Markov chain Monte Carlo and its Application to some Engineering Problems

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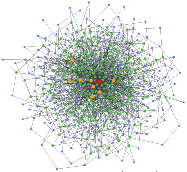
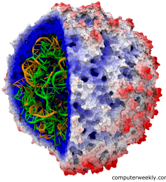
MCMC Revolution

P. Diaconis (2009), "The Markov chain Monte Carlo revolution":

> *...asking about applications of Markov chain Monte Carlo (MCMC) is a little like asking about applications of the quadratic formula... you can take any area of science, from hard to social, and find a burgeoning MCMC literature specifically tailored to that area.*



slowmuse.wordpress.com



computerweekly.com

The main goal of this talk: To demonstrate how MCMC algorithms can be used for solving engineering problems

Outline

1. What problems is MCMC meant to solve?
2. Why is MCMC useful in Engineering?
3. How does MCMC work?
4. MCMC applications to Reliability Problem
5. Summary

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Purpose of MCMC

Problem: To estimate

$$I = \int_{\Theta} h(\theta)\pi(\theta)d\theta$$

- $\Theta \subseteq \mathbb{R}^d$ parameter space
- $h : \Theta \to \mathbb{R}$ function of interest
- $\pi(\theta)$ "target" PDF on Θ

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- d is small $(d = 1, 2, 3) \Rightarrow$ numerical integration
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Typical Case in Applications:

- d is large $(d \sim 10^2 - 10^3)$
- $\pi(\theta)$ is known only up to a constant, $\pi(\theta) = cf(\theta)$

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Solution: Use an appropriate MCMC method

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1. What problems is MCMC meant to solve?
2. Why is MCMC useful in Engineering?
   - Bayesian Inference
   - Optimal Stochastic Design
   - Reliability Problem
3. How does MCMC work?
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Bayesian Inference

- $\mathcal{M}$ the assumed model class for the target dynamic system:
  - set of I/O probability models $p(y|\theta, u)$ $\xrightarrow{u} \boxed{\text{System}} \xrightarrow{y}$
  - $\theta \in \Theta$ the uncertain model parameters
  - prior PDF $\pi_0(\theta)$ over Θ

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Bayesian approach:

- Update $\pi_0(\theta)$ to posterior PDF $\pi(\theta|\mathcal{D})$ via Bayes' theorem:

$$\pi(\theta|\mathcal{D}) = L(\mathcal{D}|\theta)\pi_0(\theta)/\mathcal{Z}$$

- $\mathcal{D}$ the measured data from the system
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Problems:

- Evidence

$$\mathcal{Z} = \int_\Theta L(\mathcal{D}|\theta)\pi_0(\theta)d\theta$$

- Posterior expectations

$$\mathbb{E}_\pi[h] = \int_\Theta h(\theta)\pi(\theta|\mathcal{D})d\theta$$

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$$\mathbb{E}_\pi[h(\varphi,\theta)] = \int_\Theta h(\varphi,\theta)\pi(\theta|\varphi)d\theta$$

- $h(\varphi,\theta)$ a performance function of the system, e.g. stress in a component
- $\pi(\theta|\varphi)$ a PDF, which incorporates available knowledge about the system

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Problem:

$$\varphi^* = \arg\min_{\varphi \in \Phi} \mathbb{E}_\pi[h(\varphi, \theta)]$$

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Notation:

- $\theta \in \mathbb{R}^d$ represents the uncertain input load
  - θ is a stochastic vector and has joint PDF π
- $F \subset \mathbb{R}^d$ a failure domain (unacceptable performance)

$$F = \{\theta : G(\theta) \geq b^*\}$$

- $G(\theta)$ a performance function
- b^* a critical threshold for performance
- $I_F(\theta) = 1$ if $\theta \in F$ and $I_F(\theta) = 0$ if $\theta \notin F$

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3. How does MCMC work?
   - Markov chains
   - Markov chain Monte Carlo
   - Metropolis-Hastings algorithm
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MCMC: The Main Idea

- Monte Carlo method

$$\int_{\Theta} h(\theta)\pi(\theta)d\theta \approx \frac{1}{N}\sum_{i=1}^{N} h(\theta_i), \quad \theta_i \overset{i.i.d}{\sim} \pi$$

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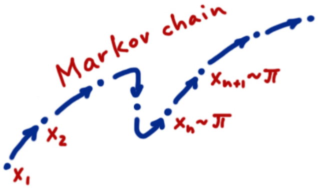
- MCMC samples from π and computes integrals using Markov chains:



$$\int_{\Theta} h(\theta)\pi(\theta)d\theta \approx \frac{1}{N-N_0}\sum_{i=N_0+1}^{N} h(x_i)$$

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Definition

Markov chain is a sequence of stochastic vectors $x_0, x_1, x_2, \dots$ such that

$$P(x_{n+1} \in A | x_0, \dots, x_n) = P(x_{n+1} \in A | x_n) \equiv K(x_n, A)$$

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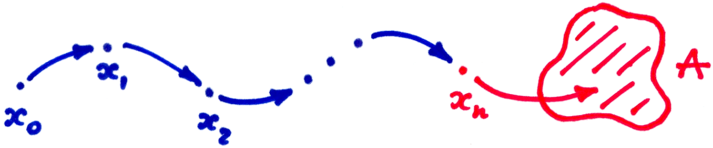

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The central result: Let K be a transition kernel with a stationary distribution π where K satisfies certain "ergodic conditions", then

- π is the unique stationary distribution
- $x_n \sim \pi$, when $n \to \infty$

Markov chain Monte Carlo

MCMC methods: The stationary distribution π is given:

it is the target distribution we want to sample from

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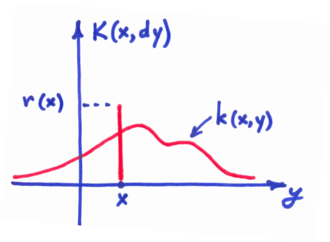

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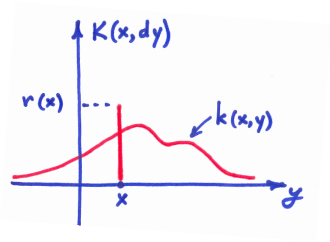

- $K(x,dy) = k(x,y)dy + r(x)\delta_x(dy)$

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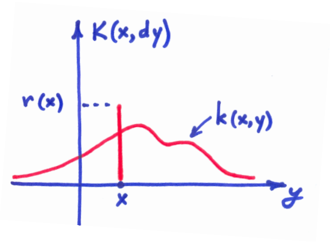

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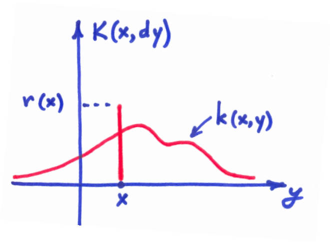

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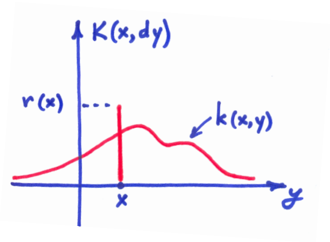

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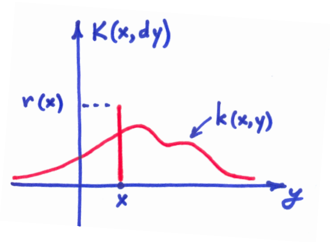

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- $r(x) = 1 - \int k(x, y)dy$ probability that the chain remains at x
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The central result: If k satisfies the detailed balance equation

$$\pi(x)k(x, y) = \pi(y)k(y, x)$$

then π is the stationary distribution for K

Metropolis-Hastings algorithm

$$\boxed{k_{MH}(x,y) = S(y|x)a(x,y)}$$

- $S(y|x)$ proposal distribution
- $a(x,y)$ acceptance probability

$$a(x,y) = \min\left\{1, \frac{\pi(y)S(x|y)}{\pi(x)S(y|x)}\right\}$$

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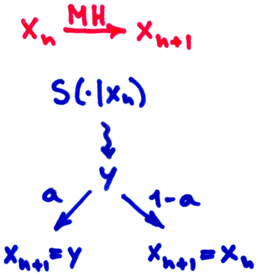

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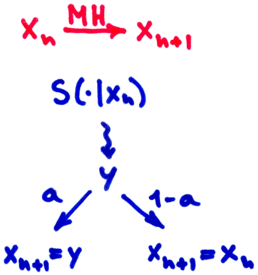

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  - Statistical mechanics
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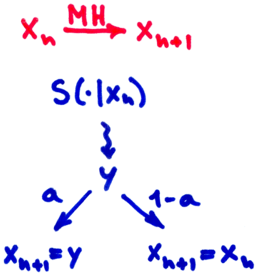

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- W.K. Hastings, 1970
  - Generalization of the M-algorithm
  - Markov chains come into play
  - Non-symmetric proposals
  - Different acceptance probabilities

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4. MCMC applications to Reliability Problem
    - Subset Simulation
    - Enhancements for Subset Simulation
5. Summary

Reliability Problem

Reliability Problem: To estimate the probability of failure p_F

$$p_F = P(\theta \in F) = \int_{\mathbb{R}^d} \pi(\theta) I_F(\theta) d\theta$$

Notation:

- $\theta \in \mathbb{R}^d$ is a stochastic vector with the joint PDF π
- $F \subset \mathbb{R}^d$ is a failure domain, $F = \{\theta : G(\theta) \geq b^*\}$
- $I_F(\theta) = 1$ if $\theta \in F$ and $I_F(\theta) = 0$ if $\theta \notin F$

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We need MCMC based simulation methods

Subset Simulation

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$$\mathbb{R}^d = F_0 \supset F_1 \supset \ldots \supset F_m = F$$

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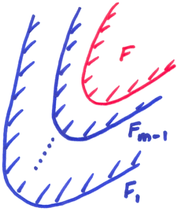
$$F_i = \{\theta : G(\theta) \geq b_i^*\}$$

$$b_1^* < b_2^* < \ldots < b_m^* = b^*$$



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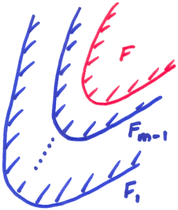
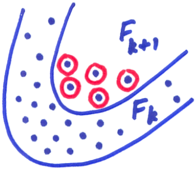


$$p_F = \prod_{k=0}^{m-1} P(F_{k+1}|F_k)$$

$$P(F_{k+1}|F_k) \approx \frac{1}{N}\sum_{i=1}^{N} I_{F_{k+1}}(\theta_k^{(i)})$$

$$\theta_k^{(i)} \sim \pi(\theta|F_k) = \frac{\pi(\theta) I_{F_k}(\theta)}{P(F_k)}$$



Subset Simulation

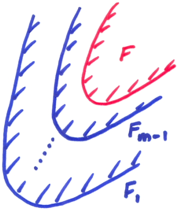
S.K. Au & J.L. Beck (PEM, 2001)

$$\mathbb{R}^d = F_0 \supset F_1 \supset \ldots \supset F_m = F$$

$$F = \{\theta : G(\theta) \geq b^*\}$$

$$F_i = \{\theta : G(\theta) \geq b_i^*\}$$

$$b_1^* < b_2^* < \ldots < b_m^* = b^*$$



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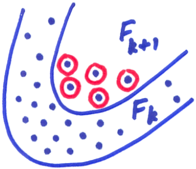

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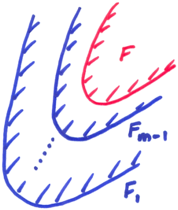

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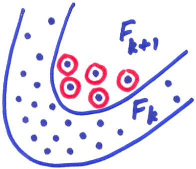

- How to sample from $\pi(\cdot|F_k)$?
- Use an appropriate MCMC alg

Modified Metropolis-Hastings algorithm

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Standard Metropolis-Hastings algorithm is not efficient in high dimensions

- Generate candidate state y

  For each $j = 1 \dots N$:

  - Simulate $\hat{y}^j \sim S^j(\cdot|x_n^j)$
  - Compute the acceptance probability

$$a^j(x_n^j, \hat{y}^j) = \min\left\{1, \frac{\pi_j(\hat{y}^j)}{\pi_j(x_n^j)}\right\}$$

  - Accept/Reject $\hat{y}^j$

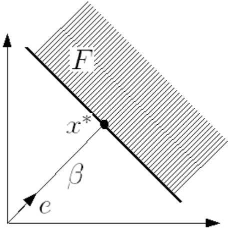
$$y^j = \begin{cases} \hat{y}^j, & \text{with prob. } a^j(x_n^j, \hat{y}^j) \\ x_n^j, & \text{with prob. } 1 - a^j(x_n^j, \hat{y}^j) \end{cases}$$

- Accept/Reject y

$$x_{n+1} = \begin{cases} y, & \text{if } y \in F_i \\ x_n, & \text{if } y \notin F_i \end{cases}$$

Efficiency of Subset Simulation

- Linear Problem
  - $F \subset \mathbb{R}^d$ is a hyperplane
  - $d = 1000$
  - $p_F = 10^{-k}$, $k = 3, 4, 5, 6$



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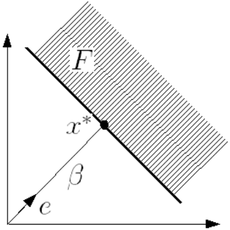

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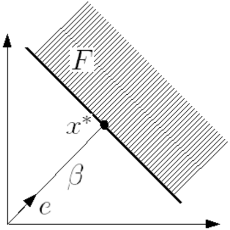

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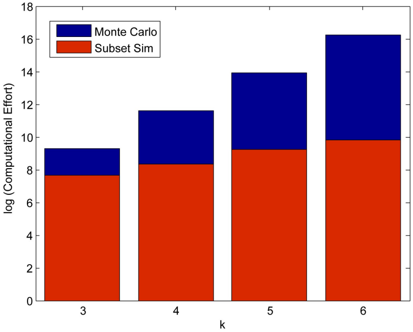
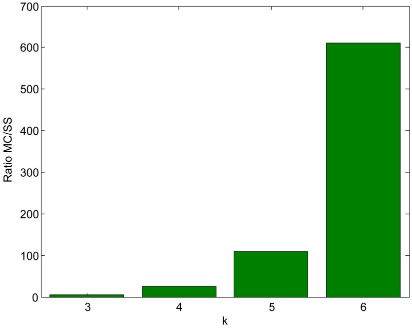
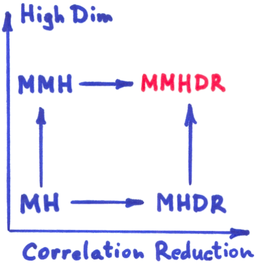




Outline

1. What problems is MCMC meant to solve?
2. Why is MCMC useful in Engineering?
3. How does MCMC work?
4. MCMC applications to Reliability Problem
    - Subset Simulation
    - Enhancements for Subset Simulation
        - Modified Metropolis-Hastings algorithm with Delayed Rejection
        - Bayesian post-processor for Subset Simulation
5. Summary

Modifications of the Metropolis-Hastings algorithm



- Modified MH (MMH) algorithm
  - S.K. Au & J.L. Beck, 2001
- MH algorithm with delayed rejection (MHDR)
  - L. Tierney & A. Mira, 1999
- Modified Metropolis-Hastings algorithm with delayed rejection (MMHDR)
  - K.M. Zuev & L.S. Katafygiotis, 2011

Metropolis-Hastings algorithm with Delayed Rejection

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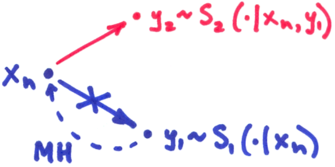

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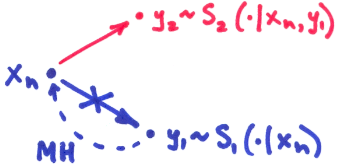

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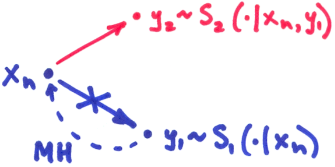

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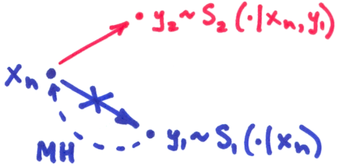

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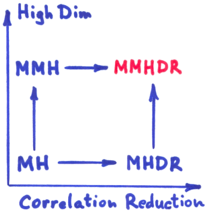
Modified MH algorithm with Delayed Rejection



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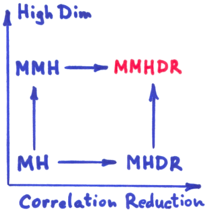
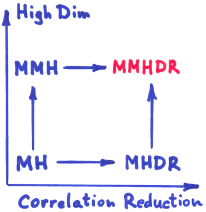


Features of the Algorithm:

Modified MH algorithm with Delayed Rejection



Features of the Algorithm:

- Samples generated by MMHDR are less correlated then samples generated by MMH.

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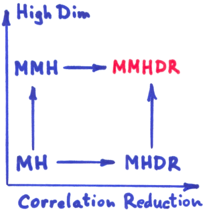

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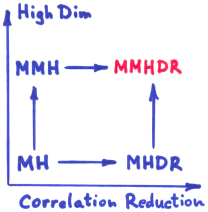

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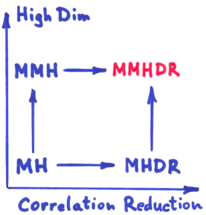

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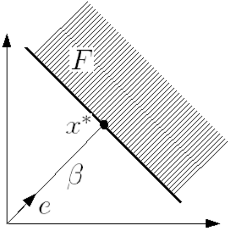
- With fixed computational effort:
  - MMH: more Markov chains with more correlated states
  - MMHDR: fewer Markov chains with less correlated states

Example

- Linear problem



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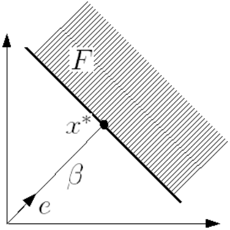

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  - $p_F = 10^{-5}$, $\beta = 4.265$

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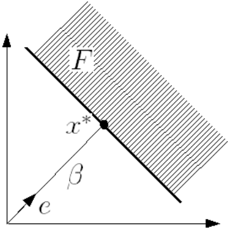

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  - MMH: $S^j(\cdot|x_0^j) = \mathcal{N}(x_0^j, 1)$
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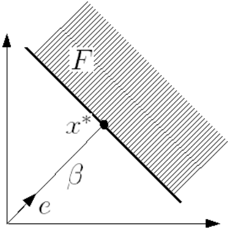

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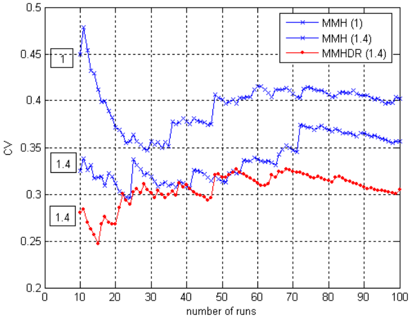

MMH(1): SS + MMH, $n = 10^3$

MMHDR(1.4): SS + MMHDR, $n = 10^3$

MMH(1.4): SS + MMH, $n = 1450$

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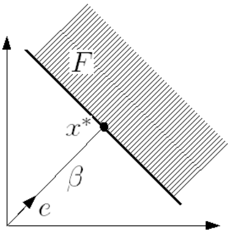

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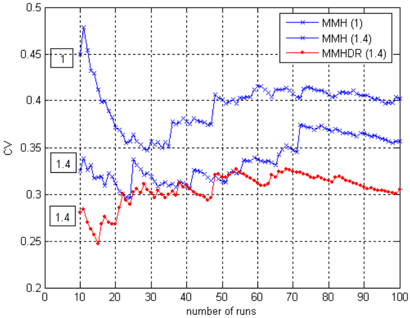

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Reduction in CV is 11%

“Bayesianization” of Subset Simulation

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3. Obtain the posterior PDF $p(p_F| \cup_{k=0}^{m-1} \mathcal{D}_k)$ of $p_F = \prod_{k=1}^{m} p_k$ from $p(p_1|\mathcal{D}_0), \ldots, p(p_m|\mathcal{D}_{m-1})$.

Prior and Posterior for $p_k = P(F_k|F_{k-1})$

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     $\Rightarrow$ Bayes' Theorem (1763):

$$p(p_k|\mathcal{D}_{k-1}) = \frac{p_k^{n_k}(1-p_k)^{N-n_k}}{B(n_k+1, N-n_k+1)}$$

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   - In fact, $\theta_{k-1}^{(1)}, \ldots, \theta_{k-1}^{(N)}$ are MCMC samples (for $k \geq 2$)
     $\Rightarrow \theta_{k-1}^{(1)}, \ldots, \theta_{k-1}^{(N)} \sim \pi(\cdot|F_{k-1})$, however, they are not independent

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Posterior PDF for p_F

Last step: To find the PDF of $p_F = \prod_{k=1}^{m} p_k$, given the PDFs of all factors

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Idea: To approximate p_F by a single beta variable

Theorem (Da-Yin Fan, 1991)

Let $X_1, \ldots, X_m$ be beta variables, $X_k \sim Beta(a_k, b_k)$, and $Y = X_1 X_2 \ldots X_m$. Then Y is approximately distributed as $\tilde{Y} \sim Beta(a, b)$, where

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Posterior PDF for p_F

Last step: To find the PDF of $p_F = \prod_{k=1}^{m} p_k$, given the PDFs of all factors

$$p_k \sim \mathcal{B}e(n_k + 1, N - n_k + 1)$$

Idea: To approximate p_F by a single beta variable

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Nice property of this approximation: $\mathbb{E}[\tilde{Y}] = \mathbb{E}[Y]$, $\mathbb{E}[\tilde{Y}^2] = \mathbb{E}[Y^2]$

Bayesian post-processor for Subset Simulation

$$\boxed{\text{Point estimate } \hat{p}_F^{SS} \rightsquigarrow \text{ PDF } p^{SS+}(p_F) = \mathcal{B}e(p_F|a,b)}$$

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- The PDF p^{SS+} can be fully used for life-cost analyses, decision making, etc.

$$\mathbb{E}[\mathrm{Loss}(p_F)] = \int \mathrm{Loss}(p_F) p^{SS+}(p_F) dp_F$$

Elasto-Plastic Structure Subjected to Ground Motion

S.K. Au (Computers & Structures, 2005):

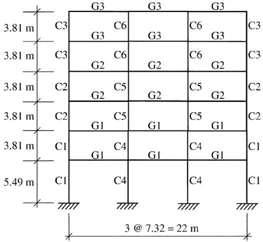
- 2D moment-resisting steel frame
- Synthetic ground motion $a = a(Z)$
  - $Z = (Z_1, \ldots, Z_d) \overset{i.i.d}{\sim} \mathcal{N}(0,1)$
  - $\xrightarrow{Z} \boxed{\text{Filter}} \xrightarrow{a(Z)}$
  - $d = 1001$
- Failure domain:

$$F = \{Z \in \mathbb{R}^d : \delta_{\max}(Z) > b\}$$

$$\delta_{\max} = \max_{i=1,\ldots,6} \delta_i$$

δ_i is the maximum absolute interstory drift ratio of the i^{th} story within the duration of study, 30 s

$$b = 0.5\% \Rightarrow p_F \approx 8.9 \times 10^{-3}$$



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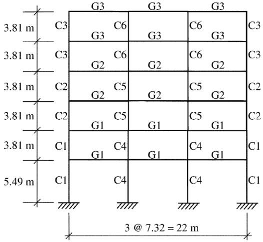

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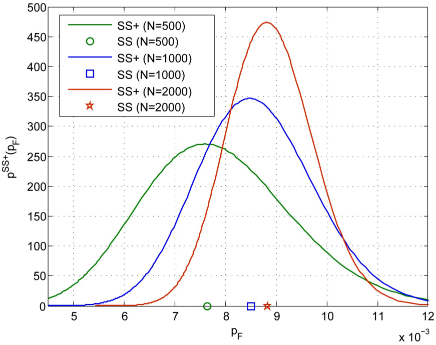

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- MCMC algorithms computes multi-dimensional integrals using Markov chains
- MCMC-based methods can be very useful for solving engineering problems
  - Reliability Engineering
- Subset Simulation (Au & Beck, 2001)
  - a very efficient MCMC method for estimation of small failure probabilities
- Enhancements for Subset Simulation
  - MMHDR = MMH (Au & Beck, 2001) + MHDR (Tierney & Mira, 1999)
  - Bayesian post-processor for Subset Simulation

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Thank you for attention!