BIOS 731
Advanced Statistical Computing

Fall 2022

lecture 11
Introduction to MCMC

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Motivation

- Generate random samples from arbitrary probability distributions.
- Ideally, the random samples are i.i.d.
  - Independent
  - Identically distributed
- Extremely hard problem especially for high dimensional distributions.

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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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What is Monte Carlo

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What is Monte Carlo?

- Rely on repeated sampling to study the results of a experiment or study the properties of certain procedure.
  - Often used in complex and uncertain scenarios
  - Difficult to formulate, high correlation.
  - Cheap
  - Take advantage of faster computers
- History
  - John von Neumann, Stanislaw Ulam, Nicholas Metropolis

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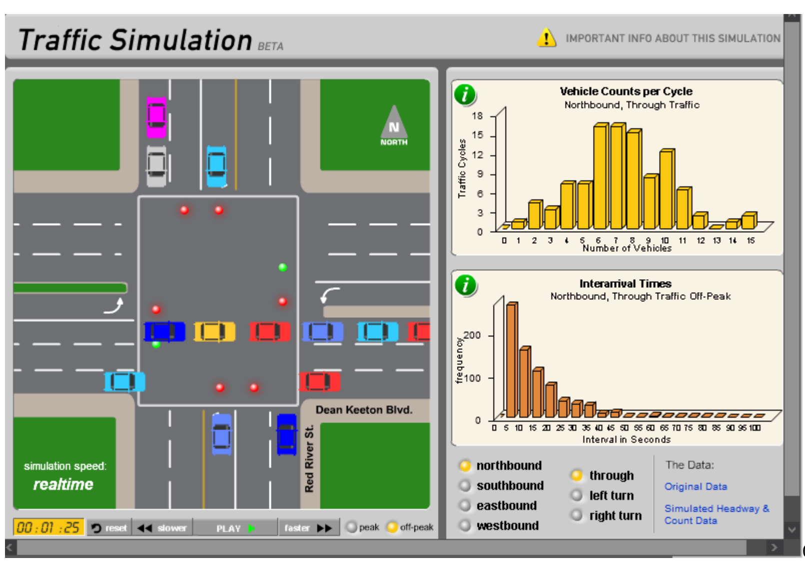
How simulation works?



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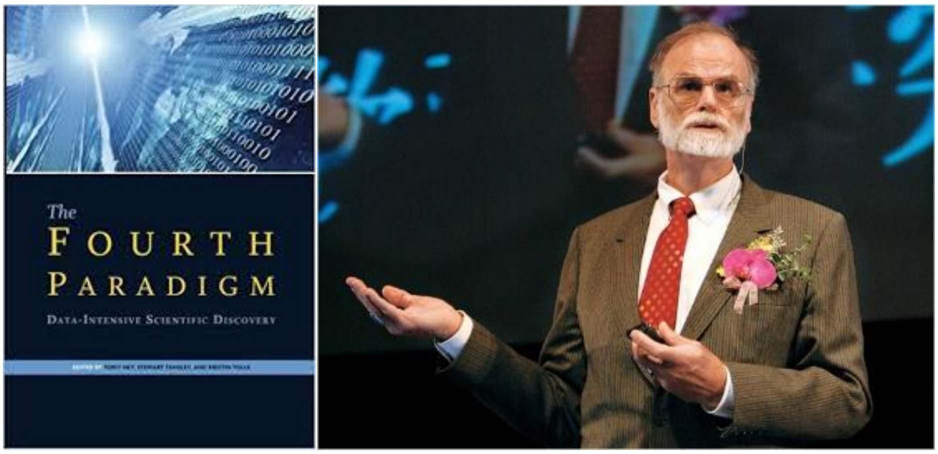
https://www.caee.utexas.edu/prof/kockelman/IntersectionSimulations/index.html#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FOURTH
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DATA-INTENSIVE SCIENTIFIC DISCOVERY

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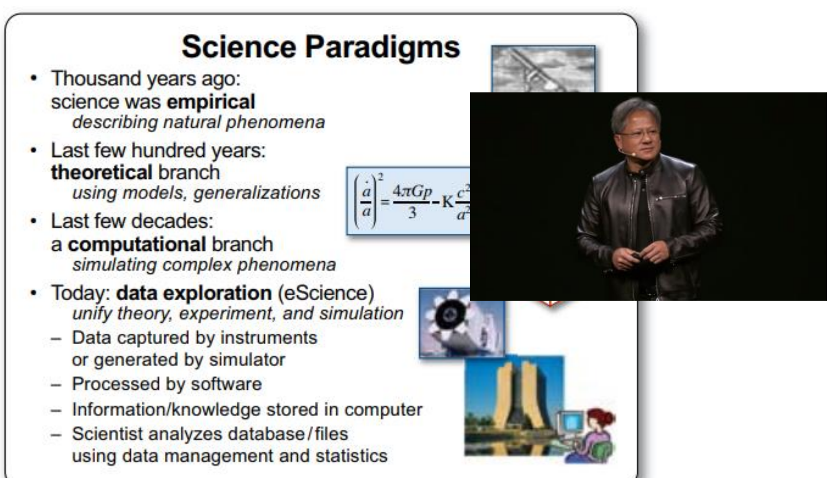
Science Paradigms
• Thousand years ago:
science was **empirical**
describing natural phenomena
• Last few hundred years:
theoretical branch
using models, generalizations
• Last few decades:
a **computational** branch
simulating complex phenomena
• Today: **data exploration** (eScience)
unify theory, experiment, and simulation
– Data captured by instruments
or generated by simulator
– Processed by software
– Information/knowledge stored in computer
– Scientist analyzes database/files
using data management and statistics

FIGURE 1

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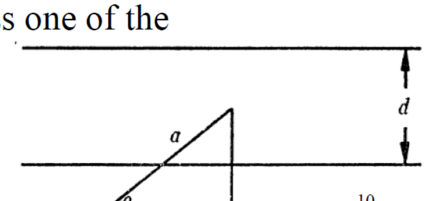
Applications of Monte Carlo

- Optimization
- Numerical integration
- Generate random samples

Buffon's needle

Georges-Louis Leclerc, Comte de Buffon (1707-1788)

Given a needle of length a and an infinite grid of parallel lines with common distance d between them, what is the probability $P(E)$ that a needle, tossed at the grid randomly, will cross one of the parallel lines?



Buffon's needle

- Assume $a < d$

$$P(E) = \int_0^\pi \frac{a \sin\theta d\theta}{\pi d} = (a/\pi d)\int_0^\pi \sin\theta d\theta = 2a/\pi d.$$

http://web.student.tuwien.ac.at/~e9527412/buffon.html

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Motivation

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

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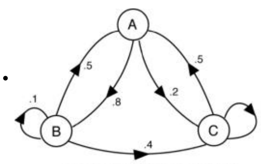
Markov chain

- 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 property,



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

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

- 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*→ *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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Examples

$$P(X \mid E, \beta, \sigma^2) \propto \prod_{k=1}^{K} \prod_{E(i)=k} \prod_{j=1}^{M} \left(\left(\sigma_{kj}^2\right)^{-\frac{1}{2}} e^{-\frac{1}{2\sigma_{kj}^2}\left(x_{ij}-\beta_{kj}\right)^2} \right)$$

$$P(X \mid E) = \prod_{k=1}^{K} \prod_{j=1}^{M} \iint \prod_{E(i)=k} P\left(x_{ij} \mid \beta_{kj}, \sigma_{kj}^2\right) p\left(\beta_{kj} \mid \beta_0, \sigma_{kj}^2\right) p\left(\sigma_{kj}^2\right) d\beta_{kj} d\sigma_{kj}^2$$

$$= \prod_{k=1}^{K} \prod_{j=1}^{M} \left[\frac{b^a}{\Gamma(a)} \frac{(2\pi)^{-\frac{n_k}{2}}}{\sqrt{n_k+1}} \frac{\Gamma\left(\frac{n_k}{2}+a\right)}{\left(b+\frac{1}{2}\left(\sum_{E(i)=k} x_{ij}^2 + \beta_0^2 - \frac{\left(\sum_{E(i)=k} x_{ij} + \beta_0\right)^2}{n_k+1}\right)\right)^{\frac{n_k}{2}+a}} \right]$$

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Bayesian Inference

Genotype $Y = (y_1, \ldots, y_n)$

Haplotype $Z = (z_1, \ldots, z_n)$

Frequency $\Theta = (\theta_1, \ldots, \theta_m)$

Prior $\theta \sim Dirichlet(\beta)$

$$P(Y, Z, \Theta) = \prod_{i=1}^{n} \theta_{z_{i1}} \theta_{z_{i2}} \prod_{g=1}^{m} \theta_g^{\beta_g - 1}$$

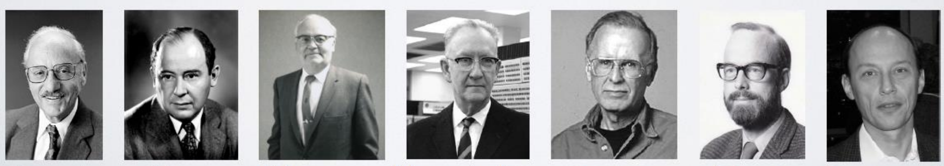
History

- 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.

THE TOP 10 LIST

1946: The Metropolis Algorithm
1947: Simplex Method
1950: Krylov Subspace Method
1951: The Decompositional Approach to Matrix Computations
1957: The Fortran Optimizing Compiler
1959: QR Algorithm
1962: Quicksort
1965: Fast Fourier Transform
1977: Integer Relation Detection
1987: Fast Multipole Method



Dantzig von Neumann Hestenes Householder Backus Hoare Greengard

Metropolis algorithm

- Direct sampling from the target distribution is difficult,
- 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 $U \sim \mathit{Uniform}\ (0,1)$,
  - If $U \leq \alpha\ (X,Y)$, set $X_i = y$,
  - Otherwise $X_i = x$.

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 $\alpha(x,y) = \min\left(1, \dfrac{\pi(y)q(y,x)}{\pi(x)q(x,y)}\right)$.

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 $y \sim T(x_t, y)$ (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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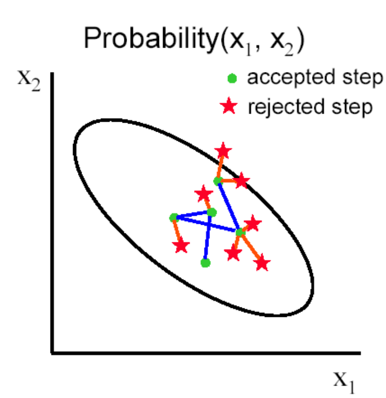
Remarks

- 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.

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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

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

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Illustration of Metropolis-Hastings

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

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

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

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

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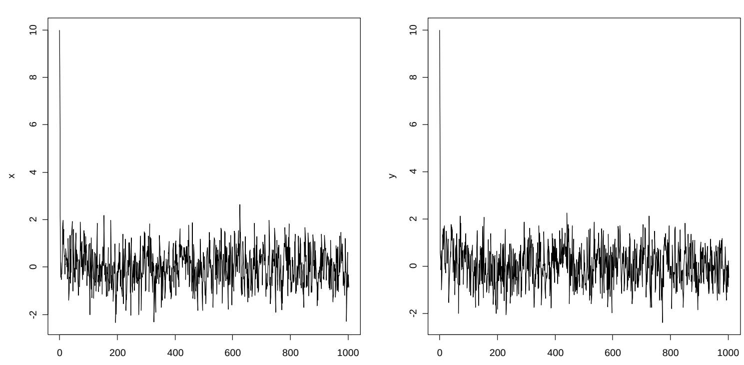
Convergence

- Trace plot Good



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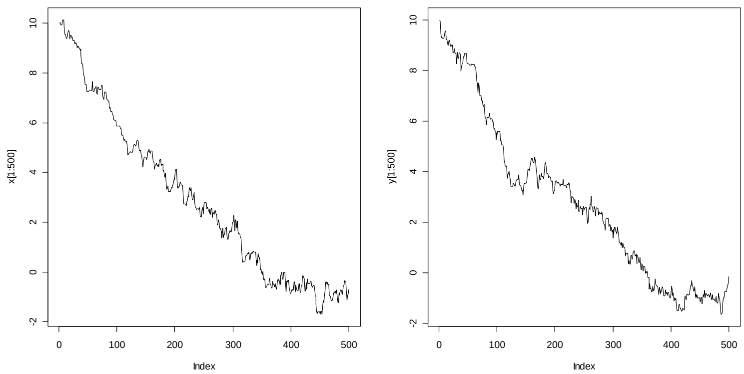
Convergence

- Trace plot Bad



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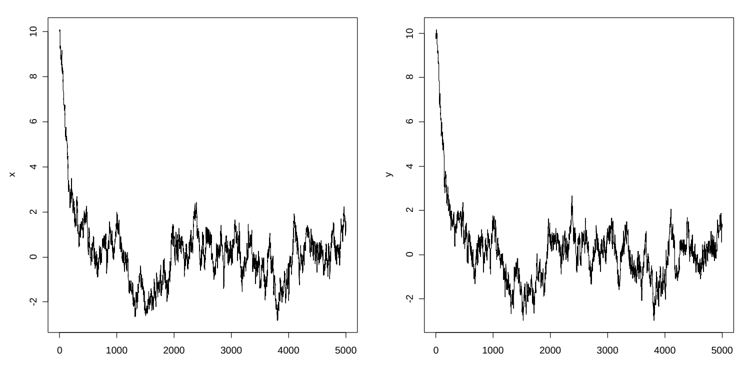
Convergence

- Trace plot



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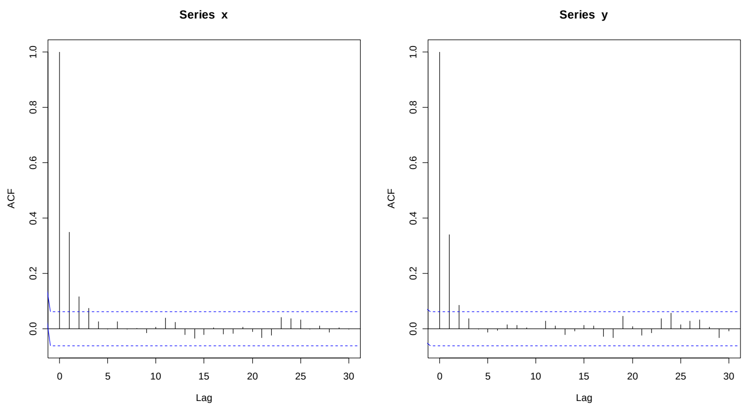
Convergence

- Autocorrelation plot Good



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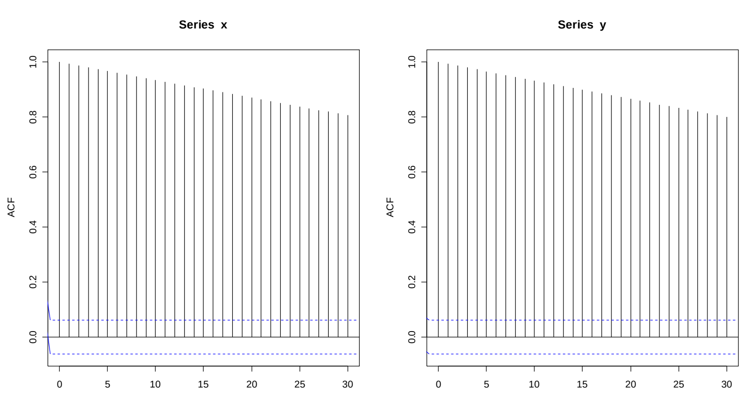
Convergence

- Autocorrelation plot Bad

s = 0.5



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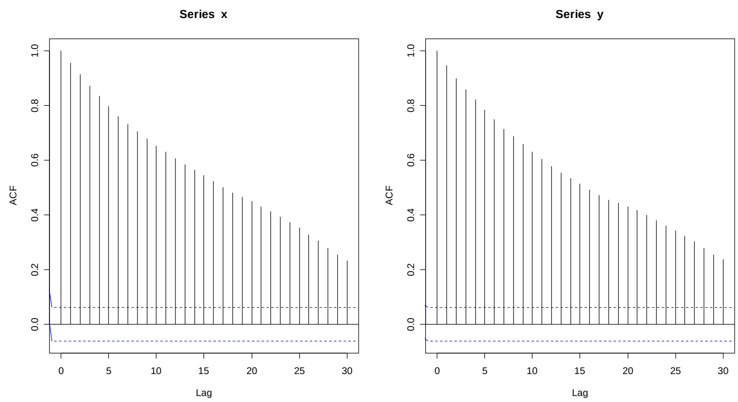
Convergence

- 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

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

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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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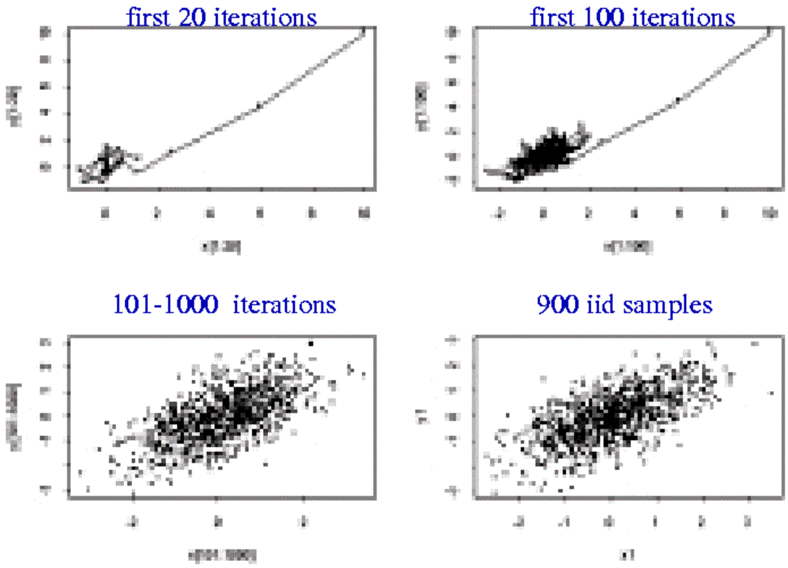

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References

- 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