Gradient-Free Optimal Postprocessing of MCMC Output

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Overview

Problem

Develop a computationally efficient algorithm for summarising the output of a Markov Chain Monte Carlo simulation.

Motivation

Uncertainty quantification in a multi-stage simulation of the functioning of the human heart.

Existing solution

The optimisation algorithm of Riabiz et al. (2022) to select a subsample of MCMC output that minimises a measure of proximity to the target distribution (kernel Stein discrepancy), which requires the gradients of the log-posterior and is thus expensive.

Proposal

Modify the algorithm of Riabiz et al. (2022) to use the gradient-free kernel Stein discrepancy of Fisher and Oates (2024).

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Markov Chain Monte Carlo

Markov chain Monte Carlo (MCMC) are a popular class of algorithms for sampling from complex probability distributions.

Given a target distribution P defined on a state space $\mathcal{X}$, an MCMC algorithm proceeds by constructing a chain of random variables $(X_i)_{i=0}^{\infty}$ which satisfy the Markov property:

$$\mathbb{P}(X_{i+1} \in A | X_0, \dots, X_i) = \mathbb{P}(X_{i+1} \in A | X_i) \quad \text{for any measurable } A \in \mathcal{X}.$$

Viewed as a function, the right-hand side above is called the Markov transition kernel and is denoted

$$R(A|x) \coloneqq \mathbb{P}(X_{i+1} \in A | X_i = x).$$

The transition kernel R is selected so that it is easy to sample from and to ensure asymptotic convergence to the target distribution P:

$$P_i \xrightarrow{d} P \quad \text{as} \quad i \to \infty.$$

A sample of size n is a realisation $(x_i)_{i=0}^{n}$ of the first n variables in the chain, which is constructed sequentially.

Challenges of running MCMC

1. Dependency on the starting point of a chain
   - $\Rightarrow$ detection and removal of burn-in
   - $\Rightarrow$ running multiple chains
2. Efficient traversal of the target domain
   - $\Rightarrow$ calibration of the scale of the proposal distribution
3. Exploring the modes of a multimodal distribution
   - $\Rightarrow$ calibration of the scale of the proposal distribution
   - $\Rightarrow$ running multiple chains
4. Convergence detection
   - $\Rightarrow$ convergence diagnostics
   - $\Rightarrow$ running multiple chains
5. Autocorrelation between samples in a chain
   - $\Rightarrow$ thinning
6. Summarising the sample for further expensive processing
   - $\Rightarrow$ thinning

Thinning

Problem

Given MCMC output $(x_i)_{i=1}^n$ of length n, identify $m \ll n$ indices $\pi(j) \in \{1, \ldots, n\}$ with $j \in \{1, \ldots, m\}$, such that the approximation provided by the subset of samples

$$\frac{1}{m} \sum_{j=1}^{m} \delta(x_{\pi(j)})$$

is closest to the target distribution.

We need a measure of proximity of the selected subsample to the target distribution.

Measure of proximity

Integral probability metric

An integral probability metric between two distributions P and P' is defined as

$$\mathcal{D}_{\mathcal{F}}(P, P') := \sup_{f \in \mathcal{F}} \left| \int_{\mathcal{X}} f \, \mathrm{d}P - \int_{\mathcal{X}} f \, \mathrm{d}P' \right|,$$

where $\mathcal{X}$ is a measurable space on which both P and P' are defined and $\mathcal{F}$ is a set of test functions.

The metric is said to be *measure-determining* if

$$\mathcal{D}_{\mathcal{F}}(P, P') = 0 \quad \text{iff} \quad P = P',$$

and it offers *convergence control* if

$$\mathcal{D}_{\mathcal{F}}(P, P'_m) \to 0 \quad \text{implies} \quad P'_m \xrightarrow{d} P$$

as $m \to \infty$, for any sequence of distributions P'_m.

Measure of proximity

Integral probability metric

An integral probability metric between two distributions P and P' is defined as

$$\mathcal{D}_{\mathcal{F}}(P, P') := \sup_{f \in \mathcal{F}} \left| \int_{\mathcal{X}} f \, \mathrm{d}P - \int_{\mathcal{X}} f \, \mathrm{d}P' \right|,$$

where $\mathcal{X}$ is a measurable space on which both P and P' are defined and $\mathcal{F}$ is a set of test functions.

However, it is difficult to compute in practice:

- the integral $\int_{\mathcal{X}} f \, \mathrm{d}P$ is often intractable,
  - $\Rightarrow$ Gorham and Mackey (2015): use infinitesimal generator of the overdamped Langevin diffusion to eliminate $\int_{\mathcal{X}} f \, \mathrm{d}P$.
- the supremum requires optimisation.
  - $\Rightarrow$ Gorham and Mackey (2017): use reproducing kernel Hilbert spaces to obtain the supremum in closed form.

Kernel Stein discrepancy

Kernel Stein discrepancy (KSD)

$$\mathcal{D}_P^2(P') := \iint_{\mathcal{X}} k_P(x,y)\,\mathrm{d}p'(x)\,\mathrm{d}p'(y),$$

If P' is a discrete distribution, this becomes

$$\mathcal{D}_P^2\left(\frac{1}{n}\sum_{i=1}^{n}\delta(x_i)\right) = \frac{1}{n^2}\sum_{i,j=1}^{n} k_P(x_i,x_j),$$

where

$$\begin{aligned} k_P(x,y) :=& (\nabla_x \cdot \nabla_y) k(x,y) \\ &+ \langle \nabla_x k(x,y), \nabla_y \log p(y)\rangle + \langle \nabla_y k(x,y), \nabla_x \log p(x)\rangle \\ &+ k(x,y)\langle \nabla_x \log p(x), \nabla_y \log p(y)\rangle. \end{aligned}$$

The typical choice for $k(x,y)$ is the inverse multiquadric kernel:

$$k(x,y) = \left(c^2 + \|\Gamma^{-1/2}(x-y)\|\right)^{\beta}.$$

Stein thinning

Riabiz et al. (2022) propose a greedy algorithm to select points from the sample that minimise the KSD at each iteration:

Algorithm 1: Stein thinning.

Data:

sample $(x_i)_{i=1}^n$ from MCMC,

gradients $(\nabla \log p(x_i))_{i=1}^n$

desired cardinality $m \in \mathbb{N}$

Result: Indices π of a sequence $(x_{\pi(j)})_{j=1}^m$ where $\pi(j) \in \{1, \ldots, n\}$.

for $j = 1, \ldots, m$ **do**

$$\pi(j) \in \underset{i=1,\ldots,n}{\arg\min} \frac{k_P(x_i, x_i)}{2} + \sum_{j'=1}^{j-1} k_P(x_{\pi(j')}, x_i)$$

end

Stein thinning (continued)

The complication in using Stein thinning comes from the need to calculate gradients of the log-posterior to evaluate the kernel:

$$
\begin{aligned}
k_P(x, y) :=& (\nabla_x \cdot \nabla_y) k(x, y) \\
& + \langle \nabla_x k(x, y), \nabla_y \log p(y) \rangle + \langle \nabla_y k(x, y), \nabla_x \log p(x) \rangle \\
& + k(x, y) \langle \nabla_x \log p(x), \nabla_y \log p(y) \rangle .
\end{aligned}
$$

This might be expensive, although it can be easily parallelised.

Gradient-free kernel Stein discrepancy

Fisher and Oates (2024) introduce a gradient-free version of KSD. An auxiliary distribution Q need to be chosen by the user, then the gradient-free KSD is given by

$$k_{P,Q}(x,y) = \frac{q(x)}{p(x)} \frac{q(y)}{p(y)} k_Q(x,y),$$

where

$$\begin{aligned} k_Q(x,y) :=& (\nabla_x \cdot \nabla_y) k(x,y) \\ &+ \langle \nabla_x k(x,y), \nabla_y \log q(y) \rangle + \langle \nabla_y k(x,y), \nabla_x \log q(x) \rangle \\ &+ k(x,y) \langle \nabla_x \log q(x), \nabla_y \log q(y) \rangle. \end{aligned}$$

When $k(x,y)$ is the inverse multiquadric kernel, the gradient-free KSD offers convergence control (Theorem 2 in Fisher and Oates (2024)).

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Gradient-free Stein thinning

We modify the algorithm of Riabiz et al. (2022) to minimise the gradient-free KSD of Fisher and Oates (2024):

Algorithm 2: Gradient-free Stein thinning.

Data:

sample $(x_i)_{i=1}^n$ from MCMC,

target log-densities $(\log p(x_i))_{i=1}^n$

auxiliary log-densities $(\log q(x_i))_{i=1}^n$

auxiliary gradients $(\nabla \log q(x_i))_{i=1}^n$

desired cardinality $m \in \mathbb{N}$

Result: Indices π of a sequence $(x_{\pi(j)})_{j=1}^m$ where $\pi(j) \in \{1, \ldots, n\}$.

for $j = 1, \ldots, m$ **do**

$$\pi(j) \in \operatorname*{arg\,min}_{i=1,\ldots,n} \frac{k_{P,Q}(x_i, x_i)}{2} + \sum_{j'=1}^{j-1} k_{P,Q}(x_{\pi(j')}, x_i)$$

end

Algorithm 3: Optimised gradient-free Stein thinning.

Data:

sample $(x_i)_{i=1}^n$ from MCMC,

target log-densities $(\log p(x_i))_{i=1}^n$

auxiliary log-densities $(\log q(x_i))_{i=1}^n$

auxiliary gradients $(\nabla \log q(x_i))_{i=1}^n$

desired cardinality $m \in \mathbb{N}$.

Result: Indices π of a sequence $(x_{\pi(j)})_{j=1}^m$ where $\pi(j) \in \{1, \ldots, n\}$.

Initialise an array $A[i]$ of size n

Set $A[i] = k_{P,Q}(x_i, x_i)$ for $i = 1, \ldots, n$

Set $\pi(1) = \arg\min_i A[i]$

for $j = 2, \ldots, m$ **do**

  Update $A[i] = A[i] + 2k_{P,Q}(x_{\pi(j-1)}, x_i)$ for $i = 1, \ldots, n$

  Set $\pi(j) = \arg\min_i A[i]$

end

Evaluation protocol

The following protocol was used in the evaluating the new method:

1. obtain a sample from the target distribution,
2. apply thinning to get a subsample of a given cardinality,
3. evaluate the result using an impartial metric.

Energy distance

In order to assess how well the selected sample approximates the target distribution, we use the energy distance.

Energy distance (Rizzo and Székely (2016))

The squared energy distance is defined for two distributions P and Q as

$$D_e^2(P,Q) := 2\mathbb{E}\|X - Y\| - \mathbb{E}\|X - X'\| - \mathbb{E}\|Y - Y'\|,$$

where $X, X' \sim P$ and $Y, Y' \sim Q$.

For samples $x_1, \dots, x_n$ and $y_1, \dots, y_m$ from X and Y, respectively, the corresponding statistic is given by

$$\mathcal{E}_{n,m}(P,Q) := \frac{2}{nm}\sum_{i=1}^{n}\sum_{j=1}^{m}\|x_i - y_j\| - \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\|x_i - x_j\| - \frac{1}{m^2}\sum_{i=1}^{m}\sum_{j=1}^{m}\|y_i - y_j\|.$$

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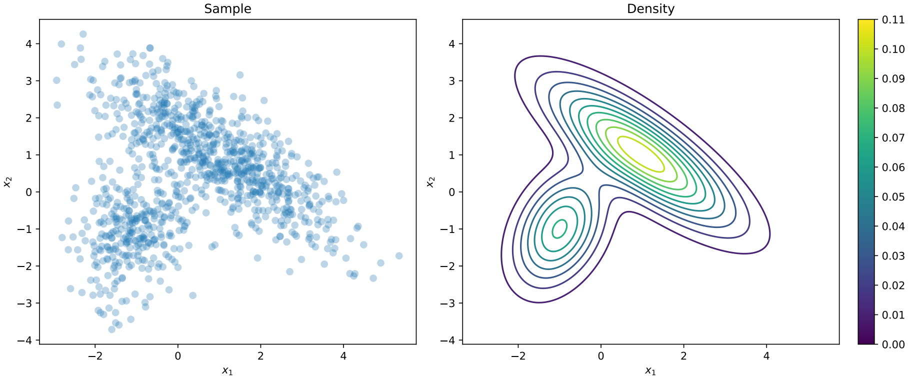
Bivariate Gaussian mixture

We use the bivariate Gaussian mixture with component weights $w = (0.3, 0.7)^T$, means $\mu_1 = (-1, -1)^T$, $\mu_2 = (1, 1)^T$ and covariances

$$\Sigma_1 = \begin{pmatrix} 0.5 & 0.25 \\ 0.25 & 1 \end{pmatrix}, \quad \Sigma_2 = \begin{pmatrix} 2 & -0.8\sqrt{3} \\ -0.8\sqrt{3} & 1.5 \end{pmatrix}.$$

We obtain 1000 points by directly drawing from the target distribution:

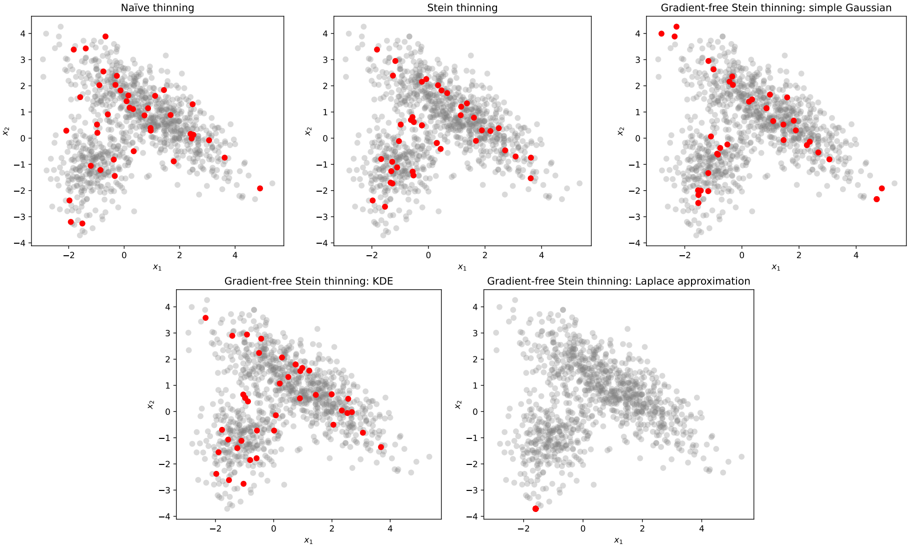


Bivariate Gaussian mixture: thinning approaches

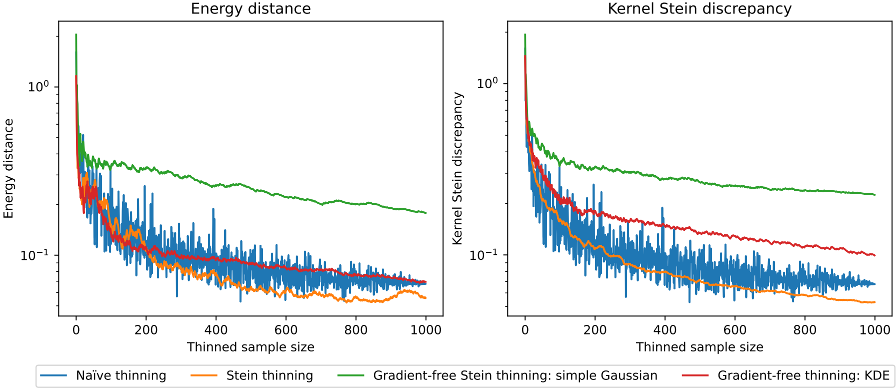
We evaluate the following approaches:

- naïve thinning,
- standard Stein thinning,
- gradient-free Stein thinning with different choices of Q:
  - multivariate Gaussian using the sample mean and covariance,
  - Laplace approximation,
  - KDE approximation.

Bivariate Gaussian mixture: thinning results



Bivariate Gaussian mixture: comparison of approaches



Lotka-Volterra inverse problem

The Lotka-Volterra model describes the evolution of an idealised ecosystem with two species: predator and prey.
Let u_1 be the size of the prey population and u_2 the size of the predator population. The model then postulates the following dynamic:

$$\frac{\mathrm{d}u_1}{\mathrm{d}t} = \theta_1 u_1 - \theta_2 u_1 u_2,$$
$$\frac{\mathrm{d}u_2}{\mathrm{d}t} = -\theta_3 u_2 + \theta_4 u_1 u_2,$$

with $\theta_1, \ldots, \theta_4 > 0$.
The inverse problem: given a noisy realisation

$$y(t) = \begin{pmatrix} u_1(t) \\ u_2(t) \end{pmatrix} + \varepsilon(t),$$

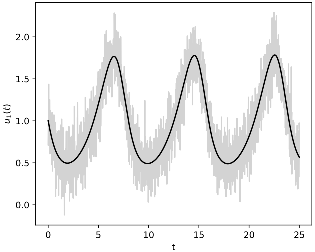
infer $\theta = (\theta_1, \ldots, \theta_4)^T$ that best describes the observed behaviour.

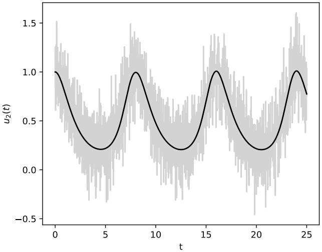
Lotka-Volterra inverse problem: synthetic data

Lotka-Volterra model

$$\frac{\mathrm{d}u_1}{\mathrm{d}t} = \theta_1 u_1 - \theta_2 u_1 u_2,$$
$$\frac{\mathrm{d}u_2}{\mathrm{d}t} = -\theta_3 u_2 + \theta_4 u_1 u_2,$$

We solve the equations with parameters $\theta^* = (0.67, 1.33, 1, 1)^T$ and initial values $u(0) = (1, 1)^T$, and add bivariate i.i.d. Gaussian noise $\varepsilon(t) \sim \mathcal{N}(0, \mathrm{diag}(0.2^2, 0.2^2))$:





Lotka-Volterra inverse problem: Bayesian inference

Assuming independent observations, we take the likelihood to be

$$\mathcal{L}(\theta) = \prod_{i=1}^{N} \phi_i(u(t_i;\theta)),$$

where

$$\phi_i(u(t_i;\theta)) \propto \exp\left(-\frac{1}{2}(y(t_i) - u(t_i;\theta))^T C^{-1}(y(t_i) - u(t_i;\theta))\right)$$

with $C = \mathrm{diag}(0.2^2, 0.2^2)$.
Since $\theta_k > 0$, we put independent log-normal priors on each θ_k:

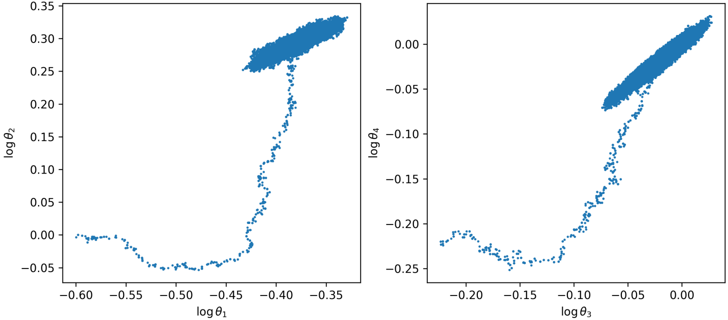
$$\pi(\theta) \propto \exp\left(-\frac{1}{2}(\log\theta)^T(\log\theta)\right).$$

By the Bayes theorem, the posterior is then

$$p(\theta) \propto \mathcal{L}(\theta)\pi(\theta).$$

Lotka-Volterra inverse problem: MCMC sample

The inference is performed using the Metropolis-Hastings algorithm with the starting points taken from Riabiz et al. (2022).
Since the parameters θ_k of the Lotka-Volterra model are positive, we run MCMC in the log-space by applying the reparameterisation $\zeta_k = \log \theta_k$.
We run 500,000 iterations of the algorithm for each chain.
The sample from the first chain is shown here for illustration:



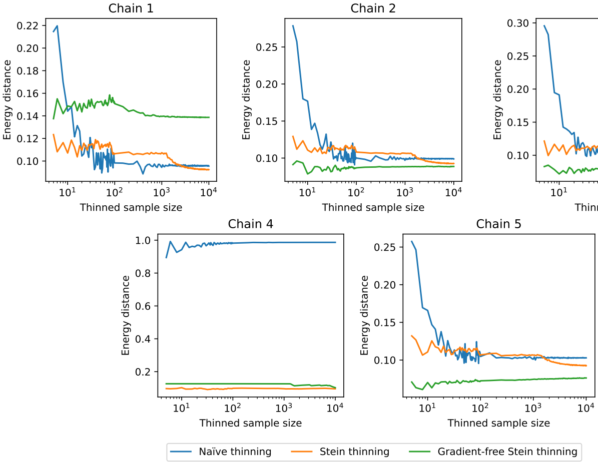
Lotka-Volterra inverse problem: thinning approaches

We evaluate the following approaches:

- naïve thinning,
- standard Stein thinning,
- gradient-free Stein thinning with different choices of Q:
  - multivariate Gaussian using the sample mean and covariance,
  - Laplace approximation - fails as in bivariate Gaussian case,
  - KDE approximation - computationally expensive.

Lotka-Volterra inverse problem: comparison of approaches

Gradient-free thinning using a multivariate Gaussian with the sample mean and covariance matrix performs comparably with the gradient-based approach, notably for chain 4, when compared using the energy distance:



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Contribution

The project makes three contributions:

- implementation of the gradient-free Stein thinning algorithm in the Python library `stein-thinning`,
- evaluation of the performance of the proposed algorithm,
- improvement of the computational efficiency of the existing Stein thinning algorithm from $O(nm^2)$ to $O(nm)$, where n is the input sample size and m is the desired thinned sample size.

Conclusions

- The gradient-free approach is feasible and performs similarly to the Stein thinning algorithm of Riabiz et al. (2022) for small thinned sample sizes.
- The performance of the algorithm depends crucially on the choice of the auxiliary distribution. For example, even in the highly favourable setting of i.i.d. samples from a Gaussian mixture, choosing the auxiliary distribution based on the Laplace approximation fails to produce a thinned sample.
- The simple multivariate Gaussian distribution using the sample mean and covariance offered a good starting point in our experiments, however bespoke treatment might be required for more complex problems.
- In deciding whether to use the new algorithm as opposed to the gradient-based approach, the effort involved in selecting a good auxiliary distribution must be weighed against the computational cost of obtaining gradients.

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Further Research

- Parallelise the computation of KDE.
- Perform thinning in a lower-dimensional space.
- Investigate the behaviour of Stein thinning for large thinned sample sizes.
- Compare the performance of the approaches in terms of estimating the true parameters of the Lotka-Volterra model.
- Run an experiment with randomised starting points.
- Repeat the experiments with more advanced MCMC algorithms.
- Check how running a gradient-free MCMC sampling algorithm (such the random-walk Metropolis-Hastings) followed by Stein thinning of the sample compares to running a gradient-based sampling algorithm (e.g. HMC).
- Provide theoretical justification for gradient-free Stein thinning.
- Explore other gradient-free alternatives.

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References

W. Y. Chen, A. Barp, F.-X. Briol, J. Gorham, M. Girolami, L. Mackey, and Chris. J. Oates. Stein Point Markov Chain Monte Carlo. In *Proceedings of the 36th International Conference on Machine Learning*, pages 1011–1021, Long Beach, California, 2019. PLMR.

M. A. Fisher and C. J. Oates. Gradient-Free Kernel Stein Discrepancy. In *Proceedings of the 37th International Conference on Neural Information Processing Systems*, pages 23855–23885, May 2024.

J. Gorham and L. Mackey. Measuring Sample Quality with Stein's Method. In *Advances in Neural Information Processing Systems*, volume 28, pages 226–234. MIT Press, 2015.

J. Gorham and L. Mackey. Measuring Sample Quality with Kernels. In *Proceedings of the 34th International Conference on Machine Learning*, pages 1292–1301, Sydney, Australia, 2017. PLMR.

M. Riabiz, W. Y. Chen, J. Cockayne, P. Swietach, S. A. Niederer, L. Mackey, and Chris. J. Oates. Optimal Thinning of MCMC Output. *Journal of the Royal Statistical Society Series B: Statistical Methodology*, 84(4):1059–1081, September 2022.

M. L. Rizzo and G. J. Székely. Energy Distance. *WIREs Computational Statistics*, 8(1):27–38, January 2016.

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Stein discrepancy

Integral probability metric

An integral probability metric between two distributions P and P' is defined as

$$\mathcal{D}_{\mathcal{F}}(P, P') := \sup_{f \in \mathcal{F}} \left| \int_{\mathcal{X}} f \, \mathrm{d}P - \int_{\mathcal{X}} f \, \mathrm{d}P' \right|,$$

where $\mathcal{X}$ is a measurable space on which both P and P' are defined and $\mathcal{F}$ is a set of test functions.

Idea

Avoid the need to evaluate $\int_{\mathcal{X}} f \, \mathrm{d}P$ by choosing a set of functions $\mathcal{F}$ such that $\int_{\mathcal{X}} f \, \mathrm{d}P = 0$ for all $f \in \mathcal{F}$.

Stein discrepancy (continued)

Gorham and Mackey (2015) use the infinitesimal generator of the overdamped Langevin diffusion to eliminate the integral $\int_{\mathcal{X}} f \,\mathrm{d}P$.

Infinitesimal generator

The infinitesimal generator $\mathcal{L}$ of a stochastic process $(Z_t)_{t\geq 0}$ is given by

$$(\mathcal{L}u)(x) := \lim_{t\to 0} \frac{\mathbb{E}[u(Z_t)|Z_0 = x] - u(x)}{t} \quad \text{for } u : \mathbb{R}^d \to \mathbb{R}.$$

Overdamped Langevin diffusion

The overdamped Langevin diffusion is a stochastic process defined by

$$\mathrm{d}Z_t = \frac{1}{2}\nabla \log p(Z_t)\,\mathrm{d}t + \mathrm{d}W_t,$$

where p is the density of P and W_t is the standard Brownian motion.

Stein discrepancy (continued)

The infinitesimal generator of an overdamped Langevin diffusion:

$$(\mathcal{L}_P u)(x) = \frac{1}{2}\langle \nabla u(x), \nabla \log p(x)\rangle + \frac{1}{2}\langle \nabla, \nabla u(x)\rangle.$$

Denoting $g = \frac{1}{2}\nabla u$, Gorham and Mackey (2015) obtain the Stein operator

$$\mathcal{A}_P g := \langle g, \nabla \log p\rangle + \langle \nabla, g\rangle = \langle p^{-1}\nabla, pg\rangle,$$

and demonstrate that

$$\int_{\mathcal{X}} \mathcal{A}_P g \,\mathrm{d}P = 0$$

for a suitably chosen set $\mathcal{G}$, enabling them to rewrite the expression for the integral probability metric as

$$\mathcal{D}_{P,\mathcal{G}}(P') = \sup_{g\in\mathcal{G}} \left| \int_{\mathcal{X}} \mathcal{A}_P g \,\mathrm{d}P' \right|$$

Stein discrepancy (continued)

Using the Langevin Stein operator, the integral probability metric specialises to

Stein discrepancy

$$\mathcal{D}_{P,\mathcal{G}}(P') = \sup_{g \in \mathcal{G}} \left| \int_{\mathcal{X}} \mathcal{A}_P g \, \mathrm{d}P' \right|$$

The difficulty evaluating the supremum still remains.

Idea

Employ the kernel trick to eliminate the supremum in the expression for the integral probability metric.

Reproducing kernel Hilbert space

A *Hilbert space* is a vector space V equipped with the inner product operation $\langle \cdot, \cdot \rangle$ and its induced norm $\| \cdot \|$ satisfying $\|v\|^2 = \langle v, v \rangle$ for all $v \in V$, if it is complete:

$$\sum_{i=1}^{\infty} \|v_i\| < \infty \quad \text{implies} \quad \sum_{i=1}^{\infty} v_i \in V$$

for any sequence $v_i \in V$.
A Hilbert space $\mathcal{H}$ of real-valued functions defined on a set $\mathcal{X}$ is called a *reproducing kernel Hilbert space (RKHS)* if there exists a function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ such that:

- for every $x \in \mathcal{X}$, the function $k(x, \cdot)$ belongs to $\mathcal{H}$,
- k satisfies the reproducing property $\langle f(\cdot), k(\cdot, x) \rangle = f(x)$ for any $f \in \mathcal{H}$ and $x \in \mathcal{X}$.

We denote $\mathcal{H}(k)$ the RKHS with kernel k.

Kernel Stein discrepancy

Taking the unit-ball in a Cartesian product of d copies $\mathcal{H}(k)$

$$\mathcal{G} := \left\{ \mathrm{g} : \mathbb{R}^d \to \mathbb{R}^d \,\middle|\, \sum_{i=1}^{d} \|g_i\|^2_{\mathcal{H}(k)} \leq 1 \right\},$$

Proposition 2 in Gorham and Mackey (2017) shows that the Stein discrepancy becomes

$$\mathcal{D}^2_P(P') := \mathcal{D}_{P,\mathcal{G}}(P') = \iint_{\mathcal{X}} k_P(x,y)\,\mathrm{d}p'(x)\,\mathrm{d}p'(y),$$

where p' is the density of P', and $k_P(x,y)$ is given by

$$\begin{aligned} k_P(x,y) :=& (\nabla_x \cdot \nabla_y) k(x,y) \\ &+ \langle \nabla_x k(x,y), \nabla_y \log p(y) \rangle + \langle \nabla_y k(x,y), \nabla_x \log p(x) \rangle \\ &+ k(x,y) \langle \nabla_x \log p(x), \nabla_y \log p(y) \rangle. \end{aligned}$$

Kernel Stein discrepancy (KSD)

$$\mathcal{D}_P^2(P') := \iint_{\mathcal{X}} k_P(x, y) \, \mathrm{d}p'(x) \, \mathrm{d}p'(y),$$

If P' is a discrete distribution, this becomes

$$\mathcal{D}_P^2 \left(\frac{1}{n} \sum_{i=1}^{n} \delta(x_i) \right) = \frac{1}{n^2} \sum_{i,j=1}^{n} k_P(x_i, x_j),$$

where

$$\begin{aligned} k_P(x, y) :=& (\nabla_x \cdot \nabla_y) k(x, y) \\ &+ \langle \nabla_x k(x, y), \nabla_y \log p(y) \rangle + \langle \nabla_y k(x, y), \nabla_x \log p(x) \rangle \\ &+ k(x, y) \langle \nabla_x \log p(x), \nabla_y \log p(y) \rangle. \end{aligned}$$

The typical choice for $k(x, y)$ is the inverse multiquadric kernel:

$$k(x, y) = \left(c^2 + \|\Gamma^{-1/2}(x - y)\| \right)^{\beta}.$$

Inverse multiquadric kernel

The common choice of the kernel k is the inverse multiquadric kernel (IMQ)

$$k(x, y) = \left(c^2 + \|\Gamma^{-1/2}(x - y)\|\right)^{\beta}.$$

When $\beta \in (-1, 0)$ and $\Gamma = I$, Gorham and Mackey (2017) demonstrate that $\mathcal{D}_P(P')$ provides convergence control (Theorem 8). Theorem 4 in Chen et al. (2019) justifies the introduction of Γ in IMQ.

Lotka-Volterra inverse problem: MCMC

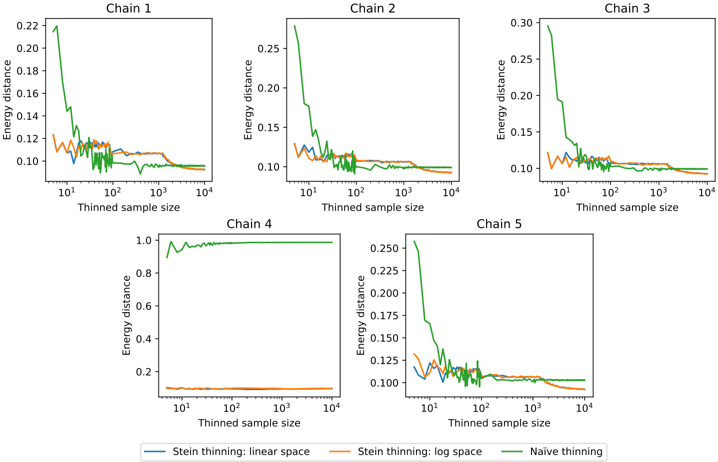
The inference is performed using the Metropolis-Hastings algorithm with the starting points taken from Riabiz et al. (2022):

Chain	θ_1	θ_2	θ_3	θ_4
1	0.55	1	0.8	0.8
2	1.5	1	0.8	0.8
3	1.3	1.33	0.5	0.8
4	0.55	3	3.	0.8
5	0.55	1	1.5	1.5

Since the parameters θ_k of the Lotka-Volterra model are positive, we run MCMC in the log-space by applying the reparameterisation $\zeta_k = \log \theta_k$. We run 500,000 iterations of the algorithm for each chain.

Lotka-Volterra inverse problem: Stein thinning

We have a choice of applying thinning in linear or logarithmic space, however the energy distance comparison indicates no discernible difference, so we proceed to use the logarithmic space.



Lotka-Volterra inverse problem: comparison of approaches

Gradient-free thinning offers a significant improvement over naïve thinning in terms of KSD: