Informed Subsampling MCMC: Approximated Bayesian Inference for Large Datasets

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Outline of talk

- Introduction/overview of literature on the Bayesian inference for tall data
- Generally, two types of approaches:
 - Divide-and-conquer: partition the data into subsets, process each batch separately and then combine the inferences.
 - Sub-sampling strategies: reduce the computational burden of Metropolis-Hastings.
- Our approach falls under the category of sub-sampling strategies.
- ► The main idea is to fix the subset size n ≪ N and to focus on those sub-samples that are similar to the full data, in terms of how close the summary statistics of the sub-sample is to summary statistics of the full data.

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 It therefore shares some similarities with Approximate Bayesian Computation.

Outlines

Introduction

Some results on exponential models

Generalization of the approach beyond the exponential case

Illustration

Metropolis-Hastings sampler in Big Data problems

Consider the posterior distribution

$$\pi(\theta \mid Y_1, \ldots, Y_N) \propto f(Y_1, \ldots, Y_N \mid \theta) p(\theta)$$

where $f(\cdot | Y_1, \ldots, Y_N)$ is the likelihood model and p the prior distribution.

• Metropolis-Hastings simulates a Markov chain $\{\theta_k\}_k$ targeting $\pi(\cdot | Y_1, \ldots, Y_N)$, transition $\theta_k \to \theta_{k+1}$ follows:

(1) draw
$$\tilde{\theta} \sim Q(\theta_k, \cdot)$$

(2) set $\theta_{k+1} = \tilde{\theta}$ with probability

$$A(\theta_k, \tilde{\theta}) = 1 \land \frac{f(\tilde{\theta} \mid Y_1, \dots, Y_N) p(\tilde{\theta}) Q(\tilde{\theta}, \theta_k)}{f(\theta_k \mid Y_1, \dots, Y_N) p(\theta_k) Q(\theta_k, \tilde{\theta})}$$

and $\theta_{k+1} = \theta_k$ w.p. $1 - A(\theta_k, \tilde{\theta})$.

Another way of looking at the MH algorithm

Transition
$$\theta_k \to \theta_{k+1}$$
 follows:
(1) draw $\tilde{\theta} \sim Q(\theta_k, \cdot)$ and $W_k \sim unif(0, 1)$
(2-a) Let $E_k^{(N)}$ be the event
 $E_k^{(N)}(\theta_k, \tilde{\theta}, W_k) = \left\{ W_k \le 1 \land \frac{f(\tilde{\theta} \mid Y_1, \dots, Y_N) p(\tilde{\theta}) Q(\tilde{\theta}, \theta_k)}{f(\theta_k \mid Y_1, \dots, Y_N) p(\theta_k) Q(\theta_k, \tilde{\theta})} \right\}$
(2-b) Set
 $\theta_{k+1} = \left\{ \begin{array}{l} \tilde{\theta} & \text{if } E_k^{(N)}(\theta_k, \tilde{\theta}, W_k) \\ \theta_k & \text{otherwise} \end{array} \right.$

 \Rightarrow A MH transition is thus a statistical hypothesis test: does $E_k^{(N)}$ occur or not?

Making the decision with sub-samples of data?

- Is it possible to make the same decision as MH (with a large probability), without computing f(θ̃ | Y₁,..., Y_N)?
- ▶ Make the decision to accept/reject $\tilde{\theta}$ based on a subset of $n \ll N$ data:

$$E_{k}^{(n)}(\theta_{k},\tilde{\theta},W_{k}) = \left\{ W_{k} \leq 1 \land \frac{f(\tilde{\theta} \mid Y_{1}^{*},\ldots,Y_{n}^{*})p(\tilde{\theta})Q(\tilde{\theta},\theta_{k})}{f(\theta_{k} \mid Y_{1}^{*},\ldots,Y_{n}^{*})p(\theta_{k})Q(\theta_{k},\tilde{\theta})} \right\}$$

rather than on $E_k^{(N)}$.

Making the decision with sub-samples of data?

- Austerity in MCMC land: Cutting the M–H budget, Korattikara et al, 2013
- Towards scaling up MCMC: an adaptive subsampling approach, Bardenet et al, 2014
- On MCMC methods for tall data, Bardenet et al, 2015
- Random Projections in MCMC for tall data, Bardenet et al, 2016

However, these methods are no longer exact in that the chain $\{\theta_k\}_k$ does not admit $\pi(\cdot | Y_1, \ldots, Y_N)$ as stationary distribution.

First approach: Austerity in MCMC land, Korattikara 2013

Rewriting $E_k^{(N)}$ in case of *i.i.d.* data

$$E_{k}^{(N)}(\theta_{k},\tilde{\theta},W_{k}) = \left\{ \underbrace{\frac{1}{N} \log \left(W_{k} \frac{p(\tilde{\theta})Q(\tilde{\theta},\theta_{k})}{p(\theta_{k})Q(\theta_{k},\tilde{\theta})} \right)}_{\mu_{0}} \leq \underbrace{\frac{1}{N} \sum_{\ell=1}^{N} \log \frac{f(\tilde{\theta} \mid Y_{\ell})}{f(\theta_{k} \mid Y_{\ell})}}_{\mu} \right\}$$

- draw without replacement *n* data Y_1^*, \ldots, Y_n^*
- calculate $\tilde{\mu}^{(n)} = n^{-1} \sum_{\ell=1}^{n} \log \frac{f(\tilde{\theta} \mid Y_{\ell}^{*})}{f(\theta_{k} \mid Y_{\ell}^{*})}$
- ▶ test $H_0^{(n)} = \{\mu_0 = \tilde{\mu}^{(n)}\}$ vs $H_1^{(n)} = \{\mu_0 \neq \tilde{\mu}^{(n)}\}$
- ▶ subsample data until $\mathbb{P}(H_1^{(n)}) > 1 \epsilon$
- make decision using $\tilde{\mu}^{(n)}$ instead of μ :

$$E_k^{(n)}(\theta_k, \tilde{\theta}, W_k) = \left\{ \mu_0 \leq \tilde{\mu}^{(n)} \right\}$$

(日)(1)

Second approach: Confidence sampler (Bardenet et al, 2014, 2015)

Assume that a concentration inequality exists for the model, i.e

$$orall \, n \leq {\sf N} \ , \exists \, {\sf c}_n > 0, \, \delta_n \in (0,1) \, , \qquad \mathbb{P}\left(\left| \mu - ilde{\mu}^{(n)}
ight| \leq {\sf c}_n
ight) \geq 1 - \delta_n \, .$$

For example, choose $\delta_n \in (0, 1)$ and c_n is defined as

$$c_n(\delta_n) = \sigma_{n,\theta,\tilde{\theta}} \sqrt{\frac{2\log(3/\delta_n)}{n}} + \frac{6C_{\theta,\tilde{\theta}}\log(3/\delta_n)}{n}$$

where

 \Rightarrow draw data Y_1^*, \ldots, Y_n^* such that as soon as:

$$\left|\tilde{\mu}^{(n)}-\mu_0\right|>c_n$$

then decisions based on $E_k^{(n)}$ and $E_k^{(N)}$ are the same with probability $1 - \delta_n$.

Subsampling approaches

- Subsampling approaches share the same philosophy: Draw more data until a decision replicating MH can be made with a level of confidence.
- ► Bardenet et al.'s works offer more theoretical guarantees (*e.g* ergodicity, quantification of the error,...) But comes at the price of more intermediate calculations $\sigma_{n,\theta,\tilde{\theta}}$ and $C_{\theta,\tilde{\theta}}$.
- Critically, the adaptive subset size *n* tends to *N* as the chain is close to equilibrium.

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Consensus Monte Carlo (Scott et al, 2013)

This approach exploits parallel computing in a very natural way.

Split the dataset into S (independent) batches Y_{1:N} = Y₁,..., Y_S and note that

$$\pi(\theta \mid Y_1, \ldots, Y_N) \propto \prod_{i=1}^{S} f(\mathbf{Y}_i) p(\theta)^{1/S}$$

- Generate *S* independent Markov chains (in parallel) targeting $\{\pi(\theta \mid \mathbf{Y}_i) \propto f(\mathbf{Y}_i) p(\theta)^{1/S}\}_{i=1}^{S}$
- Derive a weighted average of the S chains

$$\theta_k = \left\{\sum_{i=1}^S W_i\right\}^{-1} \sum_{i=1}^S W_i \theta_k^{(i)}$$

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This is justifiable when π is Gaussian, but questions about the convergence of {θ_k}_k and the choice of {W_i}^S_{i=1} remains open

Exact methods

MCMC methods producing a chain that admits $\pi(\theta \mid Y_1, \ldots, Y_N)$ as invariant distribution:

- Using unbiased estimate of f(θ | Y_{1:N}) Pseudo-Marginal literature: Andrieu & Vihola 2012, Doucet et al 2012, Quiroz et al, 2016
- A sub-optimal M–H transition kernel Accelerating M–H algorithms: Delayed acceptance with prefetching, Banterle et al, 2014
- An auxiliary variable MCMC, under strong assumptions FireFly Monte Carlo: Exact MCMC with subsets of data, MacLaurin et al, 2014

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An alternative approach

Definition

Let K be the M–H kernel targeting $\pi(\cdot | Y_1, ..., Y_N)$ Let $U \subset \{1, ..., N\}$ and K_U be the M–H kernel targeting $\pi(\cdot | Y_U)$

Assumption

$$au(K) = \mathcal{O}(N)$$
 and for $U = \{1, \dots, n\}$, $au(K_U) = \mathcal{O}(n)$

For a given CPU budget τ_0 :

- the number of M-H iterations is fixed (potentially low if $N \gg 1$)
- can we derive an algorithm that achieves an arbitrary large number of iterations for a small subset size n?

Inference based on *subposteriors*

Definition

Let Y_U be a subset of $Y_{1:N}$ of size n and $\overline{\pi}_n$ be a scaled subposterior

 $\bar{\pi}_n(\theta \mid Y_U) \propto f(Y_U \mid \theta)^{N/n} p(\theta)$

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Exponential family: an optimality result

Assume that f belongs to the curved exponential family

$$f(y | \theta) \propto \psi(\theta) \exp\{\phi(\theta)^{\mathsf{T}} S(y)\}.$$

Definition

For any subset $U \in U_n$, define the vector of sufficient statistics between the whole dataset and the sub-sample Y_U as:

$$\Delta_n(\boldsymbol{U}) = \sum_{k=1}^N S(y_k) - \frac{N}{n} \sum_{k \in \boldsymbol{U}} S(y_k)$$

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Exponential family: an optimality result

The KL divergence between two measure π and $\overline{\pi}$ is defined as $KL(\pi, \overline{\pi}) = \mathbb{E}_{\pi} \{ \log \pi(\theta) / \overline{\pi}(\theta) \}.$

Proposition

For any $U \in U_n$, the following inequality holds:

$$\operatorname{KL}(\pi, \overline{\pi}_n(\,\cdot \mid Y_U)) \leq B(Y, U),$$

where

$$B(Y, U) = \log \mathbb{E}_{\pi} \exp \left\{ \left\| \mathbb{E}_{\pi}(\phi(\theta)) - \phi(\theta) \right\| \left\| \Delta_{n}(U) \right\| \right\}$$

Corollary

1. For any subset $U \in U_n$ such that $(1/N) \sum_{k=1}^N S(Y_k) = (1/n) \sum_{k \in U} S(Y_k)$, then $\pi = \overline{\pi}(\cdot | Y_U) \pi$ -almost everywhere.

2. Let $(U_1, U_2) \in \mathcal{U}_n^2$. Assume $\|\Delta_n(U_1)\| \le \|\Delta_n(U_2)\|$, then $B(Y, U_1) \le B(Y, U_2)$.

Optimal result in asymptotic regime (when $N \to \infty$)

If a Bernstein-von Mises theorem holds for π , *i.e* π can be approximated by a Normal distribution $\tilde{\pi} = N(\theta^{\mathsf{MLE}}, (1/N)\{I(\theta^{\mathsf{MLE}})\}^{-1}).$

Definition

Define $\widehat{\mathsf{KL}}_n(U)$ as the Kullback-Leibler divergence between the asymptotic approximation of π and $\overline{\pi}_n(\cdot | Y_U)$:

$$\widehat{\mathsf{KL}}_n(U) = \mathbb{E}_{ ilde{\pi}} \log rac{\pi(heta \mid Y)}{ar{\pi}_n(heta \mid Y_U)} \,.$$

Proposition

Let $(U_1, U_2) \in \mathcal{U}_n^2$. Assume that for all $i \in \{1, \ldots, d\}$, $|\Delta_n(U_1)^{(i)}| \le |\Delta_n(U_2)^{(i)}|$, where $|\Delta_n(U_1)^{(i)}|$ refers to the *i*-th element of $\Delta_n(U_1)$. Then $\widehat{\mathsf{KL}}_n(U_1) \le \widehat{\mathsf{KL}}_n(U_2)$.

 \Rightarrow This is a stronger result on partial ordering on subsets not on the KL bound but on the KL itself.

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Example (Toy Example: probit model) Simulate N = 10,000 observations Y_1, \ldots, Y_N

•
$$X_k \sim \mathcal{N}(\theta, 1)$$

$$Y_k \mid X_k = \delta_{(X_k > 0)}(\cdot)$$

$$\pi(\theta \mid Y_{1:N}) \propto p(\theta)(1 - \alpha(\theta))^N (\alpha(\theta)/1 - \alpha(\theta))^{\sum_{k=1}^N Y_k} ar{\pi}_n(\theta \mid Y_U) \propto p(\theta)(1 - \alpha(\theta))^N (\alpha(\theta)/1 - \alpha(\theta))^{\frac{N}{n} \sum_{k \in U} Y_k}$$

where
$$\alpha(\theta) = \mathbb{P}\{X_k > 0 \mid X_k \sim \mathcal{N}(\theta, 1)\}.$$

Define

$$|\Delta_n(U)| = \left|\sum_{k=1}^N Y_k - \frac{N}{n}\sum_{k\in U} Y_k\right|$$

(note that $\sum_{k=1}^{N} Y_k$ is a sufficient statistics.)

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Probit Example: n = 100



Figure: Sub-posteriors with different subsets U of size n = 100.

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Probit Example: n = 1,000



Figure: Sub-posteriors with different subsets U of size n = 1,000.

$\ \Delta_n(U)\ $	$KL(\pi, \tilde{\pi}_n(\cdot \mid Y_U))$	B(Y, U)
4	0.004	0.04
14	0.11	0.18
26	0.19	0.29
34	0.41	0.54

Table: Comparison of the KL divergence between π and some sub-posterior distributions with different $\|\Delta_n(U)\|$.

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From summary statistics to sufficient statistics

 $y \mapsto f(y \mid \theta)$ is now any likelihood model and the data are no longer assumed to be independent.

Definition

Let

• $S : Y \rightarrow S$ be a mapping of summary statistics

$$\Delta_n(U) = S(Y_1, \ldots, Y_N) - \frac{N}{n}S(Y_U)$$

• \mathcal{U}_n be the set of all possible subset of $\{1, \ldots, N\}$ of size n

For each $U \in \mathcal{U}_n$, a weight $\nu_{n,\epsilon}(U)$ is assigned to the subset of data Y_U

$$u_{n,\epsilon}(U) \propto \exp\left\{-\epsilon \|\Delta_n(U)\|^2\right\} \,.$$

- $\blacktriangleright~\epsilon \rightarrow \infty:$ all the subsets have the same weight
- $\blacktriangleright~\epsilon \rightarrow$ 0: the mass is centered on the most representative subset

Informed Subsampling MCMC

Recall that Metropolis-Hastings produces a chain $\{\theta_k\}_k$

(*i*)
$$\tilde{\theta} \sim Q(\theta, \cdot)$$
 (*ii*) $A(\theta, \tilde{\theta}) = 1 \wedge \frac{f(\tilde{\theta} \mid Y_1, \dots, Y_N)p(\tilde{\theta})Q(\tilde{\theta}, \theta)}{f(\theta \mid Y_1, \dots, Y_N)p(\theta)Q(\theta, \tilde{\theta})}$

Our idea is to define a chain $\{\theta_k\}_k$ that evolves as follows:

(*i*)
$$\tilde{\theta} \sim Q(\theta, \cdot)$$
 (*ii*) $A(\theta, \tilde{\theta}) = 1 \wedge \frac{f(\tilde{\theta} \mid Y_U)p(\tilde{\theta})Q(\tilde{\theta}, \theta)}{f(\theta \mid Y_U)p(\theta)Q(\theta, \tilde{\theta})}$

This chain targets $\bar{\pi}_n(\theta \mid Y_U)$ which is of little interest, since likely to be far from π (see probit Example).

Informed Subsampling MCMC

Based on the analysis of exponential models, we consider the following algorithm. It produces a chain $\{\theta_k, U_k\}_k$ as follows.

- 1. Update the subset:
 - 1.1 propose $U' \sim R(U_k, \cdot)$
 - 1.2 set U_{k+1} with probability $1 \wedge \exp \{\epsilon (\|\Delta_n(U_k)\| \|\Delta_n(U')\|)\}$
- 2. Update the parameter:

2.1 propose $\theta' \sim Q(\theta_k, \cdot)$ 2.2 set θ_{k+1} with probability $\tilde{A}(\theta, \theta' | U_{k+1}) = 1 \wedge \tilde{\alpha}(\theta, \theta' | U_{k+1})$ where

$$ilde{lpha}(heta, heta'|U) = rac{f(heta'\mid Y_{U_{k+1}}) p(heta') Q(heta', heta)}{f(heta\mid Y_{U_{k+1}}) p(heta) Q(heta, heta')}\,.$$

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Note that the first step is independent of θ_k .

In fact, it is straightforward to show that $\{U_k\}_k$ is ν_n -reversible Markov chain.

Convergence of perturbed Markov chains

Consider a Metropolis-Hastings algorithm whose ratio $\alpha(\theta, \theta')$ is perturbed through some noisy auxiliary variables $U: \tilde{\alpha}(\theta, \theta' \mid U)$.

Proposition (Alquier 2016, Corollary 2.3)

If we can bound the expected error between α and $\tilde{\alpha}$ s.t.

$$\mathbb{E}\left\{\left|\alpha(\theta,\theta') - \tilde{\alpha}(\theta,\theta' \mid U)\right|\right\} \leq \delta(\theta,\theta')\,,$$

then:

$$\lim_{n \to \infty} \|\pi - \mu \tilde{P}^n\| \le \kappa \sup_{\theta \in \Theta} \int_{\Theta} Q(\theta, \mathrm{d}\theta') \delta(\theta, \theta'), \qquad (1)$$

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where

- P
 is the transition kernel of the noisy algorithm
- κ is a constant depending on the efficiency of the non-noisy Metropolis Hastings chain.

Convergence of $\{\theta_k\}_k$

We cast the analysis of Informed Subsampling chain $\{\theta_k\}_k$ in the noisy MCMC framework.

Proposition

Under regularity assumption on the function $\theta \mapsto f(Y_U | \theta)^{N/n} / f(Y | \theta)$, there is a constant λ such that

$$\mathbb{E}_{
u}igg\{ig|lpha(heta, heta')- ilde{lpha}(heta, heta'\,|\,m{U})ig|igg\}\leqlpha(heta, heta')\lambda\| heta- heta'\|\Phi(heta)\,,$$

where

$$\Phi(\theta) = \mathbb{E}_{\nu} \left\{ \frac{f(Y \mid \theta)}{f(Y_U \mid \theta)^{N/n}} \right\} \propto \sum_{U \in \mathcal{U}_n} \nu(U) \frac{f(Y \mid \theta)}{f(Y_U \mid \theta)^{N/n}}$$

The RHS's expectation can be unstable if an unappropriate weight distribution is used.

Convergence of $\{\theta_k\}_k$

Proposition

For exponential models, we prove the following:

$$\frac{f(Y \mid \theta)}{f(Y_U \mid \theta)^{N/n}} = o(1/\nu(U)).$$

and thus $\Phi(\theta)$ is bounded.

For general models, this proposition serves as a way to validate summary statistics:

Rule

Let f be a general likelihood model and S a possible summary statistics vector. If there is a β such that

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|\log f(Y | \theta) - (N/n) \log f(Y_U | \theta)| \leq \beta ||\Delta_n(U)||,
```

then S is sensible choice of summary statistics.

Outlines

Introduction

Some results on exponential models

Generalization of the approach beyond the exponential case

Illustration

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Example 1: estimation of template shapes

Data are of handwritten digits (MNIST database)



Figure: example of data

- The dataset contains N = 10,000 images of size 16x16
- Each image belongs to a class $I_k \in \{1, \dots, 5\}$ assumed to be known
- The model can be written as:

$$I_k = i, \quad Y_k = \phi(heta_i) + \sigma^2 \varepsilon_k, \qquad \varepsilon_k \sim \mathcal{N}(0, 1).$$

Example 1: estimation of template shapes

- Computational budget: $\tau_0 = 60$ mins.,
- ▶ We compare M-H and LWA-MCMC with subset of n = 100 digits, $\epsilon = 1$ and $S(U) = (S_1(U), \dots, S_5(U))$ with $S_i(U) = \sum_{k \in U} I_k$
- ► $\tau_{\rm MH} = 41.2$ secs and $\tau_{\rm Informed Subsampling-MCMC} = 0.7$ secs (60 × faster)



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Example 1: estimation of template shapes

Consider the metric $d(t) = \sum_{i=1}^{5} \left\| \theta_i^* - \frac{1}{L(t)} \sum_{\ell=1}^{L(t)} \theta_{i,\ell} \right\|$, where:

- L(t) is the number of iterations completed at time t
- θ_i^* is the map of model *i* (estimated from stochastic EM)



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Example 1: Sampling at stationarity



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Figure: Comparing the true and approximate marginal distribution of one parameter of θ_1 (left) and one parameter of θ_5 (right)

Example 2: Auto regressive model Example (AR(2))

An AR(2) model, parameterized by $\theta = (\theta_1 \, \theta_2, \theta_3)$

$$y_t = \theta_1 y_{t-1} + \theta_2 y_{t-2} + \zeta_t, \quad \zeta_t \sim \mathcal{N}(0, \theta_3^2).$$

- Simulation of a TS of $N = 10^6$ observations,
- Approximate inference with $n \in \{10^2, 10^3\}$
- Different Summary statistics are tried:
 - S(y') = {ρ₁(y'),..., ρ₅(y')} where ρ_i(y') is the *i*-th lag sample autocorrelation
 - S(y') = θ^{YW}(y'), the estimation of θ via Yule Walker method based on data y'

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- ▶ Different *e* were used.
- Our approach is tested versus MH implementation (prior, proposal, etc.) proposed in Chib, Understanding Metropolis

Samples from $\pi(\cdot | y)$ were obtained via MH on the whole dataset (a laborious work!).

Example 2: validation of summary statistics

Try S defined as the estimated ACF (first 5 coefficients)



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 \Rightarrow *S* rejected, $\phi(\theta)$ is unstable.

Example 2: validation of summary statistics

Try S defined as the Yule Walker coefficients



 \Rightarrow S accepted since the log ratio does not grow faster than linearly in $||S(Y) - (N/n)S(Y_U)||$.

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Example 2: marginal inference of θ_1 (n = 100)



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Example 2: marginal inference θ_1 (n = 1,000)



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Example 2: marginal inference θ_1 (n = 1,000)



Comparing with inference provided by a subposterior $\tilde{\pi}_n(\theta_1 | Y_U)$ given a fixed subset U: green is the best subset (as per measured by S) and gray is a subset picked at random.

Example 2: joint inference (θ_2, θ_3)



Figure: Samples from $\pi(\theta_2, \theta_3 | Y)$ obtained using Metropolis-Hastings (blue) and from $\tilde{\pi}_n(\theta_2, \theta_3 | Y)$ obtained using Informed Subsampling MCMC (green), with n = 100 (left) and n = 1,000 right.

Conclusions

"Uninformed" Subsampling MCMC

- Are designed so as to control locally the decision error wrt to the MH algorithm.
- Checking conditions in which this framework applies may be difficult in practice.
- The number of likelihood evaluation is not fixed, questioning the computational efficiency.
- Subsample the data uniformly at random
- By contrast, our Informed Subsampling MCMC scheme
 - ► Allows to control deterministically the MH transition complexity.
 - Subsamples according to their fidelity to this full dataset, through summary statistics.
 - Allows to control only asymptotically the distance between the chain distribution and the true posterior.