

Use of Importance sampling with MCMC algorithms

J. Rousseau

CEREMADE, Université Paris-Dauphine

Warwick

Joint work with C. Guihennec, R. McVinish, K. Mengersen,
D. Nur

- 1 General ideas
 - Motivation
 - Framework
- 2 Theoretical properties
 - Limit results
 - Behaviour of the weights
 - Stabilization by recentering
- 3 Some simulated examples
 - test in regression

- 1 General ideas
 - Motivation
 - Framework
- 2 Theoretical properties
 - Limit results
 - Behaviour of the weights
 - Stabilization by recentering
- 3 Some simulated examples
 - test in regression

Motivation

► Repeated MCMC under different samples :

- Bayesian p -values. X^o = observed sample

Let $H_\pi(X) = E^\pi[h(\theta)|X]$ be a test statistic and

$P[H(X) > H(X^o)] = p(X^o)$: a p value to evaluate $p(X^o)$
compute

- For $j = 1, \dots, J$ $X^{(j)} \sim P$ and compute $H(X^{(j)})$

BUT... $H(X^{(t)})$ evaluated using MCMC $\forall t \rightarrow$ Time consuming

- Bayesian cross validation : Need of computing $H(X^{(-l)})$, where $X^{(-l)} \subset X$ for many $(-l)$.

- Evaluation of procedures by simulations

► **prior sensitivity analysis** : Need to compute $H_{\pi_j}(X)$ for different π_j .

Motivation

► Repeated MCMC under different samples :

- Bayesian p -values. X^o = observed sample

Let $H_\pi(X) = E^\pi[h(\theta)|X]$ be a test statistic and

$P[H(X) > H(X^o)] = p(X^o)$: a p value to evaluate $p(X^o)$
compute

- For $j = 1, \dots, J$ $X^{(j)} \sim P$ and compute $H(X^{(j)})$
-

$$\hat{p}(X^o) = \frac{1}{J} \sum_{j=1}^J \mathbb{I}_{H(X^{(j)}) > H(X^o)}$$

BUT... $H(X^{(t)})$ evaluated using MCMC $\forall t \rightarrow$ Time consuming

- Bayesian cross validation : Need of computing $H(X^{(-l)})$, where $X^{(-l)} \subset X$ for many $(-l)$.
- Evaluation of procedures by simulations

► **prior sensitivity analysis** : Need to compute $H_{\pi_j}(X)$ for different π_j .

Outline

- 1 General ideas
 - Motivation
 - Framework
- 2 Theoretical properties
 - Limit results
 - Behaviour of the weights
 - Stabilization by recentering
- 3 Some simulated examples
 - test in regression

- **Bayesian model**

$$X \sim f_{\theta}, \quad \theta \in \Theta, \quad \theta \sim \pi,$$

- **Object of interest** $H_{\pi}(X) = E^{\pi}[h(\theta)|X]$

- **Evaluation with MCMC** $(\theta^t)_{t=1}^T = \text{MC}(\pi(\cdot|X))$

$$\hat{H}_{\pi}(X) = \frac{1}{T} \sum_t h(\theta^t)$$

- **New sample** : $Y \stackrel{d}{=} X$

$$H_{\pi}(Y) = \frac{\int_{\Theta} h(\theta) [f(Y|\theta)/f(X|\theta)] d\pi(\theta|X)}{\int_{\Theta} [f(Y|\theta)/f(X|\theta)] d\pi(\theta|X)}$$

$$H_{\pi}(Y) = \frac{\int_{\Theta} h(\theta) [f(Y|\theta)/f(X|\theta)] d\pi(\theta|X)}{\int_{\Theta} [f(Y|\theta)/f(X|\theta)] d\pi(\theta|X)}$$

So **No need to run a new MCMC** : use IS on $(\theta^t)_t$:

$$\hat{H} = \frac{\sum_{t=1}^T h(\theta^t) w(\theta^t, y, x)}{\sum_{t=1}^T w(\theta^t, y, x)} = \frac{\bar{h}\bar{w}}{\bar{w}},$$

where

$$w(\theta, y, x) = \frac{f_{\theta^t}(y)}{f_{\theta^t}(x)}, \quad \text{or} \quad w(\theta, \pi', \pi) = \frac{\pi'(\theta)}{\pi(\theta)},$$

- ▶ **Much quicker**
- ▶ **How good/bad is it ?**

Outline

- 1 General ideas
 - Motivation
 - Framework
- 2 Theoretical properties
 - Limit results
 - Behaviour of the weights
 - Stabilization by recentering
- 3 Some simulated examples
 - test in regression

Convergence

► Back to the theory on MCMC convergence :

- Consistency (in T) : OK if MC ergodic
- rate : In the original MC : estimation of the function

$$\tilde{h}(\theta) = h(\theta) \frac{f(Y|\theta)}{f(X|\theta)}$$

Usual tools • Asymptotic Variance

$$\gamma^2 = \frac{m_\pi(x)^2}{m_{\pi'}(y)^2} \left[H_\pi^2 \text{var}(\bar{w}) + \text{var}(h\bar{w}) - 2\text{cov}(\bar{w}, h\bar{w}) H_\pi \right].$$

- Variance estimation : Same as var as

$$Z(\theta_t) = \frac{\mathbb{E}_\pi(h(\theta)w(\theta))}{\mathbb{E}_\pi(w(\theta))} \left(\frac{w(\theta_t)}{\mathbb{E}_\pi(w(\theta))} - \frac{h(\theta_t)w(\theta_t)}{\mathbb{E}_\pi(h(\theta)w(\theta))} \right)$$

Outline

- 1 General ideas
 - Motivation
 - Framework
- 2 Theoretical properties
 - Limit results
 - **Behaviour of the weights**
 - Stabilization by recentering
- 3 Some simulated examples
 - test in regression

Behaviour of the weights

$$w(\theta, y, x) = \frac{f_{\theta^t}(y)}{f_{\theta^t}(x)}, \quad \tilde{w}(\theta) = \pi(\theta|x)/\pi(\theta|y)$$

$$x = (x_1, \dots, x_n) \stackrel{d}{=} y = (y_1, \dots, y_n) + \text{regul. condits} \Rightarrow$$

$$\tilde{w}(\theta) = e^{n(\hat{\theta}^x - \hat{\theta}^y)' I(\theta_0)(\theta - \hat{\theta}^x)} (1 + O(n^{-1/2})),$$

$$\text{var}_{as}(\tilde{w}(\theta) \mid x, y) = \exp \left\{ n(\hat{\theta}^x - \hat{\theta}^y)' I(\theta_0)(\hat{\theta}^x - \hat{\theta}^y) \right\} - 1.$$

► **Stability** $\hat{\theta}^x \neq \hat{\theta}^y \longrightarrow \text{Instability.}$

Outline

- 1 General ideas
 - Motivation
 - Framework
- 2 Theoretical properties
 - Limit results
 - Behaviour of the weights
 - **Stabilization by recentering**
- 3 Some simulated examples
 - test in regression

Stabilization by recentering

► Simple stabilization

$$\theta'_t = \theta_t + \hat{\theta}^y - \hat{\theta}^x, \quad w'(\theta_t) = \frac{\pi(\theta'_t)f(y^n|\theta'_t)}{\pi(\theta_t)f(x^n|\theta_t)} = 1 + O_P(n^{-1/2})$$

- Very effective if posterior not too strongly multimodal
- Often $\hat{\theta}^x$ complicated to calculate : Two-step procedure

► Compute centering

$$\tilde{\theta}^y = \frac{\sum_t \theta_t w_t}{\sum_t w_t}$$

► Apply centering

$$\theta'_t = \theta_t + \tilde{\theta}^y - \tilde{\theta}^x$$

- **Conditions** x and y have marginally the same distribution but are not nece. indpdt.

see also MacEachern+Perrugia

Outline

- 1 General ideas
 - Motivation
 - Framework
- 2 Theoretical properties
 - Limit results
 - Behaviour of the weights
 - Stabilization by recentering
- 3 Some simulated examples
 - test in regression

Regression example (explicit calculations)

► **Problem** : Test for

$$H_0 : Y_i \sim \mathcal{N}(\beta_0, \sigma^2) \quad H_1 : Y_i \sim \mathcal{N}(\beta_0 + \beta_1 x_i, \sigma^2)$$

► **test procedure** : $|\beta_1| < \epsilon$ versus $|\beta_1| \geq \epsilon \Rightarrow$

$$H_0 \quad \text{iff } H(Y) = E^\pi \left[\beta_1^2 | Y \right] < \epsilon$$

► **pb** : **Choice of ϵ ?** \Rightarrow use of p -value

Under H_0 $\theta = (\beta_0, \sigma)$ unknown \Rightarrow Use of conditional predictive p -value (Bayarri+Berger, Robbins et al., Robert + Rousseau, Fraser + Rousseau)

$$p(Y^0) = \int_{\Theta} P_{\theta}[H(Y) > H(Y^0) | \hat{\theta}] d\pi_0(\theta | \hat{\theta}) = P_{\theta}[H(Y) > H(Y^0) | \hat{\theta}]$$

Special case here : $\pi(\beta_0, \beta_1, \sigma) \propto 1/\sigma$ and $n = 250$.

$$H(y) = \mathbb{E}_{\pi} \left(\beta_1^2 \mid y, x \right) = \hat{\beta}_1^2 + \frac{\sum (y_i - \hat{y}_i)^2}{(n-4) \sum (x_i - \bar{x})^2},$$

► **Algorithm for each p -value**

- $[Y^1 | \hat{\beta}_0, \hat{\sigma}] \sim f(Y | \hat{\theta}) = \mathcal{U}_E + \text{MCMC } \pi(\psi | Y^1) \quad \psi = (\beta_0, \beta_1, \sigma),$

$$\rightarrow \psi^t, \quad t = 1, \dots, T$$

- For $j = 2, \dots, J$ Simulate $[Y^j | \hat{\beta}_0, \hat{\sigma}] \stackrel{iid}{\sim} f(Y | \hat{\theta})$
- $\forall j = 2, \dots, J$ compute $w_t(\psi^t, Y^j, Y^1)$ and $\hat{\psi}^j$ and

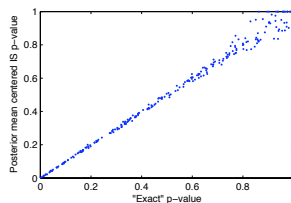
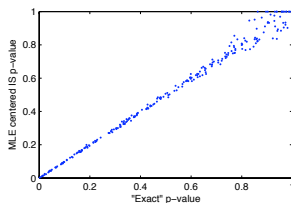
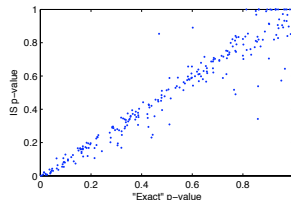
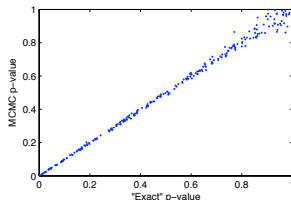
$$H_S(Y^j) = \frac{\sum_t w_t (\beta_1^t)^2}{\sum_t w_t}, \quad \text{and also } \mathbb{E}_{\pi} \left(\beta_1^2 \mid Y^j \right)$$

$$H_{CS1} = \frac{\sum_t w'_t ((\beta_1^t)')^2}{\sum_t w'_t}, \quad (\psi^t)' = \psi^t + \hat{\psi}^j - \hat{\psi}^1$$

$$H_{CS2} = \frac{\sum_t w''_t ((\beta_1^t)'')^2}{\sum_t w''_t}, \quad (\psi^t)'' = \psi^t + E^{\pi}[\psi | Y^j] - E^{\pi}[\psi | Y^1]$$

Results

250 p -values and for each : $J = 1000$ (M.C samples) and $T = 10^5$ (MCMC samples) with burn-in = 1000



Weights

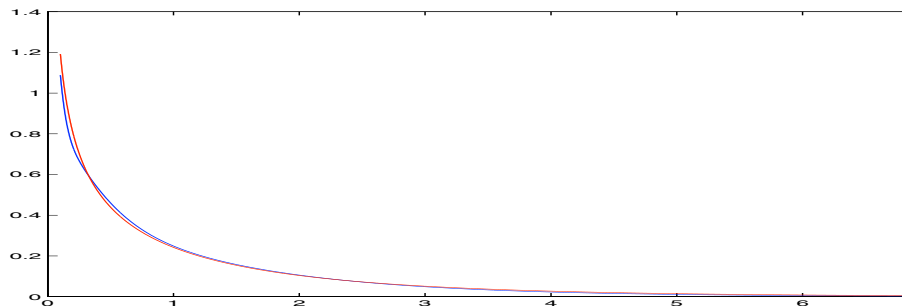


FIG.: Blue line is a kernel density estimate of the calculated variance of the normalised IS weights. Red line is the density of a χ_1^2 distribution.

- Weights : close to asymptotic

- Weights : close to asymptotic
- IS simple : OK but not marvelous

- Weights : close to asymptotic
- IS simple : OK but not marvelous
- IS recentered (MLE or posterior) : much better

- Weights : close to asymptotic
- IS simple : OK but not marvelous
- IS recentered (MLE or posterior) : much better
- posterior distribution : close to Gaussian \Rightarrow perfect for recentering.

GOF : Nonparametric example

► Problem

$$H_0 : f_* \in \mathcal{F} \quad \text{against} \quad H_1 : f_* \notin \mathcal{F}, \quad \mathcal{F} = \{f_\theta, \theta \in \Theta \subset \mathbb{R}^d\}$$

► Nonparametric model for \mathcal{F}^c (VW+RR+R)

$$F(y \mid \theta) \sim G_\psi, \quad \psi \in \mathcal{S} \quad \text{on } [0, 1] \quad \exists \psi_0; g_{\psi_0} \equiv 1$$

If $Y \sim f_\theta$ then $F(Y \mid \theta) \sim \mathcal{U}(0, 1)$. Model :

$$f_*(y \mid \theta, \psi) = f(y \mid \theta)g(F(y \mid \theta) \mid \psi), \theta \in \Theta, \quad \psi \in \mathcal{S}$$

► prior on H_1

$$d\pi_1(\theta, \psi) = d\pi_0(\theta)d\pi(\psi)$$

- ▶ **Test statistic** (Bayesian) $H(x) = \mathbb{E}_{\pi_1}[d(1, g(\cdot | \psi)) | x]$
- ▶ **p-value**

$$p(x^0) = \int_{\Theta} P_{\theta}[H(y) > H(x^0) | \hat{\theta}] \pi_0(\theta) d\theta$$

- ▶ **Set up here** $f_{\theta} \equiv \exp(\theta)$ $\pi_0 = \Gamma(\gamma_1, \gamma_2)$ $\pi_1 =$ mixture of triangular distributions (fixed partition, random weights)
 $\psi = (k, \omega)$, $k \in \mathbb{N}$, $\omega \in \mathcal{S}_k = \{z \in [0, 1]^k; \sum_{i=0}^k z_i = 1\}$,

$$g(y | \omega, k) = \sum_{i=0}^k \omega_i h_i(y; k), \quad \pi(k) = C(\rho) \rho^k, \quad k \geq 1,$$
$$\pi(\omega | k) = \mathcal{D}(\alpha_{0,k}, \dots, \alpha_{k,k}),$$

Algorithm

- $y^1 | \hat{\theta}^x \sim f(y | \hat{\theta}^y = \hat{\theta}^x)$

Algorithm

- $y^1 | \hat{\theta}^x \sim f(y | \hat{\theta}^y = \hat{\theta}^x)$
- **MCMC** = RJMCMC $\eta^t = (\theta^t, k^t, \omega^t)$ for $\pi(\eta | y^1)$

Compute $H(y^1)$

Algorithm

- $y^1 | \hat{\theta}^x \sim f(y | \hat{\theta}^y = \hat{\theta}^x)$
- **MCMC** = RJMCMC $\eta^t = (\theta^t, k^t, \omega^t)$ for $\pi(\eta | y^1)$

Compute $H(y^1)$

- $\forall j = 2, \dots, J$ $y^j \stackrel{d}{=} y^1$ (iid)

Compute $w_t(\eta^t, y^j, y^1) \Rightarrow H(y^j) \Rightarrow p(x^0) = \frac{\sum_j \mathbb{1}_{H(y^j) > H(x^0)}}{J}$

Algorithm

- $y^1 | \hat{\theta}^x \sim f(y | \hat{\theta}^y = \hat{\theta}^x)$
- **MCMC** = RJMCMC $\eta^t = (\theta^t, k^t, \omega^t)$ for $\pi(\eta | y^1)$

Compute $H(y^1)$

- $\forall j = 2, \dots, J$ $y^j \stackrel{d}{=} y^1$ (iid)

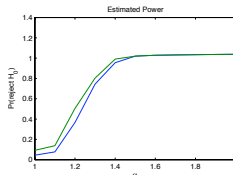
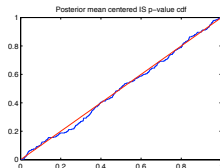
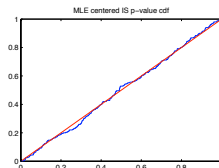
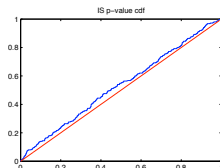
Compute $w_t(\eta^t, y^j, y^1) \Rightarrow H(y^j) \Rightarrow p(x^0) = \frac{\sum_j \mathbb{I}_{H(y^j) > H(x^0)}}{J}$

- Recentering : only on $k = 2$: MLE or posterior mean of (θ, w_1) Because

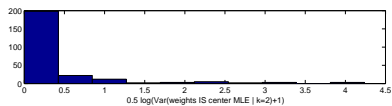
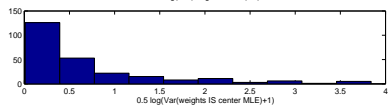
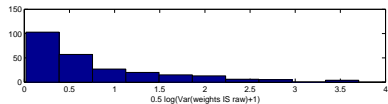
$$P^\pi[k = 2 | y_1, \dots, y_n] = 1 + o_P(1), \quad \text{if } y = (y_1, \dots, y_n) \in H_0$$

results

$n = 250$, $x^0 \sim \exp(1/4)$, $J = 1000$, $T = 100000$ with burn-in = 5000 and 250 p -values



weights



- IS in MCMC for repeated sampling : promising

conclusion

- IS in MCMC for repeated sampling : promising
- curse of dimensionality not so severe

conclusion

- IS in MCMC for repeated sampling : promising
- curse of dimensionality not so severe
- Much quicker

conclusion

- IS in MCMC for repeated sampling : promising
- curse of dimensionality not so severe
- Much quicker
- possible simple improvements : recentering (+ rescaling)

conclusion

- IS in MCMC for repeated sampling : promising
- curse of dimensionality not so severe
- Much quicker
- possible simple improvements : recentering (+ rescaling)
- Other improvements : If data set y^j too different from y^1 IS not too good : consider (y^1, \dots, y^{J_0}) Guihenneuc et al.
 - for each : 1 MCMC
 - New y^j : choose *best* $y^l, l = 1, \dots, J_0$ compute IS with it.

conclusion

- IS in MCMC for repeated sampling : promising
- curse of dimensionality not so severe
- Much quicker
- possible simple improvements : recentering (+ rescaling)
- Other improvements : If data set y^j too different from y^1 IS not too good : consider (y^1, \dots, y^{J_0}) Guihenneuc et al.
 - for each : 1 MCMC
 - New y^j : choose *best* $y^l, l = 1, \dots, J_0$ compute IS with it.
- Excellent for prior sensitivity analysis

- IS in MCMC for repeated sampling : promising
- curse of dimensionality not so severe
- Much quicker
- possible simple improvements : recentering (+ rescaling)
- Other improvements : If data set y^j too different from y^1 IS not too good : consider (y^1, \dots, y^{J_0}) Guihenneuc et al.
 - for each : 1 MCMC
 - New y^j : choose *best* $y^l, l = 1, \dots, J_0$ compute IS with it.
- Excellent for prior sensitivity analysis
- Non stationarity \Rightarrow bad.