

Uncertainty and statistics

Part IV

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Recall the typical problem setup

- ★ Have a model for stochastic variables, $x_1, \dots, x_n, y_1, \dots, y_m$
 - we have a formula for $p(x_1, \dots, x_n, y_1, \dots, y_m)$
 - we have observed y_1, \dots, y_m
 - distribution of interest

$$p(x_1, \dots, x_n | y_1, \dots, y_m) = \frac{p(x_1, \dots, x_n, y_1, \dots, y_m)}{p(y_1, \dots, y_m)}$$

where

$$p(y_1, \dots, y_m) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} p(x_1, \dots, x_n, y_1, \dots, y_m) dx_1 \cdots dx_n$$

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- common to write

$$p(x_1, \dots, x_n | y_1, \dots, y_m) \propto p(x_1, \dots, x_n, y_1, \dots, y_m)$$

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- ★ Focus today:
 - Monte Carlo sampling

$$(x_1, \dots, x_n) \sim p(x_1, \dots, x_n | y_1, \dots, y_m)$$

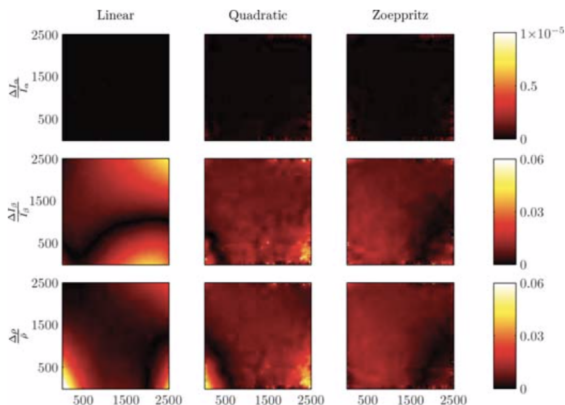
- MCMC, Metropolis–Hastings algorithm, Gibbs sampling

Plan for today

- ★ Introduce two example situations
 - Rabben, T.E., Tjelmeland, H. and Ursin, B. (2008). Non-linear Bayesian joint inversion of seismic reflection coefficients, Geophysical Journal International.
 - Tjelmeland, H., Luo, X. and Fjeldstad, T. (2019). A Bayesian model for lithology/fluid class prediction using a Markov mesh prior fitted from a training image, Geophysical Prospecting.
- ★ The Metropolis–Hastings algorithm
 - the algorithm, proposal distribution
 - toy examples, intuition
 - random walk proposals, Gibbs proposals
 - what is converging?
 - reversible jump Metropolis–Hastings
- ★ Metropolis–Hastings for the two example situations
 - proposal distribution
 - results

Inversion of seismic reflection coefficients

- ★ Reference: Rabben, T.E., Tjelmeland, H. and Ursin, B. (2008). Non-linear Bayesian joint inversion of seismic reflection coefficients, Geophysical Journal International.

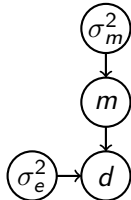


Inversion of seismic reflection coefficients

★ Variables in the problem:

- $m = \{m_{ij}; i = 1, \dots, n_y, j = 1, \dots, n_x\}$, $m_{ij} = \left\{ \frac{\Delta I_\alpha}{I_\alpha}, \frac{\Delta I_\beta}{I_\beta}, \frac{\Delta \rho}{\bar{\rho}} \right\}_{ij}$
- $d = \{d_{ij}, i = 1, \dots, n_y, j = 1, \dots, n_x\}$, $d_{ij} = \{r_{PP}(\theta), r_{PS}(\theta)\}_{ij}$
for $\theta = 0^\circ$ (only PP), $20^\circ, 40^\circ, 55^\circ$
- σ_m^2 : variance of m_{ij}
- σ_e^2 : variance of $d_{ij}|m$

★ Structure of stochastic model



$$p(m, d, \sigma_m^2, \sigma_e^2) = p(\sigma_m^2)p(\sigma_e^2)p(m|\sigma_m^2)p(d|m, \sigma_e^2)$$

Inversion of seismic reflection coefficients

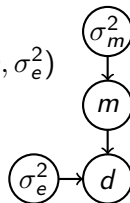
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★ Model components

- $m|\sigma_m^2 \sim N(\mu_m, \sigma_m^2 S_m)$
- $d|m, \sigma_e^2 \sim N(f(m), \sigma_e^2 S_e)$

$$d = f(m) + e, e \sim N(0, \sigma_e^2 S_e)$$

- $\sigma_m^2 \sim \text{IG}(\alpha_m, \beta_m)$
- $\sigma_e^2 \sim \text{IG}(\alpha_e, \beta_e)$



Inversion of seismic reflection coefficients

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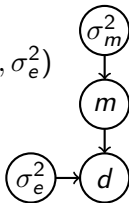
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★ Use three versions for $f(m)$

– Zoeppritz equations

– quadratic approximation of the Zoeppritz equations

– linear approximation of the Zoeppritz equations



Quadratic approximation of the Zoepritz equations

$$\begin{aligned}
 r_{PP} = & \frac{1}{2 \cos^2 \theta_p} \frac{\Delta I_\alpha}{\bar{I}_\alpha} - 4 \sin^2 \theta_s \frac{\Delta I_\beta}{\bar{I}_\beta} - \frac{1}{2} \tan^2 \theta_p (1 - 4\gamma^2 \cos^2 \theta_p) \frac{\Delta \rho}{\bar{\rho}} \\
 & + \tan \theta_p \tan \theta_s \left\{ 4\gamma^2 (1 - (1 + \gamma^2) \sin^2 \theta_p) \left(\frac{\Delta I_\beta}{\bar{I}_\beta} \right)^2 \right. \\
 & - 4\gamma^2 \left[1 - \left(\frac{3}{2} + \gamma^2 \right) \sin^2 \theta_p \right] \left(\frac{\Delta I_\beta}{\bar{I}_\beta} \frac{\Delta \rho}{\bar{\rho}} \right) \\
 & \left. + \left[\gamma^2 (1 - (2 + \gamma^2) \sin^2 \theta_p) - \frac{1}{4} \right] \left(\frac{\Delta \rho}{\bar{\rho}} \right)^2 \right\}
 \end{aligned}$$

$$\begin{aligned}
 r_{PS} = & \sqrt{\tan \theta_p \tan \theta_s} \left\{ \left[(1 - \cos \theta_s (\cos \theta_s + \gamma \cos \theta_p)) \left(2 \frac{\Delta I_\beta}{\bar{I}_\beta} - \frac{\Delta \rho}{\bar{\rho}} \right) - \frac{1}{2} \frac{\Delta \rho}{\bar{\rho}} \right] \right. \\
 & + \frac{1}{2} \left[(1 - \cos \theta_s (\cos \theta_s - \gamma \cos \theta_p)) \left(2 \frac{\Delta I_\beta}{\bar{I}_\beta} - \frac{\Delta \rho}{\bar{\rho}} \right) - \frac{1}{2} \frac{\Delta \rho}{\bar{\rho}} \right] \\
 & \times \left[\frac{1}{2 \cos^2 \theta_p} \frac{\Delta I_\alpha}{\bar{I}_\alpha} + \left(\frac{1}{2 \cos^2 \theta_s} - 8 \sin^2 \theta_s \right) \frac{\Delta I_\beta}{\bar{I}_\beta} \right. \\
 & \left. \left. + \left(4 \sin^2 \theta_s - \frac{1}{2} (\tan^2 \theta_p + \tan^2 \theta_s) \right) \frac{\Delta \rho}{\bar{\rho}} \right] \right\},
 \end{aligned}$$

Inversion of seismic reflection coefficients

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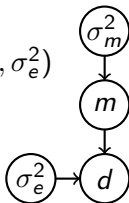
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Inversion of seismic reflection coefficients

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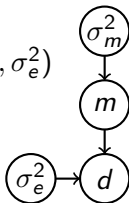
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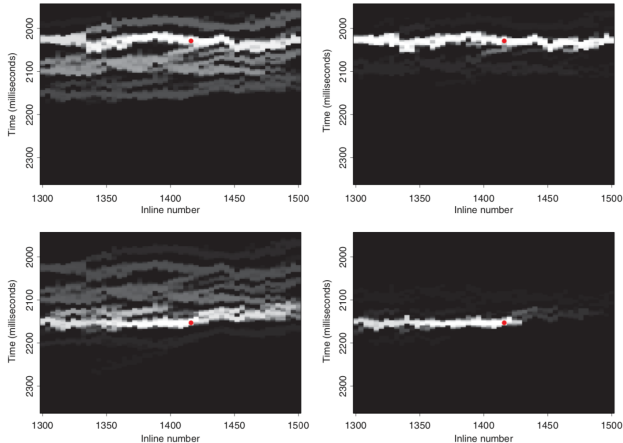
★ Distribution of interest

$$p(m, \sigma_m^2, \sigma_e^2 | d) \propto p(m, d, \sigma_m^2, \sigma_e^2)$$



Lithology/fluid class prediction using a Markov mesh prior

- ★ Reference: Tjelmeland, H., Luo, X. and Fjeldstad, T. (2019). A Bayesian model for lithology/fluid class prediction using a Markov mesh prior fitted from a training image, Geophysical Prospecting.



Lithology/fluid class prediction using a Markov mesh prior

- ★ Variables in the problem:

- $\kappa = \{\kappa_{ij}; i = 1, \dots, n_y, j = 1, \dots, n_x\}$, $\kappa_{ij} \in \{0, 1\}$ (shale, oil sand)
- $m = \{m_{ij}; i = 1, \dots, n_y, j = 1, \dots, n_x\}$, $m_{ij} = (\text{impedance}, v_p/v_s)_{ij}$
- $d = \{d_{ij}; i = 1, \dots, n_y, j = 1, \dots, n_x\}$, $d_{ij} = (\text{near offset}, \text{far offset})_{ij}$
- θ : parameters vector describing stochastic model for κ (fixed)

- ★ Structure of the stochastic model



$$p(\kappa, m, d|\theta) = p(\kappa|\theta)p(m|\kappa)p(d|m)$$

Lithology/fluid class prediction using a Markov mesh prior

★ Recall: $p(\kappa, m, d|\theta) = p(\kappa|\theta)p(m|\kappa)p(d|m)$



★ Model components

- $\kappa|\theta \sim$ Markov mesh model
- $m_{ij}|\kappa \sim N(\mu_{\kappa_{ij}}, \Sigma_{\kappa_{ij}})$
- $d|m \sim N(WADm, \Sigma_{\varepsilon})$

$$d = WADm + \varepsilon, \varepsilon \sim N(0, \Sigma_{\varepsilon})$$

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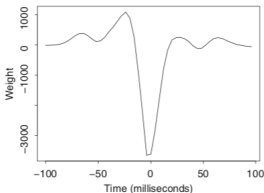
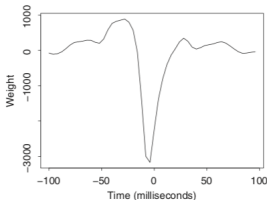


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wavelet for near offset wavelet for far offset



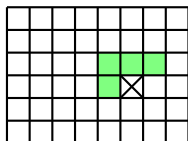
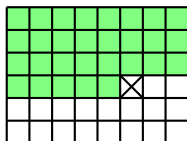
Markov mesh model

- ★ Order the nodes in lexicographical order from 1 to $n = n_x \cdot n_y$

$$p(\kappa|\theta) = \prod_{i=1}^n p(\kappa_i|\kappa_{<i}, \theta)$$

- ★ Conditional independence (Markov) assumption

$$p(\kappa|\kappa_{<i}, \theta) = p(\kappa_i|\kappa_{\nu_i}, \theta)$$



- ★ Thus

$$p(\kappa|\theta) = \prod_{i=1}^n p(\kappa_i|\kappa_{\nu_i}, \theta)$$

Markov mesh model

- ★ Recall:

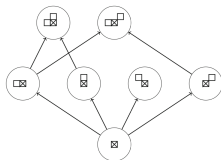
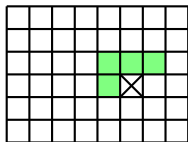
$$p(\kappa|\theta) = \prod_{i=1}^n p(\kappa_i|\kappa_{\nu_i}, \theta)$$

- ★ Reformulation of $p(\kappa_i|\kappa_{\nu_i}, \theta)$

$$\theta_i(\kappa_{\nu_i}) = \ln \left(\frac{p(\kappa_i = 1|\kappa_{\nu_i}, \theta)}{1 - p(\kappa_i = 1|\kappa_{\nu_i}, \theta)} \right)$$

$$\theta_i(\kappa_{\nu_i}) = \sum_{\lambda \subseteq \kappa_{\nu_i}} \beta(\lambda)$$

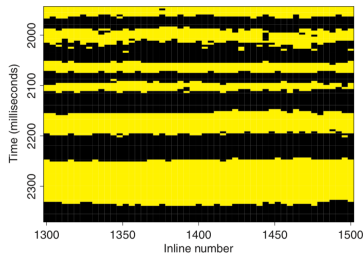
- ★ Limit the number of model parameters by setting some $\beta(\lambda) = 0$



- ★ $\theta = (\nu_i; \beta(\lambda), \nu_i \subseteq \nu_i)$

How to specify θ ?

- ★ Values in θ does not have a simple interpretation
 - difficult to set values consistent with prior knowledge
- ★ Use a training image
 - hand drawn or from area with similar geological origin
 - contain information about typical spatial structures



- ★ Let θ be a Monte Carlo sample from

$$p(\theta|\text{training image}) \propto p(\theta)p(\text{training image}|\theta)$$

Lithology/fluid class prediction using a Markov mesh prior

★ Recall: $p(\kappa, m, d|\theta) = p(\kappa|\theta)p(m|\kappa)p(d|m)$



★ Model components

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★ Distribution of interest

$$p(\kappa, m|\theta, d) \propto p(\kappa, m, d|\theta)$$

- can analytically integrate over m to find formula for

$$p(\kappa|\theta, d) \propto p(\kappa, d|\theta)$$

Markov chain Monte Carlo

- ★ Have a model for stochastic variables, $x_1, \dots, x_n, y_1, \dots, y_m$
 - we have a formula for $p(x_1, \dots, x_n, y_1, \dots, y_m)$
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- ★ Note: The y 's are observed numbers

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- ★ Note: The y 's are observed numbers
- ★ We now simplify the notation and write

$$p(x) = p(x_1, \dots, x_n) = c \cdot h(x) \quad \text{in stead of} \quad p(x_1, \dots, x_n | y_1, \dots, y_m)$$

- we have a formula for $h(x) = p(x_1, \dots, x_n, y_1, \dots, y_m)$
- we don't know the value of c

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- we have a formula for $h(x) = p(x_1, \dots, x_n, y_1, \dots, y_m)$
 - we don't know the value of c
- ★ So the goal is to generate a Monte Carlo sample

$$x \sim p(x) = c \cdot h(x)$$

Markov chain Monte Carlo

- ★ Want a Monte Carlo sample from

$$x \sim p(x) = c \cdot h(x)$$

- ★ Metropolis–Hastings algorithm: Generate x^1, x^2, \dots as follows

1. Generate/set x^1 somehow
2. For $k = 2, 3, \dots, K$
 - (a) Generate a potential new values $z^k \sim q(z^k|x^{k-1})$
 - (b) Compute acceptance probability

$$\alpha(z^k|x^{k-1}) = \min \left\{ 1, \frac{p(z^k)}{p(x^{k-1})} \cdot \frac{q(x^{k-1}|z^k)}{q(z^k|x^{k-1})} \right\}$$

- (c) Generate $u^k \sim \text{Uniform}[0, 1]$
 - (d) If ($u^k \leq \alpha(z^k|x^{k-1})$)
 $x^k = z^k$ (accept z^k)
else
 $x^k = x^{k-1}$ (reject z^k)
3. End

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3. End

- ★ For k large enough, x^k is (approximately) from $p(x)$

Random walk proposal

- ★ Target distribution: $p(x)$
- ★ Proposal distribution: $z^k \sim q(z^k|x^{k-1})$
- ★ Acceptance probability:

$$\alpha(z^k|x^{k-1}) = \min \left\{ 1, \frac{p(z^k)}{p(x^{k-1})} \cdot \frac{q(x^{k-1}|z^k)}{q(z^k|x^{k-1})} \right\}$$

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- ★ Random walk proposal:

$$z_i^k = x_i^{k-1} + \varepsilon_i, \quad \varepsilon_i \sim \mathbf{N}(0, \sigma^2)$$

- formula for the proposal distribution

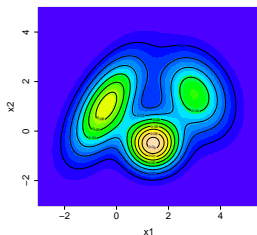
$$q(z^k|x^{k-1}) = \frac{1}{(2\pi\sigma^2)^{\frac{n}{2}}} \exp \left\{ -\frac{1}{2\sigma^2} (z^k - x^{k-1})^T (z^k - x^{k-1}) \right\}$$

- acceptance probability

$$\alpha(z^k|x^{k-1}) = \min \left\{ 1, \frac{p(z^k)}{p(x^{k-1})} \right\}$$

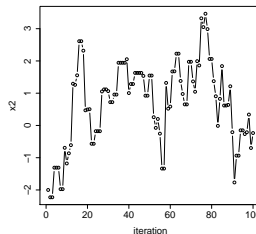
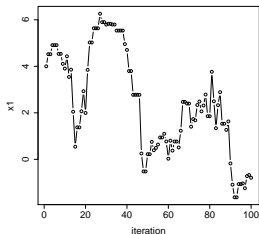
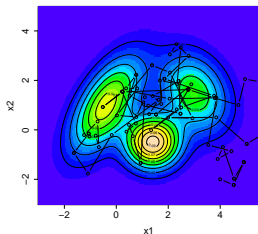
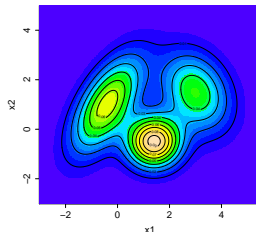
Toy example: Random walk proposal

- ★ Target distribution: $p(x)$
- ★ Start with $x^1 = (4, -2)$
- ★ Random walk proposal with $\sigma = 1.0$
- ★ Run $K = 100$ iterations



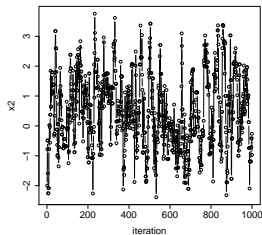
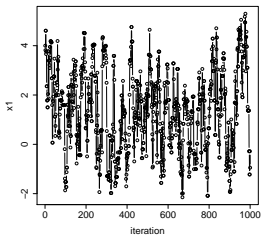
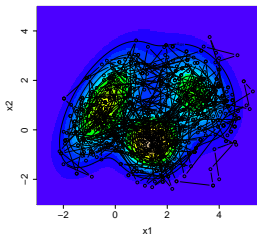
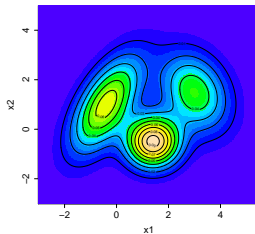
Toy example: Random walk proposal

- ★ Target distribution: $p(x)$
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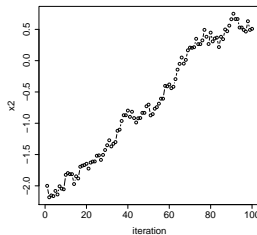
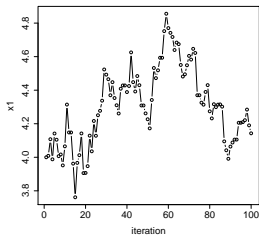
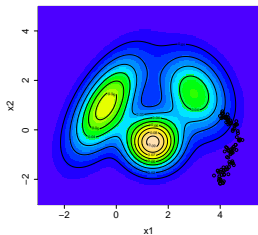
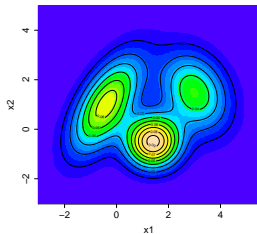
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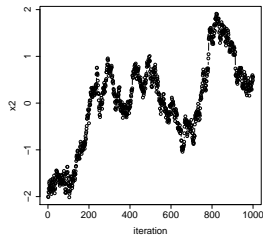
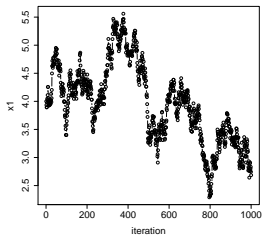
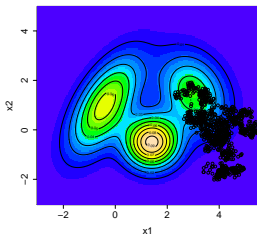
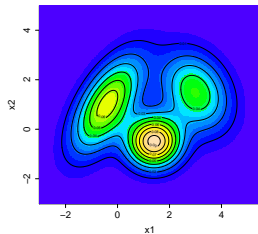
Toy example: Random walk proposal

- ★ Target distribution: $p(x)$
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- ★ Random walk proposal with $\sigma = 0.1$
- ★ Run $K = 100$ iterations



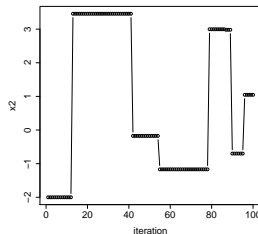
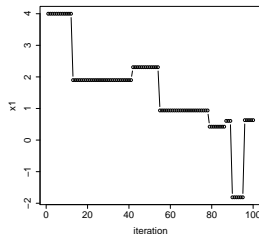
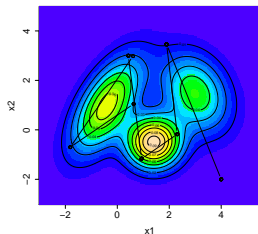
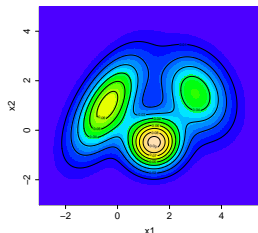
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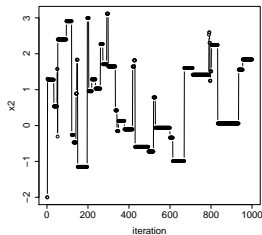
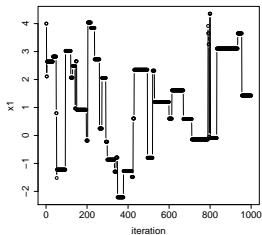
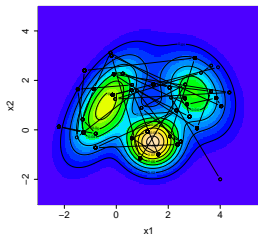
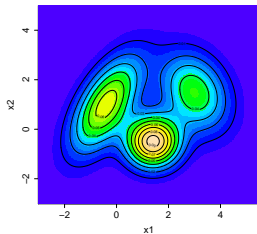
Toy example: Random walk proposal

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Gibbs sampling

- ★ Target distribution: $p(x)$
- ★ Proposal distribution: $z^k \sim q(z^k|x^{k-1})$
- ★ Acceptance probability:

$$\alpha(z^k|x^{k-1}) = \min \left\{ 1, \frac{p(z^k)}{p(x^{k-1})} \cdot \frac{q(x^{k-1}|z^k)}{q(z^k|x^{k-1})} \right\}$$

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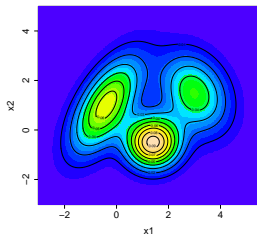
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- ★ Gibbs proposal:
 - sample $i \sim \text{Uniform}\{1, \dots, n\}$
 - sample $z_i^k \sim p(x_i|x_1^{k-1}, \dots, x_{i-1}^{k-1}, x_{i+1}^{k-1}, \dots, x_n^{k-1})$
 - set $z_j^k = x_j^{k-1}$ for $j \neq i$
 - acceptance probability

$$\alpha(z^k|x^{k-1}) = 1$$

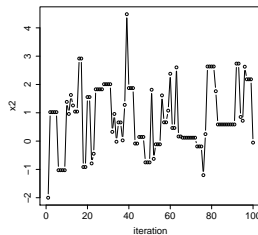
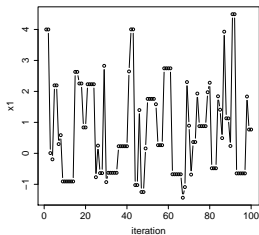
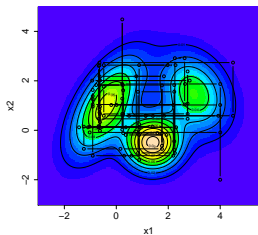
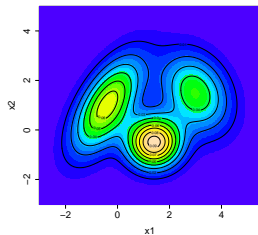
Toy example: Gibbs sampling

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- ★ Run $K = 100$ iterations



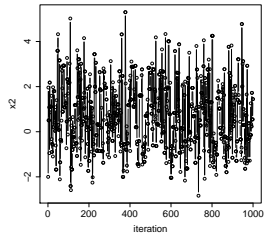
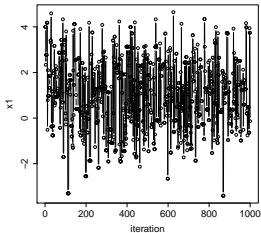
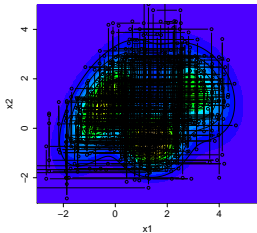
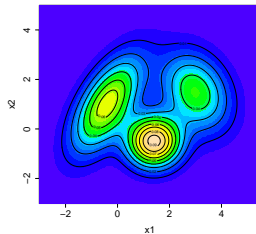
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Toy example: Gibbs sampling

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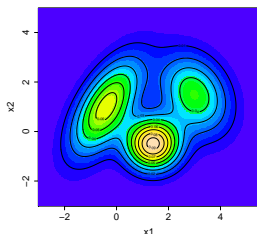


Toy example: Combine Gibbs and random walk

- ★ Target distribution: $p(x)$
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$$z_2^k = x_2^{k-1} + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, 1)$$

- ★ Run $K = 100$ iterations

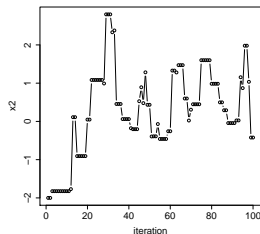
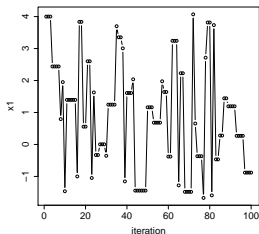
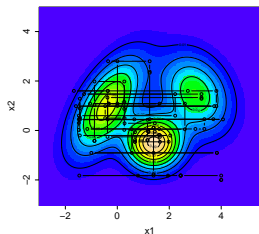
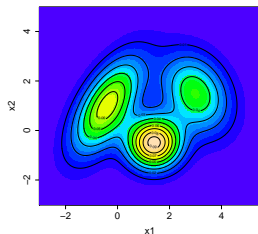


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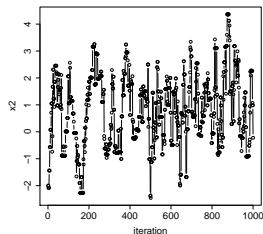
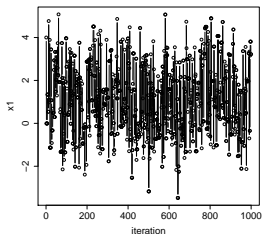
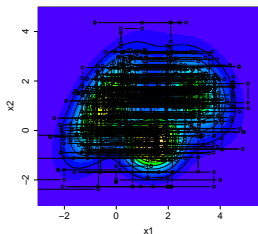
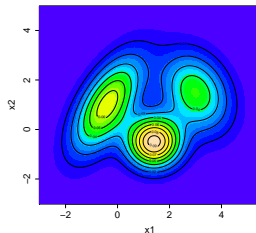


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Convergence of the Metropolis–Hastings algorithm

- ★ Note: It is not x^k that is converging
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 - we can only look at and plot x^k
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 - the convergence can be extremely slow — not useful!
 - to choose a good proposal distribution for a given distribution often requires experience
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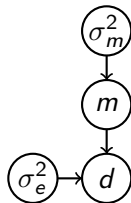
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- ★ Reversible jump Metropolis–Hastings
 - also the dimension of x is stochastic
 - the number of stochastic variables is a stochastic variable

Inversion of seismic reflection coefficients

- ★ Reference: Rabben, T.E., Tjelmeland, H. and Ursin, B. (2008). Non-linear Bayesian joint inversion of seismic reflection coefficients, Geophysical Journal International.
- ★ Distribution of interest

$$p(m, \sigma_m^2, \sigma_e^2 | d) \propto p(m, d, \sigma_m^2, \sigma_e^2)$$

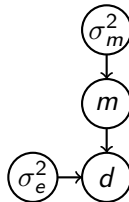
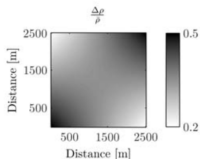
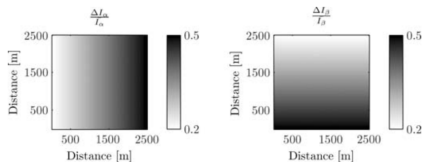


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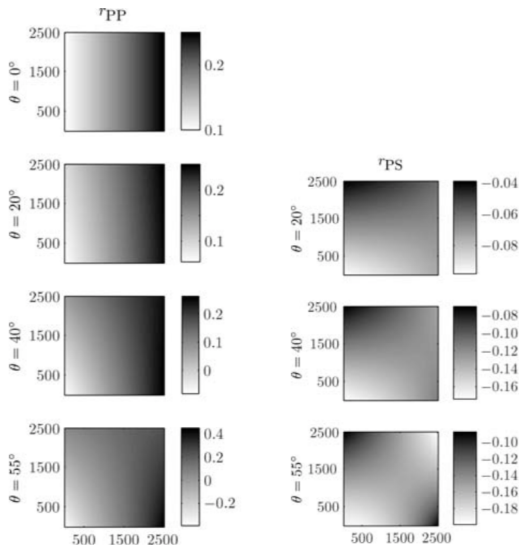
$$p(m, \sigma_m^2, \sigma_e^2 | d) \propto p(m, d, \sigma_m^2, \sigma_e^2)$$

- ★ Simulation example: Reference contrasts



Simulation example: Observations

- ★ "Observed" PP and PS reflection coefficients using the Zoeppritz model



Proposal distributions

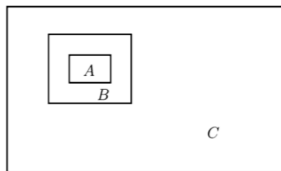
★ Target distribution:

$$p(m, \sigma_m^2, \sigma_e^2 | d) \propto p(m, d, \sigma_m^2, \sigma_e^2)$$

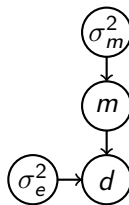
★ Proposal distributions:

- Gibbs proposal for σ_m^2
- Gibbs proposal for σ_e^2
- proposal for m_A based on a linearised model

$$p^{\text{lin}}(m_A | m_B, \sigma_m^2, \sigma_e^2)$$

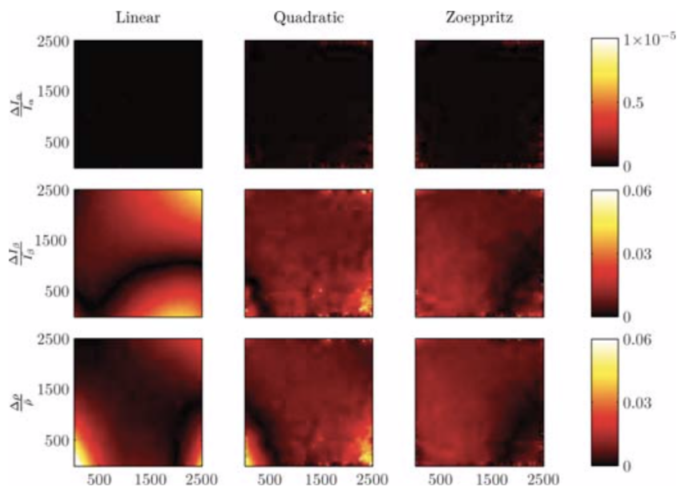


note: the acceptance probability is correcting the error done when proposing from a linearised model and by not conditioning on m_c



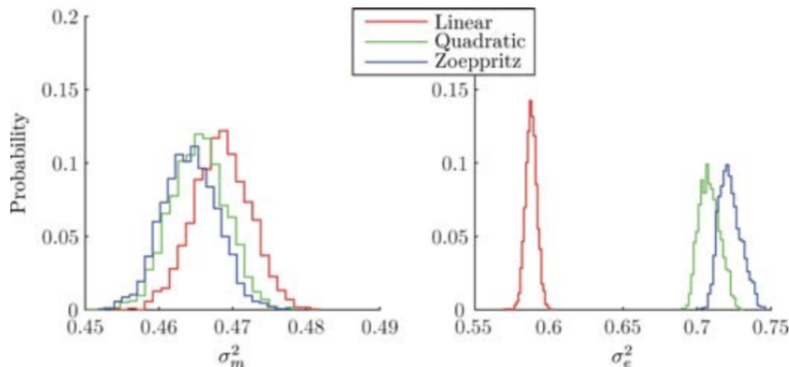
Inversion of seismic reflection coefficients: Results

- ★ Resulting bias in inverted reflection coefficients
 - recall: results for three forward functions



Inversion of seismic reflection coefficients: Results

- ★ Distribution of σ_m^2 and σ_e^2
 - recall: results for three forward functions



Lithology/fluid class prediction using a Markov mesh prior

- ★ Reference: Tjelmeland, H., Luo, X. and Fjeldstad, T. (2019). A Bayesian model for lithology/fluid class prediction using a Markov mesh prior fitted from a training image, Geophysical Prospecting.
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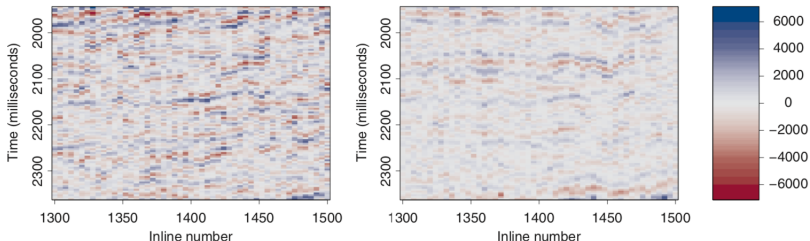
$$p(\kappa|\theta, d) \propto p(\kappa, d|\theta)$$

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- ★ Near (left) and far (right) offset seismic data

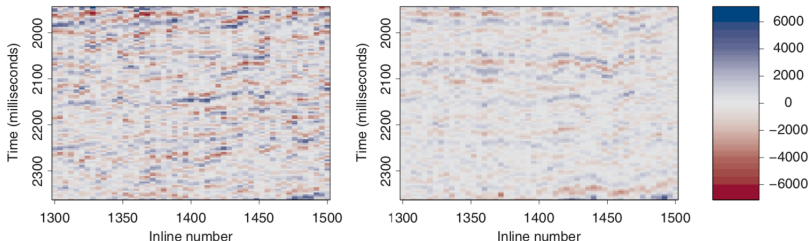


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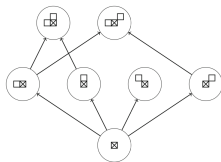
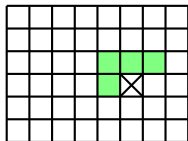
- ★ Near (left) and far (right) offset seismic data



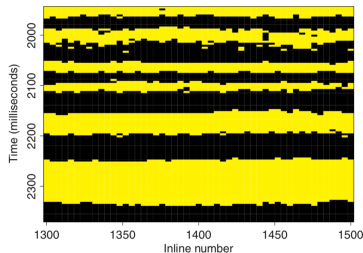
- ★ First: Construction of the prior, $p(\kappa|\theta)$

Prior $p(\kappa)$

- ★ Recall: Markov mesh, $\theta = (\nu_i; \beta(\lambda), \nu_i \subseteq \nu_j)$



- ★ Training image

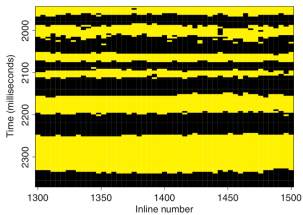


- ★ Use reversible jump Metropolis–Hastings to sample from

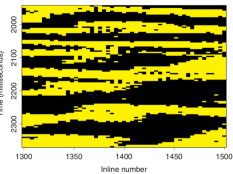
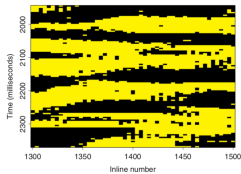
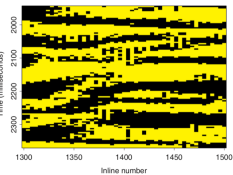
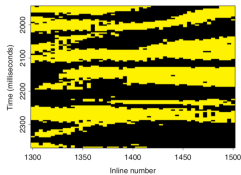
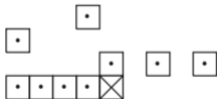
$$p(\theta | \text{training image}) \propto p(\theta) p(\text{training image} | \theta)$$

The fitted prior

- ★ Training image



- ★ Neighbourhood and Monte Carlo samples



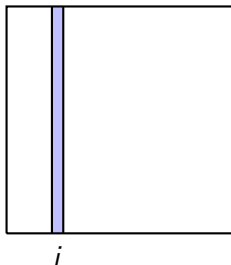
Proposal distributions

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- ★ Proposal distributions

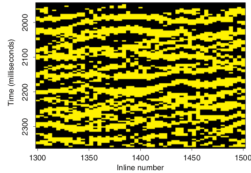
- Gibbs proposal for $\kappa_i = (\kappa_{ij}, j = 1, \dots, nx)$



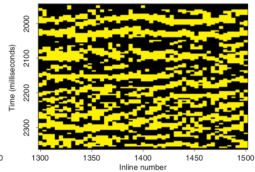
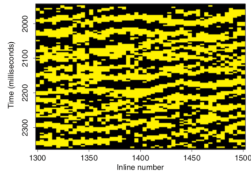
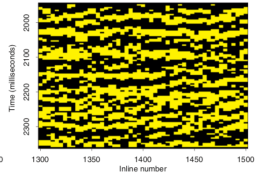
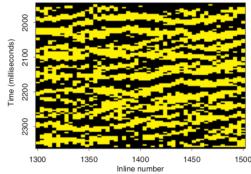
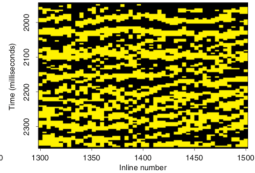
Lithology/fluid class prediction: Results

- ★ Monte Carlo samples from posterior

Markov mesh prior



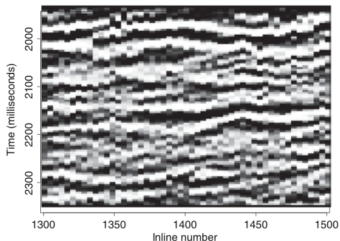
Simpler prior



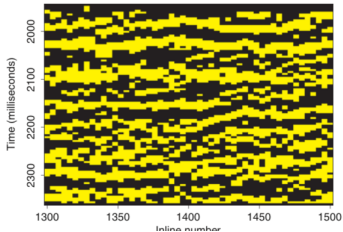
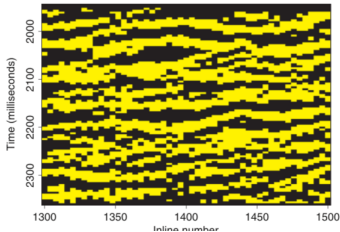
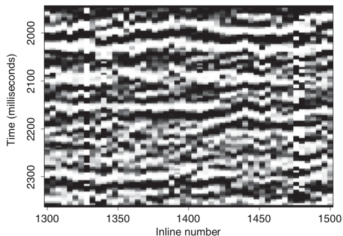
Lithology/fluid class prediction: Results

- ★ Marginal probabilities and most probable value

Markov mesh prior



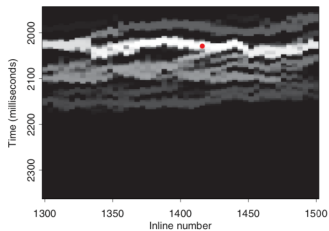
Simpler prior



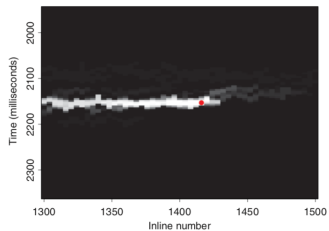
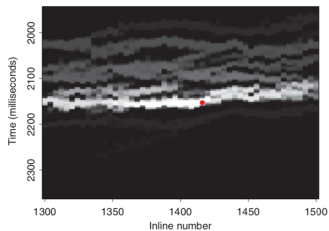
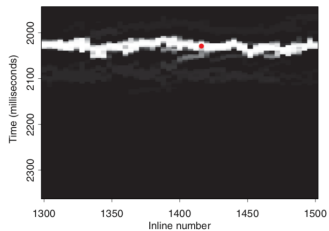
Lithology/fluid class prediction: Results

- ★ Probabilities for connectivity

Markov mesh prior



Simpler prior



Markov chain Monte Carlo summary

- ★ Metropolis–Hastings is extremely flexible
 - can sample from almost any distribution
- ★ Metropolis–Hastings can be reasonable fast or extremely slow
- ★ If you can sample without using Metropolis–Hastings:
 - do not use Metropolis–Hastings
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- ★ Next Friday: Alternatives to MCMC for specific classes of models