

Bayesian Computation Using Design of Experiments-Based Interpolation Technique

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(with discussions)

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Bayesian Computation

- Many intractable high-dimensional integrals
 - Posterior distribution
 - Posterior summaries
 - Marginal posterior distributions
 - Posterior predictive distributions
- Use approximation methods

Deterministic Methods

- Laplace's Approximation (e.g. Tierney and Kadane 1986)
 - May not be accurate.
- Gaussian Quadrature (e.g. Naylor and Smith 1982)
 - Can produce accurate results.
 - Cannot be used for high dimensions.

Simulation-Based Methods

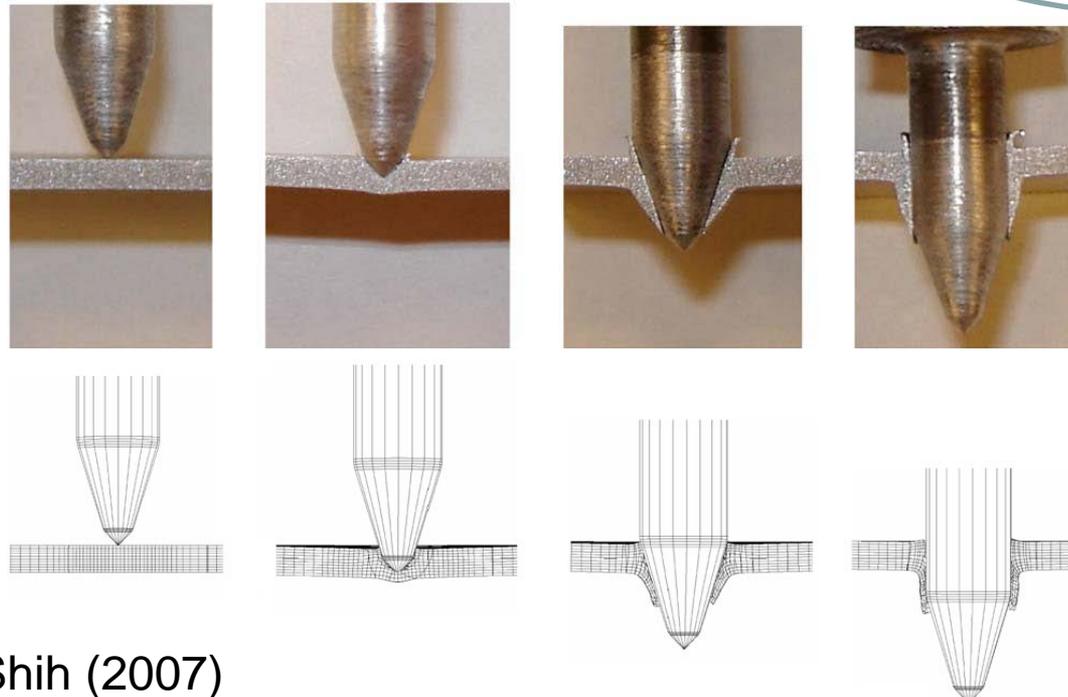
- MC/MCMC (Metropolis et al. 1953, Hastings 1970, Geman and Geman 1984, Gelfand and Smith 1990, ...)
 - Can obtain results with arbitrary precision
 - Suffer less from the curse of dimensionality
 - Convergence issues
 - High computational cost when dealing with computationally expensive posteriors

Examples of computationally expensive posteriors

- Model calibration

$$\min_{\theta} \sum_{i=1}^n \{y_i - f(x_i; \theta)\}^2$$

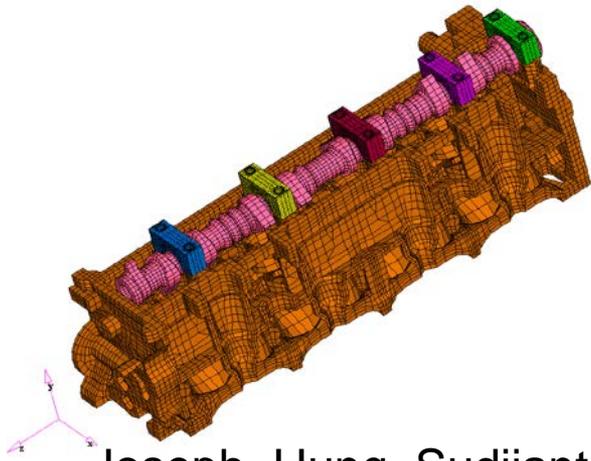
Expensive



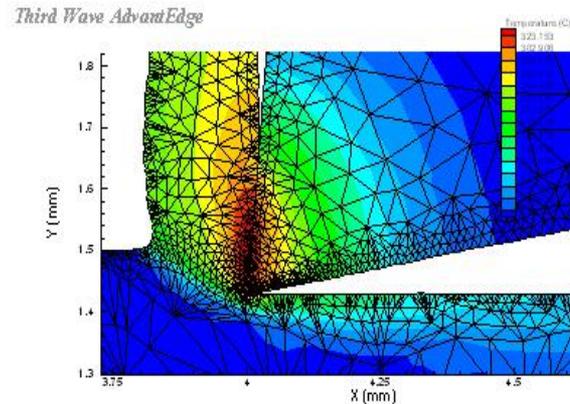
Miller and Shih (2007)

Examples-continued

- Geostatistics/Spatial statistics/Computer experiments



Joseph, Hung, Sudjianto (2008)



Hung, Joseph, Melkote (2009)

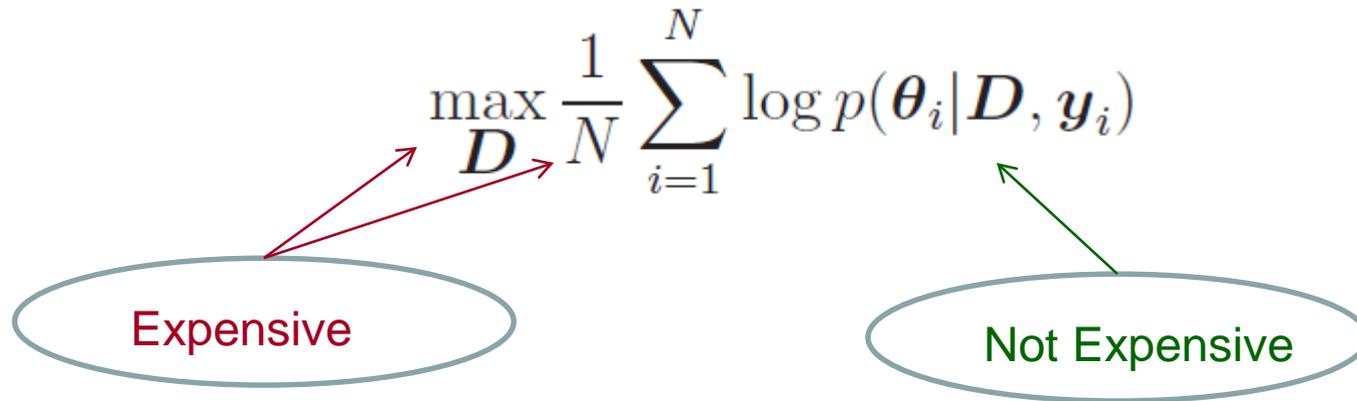
$$f(\mathbf{x})|\mu, \sigma^2, \boldsymbol{\theta} \sim GP(\mu, \sigma^2 \mathbf{R}(\cdot; \boldsymbol{\theta}))$$

$$p(\mathbf{y}|\mu, \sigma^2, \boldsymbol{\theta}) \propto \frac{1}{\sigma^n |\mathbf{R}(\boldsymbol{\theta})|^{1/2}} \exp\left\{-\frac{1}{2\sigma^2} (\mathbf{y} - \mu \mathbf{1})' \mathbf{R}(\boldsymbol{\theta})^{-1} (\mathbf{y} - \mu \mathbf{1})\right\}$$

Expensive

Examples-continued

- Inexpensive likelihood, but appearing within some algorithms.
- Simulation-based nonlinear optimal design (Muller 1999)



New Deterministic Method

- **Design of Experiments-based Interpolation technique (DoIt)**
 - Design of experiments
 - Interpolation methods (e.g., kriging)
- **Advantages**
 - Can obtain results with arbitrary precision
 - Suffer less from the curse of dimensionality
 - Works much faster than MC/MCMC
- **Disadvantages**
 - Small to moderate number dimensions
 - Continuous parameters

Earlier Work

- Bayes-Hermite Quadrature
 - O'Hagan (1991)
 - Kennedy (1998)
 - Rasmussen and Ghahramani (2003)
- Hybrid Monte Carlo using Gaussian Process Models
 - Rasmussen (2003)
 - Bliznyuk et al. (2008)
 - Henedrson et al. (2008)
 - Fielding, Nott, and Liong (2011)

Laplace's Approximation

- Bayesian model:

$$\mathbf{y}|\boldsymbol{\theta} \sim p(\mathbf{y}|\boldsymbol{\theta})$$

$$\boldsymbol{\theta} \sim p(\boldsymbol{\theta})$$

- Unnormalized posterior: $h(\boldsymbol{\theta}) \propto p(\mathbf{y}|\boldsymbol{\theta})p(\boldsymbol{\theta})$

$$\hat{\boldsymbol{\theta}} = \operatorname{argmax}_{\boldsymbol{\theta}} h(\boldsymbol{\theta})$$

$$h(\boldsymbol{\theta}) \approx h(\hat{\boldsymbol{\theta}}) \exp\left\{-\frac{1}{2}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})' \boldsymbol{\Sigma}^{-1}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})\right\}$$

$$\boldsymbol{\theta}|\mathbf{y} \sim^a N(\hat{\boldsymbol{\theta}}, \boldsymbol{\Sigma})$$

$$\boldsymbol{\Sigma} = [-\nabla^2 \log(h(\hat{\boldsymbol{\theta}}))]^{-1}$$

DoIt

- Unnormalized normal density function:

$$g(\boldsymbol{\theta}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \exp\left\{-\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1}(\boldsymbol{\theta} - \boldsymbol{\mu})\right\}$$

- Experimental design:

$$D = \{\boldsymbol{\nu}_1, \dots, \boldsymbol{\nu}_m\}$$

- DoIt:

$$h(\boldsymbol{\theta}) \approx \sum_{i=1}^m c_i g(\boldsymbol{\theta}; \boldsymbol{\nu}_i, \boldsymbol{\Sigma})$$

- Kriging, Radial Basis Function,...

DoIt-continued

- Evaluations: $\mathbf{h} = (h_1, \dots, h_m)'$, where $h_i = h(\boldsymbol{\nu}_i)$
- To get interpolation:

$$\mathbf{G}\mathbf{c} = \mathbf{h},$$

where $\mathbf{c} = (c_1, \dots, c_m)'$ and $G_{ij} = g(\boldsymbol{\nu}_i; \boldsymbol{\nu}_j, \boldsymbol{\Sigma})$

$$\tilde{\mathbf{c}} = \mathbf{G}^{-1}\mathbf{h}$$

- Let $\mathbf{g}(\boldsymbol{\theta}) = (g(\boldsymbol{\theta}; \boldsymbol{\nu}_1, \boldsymbol{\Sigma}), \dots, g(\boldsymbol{\theta}; \boldsymbol{\nu}_m, \boldsymbol{\Sigma}))'$

$$\tilde{h}(\boldsymbol{\theta}) = \tilde{\mathbf{c}}'\mathbf{g}(\boldsymbol{\theta})$$

DoIt-continued

- Marginal likelihood

$$\begin{aligned}\int \tilde{h}(\boldsymbol{\theta}) d\boldsymbol{\theta} &= \tilde{\mathbf{c}}' \int \mathbf{g}(\boldsymbol{\theta}) d\boldsymbol{\theta} \\ &= (2\pi)^{d/2} |\boldsymbol{\Sigma}|^{1/2} \tilde{\mathbf{c}}' \mathbf{1}\end{aligned}$$

- Posterior distribution

$$\tilde{p}(\boldsymbol{\theta}|\mathbf{y}) \approx \frac{\tilde{\mathbf{c}}' \mathbf{g}(\boldsymbol{\theta})}{(2\pi)^{d/2} |\boldsymbol{\Sigma}|^{1/2} \tilde{\mathbf{c}}' \mathbf{1}} = \frac{\tilde{\mathbf{c}}' \boldsymbol{\phi}(\boldsymbol{\theta})}{\tilde{\mathbf{c}}' \mathbf{1}}$$

$$\tilde{p}(\boldsymbol{\theta}|\mathbf{y}) \approx \frac{\sum_{i=1}^m \tilde{c}_i \boldsymbol{\phi}(\boldsymbol{\theta}; \boldsymbol{\nu}_i, \boldsymbol{\Sigma})}{\sum_{i=1}^m \tilde{c}_i}$$

Example

- Bayesian model:

$$y|\theta \sim \text{Poisson}(\theta),$$

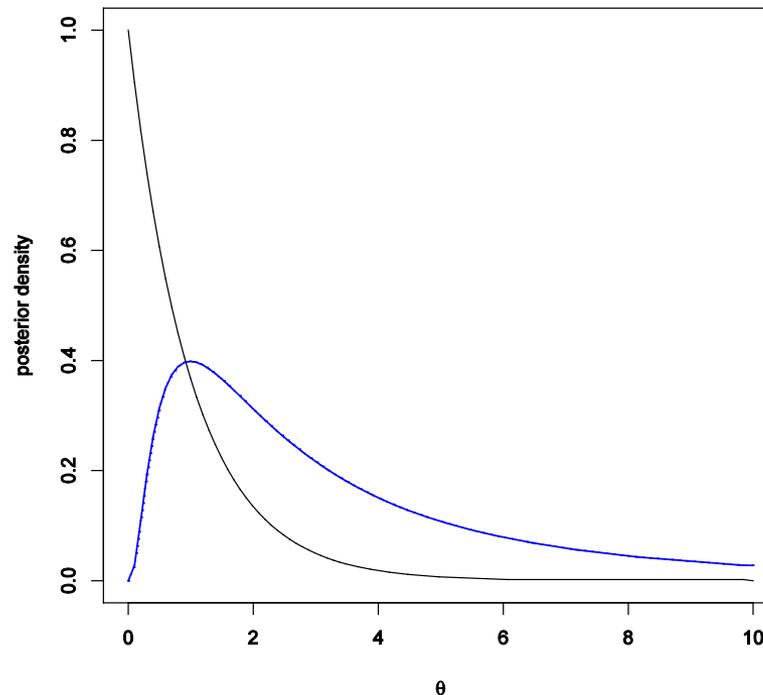
$$p(\theta) \propto 1.$$

- For $y=0$, posterior distribution:

$$\theta|y \sim \text{Exp}(1).$$

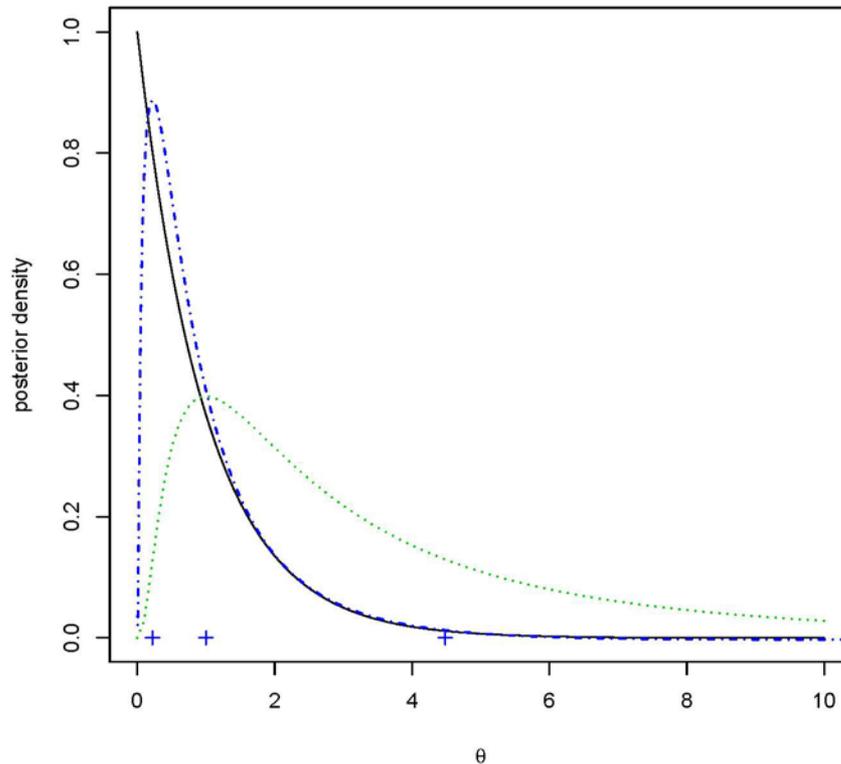
Example-continued

- Laplace's approximation: $\gamma = \log(\theta)$
- $\hat{\gamma} = 0$ and $\hat{\sigma}^2 = 1$: $\theta|y \sim^a \text{log-normal}(0, 1)$.



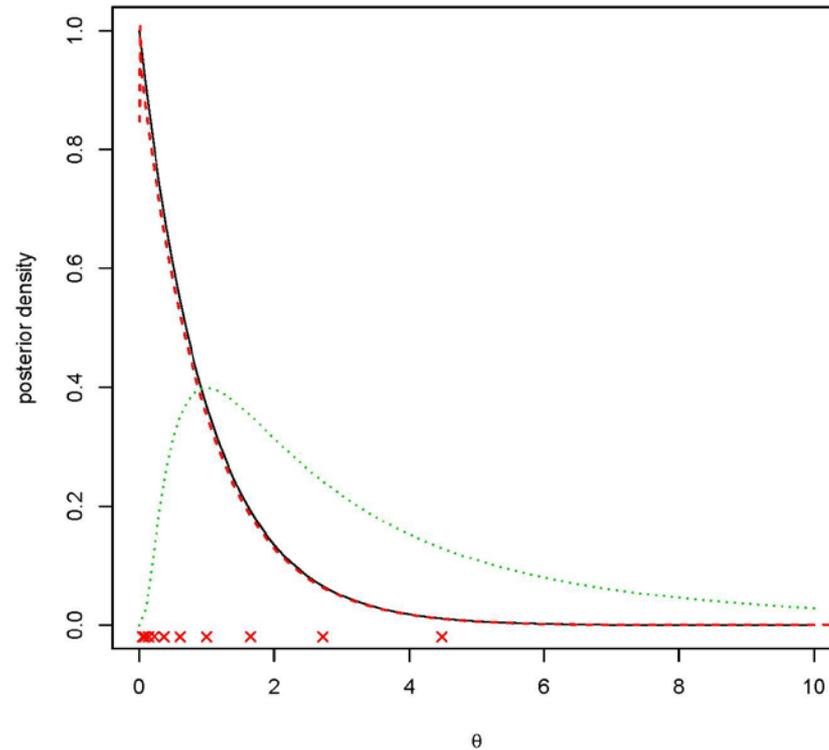
Example-continued

- DoIt : $\nu_1 = \hat{\gamma}$, $\nu_2 = \hat{\gamma} - 1.5\sigma$, and $\nu_2 = \hat{\gamma} + 1.5\sigma$



Example-continued

- DoIt : 10 equally spaced points from $\hat{\gamma} - 3\sigma$ to $\hat{\gamma} + 1.5\sigma$



A Result

Theorem 1: If $h(\boldsymbol{\theta})$ is continuous, then for any $\alpha \in (0, 1)$ and any $\epsilon > 0$, there exists a finite number of points $D = \{\nu_1, \dots, \nu_m\}$ in Θ such that

$$\left| \frac{\hat{h}(\boldsymbol{\theta}) / \int_{\Theta} \hat{h}(\boldsymbol{\theta}) d\boldsymbol{\theta}}{h(\boldsymbol{\theta}) / \int_{\Theta} h(\boldsymbol{\theta}) d\boldsymbol{\theta}} - 1 \right| < \epsilon \quad (6)$$

for all $\boldsymbol{\theta} \in \Theta$, where $\hat{h}(\boldsymbol{\theta})$ is any continuous and uniformly convergent interpolator of $h(\boldsymbol{\theta})$ on D and Θ is the $(1 - \alpha)$ highest posterior density (HPD) credible set.

As $\alpha \rightarrow 0$,

$$\frac{\hat{h}(\boldsymbol{\theta}) / \int_{\Theta} \hat{h}(\boldsymbol{\theta}) d\boldsymbol{\theta}}{h(\boldsymbol{\theta}) / \int_{\Theta} h(\boldsymbol{\theta}) d\boldsymbol{\theta}} \rightarrow \tilde{p}(\boldsymbol{\theta}|\mathbf{y})/p(\boldsymbol{\theta}|\mathbf{y}),$$

and as $\epsilon \rightarrow 0$,

$$\tilde{p}(\boldsymbol{\theta}|\mathbf{y})/p(\boldsymbol{\theta}|\mathbf{y}) \rightarrow 1.$$

Unknown Posterior Mode

- Assume that $\Sigma = \text{diag}\{\sigma_1^2, \dots, \sigma_d^2\}$
- Leave-one-out cross validation: $e_i = h_i - \tilde{h}_{(i)i}$
- From the kriging literature

$$e_i = \frac{(\mathbf{G}^{-1})_{ii}}{(\mathbf{G}^{-1})_{ii}} \mathbf{h}$$

- Minimize

$$MSCV = \frac{1}{m} \mathbf{e}' \mathbf{e}.$$

- or

$$WMSCV = \frac{1}{m} \mathbf{e}' \text{diag}(\mathbf{G}^{-1}) \mathbf{e}$$

Example

- Bayesian model:

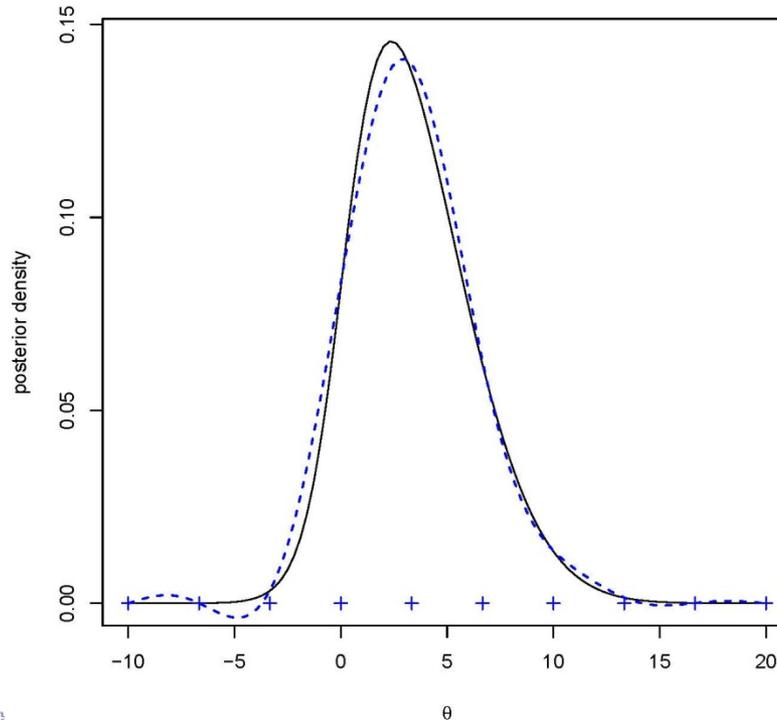
$$y|\theta \sim \text{Bernoulli}(\{1 + \exp(-\theta)\}^{-1}),$$

$$\theta \sim N(\mu, \tau^2).$$

- Suppose $y = 1$, $\mu = 1$ and $\tau = 4$.

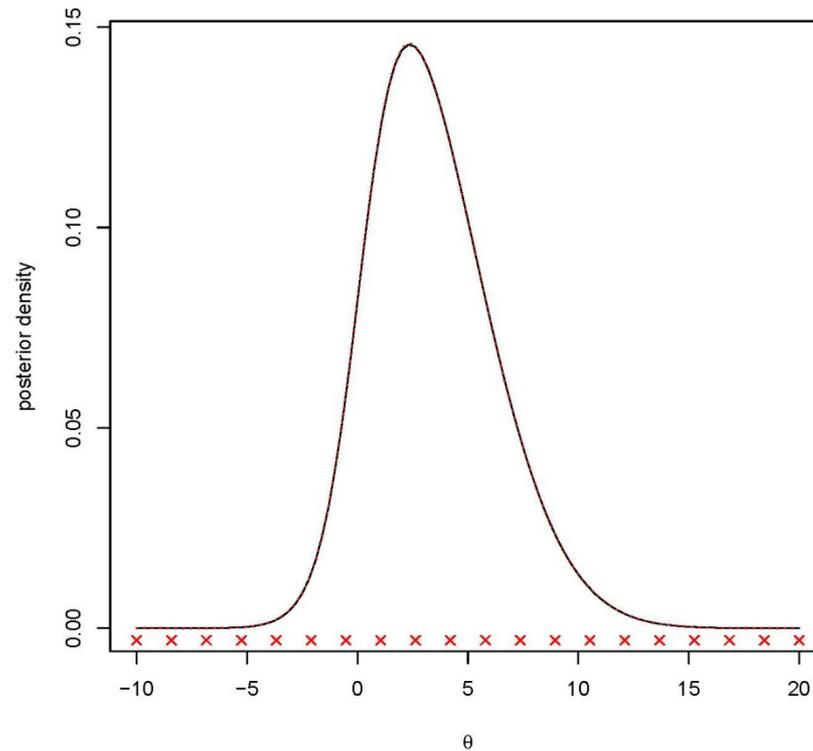
Example-continued

- Suppose we sample 10 equally spaced points from -10 to 20.
- Minimizing $WMSCV$: $\hat{\sigma}^2 = 9.30$



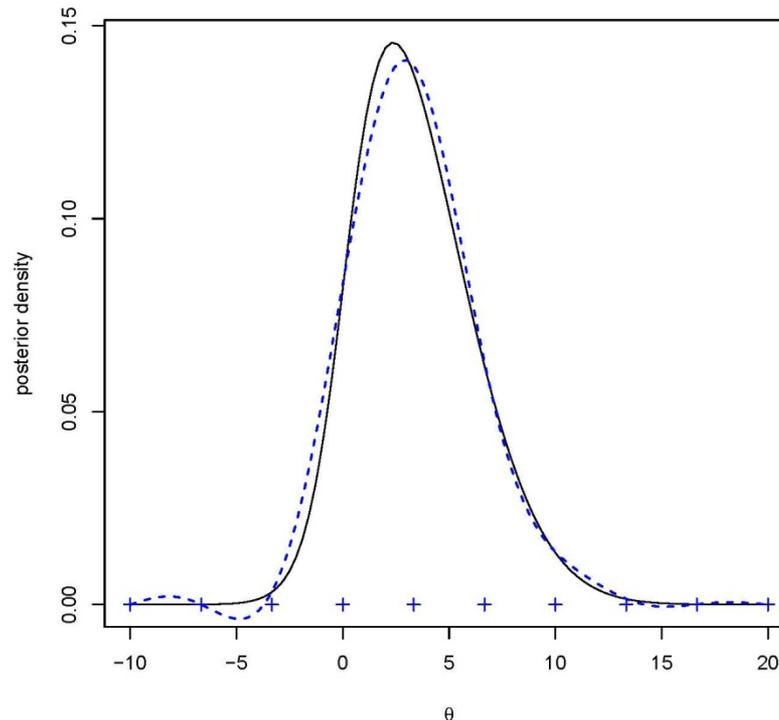
Example-continued

- $m=20$



Negativity Problem

- The coefficients \tilde{c}_i can be negative and can lead to negative posterior density values.



Mixture Normal Approximation

- Restrict c_i 's to be nonnegative:

$$\min_{\mathbf{c} \geq \mathbf{0}} (\mathbf{h} - \mathbf{G}\mathbf{c})' \mathbf{G}^{-1} (\mathbf{h} - \mathbf{G}\mathbf{c})$$

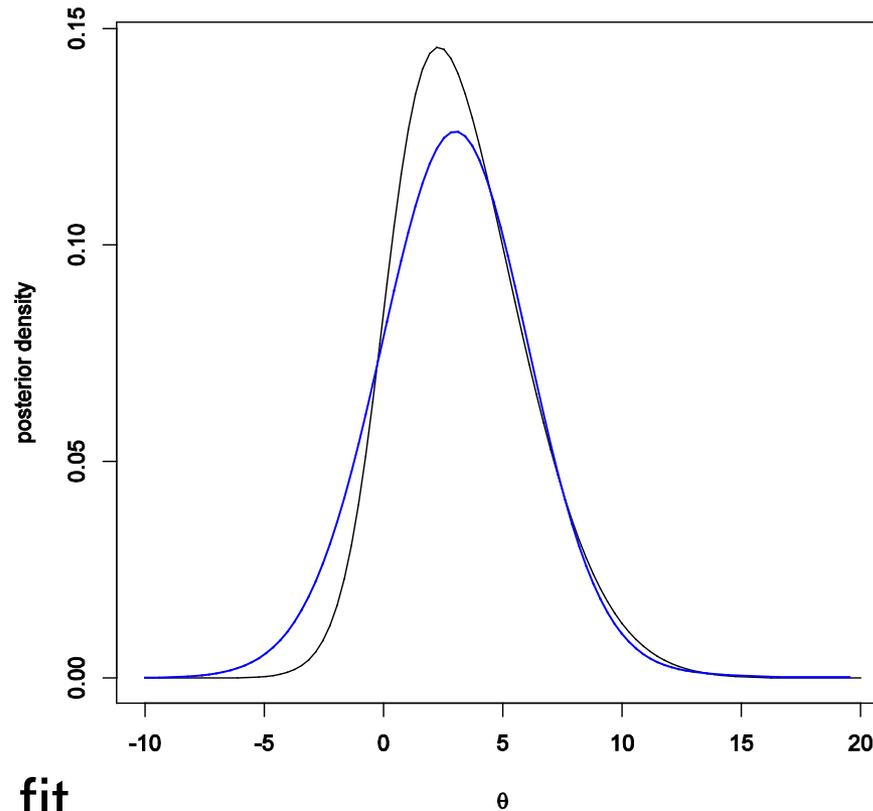
- Quadratic program.
- Then, DoIt

$$\hat{p}(\boldsymbol{\theta} | \mathbf{y}) \approx \frac{\hat{\mathbf{c}}' \phi(\boldsymbol{\theta}; \boldsymbol{\Sigma})}{\hat{\mathbf{c}}' \mathbf{1}}$$

becomes a mixture normal approximation.

Mixture Normal Approximation

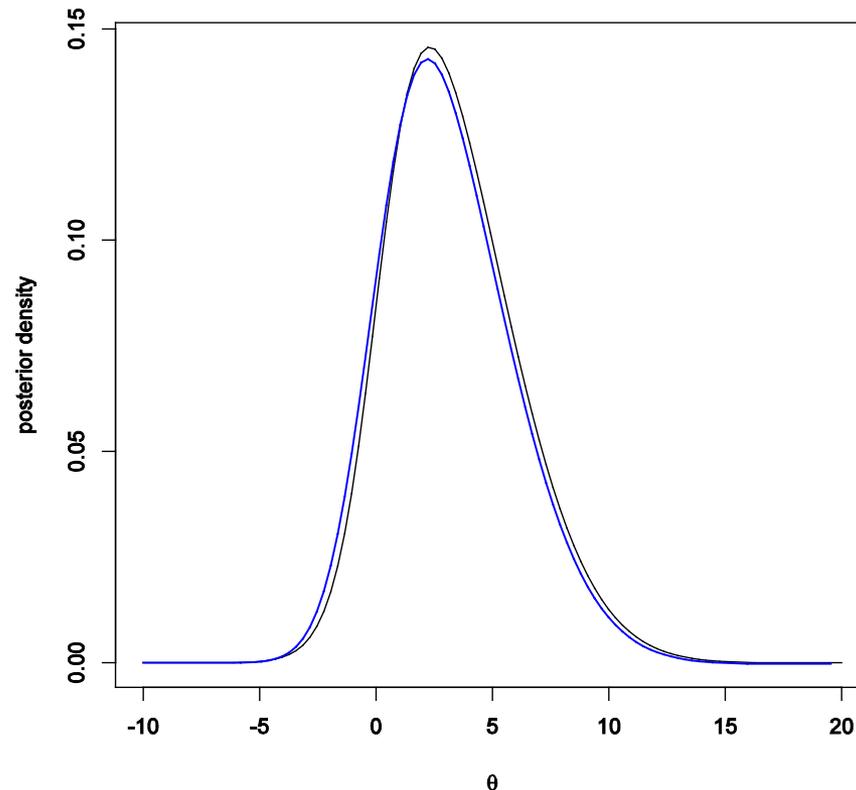
- $m=10$



- Not a good fit.

Mixture Normal Approximation

- $m=20$



- Better, but not good enough.

Improved DoIt

- DoIt :

$$h(\boldsymbol{\theta}) \approx \sum_{i=1}^m \hat{c}_i g(\boldsymbol{\theta}; \boldsymbol{\nu}_i, \boldsymbol{\Sigma}) \left\{ a + \sum_{i=1}^m b_i g(\boldsymbol{\theta}; \boldsymbol{\nu}_i, \boldsymbol{\Lambda}) \right\}$$

- Let $z_i = h(\boldsymbol{\nu}_i) / \hat{\mathbf{c}}' \mathbf{g}(\boldsymbol{\nu}_i; \boldsymbol{\Sigma})$ for $i = 1, \dots, m$.

- Then, $\hat{\mathbf{b}} = \mathbf{G}(\boldsymbol{\Lambda})^{-1}(\mathbf{z} - a\mathbf{1})$

- New approximation:

$$\hat{h}(\boldsymbol{\theta}) = \hat{\mathbf{c}}' \mathbf{g}(\boldsymbol{\theta}; \boldsymbol{\Sigma}) \{ a + \hat{\mathbf{b}}' \mathbf{g}(\boldsymbol{\theta}; \boldsymbol{\Lambda}) \}$$

Improved DoIt-continued

$$\begin{aligned}\int \hat{h}(\boldsymbol{\theta}) d\boldsymbol{\theta} &= a \hat{\mathbf{c}}' \int g(\boldsymbol{\theta}; \boldsymbol{\Sigma}) d\boldsymbol{\theta} + \hat{\mathbf{c}}' \int g(\boldsymbol{\theta}; \boldsymbol{\Sigma}) g(\boldsymbol{\theta}; \boldsymbol{\Lambda})' d\boldsymbol{\theta} \hat{\mathbf{b}} \\ &= a \hat{\mathbf{c}}' (2\pi)^{d/2} |\boldsymbol{\Sigma}|^{1/2} \mathbf{1} + \hat{\mathbf{c}}' (2\pi)^{d/2} \frac{|\boldsymbol{\Sigma} \boldsymbol{\Lambda}|^{1/2}}{|\boldsymbol{\Sigma} + \boldsymbol{\Lambda}|^{1/2}} \mathbf{G}(\boldsymbol{\Sigma} + \boldsymbol{\Lambda}) \hat{\mathbf{b}}\end{aligned}$$

$$a = \int \hat{z}(\boldsymbol{\theta}) \frac{\hat{\mathbf{c}}' \phi(\boldsymbol{\theta}; \boldsymbol{\Sigma})}{\hat{\mathbf{c}}' \mathbf{1}} d\boldsymbol{\theta} = \frac{\int \hat{h}(\boldsymbol{\theta}) d\boldsymbol{\theta}}{(2\pi)^{d/2} |\boldsymbol{\Sigma}|^{1/2} \hat{\mathbf{c}}' \mathbf{1}}$$

$$a = \frac{\hat{\mathbf{c}}' \mathbf{G}(\boldsymbol{\Sigma} + \boldsymbol{\Lambda}) \mathbf{G}(\boldsymbol{\Lambda})^{-1} \mathbf{z}}{\hat{\mathbf{c}}' \mathbf{G}(\boldsymbol{\Sigma} + \boldsymbol{\Lambda}) \mathbf{G}(\boldsymbol{\Lambda})^{-1} \mathbf{1}}$$

Improved DoIt-continued

$$\int \hat{h}(\boldsymbol{\theta}) d\boldsymbol{\theta} = a(2\pi)^{d/2} |\boldsymbol{\Sigma}|^{1/2} \hat{\mathbf{c}}' \mathbf{1}$$

$$\hat{p}(\boldsymbol{\theta} | \mathbf{y}) \approx \frac{\hat{\mathbf{c}}' \phi(\boldsymbol{\theta}; \boldsymbol{\Sigma})}{\hat{\mathbf{c}}' \mathbf{1}} \{1 + \hat{\mathbf{b}}' \mathbf{g}(\boldsymbol{\theta}; \boldsymbol{\Lambda}) / a\}$$

- $\boldsymbol{\Lambda}$ can be obtained using cross validation.

Improved DoIt-continued

Let $V = \Sigma(\Sigma + \Lambda)^{-1}\Lambda$ and $\mu_{ij} = V(\Sigma^{-1}\nu_i + \Lambda^{-1}\nu_j)$

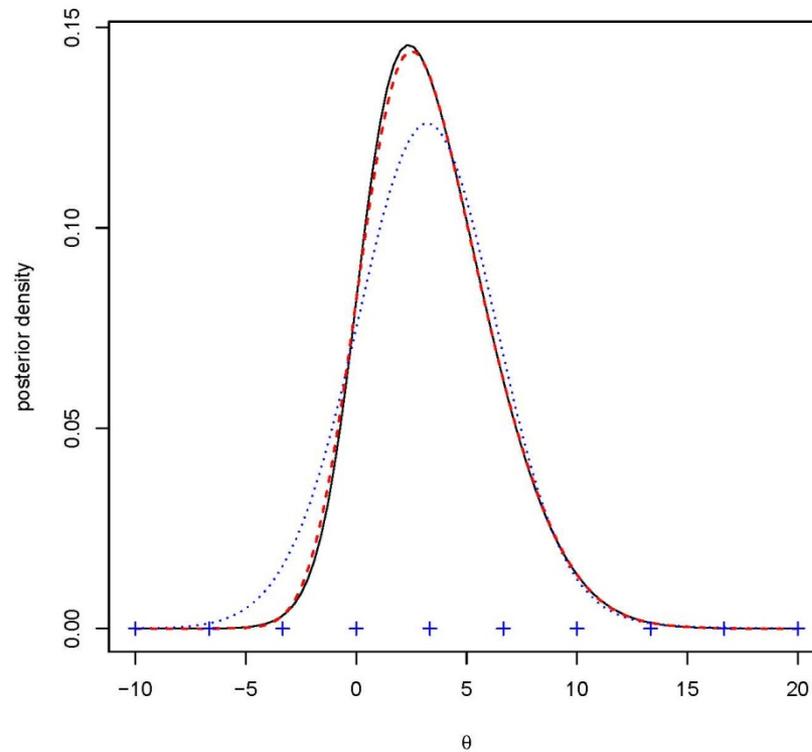
$$\hat{p}(\theta|\mathbf{y}) \approx \frac{\sum_{i=1}^m \hat{c}_i \phi(\theta; \nu_i, \Sigma) + \sum_{i=1}^m \sum_{j=1}^m d_{ij} \phi(\theta; \mu_{ij}, V)}{\sum_{i=1}^m \hat{c}_i}$$

- where

$$d_{ij} = \frac{\hat{c}_i \hat{b}_j |\Lambda|^{1/2}}{a |\Sigma + \Lambda|^{1/2}} g(\nu_i; \nu_j, \Sigma + \Lambda).$$

Binary Data Example

- $m=10$



Another Example

- Marin and Robert (2007)

$$y|\theta \sim \text{Cauchy}(\theta, 1),$$

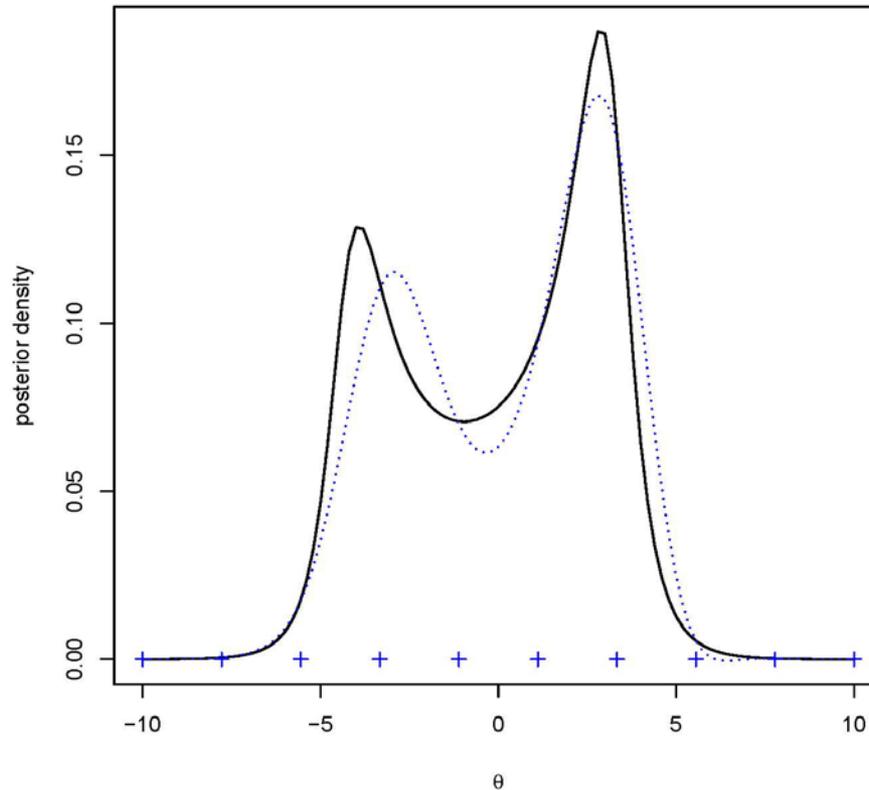
$$\theta \propto N(0, (\sqrt{10})^2).$$

- Unnormalized posterior:

$$h(\theta) = \frac{\exp(-\theta^2/20)}{\prod_{i=1}^2 (1 + (y_i - \theta)^2)}.$$

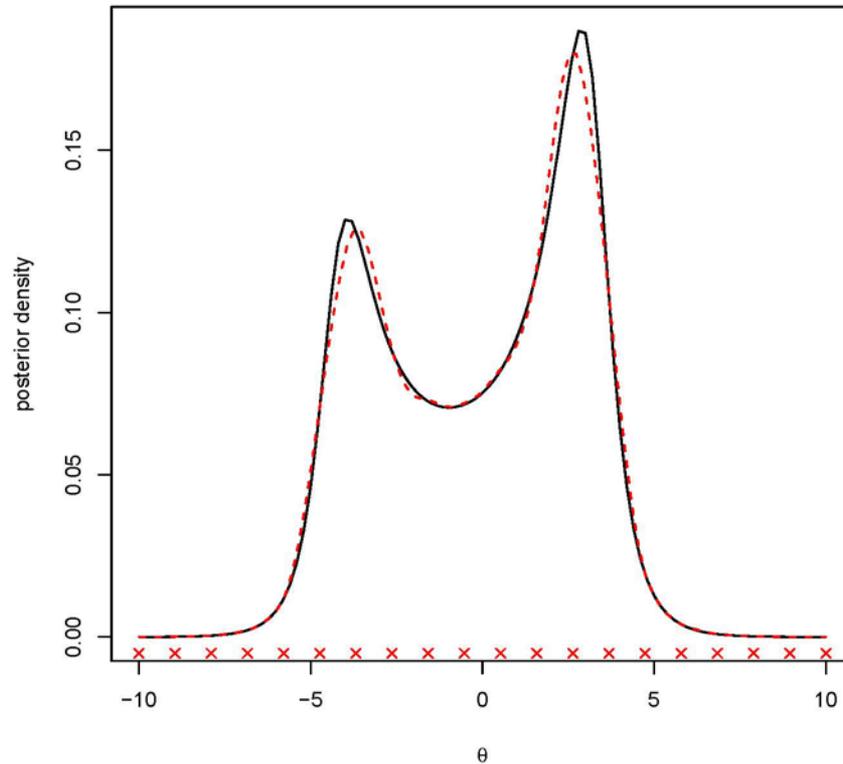
Example-continued

Suppose we sample 10 equally spaced points from -10 to 10 .



Example-continued

- $m=20$



Marginal Posterior Distributions

- Using properties of multivariate normal distribution:

$$\hat{p}(\theta_k | \mathbf{y}) \approx \frac{\sum_{i=1}^m \hat{c}_i \phi(\theta_k; \nu_{ik}, \Sigma_{kk}) + \sum_{i=1}^m \sum_{j=1}^m d_{ij} \phi(\theta_k; \mu_{ijk}, \mathbf{V}_{kk})}{\sum_{i=1}^m \hat{c}_i}$$

Posterior Summaries

$$E(\boldsymbol{\theta}|\mathbf{y}) = \bar{\boldsymbol{\theta}} \approx \frac{\sum_{i=1}^m \hat{c}_i \boldsymbol{\nu}_i + \sum_{i=1}^m \sum_{j=1}^m d_{ij} \boldsymbol{\mu}_{ij}}{\sum_{i=1}^m \hat{c}_i}$$

$$\text{var}(\boldsymbol{\theta}|\mathbf{y}) \approx \frac{\sum_{i=1}^m \hat{c}_i (\boldsymbol{\nu}_i \boldsymbol{\nu}_i' + \boldsymbol{\Sigma}) + \sum_{i=1}^m \sum_{j=1}^m d_{ij} (\boldsymbol{\mu}_{ij} \boldsymbol{\mu}_{ij}' + \mathbf{V})}{\sum_{i=1}^m \hat{c}_i} - \bar{\boldsymbol{\theta}} \bar{\boldsymbol{\theta}}'$$

Posterior Expectation

- More generally,

$$\begin{aligned}\xi &= E\{f(\boldsymbol{\theta})|\mathbf{y}\} \\ &\approx \int f(\boldsymbol{\theta}) \frac{\hat{\mathbf{c}}' \phi(\boldsymbol{\theta}; \boldsymbol{\Sigma})}{a \hat{\mathbf{c}}' \mathbf{1}} \{a + \hat{\mathbf{b}}' \mathbf{g}(\boldsymbol{\theta}; \boldsymbol{\Lambda})\} d\boldsymbol{\theta}\end{aligned}$$

for some function $f(\boldsymbol{\theta})$.

- Use approximations.

Posterior Expectation-continued

- First, let $z(\boldsymbol{\theta}) = a + \hat{\mathbf{b}}' \mathbf{g}(\boldsymbol{\theta}; \boldsymbol{\Lambda})$ and $f^*(\boldsymbol{\theta}) = f(\boldsymbol{\theta})z(\boldsymbol{\theta})$.

$$\xi \approx \frac{1}{a\hat{\mathbf{c}}'\mathbf{1}} \sum_{i=1}^m \hat{c}_i \int f^*(\boldsymbol{\theta}) \phi(\boldsymbol{\theta}; \boldsymbol{\nu}_i, \boldsymbol{\Sigma}) d\boldsymbol{\theta}$$

- Let $\mathbf{f}^* = (f^*(\boldsymbol{\nu}_1), \dots, f^*(\boldsymbol{\nu}_m))' = \mathbf{f} \odot \mathbf{z}$

- Approximate $f^*(\boldsymbol{\theta})$ using a kriging predictor:

$$f^*(\boldsymbol{\theta}) = \alpha z(\boldsymbol{\theta}) + \mathbf{g}(\boldsymbol{\theta}; \boldsymbol{\Omega})' \mathbf{G}(\boldsymbol{\Omega})^{-1} (\mathbf{f}^* - \alpha \mathbf{z})$$

Posterior Expectation-continued

$$\xi \approx \alpha + \frac{|\Omega|^{1/2}}{a\hat{c}'\mathbf{1}|\Omega + \Sigma|^{1/2}}\hat{c}'G(\Omega + \Sigma)G(\Omega)^{-1}(f^* - \alpha z)$$

- Choose $\alpha = \xi$ (Joseph 2006),

$$\xi \approx \frac{\hat{c}'G(\Omega + \Sigma)G(\Omega)^{-1}f^*}{\hat{c}'G(\Omega + \Sigma)G(\Omega)^{-1}z}$$

- Take $\Omega = \Lambda$,

$$\xi \approx \frac{\hat{c}'G(\Sigma + \Lambda)G(\Lambda)^{-1}f^*}{\hat{c}'G(\Sigma + \Lambda)G(\Lambda)^{-1}z}$$

Example

- Posterior predictive density in the binary data example:

$$y|\mathbf{y} \sim \text{Bernoulli}(\xi),$$

where

$$\xi = E(\{1 + \exp(-\theta)\}^{-1}|\mathbf{y}).$$

- Numerical integration: $\xi = .8496$
- Kriging approximation: $\xi \approx .8478$
- First order approximation: $\xi \approx \{1 + \exp(-\hat{\theta})\}^{-1} = .914$

Experimental Design

- Initial space-filling design
- Sequential design

Space-Filling Design

- By Laplace's approximation

$$\boldsymbol{\theta} | \mathbf{y} \sim^a N(\hat{\boldsymbol{\theta}}, \boldsymbol{\Sigma})$$

- Transform:

$$\boldsymbol{\alpha} = \boldsymbol{\Sigma}^{-1/2}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})$$

- Then,

$$\boldsymbol{\alpha} | \mathbf{y} \sim^a N(\mathbf{0}, \mathbf{I})$$

First choose a design $\mathbf{D}^* = (\boldsymbol{\nu}_1^*, \dots, \boldsymbol{\nu}_m^*)'$ from $(0, 1)^d$

$$\mathbf{D} = (\hat{\boldsymbol{\theta}} + \boldsymbol{\Sigma}^{1/2} \Phi^{-1}(\boldsymbol{\nu}_1^*), \dots, \hat{\boldsymbol{\theta}} + \boldsymbol{\Sigma}^{1/2} \Phi^{-1}(\boldsymbol{\nu}_m^*))'$$

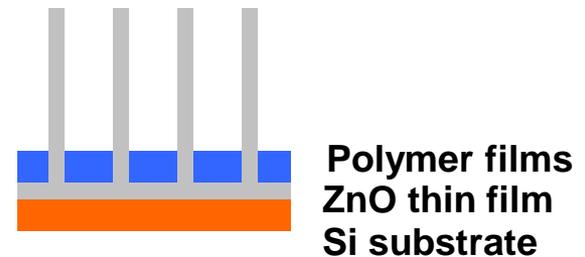
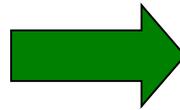
Space-Filling Design-continued

- Latin Hypercube Design (LHD)
- Maximin LHD (Morris and Mitchell 1995)
- Let $\boldsymbol{\nu}_1^* = .5 = (.5, \dots, .5)'$
- Find the remaining $m-1$ points by minimizing

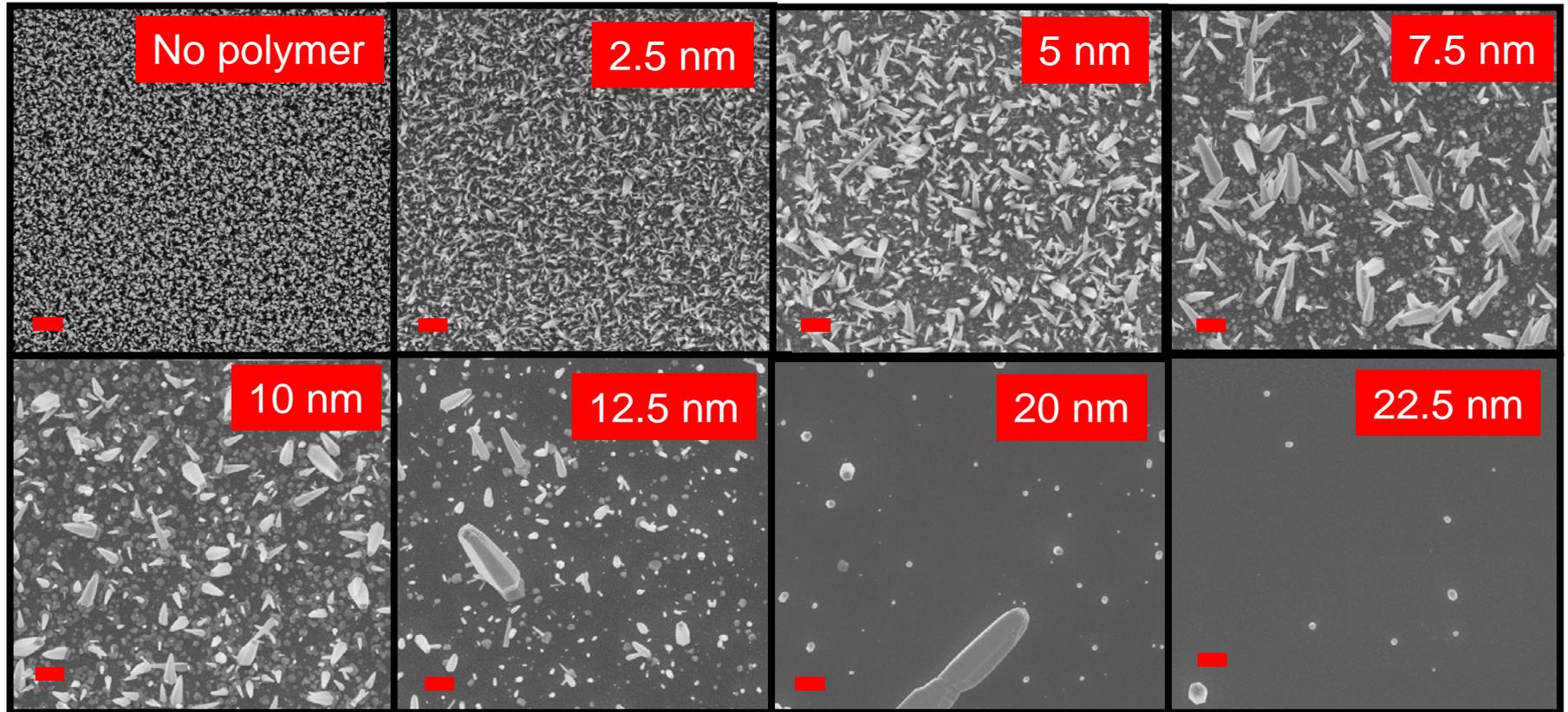
$$\left\{ \sum_{i=2}^m \sum_{j=2}^m 1/d^k(\boldsymbol{\nu}_i^*, \boldsymbol{\nu}_j^*) \right\}^{1/k}$$

Example: Density Control of Nanowires

- Dasgupta, Weintraub, and Joseph (2011)



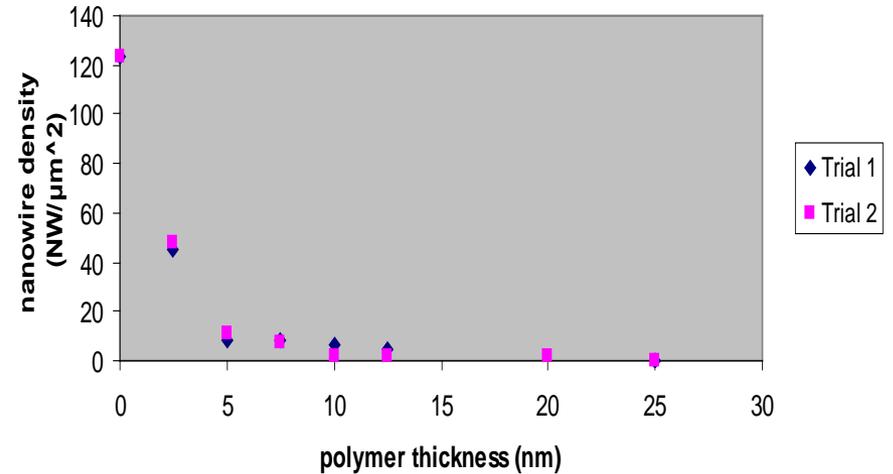
Results (1st set of experiments)



(All images at 5000x magnification; \blacksquare = 1 μm)

Experimental Data

# Bi Layers	Thickn ess (nm)	Density (NW/ μm^2)	
		Trial 1	Trial 2
0	0.0	123	123
1	2.5	46	48
2	5.0	8	11
3	7.5	8	7
4	10.0	7	2
5	12.5	5	1
8	20.0	2	-
10	25.0	0	0



Example-continued

- Density of nanowires (y)
- Thickness of polymer films (x)

$$y_{ij} | \boldsymbol{\theta}, \mathbf{u} \sim \text{Poisson}(\mu(x_i))$$

$$\mu(x_i) = [\theta_1 \exp(-\theta_2 x_i^2) + \theta_3 \{1 - \exp(-\theta_2 x_i^2)\} \Phi(-x_i/\theta_4)] u_i$$

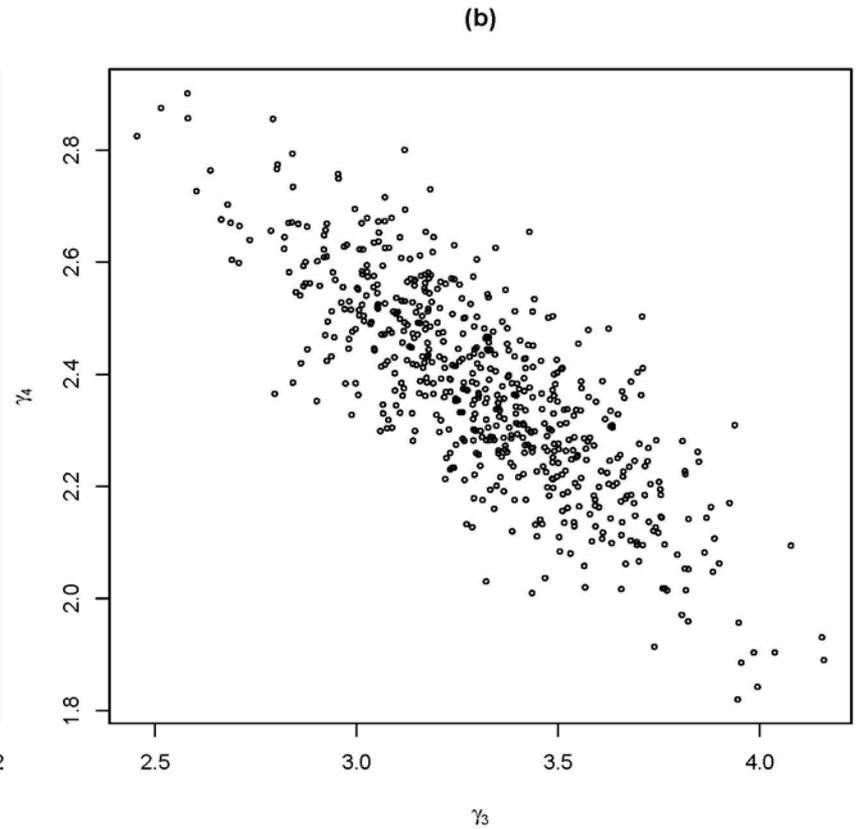
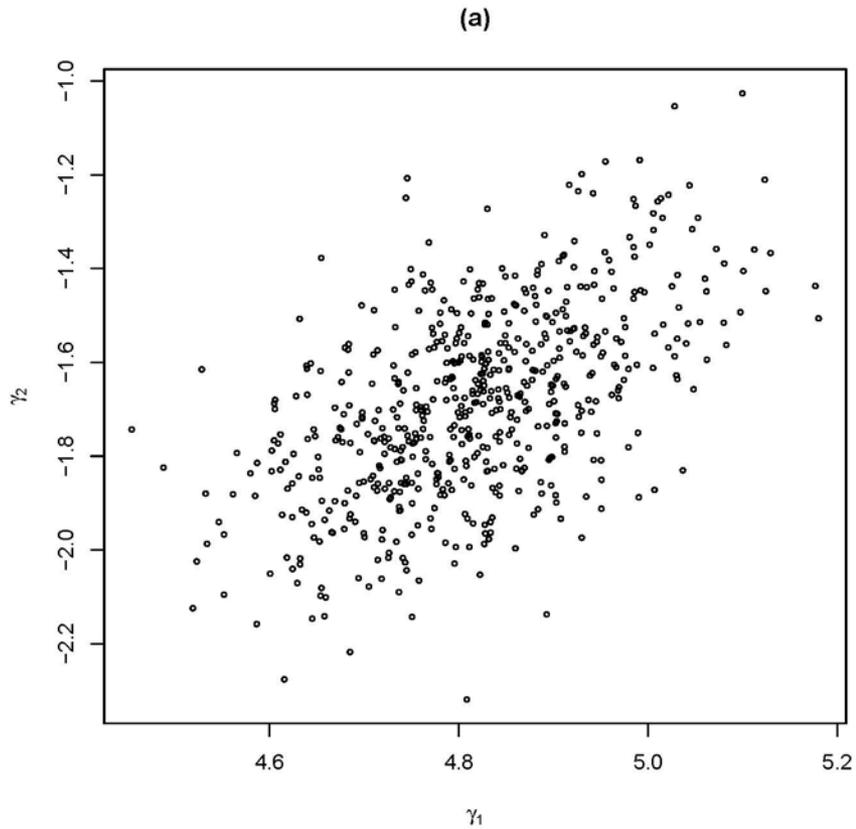
for $i = 1, \dots, 8$ and $j = 1, 2$.

- Let $\gamma_i = \log(\theta_i)$ for $i = 1, \dots, 4$.
and $\alpha_i = \log(u_i)$ for $i = 1, \dots, 8$
- Prior: $p(\boldsymbol{\gamma}) \propto 1$, and $\alpha_i \sim^{iid} N(0, .1^2)$

Example-continued

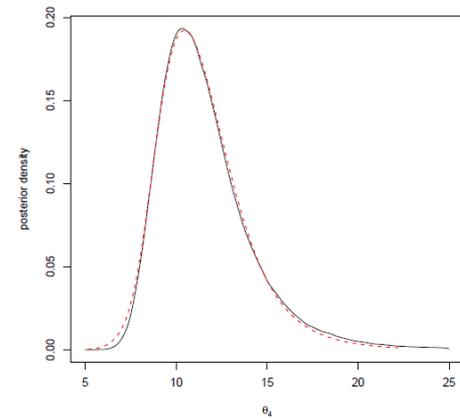
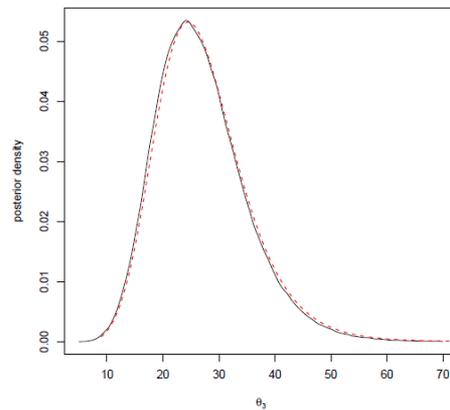
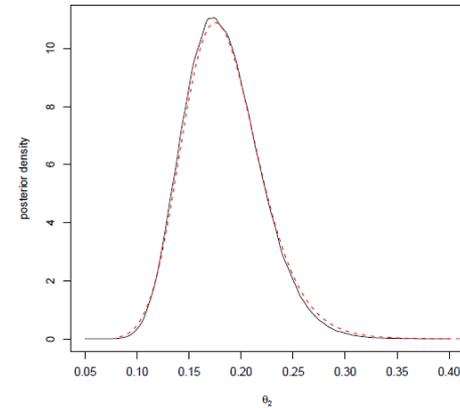
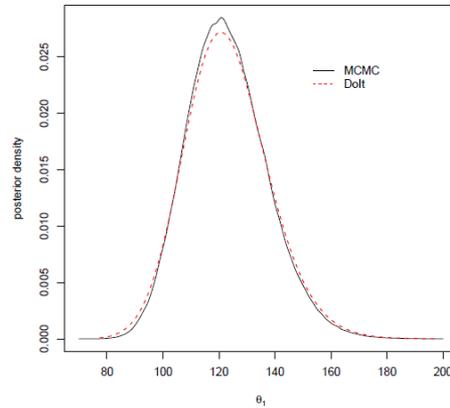
- Posterior mode: $\hat{\gamma} = (4.82, -1.69, 3.32, 2.37)'$
 $\hat{\alpha} = (-0.003, 0.005, -0.008, 0.014, -0.007, -0.007, 0.011, -0.005)'$
- Σ obtained through numerical differentiation.
- $m = 50 \times 12 = 600$
- MmLHD
- $D = (\hat{\theta} + \Sigma^{1/2}\Phi^{-1}(\nu_1^*), \dots, \hat{\theta} + \Sigma^{1/2}\Phi^{-1}(\nu_m^*))'$

Example-continued



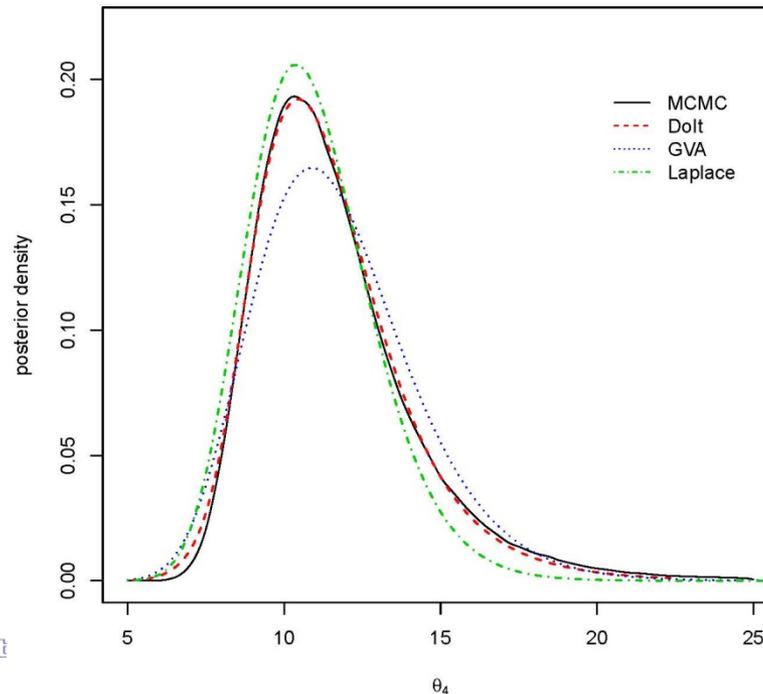
Example-continued

- Metropolis algorithm with 3,000,000 samples (black line).



Comparison

- Quadrature method: didn't converge!
- Gaussian Variational Approximation (GVA) (Ormerod and Wand 2012)



Sequential Design

- Add points one-by-one to improve approximation.
- Optimal design theory: add the new point at a location with the largest prediction uncertainty.
- DoIt can be viewed as a simple kriging predictor given $\hat{c}'g(\theta; \Sigma)$.
- Conditional prediction variance is

$$(\hat{c}'g(\theta; \Sigma))^2 \{1 - g(\theta; \Lambda)'G^{-1}(\Lambda)g(\theta; \Lambda)\}$$

$$\nu_{m+1} = \underset{\theta}{\operatorname{arg\,max}} (\hat{c}'g(\theta; \Sigma))^2 \{1 - g(\theta; \Lambda)'G^{-1}(\Lambda)g(\theta; \Lambda)\}$$

Sequential Design-continued

- Let $v_{(i)}$ be the leave-one-out estimate of the prediction variance

$$v_{(i)} \approx \left(h_i + l_i - \frac{G_i^{-1}(\Sigma)}{G_{ii}^{-1}(\Sigma)} (\mathbf{h} + \mathbf{l}) \right)^2 \frac{1}{G_{ii}^{-1}(\Lambda)}$$

for $i = 1, \dots, m$, where $\mathbf{l} = \mathbf{G}(\Sigma)\hat{\mathbf{c}} - \mathbf{h}$

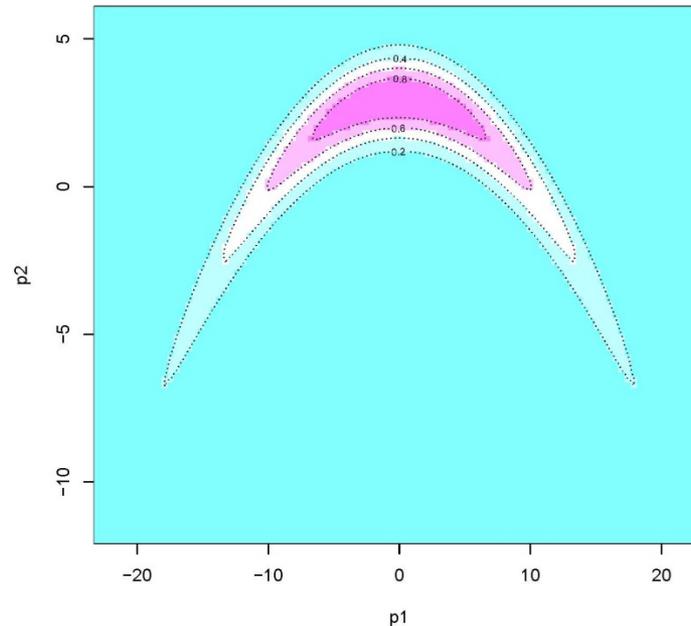
Let $i^* = \arg \max_i v_{(i)}$.

- Optimize in the neighborhood of v_{i^*}

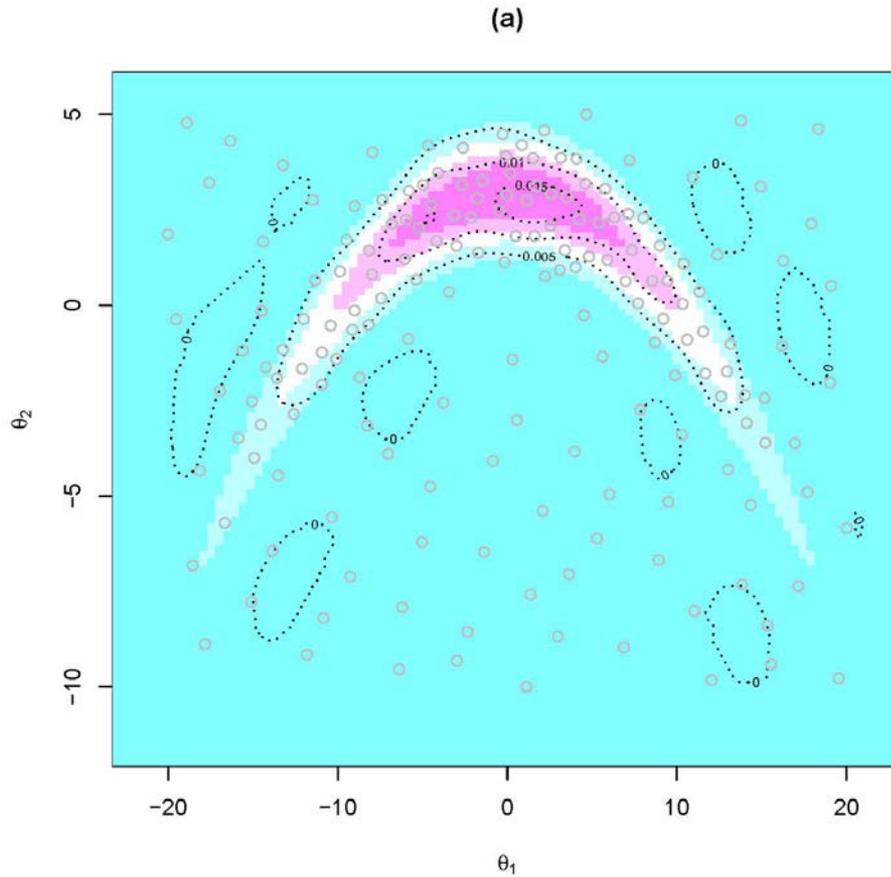
Example

- Haario, Saksman, and Tamminen (2001)

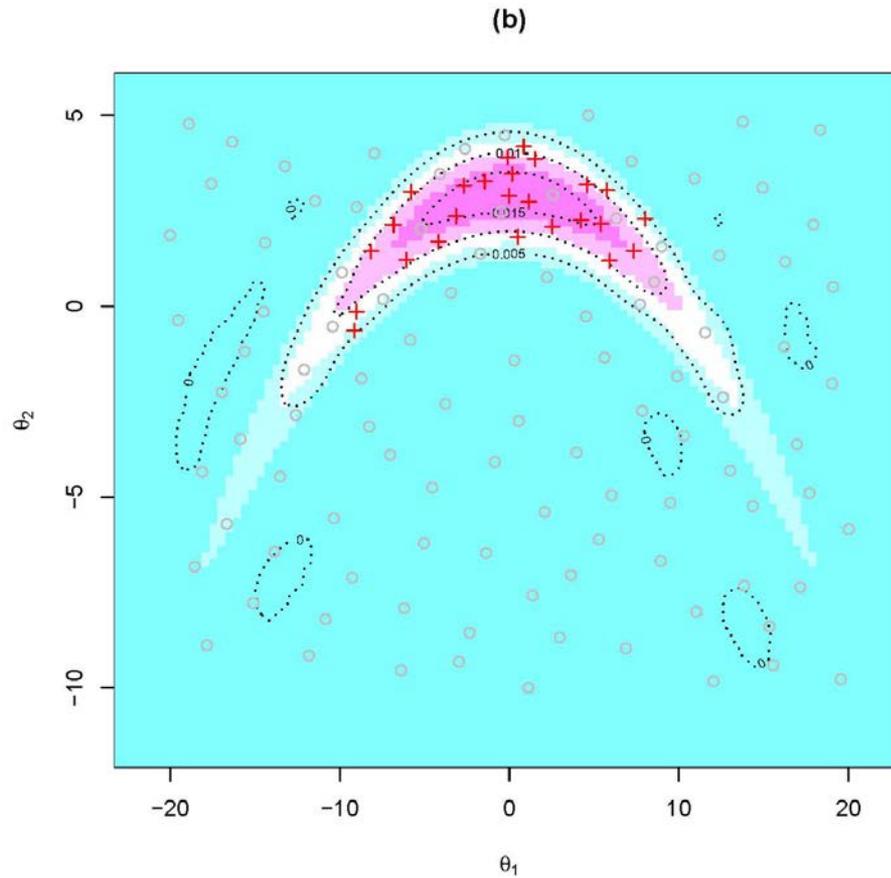
$$p(\boldsymbol{\theta}|\mathbf{y}) = \phi \left((\theta_1, \theta_2 + .03\theta_1^2 - 3)'; (0, 0)', \text{diag}\{100, 1\} \right)$$



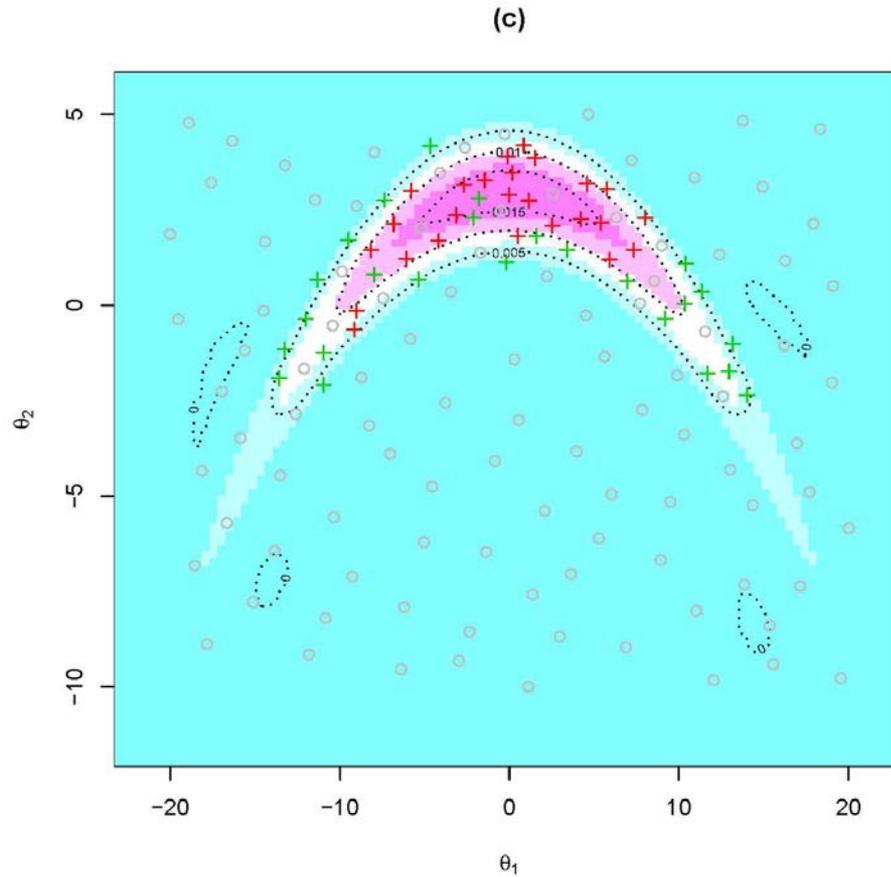
$m=100$



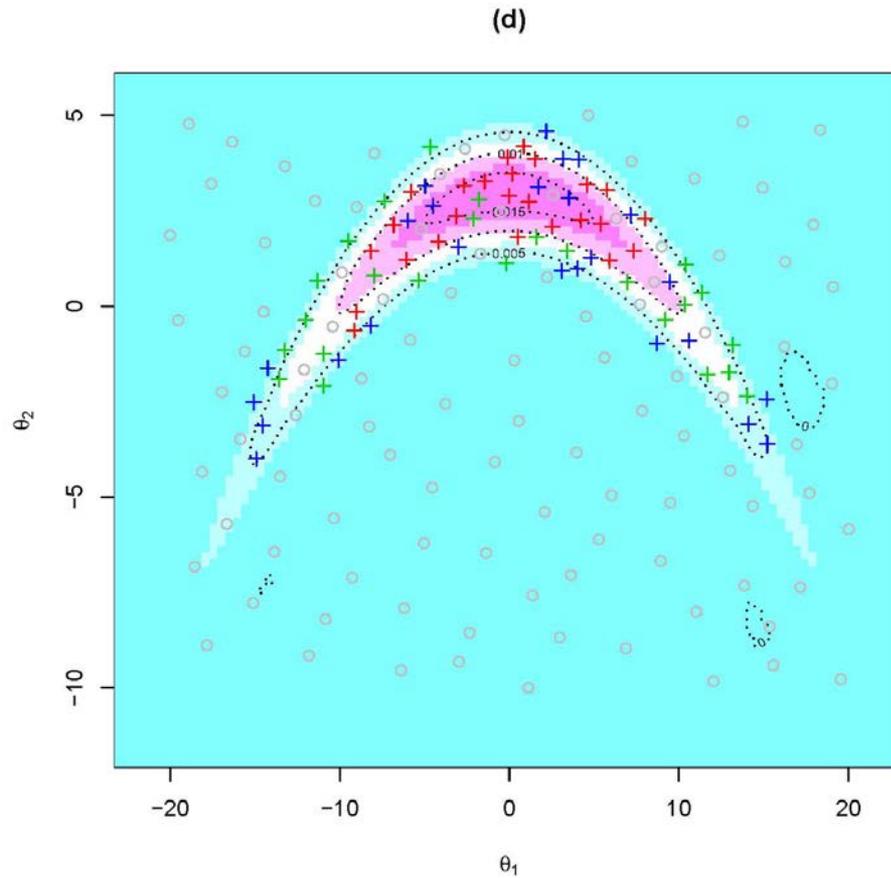
$$m=100+25$$



$$m=100+50$$



$$m=100+75$$

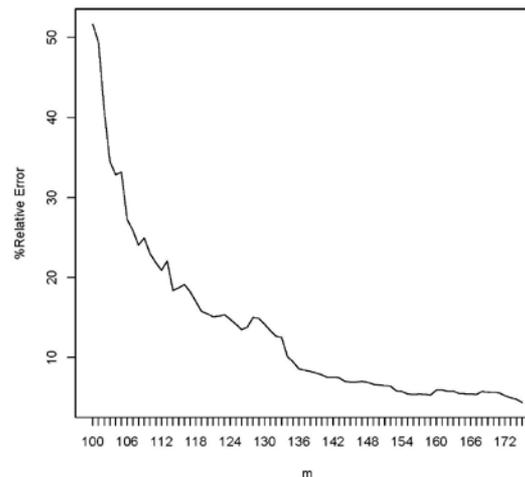


Example-continued

- % Relative Error: $\%RE = \frac{\overline{|cv|}}{\bar{h}} \times 100,$

where $\overline{|cv|} = E(|cv(\boldsymbol{\theta})| | \mathbf{y})$ and $\bar{h} = E(h(\boldsymbol{\theta}) | \mathbf{y})$

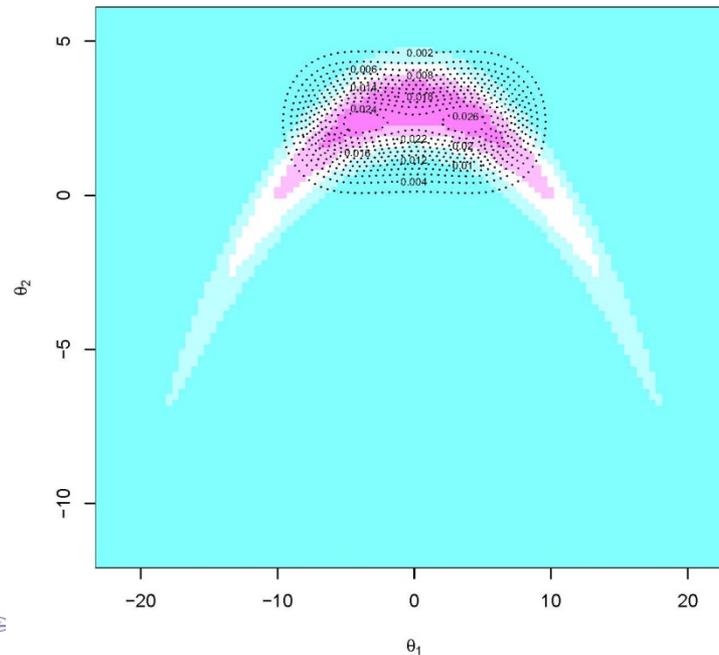
$$cv_i = h_i - \left(h_i + l_i - \frac{G_i^{-1}(\Sigma)}{G_{ii}^{-1}(\Sigma)}(h + l) \right) \left(\frac{h_i}{h_i + l_i} - \frac{G_i^{-1}(\Lambda)}{G_{ii}^{-1}(\Lambda)} \left(\frac{h}{h + l} - a1 \right) \right)$$



Comparison: Variational Bayes

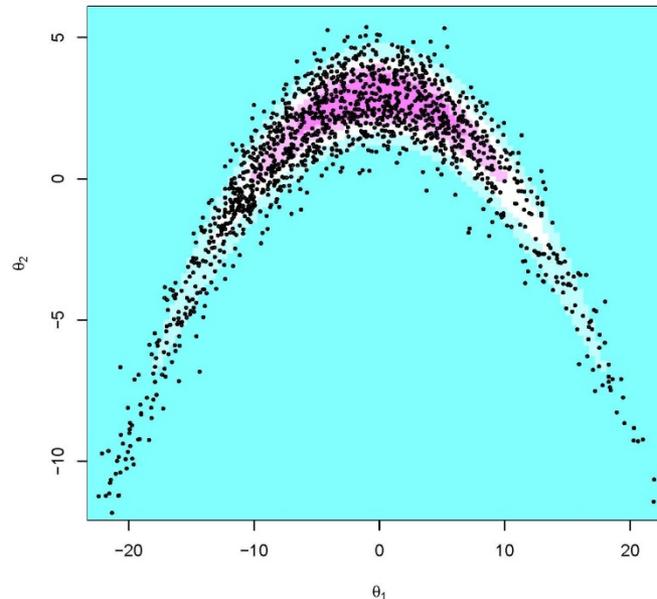
$$\hat{p}_{VB}(\boldsymbol{\theta}|\mathbf{y}) = q_1(\theta_1)\phi(\theta_2; \mu_2, \sigma_2^2),$$

where $q_1(\theta_1) \propto \exp\{-.5[\theta_1^2/100 + (\mu_2 + .03\theta_1^2 - 3)^2]\}$,
 $\mu_2 = -.03(\mu_1^2 + \sigma_1^2) + 3$, and $\sigma_2^2 = 1$.



Comparison: Hybrid MCMC

- Fielding, Nott, and Liong (2011)



- CPU time: Hybrid MCMC=90 mins, Dolt=3 mins.

Discussion from Dagupta and Meng: connections to QMC

- Experimental design
 - QMC: low discrepancy sequence in $[0,1]^d$
 - Dolt: initial space-filling design+ sequential design
- Posterior summaries
 - QMC: Monte Carlo average
 - Dolt: smooth interpolation + analytical evaluation
- Dolt is likely to perform better than QMC when the posterior densities are smooth.

Numerical Comparison

- Binary data example

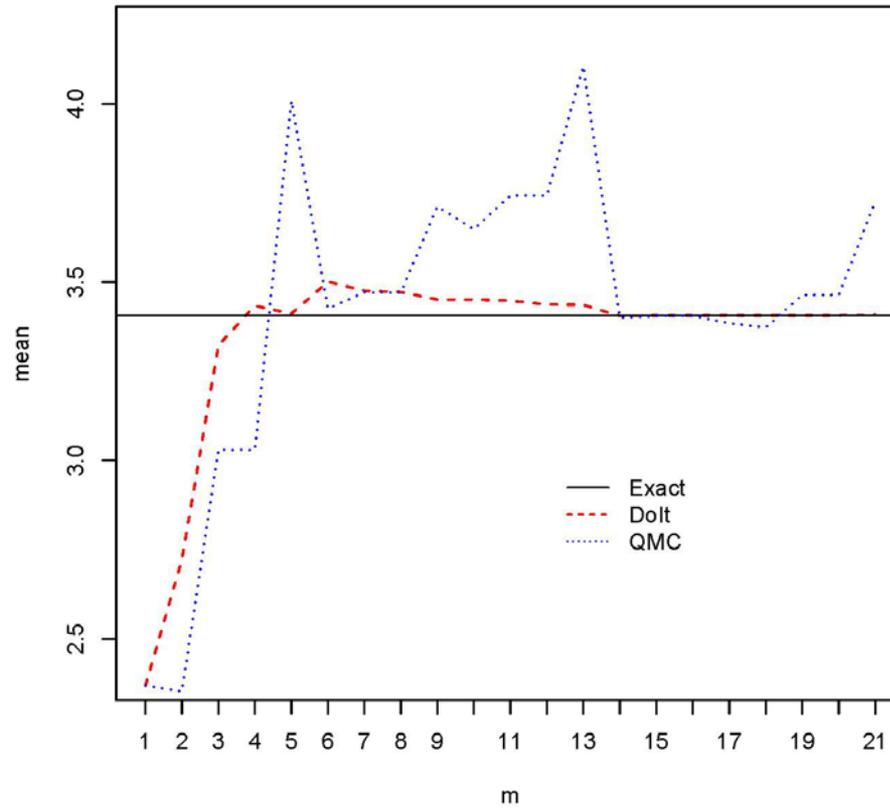
$$y|\theta \sim \text{Bernoulli}(\{1 + \exp(-\theta)\}^{-1}),$$

$$\theta \sim N(\mu, \tau^2).$$

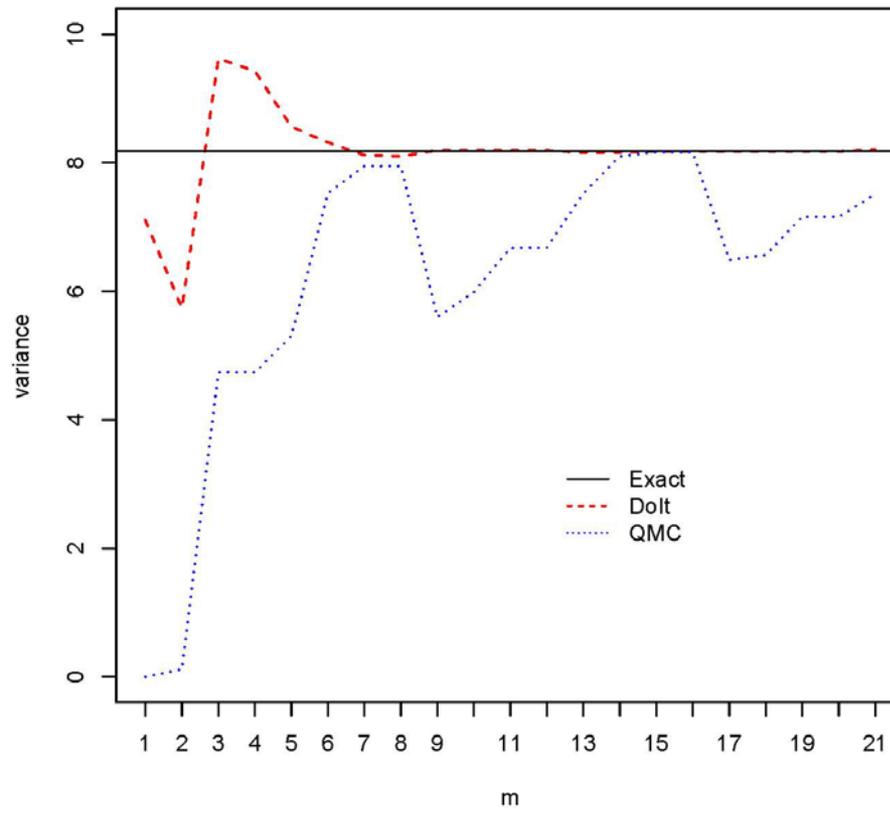
- Laplace approximation: $N(2.37, 2.67^2)$
- van der Corput sequence: $\frac{1}{2}, \frac{1}{4}, \frac{3}{4}, \dots$ and re-scaled to $[2.37-15, 2.37+15]$.

$$\hat{\theta}_{QMC} = E(\theta|y)_{QMC} = \frac{\sum_{i=1}^m h_i \nu_i}{\sum_{i=1}^m h_i} \quad \text{and} \quad \text{var}(\theta|y)_{QMC} = \frac{\sum_{i=1}^m h_i (\nu_i - \hat{\theta}_{QMC})^2}{\sum_{i=1}^m h_i}.$$

Posterior Mean



Posterior Variance



Hierarchical Models

- May contain very large number of parameters
- Not easy to find a good space-filling design in high dimensions.
 - Make use of the hierarchical structure.

$$y|\theta \sim p(y|\theta), \theta|\eta \sim p(\theta|\eta), \text{ and } \eta \sim p(\eta).$$

Hierarchical Models-continued

- Suppose we can obtain explicit expression of

$$p(\mathbf{y}|\boldsymbol{\eta}) = \int p(\mathbf{y}|\boldsymbol{\theta})p(\boldsymbol{\theta}|\boldsymbol{\eta}) d\boldsymbol{\theta},$$

- And have the conditional distribution

$$p(\boldsymbol{\theta}|\boldsymbol{\eta}, \mathbf{y}) \propto p(\mathbf{y}|\boldsymbol{\theta})p(\boldsymbol{\theta}|\boldsymbol{\eta})$$

- Use DoIt : $\hat{p}(\boldsymbol{\eta}|\mathbf{y}) \approx \frac{\hat{\mathbf{c}}' \phi(\boldsymbol{\eta}; \boldsymbol{\Sigma})}{\hat{\mathbf{c}}' \mathbf{1}} \{1 + \hat{\mathbf{b}}' \mathbf{g}(\boldsymbol{\eta}; \boldsymbol{\Lambda})/a\}$.

- Then, $\hat{p}(\boldsymbol{\theta}|\mathbf{y}) \approx \frac{\hat{\mathbf{c}}' \mathbf{G}(\boldsymbol{\Sigma} + \boldsymbol{\Lambda}) \mathbf{G}(\boldsymbol{\Lambda})^{-1} p^*(\boldsymbol{\theta})}{\hat{\mathbf{c}}' \mathbf{G}(\boldsymbol{\Sigma} + \boldsymbol{\Lambda}) \mathbf{G}(\boldsymbol{\Lambda})^{-1} \mathbf{z}}$

where $p^*(\boldsymbol{\theta}) = (p(\boldsymbol{\theta}|\boldsymbol{\nu}_1, \mathbf{y}), \dots, p(\boldsymbol{\theta}|\boldsymbol{\nu}_m, \mathbf{y}))' \odot \mathbf{z}$

Example 1: A Longitudinal Data Analysis

- Orthodontic measurements on 27 children (Phinheiro and Bates 2000)

$$y_{ij} | \beta, u_i, \sigma_\epsilon^2 \sim^{ind.} N(\beta_0 + u_i + \beta_1 age_{ij} + \beta_2 sex_i, \sigma_\epsilon^2),$$

$$u_i | \sigma_u^2 \sim^{iid} N(0, \sigma_u^2),$$

$$\beta \sim N(\mathbf{0}, 10^8 \mathbf{I}_3),$$

$$\sigma_\epsilon^2, \sigma_u^2 \propto^{ind.} IG(.01, .01),$$

for $i = 1, \dots, 27$ and $j = 1, \dots, 4$.

- **32 parameters**

Longitudinal Data-continued

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u} + \boldsymbol{\epsilon}$$

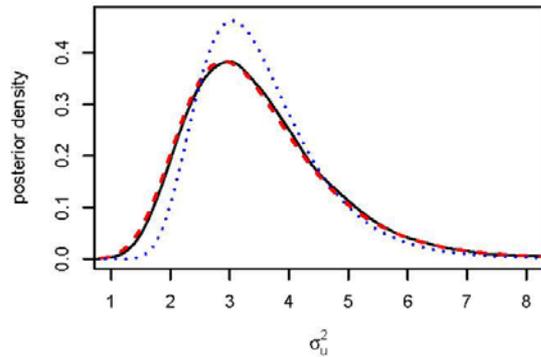
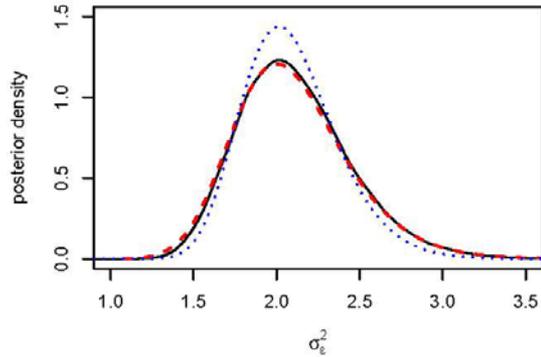
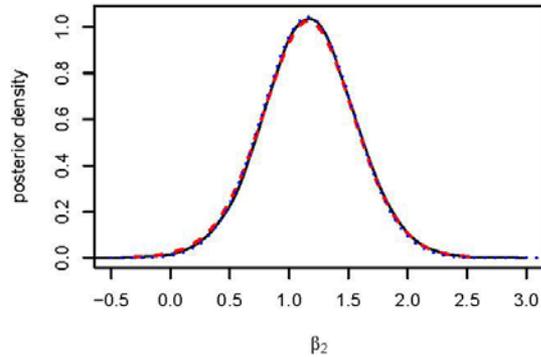
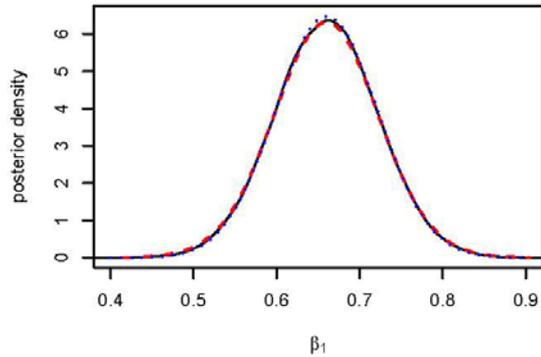
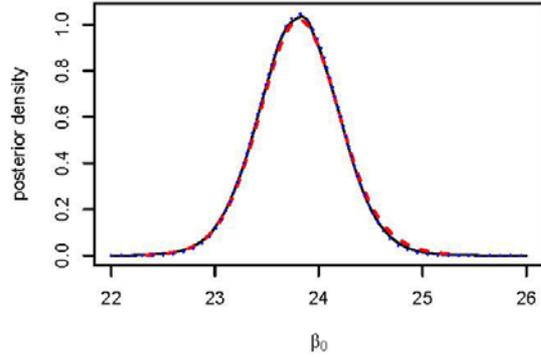
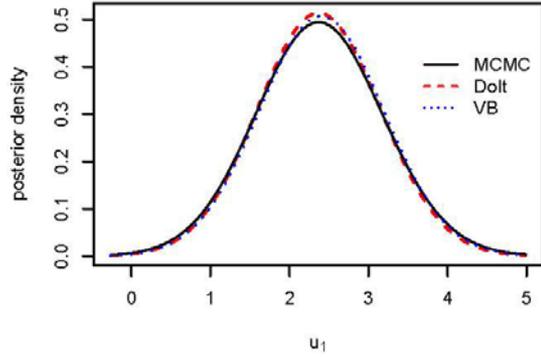
- Integrating out \mathbf{u}

$$\mathbf{y}|\boldsymbol{\beta}, \sigma_{\epsilon}^2, \sigma_u^2 \sim N(\mathbf{X}\boldsymbol{\beta}, \sigma_{\epsilon}^2 \mathbf{I}_{108} + \sigma_u^2 \mathbf{Z}\mathbf{Z}')$$

- Also,

$$\mathbf{u}|\boldsymbol{\beta}, \sigma_{\epsilon}^2, \sigma_u^2, \mathbf{y} \sim N\left(\left(\mathbf{Z}'\mathbf{Z} + \frac{\sigma_{\epsilon}^2}{\sigma_u^2} \mathbf{I}_{27}\right)^{-1} \mathbf{Z}'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}), \left(\mathbf{Z}'\mathbf{Z} + \frac{\sigma_{\epsilon}^2}{\sigma_u^2} \mathbf{I}_{27}\right)^{-1}\right)$$

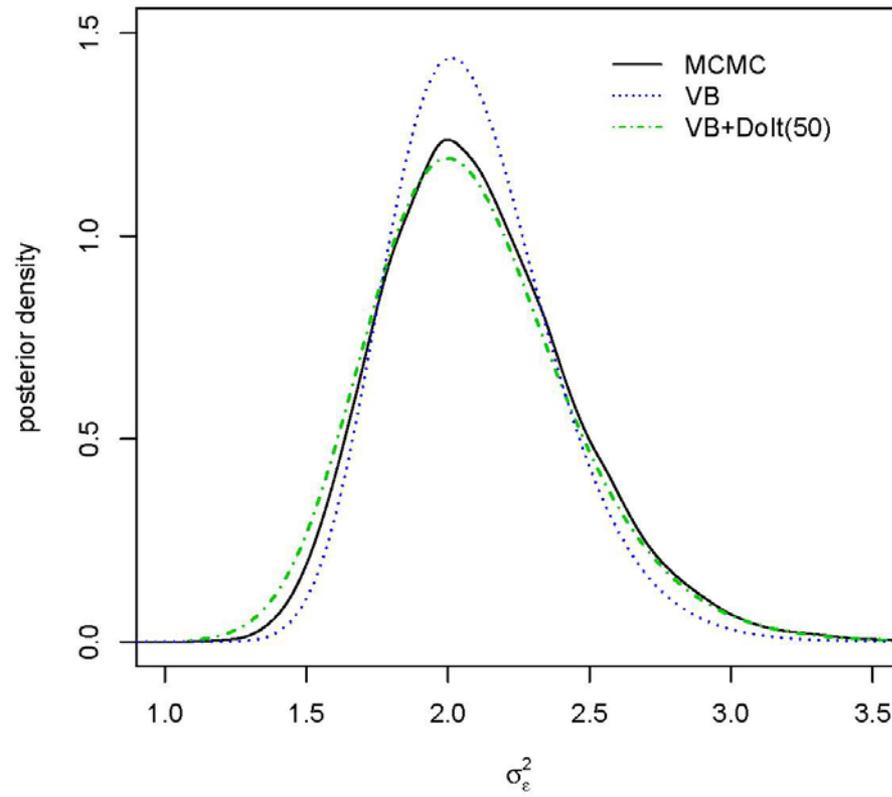
- DoIt : 250-run MmLHD in **5 dimensions**



Discussion from Ormerod & Wand

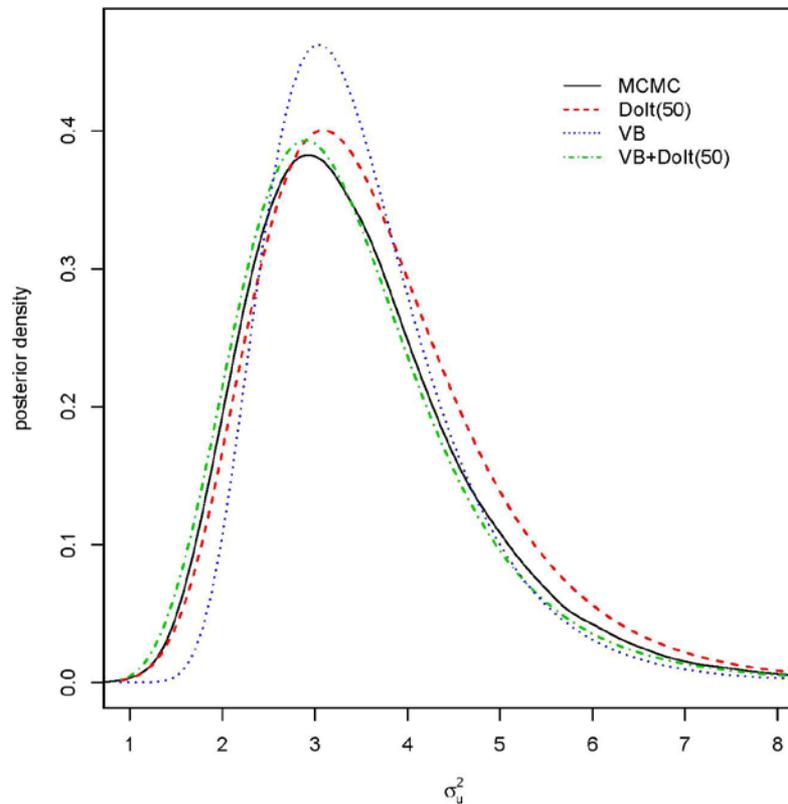
- VB approximation can be improved using the grid-based variational approximation method in Ormerod (2011).
- Dolt can be used for the same purpose!
 - Center the experimental design using VB estimates.

VB+DoIt



VB+DoIt

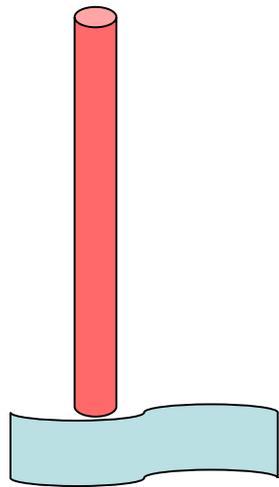
- VB can be used to improve DoIt, whenever VB implementation is readily available.



Example 2: LAMM

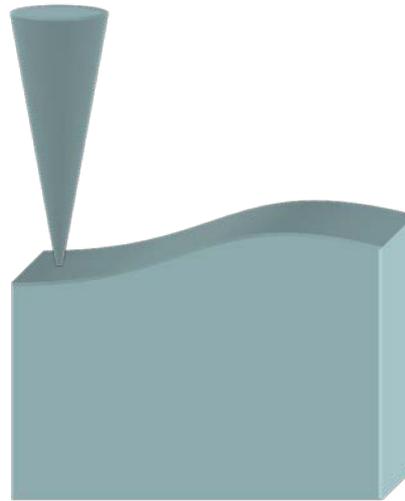
Laser assisted mechanical micromachining (LAMM) integrates *thermal softening* with *mechanical micro cutting*

(Singh, Joseph, and Melkote 2011)



Laser heating

+



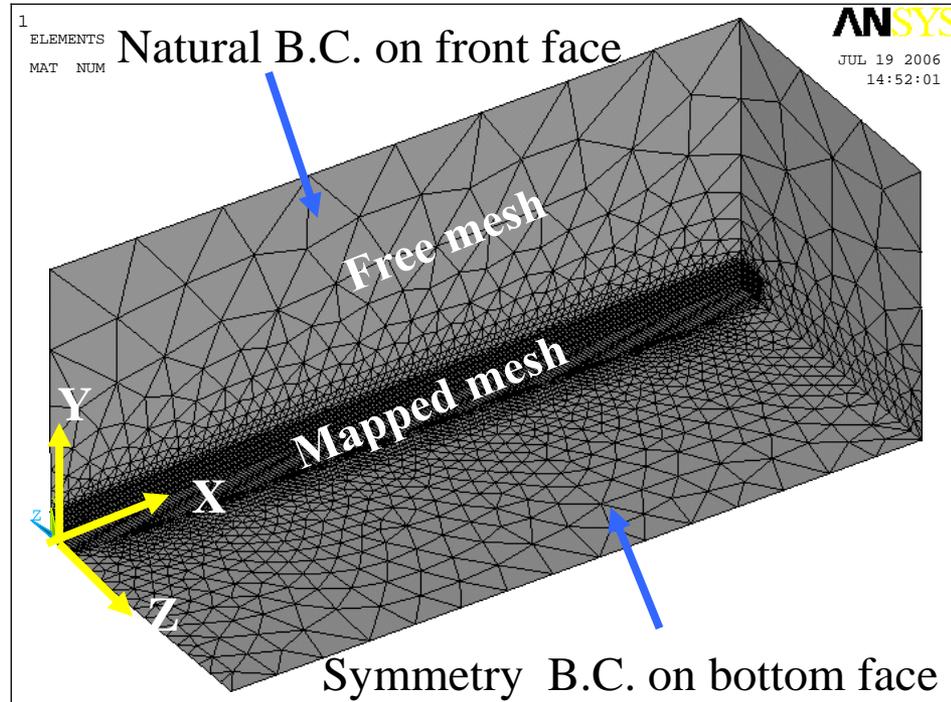
Mechanical micromachining

= LAMM

Objective

Find optimum processing conditions that minimize cutting/thrust forces and thermal damage.

Thermal Model



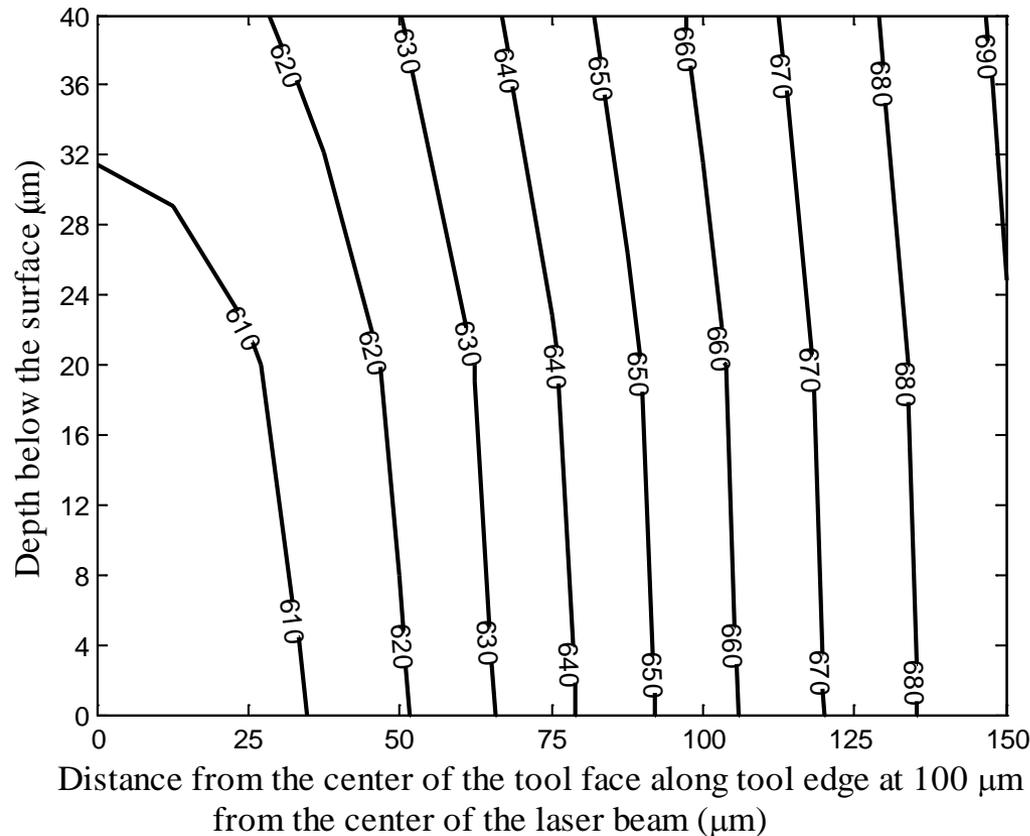
- Mapped dense mesh ($25 \mu\text{m} \times 12.5 \mu\text{m} \times 20 \mu\text{m}$)
- An 8 noded 3-D thermal element (Solid70) is used
- Gaussian distribution of heat flux applied to a 5x5 element matrix which sweeps the mesh on the front face

Shear Flow Strength

$$\sigma(\varepsilon, \dot{\varepsilon}, T, HRC) = \left(A + B\varepsilon^n + C \ln(\varepsilon + \varepsilon_0) + D \right) \left(1 + E \ln \left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} \right) \right) \left(1 - (T^*)^m \right)$$

Yan et al., 2007

$$S = \sigma / \sqrt{3}$$



10W laser power, 10 mm/min speed 100 μm laser-tool distance
and 110 μm spot size

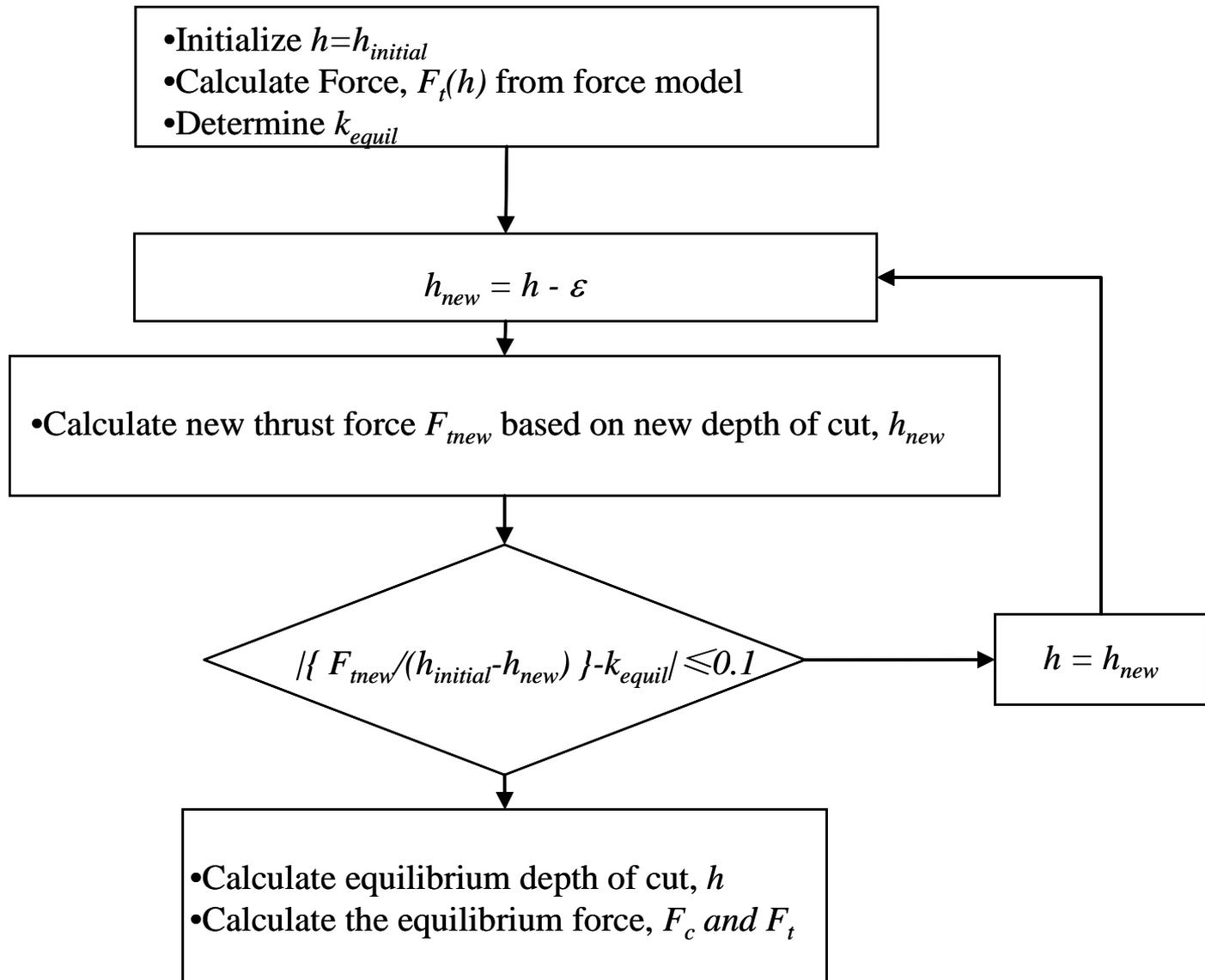
Forces

- Cutting and thrust forces,

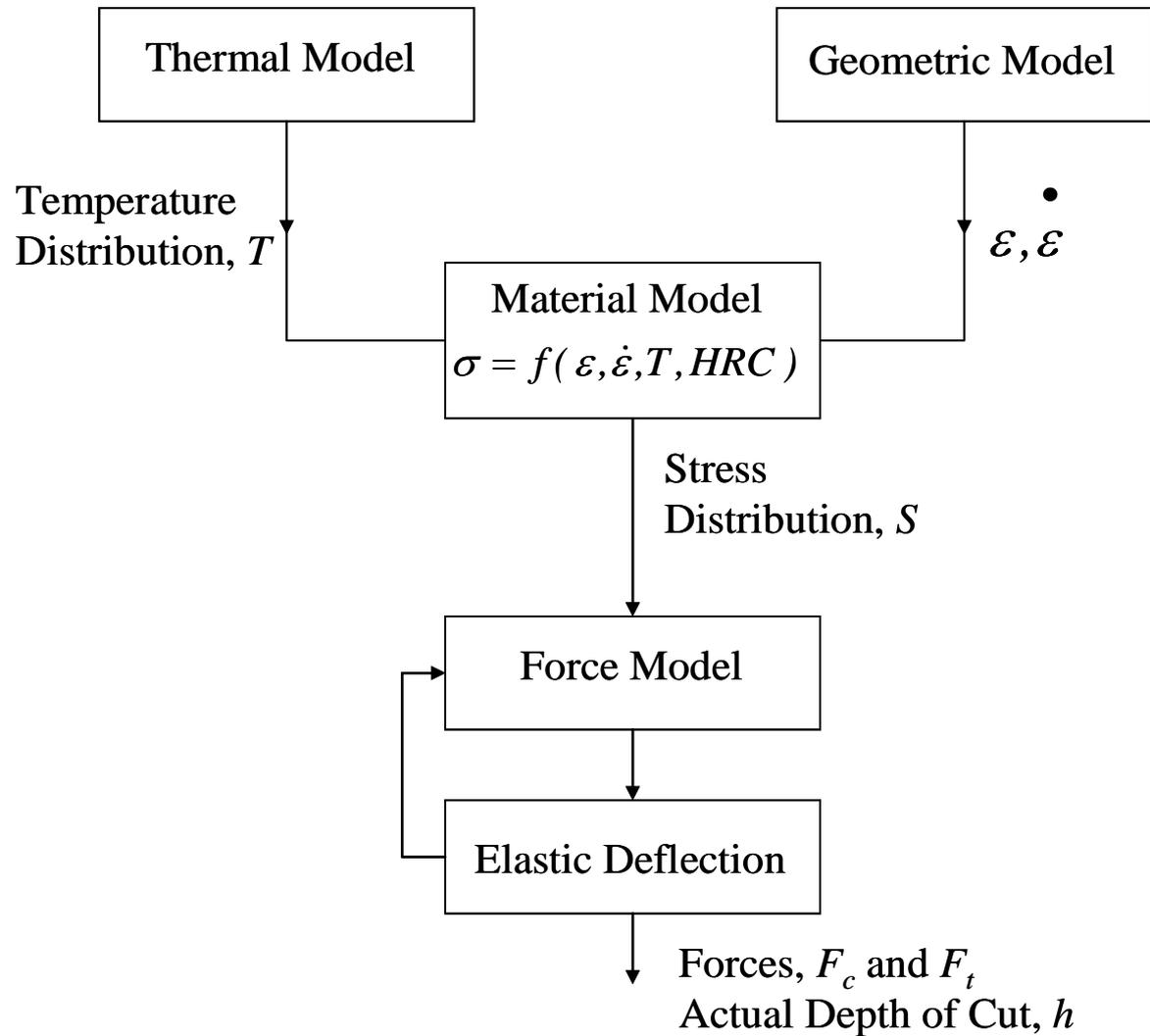
$$F_c = \{ (h - p) \cot \phi + h + r_n \sin \theta - (k - 1) \delta \} \sum_{i=1}^n \bar{S}(i) w(i)$$

$$F_t = \{ (h - p) \cot \phi - h + r_n \sin \theta + (k - 1) \delta \cot \psi \} \sum_{i=1}^n \bar{S}(i) w(i)$$

Equilibrium Forces/Deflection



Force model



LAMM-continued

$$y_i = \theta(\mathbf{x}_i)$$

$$\theta(\mathbf{x}) \sim GP(\mu, \tau^2 r), \quad r(\mathbf{x}_i, \mathbf{x}_j) = \exp\left\{-\sum_{k=1}^4 \alpha_k (x_{ik} - x_{jk})^2\right\}$$

$$p(\mu, \tau^2) \propto 1/\tau^2$$

$$\gamma_i = \log(\alpha_i) \sim^{iid} N(0, 1).$$

LAMM-continued

- Unnormalized posterior

$$\begin{aligned}h(\theta(\mathbf{x}), \mu, \tau^2, \gamma) &\propto p(\mathbf{y}|\theta(\mathbf{x}), \mu, \tau^2, \gamma)p(\theta(\mathbf{x})|\mu, \tau^2, \gamma)p(\mu, \tau^2)p(\gamma), \\ &= p(\theta(\mathbf{x})|\mu, \tau^2, \gamma, \mathbf{y})p(\mathbf{y}|\mu, \tau^2, \gamma)p(\mu, \tau^2)p(\gamma)\end{aligned}$$

- Integrating out $\theta(\mathbf{x})$, μ , and τ^2 ,

$$h(\gamma) = |\mathbf{R}|^{-1/2}(\mathbf{1}'\mathbf{R}^{-1}\mathbf{1})^{-1/2}[(\mathbf{y} - \hat{\mu}\mathbf{1})'\mathbf{R}^{-1}(\mathbf{y} - \hat{\mu}\mathbf{1})]^{-(n-1)/2}$$

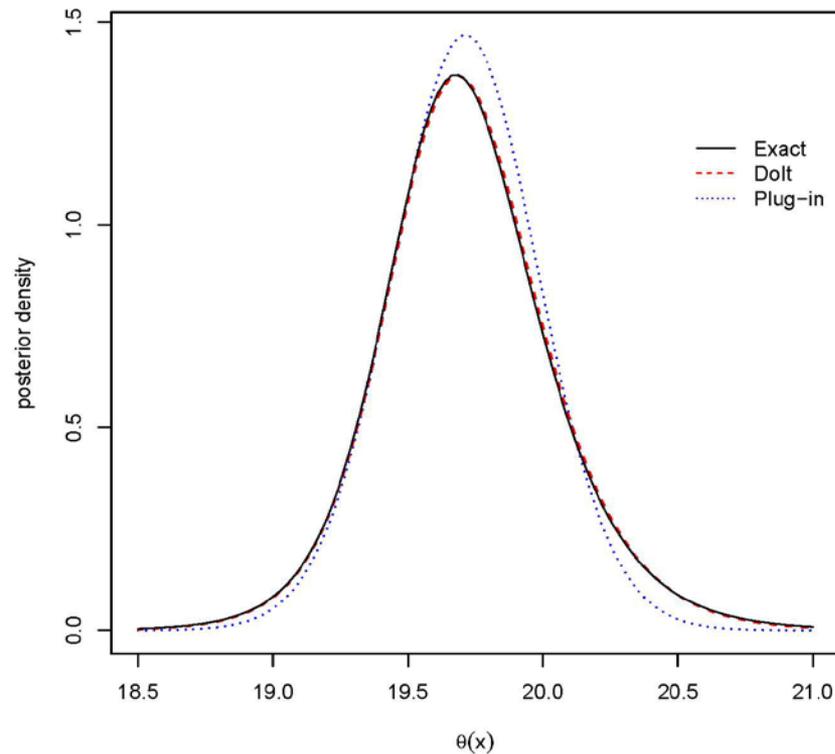
LAMM-continued

- Conditional distribution: $\frac{\theta(\mathbf{x}) - \hat{\theta}(\mathbf{x})}{\sqrt{V(\mathbf{x})}} | \gamma, \mathbf{y} \sim t_{n-1},$

$$\begin{aligned}\hat{\theta}(\mathbf{x}) &= \hat{\mu} + \mathbf{r}(\mathbf{x})' \mathbf{R}^{-1} (\mathbf{y} - \hat{\mu} \mathbf{1}), \\ V(\mathbf{x}) &= \hat{\tau}^2 \left(1 - \mathbf{r}(\mathbf{x})' \mathbf{R}^{-1} \mathbf{r}(\mathbf{x}) + \frac{\{1 - \mathbf{r}(\mathbf{x})' \mathbf{R}^{-1} \mathbf{1}\}^2}{\mathbf{1}' \mathbf{R}^{-1} \mathbf{1}} \right), \\ \hat{\mu} &= \frac{\mathbf{1}' \mathbf{R}^{-1} \mathbf{y}}{\mathbf{1}' \mathbf{R}^{-1} \mathbf{1}}, \\ \hat{\tau}^2 &= \frac{1}{n-1} (\mathbf{y} - \hat{\mu} \mathbf{1})' \mathbf{R}^{-1} (\mathbf{y} - \hat{\mu} \mathbf{1}).\end{aligned}$$

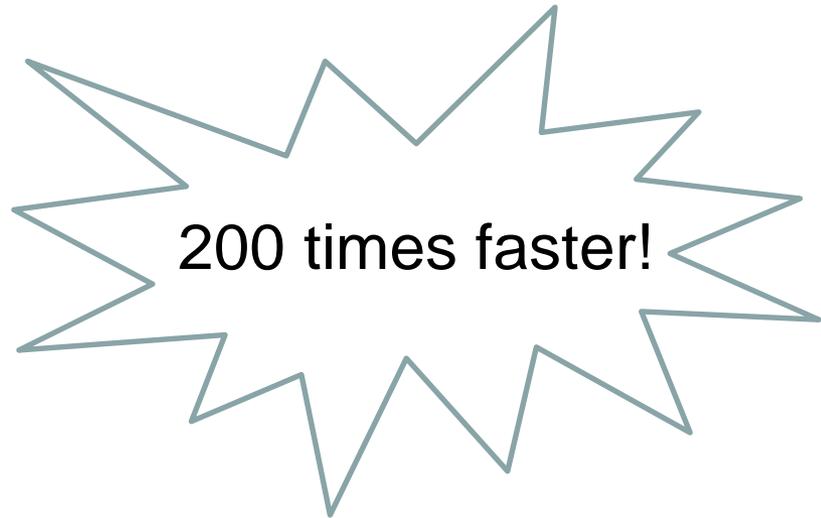
LAMM-continued

- DoIt : $m=100$ (red), MCMC: $m=100,000$ (black)



LAMM-continued

- Computational time
 - DoIt = 3 seconds
 - MCMC=10 minutes



- Computationally expensive likelihood.
 - Computational complexity: $O(n^3)$.
 - Here $n=48$.

Conclusions

- A new deterministic approximation method using **design of experiments** and **interpolation** techniques.
 - Very general.
 - Can obtain the results with arbitrary precision.
 - Suffer less from the curse of dimensionality compared to lattice-based quadrature methods.
 - Some of the very large hierarchical problems can be solved efficiently.
 - Very fast!
 - Almost a black box method (no extra programming or derivations are needed).

Conclusions

- Disadvantages
 - Not as flexible as MCMC.
 - Not easy to find good space-filling designs in high dimensions.
 - Can handle only continuous parameters.
 - Cannot ensure nonnegativity of the posterior density.

Nonnegative Dolt

- Joseph, *Technometrics*, 2013, February.

Let $\hat{\mathbf{c}} = \mathbf{b}$, $\Lambda = \Sigma$, and $a = 0$.

$$h(\boldsymbol{\theta}) \approx \left\{ \sum_{i=1}^m b_i g(\boldsymbol{\theta}; \boldsymbol{\nu}_i, \Sigma) \right\}^2,$$

which will always be nonnegative!

$$\sqrt{h(\boldsymbol{\theta})} \approx \sum_{i=1}^m b_i g(\boldsymbol{\theta}; \boldsymbol{\nu}_i, \Sigma)$$

Future Research

- Fast generation of design points at high probability regions.
 - Need a better design strategy.
- Fast approximation using local versions of Σ .
 - Need a better modeling strategy.
- Topics for future research!

Conclusions

If you have a Bayesian problem, then just

Do It !