Post-Processing of MCMC

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Setting

We can't simulate directly from π so instead we've used another approach to get samples $\{\theta^{(i)}\}_{i=1}^N$, such as

- Standard MCMC
- Biased MCMC
- Any other mechanism for coming up with samples (even if the samples are correlated or weighted[1])

Our probability mass function for these samples[2] is denoted Q.

[1] Typically a simple extension but not covered here

[2] $Q = \frac{1}{N}\sum_{i=1}^N \delta_{\theta^{(i)}}$ where $\delta_{\theta^{(i)}}$ puts all probability mass on $\theta^{(i)}$

Outline

We will cover

- **Sample quality:**
  - Measuring sample quality with the kernel Stein discrepancy
  - Testing if $\{\theta^{(i)}\}_{i=1}^{N} \sim \pi$ with kernel Stein goodness of fit tests
- **Choosing samples:**
  - Selecting a subset of samples with Stein thinning
- **Improving estimates:**
  - Improving upon $\widehat{\mathbb{E}_\pi[f(\theta)]} = \frac{1}{N}\sum_{i=1}^{N} f(\theta^{(i)})$ with Stein-based control variates.

Measuring Sample Quality
with the kernel Stein discrepancy (KSD)

Setting

Our goal is usually to estimate posterior expectations, $\mathbb{E}_\pi[f(\theta)]$.

If we could calculate it, we would like to use

$$d_f(Q, \pi) = \mathbb{E}_Q[f(\theta)] - \mathbb{E}_\pi[f(\theta)]$$

as a measure of performance.

This may be fine if there is only interest in a single f but it doesn't track non-convergence because $d_f(Q, \pi) \to 0$ doesn't imply $Q \to \pi$. Let's discuss why.

Setting

To assess general sample quality, we would like to calculate

$$d_{\mathcal{F}}(Q, \pi) = \sup_{f \in \mathcal{F}} \left[\mathbb{E}_Q[f(\theta)] - \mathbb{E}_\pi[f(\theta)] \right].$$

Note that sup is the supremum or the "least upper bound".

To be convergence-determining, we need $\mathcal{F}$ to be sufficiently large.

Setting

This,

$$d_{\mathcal{F}}(Q, \pi) = \sup_{f \in \mathcal{F}} \left[\mathbb{E}_Q[f(\theta)] - \mathbb{E}_\pi[f(\theta)] \right],$$

is the definition of an *integral probability metric (IPM)*. Some well-known IPM's include maximum mean discrepancy (MMD), Wasserstein distance and Kolmogorov distance.

This raises three follow-up questions

1. How can we circumvent $\mathbb{E}_\pi[f(\theta)]$?
2. How should we select our class of test functions?
3. Is our final discrepancy convergence-determining?

Circumventing $\mathbb{E}_\pi[f(\theta)]$

There is a construction that gives us $\mathbb{E}_\pi[f(\theta)] = 0$ called the Stein operator $\mathcal{A}$.

If we pick $f = \mathcal{A}g$ then $\mathbb{E}_\pi[f(\theta)] = \mathbb{E}_\pi[\mathcal{A}g(\theta)] = 0$.

We will use the Langevin Stein operator[1]

$$\mathcal{A}g(\theta) = \nabla_\theta \cdot g(\theta) + \nabla \log \pi(\theta|y) \cdot g(\theta)$$

where g is an $\mathbb{R}^d$-valued function.

[1] Stein (1972), Gorman and Mackey (2015)

Circumventing $\mathbb{E}_\pi[f(\theta)]$

Other Stein operators can be developed using the generator method of Barbour (1988, 1990):

1. Identify a Markov process $(\theta_t)_{t\geq 0}$ with stationary distribution π
   E.g. the Langevin diffusion $\mathrm{d}\theta(t) = \nabla_\theta \log \pi(\theta|y)\mathrm{d}t/2 + \mathrm{d}b(t)$ where $b(t)$ is Brownian motion.
2. Under mild conditions, the infinitesimal generator

$$\mathcal{A}g(x) = \lim_{t\to 0} \frac{\mathbb{E}[g(\theta_t|\theta_0 = x] - g(x)}{t}$$

   satisfies $\mathbb{E}_\pi[\mathcal{A}g(\theta)] = 0$.

Circumventing $\mathbb{E}_\pi[f(\theta)]$

The new discrepancy looks like this:

$$
\begin{aligned}
d_{\mathcal{F}}(Q, \pi) &= \sup_{f \in \mathcal{F}} \left[\mathbb{E}_Q[f(\theta)] - \mathbb{E}_\pi[f(\theta)]\right] \\
&= \sup_{g \in \mathcal{G}} \left[\mathbb{E}_Q[\mathcal{A}g(\theta)] - \mathbb{E}_\pi[\mathcal{A}g(\theta)]\right] \\
&= \sup_{g \in \mathcal{G}} \mathbb{E}_Q[\mathcal{A}g(\theta)] \\
&:= d_{\mathcal{G}}(Q, \mathcal{A}, \pi)
\end{aligned}
$$

Now we need to pick a large enough $\mathcal{G}$ for which we can compute this discrepancy.

Class Selection (RKHS's)

Gorham and Mackey (2017) use *reproducing kernels* $k : \Theta \times \Theta \to \mathbb{R}$.

- For a kernel to be *reproducing*, it needs to be symmetric, i.e. $k(\theta, \theta') = k(\theta', \theta)$, and the kernel matrix $[K]_{ij} = k(\theta^{(i)}, \theta^{(j)})$ needs to be positive semi-definite. Some examples:
  - Polynomial kernel $k(\theta, \theta') = \sum_{j=1}^{J} P_j(\theta) P_j(\theta')$
  - Gaussian kernel: $k(\theta, \theta') = e^{-\|\theta - \theta'\|_2^2/(2\sigma)}$
- Such kernels induce a unique reproducing kernel Hilbert space $\mathcal{K}_k = \{h : h(\theta) = \sum_{i=1}^{N} c_i k(\theta^{(i)}, \theta)\}$ with norm $\|h\|_{\mathcal{K}_k} = \sqrt{\sum_{i=1}^{N} \sum_{j=1}^{N} c_i c_j k(\theta^{(i)}, \theta^{(j)})}$
  - Polynomial kernel $\mathcal{K}_k = \text{span}\{P_j\}_{j=1,\ldots,J}$
  - Gaussian kernel: $\mathcal{K}_k =$ (hard to write down but it has infinite span!)

Class Selection (RKHS's)

These methods give us the ability to have an infinite span for $\mathcal{G}$ while being computable.

Our functions $g \in \mathcal{G}$ need to be $\mathbb{R}^d$-valued functions and the space needs to be constrained:

$$\mathcal{G} =: \{g = (g_1, \ldots, g_d) \mid \|v\| \leq 1 \text{ for } v_j = \|g_j\|_{\mathcal{K}_k}\}$$

where $g_i \in \mathcal{K}_k$ for $i = 1, \ldots, d$.

This video explains more about RKHS's:
`https://www.youtube.com/watch?v=KZZD5sBwGCA`

Class Selection (RKHS's)

Under these choices, it can be shown that

$$d_{\mathcal{G}}(Q, \mathcal{A}, \pi) = \sup_{g \in \mathcal{G}} \mathbb{E}_Q[\mathcal{A}_\pi g(\theta)]$$

$$= \sqrt{\frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} k_0(\theta^{(i)}, \theta^{(j)})},$$

where

$$= \sqrt{\mathbb{E}_{\theta \sim Q, \theta' \sim Q}[k_0(\theta, \theta')]}$$

$$\begin{aligned} k_0(\theta, \theta') &= \mathcal{A}_\theta \mathcal{A}_{\theta'} k(\theta, \theta') \\ &= \text{trace}(\nabla_\theta \nabla_{\theta'} k(\theta, \theta')) + \nabla_\theta \log \pi(\theta|y) \cdot \nabla_{\theta'} k(\theta, \theta') \\ &\quad + \nabla_{\theta'} \log \pi(\theta'|y) \cdot \nabla_\theta k(\theta, \theta') + k(\theta, \theta') \nabla_\theta \log \pi(\theta|y) \cdot \nabla_{\theta'} \log \pi(\theta'|y). \end{aligned}$$

This discrepancy is called the kernel Stein discrepancy (KSD).

Convergence Determining?

The KSD can be computed at $\mathcal{O}(N^2)$ complexity given $\{\theta^{(i)}, \nabla_\theta \log \pi(\theta^{(i)}|y)\}_{i=1}^N$.

Now we have a computable discrepancy but when is it convergence determining? Stein's method requires thats we

- Lower bound the KSD to establish that $d_{\mathcal{G}}(Q, \mathcal{A}, \pi) \to 0$ only if $Q \to \pi$
- Upper bound the KSD to establish that $d_{\mathcal{G}}(Q, \mathcal{A}, \pi) \to 0$ if $Q \to \pi$

Both are needed. The quick answer is that it depends on the kernel choice, $k(\theta, \theta')$, and on the target, π.

Convergence Determining?

The recommended kernel for detecting non-convergence is the inverse multiquadric kernel (IMQ),

$$k(\theta, \theta') = (c^2 + \|\theta - \theta'\|_2^2)^{\beta},$$

with $\beta = -0.5$ and $c = 1$.

An Example

Problems with Gaussian & Matérn kernels: Figure 2 from Gorham & Mackey (2017)[1]:

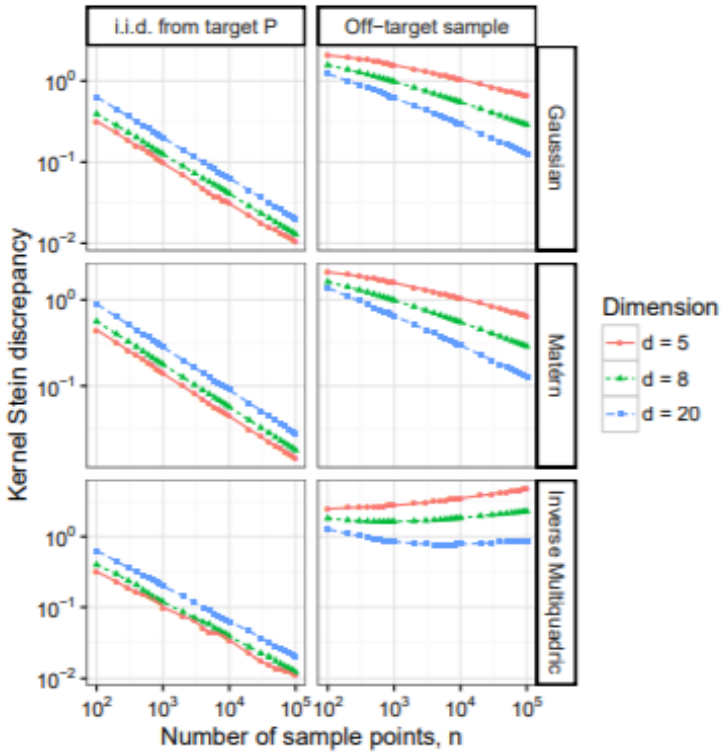


Figure 2. Gaussian and Matérn KSDs are driven to 0 by an off-target sequence that does not converge to the target $P = \mathcal{N}(0, I_d)$ (see Section 4.2). The IMQ KSD does not share this deficiency.

An Example

Figure 1 from Nemeth & Fearnhead (2021)[1]:

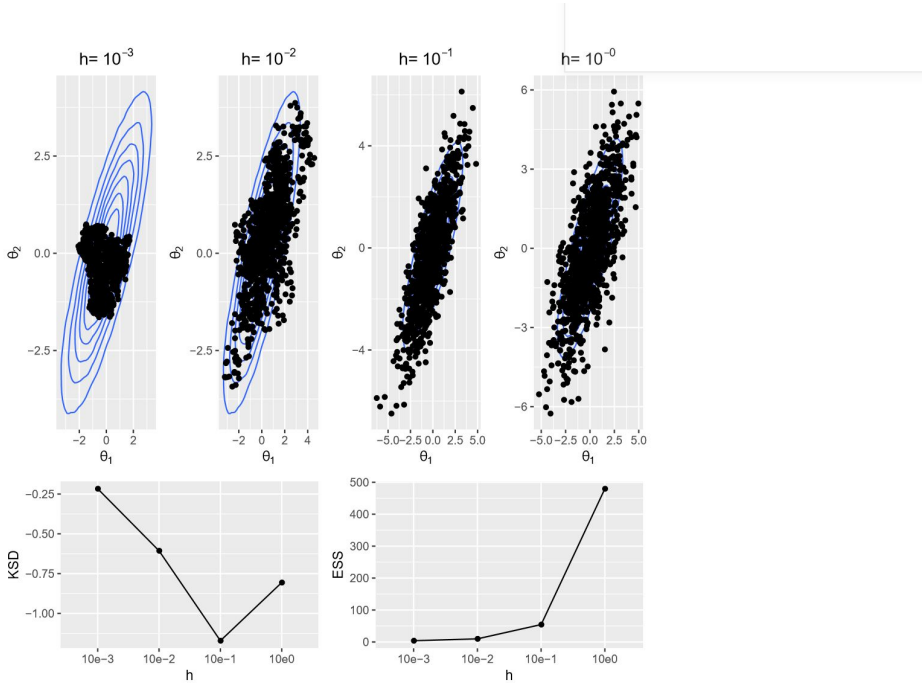


Figure 1: Top: Samples generated from the Langevin dynamics (7) are plotted over the bivariate Gaussian target. The samples are thinned to 1,000 for the ease of visualisation. Bottom: The kernel Stein discrepancy (log10) and effective sample size are calculated for each Markov chain with varying step size parameter h.

[1] Nemeth, C., & Fearnhead, P. (2021). Stochastic gradient Markov chain Monte Carlo. Journal of the American Statistical Association, 116(533), 433-450.

Running Example

Let's take a look at the radiata pine example.

Summary

- KSD can be used to compare the quality of samples from various methods
- This includes standard MCMC, biased MCMC, deterministic points, ...
- There is theory that tells us it's convergence-determining for some settings
  - Consider looking at the paper if you're not sure about your example
  - Even if the theory doesn't hold, it may still be practically useful.

Testing if $\{\theta^{(i)}\}_{i=1}^{N} \sim \pi$
with kernel Stein goodness of fit (GoF) tests

A goodness of fit test

Chwialkowski et al (2016)[1] designed a method to test if $\{\theta^{(i)}\}_{i=1}^N$ are generated from π using similar ideas to the KSD method.

We now think of the samples $\{\theta^{(i)}\}_{i=1}^N$ as coming from some unknown distribution Q. Therefore KSD is a random variable.

Applications: - biased MCMC (are the samples of the desired quality?) - standard MCMC - an alternative to standard normality tests - any time we want to test if $\{\theta^{(i)}\}_{i=1}^N \sim \pi$.

[1] Chwialkowski, K., Strathmann, H., & Gretton, A. (2016). A kernel test of goodness of fit. ICML

The test

Our hypotheses are:

$$H_0 : \{\theta^{(i)}\}_{i=1}^N \sim \pi$$
$$H_a : \{\theta^{(i)}\}_{i=1}^N \not\sim \pi$$

The test statistic, its distribution and the procedure are slightly different depending on whether we do[1] or don't[2] have autocorrelation.

We estimate quantiles of the test statistic under H_0 using a form of bootstrapping.

[1] Liu, Q., Lee, J., & Jordan, M. (2016). A kernelized Stein discrepancy for goodness-of-fit tests. ICML

[2] Chwialkowski, K., Strathmann, H., & Gretton, A. (2016). A kernel test of goodness of fit. ICML

Without Correlation

Our test statistic[3] is $\widetilde{\text{KSD}^2}$.

The kernel test of goodness of fit with significance level α:

1. Calculate the test statistic KSD^2
2. Obtain M sets of bootstrap samples $\{B_n^{(m)}\}$.
3. If KSD^2 exceeds the $1-\alpha$ empirical quantile of these samples, reject H_0.

[3] The tilde denotes a slight difference compared to KSD: we don't include $k(\theta, \theta)$ terms.

With Correlation: Wild Bootstrap

To take into account correlation, the procedure involves using a Markov chain taking values in $\{-1, 1\}$ starting from $W_1 = 1$ and following

$$W_t = 1(U_t > a)W_{t-1} - 1(U_t < a)W_{t-1}$$

where $U_t \sim U(0, 1)$ and a is the probability of W_t changing sign. The tuning parameter a should be chosen based on the level of autocorrelation ($a = 0.5$ for iid data).

The bootstrapped V-statistic is

$$B_n = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} W_i W_j k_0(x_i, x_j).$$

With Correlation: Wild Bootstrap

The kernel test of goodness of fit with significance level α:

1. Calculate the test statistic KSD^2
2. Obtain M sets of wild bootstrap samples $\{B_n^{(m)}\}$.
3. If KSD^2 exceeds the $1-\alpha$ empirical quantile of these samples, reject H_0.

Intuition: There is some theory[1] that says nB_n is a good approximation of $n\text{KSD}^2$ under the null. Under the alternative, $\text{KSD}^2 \to c$ for some $c > 0$ while $B_n \to 0$, resulting in almost sure rejection of the null.

[1] The theory assumes a basic regularity condition and holds for iid observations and geometrically ergodic Markov chains.

In practice

In practice,

- The kernel $k(\theta, \theta')$ can affect the statistical power (prob. of rejecting H_0 when the alternative is true).
- Choosing the tuning parameter a too high (underestimating the correlation) leads to overly conservative p-values but choosing it too low decreases power.

In practice

Chwialkowski et al (2016) recommend a mixture of thinning and adjusting the tuning parameter *a*...

hypothesis. In a general, we recommend to thin a chain so that $Cor(X_t, X_{t-1}) < 0.5$, set $a_n = 0.1/k$, and run test with at least $max(500k, d100)$ data points, where $k < 10$, and d is data dimensionality[3].

[3] We recommend men should drink no more than 68 units of alcohol per week, no more than 34 units in any given day, and have at least 1 alcohol-free day.

Choosing Which Samples to Use
with Stein thinning

Stein Thinning

The method of Riabiz et al (2020)[1] develop an approach to select a subset of m samples from our N samples ($m \ll N$) by minimising the KSD.

The goal is to select the subsample which minimises the KSD:

$$\begin{aligned} S &= \underset{S \subset \{1,\dots,N\}, |S|=m}{\arg\min} \; d_{\mathcal{G}}(Q_m, \mathcal{A}, \pi) \\ &= \underset{S \subset \{1,\dots,N\}, |S|=m}{\arg\min} \; d_{\mathcal{G}}(\frac{1}{m}\sum_{i \in S} \delta_{\theta^{(i)}}, \mathcal{A}, \pi) \end{aligned}$$

This is an expensive combinatorial problem. A greedy minimisation based on selecting one sample at a time works well.

[1] Riabiz, M., Chen, W., Cockayne, J., Swietach, P., Niederer, S. A., Mackey, L., & Oates, C. (2020). Optimal thinning of MCMC output. arXiv preprint arXiv:2005.03952.

Stein Thinning

I recommend going to the website

`http://stein-thinning.org/`

Stein thinning is bias-removing in some contexts (we can get KSD $\to 0$ as $m, n \to \infty$ for certain non π-invariant Markov chains).

We can also use all of the samples or a weighted set of samples (related to the next section). Rob Salomone (next week) has done some related work!

Improving Estimates
using Stein-based control variates

Setting

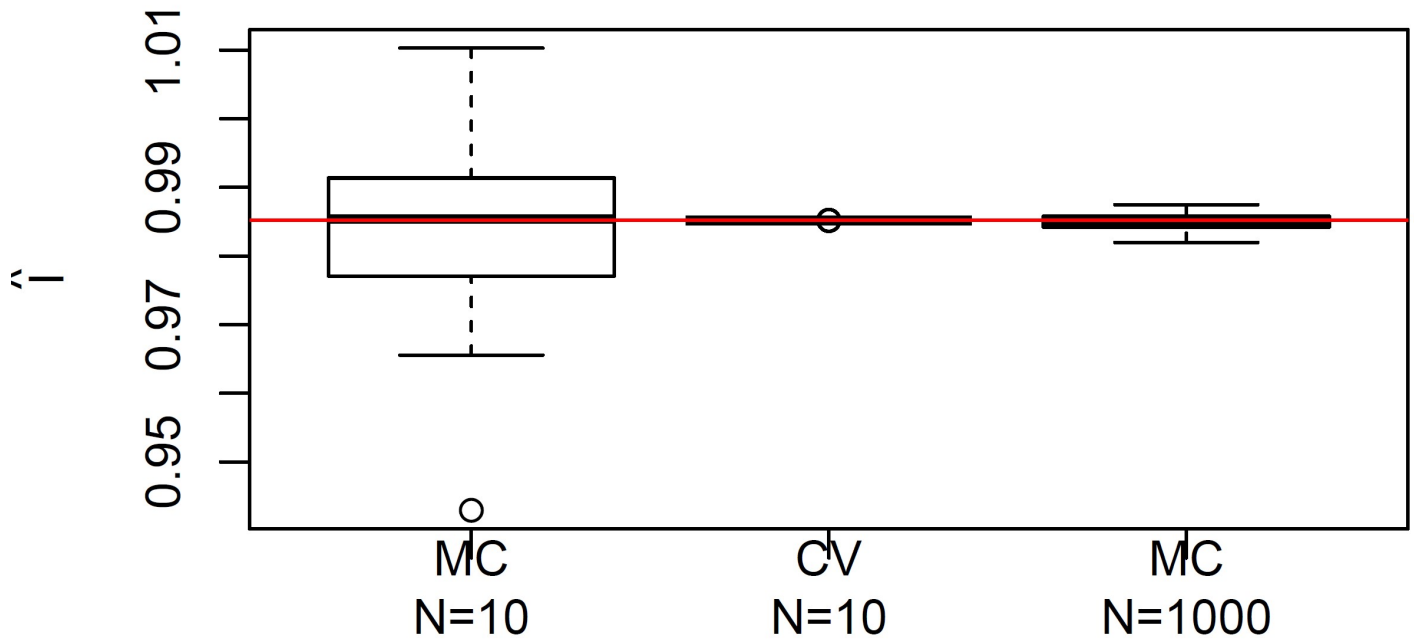
We have samples $\{\theta^{(i)}\}_{i=1}^N$ and gradients $\{\nabla_\theta \log \pi(\theta^{(i)}|y)\}_{i=1}^N$ and we want to evaluate

$$I = \mathbb{E}_\pi[f(\theta)] = \int_\Omega f(\theta)\pi(\theta|y)d\theta.$$

We now focus on improving upon the vanilla estimate $\hat{I} = \frac{1}{N}\sum_{i=1}^N f(\theta^{(i)})$, which often has high variance and/or bias.

This Section

Example comparisons



All methods I'll talk about are in the R package ZVCV.

Control Variates

In control variates, we replace the Monte Carlo estimator with

$$\hat{I}_{\text{CV}} = \frac{1}{N}\sum_{i=1}^{N}\left[f(\theta^{(i)}) - \tilde{f}(\theta^{(i)})\right] + \int_{\Omega}\tilde{f}(\theta)\pi(\theta|y)\mathrm{d}\theta.$$

Control Variates

The intuition for i.i.d. samples from π:

- $\mathbb{E}_\pi[\hat{I}_{\text{CV}}] = I$
- $\mathbb{V}_\pi[\hat{I}_{\text{CV}}] \ll \mathbb{V}_\pi[\hat{I}_{\text{MC}}]$ because

$$\mathbb{V}_\pi[f(\theta) - \tilde{f}(\theta)] = \mathbb{V}_\pi[f(\theta)] + \mathbb{V}_\pi[\tilde{f}(\theta)] \underline{\underline{-2\mathbb{COV}_\pi[f(\theta), \tilde{f}(\theta)]}}$$

Stein Control Variates

Desiderata for control variates:

1. Ability to evaluate $\mathbb{E}_\pi[f(\theta)] = \int_\Omega \tilde{f}(\theta)\pi(\theta|y)\mathrm{d}\theta$
2. Easy to compute $\tilde{f}$ at $\{\theta^{(i)}\}_{i=1}^N$
3. Reduced variance: $\sigma^2(f - \tilde{f}) \ll \sigma^2(f)$

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3. Reduced variance: $\sigma^2(f - \tilde{f}) \ll \sigma^2(f)$

Control variates based on the Langevin Stein operator can satisfy these.

Stein Control Variates

Oates et al (2017) propose to use

$$\tilde{f}(\theta) = a + \mathcal{A}g(\theta),$$

where $a \in \mathbb{R}$, g is a user-specified function and $\mathcal{A}$ is a Stein operator:

$$\mathcal{A}g(\theta) = \nabla_\theta \cdot g(\theta) + \nabla \log \pi(\theta|y) \cdot g(\theta) \text{ for } g : \Theta \to \mathbb{R}^d$$
$$\mathcal{A}g(\theta) = \Delta_\theta g(\theta) + \nabla \log \pi(\theta|y) \cdot \nabla_\theta g(\theta) \text{ for } g : \Theta \to \mathbb{R}$$

which signifies that $\mathbb{E}_\pi[\mathcal{A}g(\theta)] = 0$ under regularity conditions on g and π.

The challenge is to choose g so that $\sigma^2(f - \tilde{f}) \ll \sigma^2(f)$. The key is to select $g \in \mathcal{G}$ by optimising some criterion.

Zero-Variance Control Variates: Polynomial $\mathcal{G}$

Assaraf and Caffarel (1999) and Mira et al. (2013) choose $\mathcal{G}$ to be the class of rth order polynomials.

Zero-Variance Control Variates: Polynomial $\mathcal{G}$

Assaraf and Caffarel (1999) and Mira et al. (2013) choose $\mathcal{G}$ to be the class of rth order polynomials.

$P(\theta) = \beta_0 + \beta_1 \theta + \beta_2 \theta^2$

This leads to

$$\begin{aligned}\tilde{f}(\theta) &= a + \mathcal{A}P(\theta) \\ &= a + \sum_{j=1}^{J} \beta_j \mathcal{A}P_j(\theta), \\ &= a + \beta^T x(\theta),\end{aligned}$$

where $\beta \in \mathbb{R}^J$ is the polynomial coefficients and $x(\theta) \in \mathbb{R}^J$ is a vector of terms involving θ and $\nabla_\theta \log \pi(\theta|y)$.

Zero-Variance Control Variates: Polynomial $\mathcal{G}$

A common approach to estimating (a, β) is OLS,

$$(\hat{a}, \hat{\beta}) \in \underset{\substack{a \in \mathbb{R} \\ \beta \in \mathbb{R}^J}}{\arg\min} \sum_{i=1}^{N} \left[f(\theta^{(i)}) - a - \beta^\top x(\theta^{(i)}) \right]^2,$$

so $(\hat{a}, \hat{\beta})^\top = (X^\top X)^{-1} X^\top f$ and the resulting estimator is

$$\hat{I}_{\text{ZVCV}} = \frac{1}{N} \sum_{i=1}^{N} \left[f(\theta^{(i)}) - \hat{\beta}^\top x(\theta^{(i)}) \right] = \hat{a}.$$

Zero-Variance Control Variates: Polynomial $\mathcal{G}$

$$\log \pi(\theta) = -\frac{1}{2}\log(2\pi) - (\theta-5)^2/2$$
$$\nabla_\theta \log \pi(\theta) = -2(\theta-5)/2 = -(\theta-5)$$

Let's implement this to estimate some expectations for a unit normal distribution $\pi(\theta) = \frac{1}{\sqrt{2\pi}} e^{-(\theta-5)^2/2}$ where $\{\theta^{(i)}\}_{i=1}^{10} \overset{iid}{\sim} \pi$.

$$P(\theta) = \beta_0 + \beta_1 \theta$$
$$\widetilde{f}(\theta) = a + A P(\theta) \quad (A \to \Delta)$$
$$= a + \Delta P(\theta) + \nabla \log \pi(\theta) \cdot \nabla P(\theta) \quad (\nabla P(\theta) \to \beta_1)$$
$$= a + \nabla \log \pi(\theta) \cdot \beta_1$$
$$= a + \beta_1(-(\theta-5))$$

Control Functionals: RKHS $\mathcal{G}$

Oates et al. (2017) set $\mathcal{G}$ to be a reproducing kernel hilbert space $\mathcal{K}_k$.

$$(\hat{a}, \hat{g}) \in \underset{\substack{a \in \mathbb{R} \\ g \in \mathcal{K}_k}}{\arg\inf} \frac{1}{N} \sum_{i=1}^{N} \left[f(\theta^{(i)}) - a - \mathcal{A}g(\theta^{(i)}) \right]^2 + \lambda \|g\|^2_{\mathcal{K}_k}$$

In practice, performing CF amounts to choosing a kernel $k(\theta, \theta')$, estimating its parameters and solving the N by N linear system:

$$\hat{I}_{\text{CF}} = \frac{1^T (K_0 + \lambda N I)^{-1} f}{1^T (K_0 + \lambda N I)^{-1} 1}$$

where $f_i = f(\theta^{(i)})$ and $[K_0]_{i,j} = \mathcal{A}_x \mathcal{A}_y k(x, y)|_{x=\theta^{(i)}, y=\theta^{(j)}}$.

The estimator can also be thought of as the posterior mean with a Gaussian process prior $f \sim \mathcal{GP}(0, K_0)$.

Semi-Exact Control Functionals

The interpolant takes the form

$$\tilde{f}(\theta) = b_0 + \underbrace{\sum_{j=1}^{J-1} b_j \mathcal{A} P_j(\theta)}_{\text{related to ZV-CV}} + \underbrace{\sum_{i=1}^{N} a_i k_0(\theta, \theta^{(i)})}_{\text{related to CF}} .$$

where $\{P_j\}_{j=1}^{J-1}$ is a polynomial basis

Semi-Exact Control Functionals

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where $\{P_j\}_{j=1}^{J-1}$ is a polynomial basis and the coefficients a and b are selected such that

1. $\tilde{f} = f$ whenever $f \in \text{span}(1, \mathcal{A}P_1, \ldots, \mathcal{A}P_{J-1})$
2. $\tilde{f}(\theta^{(i)}) = f(\theta^{(i)})$ for $i = 1, \ldots, N$

This is estimating the posterior mean using a GP prior $f \sim \mathcal{GP}(\sum_{j=1}^{J-1} b_j \mathcal{A}P_j, K_0)$

Semi-Exact Control Functionals

Estimation of a and b amounts to solving the linear system

$$\begin{bmatrix} K_0 & P \\ P^T & 0 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix},$$

where

$$P = \begin{bmatrix} 1 & \mathcal{A}P_1(\theta^{(1)}) & \cdots & \mathcal{A}P_J(\theta^{(1)}) \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \mathcal{A}P_1(\theta^{(N)}) & \cdots & \mathcal{A}P_J(\theta^{(N)}) \end{bmatrix} \text{ and } \quad f = \begin{bmatrix} f(\theta^{(1)}) \\ \vdots \\ f(\theta^{(N)}) \end{bmatrix}.$$

Semi-Exact Control Functionals

The estimator is

$$\begin{aligned}\hat{I}_{\text{SECF}} &= \frac{1}{N}\sum_{i=1}^{N}\left[f(\theta^{(i)}) - \tilde{f}(\theta^{(i)})\right] + \int_{\Omega}\tilde{f}(\theta)\pi(\theta|y)\mathrm{d}\theta \\ &= \int_{\Omega}\tilde{f}(\theta)\pi(\theta|y)d\theta \\ &= \hat{b}_0 \\ &= e_1^T(P^T K_0^{-1} P)^{-1} P^T K_0^{-1} f\end{aligned}$$

Summary of Theory

- The polynomial approaches (ZV-CV and SECF) are exact for all rth order polynomials in the Bernstein-von-Mises (Bayesian big data) limit
- The kernel-based approaches (CF and SECF) offer consistency:

$$\hat{I}_{\text{SECF}} \to I \text{ in probability as } N \to \infty,$$

under certain conditions even in the biased sampling setting where the Markov chain is not π-invariant and the potential for improved convergence rates.

Example Bias-Correction

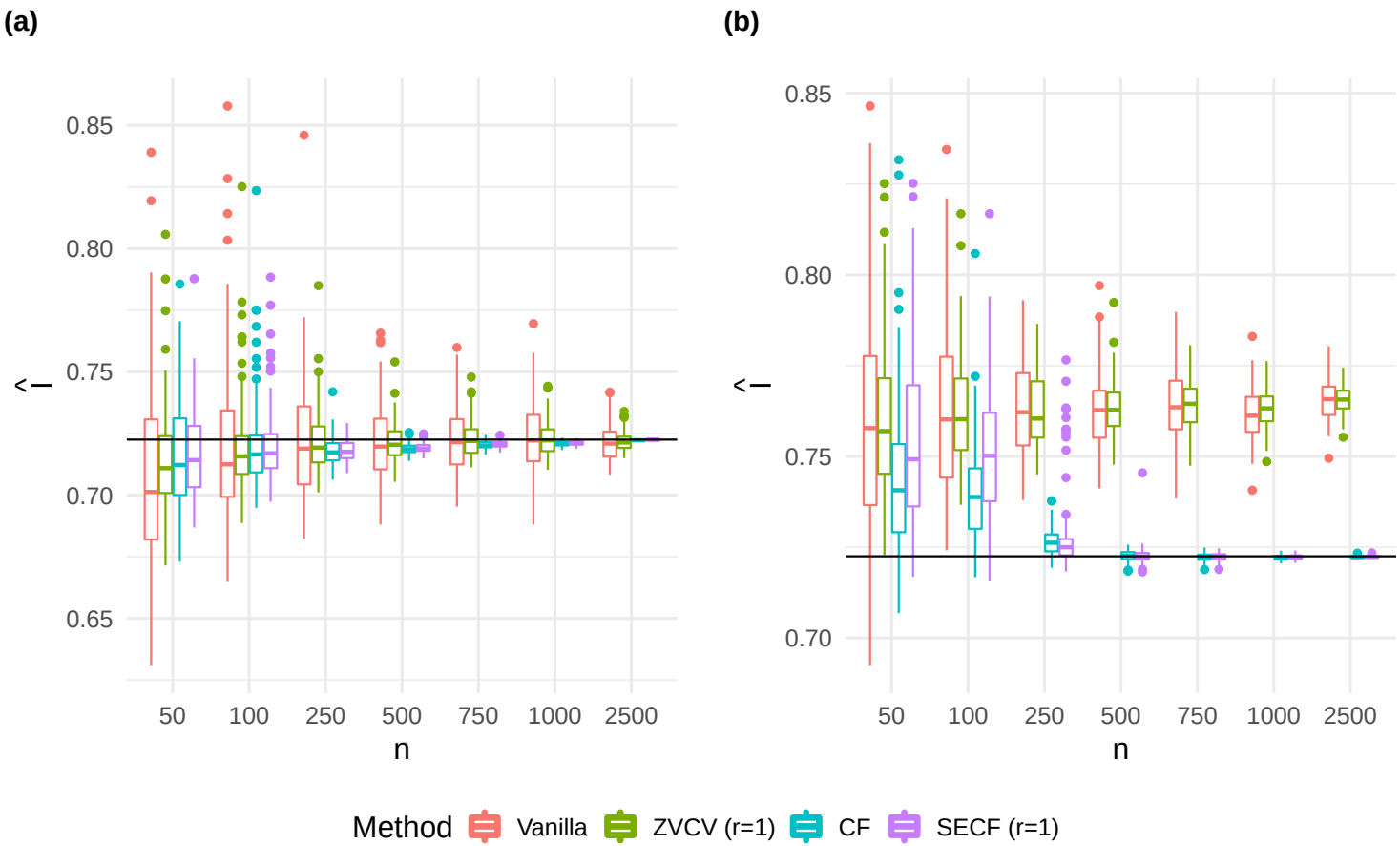

Figure: Boxplots of 100 estimates of an expectation when (a) MALA and (b) ULA are used for sampling. The black horizontal line is the gold standard.

R package

ZVCV is available on CRAN.

ZVCV_package {ZVCV} R Documentation

Zero-Variance Control Variates

Description

This package can be used to perform post-hoc variance reduction of Monte Carlo estimators when the derivatives of the log target are available. The main functionality is available through the following functions. All of these use a set of N d-dimensional samples along with the associated derivatives of the log target. You can evaluate posterior expectations of k functions.

- `zvcv`: For estimating expectations using (regularised) zero-variance control variates (ZV-CV, Mira et al, 2013; South et al, 2018). This function can also be used to choose between various versions of ZV-CV using cross-validation.
- `CF`: For estimating expectations using control functionals (CF, Oates et al, 2017).
- `SECF`: For estimating expectations using semi-exact control functionals (SECF, South et al, 2020).
- `aSECF`: For estimating expectations using approximate semi-exact control functionals (aSECF, South et al, 2020).
- `CF_crossval`: CF with cross-validation tuning.
- `SECF_crossval`: SECF with cross-validation tuning.
- `aSECF_crossval`: aSECF with cross-validation tuning.

ZV-CV is exact for polynomials of order at most `polyorder` under Gaussian targets and is fast for large N (although setting a limit on `polyorder` through `polyorder_max` is recommended for large N). CF is a non-parametric approach that offers better than the standard Monte Carlo convergence rates. SECF has both a parametric and a non-parametric component and it offers the advantages of both for an additional computational cost. The cost of SECF is reduced in aSECF using nystrom approximations and conjugate gradient.

Helper functions

Running Example

Let's take a look at the radiata pine example.

Summary

Summary

We have covered

- **Sample quality:**
  - Measuring sample quality with the kernel Stein discrepancy
  - Testing if $\{\theta^{(i)}\}_{i=1}^N \sim \pi$ with kernel Stein goodness of fit tests
- **Choosing samples:**
  - Selecting a subset of samples with Stein thinning
- **Improving estimates:**
  - Improving upon $\widehat{\mathbb{E}_\pi[f(\theta)]} = \frac{1}{N}\sum_{i=1}^N f(\theta^{(i)})$ with Stein-based control variates.

All methods used $\{\theta^{(i)}, \nabla_\theta \log \pi(\theta^{(i)}|y)\}_{i=1}^N$.

Advert

Do you want 80 hours of paid RA work?[1]

- Write a vignette on ZVCV + RStan
- Try out some of these methods
- ...

I'm also doing research on a fast alternative to KSD.

[1] QUT may make this difficult for external applicants, sorry.

Additional Resources

- This talk by the creator of the KSD: `https://www.youtube.com/watch?v=nVTL2yH_VOk`
- The review paper and references within: South, L. F., Riabiz, M., Teymur, O., & Oates, C. (2021). Post-Processing of MCMC. *arXiv preprint arXiv:2103.16048*.
- The review paper and references within: Anastasiou, A., Barp, A., Briol, F. X., Ebner, B., Gaunt, R. E., Ghaderinezhad, F., Gorham, J., Gretton, A., Ley, C., Liu, Q., Mackey, L., Oates, C. J., Reinert, G. & Swan, Y. (2021). Stein's Method Meets Statistics: A Review of Some Recent Developments. *arXiv preprint arXiv:2105.03481*.

Boundary/tail condition

$$\begin{aligned}
\mathbb{E}_\pi[\mathcal{A}g(\theta)] &= \int_\Omega \mathcal{A}g(\theta)\pi(\theta|y)\mathrm{d}\theta \\
&= \int_\Omega \nabla_\theta \cdot (\pi(\theta|y)\nabla_\theta g(\theta))\,\mathrm{d}\theta \\
&= \oint_{\delta\Omega} \pi(\theta|y)\nabla_\theta g(\theta) \cdot n(\theta) S(\mathrm{d}\theta)
\end{aligned}$$

where the last line is by the divergence theorem.

Convergence Determining?

Upper bound: Under regularity conditions, we have that $d_{\mathcal{G}}(Q, \mathcal{A}, \pi) \to 0$ when the Wasserstein distance between Q and π goes to zero.
Lower bound: Kernels with rapidly decaying tails can lead to $d_{\mathcal{G}}(Q, \mathcal{A}, \pi) \to 0$ even when $Q \not\to \pi$.

The conditions required for $d_{\mathcal{G}}(Q, \mathcal{A}, \pi) \to 0$ only if $Q \to \pi$ are:

- $d = 1$: π is "distantly dissipative"[1] and k is sufficiently regular[2]
- $d > 1$: All of the above plus k does not decay more rapidly than the score function grows.

KSD fails to detect non-convergence for bounded scores.

[1] A relaxation of log-concavity covering many distributions of interest including Bayesian logistic & student's t regression with Gaussian priors, Gaussian mixtures with common variance and more

[2] $k(\theta, \theta') = \Phi(\theta - \theta')$ for Φ with continuous second order derivatives and a non-vanishing generalised Fourier transform.