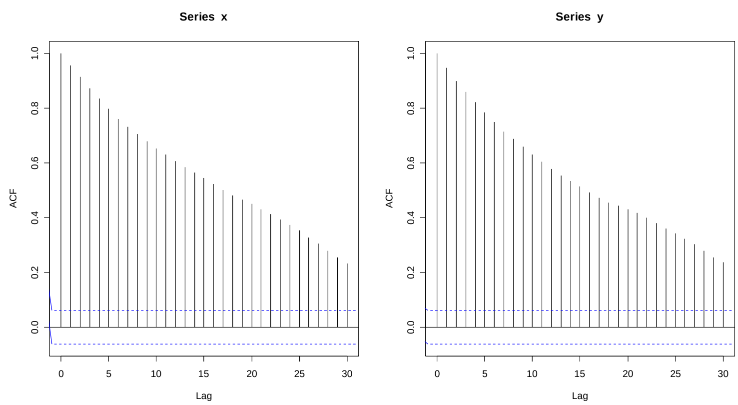
- Autocorrelation plot   Bad   **s = 0.5**



Convergence

- Autocorrelation plot Okay

s = 3.0



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References

- Metropolis et al. 1953,
- Hastings 1973,
- Tutorial paper:

  Chib and Greenberg (1995). Understanding the Metropolis--Hastings Algorithm. *The American Statistician* **49**, 327-335.

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Gibbs Sampler

- Purpose: Draw random samples form a joint distribution (high dimensional)

$$x = (x_1, x_2, ..., x_n) \text{ Target } \pi(x)$$

- Method: Iterative conditional sampling

$$\forall i, \text{ draw } x_i \sim \pi(x_i \mid x_{[-i]})$$

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Illustration of Gibbs Sampler

- Suppose the target distribution is:

$$(X, Y) \sim N\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}\right)$$

- Gibbs sampler:

$$[X \mid Y = y] \sim N(\rho y, 1 - \rho^2)$$
$$[Y \mid X = x] \sim N(\rho x, 1 - \rho^2)$$

Start from, say, (X,Y)=(10,10), we can take a look at the trajectories. We took ρ=0.6.

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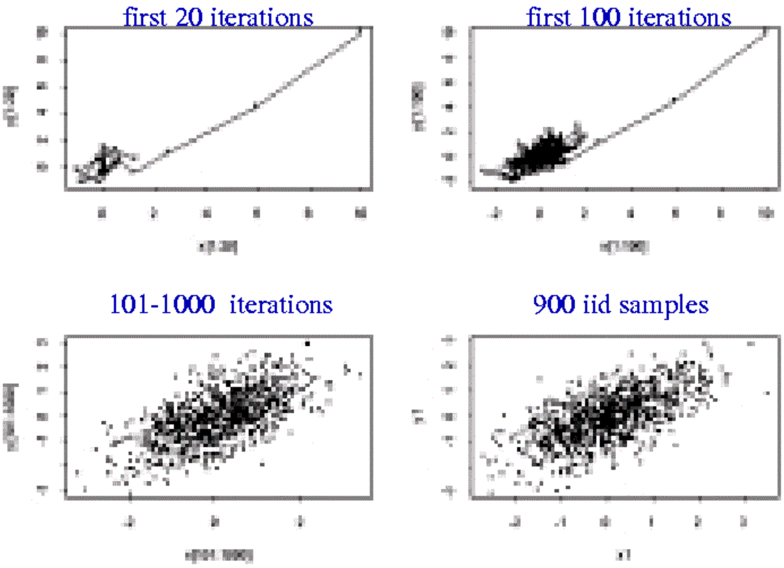

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References

- Geman and Geman 1984,
- Gelfand and Smith 1990,
- Tutorial paper:

  Casella and George (1992). Explaining the Gibbs sampler. *The American Statistician*, **46**, 167-174.

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Remarks

- Gibbs Sampler is a special case of Metropolis-Hastings
- Compare to EM algorithm, Gibbs sampler and Metropolis-Hastings are stochastic procedures
- Verify convergence of the sequence
- Require Burn in
- Use multiple chains

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