Inference from iterative simulation using multiple sequences

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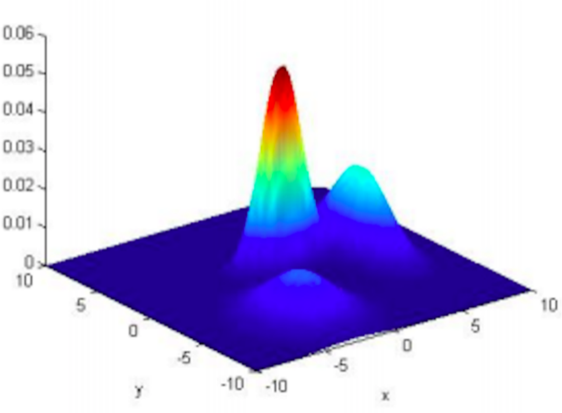
April 2, 2015

Motivation



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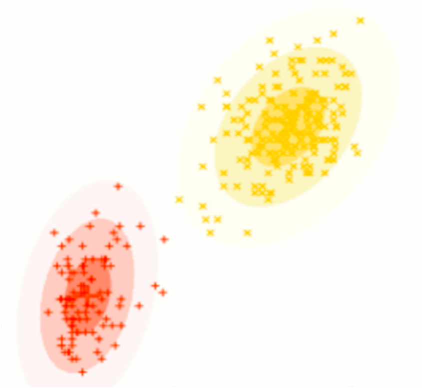

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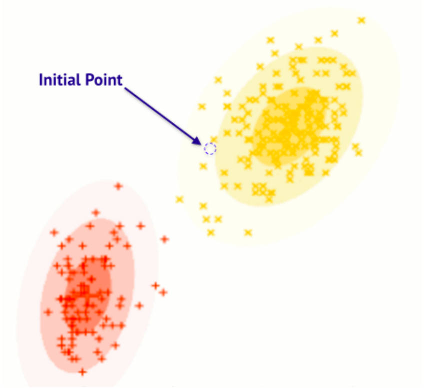

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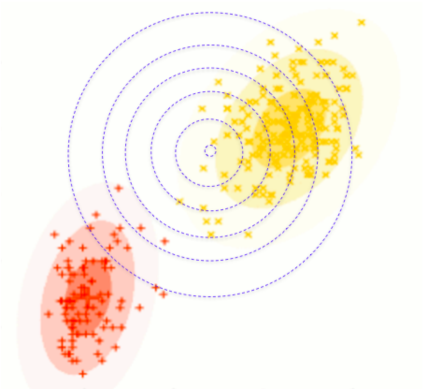

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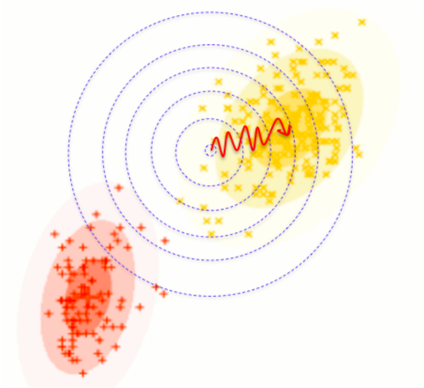
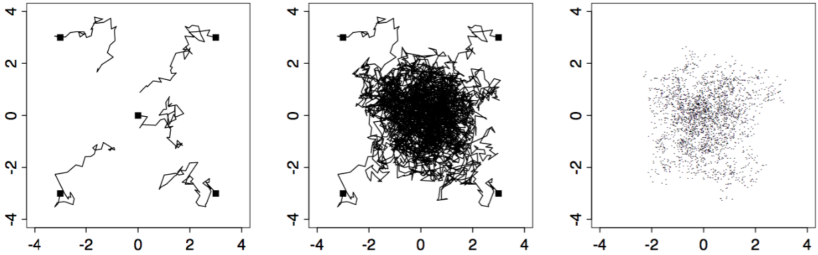


Iterative simulation using multiple sequences



Choosing initial points

1. Locate the modes using EM
2. Sample N points from a mixture of t-distributions centered at the modes
3. Sharpen the overdispersed approximation using sequential importance resampling (SIR; Rubin, 1987)
   - Gives m samples, one for starting each chain, from the set of N

Monitoring convergence

1. Gelman-Rubin diagnostic ($\hat{R}$)
2. Effective number of simulation draws ($\hat{n}_{eff}$)

Other diagnostics:

- Visuals: traceplots, autocorrelation plots, empirical density plots
- Acceptance rate
- Heidelberg and Welch diagnostic (1983)
- Geweke diagnostic (1992)
- Raftery and Lewis diagnostic (1992)

Procedure

- Run $m \geq 2$ sequences of length $2n$ from the starting values and discard the first n draws in each sequence

For each parameter of interest:

1. Calculate the between- and within-sequence variances
2. Estimate the total variance using a combining rule
3. Compute a ratio of variances $\sqrt{\hat{R}}$, known as the *potential scale reduction factor* (Gelman and Rubin, 1992)

Continue running chains until PSRF is sufficiently close to 1 for all (or "enough") estimands.

Within-sequence variance

For each scalar estimand ψ, let ψ_{ij} be the i^{th} estimand (p estimands) from the j^{th} chain (m chains)

$$W = \frac{1}{m}\sum_{j=1}^{m} s_j^2$$

where

$$s_j^2 = \frac{1}{n-1}\sum_{j=1}^{n}(\psi_{ij} - \bar{\psi}_{.j})^2, \ \bar{\psi}_{.j} = \frac{1}{n}\sum_{i=1}^{n}\psi_{ij}$$

Between-sequence variance

$$B/n = \frac{1}{m-1}\sum_{j=1}^{m}(\bar{\psi}_{.j} - \bar{\psi}_{..})^2$$

where

$$\bar{\psi}_{.j} = \frac{1}{n}\sum_{i=1}^{n}\psi_{ij},\ \ \bar{\psi}_{..} = \frac{1}{m}\sum_{j=1}^{m}\psi_{.j}$$

Total variance

Estimate $\mathrm{var}(\psi|y)$, the marginal posterior variance of the estimator, by a weighted average of W and B

$$\hat{var}^{+}(\psi|y) = \frac{n-1}{n} W + B/n$$

- Consistency guarantee!

Total variance

Estimate $\mathrm{var}(\psi|y)$, the marginal posterior variance of the estimator, by a weighted average of W and B

$$\hat{var}^+(\psi|y) = \frac{n-1}{n}W + B/n$$

- Consistency guarantee!
- For finite n, $\hat{var}^+(\psi|y)$ will underestimate the true variance.

Using

$$\widehat{V} = \hat{var}^+(\psi|y) + (1/m)B/n$$

adjusts for the uncertainty in estimating $\bar{\psi}_{..}$ (Rubin, 1987; Ch. 4)

Potential scale reduction factor

$$\sqrt{\hat{R}} = \sqrt{\frac{\widehat{V}}{W}}$$

- $\widehat{V}$ *overestimates* the true variance of the target distribution
- W *underestimates* the true variance of the target distribution
- If $\sqrt{\hat{R}}$ is high (say, greater than 1.1), then we have reason to believe that the chains have not converged

Evolution of $\hat{R}$

$$\sqrt{\hat{R}} = \sqrt{\frac{\hat{V}}{W}}$$ Gelman and Rubin (1992)

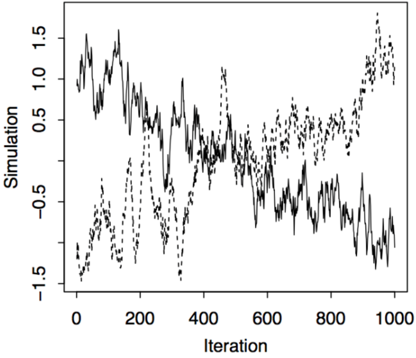
$$\sqrt{\hat{R}} = \sqrt{\frac{\hat{var}^{+}(\psi|y)}{W}}$$ BDA1 (1995)

$$\hat{R}^{p} = \frac{n-1}{n} + \frac{m+1}{m} \max_{a} \frac{a^{T}\widehat{V}_{cov}a}{a^{T}W_{cov}a}$$ Brooks and Gelman (1998)

$$\hat{R}_{split} = \sqrt{\frac{\hat{var}^{+}(\psi|y)}{W}}$$ on *split chains*, BDA3 (2013)

Unsplit-$\hat{R}$ and split-$\hat{R}$

The unsplit-$\hat{R}$ would not correctly diagnose the poor convergence in nonstationarity as below:



Effective number of simulation draws

1. Account for ρ_t, autocorrelation of the sequence ψ at lag t
2. Define the effective sample size as:

$$n_{eff} = \frac{mn}{1+2\sum_{t=1}^{\infty} \rho_t}$$

3. Estimate autocorrelations:

$$\hat{\rho}_t = 1 - \frac{V_t}{2\widehat{var}^+(\psi|y)}$$

4. Compute a positive partial sum for autocorrection:

$$\hat{n}_{eff} = \frac{mn}{1+2\sum_{t=1}^{T} \hat{\rho}_t}$$

Where the Gelman-Rubin diagnostic fails

- Full coverage: If important areas of the target distribution were not captured by the starting distribution and are not easily reachable by the proposals...
- Computational efficiency: Given finite runtime constraints, how to assess the time it takes to get mn desired samples?
- Precognition: Can we assess the the rate of convergence before the actual convergence of the chains?

Other ideas: Markov-normal based analysis

(Liu and Rubin, 1996; Liu and Rubin, 2002)

Assumption: Target distribution of the simulated Markov chains is approximately normal.

1. Obtain ML estimates of the target distribution from multiple sequences *before their convergence*
2. Use pre-convergence ML estimates to *define a restarting distribution for the simulations*, *assess convergence rate*, and/or *analyze problematic areas in the simulation*

Other ideas: Markov-normal based analysis

Suppose all transition distributions for chains are

$$X_j^{(t)}|(X_j^{(t-1)}, \ldots, X_j^{(0)} \sim N_d(\beta X_j^{(t-1)} + \gamma, \Delta), t = 1, 2, \ldots$$

This is the $AR(1)$ multivariate time-series model, and the target distribution is

$$N_d(\beta\mu + \gamma, \beta\Psi\beta^T + \Delta)$$

Other ideas: Markov-normal based analysis

We have

$$(X^{(t)} - \mu) = \beta(X^{(t-1)} - \mu) + \epsilon^{(t)},\ \ \epsilon^{(t)} \sim N_d(0, \Delta)$$

- $X^{(t)}$'s are independent of $\epsilon^{(t)}$
- $\mathrm{Cov}(X^{(t)}, X^{(t-1)}) = \beta\Psi$
- Correlation of normalized values $\mathrm{Cor}(\Psi^{-1/2}X^{(t)}, \Psi^{-1/2}X^{(t-1)}) = \Psi^{-1/2}\beta\Psi^{1/2}$

Other ideas: Markov-normal based analysis

The rate of convergence of $P^{(t)}(X)$ to $P(X)$ is the *spectral radius* of the matrix β: $\max_{|\lambda|}\{|\lambda_i(\beta)|\}$. This can be difficult to compute (possibly complex number).

Alternatively consider the square root of the spectral radius ρ of the PSD matrix

$$M = (\mathrm{Cor}(\Psi^{-1/2}X^{(t)}, \Psi^{-1/2}X^{(t-1)}))(\mathrm{Cor}(\Psi^{-1/2}X^{(t)}, \Psi^{-1/2}X^{(t-1)}))^T$$
$$= \Psi^{-1/2}\beta\Psi\beta^T\Psi^{-1/2}$$

Other ideas: Markov-normal based analysis

Consider

$$S = I - M = \Psi^{-1/2} \Delta \Psi^{-1/2}$$

the *squared speed matrix* of the underlying MCMC scheme.

- S is related to the fraction of observed information: $\operatorname{Var}(X) / \operatorname{Var}(X | X^{(t)})$
- Intuition: the larger the within-variance covariance matrix Δ with respect to the target covariance matrix Ψ, the faster the algorithm converges because the fraction of missing information is less

Other ideas: Markov-normal based analysis

Let $Z^{(t)} = \Psi^{-1/2}(X^{(t)} - \mu)$. Then $Z^{(t)}|Z^{(t-1)} \sim N_d(0, S)$.

- If the eigenvalues of S are all 1, converges in one step; if zero, then MCMC scheme never converges
- The eigenvalues govern the rate of convergence in each dimension, and the minimal eigenvalue is the slowest

$$\rho = (1 - \lambda_1)^{1/2}$$

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