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Joint work with Nicolas Chopin and Jean-Michel Marin

Outline



Introduction

- 2 Importance sampling solutions
- 3 Cross-model solutions
- 4 Nested sampling





Introduction

-Bayes factor

Bayes factor

Definition (Bayes factors)

For testing hypotheses H_0 : $\theta \in \Theta_0$ vs. H_a : $\theta \notin \Theta_0$, under prior

 $\pi(\Theta_0)\pi_0(\theta) + \pi(\Theta_0^c)\pi_1(\theta)\,,$

central quantity

$$B_{01} = \frac{\pi(\Theta_0|x)}{\pi(\Theta_0^c|x)} \Big/ \frac{\pi(\Theta_0)}{\pi(\Theta_0^c)} = \frac{\int_{\Theta_0} f(x|\theta)\pi_0(\theta)d\theta}{\int_{\Theta_0^c} f(x|\theta)\pi_1(\theta)d\theta}$$
[Jeffreys, 1939]

-Introduction

-Bayes factor

Self-contained concept

Outside decision-theoretic environment:

- $\bullet\,$ eliminates impact of $\pi(\Theta_0)$ but depends on the choice of (π_0,π_1)
- Bayesian/marginal equivalent to the likelihood ratio
- Jeffreys' scale of evidence:
 - if $\log_{10}(B_{10}^{\pi})$ between 0 and 0.5, evidence against H_0 weak,
 - if $\log_{10}(B_{10}^{\pi}) \ 0.5$ and 1, evidence substantial,
 - if $\log_{10}(B_{10}^{\pi}) \ 1$ and 2, evidence *strong* and
 - if $\log_{10}(B_{10}^{\pi})$ above 2, evidence *decisive*
- Requires the computation of the marginal/evidence under both hypotheses/models

Introduction

└─ Model choice

Model choice and model comparison

Choice between models

Several models available for the same observation

$$\mathfrak{M}_i: x \sim f_i(x|\theta_i), \qquad i \in \mathfrak{I}$$

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where $\ensuremath{\mathfrak{I}}$ can be finite or infinite

Introduction

└─ Model choice

Bayesian resolution

Probabilise the entire model/parameter space

- allocate probabilities p_i to all models \mathfrak{M}_i
- define priors $\pi_i(heta_i)$ for each parameter space Θ_i
- compute

$$\pi(\mathfrak{M}_i|x) = \frac{p_i \int_{\Theta_i} f_i(x|\theta_i) \pi_i(\theta_i) \mathrm{d}\theta_i}{\sum_j p_j \int_{\Theta_j} f_j(x|\theta_j) \pi_j(\theta_j) \mathrm{d}\theta_j}$$

 take largest \(\mathcal{m}_i | x)\) to determine "best" model, or use averaged predictive

$$\sum_{j} \pi(\mathfrak{M}_{j}|x) \int_{\Theta_{j}} f_{j}(x'|\theta_{j}) \pi_{j}(\theta_{j}|x) \mathrm{d}\theta_{j}$$

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Introduction

Evidence

Evidence

All these problems end up with a similar quantity, the evidence

$$\mathfrak{Z} = \int \pi(\theta) L(\theta) \, \mathrm{d}\theta,$$

aka the marginal likelihood.

Importance sampling solutions

Regular importance

Bridge sampling

lf

$$\begin{array}{rcl} \pi_1(\theta_1|x) & \propto & \tilde{\pi}_1(\theta_1|x) \\ \pi_2(\theta_2|x) & \propto & \tilde{\pi}_2(\theta_2|x) \end{array}$$

live on the same space, then

$$B_{12} \approx \frac{1}{n} \sum_{i=1}^{n} \frac{\tilde{\pi}_1(\theta_i | x)}{\tilde{\pi}_2(\theta_i | x)} \qquad \theta_i \sim \pi_2(\theta | x)$$

[Gelman & Meng, 1998; Chen, Shao & Ibrahim, 2000]

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Importance sampling solutions

Regular importance

(Further) bridge sampling

In addition

$$B_{12} = \frac{\int \tilde{\pi}_2(\theta|x)\alpha(\theta)\pi_1(\theta|x)d\theta}{\int \tilde{\pi}_1(\theta|x)\alpha(\theta)\pi_2(\theta|x)d\theta} \qquad \forall \alpha(\cdot)$$

$$\approx \frac{\frac{1}{n_1} \sum_{i=1}^{n_1} \tilde{\pi}_2(\theta_{1i}|x) \alpha(\theta_{1i})}{\frac{1}{n_2} \sum_{i=1}^{n_2} \tilde{\pi}_1(\theta_{2i}|x) \alpha(\theta_{2i})} \qquad \theta_{ji} \sim \pi_j(\theta|x)$$

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Importance sampling solutions

Regular importance

Optimal bridge sampling

The optimal choice of auxiliary function α

$$\alpha^{\star} = \frac{n_1 + n_2}{n_1 \tilde{\pi}_1(\theta|x) + n_2 \tilde{\pi}_2(\theta|x)}$$

leading to

$$\widehat{B}_{12} \approx \frac{\frac{1}{n_1} \sum_{i=1}^{n_1} \frac{\widetilde{\pi}_2(\theta_{1i}|x)}{n_1 \widetilde{\pi}_1(\theta_{1i}|x) + n_2 \widetilde{\pi}_2(\theta_{1i}|x)}}{\frac{1}{n_2} \sum_{i=1}^{n_2} \frac{\widetilde{\pi}_1(\theta_{2i}|x)}{n_1 \widetilde{\pi}_1(\theta_{2i}|x) + n_2 \widetilde{\pi}_2(\theta_{2i}|x)}}$$

Back later!

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Importance sampling solutions

Harmonic means

Approximating \mathfrak{Z} from a posterior sample

Use of the identity

$$\mathbb{E}^{\pi}\left[\left.\frac{\varphi(\theta)}{\pi(\theta)L(\theta)}\right|x\right] = \int \frac{\varphi(\theta)}{\pi(\theta)L(\theta)} \frac{\pi(\theta)L(\theta)}{\mathfrak{Z}} \,\mathrm{d}\theta = \frac{1}{\mathfrak{Z}}$$

no matter what the proposal $\varphi(\theta)$ is. [Gelfand & Dey, 1994; Bartolucci et al., 2006]

Direct exploitation of MCMC output

▶ RB-RJ

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Importance sampling solutions

Harmonic means

Comparison with regular importance sampling

Harmonic mean: Constraint opposed to usual importance sampling constraints: $\varphi(\theta)$ must have lighter (rather than fatter) tails than $\pi(\theta)L(\theta)$ for the approximation

$$\widehat{\mathfrak{Z}_1} = 1 \middle/ \frac{1}{T} \sum_{t=1}^T \frac{\varphi(\theta^{(t)})}{\pi(\theta^{(t)})L(\theta^{(t)})}$$

to have a finite variance.

E.g., use finite support kernels (like Epanechnikov's kernel) for arphi

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E.g., use finite support kernels (like Epanechnikov's kernel) for φ

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Importance sampling solutions

Harmonic means

Comparison with regular importance sampling (cont'd)

Compare $\widehat{\mathfrak{Z}_1}$ with a standard importance sampling approximation

$$\widehat{\mathfrak{Z}_2} = \frac{1}{T} \sum_{t=1}^T \frac{\pi(\theta^{(t)})L(\theta^{(t)})}{\varphi(\theta^{(t)})}$$

where the $\theta^{(t)}$'s are generated from the density $\varphi(\theta)$ (with fatter tails like t's)

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Importance sampling solutions

Harmonic means

Approximating \mathfrak{Z} using a mixture representation

Bridge sampling redux

Design a specific mixture for simulation [importance sampling] purposes, with density

$$\tilde{\varphi}(\theta) \propto \omega_1 \pi(\theta) L(\theta) + \varphi(\theta) \,,$$

where $\varphi(\theta)$ is arbitrary (but normalised) Note: ω_1 is not a probability weight

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Importance sampling solutions

Harmonic means

Approximating \mathfrak{Z} using a mixture representation (cont'd)

Corresponding MCMC (=Gibbs) sampler

At iteration t

(1) Take $\delta^{(t)} = 1$ with probability

$$\omega_1 \pi(\theta^{(t-1)}) L(\theta^{(t-1)}) \Big/ \left(\omega_1 \pi(\theta^{(t-1)}) L(\theta^{(t-1)}) + \varphi(\theta^{(t-1)}) \right)$$

and $\delta^{(t)} = 2$ otherwise;

- ② If $\delta^{(t)} = 1$, generate $\theta^{(t)} \sim \mathsf{MCMC}(\theta^{(t-1)}, \theta^{(t)})$ where $\mathsf{MCMC}(\theta, \theta')$ denotes an arbitrary MCMC kernel associated with the posterior $\pi(\theta|x) \propto \pi(\theta)L(\theta)$;
- ③ If $\delta^{(t)} = 2$, generate $\theta^{(t)} \sim \varphi(\theta)$ independently

Importance sampling solutions

Harmonic means

Approximating \mathfrak{Z} using a mixture representation (cont'd)

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and $\delta^{(t)} = 2$ otherwise;

- (2) If $\delta^{(t)} = 1$, generate $\theta^{(t)} \sim \mathsf{MCMC}(\theta^{(t-1)}, \theta^{(t)})$ where $\mathsf{MCMC}(\theta, \theta')$ denotes an arbitrary MCMC kernel associated with the posterior $\pi(\theta|x) \propto \pi(\theta)L(\theta)$;
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Importance sampling solutions

Harmonic means

Evidence approximation by mixtures

Rao-Blackwellised estimate

$$\hat{\xi} = \frac{1}{T} \sum_{t=1}^{T} \omega_1 \pi(\theta^{(t)}) L(\theta^{(t)}) \Big/ \omega_1 \pi(\theta^{(t)}) L(\theta^{(t)}) + \varphi(\theta^{(t)}),$$

converges to $\omega_1 \mathfrak{Z} / \{\omega_1 \mathfrak{Z} + 1\}$ Deduce $\hat{\mathfrak{Z}}_3$ from $\omega_1 \hat{\mathfrak{Z}}_3 / \{\omega_1 \hat{\mathfrak{Z}}_3 + 1\} = \hat{\xi}$ ie

$$\hat{\mathfrak{Z}}_{3} = \frac{\sum_{t=1}^{T} \omega_{1} \pi(\theta^{(t)}) L(\theta^{(t)}) / \omega_{1} \pi(\theta^{(t)}) L(\theta^{(t)}) + \varphi(\theta^{(t)})}{\sum_{t=1}^{T} \varphi(\theta^{(t)}) / \omega_{1} \pi(\theta^{(t)}) L(\theta^{(t)}) + \varphi(\theta^{(t)})}$$

[Bridge sampler]

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[Bridge sampler]

Importance sampling solutions

Chib's solution

Chib's representation

Direct application of Bayes' theorem: given ${\bf x}\sim f_k({\bf x}|\theta_k)$ and $\theta_k\sim \pi_k(\theta_k)$,

$$m_k(\mathbf{x}) = \frac{f_k(\mathbf{x}|\theta_k) \, \pi_k(\theta_k)}{\pi_k(\theta_k|\mathbf{x})} \,,$$

Use of an approximation to the posterior

$$\hat{m}_k(\mathbf{x}) = \frac{f_k(\mathbf{x}|\theta_k^*) \, \pi_k(\theta_k^*)}{\hat{\pi}_k(\theta_k^*|\mathbf{x})} \, .$$

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Importance sampling solutions

Chib's solution

Case of latent variables

For missing variable \mathbf{z} as in mixture models, natural Rao-Blackwell estimate

$$\hat{\pi_k}(\theta_k^*|\mathbf{x}) = \frac{1}{T} \sum_{t=1}^T \pi_k(\theta_k^*|\mathbf{x}, \mathbf{z}_k^{(t)}),$$

where the $\mathbf{z}_{k}^{(t)}$'s are the latent variables simulated by a Gibbs sampler.

Importance sampling solutions

Chib's solution

Compensation for label switching

For mixture models, $\mathbf{z}_k^{(t)}$ usually fails to visit all configurations in a balanced way, despite the symmetry predicted by the theory

$$\pi_k(\theta_k | \mathbf{x}) = \pi_k(\sigma(\theta_k) | \mathbf{x}) = \frac{1}{k!} \sum_{\sigma \in \mathfrak{S}} \pi_k(\sigma(\theta_k) | \mathbf{x})$$

for all σ 's in \mathfrak{S}_k , set of all permutations of $\{1, \ldots, k\}$. Consequences on numerical approximation, biased by an order k! Recover the theoretical symmetry by using

$$\tilde{\pi_k}(\theta_k^*|\mathbf{x}) = \frac{1}{T \, k!} \sum_{\sigma \in \mathfrak{S}_k} \sum_{t=1}^T \pi_k(\sigma(\theta_k^*)|\mathbf{x}, \mathbf{z}_k^{(t)}) \,.$$

[Berkhof, Mechelen, & Gelman, 2003]

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[Berkhof, Mechelen, & Gelman, 2003]

Cross-model solutions

Reversible jump

Reversible jump

Idea: Set up a proper measure–theoretic framework for designing moves between models \mathfrak{M}_k

[Green, 1995] Create a reversible kernel \mathfrak{K} on $\mathfrak{H} = \bigcup_k \{k\} \times \Theta_k$ such that

$$\int_A \int_B \mathfrak{K}(x,dy) \pi(x) dx = \int_B \int_A \mathfrak{K}(y,dx) \pi(y) dy$$

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for the invariant density π [x is of the form $(k, heta^{(k)})]$

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Cross-model solutions

-Reversible jump

Local moves

For a move between two models, \mathfrak{M}_1 and \mathfrak{M}_2 , the Markov chain being in state $\theta_1 \in \mathfrak{M}_1$, denote by $\mathfrak{K}_{1\to 2}(\theta_1, d\theta)$ and $\mathfrak{K}_{2\to 1}(\theta_2, d\theta)$ the corresponding kernels, under the *detailed balance condition*

$$\pi(d\theta_1)\,\mathfrak{K}_{1\to 2}(\theta_1,d\theta) = \pi(d\theta_2)\,\mathfrak{K}_{2\to 1}(\theta_2,d\theta)\,,$$

and take, wlog, $\dim(\mathfrak{M}_2) > \dim(\mathfrak{M}_1)$.

Proposal expressed as

 $\theta_2 = \Psi_{1 \to 2}(\theta_1, v_{1 \to 2})$

where $v_{1\rightarrow 2}$ is a random variable of dimension $\dim(\mathfrak{M}_2) - \dim(\mathfrak{M}_1)$, generated as

$$v_{1\to 2} \sim \varphi_{1\to 2}(v_{1\to 2}).$$

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Cross-model solutions

Reversible jump

Local moves (2)

In this case, $q_{1\rightarrow 2}(\theta_1, d\theta_2)$ has density

$$\varphi_{1\to 2}(v_{1\to 2}) \left| \frac{\partial \Psi_{1\to 2}(\theta_1, v_{1\to 2})}{\partial(\theta_1, v_{1\to 2})} \right|^{-1},$$

by the Jacobian rule.

Reverse importance link

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If probability $\varpi_{1\to 2}$ of choosing move to \mathfrak{M}_2 while in \mathfrak{M}_1 , acceptance probability reduces to

$$\alpha(\theta_1, v_{1 \to 2}) = 1 \wedge \frac{\pi(\mathfrak{M}_2, \theta_2) \, \varpi_{2 \to 1}}{\pi(\mathfrak{M}_1, \theta_1) \, \varpi_{1 \to 2} \, \varphi_{1 \to 2}(v_{1 \to 2})} \left| \frac{\partial \Psi_{1 \to 2}(\theta_1, v_{1 \to 2})}{\partial(\theta_1, v_{1 \to 2})} \right|$$

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Cross-model solutions

Reversible jump

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Cross-model solutions

Reversible jump

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Cross-model solutions

Saturation schemes

Alternative

Saturation of the parameter space $\mathfrak{H} = \bigcup_k \{k\} \times \Theta_k$ by creating

- \bullet a model index M
- pseudo-priors $\pi_j(\theta_j|M=k)$ for $j \neq k$

[Carlin & Chib, 1995]

Validation by

$$\pi(M = k|y) = \int P(M = k|y, \theta) \pi(\theta|y) d\theta = \mathfrak{Z}_k$$

where the (marginal) posterior is

$$\begin{aligned} \pi(\theta|y) &= \sum_{k=1}^{D} \pi(\theta, M = k|y) \\ &= \sum_{k=1}^{D} \varrho_k \, m_k(y) \, \pi_k(\theta_k|y) \prod_{j \neq k} \pi_j(\theta_j|M = k) \, . \end{aligned}$$

Cross-model solutions

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[Carlin & Chib, 1995]

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$$\pi(\theta|y) = \sum_{k=1}^{D} \pi(\theta, M = k|y)$$
$$= \sum_{k=1}^{D} \varrho_k m_k(y) \pi_k(\theta_k|y) \prod_{j \neq k} \pi_j(\theta_j|M = k).$$

Cross-model solutions

└─ Saturation schemes

MCMC implementation

Run a Markov chain $(M^{(t)},\theta_1^{(t)},\ldots,\theta_D^{(t)})$ with stationary distribution $\pi(\theta,M=k|y)$ by

1 Pick $M^{(t)} = k$ with probability $P(\theta^{(t-1)}, M = k|y)$

Q Generate \$\theta_k^{(t-1)}\$ from the posterior \$\pi_k(\theta_k|y)\$ [or MCMC step]
Q Generate \$\theta_j^{(t-1)}\$ (\$j \neq k\$) from the pseudo-prior \$\pi_j(\theta_j|M = k\$)\$
Approximate \$\pi(M = k|y) = \mathcal{J}_k\$ by

$$\check{\varrho}_k(y) \propto \varrho_k \sum_{t=1}^T f_k(y|\theta_k^{(t)}) \pi_k(\theta_k^{(t)}) \prod_{j \neq k} \pi_j(\theta_j^{(t)}|M=k) \\ \Big/ \sum_{\ell=1}^D \varrho_\ell f_\ell(y|\theta_\ell^{(t)}) \pi_\ell(\theta_\ell^{(t)}) \prod_{j \neq \ell} \pi_j(\theta_j^{(t)}|M=\ell)$$

Cross-model solutions

└─ Saturation schemes

MCMC implementation

Run a Markov chain $(M^{(t)}, \theta_1^{(t)}, \dots, \theta_D^{(t)})$ with stationary distribution $\pi(\theta, M = k|y)$ by

 $\textcircled{0} \ \mbox{Pick } M^{(t)} = k \ \mbox{with probability } P(\theta^{(t-1)}, M = k | y)$

- ⁽²⁾ Generate $\theta_k^{(t-1)}$ from the posterior $\pi_k(\theta_k|y)$ [or MCMC step]
- 3 Generate $\theta_j^{(t-1)}$ $(j \neq k)$ from the pseudo-prior $\pi_j(\theta_j | M = k)$

$$\check{\varrho}_k(y) \propto \varrho_k \sum_{t=1}^T f_k(y|\theta_k^{(t)}) \pi_k(\theta_k^{(t)}) \prod_{j \neq k} \pi_j(\theta_j^{(t)}|M=k) \\ \Big/ \sum_{\ell=1}^D \varrho_\ell f_\ell(y|\theta_\ell^{(t)}) \pi_\ell(\theta_\ell^{(t)}) \prod_{j \neq \ell} \pi_j(\theta_j^{(t)}|M=\ell)$$

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Cross-model solutions

└─ Saturation schemes

MCMC implementation

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 $\textcircled{0} \ \ \mbox{Pick} \ M^{(t)} = k \ \mbox{with probability} \ P(\theta^{(t-1)}, M = k | y)$

2 Generate θ_k^(t-1) from the posterior π_k(θ_k|y) [or MCMC step]
3 Generate θ_i^(t-1) (j ≠ k) from the pseudo-prior π_j(θ_j|M = k)

Approximate $\pi(M = k|y) = \mathfrak{Z}_k$ by

$$\check{\varrho}_k(y) \propto \varrho_k \sum_{t=1}^T f_k(y|\theta_k^{(t)}) \pi_k(\theta_k^{(t)}) \prod_{j \neq k} \pi_j(\theta_j^{(t)}|M=k) \\ \left/ \sum_{\ell=1}^D \varrho_\ell f_\ell(y|\theta_\ell^{(t)}) \pi_\ell(\theta_\ell^{(t)}) \prod_{j \neq \ell} \pi_j(\theta_j^{(t)}|M=\ell) \right.$$

Cross-model solutions

Implementation error

Scott's (2002) proposal

Suggest estimating P(M = k|y) by

$$\tilde{\varrho}_k(y) \propto \varrho_k \sum_{t=1}^T \left\{ f_k(y|\theta_k^{(t)}) \middle/ \sum_{j=1}^D \varrho_j f_j(y|\theta_j^{(t)}) \right\} \,,$$

based on D simultaneous and independent MCMC chains

$$(\theta_k^{(t)})_t, \qquad 1 \le k \le D,$$

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with stationary distributions $\pi_k(\theta_k|y)$ [instead of above joint]

Cross-model solutions

Implementation error

Scott's (2002) proposal

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$$\tilde{\varrho}_k(y) \propto \varrho_k \sum_{t=1}^T \left\{ f_k(y|\theta_k^{(t)}) \middle/ \sum_{j=1}^D \varrho_j f_j(y|\theta_j^{(t)}) \right\} \,,$$

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Cross-model solutions

Implementation error

Congdon's (2006) extension

Selecting flat [prohibited!] pseudo-priors, uses instead

$$\hat{\varrho}_k(y) \propto \varrho_k \sum_{t=1}^T \left\{ f_k(y|\theta_k^{(t)}) \pi_k(\theta_k^{(t)}) \middle/ \sum_{j=1}^D \varrho_j f_j(y|\theta_j^{(t)}) \pi_j(\theta_j^{(t)}) \right\} \,,$$

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where again the $\theta_k^{(t)}$'s are MCMC chains with stationary distributions $\pi_k(\theta_k|y)$

Cross-model solutions

Implementation error

Examples

Example (Model choice)

Model $\mathfrak{M}_1: y|\theta \sim \mathcal{U}(0,\theta)$ with prior $\theta \sim \mathcal{E}xp(1)$ is versus model $\mathfrak{M}_2: y|\theta \sim \mathcal{E}xp(\theta)$ with prior $\theta \sim \mathcal{E}xp(1)$. Equal prior weights on both models: $\varrho_1 = \varrho_2 = 0.5$.

Approximations of $\pi(M = 1|y)$: Scott's (2002) (green), and Congdon's (2006) (brown) $(N = 10^6 \text{ simulations}).$

Cross-model solutions

Implementation error

Examples

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Cross-model solutions

Implementation error

Examples (2)



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Cross-model solutions

Implementation error

Examples (3)

Example (Model choice (3)) Model $\mathfrak{M}_1: y \sim \mathcal{N}(0, 1/\omega)$ with $\omega \sim \mathcal{E}xp(a)$ vs. $\mathfrak{M}_2: \exp(y) \sim \mathcal{E}xp(\lambda)$ with $\lambda \sim \mathcal{E}xp(b)$.

Comparison of Congdon's (2006) (brown and dashed lines) with $\pi(M = 1|y)$ when (a, b) is equal to (.24, 8.9), (.56, .7), (4.1, .46) and (.98, .081), resp. $(N = 10^4$ simulations).



-Nested sampling

Purpose

Nested sampling: Goal

Skilling's (2007) technique using the one-dimensional representation:

$$\mathfrak{Z} = \mathbb{E}^{\pi}[L(\theta)] = \int_0^1 \varphi(x) \, \mathrm{d}x$$

with

$$\varphi^{-1}(l) = P^{\pi}(L(\theta) > l).$$

Note; $\varphi(\cdot)$ is intractable in most cases.

-Nested sampling

- Implementation

Nested sampling: First approximation

Approximate \mathfrak{Z} by a Riemann sum:

$$\widehat{\mathfrak{Z}} = \sum_{i=1}^{j} (x_{i-1} - x_i)\varphi(x_i)$$

where the x_i 's are either:

• deterministic: $x_i = e^{-i/N}$

or random:

$$x_0 = 0, \quad x_{i+1} = t_i x_i, \quad t_i \sim \mathcal{B}e(N, 1)$$

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so that $\mathbb{E}[\log x_i] = -i/N$.

└─ Nested sampling

- Implementation

Extraneous white noise

Take

$$\begin{split} \mathfrak{Z} &= \int e^{-\theta} \, \mathrm{d}\theta = \int \frac{1}{\delta} \, e^{-(1-\delta)\theta} \, e^{-\delta\theta} = \mathbb{E}_{\delta} \left[\frac{1}{\delta} \, e^{-(1-\delta)\theta} \right] \\ \hat{\mathfrak{Z}} &= \frac{1}{N} \, \sum_{i=1}^{N} \, \delta^{-1} \, e^{-(1-\delta)\theta_{i}}(x_{i-1} - x_{i}) \,, \quad \theta_{i} \sim \mathcal{E}(\delta) \, \mathbb{I}(\theta_{i} \leq \theta_{i-1}) \end{split}$$

└─ Nested sampling

- Implementation

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└─ Nested sampling

- Implementation

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N	deterministic	random	
50	4.64	10.5	-
	4.65	10.5	
100	2.47	4.9	Comparison of variances and MSEs
	2.48	5.02	
500	.549	1.01	
	.550	1.14	

-Nested sampling

Implementation

Nested sampling: Second approximation

Replace (intractable) $\varphi(x_i)$ by φ_i , obtained by

Nested sampling

Start with N values θ_1,\ldots,θ_N sampled from π

At iteration *i*,

- 1) Take $\varphi_i = L(\theta_k)$, where θ_k is the point with smallest likelihood in the pool of θ_i 's
- 2 Replace θ_k with a sample from the prior constrained to $L(\theta) > \varphi_i$: the current N points are sampled from prior constrained to $L(\theta) > \varphi_i$.

-Nested sampling

Implementation

Nested sampling: Second approximation

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-Nested sampling

Implementation

Nested sampling: Third approximation

Iterate the above steps until a given stopping iteration j is reached: e.g.,

- observe very small changes in the approximation $\widehat{\mathfrak{Z}}$;
- reach the maximal value of $L(\theta)$ when the likelihood is bounded and its maximum is known;
- truncate the integral \mathfrak{Z} at level ϵ , i.e. replace

$$\int_0^1 \varphi(x) \, \mathrm{d}x \qquad \text{with} \qquad \int_\epsilon^1 \varphi(x) \, \mathrm{d}x$$

-Nested sampling

Error rates

Approximation error

$$\begin{aligned} \operatorname{Error} &= \widehat{\mathfrak{Z}} - \mathfrak{Z} \\ &= \sum_{i=1}^{j} (x_{i-1} - x_i) \varphi_i - \int_0^1 \varphi(x) \, \mathrm{d}x = -\int_0^{\epsilon} \varphi(x) \, \mathrm{d}x \\ &+ \left[\sum_{i=1}^{j} (x_{i-1} - x_i) \varphi(x_i) - \int_{\epsilon}^1 \varphi(x) \, \mathrm{d}x \right] \quad \text{(Quadrature Error)} \\ &+ \left[\sum_{i=1}^{j} (x_{i-1} - x_i) \left\{ \varphi_i - \varphi(x_i) \right\} \right] \quad \text{(Stochastic Error)} \end{aligned}$$

[Dominated by Monte Carlo!]

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Nested sampling

Error rates

A CLT for the Stochastic Error

The (dominating) stochastic error is $O_P(N^{-1/2})$:

$$N^{1/2} \{ \mathsf{Stochastic Error} \} \xrightarrow{\mathcal{D}} \mathcal{N} \left(0, V \right)$$

with

$$V = -\int_{s,t\in[\epsilon,1]} s\varphi'(s)t\varphi'(t)\log(s\vee t)\,\mathrm{d}s\,\mathrm{d}t.$$

[Proof based on Donsker's theorem]

The number of simulated points equals the number of iterations j, and is a multiple of N: if one stops at first iteration j such that $e^{-j/N} < \epsilon$, then: $j = N \lceil -\log \epsilon \rceil$.

Nested sampling

Error rates

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-Nested sampling

Impact of dimension

Curse of dimension

For a simple Gaussian-Gaussian model of dimension $\dim(\theta) = d$, the following 3 quantities are O(d):

- asymptotic variance of the NS estimator;
- number of iterations (necessary to reach a given truncation error);
- 3 cost of one simulated sample.
- Therefore, CPU time necessary for achieving error level e is

 $O(d^3/e^2)$

-Nested sampling

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Nested sampling

└─ Constraints

Sampling from constr'd priors

Exact simulation from the constrained prior is intractable in most cases!

Skilling (2007) proposes to use MCMC, but:

- this introduces a bias (stopping rule).
- if MCMC stationary distribution is unconst'd prior, more and more difficult to sample points such that L(θ) > l as l increases.

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If implementable, then slice sampler can be devised at the same cost!

-Nested sampling

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-Nested sampling

Constraints

Illustration of MCMC bias



Log-relative error against d (*left*), avg. number of iterations (*right*) vs dimension d, for a Gaussian-Gaussian model with d parameters, when using T = 10 iterations of the Gibbs sampler.

-Nested sampling

Importance variant

A IS variant of nested sampling

Consider instrumental prior $\tilde{\pi}$ and likelihood \tilde{L} , weight function

$$w(\theta) = \frac{\pi(\theta)L(\theta)}{\widetilde{\pi}(\theta)\widetilde{L}(\theta)}$$

and weighted NS estimator

$$\widehat{\mathfrak{Z}} = \sum_{i=1}^{j} (x_{i-1} - x_i)\varphi_i w(\theta_i).$$

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Then choose $(\tilde{\pi}, L)$ so that sampling from $\tilde{\pi}$ constrained to $\tilde{L}(\theta) > l$ is easy; e.g. $\mathcal{N}(c, I_d)$ constrained to $\|c - \theta\| < r$.

-Nested sampling

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Mixture example

Benchmark: Target distribution

Posterior distribution on (μ, σ) associated with the mixture

$$p\mathcal{N}(0,1) + (1-p)\mathcal{N}(\mu,\sigma),$$

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when p is known
Mixture example

Experiment

- n observations with $\mu = 2$ and $\sigma = 3/2$,
- Use of a uniform prior both on (-2, 6) for μ and on (.001, 16) for $\log \sigma^2$.
- occurrences of posterior bursts for $\mu = x_i$
- computation of the various estimates of 3



Mixture example

Experiment (cont'd)



MCMC sample for n = 16 observations from the mixture.

Nested sampling sequence with M = 1000 starting points.

Mixture example

Experiment (cont'd)



MCMC sample for n = 50 observations from the mixture.

Nested sampling sequence with M = 1000 starting points.

Mixture example

Comparison

Monte Carlo and MCMC (=Gibbs) outputs based on $T=10^4$ simulations and numerical integration based on a 850×950 grid in the (μ,σ) parameter space.

Nested sampling approximation based on a starting sample of M=1000 points followed by at least 103 further simulations from the constr'd prior and a stopping rule at 95% of the observed maximum likelihood.

Constr'd prior simulation based on 50 values simulated by random walk accepting only steps leading to a lik'hood higher than the bound

Mixture example

Comparison (cont'd)



Graph based on a sample of 10 observations for $\mu=2$ and $\sigma=3/2$ (150 replicas).

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Mixture example

Comparison (cont'd)



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Graph based on a sample of 50 observations for $\mu=2$ and $\sigma=3/2$ (150 replicas).

Mixture example

Comparison (cont'd)



Graph based on a sample of 100 observations for $\mu=2$ and $\sigma=3/2$ (150 replicas).

Mixture example

Comparison (cont'd)

Nested sampling gets less reliable as sample size increases Most reliable approach is mixture $\hat{\mathfrak{Z}}_3$ although harmonic solution $\hat{\mathfrak{Z}}_1$ close to Chib's solution [taken as golden standard] Monte Carlo method $\hat{\mathfrak{Z}}_2$ also producing poor approximations to \mathfrak{Z} (Kernel ϕ used in $\hat{\mathfrak{Z}}_2$ is a t non-parametric kernel estimate with standard bandwidth estimation.)