Bayesian inference for spatial GP models: Part 2

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February 23, 2018

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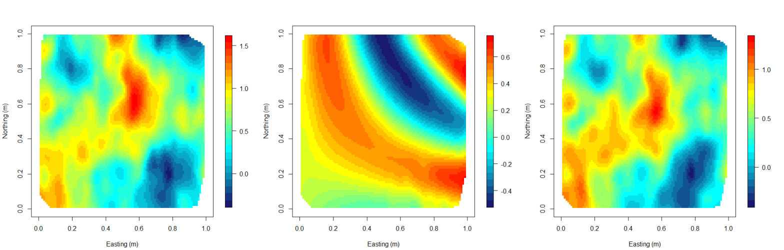
Review of last lecture

- Gibbs sampler: Generate samples from $p(X_1, X_2)$ by iteratively generating samples from $p(X_1^{(t)}|X_2^{(t-1)})$ and $p(X_2^{(t)}|X_1^{(t)})$
- Implementing our own Gibbs sampler for the unmarginalized model: $y \sim N(X\beta + w, \tau^2 I)$, $w \sim N(0, \sigma^2 R(\phi))$
    - Assume ϕ is known
    - Priors: $\sigma^2 \sim IG(a_\sigma, b_\sigma)$, $\tau^2 \sim IG(a_\tau, b_\tau)$ and $\beta \sim N(\mu, V)$
    - Full conditionals:

$$
\begin{aligned}
\beta \,|\, \sigma^2, \tau^2, w, y &\sim N(\mu^*, V^*) \\
w \,|\, \sigma^2, \tau^2, \beta, y &\sim N(m, C^*) \\
\sigma^2 \,|\, \beta, \tau^2, w, y &\sim IG(a_\sigma^*, b_\sigma^*) \\
\tau^2 \,|\, \beta, \sigma^2, w, y &\sim IG(a_\tau^*, b_\tau^*)
\end{aligned}
$$

Data analysis

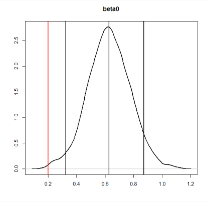
- Dataset 3 from Lecture 1
- True model: $y(s) \sim N(0.2 - 0.3x(s) + w(s), 0.01)$,
  $w(s) \sim GP,\ Cov(w(s_i), w(s_j)) = 0.25 * exp(-2||s_i - s_j||)$



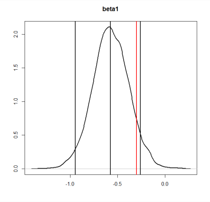
$y(s)$ $x(s)$ $w(s)$

Parameter posteriors

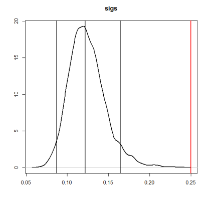
- ϕ is kept fixed at 4.23 (estimated value from variogram fitting)
- Gibbs sampler for w, β, σ^2 and τ^2



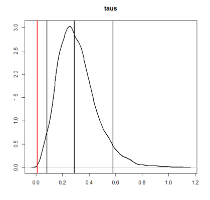
β_0



β_1

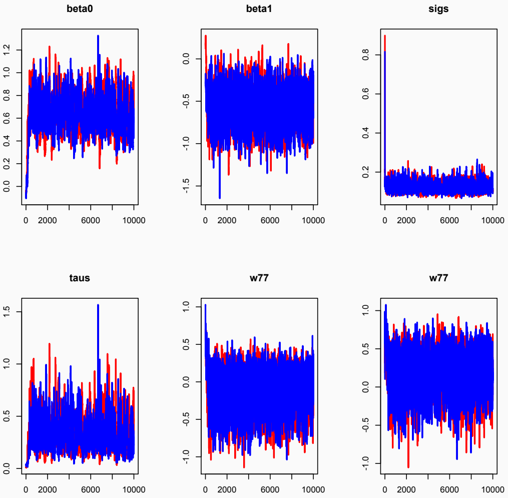


σ^2



τ^2

Convergence diagnostics: Trace plots



Convergence diagnostics: Gelman-Rubin shrink factor

- Run chains of length N with overdispersed initial values
- Discard the first N_b draws of each chain as burn-in
- For each variable θ, calculate the within-chain variance $W = \frac{1}{m}\sum_{j=1}^{m}\frac{1}{N-N_b-1}\sum_{i=N_b+1}^{N}(\theta^{(ij)} - \bar{\theta}_j)^2$
- For each variable θ, calculate the between-chain variance $B = \frac{N-N_b}{m-1}\sum_{j=1}^{m}(\bar{\theta}_j - \bar{\theta})^2$ where $\bar{\theta} = \frac{1}{m}\sum_{j=1}^{m}\bar{\theta}_j$
- Calculate the Gelman-Rubin shrink factor as $R = \sqrt{\frac{(1-\frac{1}{N-N_b})W + \frac{1}{N-N_b}B}{W}}$
- $R > 1.1$ or 1.2 indicates lack of convergence
- *coda* package in R gives the GR-shrink factors for each variable

Convergence diagnostics: Gelman-Rubin shrink factor

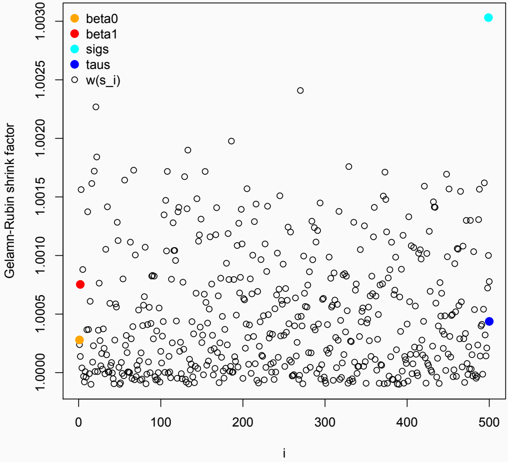


Figure: GR shrink factor for dataset 3

Convergence diagnostics: Plots of Gelman-Rubin shrink factor

- Plots of GR shrink factor against MCMC iteration number can help determine the burn-in

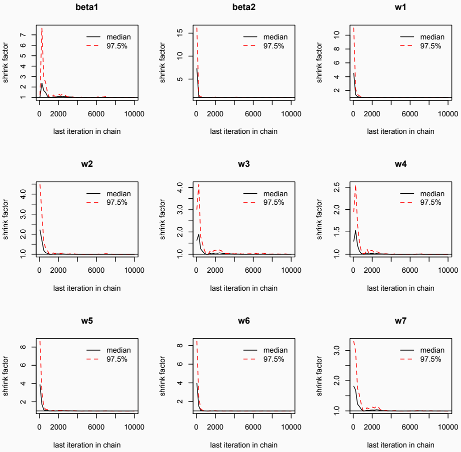


Figure: GR shrink factor a a function of MCMC iteration for dataset 3

Convergence diagnostics: Plots of Gelman-Rubin shrink factor

- Plots of GR shrink factor against MCMC iteration number can help determine the burn-in

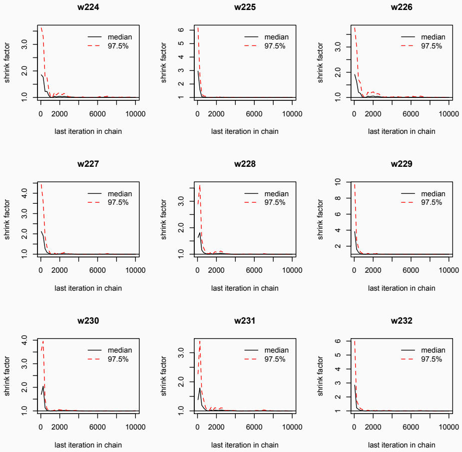
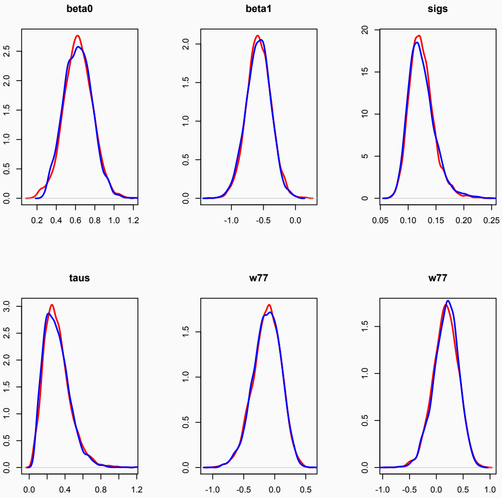


Figure: GR shrink factor a a function of MCMC iteration for dataset 3

Convergence diagnostics: Density plots



Model comparison using Bayesian output

- With holdout data we can use RMSPE (using posterior means or medians), out-of-sample CP (coverage probability) and CIW (confidence interval width) based on posterior quantiles

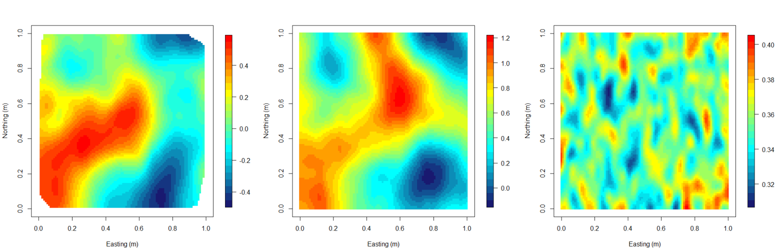
Model comparison using Bayesian output

- Deviance Information Criterion (DIC) (Spiegelhalter, 2002) uses the posterior samples for model comparison
- DIC for the model $l(y|\theta)$ is based on the deviance $D(y, \theta) = -2 \log l(y|\theta)$
- $\bar{D}(y) = E(D(y, \theta)|\theta) \approx \frac{1}{N} \sum_{i=1}^{N} D(y, \theta^{(i)})$
- $p_D = \bar{D}(y) - D(y, \bar{\theta})$ where $\bar{\theta} = E(\theta|y) \approx \frac{1}{N} \sum_{i=1}^{N} \theta^{(i)}$
- $DIC = \bar{D}(y) + p_D$
- The p_D term can be interpreted as effective number of parameters in the model and hence penalizes more complex models (similarity to AIC and BIC)

Posterior predictive distributions

- For the unmarginalized model, posterior samples for $w(s)$ are already generated for all s in the training data locations S
- Posterior predictive distributions $\tilde{y}(s)$ can be obtained using composition sampling:
  - If $s_0 \notin S$, generate samples from $w(s_0) \mid y$ using $w(s_0)^{(j)} \mid \cdot \sim N(c(s_0)' C^{-1} w^{(j)}, \sigma^{2(j)}(1 - r(s_0)' R^{-1} r(s_0)))$
  - $r(s_0) = cor(w(s_0), w)$ and $R = cor(w)$
  - If ϕ was also sampled, replace r and R by $c^{(j)}$ and $C^{(j)}$
  - For any s, generate $\tilde{y}(s)^{(j)} = N(x(s)' \beta^{(j)}, \tau^{2(j)})$

Posterior surfaces



$w(s) \mid y$ $\qquad$ $\tilde{y}(s) \mid y$ $\qquad$ $var(\tilde{y}(s) \mid y)$

Marginalized model

- Unmarginalized model has n additional parameters (w)
- May lead to slow MCMC convergence
- Marginalized model: $y \sim N(X\beta, \sigma^2 R(\phi) + \tau^2 I)$
- Pros: Only $p + 3$ parameters
- Cons: Even the full conditionals are not useful (except for β)
- How to do MCMC?

Metropolis algorithm

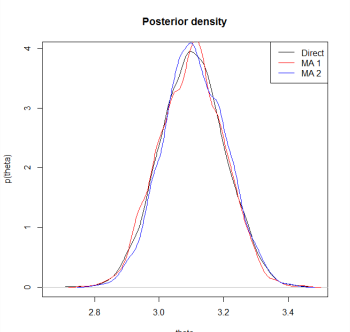
- We want to draw sample from a density $p(\theta) = f(\theta)/K$
- Begin with an initial θ^0
- Choose a function $q(x \mid y)$ such that
  - $q(x \mid y)$ is a valid density function in x for every value of y
  - $q(x \mid y) = q(y \mid x)$
  - e.g. $q(x \mid y) \sim N(x \mid y, \lambda) = \frac{1}{\sqrt{2\pi\lambda}} \exp(-\frac{1}{2\lambda}(x-y)^2)$
  - If θ is multivariate one can choose $q(x \mid y) \sim N(x \mid y, \Sigma)$
- q is called the proposal density
- If θ is multivariate, choose q to be a multivariate proposal density

Metropolis algorithm

- At the i^{th} iteration, generate θ^* from $q(\cdot \mid \theta_{i-1})$
- Calculate the ratio $r = f(\theta^*)/f(\theta_{i-1})$
- If $r \geq 1$, accept the new value i.e $\theta_i = \theta^*$
- If $r < 1$:
    - Accept the new value i.e $\theta_i = \theta^*$ with probability r
    - Keep the old value i.e $\theta_i = \theta_{i-1}$ with probability $1 - r$
- The sample $(\theta_i)_{i=N_b}^{N}$ is a sample from $p(\theta)$ where N_b is a burn-in period used
- An overall rate of acceptance around $30\% - 50\%$ is desirable (controlled by the tuning parameter λ)

Example

- $Y_i \overset{\text{iid}}{\sim} N(\theta, \sigma^2)$ for $i = 1, \ldots, n$ where $\theta = 3$ (unknown), $\sigma^2 = 1$(known) and $n = 100$
- Prior: $\theta \sim N(\mu, \tau^2)$ where $\mu = 0$ and $\tau^2 = 10$
- Metropolis algorithm:
$p(\theta \mid Y) \propto \exp(-\frac{n}{2\sigma^2}\left(\bar{y} - \theta)^2 - \frac{1}{2\tau^2}(\theta - \mu)^2\right)$
- Direct approach: $\theta \mid Y \sim N\left(\frac{\frac{n\bar{y}}{\sigma^2} + \frac{\mu}{\tau^2}}{\frac{n}{\sigma^2} + \frac{1}{\tau^2}}, \frac{1}{\frac{n}{\sigma^2} + \frac{1}{\tau^2}}\right)$

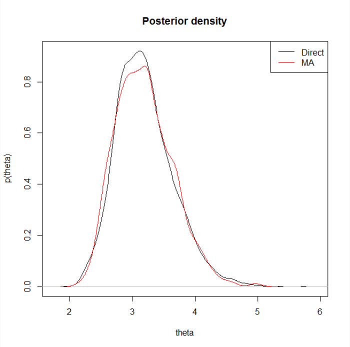


Jacobian adjustment

- Often the parameter of interest θ is not supported on the entire real line but on a part of it e.g. $[0, 1]$, $(0, \infty)$ etc.
- The normal proposal density is easy to use but has the entire real line as support
- One can choose a transformation g such that $\eta = g(\theta)$ is supported on the real line
- Generate new η^* using the normal proposal density
- Use the inverse transformation to obtain $\theta^* = g^{-1}(\eta^*)$
- The likelihood for η will be given by $p(\eta) = p(\theta)/|g'(\theta)|$
- Calculate
  $r = p(\eta^*)/p(\eta_{i-1}) = p(\theta^*)/p(\theta_{i-1}) \times |g'(\theta_{i-1})|/|g'(\theta^*)|$

Example

- $Y_i \overset{\text{iid}}{\sim} N(0, \sigma^2)$ for $i = 1, \ldots, n$ where $\sigma^2 = 4$ (unknown)
- σ^2 is supported on $(0, \infty)$. So, we use log transformation
- Prior: $\sigma^2 \sim \text{IG}(\alpha, \beta)$ where $\alpha = 2$ and $\beta = 1$
- Metropolis algorithm:
  $p(\sigma^2 \mid Y) \propto (\sigma^2)^{-1-\alpha-n/2} \exp(-(\beta + \sum_{i=1}^n y_i^2/2)/\sigma^2)$
- Direct approach:
  $\sigma^2 \mid Y \sim \text{Inverse Gamma}(\alpha + n/2, \beta + \sum_{i=1}^n y_i^2/2)$



Metropolis-Hastings Algorithm

- Allows for asymmetric proposal densities
- We want to draw sample from a density $p(\theta) = f(\theta)/K$
- Let $q(x \mid y)$ denote the proposal density
- Calculate the ratio $r = \frac{f(\theta^*)q(\theta_{i-1} \mid \theta^*)}{f(\theta_{i-1})q(\theta^* \mid \theta_{i-1})}$
- Useful if f is asymmetric
- Reduces to Metropolis algorithm is q is symmetric

Metropolis within Gibbs

- For the marginalized model, doing MH for the entire vector $(\beta', \sigma^2, \tau^2, \phi)'$ may be slow if p is large
- Also, β has nice normal full conditionals

- One can use a Metropolis Random Walk (RW) step for the univariate full conditional target densities inside the Gibbs sampler

- Example: MCMC steps for the marginalized model:
  (a) Gibbs for β: $\beta^{(j)} \sim N((X'X)^{-1}X'y, \tau^{2(j-1)}(X'X)^{-1})$

  (b) RW for ϕ from target density
  $N(y \,|\, X\beta^{(j)}, \sigma^{2(j-1)}R(\phi) + \tau^{2(j-1)}I) \times p(\phi)$

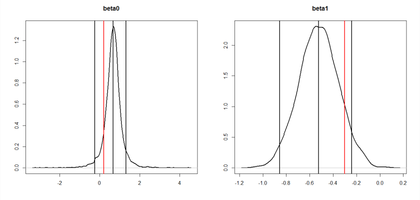
  (c) RW for σ^2 from $N(y \,|\, X\beta^{(j)}, \sigma^2 R(\phi^{(j)}) + \tau^{2(j-1)}I) \times p(\sigma^2)$

  (d) RW for τ^2 from target density
  $N(y \,|\, X\beta^{(j)}, \sigma^{2(j)}R(\phi^{(j)}) + \tau^2 I) \times p(\phi)$

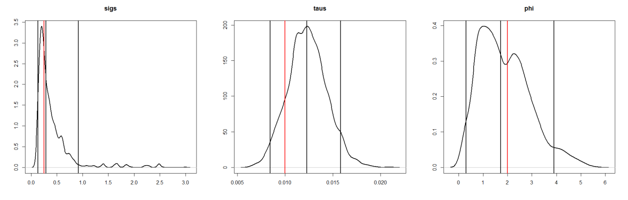
Nimble package

- `https://r-nimble.org/`
- Implements the MCMC for you
- You only need to specify the model and initialize the MCMC !
- We run the MCMC for the marginalized model for dataset 3 in Nimble

Parameter posteriors



β_0 β_1



σ^2 τ^2 ϕ

Recovering w

- The marginalized model integrates out the w's
- We can recover them after the MCMC
- $w \mid y, \beta, \sigma^2, \tau^2, \phi \sim N(V_w(y - X\beta)/\tau^2, V_w)$ where $V_w = (I/\tau^2 + R(\phi)^{-1}/\sigma^2)^{-1}$
- Use composition sampling

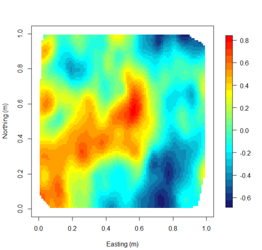


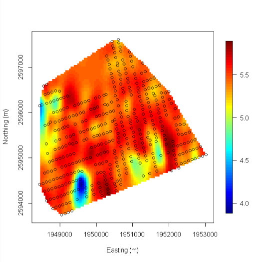
Figure: $w(\mathbf{s}) \mid y$

Predictions for the marginalized model

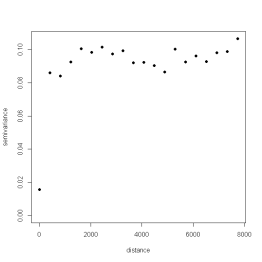
- Two ways to do predict $\tilde{y}(s) \,|\, y$ using composition sampling
- If you have already recovered w
  - Similar to the unmarginalized model
  - Generate $w(s_0) \,|\, w, params$ and then $\tilde{y}(s_0) \,|\, w(s_0), params$
- Direct approach (not requiring samples of w):
  - $c(s_0) = cov(w(s_0), w)$ and $\Sigma = \sigma^2 R(\phi) + \tau^2 I$
  - Generate samples of $\tilde{y}(s_0) \,|\, y, params \sim N(x(s_0)'\beta + c(s_0)'\Sigma^{-1}(y - X\beta), \sigma^2 + \tau^2 - c(s_0)'\Sigma^{-1}c(s_0))$

BEF data analysis in spBayes

- Dataset available in spBayes on long-term research studies on the Bartlett Experimental Forest, Bartlett, NH
- Forest inventory data for 437 locations
- Variables include species specific basal area and biomass; inventory plot coordinates; slope; elevation; and tasseled cap brightness (TC1), greenness (TC2), and wetness (TC3) components from spring, summer, and fall 2002 Landsat images



log biomass



Variogram

MCMC free Bayesian inference

- The marginalized model can be reparametrized as: $N(y, X\beta, \sigma^2(R(\phi) + \alpha I))$ where $\alpha = \tau^2/\sigma^2$
- If ϕ and α is fixed, we can do exact conjugate sampling
- *bayesGeostatExact* does that
- Fixed values of ϕ and α can be chosen from the variogram

	2.5%	25%	50%	75%	97.5%
(Intercept)	-0.624	0.267	0.728	1.182	2.079
Elevation	0.000	0.001	0.001	0.001	0.001
Slope	-0.017	-0.013	-0.011	-0.008	-0.004
Brightness	-0.001	0.006	0.010	0.013	0.021
Greenness	0.000	0.004	0.007	0.009	0.014
Wetness	0.015	0.021	0.024	0.028	0.034
σ^2	0.072	0.079	0.083	0.087	0.094
τ^2	0.014	0.016	0.016	0.017	0.019

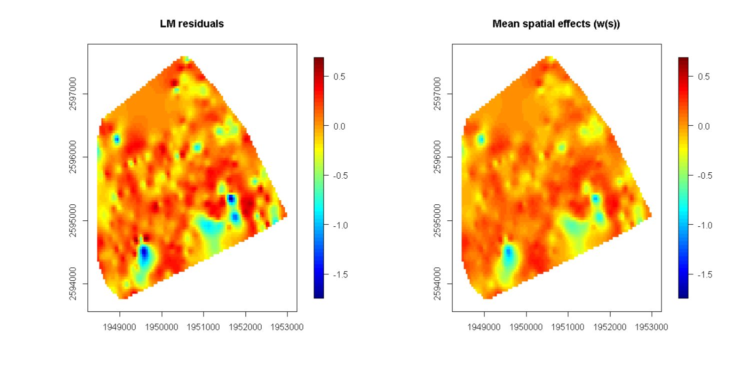
Full Bayesian inference

- *spLM* function
- Even marginalizes out β to make the chain only 3 dimensional

	2.5%	25%	50%	75%	97.5%
(Intercept)	-0.253	0.937	1.586	2.069	3.189
Elevation	0.000	0.000	0.000	0.001	0.001
Slope	-0.017	-0.011	-0.008	-0.005	0.002
Brightness	-0.005	0.006	0.010	0.015	0.025
Greenness	-0.005	0.003	0.005	0.008	0.014
Wetness	0.007	0.015	0.019	0.023	0.032
σ^2	0.042	0.074	0.086	0.095	0.108
τ^2	0.005	0.010	0.015	0.030	0.063
ϕ	0.004	0.008	0.010	0.012	0.016

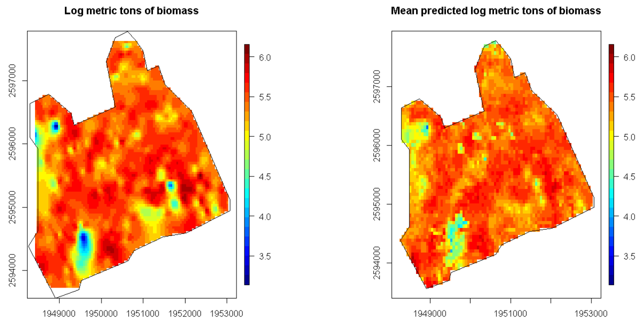
Recovery of $w(s)$

- *spRecover* function recovers both β and w



Kriging

- *spPredict* function



What we covered today

- Convergence diagnostics
- Model comparison using Bayesian output
- MH algorithm
- Writing your on MCMC
- Using Nimble package to run the MCMC
- Spatial predictions from Bayesian output
- MCMC-free and fully Bayesian spatial analysis using spBayes package

References

- Expository article on Gibbs sampler: Casella, G. and George, E.I. (1992), Explaining the Gibbs Sampler, The American Statistician, 46, 167-174.
- Expository article on MH algorithm: Chib, S. and Greenberg, E. (1995), Understanding the Metropolis-Hastings Algorithm, The American Statistician, 49, 327-335.
- DIC Spiegelhalter, D. J., and Best, N. G., and Carlin, B. P., and van der Linde, A. (2002). *Bayesian measures of model complexity and fit* Journal of the Royal Statistical Society, Series B. 64 (4), 583-63
- Great slides on convergence diagnostics of Markov Chains `http://patricklam.org/teaching/convergence_print.pdf`
- Gelfand, A. E. , and Smith. A. F. M. (1990). *Sampling-Based Approaches to Calculating Marginal Densities.* Journal of the American Statistical Association, 85(410), 398–409.
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