BAYESIAN IDEAS FOR DISCRETE EVENT SIMULATION: WHY, WHAT AND HOW

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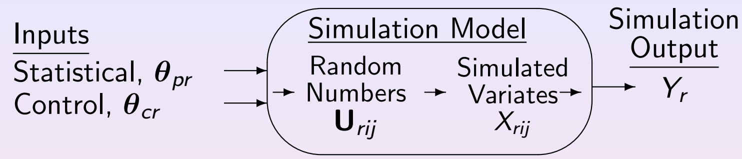
Why Bayesian methods in Simulation?



$$Y_r = g(\boldsymbol{\theta}_p, \boldsymbol{\theta}_c; \mathbf{U}_r)$$

- Example: Single Server Queue (M/M/1): $\boldsymbol{\theta}_p = (\lambda, \mu_i) =$ arrival and service rates (server $i = 1, 2$)
- Output: $Y \approx \lambda/(\mu_i - \lambda)$ + noise
- Simulation: Analyze stochastic processes via sample path generation. Inform decisions: pick control parameter $\boldsymbol{\theta}_c$, to estimate or to optimize value $h(E[Y \mid \boldsymbol{\theta}_p, \boldsymbol{\theta}_c])$
- Bayesian as alternative to frequentist

Why Bayesian methods?

- Glynn (1986): *Uncertainty analysis*. Not $\alpha = h(E[Y])$, but

$$\alpha(\theta) = h(E[Y \mid \theta])$$

- Unknown parameters, $p(\theta)$, data from modeled system to update
  1. Mean $E[\alpha(\Theta)]$
  2. Distribution of $\alpha(\Theta)$ induced by Θ
  3. Credible set: θ_{lo}, θ_{hi} so $p([h(\theta_{lo}), h(\theta_{hi})]) = 95\%$
- Chick (1997): Reviewed work to that date.
- Suggested broader range of application.
  1. *Ranking and selection*
  2. *Response surface modeling*
  3. *Experimental design*

The Point of Today

- Review some basic concepts of subjective probability, Bayesian statistics, decision theory.
- Identify several applications to simulation experiments.
- Summarize some implementation issues.
- Identify some areas for future work.

Related work

See the WSC (2006) paper and chapter in Henderson and Nelson book for a long (but incomplete) citation list for work over the last 10 years on:

- Formal Bayes or decision theoretic theory
- Applications: scheduling, insurance, finance, traffic modeling, public health, waterway safety, supply chain and other areas
- Bayes and deterministic simulations
- Favorite books on subjective and Bayesian probability and decision theory

Public Policy and Health Economics: increasingly uses simulation (in addition to decision trees, Markov chains), and *increasingly* requires *probabilistic sensitivity analysis*.

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Outline

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Getting down to brass tacks

Probability of 7 heads in the first 10 flips?

How to approach the problem...

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Getting down to brass tacks

Probability of 7 heads in the first 10 flips?

Comte d'Alembert (18th cent.)

- Indifference says maybe $1/11$?
- But wait, for one flip, probability of heads is $1/2$?

See Savage (1972) and Kreps (1988).

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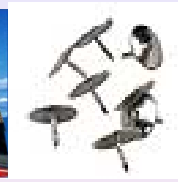
Getting down to brass tacks



Probability of 7 heads in the first 10 flips?

Dwight (an unreconstructed frequentist)

- $\frac{10!}{7!3!}\theta^7(1-\theta)^3$, where $\theta = \lim_{n\to\infty} \frac{X_1+\ldots+X_n}{n}$ (a.e.).
- If we rent Madison Square garden and flip the tack repeatedly, I can estimate θ for you.
- What confidence and how accurately do you need to know θ?

Hmmm. . .

Getting down to brass tacks

Probability of 7 heads in the first 10 flips?

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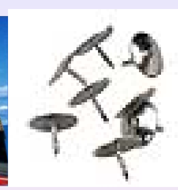
Let's reformulate the question . . .

Why am I a Bayesian?



Will you accept the following bet *now*? You get \$100 if there are 7 heads, but you pay \$5 if not.

more from Dwight

- I can't answer until I have a good idea of what θ is.
- Guessing wouldn't be scientific.

Why am I a Bayesian?


Ralph

Probability of 7 heads in the first 10 flips?

- I'm willing to use probability for personal judgments
- $\int_0^1 \frac{10!}{7!3!}\theta^7(1-\theta)^3\pi(\theta)d\theta$, where $\pi(\theta)$ is a *prior probability*.
- I'll update with *Bayes' rule*, to get *posterior probability*

$$p(\theta \mid \mathbf{x}_n) = \frac{\pi(\theta)p(\mathbf{x}_n \mid \theta)}{p(\mathbf{x}_n)} = \frac{\pi(\theta)\prod_{i=1}^n p(x_i \mid \theta)}{\int p(\mathbf{x}_n \mid \theta)d\pi(\theta)}$$

Why am I a Bayesian?

Lenny

Probability of 7 heads in the first 10 flips?

- Fair bets: I set $p(E_1) > p(E_2)$ if I prefer the first bet:

- Exchangeability (weaker than i.i.d.)

$$p(x_1, x_2, \ldots, x_n) = p(x_{s_1}, x_{s_2}, \ldots, x_{s_n})$$

for permutations s on $\{1, 2, \ldots, n\}$ for arbitrary n.

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Why am I a Bayesian?

Lenny

- Exchangeability plus conceptually infinite N *imply*

$$\lim_{N\to\infty} p(7 \text{ heads in first 10 flips}) = \int_0^1 \frac{10!}{7!3!}\theta^7(1-\theta)^3 dF(\theta)$$

- de Finetti (1990)-like representation
- Ralph assumed conditional i.i.d., while Lenny *derives* formula from exchangeability
- Probability defined by bet preferences, not repeated outcomes

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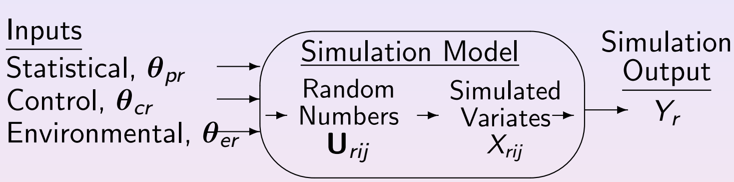
Implication for Simulation: $Y_r = g(\boldsymbol{\theta}_p, \boldsymbol{\theta}_e, \boldsymbol{\theta}_c; \mathbf{U}_r)$



- Input selection: Infinite exchangeable sequence X_{ij} from modeled system to infer ith statistical input, $\boldsymbol{\theta}_{pi}$

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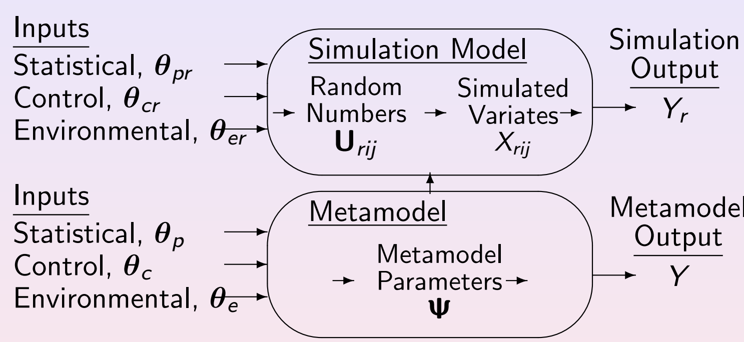
Implication for Simulation: $Y_r = g(\boldsymbol{\theta}_p, \boldsymbol{\theta}_e, \boldsymbol{\theta}_c; \mathbf{U}_r)$



- Input selection: Infinite exchangeable sequence X_{ij} from modeled system to infer ith statistical input, $\boldsymbol{\theta}_{pi}$
- Metamodeling: Infinite exchangeable Y_r to infer $\boldsymbol{\Psi}$.

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Part of the process

- Establish exchangeability arguments, posit potential likelihood functions for observables, given unknown quantities
- Assess prior distributions for unknown quantities
- Relevant asymptotic theorems
- Decisions, loss, and value of information
  - ranking and selection,
  - other experimental design issues

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Subjective Methods

We need a prior distribution for unknown parameters.
For a Bernoulli outcome . . . de Finetti (1990), Savage (1972) require *You* to assess your personal belief, $\pi(\theta)$ to describe $p(\Theta \leq \theta)$

- Important gain in flexibility
- Consistent with expected value decision theory
- Kahneman, Slovic, and Tversky (1982) describe difficulties with elicitation . . .

Some seek 'automated' methods . . .

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Principle of Indifference

For finite exchangeable sequence, set

$$\theta_N = \frac{X_1 + \ldots + X_N}{N} \in \{0/N, 1/N, \ldots, (N-1)/N, 1\}$$

- Indifference: discrete uniform for finite N
- Limit: $\lim_{N\to\infty} p(\theta_N) \stackrel{\mathcal{D}}{\to} \mathtt{uniform}[0,1]$
- Laplace (1812) used $\mathtt{uniform}[0,1]$ for his prior probability that the sun would come up tomorrow

- Coordinate dependence for continuous r.v. (X_i versus $\log X_i$)

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Jeffrey's invariant prior

- $\pi(\theta) \propto |H(\theta)|^{1/2} d\theta$, where H is the expected information in one observation,

$$H(\theta) = E_X \left[-\frac{\partial^2 \log p(X \mid \theta)}{\partial \theta^2} \bigg|_\theta \right], \qquad (1)$$

  'uniform' with respect to the natural metric induced by the likelihood function (Kass 1989)
- *Jeffreys' prior* for Bernoulli sampling is $\texttt{beta}(1/2, 1/2)$
- For some likelihoods, Jeffreys' prior is improper (doesn't integrate to 1). Might be used formally

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Conjugate prior distribution

Bernoulli sampling

- Set $s_n = \sum_{i=1}^n x_i$
- Likelihood: $p(\mathbf{x}_n|\theta) \propto \theta^{s_n}(1-\theta)^{n-s_n}$
- Prior: $\pi(\theta) \propto \theta^{\alpha-1}(1-\theta)^{\beta-1}$, a $\texttt{beta}(\alpha, \beta)$ distribution
- Posterior: $\propto \theta^{\alpha+s_n-1}(1-\theta)^{\beta+n-s_n-1}$, a $\texttt{beta}(\alpha+s_n, \beta+n-s_n)$ (conjugate) distribution

Exponential family

- Likelihood: $p(x \mid \theta) = a(x)h_0(\theta)\exp\left[\sum_{j=1}^d c_j\phi_j(\theta)h_j(x)\right]$
- Canonical conjugate prior: $p(\theta) = K(\mathbf{t})[h_0(\theta)]^{n_0}\exp\left[\sum_{j=1}^d c_j\phi_j(\theta)t_j\right]$
- Posterior, given n data points: has parameters $n_0 + n$ and sum of $\mathbf{t} = (t_1, t_2, \ldots, t_d)$ and sufficient statistics (Bernardo and Smith 1994)

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'Noninformative'

- The $\texttt{uniform}[0, 1]$ distribution is conjugate for Bernoulli sampling—a $\texttt{beta}(1, 1)$ distribution.
- 'Noninformative' means 'evenly spread'—a heuristic term
- For canonical conjugate prior (for exponential family), the posterior has parameter $n_0 + n$
- Some think of $n_0 + n$ as an 'effective' number of data points
- 'Noninformative' associated with a small n_0

Others

- Jaynes (1983): maximum entropy methods
- Berger (1994), Kass and Wasserman (1996): Default rules

Useful? Actually informative?

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Classic Analogs for Infinite Exchangeable Sequences

Classical asymptotic theorems (e.g. Billingsley 1986) . . .

- laws of large numbers (LLN)
- central limit theorem (CLT)
- law of iterated logarithm (LIL)

. . . have Bayesian interpretations if considered conditional on mean and standard deviation of an infinite exchangeable sequence.

Bayesian LLN

A Bayesian extension of the LLN allows for sample averages to converge to random variables rather than to 'true' means.

Theorem (Bayesian LLN)

If $\bar{X}_n$ and $\bar{Y}_m$ are respectively the averages of n and m exchangeable random quantities X_i (the two averages may or may not have some terms in common), the probability *that*

$$|\bar{X}_n - \bar{Y}_m| > \epsilon$$

may be made arbitrarily small by taking n and m sufficiently large (de Finetti 1990, p. 216 assumes a finite variance).

Theorem (Posterior Normality)

For each n, let $p_n(\cdot)$ be the posterior pdf of the d-dimensional parameter θ_n given $\mathbf{x}_n = (x_1, \ldots, x_n)$, let $\tilde{\theta}_n$ be its mode (MAP), and define the $d \times d$ Bayesian observed information matrix Σ_n^{-1} by

$$\Sigma_n^{-1} = -\frac{\partial^2 \log p_n(\theta \mid \mathbf{x}_n)}{\partial \theta^2}\bigg|_{\tilde{\theta}_n}. \qquad (2)$$

Then $\phi_n = \Sigma_n^{-1/2}(\theta_n - \tilde{\theta}_n)$ converges in distribution to a standard (multivariate) normal random variable (Bernardo and Smith 1994, Prop 5.14 needs regularity conditions).

Frequentist analog: asserts that MLE is asymptotically normally distributed about a 'true' θ_0 (Law and Kelton 2000), *as opposed to* describing uncertainty about θ.

Outline

Decisions under uncertainty

- Uncertainty described by probability $\Rightarrow$ modeler can assess *expected value of information* (EVI) of additional data.
- EVI is useful in experimental design.
- EVI : value of resolving uncertainty with respect to a *loss function* $\mathcal{L}(d, \omega)$ that describes losses when a *decision d* is chosen when the state of nature is ω.
- Data from experiment can reduce uncertainty about ω, reduce expected loss.

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Example: What is the mean? Setup

Example adapted from de Groot (1970) illustrates key concepts used for VIP procedures (Chick and Inoue 2001b)

- Decide if unknown mean W of normal distribution (known σ^2) is smaller (decision $d = 1$) or larger ($d = 2$) than w_0.
- Exchangeable samples $\mathbf{X}_n = (X_1, X_2, \ldots, X_n)$, with $p(X_i) \sim \mathtt{Normal}\left(w, \sigma^2\right)$, given $W = w$, are available
- Goal: design experiment (choose n) to balance sampling cost (cn) and expected opportunity cost if wrong answer chosen

$$\mathcal{L}(1, w) = \begin{cases} 0 & \text{if } w \le w_0 \\ w - w_0 & \text{if } w > w_0, \end{cases}$$

$$\mathcal{L}(2, w) = \begin{cases} w_0 - w & \text{if } w \le w_0 \\ 0 & \text{if } w > w_0. \end{cases}$$

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Example: What is the mean? If we knew...

- Prior: $W \sim \mathtt{Normal}\left(\mu, 1/\tau\right)$ is conjugate. NOTE: τ is the *precision* in our uncertainty about unknown mean, W.
- Posterior: Observing $\mathbf{X}_n = \mathbf{x}_n$ would result in

$$\begin{aligned} p(w \mid \mathbf{x}_n) &\sim \mathtt{Normal}\left(z, \tau_n^{-1}\right) \\ z &= \text{posterior mean of } W = E[W \mid \mathbf{x}_n] = \frac{\tau\mu + \frac{n}{\sigma^2}\bar{x}_n}{\tau + \frac{n}{\sigma^2}} \\ \tau_n &= \text{posterior precision of } W = \tau + n/\sigma^2. \end{aligned}$$

τ_n^{-1} equals the asymptotic posterior variance approximation Σ_n from theorem

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Example: What is the mean? How much to know...

- Posterior mean z for unknown w influences the decision, but depends upon n, which is selected before $\mathbf{X}_n$ is seen.
- Conditional distribution of $\bar{X}_n$ given w is $\mathtt{Normal}\left(w, \sigma^2/n\right)$
- *Predictive distribution* $p(z)$ of the posterior mean $Z = E[W \mid \mathbf{X}_n] = (\tau\mu + \frac{n}{\sigma^2}\bar{X}_n)/\tau_n$
- Mixing over prior $\pi(w)$ implies a predictive distribution

$$\begin{aligned} Z &\sim \mathtt{Normal}\left(\mu, \tau_z^{-1}\right) \\ \tau_z &= \tau(\tau + n/\sigma^2)/(n/\sigma^2) \end{aligned}$$

Note: $\tau_z^{-1} \to 0$ when $n \to 0$ (no new information).
If $n \to \infty$, then $\mathrm{Var}[Z] \to \sigma^2$.

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Example: What is the mean? What is the risk. . .

To minimize risk (sampling cost + expected loss from potentially incorrect decision), pick n to minimizes a nested expectation

$$\rho(n) = cn + E_{\mathbf{X}_n}[E_W[\mathcal{L}(d(\mathbf{X}_n), W) \mid \mathbf{X}_n]].$$

- General technique: set $\mathcal{L}^*(d, w) = \mathcal{L}(d, w) - \mathcal{L}(1, w)$, which is 0 if $d = 1$ and is $w_0 - w$ if $d = 2$. Then

$$E_W[\mathcal{L}^*(d(\mathbf{X}_n), W) \mid \mathbf{X}_n] = \begin{cases} 0 & \text{if } d = 1 \\ w_0 - Z & \text{if } d = 2. \end{cases} \quad (3)$$

- To minimize loss in Eq. 3, assert $d(\mathbf{X}_n) = 2$ ('bigger') if posterior mean exceeds threshold, $Z > w_0$, and assert $d(\mathbf{X}_n) = 1$ ('smaller') if $Z \leq w_0$.

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Example: What is the mean? Expected loss

- Decision depends on $\mathbf{X}_n$ via Z; Z has normal distribution
- Expected loss found with standard normal loss for newsboy

$$\begin{aligned} L_N[s] &= \int_s (t - s)\phi(t)dt = \phi(s) - s(1 - \Phi(s)) \\ E[\mathcal{L}^*(d(\mathbf{X}_n), W)] &= E_{\mathbf{X}_n}[E_W[\mathcal{L}^*(d(\mathbf{X}_n), W) \mid \mathbf{X}_n]] \\ &= -\tau_z^{\frac{-1}{2}} L_N[\tau_z^{\frac{1}{2}}(w_0 - \mu)] \end{aligned}$$

- Add back $E[\mathcal{L}(1, W)]$, use prior for W

$$E[\mathcal{L}(d(\mathbf{X}_n), W)] = \tau^{\frac{-1}{2}} L_N[\tau^{\frac{1}{2}}(w_0 - \mu)] - \tau_z^{\frac{-1}{2}} L_N[\tau_z^{\frac{1}{2}}(w_0 - \mu)]$$

- EVI and EVPI

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Example: What is the mean? What is the risk. . .

- First-order optimality condition

$$\frac{\partial \rho}{\partial n} = \frac{1}{2}\tau_z^{-\frac{3}{2}}\phi[\tau_z^{\frac{1}{2}}(w_0 - \mu)] \cdot \frac{-\tau^2\sigma^2}{n^2} + c = 0$$

- For small costs $c \to 0$, the sample size is large. Since $\tau_z \to \tau$ as $n \to \infty$, the optimal sample size n is asymptotically

$$n^* \approx \left(\tau^{\frac{1}{2}}\sigma^2\phi[\tau_z^{\frac{1}{2}}(w_0 - \mu)]/(2c)\right)^{1/2}.$$

- Asymptotic approximations are a second useful tool to identify criteria-based sampling plans.
- Extensions of these ideas used to derive VIP procedures (Chick and Inoue 2001b).

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Alternate approximation

- Regular exponential family: asymptotic variance approximation Σ_n from theorem simplifies to

$$H^{-1}(\theta)/(n_0 + n),$$

where H is the expected information from one observation (Eq. 1), if canonical conjugate prior distribution is used
- Approximate effect of m new samples is to change posterior to

$$\mathtt{Normal}\left(\tilde{\theta}_n, \Sigma_n \frac{n_0 + n}{n_0 + n + m}\right).$$

- Used for OCBA (Chen 1996), sampling plans for field data (Ng and Chick 2001). Frequentist result to obtain CI of desired size (Law and Kelton 2000)

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Another loss function: discrepancy

- Kullback-Leibler discrepancy: difference between distributions
- Discrete distributions $\tilde{p}$ and p,

$$\delta(p \,||\, \tilde{p}) = \sum \tilde{p}_i \log(\tilde{p}_i / q_i).$$

- Continuous r.v. X with densities $\tilde{f}$ and $f_\theta = f(x \mid \theta)$,

$$\delta(f_\theta \,||\, \tilde{f}) = \int \tilde{f}(x) \log \frac{\tilde{f}(x)}{f(x \mid \theta)} dx.$$

- One use: loss function for eliciting probability. If you believe the distribution is $\tilde{f}$, and you lose $\delta(f \,||\, \tilde{f})$ if you provide a distribution f, then you should honestly report $\tilde{f}$ (Bernardo 1979)

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Discrepancy: Other uses

- Select design matrix $\mathbf{d}_\Theta$ of r vectors of inputs $(\boldsymbol{\theta}_{pi}, \boldsymbol{\theta}_{ei}, \boldsymbol{\theta}_{ci})$ for $i = 1, 2, \ldots, r$ with output $\mathbf{Y}$ in order to best differentiate the posterior distribution of the response parameters ψ from the prior distribution for ψ (Bayesian D-optimal, Bernardo 1979; Smith and Verdinelli 1980; Ng and Chick 2004)

$$\int p(\mathbf{Y} \mid \mathbf{d}_\Theta) \left(\int p(\psi \mid \mathbf{Y}) \log \frac{p(\psi \mid \mathbf{Y})}{p(\psi)} d\psi \right) d\mathbf{Y}$$

- Select maximum entropy prior distribution (Jaynes 1983)
- More later: input distribution selection ...

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Outline

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Why Uncertainty Analysis?

- Simple Example

$$\mu_j \rightarrow \boxed{\text{Simulation}} \rightarrow Y_j = 2\mu_j + e_j$$

- Input model: $X_\ell \sim \texttt{Normal}\left(\mu, \sigma_x^2\right)$, known σ_x^2
- Data: X_ℓ observed $(\ell = 1, 2, \ldots, n_0)$
- Run r replications with $\bar{X}_{n_0}$ input for μ
- Construct 90% CI:

$$\bar{Y}_r \pm z_{0.95} \frac{\hat{\sigma}_y}{\sqrt{r}}$$

Coverage?

If μ is known, expect coverage to be 90%. But μ is *not* known.

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CI can be meaningless (several authors...)

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$$\bar{Y}_r \pm z_{0.95} \cancel{\frac{\hat{\sigma}_y}{\sqrt{r}}} \sqrt{V_{tot}}$$

Account for parameter uncertainty

$V_{tot} = \frac{\sigma_y^2}{r} + \frac{4\sigma_x^2}{n_0}$, so try $\bar{Y}_r \pm z_{0.95}\sqrt{V_{tot}}$

Why Uncertainty Analysis?

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- Construct 90% CI:

$$\bar{Y}_r \pm z_{0.95} \cancel{\frac{\hat{\sigma}_y}{\sqrt{r}}} \sqrt{V_{tot}}$$

For *known* mean response g, input parameters $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_k)$

$V_{tot} \approx \frac{\sigma_y^2}{r} + \sum_{i=1}^k \frac{\boldsymbol{\beta}_i H(\tilde{\theta}_i)^{-1} \boldsymbol{\beta}_i^{\mathrm{T}}}{n_i}$ where gradient $\boldsymbol{\beta}_i = \frac{\partial g(\tilde{\boldsymbol{\theta}})^{\mathrm{T}}}{\partial \theta_i}\Big|_{\tilde{\boldsymbol{\theta}}}$
(asymptotics. Cheng & Holland; Ng & Chick; Wilson & Zouaoui)

Why Uncertainty Analysis? Estimate response

Inputs

$\theta_1 = (\mu_1, \lambda_1)$ →
$\theta_2 = (\mu_2, \lambda_2)$ → Simulation →
$\theta_3 = (\mu_3, \lambda_3)$ →

$$\begin{aligned} Y_r &= g(\boldsymbol{\theta}) + \sigma Z \\ &= \beta_0 + \left(\sum_{i=1}^{k} \beta_{2i-1}\mu_i + \beta_{2i}\lambda_i\right) \\ &\quad + \beta_7\mu_1\mu_2 + \beta_8\mu_1^2 + \sigma Z \end{aligned}$$

- Assess $X_{i\ell} \sim \texttt{Normal}\left(\mu_i, \lambda_i^{-1}\right)$ for ith source of randomness
- Observe data $X_{i\ell}$ are observed ($i = 1, 2, 3$; $\ell = 1, 2, \ldots, n_i$)
- Estimate *unknown* $\boldsymbol{\beta}$ with r_0 runs (e.g. CCD from DOE)

$$V_{tot} = \frac{\hat{\sigma}_y^2}{r_0} + \underbrace{\sum_{i=1}^{k} \frac{\partial g(\tilde{\boldsymbol{\theta}}_n, \tilde{\boldsymbol{\beta}}_{r_0})}{\partial \theta_i} \Sigma_{n_i} \frac{\partial g(\tilde{\boldsymbol{\theta}}_n, \tilde{\boldsymbol{\beta}}_{r_0})^{\mathrm{T}}}{\partial \theta_i}}_{V_{par}=O(n_i^{-1})} + \underbrace{\Sigma_{\boldsymbol{\beta}} \otimes \Sigma_{\boldsymbol{\theta}}}_{V_{resp}=O(n_i^{-1}r^{-1})}$$

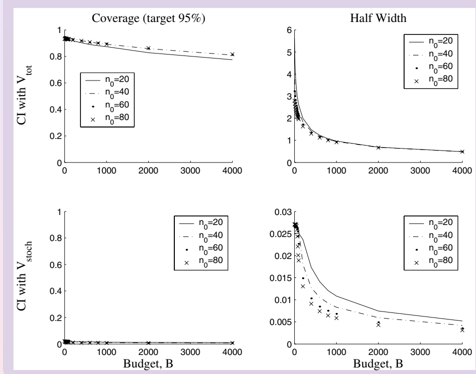
Uncertainty Analysis: Uncertainty Reduction

- Goal: Reduce uncertainty, not just quantify
  - r more replications
  - m_i more samples from source of randomness i
- Optimization:

$$\min_{r, m_i} \quad \frac{\hat{\sigma}_y^2}{r_0 + r} + \sum_{i=1}^{k} \frac{\xi_i}{n_i + m_i} + \frac{\zeta_i}{(r_0 + r)(n_i + m_i)}$$

$$r, m_i \quad \geq \quad 0$$

CI Coverage (Ng and Chick 2006)



Uncertainty Analysis

- Sensitivity analysis: $E[g(\theta)]$ as a function of θ (average out stochastic uncertainty from $\mathbf{u}$)
- Uncertainty analysis: $E[Y \mid \mathcal{E}]$, with both stochastic and parameter uncertainty, given all information $\mathcal{E}$
- Bayesian Model Average (BMA) estimates $E_Y[Y \mid \mathcal{E}]$

for $r = 1, \ldots, R$ replications
  sample parameter $\theta_r \sim p(\theta \mid \mathcal{E})$
  for $i = 1, 2, \ldots, n$
    generate output y_{ri} given input θ_r
  end loop
end loop
Generate estimate $\bar{y} = \sum_{r=1}^{R} \frac{1}{R} \sum_{i=1}^{n} \frac{y_{ri}}{n}$.

Variations on Estimating $E[Y \mid \mathcal{E}]$

- Zouaoui and Wilson (2003): decouple stochastic, parameter uncertainty; update estimate as new data becomes available with variations on BMA
- Andradóttir and Glynn (2004): biased estimates of $E[Y \mid \theta]$; quasi-random numbers; quadrature to select inputs θ_i
- Estimate distribution of conditional expectation $E[Y \mid \Theta, \mathcal{E}]$. Steckley and Henderson (2003) derive asymptotically optimal ways selecting r and n in BMA to produce a kernel density estimator (some conditions apply)

Outline

1. Getting down to brass tacks
   - Subjective and Bayesian methods
   - Assessing prior probability
   - Asymptotic Theorems
   - Decisions, loss, and value of information
   - Entropy and Kullback-Leibler Discrepancy
2. Applications
   - Uncertainty Analysis
   - Selecting from Multiple Candidate Distributions
   - Selecting the Best System
   - Metamodels
3. Implementation
4. Summary

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Basic Problem

- Which distribution/parameter to pick?
- 'Usual':
  1. Pick q candidate input distributions (e.g. exponential, gamma, Weibull, lognormal)
  2. Find MLE $\hat{\theta}_i$ for candidates $i = 1, \ldots, q$
  3. Goodness-of-fit (χ-squared, K-S, A-D) tests
- Concerns:
  1. CI coverage if MLE/best distribution selected
  2. How to select among unrejected models? . . . (Lindley 1957; Berger and Pericchi 1996)

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Bayesian Input Selection

- BMA applies without change for q candidates
  1. Put prior on $(M = m, \theta_m)$, where $m \in \{1, 2, \ldots, q\}$
  2. Compute posterior $p(m, \Theta_m|\mathcal{E})$, sample from it in BMA
- Chick (2001): stochastic process simulation context; moment matching method for commensurate prior distributions
- Zouaoui and Wilson (2004): decouple stochastic uncertainty from two types of structural uncertainty (candidate model & parameters); variance reduction for BMA; numerical analysis
- Model selected closest to the true model in sense of Kullback-Leibler divergence (Berk 1966; Bernardo and Smith 1994; Dmochowski 1999).

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Outline

1. Getting down to brass tacks
   - Subjective and Bayesian methods
   - Assessing prior probability
   - Asymptotic Theorems
   - Decisions, loss, and value of information
   - Entropy and Kullback-Leibler Discrepancy
2. Applications
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Ranking and selection procedures differ?

- What is it for?
  - Select the 'best' of a finite set
  - Best identified by mean simulation response
- What are the approaches?
  - IZ, Indifference zone:
    $P(CS) \geq 1 - \alpha$, δ^*, repeated applications of procedure
  - VIP, Bayesian value of information procedures:
    Like selection of mean bigger or smaller than threshold, Bayesian inference, loss, EVI
  - OCBA, Chen et al.:
    Heuristic, allocates samples to improve Bayesian PCS using 'thought experiment' $\sigma^2/r_0 \rightarrow \sigma^2/(r_0 + r)$
  - Economic. Chick and Gans (2005) propose a new economic approach, includes costs of replications and discounting, maximizes E[NPV] of decisions with simulation.

VIP procedures

- Motivated by 'statistical conservativeness' of IZ approaches
- Two-stage: Unknown means of several systems.
  - Opportunity cost *and* 0-1 loss ($P(CS)$)
  - Variances also unknown, different (conjugate prior, student marginal for mean)
  - Optimal solution unknown except special cases
  - Asymptotic approximation, Bonferroni bound for loss
- Sequential:
  - In theory, should improve things
  - Behrens-Fisher
  - Seems to work quite well

Procedure $\mathcal{LL}(\mathcal{B})$, for opportunity cost (linear loss)

1. Specify the first-stage sample size r_0. Take independent replications $y_{i1}, \ldots, y_{ir_0}$, for each system, $i = 1, \ldots, k$
2. Compute all first-stage sample means $\bar{x}_i = \sum_{j=1}^{r_0} y_{ij}/r_0$ and sample variances $\hat{\sigma}_i^2 = \frac{\sum_{j=1}^{r_0}(y_{ij}-\bar{x}_i)^2}{r_0-1}$, order statistics $\bar{x}_{[1]} \leq \ldots \leq \bar{x}_{[k]}$, and $\lambda_{i,k} = r_0/(\hat{\sigma}_{[k]}^2 + \hat{\sigma}_{[i]}^2)$
3. If sampling budget is B, run r_i more independent replications,

$$r_{[i]} = \frac{B + \sum_{j \in \mathcal{S}} r_0 c_j}{\sum_{j \in \mathcal{S}} \left(\frac{c_j c_{[i]} \hat{\sigma}_j^2 \eta_j}{\hat{\sigma}_{[i]}^2 \eta_{[i]}} \right)^{1/2}} - r_0$$

$\eta_{[i]} = (\lambda_{i,k})^{1/2} \frac{(r_0-1)+\lambda_{i,k}(\bar{x}_{[k]}-\bar{x}_{[i]})^2}{(r_0-1)-1} \phi_{r_0-1}[(\lambda_{i,k})^{1/2}(\bar{x}_{[k]} - \bar{x}_{[i]})]$ if $[i] \neq [k]$ and $\eta_{[k]} = \sum_{j=1}^{k-1} \eta_{[j]}$

4. Select system with largest $\bar{\bar{x}}_i = \sum_{j=1}^{r_0+r_i} y_{ij}/(r_0 + r_i)$

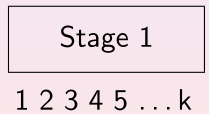
Sample Comparison with Combined Procedure, $\mathcal{C}$ (MDM)

Figure of merit	Proc.	Number of systems, k: 2	5	10	100
ANR	All	738	3,429	8,784	42,862
Empirical P(CS)	$\mathcal{C}$	0.8363	0.9140	0.9323	0.9763
	0-1($\mathcal{B}$)	0.8527*	0.9117	0.9480*	0.9937*
	$\mathcal{LL}(\mathcal{B})$	0.8500	0.9293*	0.9660*	0.9987*
Empirical frac. 'good' selections	$\mathcal{C}$	1.0000	0.9943	0.9990	1.0000
	0-1($\mathcal{B}$)	1.0000	0.9953	0.9977	0.9997
	$\mathcal{LL}(\mathcal{B})$	1.0000	0.9953	0.9993	1.0000
Expected posterior PCS	$\mathcal{C}$	0.8336	0.8379	0.8649	0.9318
	0-1($\mathcal{B}$)	0.8446*	0.8339	0.8821*	0.9717*
	$\mathcal{LL}(\mathcal{B})$	0.8470*	0.8462*	0.9022*	0.9842*
Expected bound, opp. cost	$\mathcal{C}$	0.0176	0.0138	0.0104	0.0037
	0-1($\mathcal{B}$)	0.0157*	0.0128*	0.0075*	0.0012*
	$\mathcal{LL}(\mathcal{B})$	0.0154*	0.0110*	0.0055*	0.0005*

Monotone decreasing means (MDM). * indicates statistically significant difference

VIP: Common Random Numbers

- Common random numbers (CRN) can sharpen contrasts between systems (e.g. same simulated demand pattern)
- Two-stage with screening (Chick and Inoue 2001a)
  - Run subset of systems in stage 2
  - Use 'missing data' formulas to update
  - Select from even screened systems
- Matrix intensive, heuristic provided



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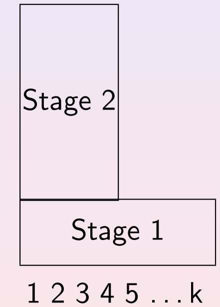

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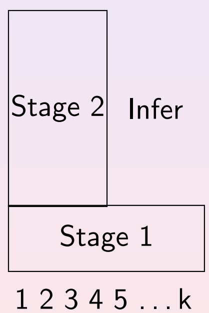

Summaries

- VIP procedures have solid basis, perform numerically quite well Chick and Inoue (2001, 2001a, 2002).
  - Matlab: All procedures (0-1 or opportunity cost loss; two-stage or independent sequential; two-stage CRN)
  - C: Independent replications, two-stage or sequential, both loss functions, *plus* variants (work in progress) to achieve Bayesian predictive targets for PCS and EOC
- Can show asymptotic relation between certain VIP and OCBA procedures
- Specific Bayesian procedures with new stopping rules highly effective (Branke, Chick, and Schmidt 2005)

Outline

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Metamodels

- Normal linear model

$$Y = \sum_{\ell=1}^{p} g_\ell(\boldsymbol{\theta})\beta_\ell + Z(\boldsymbol{\theta};\mathbf{U}) = \mathbf{g}^T(\boldsymbol{\theta})\boldsymbol{\beta} + Z(\boldsymbol{\theta};\mathbf{U}), \quad (4)$$

- Gaussian random function (GRF) - kriging

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Normal linear model

$$Y = \sum_{\ell=1}^{p} g_\ell(\boldsymbol{\theta})\beta_\ell + Z(\boldsymbol{\theta};\mathbf{U}) = \mathbf{g}^T(\boldsymbol{\theta})\boldsymbol{\beta} + Z(\boldsymbol{\theta};\mathbf{U}), \quad (5)$$

- Model
  - Known: regression functions $g_1, \ldots, g_p$
  - Unknown: coefficients $\boldsymbol{\beta}$, variance of zero-mean noise $Z(\cdot)$
- Conjugate prior $p(\boldsymbol{\beta}, \sigma^2)$ (if all factors active)
  - Inverted gamma distribution for unknown variance σ^2
  - Multivariate normal distribution for $\boldsymbol{\beta}$ given σ^2,
  - Raftery, Madigan, and Hoeting (1997) describe a relatively 'uninformative' prior distribution, 'good' results
- Identifying important factors like input distribution selection
  - 2^p candidate models
  - KL discrepancy-based design criterion balances factor identification and parameter estimation (Ng and Chick 2004)

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Gaussian random functions (GRF)

- Well-known in deterministic simulations, particularly in geostatistics (Cressie 1993; Santner et al. 2003)
- Provide flexibility that the linear model does not, and are useful when g takes a long time to compute.
- GRF for unknown nonstochastic g (no random numbers $\mathbf{u}$) is

$$Y(\boldsymbol{\theta}) = \sum_{\ell=1}^{p} g_\ell(\boldsymbol{\theta})\beta_\ell + Z(\boldsymbol{\theta}) = \mathbf{g}^T(\boldsymbol{\theta})\boldsymbol{\beta} + Z(\boldsymbol{\theta}) \quad (6)$$

for *known* regression functions $g_1, \ldots, g_p$ of $\mathbb{R}^d$, unknown regression coefficients $\boldsymbol{\beta}$, and a *zero-mean random second-order process* so that for any distinct inputs $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_m$, the vector $(Y_1, \ldots, Y_m)$ has (nonindependent) multivariate normal distribution, conditional on $\boldsymbol{\beta}$.

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Inference with GRFs

- GRF: Determined by mean $\mathbf{g}^T(\boldsymbol{\theta})\beta$ and covariance function

$$C^*(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2) = \mathrm{Cov}(Y(\boldsymbol{\theta}_1), Y(\boldsymbol{\theta}_2))$$

- Common to assume strong stationarity, so

$$C^*(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2) = C(\boldsymbol{\theta}_1 - \boldsymbol{\theta}_2)$$

- Inference for $g(\boldsymbol{\theta})$ at $\boldsymbol{\theta}_{r+1}$ not yet input to simulation model with correlation function $R(\mathbf{h}) = C(\mathbf{h})/C(0)$ for $\mathbf{h} \in \mathbb{R}^d$. Example: power exponential $R(\mathbf{h}) = \prod \exp[-|h_i/\gamma_i|^{p_i}]$ for $p_i \in [0, 2]$.
- Kriging (geostatistics) is best linear unbiased prediction (BLUP) for $g(\boldsymbol{\theta}_{r+1})$

More GRF

- Assessment of uncertainty in $g(\boldsymbol{\theta}_{r+1}) \Rightarrow$ experimental design technique to choose inputs to reduce response uncertainty (Santner et al. 2003)
- Also see tutorial by van Beers and Kleijnen (2004)
- Deterministic simulation: (Sacks et al. 1989; O'Hagan et al. 1999; Kennedy and O'Hagan 2001; Santner et al. 2003; van Beers and Kleijnen 2003).
- More work is needed for GRFs in the stochastic simulation context.

Implementation

Issues:

- Maximize (MLE $\hat{\theta}$ or MAP $\tilde{\theta}$)
- Integrate (marginal distribution $p(\theta_1 \mid \mathbf{x}_n)$ from $p(\theta_1, \theta_2 \mid \mathbf{x}_n)$), or proportionality constant $c^{-1} = \int f(\mathbf{x}_n \mid \theta) d\pi(\theta)$)
- Simulate (sample from $p(\theta \mid \mathbf{x}_n)$ to estimate $E[\alpha(\Theta)]$)

Tools:

- Newton-Raphson, Nelder-Mead, expectation-maximization (EM) algorithm, ...
- Quadrature, normal approximation, data augmentation (IP algorithm), importance sampling (IS)
- Inversion, importance sampling (IS), Markov Chain Monte Carlo (MCMC)

Evans and Swartz 1995; Tanner 1996; Gilks et al. 1996; Devroye 2006, ...

Metropolis-Hastings: An MCMC Algorithm

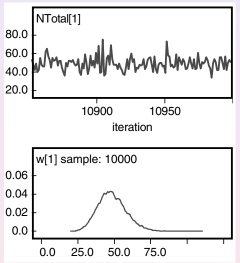
Target: Sample from $p(\theta \mid \mathcal{E})$
Capable: Easily sample from $q(\cdot \mid \theta_{t-1})$

Initialize $t = 0$, θ_0
for $t = 1, 2, \ldots$
  sample a candidate $\theta \sim q(\cdot \mid \theta_{t-1})$
  compute acceptance probability

$$\alpha(\theta_{t-1}, \theta) = \min\left\{1, \frac{p(\theta|\mathcal{E}) \cdot q(\theta_{t-1}|\theta)}{p(\theta_{t-1}|\mathcal{E}) \cdot q(\theta|\theta_{t-1})}\right\}$$

  generate an independent $u \sim \mathtt{uniform}[0, 1]$
  if $u \le \alpha(\theta_{t-1}, \theta)$ then set $\theta_t \leftarrow \theta$
    otherwise set $\theta_t \leftarrow \theta_{t-1}$
  set $t \leftarrow t + 1$
end loop

Sample path



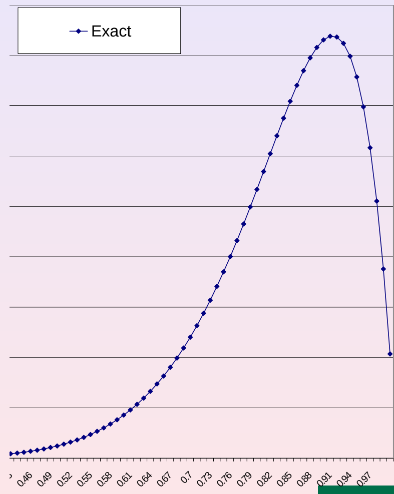
Density Estimate

Approximating Posterior Distributions: Pros and Cons

Exact Posterior

- Exact
- Good if simple closed form known
- May be hard in general (mixtures, missing data, marginal distribution, curse of dimensionality?)

Here, gene linkage example (Tanner 1996)

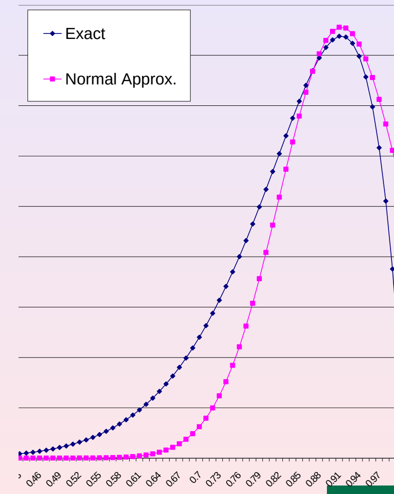


Getting down To brass tacks Applications **Implementation** S

Approximating Posterior Distributions: Pros and Cons

Asymptotic normality (from theorem)

- $\texttt{Normal}\left(\tilde{\theta}_n, \Sigma_n\right)$
- Relatively easy to compute
- Requires many data points ($n > 20d$)
- Does not model skew, etc.



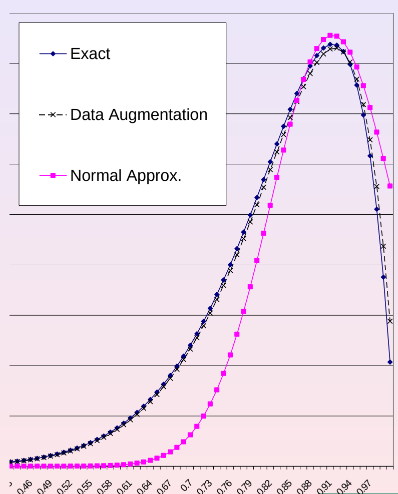
WSC'06 Bayesian Ideas for Simulation

Getting down To brass tacks Applications **Implementation** S

Approximating Posterior Distributions: Pros and Cons

Data Augmentation (IP algorithm)

- $p(\theta|\mathcal{E}) = \int p(\theta|Z,\mathcal{E})p(Z|\mathcal{E})$, average over Z = 'missing data'
  1. Set $i = 0$; $g_0(\theta)$ = current estimate of $p(\theta|\mathcal{E})$
  2. Generate $z_1, z_2, \ldots, z_m$ from $g_i(\theta)$ by
     1. Sample $\theta_1, \ldots, \theta_m$ from $g_i(\theta)$
     2. Sample $z_1, \ldots, z_m$ from $p(Z|\theta_i, \mathcal{E})$
  3. $g_{i+1}(\theta) = \sum_{j=1}^{m} p(\theta|z_j, \mathcal{E})/m$



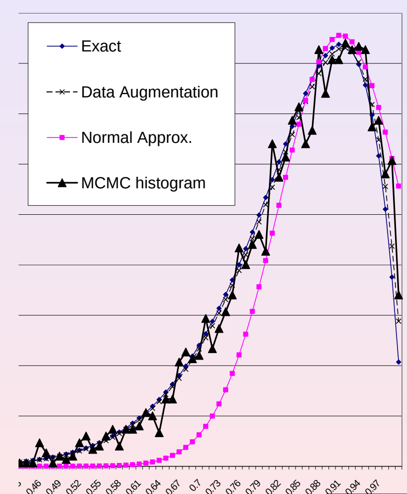
WSC'06 Bayesian Ideas for Simulation

Getting down To brass tacks Applications **Implementation** S

Approximating Posterior Distributions: Pros and Cons

MCMC with histogram

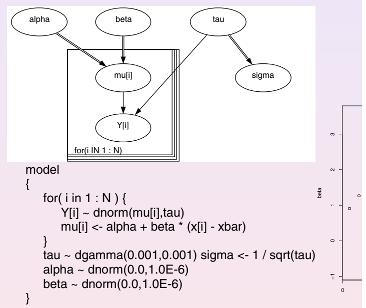
- General tool to sample (approximately) from posterior
- Complicated models possible
- Output analysis issues (convergence)
- Time-average (IP was average of distributions)
- MCMC can average distributions, too



WSC'06 Bayesian Ideas for Simulation

Some Tools

- Handcode: Matlab, C, Gauss
- WinBUGS (Spiegelhalter et al. 1996) (http://www.mrc-bsu.cam.ac.uk/bugs/welcome.shtml)
- R (http://www.r-project.org/), S-PLUS packages, BOA add-on (http://www.public-health.uiowa.edu/boa/)
- Uncertainty analysis in spreadsheet Monte Carlo applications are available (e.g. Winston 2000).
- Most DEDS Commercial Tools: cumbersome to implement BMA



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Bayesian Methods for Stochastic Process Simulation

- Themes:
  - Represent *all* uncertainty with probability, update with Bayes' rule, expected value of information for sampling decisions
  - Use simulation to efficiently estimate quantities of interest for a Bayesian analysis
- Bayesian, decision theory fits well with managerial/economic mindset
- Applications: input distribution selection, uncertainty analysis, experimental design, ranking and selection
- Asymptotic approximations helpful when exact optimal solutions are hard to find

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Research opportunities include

- More links to economics of simulation analysis
- Input modeling and uncertainty analysis (kernel estimation of conditional means; the effect of different candidate distributions on uncertainty; prior distributions elicitation; calibration/inverse problem)
- Response modeling (extend the Gaussian random field work for stochastic simulation; nonasymptotic sampling plans for input parameter inference to optimally reduce output uncertainty; reasoning about models; calibration. . .)
- Experimental design (quantiles, non-expected value goals; CRN for unknown input parameters for ranking and selection; non-Gaussian output for ranking and selection, GRFs)
- Improved computational tools (e.g. MCMC, software interop)

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