# Sampling with Stein Discrepancies

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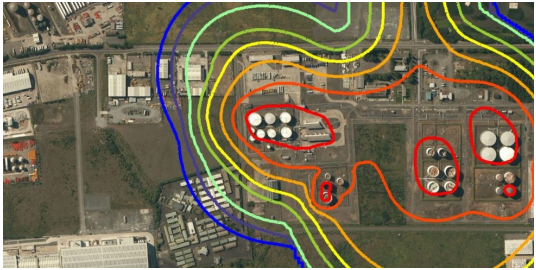
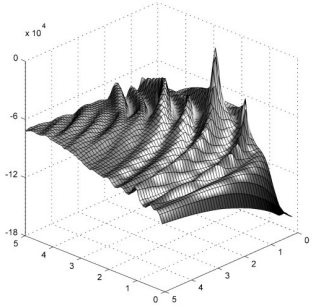
July 2022 @ MCQMC

Newcastle University

# Motivation: Bayesian Inference and Sampling

The result of integrating expert knowledge with experimental measurement is a *posterior* distribution that is implicitly defined:






The (lack of) power of computational methodology for Bayesian inference forms a bottleck, imposing a limit of the sophistication of statistical models, or types of information, than can be integrated into a scientific investigation.

This tutorial concerns a new mathematical tool, *Stein discrepancy*, which has the potential to increase the range and scope of statistical analyses that can be performed.

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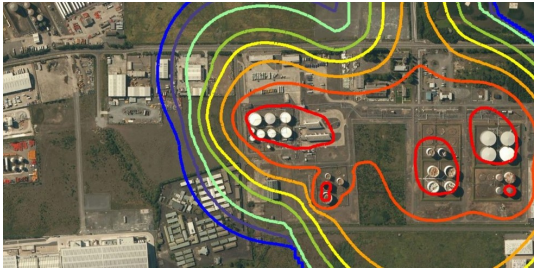

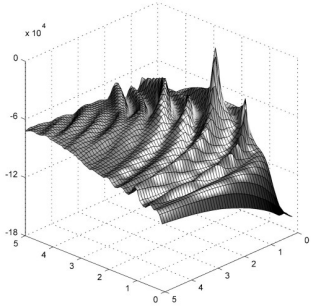


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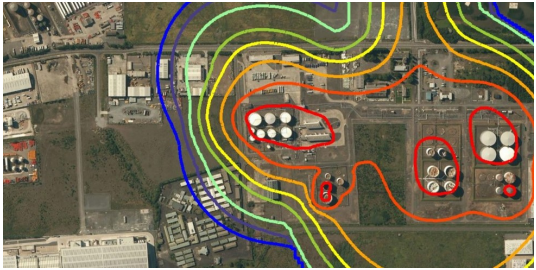

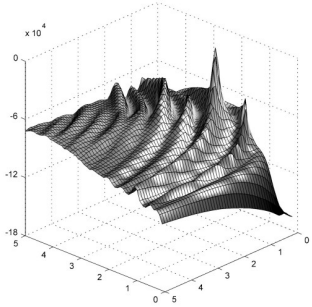


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# Outline of the Tutorial

# Measuring Sample Quality with Kernels

# Sampling

Consider general probability distributions $P$ on general domains $\mathcal{X}$.

Interested in *sampling*, which in this tutorial means approximation of the form

$$P \approx \sum_{i=1}^{n} w_i \delta(x_i)$$

for some weights $w_i \in \mathbb{R}$ and some states $x_i \in \mathcal{X}$.
[Motivation: Forward UQ.]

The quality of the approximation should be close to optimal (in some sense to be specified) for the number $n$ of states used. [Note: This is not independent sampling from $P$.]

Markov chain Monte Carlo widely used but "typically" requires $n \approx 10^3$ or $10^4$ (to run diagnostics).

Quasi Monte Carlo is highly effective for specific $P$. [Motivation: General, implicitly defined $P$.]

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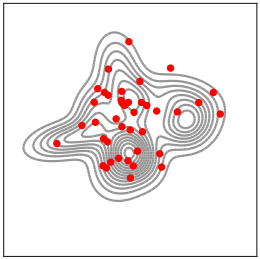

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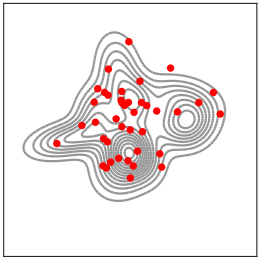

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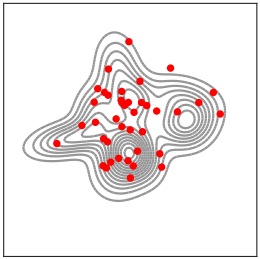

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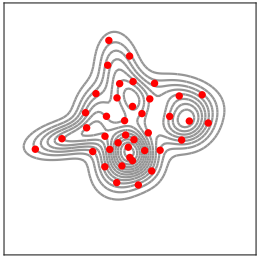

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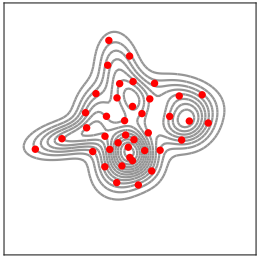

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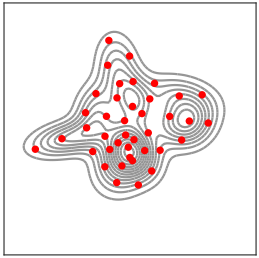

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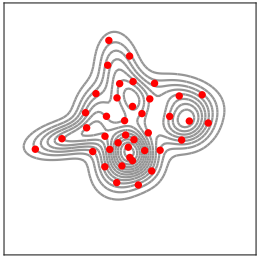

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# Measuring the Quality of a Sample

One of the most basic operations that one could hope to perform with a probability distribution is to compute expectations; i.e. to compute integrals of the form

$$\int f \mathrm{d}P, \qquad \text{or} \qquad \int f(\boldsymbol{x}) p(\boldsymbol{x}) \mathrm{d}\boldsymbol{x}$$

if the probability distribution $P$ admits a probability density function (PDF) $p(\boldsymbol{x})$.

For implicitly defined $P$, such integrals do not possess a closed form and numerical integration (also called *cubature*) will be required.

Using a sample, we arrive at a natural approximation

$$P \approx \sum_{i=1}^{n} w_i \delta(\boldsymbol{x}_i) \qquad \Longrightarrow \qquad \int f \mathrm{d}P \approx \sum_{i=1}^{n} w_i f(\boldsymbol{x}_i)$$

to the integral. This suggests designing a sample for which the *cubature error*

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# Cubature Error Representer

The basic idea is as follows: we consider the set $\mathcal{S}(k)$ of all functions of the form

$$f(\boldsymbol{x}) = \sum_{i=1}^{m} b_i k(\boldsymbol{x}, \boldsymbol{y}_i),$$

where $k$ is to be specified, the $\boldsymbol{y}_i$ are fixed states, and $n \in \mathbb{N}$. The function $k$ determines the regularity of the elements in $\mathcal{S}(k)$:

Figure: The left panel represents functions built from $k(\boldsymbol{x}, \boldsymbol{y}) = \exp(-\|\boldsymbol{x} - \boldsymbol{y}\|)$, which is non-differentiable, while the right panel corresponds to functions built from $k(\boldsymbol{x}, \boldsymbol{y}) = \exp(-\|\boldsymbol{x} - \boldsymbol{y}\|^2)$, which is smooth.

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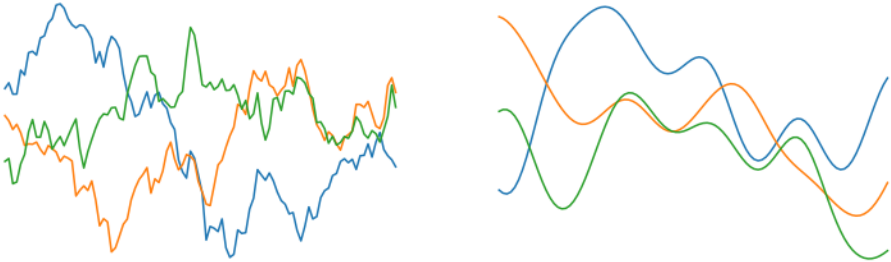

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$\mathcal{S}(k)$ is a vector space (over the reals) of functions when (pointwise) addition and scalar multiplication are defined. In addition to that, we will want to make use of an inner product

$$\langle f, g\rangle_{\mathcal{S}(k)} = \sum_{i=1}^{m}\sum_{j=1}^{n} b_i c_j k(\boldsymbol{y}_i, \boldsymbol{z}_j), \quad f(\boldsymbol{x}) = \sum_{i=1}^{m} b_i k(\boldsymbol{x}, \boldsymbol{y}_i), \quad g(\boldsymbol{x}) = \sum_{j=1}^{n} c_j k(\boldsymbol{x}, \boldsymbol{z}_j),$$

for which we must require that $k$ is *symmetric* (i.e. $\langle f, g\rangle_{\mathcal{S}(k)} = \langle g, f\rangle_{\mathcal{S}(k)}$) and *positive definite* (i.e. $\langle f, f\rangle_{\mathcal{S}(k)} > 0$ for all $f \neq 0$). This inner product is useful because it satisfies a *reproducing property*, meaning that

$$\langle f, k(\cdot, \boldsymbol{x})\rangle_{\mathcal{S}(k)} = f(\boldsymbol{x}),$$

and suggesting the formal manipulation

$$\begin{aligned}\frac{1}{n}\sum_{i=1}^{n} f(\boldsymbol{x}_i) - \int f(\boldsymbol{x})\mathrm{d}P(\boldsymbol{x}) &= \frac{1}{n}\sum_{i=1}^{n}\langle f, k(\cdot, \boldsymbol{x}_i)\rangle_{\mathcal{S}(k)} - \int \langle f, k(\cdot, \boldsymbol{x})\rangle_{\mathcal{S}(k)}\mathrm{d}P(\boldsymbol{x}) \\ &= \Bigg\langle f, \underbrace{\frac{1}{n}\sum_{i=1}^{n} k(\cdot, \boldsymbol{x}_i) - \int k(\cdot, \boldsymbol{x})\mathrm{d}P(\boldsymbol{x})}_{=e(\cdot)}\Bigg\rangle_{\mathcal{S}(k)},\end{aligned}$$

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for which we must require that $k$ is *symmetric* (i.e. $\langle f, g\rangle_{\mathcal{S}(k)} = \langle g, f\rangle_{\mathcal{S}(k)}$) and *positive definite* (i.e. $\langle f, f\rangle_{\mathcal{S}(k)} > 0$ for all $f \neq 0$). This inner product is useful because it satisfies a *reproducing property*, meaning that

$$\langle f, k(\cdot, \boldsymbol{x})\rangle_{\mathcal{S}(k)} = f(\boldsymbol{x}),$$

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$$\begin{aligned}\frac{1}{n}\sum_{i=1}^{n} f(\boldsymbol{x}_i) - \int f(\boldsymbol{x})\mathrm{d}P(\boldsymbol{x}) &= \frac{1}{n}\sum_{i=1}^{n}\langle f, k(\cdot, \boldsymbol{x}_i)\rangle_{\mathcal{S}(k)} - \int \langle f, k(\cdot, \boldsymbol{x})\rangle_{\mathcal{S}(k)}\mathrm{d}P(\boldsymbol{x}) \\ &= \Bigg\langle f, \underbrace{\frac{1}{n}\sum_{i=1}^{n} k(\cdot, \boldsymbol{x}_i) - \int k(\cdot, \boldsymbol{x})\mathrm{d}P(\boldsymbol{x})}_{=e(\cdot)}\Bigg\rangle_{\mathcal{S}(k)},\end{aligned}$$

where the *cubature error representer* $e(\cdot)$ is indepenent of $f$. Idea: Seek sample with $\|e\|_{\mathcal{S}(k)}$ small.

# Cubature Error Representer

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# Reproducing Kernel Hilbert Spaces

The main mathematical tool that we will exploit is that of a *reproducing kernel*:

**Definition 1 (Reproducing kernel Hilbert space)**

Let $\mathcal{X}$ be a set and consider a symmetric and positive definite function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. Then a *reproducing kernel Hilbert space (RKHS)* with *reproducing kernel* (or simply *kernel*) $k$ is an inner product space $\mathcal{H}(k)$ of functions $f : \mathcal{X} \to \mathbb{R}$, such that

1. $k(\cdot, x) \in \mathcal{H}(k)$ for all $x \in \mathcal{X}$
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# Reproducing Kernel Hilbert Spaces

In general it is difficult to characterise the inner product induced by a reproducing kernel, and hence the elements of the RKHS. However, there are a number of important cases where this can be carried out:

## Example 2

The linear span of a finite collection of functions $e_1(x), \ldots, e_p(x)$ can be endowed with the structure of an RKHS with reproducing kernel

$$k(x, y) = \sum_{i=1}^{p} e_i(x) e_i(y).$$

The induced inner product is

$$\langle f, g \rangle_{\mathcal{H}(k)} = b_1 c_1 + \cdots + b_p c_p, \qquad f(x) = \sum_{i=1}^{n} b_i e_i(x), \qquad g(x) = \sum_{i=1}^{n} c_i e_i(x).$$

## Example 3

The kernel

$$k(x, y) = \prod_{i=1}^{d} \left(1 + \min(1 - x_i, 1 - y_i)\right), \qquad x, y \in [0, 1]^d$$

reproduces a Hilbert space with inner product

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# Kernel Mean Embedding

Idea: Work with $\mathcal{H}(k)$ instead of $\mathcal{S}(k)$.

**Definition 4 (Kernel mean embedding)**

For a kernel $k$ and a probability distribution $P$, we call $\mu_P = \int k(\cdot, x) \mathrm{d}P(x)$ the *kernel mean embedding* of $P$ in $\mathcal{H}(k)$, whenever it is well-defined.

**Example 5**

For the kernel

$$k(x, y) = \sum_{i=1}^{p} e_i(x) e_i(y),$$

with $e_i \in L^1(P)$, we have kernel mean embedding

$$\mu_P(x) = \sum_{i=1}^{p} \Big( \underbrace{\int e_i(y) \, \mathrm{d}P(y)}_{<\infty} \Big) e_i(x) \in \mathcal{H}(k).$$

In general, when is the kernel mean embedding well-defined?

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# Kernel Mean Embedding

**Lemma 6**
*If* $\int \sqrt{k(x,x)}\mathrm{d}P(x) < \infty$ *then* $\mu_P(x) \in \mathcal{H}(k)$.

**Proof.**
Consider the linear operator $Lf = \int f(x)\mathrm{d}P(x)$ acting on $f \in \mathcal{H}(k)$. Claim that $L$ is a *bounded linear operator* from $\mathcal{H}(k)$ to $\mathbb{R}$. Indeed,

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|Lf| = \left|\int f(x)\mathrm{d}P(x)\right| &\leq \int |f(x)|\mathrm{d}P(x) && (1)\\
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*If* $\int \sqrt{k(x,x)}\mathrm{d}P(x) < \infty$ *then* $\mu_P(x) \in \mathcal{H}(k)$.

**Proof.**
Consider the linear operator $Lf = \int f(x)\mathrm{d}P(x)$ acting on $f \in \mathcal{H}(k)$. Claim that $L$ is a *bounded linear operator* from $\mathcal{H}(k)$ to $\mathbb{R}$. Indeed,

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\begin{aligned}
|Lf| = \left|\int f(x)\mathrm{d}P(x)\right| &\leq \int |f(x)|\mathrm{d}P(x) && (1)\\
&= \int |\langle f, k(\cdot, x)\rangle_{\mathcal{H}(k)}|\mathrm{d}P(x) && (2)\\
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&= \int \sqrt{k(x,x)}\mathrm{d}P(x)\|f\|_{\mathcal{H}(k)} && (4)
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where (1) is Jensen's inequality, (2) is the reproducing property, (3) is Cauchy–Schwarz, and (4) is the reproducing property again.

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Thus, from the Riesz representation theorem, there exists $h \in \mathcal{H}(k)$ such that

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# Cubature Error Representer in RKHS

In this more general setting, the cubature error representer is the difference $e = \mu_{Q_n} - \mu_P$ of two kernel mean embeddings, where $Q_n = \sum_{i=1}^n w_i \delta(\boldsymbol{x}_i)$ is the discrete distribution on which the cubature rule is based. i.e.

$$\int f \mathrm{d}P - \sum_{i=1}^n w_i f(\boldsymbol{x}_i) = \langle f, \mu_P - \mu_{Q_n} \rangle_{\mathcal{H}(k)}, \quad \mu_P = \int k(\cdot, \boldsymbol{x}) \, \mathrm{d}P(\boldsymbol{x}), \quad \mu_{Q_n} = \sum_{i=1}^n w_i k(\cdot, \boldsymbol{x}_i).$$

There are several different ways to systematically assess the performance of a cubature rule, but here we focus on a *worst case* assessment:

**Definition 7 (Maximum mean discrepancy)**

The *maximum mean discrepancy (MMD)* between two distributions $P$ and $Q$ is

$$D_k(P, Q) = \|\mu_P - \mu_Q\|_{\mathcal{H}(k)} = \sup_{\|f\|_{\mathcal{H}(k)} \leq 1} \left| \int f \mathrm{d}P - \int f \mathrm{d}Q \right|,$$

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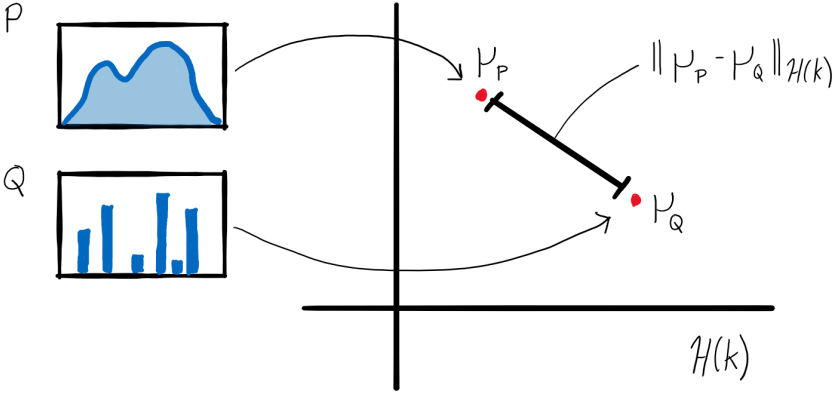


Figure: *Kernel mean embedding:* Two probability distributions $P$ and $Q$ are mapped to their respective elements $\mu_P$ and $\mu_Q$ in the RKHS $\mathcal{H}(k)$. The distance (in $\mathcal{H}(k)$) between these kernel mean embeddings $\mu_P$ and $\mu_Q$ is called the MMD between $P$ and $Q$.

# Maximum Mean Discrepancy

If $D_k(P, Q_n) = 0$, the cubature rule based on $Q_n$ will be exact for all integrands $f \in \mathcal{H}(k)$. Does this mean that $Q_n$ and $P$ are identical?

**Definition 8 (Characteristic kernel)**

A kernel $k$ is said to be *characteristic* if $D_k(P, Q) = 0$ implies $P = Q$.

**Example 9 (Polynomial kernel is not characteristic)**

From Example 2, the kernel $k(x, y) = \sum_{i=0}^{p} x^i y^i$ reproduces an RKHS whose elements are the polynomials of degree at most $p$ on the domain $\mathcal{X} = \mathbb{R}$. Thus $D_k(P, Q) = 0$ if and only if the moments $\int x^i \mathrm{d}P(x)$ and $\int x^i \mathrm{d}Q(x)$ are identical for $i = 1, \ldots, p$. In particular, $k$ is *not* a characteristic kernel.

**Example 10**

The Gaussian kernel $k(\boldsymbol{x}, \boldsymbol{y}) = \exp(-\|\boldsymbol{x} - \boldsymbol{y}\|^2)$ is a characteristic kernel on $\mathcal{X} = \mathbb{R}^d$.

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A kernel $k$ is said to have *weak convergence control* if $D_k(P, Q_n) \to 0$ implies that $Q_n \Rightarrow P$.

### Remark 1

*For a compact Hausdorff space $\mathcal{X}$, a bounded characteristic kernel $k$ has weak convergence control. This need not hold when the domain $\mathcal{X}$ is non-compact.*

Convergence control justifies attempting to minimise MMD for the purposes of quantisation and more general approximation, as we will attempt in the sequel.

### Example 12

The Gaussian kernel $k(x, y) = \exp(-\|x - y\|^2)$ controls weak convergence of probability distributions on $\mathcal{X} = [0, 1]^d$. It can also be shown that the Gaussian kernel controls weak convergence on $\mathcal{X} = \mathbb{R}^d$; this can be deduced from e.g. Theorem 7 of Simon-Gabriel et al. [2020] and the general results in Sriperumbudur et al. [2011].

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# Maximum Mean Discrepancy

MMD is a convenient measure of sample quality because it can be computed:

$$\begin{aligned} D_k(P,Q)^2 &= \|\mu_P - \mu_Q\|^2_{\mathcal{H}(k)} \\ &= \langle \mu_P - \mu_Q, \mu_P - \mu_Q \rangle_{\mathcal{H}(k)} \\ &= \langle \mu_P, \mu_P \rangle_{\mathcal{H}(k)} - 2\langle \mu_P, \mu_Q \rangle_{\mathcal{H}(k)} + \langle \mu_Q, \mu_Q \rangle_{\mathcal{H}(k)}. \end{aligned}$$

Considering for example the term $\langle \mu_P, \mu_Q \rangle_{\mathcal{H}(k)}$, we have

$$\begin{aligned} \langle \mu_P, \mu_Q \rangle_{\mathcal{H}(k)} &= \left\langle \int k(\cdot, x)\mathrm{d}P(x), \int k(\cdot, y)\mathrm{d}Q(y) \right\rangle_{\mathcal{H}(k)} \\ &= \iint \langle k(\cdot, x), k(\cdot, y) \rangle_{\mathcal{H}(k)} \mathrm{d}P(x)\mathrm{d}Q(y) = \iint k(x,y)\mathrm{d}P(x)\mathrm{d}Q(y). \end{aligned}$$

Here we have used the reproducing property, as well as using Lemma 6 to justify the exchanges of integral and inner product. Proceeding similarly with all three terms results in the expression

$$D_k(P,Q)^2 = \iint k(x,y)\mathrm{d}P(x)\mathrm{d}P(y) - 2\iint k(x,y)\mathrm{d}P(x)\mathrm{d}Q(y) + \iint k(x,y)\mathrm{d}Q(x)\mathrm{d}Q(y).$$

How to exploit MMD for sampling?

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# Sampling with Kernels

# Quantisation with Monte Carlo

The goal of *quantisation* is to find $Q$ of the form $Q_n = \frac{1}{n}\sum_{i=1}^{n} \delta(\boldsymbol{x}_i)$ such that $Q_n \approx P$.

As a simple baseline method for quantisation we consider Monte Carlo:

Figure: *Monte Carlo:* Independent samples (blue circles) from a "horseshoe" distribution $P$ (grey contours).

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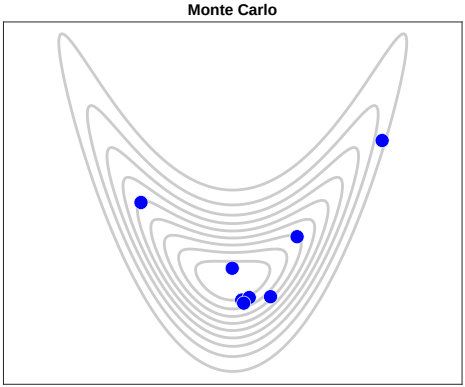


Figure: *Monte Carlo:* Independent samples (blue circles) from a "horseshoe" distribution $P$ (grey contours).

# Quantisation with Monte Carlo

## Proposition 1 (MMD of Monte Carlo)

*Let $x_1, \ldots, x_n \sim P$ be independent. Assume that $C := \int k(x, x) \mathrm{d}P(x) < \infty$. Then*

$$\mathbb{E}\left[D_k(P, Q_n)^2\right] \leq \frac{C}{n}.$$

Proof.

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# Optimal Quantisation

Monte Carlo sampling provides a consistent but potentially far from optimal quantisation of $P$.

Note that the convergence *rate* in Proposition 1 does not depend on the kernel $k$, which highlights the inefficiency of the Monte Carlo method. [But the rate is dimension-independent.]

The goal of *optimal* quantisation is to approximate $P$ as well as possible, with a fixed number of states $x_1, \ldots, x_n$.

In what follows we are going to introduce some algorithms that are **often inferior to QMC**, but have the advantage of being **applicable to general Bayesian inference tasks** with minor modification, as we will see in the sequel.

Algorithm 1 (Optimise Everything)

*Approximate a solution to*

$$\min_{(x_1,\ldots,x_n)\in\mathcal{X}\times\cdots\times\mathcal{X}} D_k\left(P, \frac{1}{n}\sum_{i=1}^{n}\delta(x_i)\right)$$

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*using a numerical global optimisation method.*

# Optimal Quantisation

Monte Carlo sampling provides a consistent but potentially far from optimal quantisation of $P$.

Note that the convergence *rate* in Proposition 1 does not depend on the kernel $k$, which highlights the inefficiency of the Monte Carlo method. [But the rate is dimension-independent.]

The goal of *optimal* quantisation is to approximate $P$ as well as possible, with a fixed number of states $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$.

In what follows we are going to introduce some algorithms that are **often inferior to QMC**, but have the advantage of being **applicable to general Bayesian inference tasks** with minor modification, as we will see in the sequel.

## Algorithm 1 (Optimise Everything)

*Approximate a solution to*

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# Optimal Quantisation

Figure: *Optimal quantisation:* Global (continuous) minimisation of MMD to select states $\{\boldsymbol{x}_i\}_{i=1}^n$ in an approximation $Q_n$ to $P$. Example due to Gräf et al. [2012].

This example is the *stippling* procedure discussed in Gräf et al. [2012], implemented using a bandlimited kernel and the nonlinear CG method. See also *minimum energy designs* and MMD *gradient flow* [Arbel et al., 2019]. Requires a good initialisation to work well.

Also requires selecting $n$ in advance - a *non-extensible* sequence of approximations to $P$.

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# Optimal Quantisation

To arrive at an extensible approximation, consider a greedy sequential algorithm:

**Algorithm 2 (Continuous Greedy Optimisation)**

*Approximate a solution to*

$$x_n \in \operatorname*{arg\,min}_{x \in \mathcal{X}} \; D_k \left( P, \frac{1}{n}\delta(x) + \frac{1}{n}\sum_{i=1}^{n-1} \delta(x_i) \right), \qquad n = 1, 2, \ldots$$

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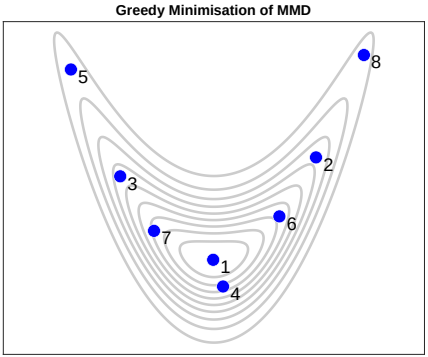


Figure: *Optimal quantisation:* Sequential (greedy) minimisation of MMD to select $n = 8$ states $\{\boldsymbol{x}_i\}_{i=1}^n$ in an approximation $Q_n$ to $P$. The numbers indicate the order in which the states $\boldsymbol{x}_i$ were selected.

However, the computation required to select the location $x_n$ becomes increasingly difficult as $n$ is increased. A computationally simpler algorithm is proposed next.

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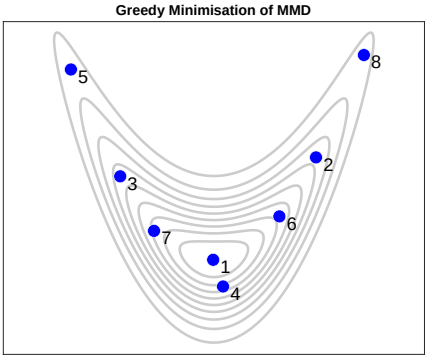


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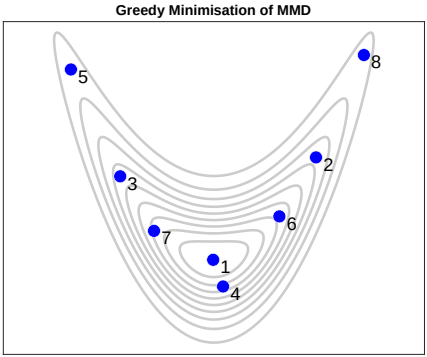


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# Optimal Quantisation

## Algorithm 3 (Discrete Greedy Optimisation)

*Let $(y_i)_{i\in\mathbb{N}}$ be a sample path from a Markov chain that is $P$-invariant. Then set*

$$x_n \in \operatorname*{arg\,min}_{x\in\{y_1,\ldots,y_N\}} D_k\left(P, \frac{1}{n}\delta(x) + \frac{1}{n}\sum_{i=1}^{n-1}\delta(x_i)\right), \qquad n = 1, 2, \ldots.$$

- Includes the case where the $y_i$ are independent samples from $P$. [Pre-empts application to the motivating Bayesian context.]
- For a sample path of length $N \gg 1$, the resulting sequence approximates that of continuous greedy optimisation (Algorithm 2).
- Under assumptions, that include sufficiently rapid mixing of the Markov chain,

$$\mathbb{E}\left[D_k(P, Q_n)^2\right] \leq \frac{C_1}{N} + \frac{C_2(1+\log(N))(1+\log(n))}{n}.$$

  See Theorem 4 in Teymur et al. [2021].
- Same rate as Monte Carlo up to log terms; recall Proposition 1. [Possibly a theoretical gap here.]

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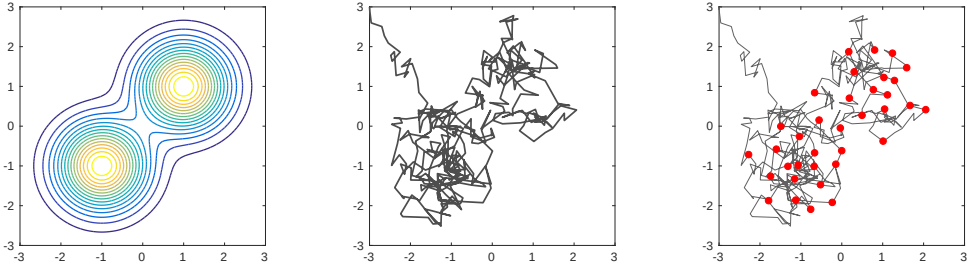


$P$ | MCMC output $(y_i)_{i=1}^N$ | Representative Subset $(x_i)_{i=1}^n$

Figure: *Optimal quantisation:* Discrete greedy optimisation of MMD to select $n = 35$ states $\{x_i\}_{i=1}^n$ in an approximation $Q_n$ to $P$.

Q: What can be done to improve the disappointing theoretical convergence rate?

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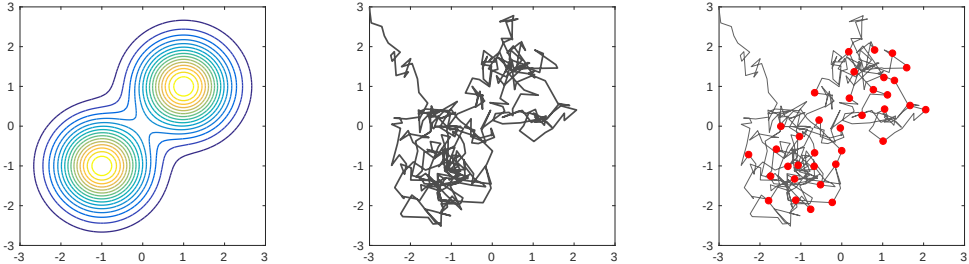


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Let's return to the case of *weighted* point sets; i.e. approximations of the form $Q_n = \sum_{i=1}^n w_i \delta(\boldsymbol{x}_i)$ for some weights $w_1, \ldots, w_n \in \mathbb{R}$.

**Lemma 13**

*Let $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in \mathcal{X}$ be distinct. The optimal weights*

$$\underset{\boldsymbol{w} \in \mathbb{R}^n}{\arg\min}\, D_k\left(P, \sum_{i=1}^n w_i \delta(\boldsymbol{x}_i)\right)$$

*are the solution of the linear system*

$$K\boldsymbol{w} = \boldsymbol{z} \tag{5}$$

*where $K_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j)$ and $z_i = \mu_P(\boldsymbol{x}_i)$.*

**Proof.**

The MMD between $P$ and $Q_n = \sum_{i=1}^n w_i \delta(\boldsymbol{x}_i)$ can be expressed as

$$D_k(P, Q_n)^2 = \iint k(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}P(\boldsymbol{x}) \mathrm{d}P(\boldsymbol{y}) - 2 \iint k(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}P(\boldsymbol{x}) \mathrm{d}Q(\boldsymbol{y}) + \iint k(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}Q(\boldsymbol{x}) \mathrm{d}Q(\boldsymbol{y})$$

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where $C = \iint k(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}P(\boldsymbol{x}) \mathrm{d}P(\boldsymbol{y})$ is independent of $\boldsymbol{w}$. This is a non-degenerate quadratic form in $\boldsymbol{w}$ (since $\boldsymbol{K}$ is a positive definite matrix), from which the result is easily verified.

# Optimal Approximation

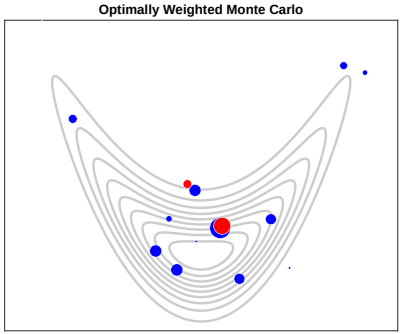


Figure: *Optimally weighted Monte Carlo samples:* The weights $w_1, \ldots, w_n$ are obtained by minimising MMD in the manner of Lemma 13. Blue indicates states $\boldsymbol{x}_i$ with positive weights $w_i > 0$, while red indicates negative weights $w_i < 0$. The size of the circles is proportional to $|w_i|$.

The linear system in (5), defining the optimal weights, can be numerically ill-conditioned and the general computational overhead is $O(n^3)$. However, several "tricks" are available, such as Karvonen and Särkkä [2018], Karvonen et al. [2019].

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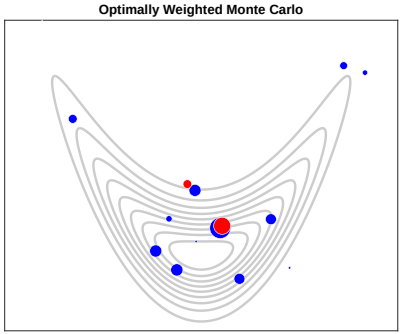


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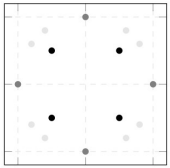

# Optimal Approximation

Do optimal weights improve convergence rates? It depends on the kernel!

**Notation:** The *multi-index* notation

$$\partial^{\alpha} f : \boldsymbol{x} \mapsto \frac{\partial^{\alpha} f(\boldsymbol{x})}{\partial \boldsymbol{x}^{\alpha}} = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \dots \partial x_d^{\alpha_d}} f(\boldsymbol{x}), \qquad \boldsymbol{\alpha} \in \mathbb{N}_0^d$$

will be used, and we let $|\boldsymbol{\alpha}| = \alpha_1 + \cdots + \alpha_d$.

Definition 14

For $s > d/2$ and (sufficiently regular) $\mathcal{X} \subset \mathbb{R}^d$, the (order $s$) Sobolev space $H^s(\mathcal{X})$ is defined to be the set of functions $f : \mathcal{X} \to \mathbb{R}$ whose mixed partial derivatives $\partial^{\alpha} f$, $|\alpha| \leq s$, exist in $L^2(\mathcal{X})$. This becomes a Hilbert space with inner product

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For $s > d/2$ and (sufficiently regular) $\mathcal{X} \subset \mathbb{R}^d$, the (order $s$) Sobolev space $H^s(\mathcal{X})$ is defined to be the set of functions $f : \mathcal{X} \to \mathbb{R}$ whose mixed partial derivatives $\partial^{\boldsymbol{\alpha}} f$, $|\boldsymbol{\alpha}| \leq s$, exist in $L^2(\mathcal{X})$. This becomes a Hilbert space with inner product

$$\langle f, g \rangle_{H^s(\mathcal{X})} = \sum_{|\boldsymbol{\alpha}| \leq s} \int \frac{\partial^{\boldsymbol{\alpha}} f(\boldsymbol{x})}{\partial \boldsymbol{x}^{\boldsymbol{\alpha}}} \frac{\partial^{\boldsymbol{\alpha}} g(\boldsymbol{x})}{\partial \boldsymbol{x}^{\boldsymbol{\alpha}}} \mathrm{d}\boldsymbol{x}.$$

A kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called a *Sobolev kernel* if there exists $0 < c_1 < c_2 < \infty$ such that, for all $f \in \mathcal{H}(k)$, we have $c_1 \|f\|_{H^s(\mathcal{X})} \leq \|f\|_{\mathcal{H}(k)} \leq c_2 \|f\|_{H^s(\mathcal{X})}$.

# Optimal Approximation

Do optimal weights improve convergence rates? It depends on the kernel!

**Notation:** The *multi-index* notation

$$\partial^{\boldsymbol{\alpha}} f : \boldsymbol{x} \mapsto \frac{\partial^{\boldsymbol{\alpha}} f(\boldsymbol{x})}{\partial \boldsymbol{x}^{\boldsymbol{\alpha}}} = \frac{\partial^{|\boldsymbol{\alpha}|}}{\partial x_1^{\alpha_1} \dots \partial x_d^{\alpha_d}} f(\boldsymbol{x}), \qquad \boldsymbol{\alpha} \in \mathbb{N}_0^d$$

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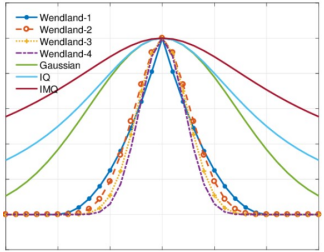
## Example 14

Let $z_+^m$ denote $\max(0, z)^m$ in shorthand. Then examples of Sobolev kernels on (sufficiently regular) $\mathcal{X} \subseteq \mathbb{R}$ include the following, due to Wendland [1998]:

| $k(x, y) \quad (r = \lvert x - y \rvert,\ x, y \in \mathbb{R})$ | order |
|---|---|
| $(1 - r)_+$ | $s = 1$ |
| $(1 - r)_+^3 (3r + 1)$ | $s = 2$ |
| $(1 - r)_+^5 (8r^2 + 5r + 1)$ | $s = 3$ |




These kernels are convenient for numerical reasons, due to their compact support, which renders $K$ a *sparse* matrix.

# Optimal Approximation

Optimal weights can accelerate convergence:

**Theorem 15 (e.g. Ehler et al. [2019])**

*Let $x_1, \ldots, x_n \sim P$ be independent and let $w = w(x_1, \ldots, x_n)$ denote optimal weights in the sense of Lemma 13. Let $k(x, y)$ be an (order $s$) Sobolev kernel. Then, under regularity conditions on the domain $\mathcal{X}$, which is of dimension $d$, and the distribution $P$, there exists a constant $0 < C < \infty$ such that*

$$\mathbb{E}\left[D_k\left(P, \sum_{i=1}^{n} w_i \delta(x_i)\right)\right] \leq C\left(\frac{\log(n)}{n}\right)^{s/d}.$$

For $s = d/2$ we recover the same rate as Proposition 1 for un-weighted Monte Carlo (up to log factors), while for $s > d/2$ we obtain faster convergence in MMD.

So surely it is a good idea to employ optimal weights? Not necessarily - the gain in rate has to out-weight the higher computational cost of $O(n^3)$. Superior error-per-cost only when $s > 3d/2$.

Numerical ill-conditioning at large $n$ also requires careful treatment. The use of points from optimal quantisation can be helpful.

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# Stein Discrepancy

# Recap: Bayesian Inference and Sampling

Recall that we aim to perform optimal quantisation of a distribution $P$ that admits a PDF $p(\boldsymbol{x})$ on $\boldsymbol{x} \in \mathbb{R}^d$, such that

$$p(\boldsymbol{x}) = \frac{\tilde{p}(\boldsymbol{x})}{Z},$$

where $\tilde{p}$ can be exactly evaluated but $Z$, and hence $p(\boldsymbol{x})$, cannot easily be evaluated or even approximated.

This setting is typical in applications of Bayesian inference, where we have

$$p(x) = \frac{\pi(x)\mathcal{L}(x)}{Z}$$

where $\pi(x)$ is a *prior* PDF, $\mathcal{L}(x)$ is a likelihood, and the implicitly defined normalisation constant $Z$ is the *marginal likelihood*.

Several methods have been developed in the statistics, applied probability, physics and machine learning literatures to approximate distributions $P$ with these characteristics, including *Markov chain Monte Carlo (MCMC)*, *sequential Monte Carlo (SMC)*, and *variational inference*. These techniques do not typically attempt *optimal* quantisation, since even the basic quantisation task can be difficult.

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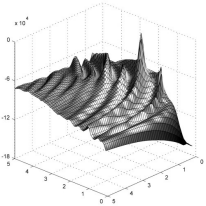


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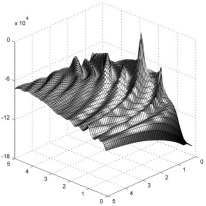


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# Stein Discrepancy

## How can our algorithms be applied?

The apparent difficulty is that we cannot compute integrals with respect to $P$, such as $\int k(\cdot, x)\mathrm{d}P(x)$, which are required for computation of MMD. A hint at a possible solution is provided by the following result:

**Lemma 16**

*Suppose $k_P : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a kernel with $\int k_P(\cdot, x)\mathrm{d}P = 0$ for all $x \in \mathcal{X}$. Then*

$$D_{k_P}(Q) = D_{k_P}(P, Q) = \sup_{\|f\|_{\mathcal{H}(k_P)} \leq 1} \left| \int f \mathrm{d}Q \right|.$$

**Proof.**

For all $f \in \mathcal{H}(k_P)$ it holds that $\int f \mathrm{d}P = 0$, whence the result. Indeed, from the reproducing property, and using Lemma 6 with Standing Assumption 1 to interchange integral with inner product, $\int f \mathrm{d}P = \int \langle f, k(\cdot, x)\rangle_{\mathcal{H}(k_P)} \mathrm{d}P(x) = \left\langle f, \int k(\cdot, x)\mathrm{d}P(x)\right\rangle_{\mathcal{H}(k_P)} = \langle f, 0\rangle_{\mathcal{H}(k_P)} = 0.$

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# Stein Discrepancy

As an example, consider a bounded linear operator

$$(\mathcal{A}_P g)(\boldsymbol{x}) = g(\boldsymbol{x}) - \int g \mathrm{d}P$$

acting on elements of an RKHS $\mathcal{H}(k)$.

If we apply $\mathcal{A}_P$ to both arguments of the kernel $k$, we obtain a Stein kernel

$$\begin{aligned} k_P(\boldsymbol{x}, \boldsymbol{y}) &= \mathcal{A}_P^{\boldsymbol{y}} \mathcal{A}_P^{\boldsymbol{x}} k(\boldsymbol{x}, \boldsymbol{y}) \\ &= k(\boldsymbol{x}, \boldsymbol{y}) - \int k(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}P(\boldsymbol{x}) - \int k(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}P(\boldsymbol{y}) + \iint k(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}P(\boldsymbol{x}) \mathrm{d}P(\boldsymbol{y}). \end{aligned} \tag{6}$$

Indeed, $\int k_P(\cdot, \boldsymbol{x}) \mathrm{d}P(\boldsymbol{x}) = \int \mathcal{A}_P^{\boldsymbol{y}} \mathcal{A}_P^{\boldsymbol{x}} k(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}P(\boldsymbol{x}) = \mathcal{A}_P^{\boldsymbol{y}} \int \mathcal{A}_P^{\boldsymbol{x}} k(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}P(\boldsymbol{x}) = \mathcal{A}_P^{\boldsymbol{y}} 0 = 0$, where interchange of $\mathcal{A}_P^{\boldsymbol{y}}$ and the integral is justified by noting that $\mathcal{A}_P^{\boldsymbol{y}}$ is a bounded linear operator and following similar reasoning to Lemma 6.

Unfortunately, the Stein kernel in (6) is not useful because it still involves the problematic integral $\int k(\cdot, \boldsymbol{x}) \mathrm{d}P(\boldsymbol{x})$. A more useful construction of a Stein kernel is needed.

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Indeed, $\int k_P(\cdot, x) \mathrm{d}P(x) = \int \mathcal{A}_P^y \mathcal{A}_P^x k(x, y) \mathrm{d}P(x) = \mathcal{A}_P^y \int \mathcal{A}_P^x k(x, y) \mathrm{d}P(x) = \mathcal{A}_P^y 0 = 0$, where interchange of $\mathcal{A}_P^y$ and the integral is justified by noting that $\mathcal{A}_P^y$ is a bounded linear operator and following similar reasoning to Lemma 6.

Unfortunately, the Stein kernel in (6) is not useful because it still involves the problematic integral $\int k(\cdot, x) \mathrm{d}P(x)$. A more useful construction of a Stein kernel is needed.

# Stein Discrepancy

As an example, consider a bounded linear operator

$$(\mathcal{A}_P g)(\boldsymbol{x}) = g(\boldsymbol{x}) - \int g \mathrm{d}P$$

acting on elements of an RKHS $\mathcal{H}(k)$.

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# Stein Operators

**Notation:** Let $\nabla f = (\partial_{x_1} f, \ldots, \partial_{x_d} f)^\top$ for differentiable functions $f : \mathbb{R}^d \to \mathbb{R}$.

### Standing Assumption 2

*The distribution $P$ admits a positive and differentiable PDF such that $x \mapsto (\nabla \log p)(x)$ is Lipschitz.*

### Definition 17 (Canonical Stein operator)

For a distribution $P$ admitting a positive and differentiable density $p$ on $\mathbb{R}^d$, we define the *canonical Stein operator*

$$(\mathcal{A}_P g)(x) = (\nabla \cdot g)(x) + g(x) \cdot (\nabla \log p)(x)$$

acting on differentiable vector field $g : \mathbb{R}^d \to \mathbb{R}^d$, where $x \in \mathbb{R}^d$.

The canonical Stein operator was introduced (for Gaussian $P$) in Stein [1972]. Importantly, observe that

$$(\nabla \log p)(x) = \frac{(\nabla p)(x)}{p(x)} = \frac{\frac{1}{Z}(\nabla \tilde{p})(x)}{\frac{1}{Z}\tilde{p}(x)} = \frac{(\nabla \tilde{p})(x)}{\tilde{p}(x)} = (\nabla \log \tilde{p})(x),$$

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Now we apply the Stein operator $\mathcal{A}_P$ to a standard kernel $k$, to obtain the following Stein kernel:

**Lemma 18**

*Suppose the kernel $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ has $(\boldsymbol{x}, \boldsymbol{y}) \mapsto \partial^{(\boldsymbol{\alpha},\boldsymbol{\beta})} k(\boldsymbol{x}, \boldsymbol{y})$ continuous and uniformly bounded for all $|\boldsymbol{\alpha}|, |\boldsymbol{\beta}| \leq 1$. Suppose $\int \|\nabla \log p(\boldsymbol{x})\| \mathrm{d}P(\boldsymbol{x}) < \infty$ and that $\sup_{\|\boldsymbol{x}\| \geq r} r^{d-1} p(\boldsymbol{x}) \to 0$ as $r \to \infty$. Then*

$$\begin{aligned} k_P(\boldsymbol{x}, \boldsymbol{y}) = \nabla_x \cdot \nabla_y k(\boldsymbol{x}, \boldsymbol{y}) + \nabla_x \log p(\boldsymbol{x}) \cdot \nabla_y k(\boldsymbol{x}, \boldsymbol{y}) + \nabla_y \log p(\boldsymbol{y}) \cdot \nabla_x k(\boldsymbol{x}, \boldsymbol{y}) \\ + (\nabla_x \log p(\boldsymbol{x})) \cdot (\nabla_y \log p(\boldsymbol{y})) k(\boldsymbol{x}, \boldsymbol{y}) \end{aligned}$$

*is a kernel with $\int k_P(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}P(\boldsymbol{y}) = 0$ for all $\boldsymbol{x} \in \mathbb{R}^d$.*

**Proof.**

First notice that

$$k_P(\boldsymbol{x}, \boldsymbol{y}) = \mathcal{A}_P^y \begin{bmatrix} \vdots \\ \nabla_{x_i} k(\boldsymbol{x}, \boldsymbol{y}) + k(\boldsymbol{x}, \boldsymbol{y}) \nabla_{x_i} \log p(\boldsymbol{x}) \\ \vdots \end{bmatrix} = \mathcal{A}_P^y g(\boldsymbol{y})$$

where, under our assumptions, (a) $\boldsymbol{y} \mapsto g(\boldsymbol{y})$ is bounded, and (b) $\boldsymbol{y} \mapsto \nabla_y \cdot g(\boldsymbol{y})$ is integrable with respect to $P$. Thus it suffices to show that $\int \mathcal{A}_P g \mathrm{d}P = 0$ for *all* vector fields $g$ for which (a) and (b) hold.

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## Proof.

Let $g$ be such a vector field, and let $B_r = \{\boldsymbol{x} \in \mathbb{R}^d : \|\boldsymbol{x}\| \leq r\}$ and $S_r = \{\boldsymbol{x} \in \mathbb{R}^d : \|\boldsymbol{x}\| = r\}$. The main idea is to apply the divergence theorem (i.e. integrate by parts):

$$\begin{aligned} \int \mathcal{A}_P g \mathrm{d}P &= \int (\nabla \cdot g) + g \cdot (\nabla \log p) \mathrm{d}P = \int (\nabla \cdot (pg))(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} \\ &= \lim_{r \to \infty} \int_{B_r} (\nabla \cdot (pg))(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} = \lim_{r \to \infty} \oint_{S_r} p(\boldsymbol{x})(g(\boldsymbol{x}) \cdot n(\boldsymbol{x})) \mathrm{d}\boldsymbol{x} \end{aligned}$$

where $n(\boldsymbol{x})$ is the outward unit normal to $S_r$ at $\boldsymbol{x}$. (The regularity assumptions ensure that the integrals $\int (\nabla \cdot g) \mathrm{d}P$ and $\int g \cdot (\nabla \log p) \mathrm{d}P$ exist.)

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## Proof.

Now

$$\begin{aligned} \oint_{S_r} p(x)(g(x) \cdot n(x)) \mathrm{d}x &\leq \|g\|_\infty \sup_{\|x\| \geq r} p(x) \oint_{S_r} \mathrm{d}x \\ &= \|g\|_\infty \sup_{\|x\| \geq r} p(x) \frac{2\pi^{d/2}}{\Gamma(d/2)} r^{d-1} \\ &\to 0 \text{ as } r \to \infty, \end{aligned}$$

where we have used the formula for the surface area of the radius $r$ sphere in $\mathbb{R}^d$.

# Kernel Stein Discrepancy

For $Q_n = \sum_{i=1}^n w_i \delta(\boldsymbol{x}_i)$ and $k_P$ defined in Lemma 18, we obtain the kernel Stein discrepancy (KSD):

$$D_{k_P}(Q_n) = \sup_{\|f\|_{\mathcal{H}(k_P)} \leq 1} \left| \int f \mathrm{d} Q_n \right| = \sqrt{\sum_{i=1}^n \sum_{j=1}^n w_i w_j k_P(\boldsymbol{x}_i, \boldsymbol{x}_j)}$$

As with MMD, we can establish properties analogous to characteristicness and convergence control for KSD. Here we focus on convergence control:

**Theorem 19 (Gorham and Mackey [2017])**

*Let $P$ be distantly dissipative [see Gorham et al., 2019]. Consider the kernel*

$$k(\boldsymbol{x}, \boldsymbol{y}) = (\sigma^2 + \|\boldsymbol{x} - \boldsymbol{y}\|^2)^{-\beta}$$

*for some fixed $\sigma > 0$ and a fixed exponent $\beta \in (0, 1)$. Then $D_{k_P}(Q_n) \to 0$ implies $Q_n \Rightarrow P$.*

However, unlike MMD, the construction of KSD suffers from *blindness to mixing proportions*; figure taken from Wenliang and Kanagawa [2020]:

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# Optimal Quantisation

**The algorithms previously described for MMD can immediately be applied to KSD!**

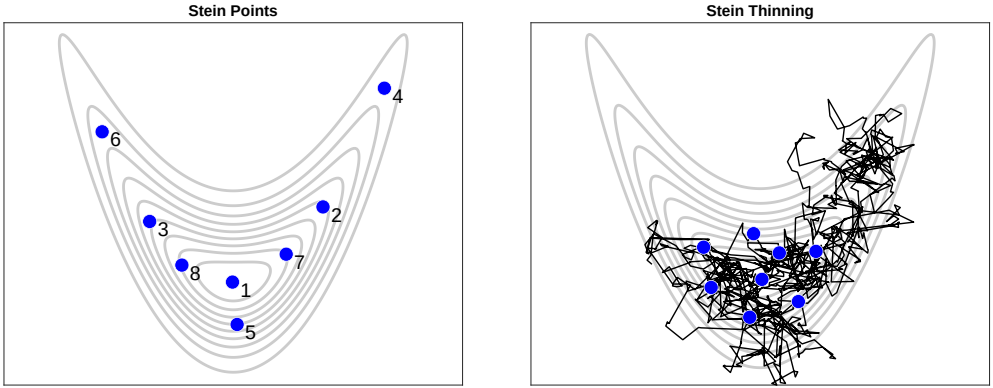


Figure: *Stein points* (left) *and Stein thinning* (right)*:* Stein points are generated by sequential (greedy) minimisation of KSD to select $n = 8$ states $\{\boldsymbol{x}_i\}_{i=1}^n$ in an approximation $Q_n$ to $P$. The numbers indicate the order in which the states $\boldsymbol{x}_i$ were selected. Stein thinning restricts the continuous inner-loop optimisation problem in Stein points to a discrete search over a MCMC sample path (black).

# Optimal Approximation

Optimal weights can again be computed, with a slight twist:

**Lemma 20**

*Let $x_1, \ldots, x_n \in \mathcal{X}$ be distinct. The optimal weights*

$$\underset{\substack{\boldsymbol{w} \in \mathbb{R}^n \\ \mathbf{1}^\top \boldsymbol{w} = 1}}{\arg\min} D_{k_P} \left( \sum_{i=1}^n w_i \delta(\boldsymbol{x}_i) \right)$$

*are $\boldsymbol{w} = (K_P^{-1}\mathbf{1})/(\mathbf{1}^\top K_P^{-1}\mathbf{1})$, where $[K_P]_{ij} = k_P(\boldsymbol{x}_i, \boldsymbol{x}_j)$. [Note the constraint $w_1 + \cdots + w_n = 1$.]*

**Proof.**

From the explicit form of MMD we have

$$D_{k_P} \left( \sum_{i=1}^n w_i \delta(\boldsymbol{x}_i) \right)^2 = \boldsymbol{w}^\top K_P \boldsymbol{w},$$

so the optimisation problem is

$$\arg\min \boldsymbol{w}^\top K_P \boldsymbol{w} \qquad \text{s.t.} \qquad \mathbf{1}^\top \boldsymbol{w} = 1.$$

This can be solved using the method of Lagrange multipliers to obtain the stated result.

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$$\underset{\substack{\boldsymbol{w} \in \mathbb{R}^n \\ \mathbf{1}^\top \boldsymbol{w} = 1}}{\arg\min} D_{k_P} \left( \sum_{i=1}^n w_i \delta(\boldsymbol{x}_i) \right)$$

*are $\boldsymbol{w} = (K_P^{-1}\mathbf{1})/(\mathbf{1}^\top K_P^{-1}\mathbf{1})$, where $[K_P]_{ij} = k_P(\boldsymbol{x}_i, \boldsymbol{x}_j)$. [Note the constraint $w_1 + \cdots + w_n = 1$.]*

**Proof.**

From the explicit form of MMD we have

$$D_{k_P} \left( \sum_{i=1}^n w_i \delta(\boldsymbol{x}_i) \right)^2 = \boldsymbol{w}^\top K_P \boldsymbol{w},$$

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This can be solved using the method of Lagrange multipliers to obtain the stated result.

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Optimal weights can again be computed, with a slight twist:

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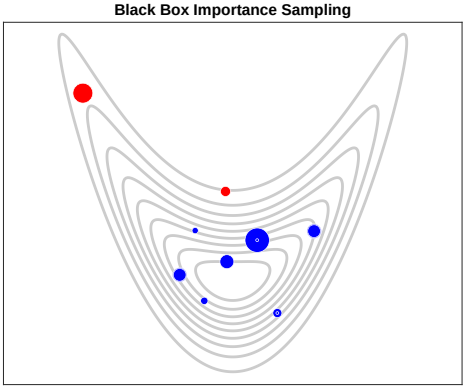


Figure: *Black box importance sampling* [Liu and Lee, 2017, Hodgkinson et al., 2020]: In black box importance sampling the weights $w_1, \ldots, w_n$ are obtained by minimising KSD in the manner of Lemma 20. Blue indicates states $\boldsymbol{x}_i$ with positive weights $w_i > 0$, while red indicates negative weights $w_i < 0$. The size of the circles is proportional to $|w_i|$.

Complexity $= O(n^3)$ and symmetry exploits fail, but $P_{\mathrm{ST}} \to P_{\mathrm{BBIS}}$ as $m \to \infty$ for $n$ fixed.

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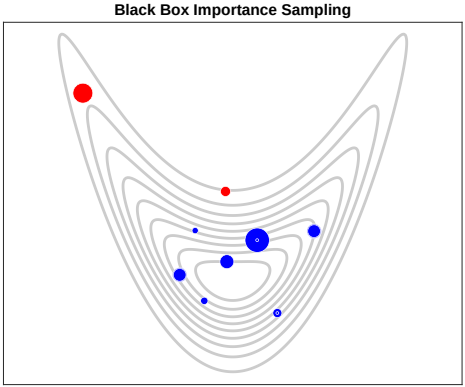


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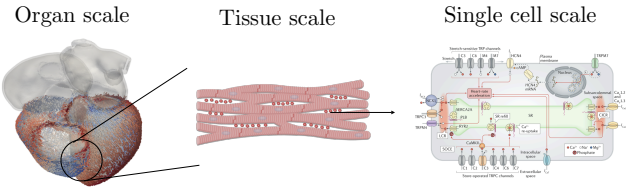
# Case Study: Cardiac Digital Twins

# Cardiac Models




- Cardiac function determined by integrated action of myocytes.
- Calcium is intracellular end-point signal driving contraction.
- **Question**: is there cell-to-cell variability?
  - "Extreme" cells might be related to pathologies (arrythmias - ventricular fibrillation)?
  - Role for ageing in the extent of heterogeneity?
  - ...

- 25 myocytes, from different rat hearts, fed in a dish.
- **Patch clamp experiment**: micropipette controls cell membrane potential, and adds a drug to
  - block transients of ions that are not calcium;
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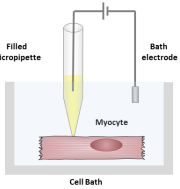

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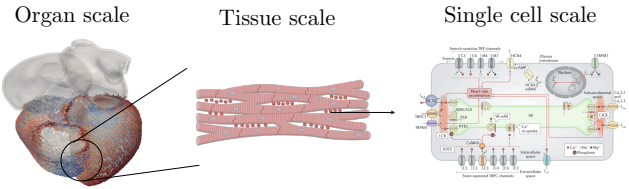


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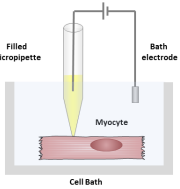

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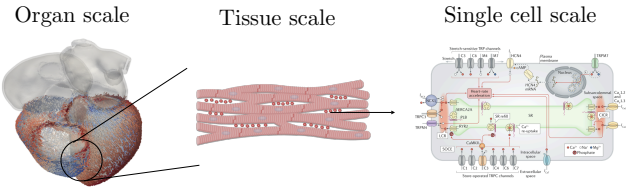


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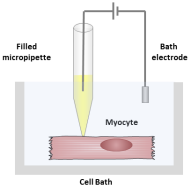

# Statistical Model

- The experiment is modelled using mass action kinetics, in the form of an ordinary differential equation (ODE) with unknown parameters denoted $\theta \in \Theta$.
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$$u(0) = u_0, \qquad \frac{\mathrm{d}u_1}{\mathrm{d}t} = f_1(t, u; \theta),$$
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  and the solution at time $t$ is denoted $u(t; \theta)$. Here $p = 6$ and $d := \dim(\Theta) = 38$.
- The data are related to the ODE via a measurement error model

$$\pi(y|\theta) := \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y_i - u_1(t_i; \theta))^2}{2\sigma^2}\right),$$

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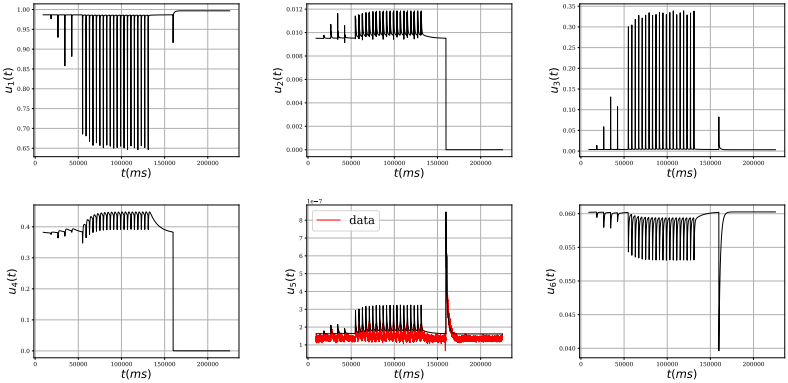


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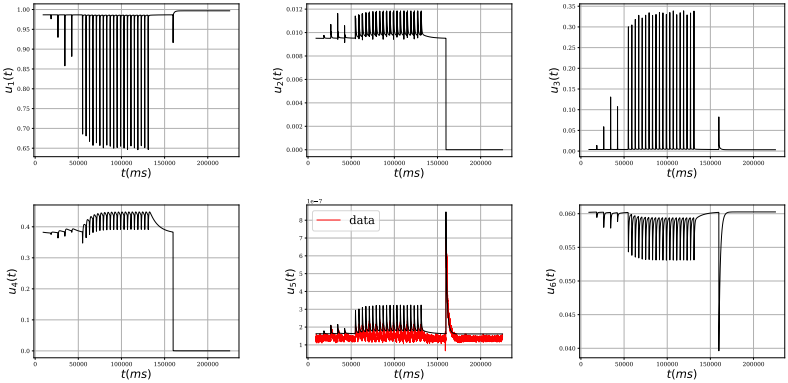


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# De-Biasing of Markov Chain Monte Carlo

MCMC samples are biased by ODE solver failure, but Stein Thinning does not require MCMC to be $P$-invariant - as long as the relevant part of the parameter space is explored:

**Theorem 21 ([Riabiz et al., 2022])**

*Let $(\theta_i)_{i\in\mathbb{N}}$ be a $Q$-invariant, time-homogeneous, reversible Markov chain, such that $P$ is absolutely continuous with respect to $Q$ and*

- *$(\theta_i)_{i\in\mathbb{N}}$ is $V$-uniformly ergodic with $V(\theta) \geq \frac{\mathrm{d}P}{\mathrm{d}Q}(\theta)\sqrt{k_P(\theta,\theta)}$*
- $\sup_{i\in\mathbb{N}} \mathbb{E}[\frac{\mathrm{d}P}{\mathrm{d}Q}(\theta_i)\sqrt{k_P(\theta_i,\theta_i)}V(\theta_i)] < \infty$
- $\exists\gamma > 0$ *s.t.* $b := \sup_{i\in\mathbb{N}} \mathbb{E}[e^{\gamma \max(1, \frac{\mathrm{d}P}{\mathrm{d}Q}(\theta_i)^2)k_P(\theta_i,\theta_i)}] < \infty$.

*Then the output of Stein Thinning satisfies*

$$\frac{1}{m}\sum_{i\in S}\delta(\theta_i) \Rightarrow P$$

*almost surely as $n, m \to \infty$ with $m \leq n$ and $\log(n) = O(m^{\beta/2})$ for some $\beta < 1$.*

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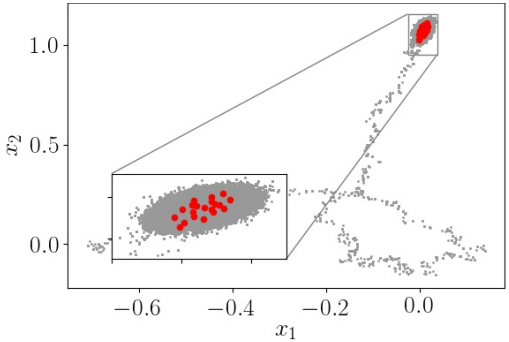
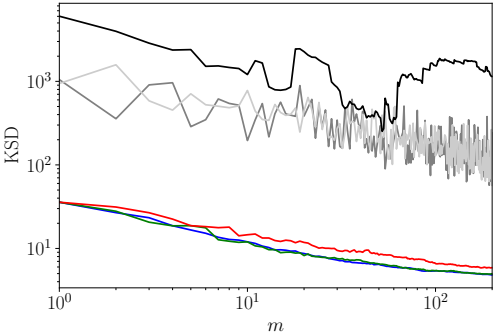
# Illustrative Application to Differential Equation Constrained Inverse Problems

Goodwin oscillator; $d = 4$ parameters to be estimated. (Red dots are Stein Thinning, while gray dots are MCMC.)




Cardiac model; $d = 38$ parameters to be esitmated. (Blue, red, and green are Stein Thinning, while black are MCMC.)



# Future Directions, Open Questions and Challenges

# Scalable Stein Thinning

Greedy selection may be sub-optimal. Also, the cost of selecting $m$ points from $n$ using Stein Thinning is high, at $O(m^2 n)$.

- A **non-myopic** algorithm selects $s$ points simultaneously.
- A **mini-batch** algorithm searches over a subset of $b \ll n$ candidates at each step.

Full details in Teymur et al. [2021].

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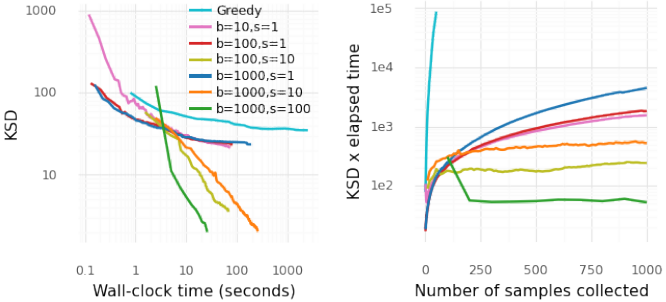


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# Gradient-Free Kernel Stein Discrepancy

Gradients can be difficult to stably compute, e.g. for ODEs and PDEs.

**Definition 22 (Gradent-free Stein operator)**

For distributions $P$ and $Q$ admitting sufficiently regular densities $p$ and $q$ on $\mathbb{R}^d$, we define the *gradient-free Stein operator*

$$(\mathcal{A}_{P,Q}\, g)(x) = \frac{q(x)}{p(x)} \left[ (\nabla \cdot g)(x) + g(x) \cdot (\nabla \log q)(x) \right]$$

acting on differentiable vector field $g : \mathbb{R}^d \to \mathbb{R}^d$, where $x \in \mathbb{R}^d$.

- The associated Stein discrepancy can be computed up to proportionality using $\tilde{p}(x) = Z \times p(x)$.
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- Sufficient conditions have been established on $q$ for convergence detection and control.

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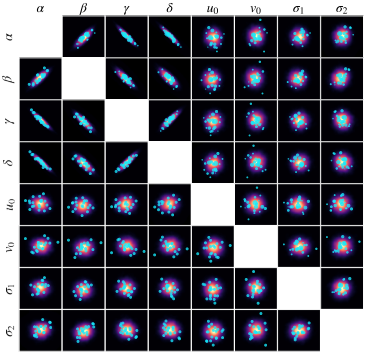
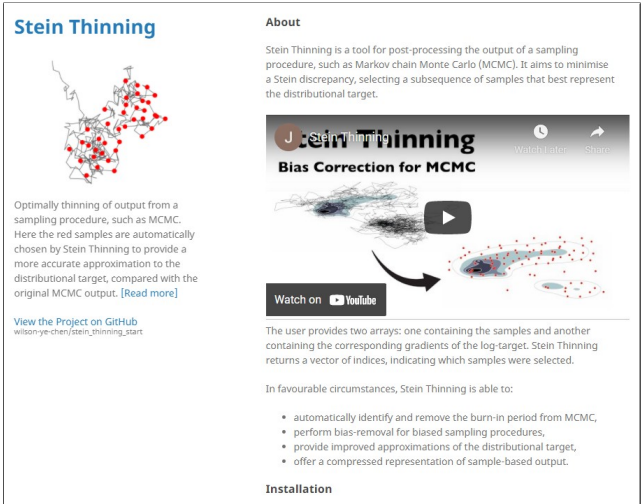
- The associated Stein discrepancy can be computed up to proportionality using $\tilde{p}(x) = Z \times p(x)$.
- The differentiability and distant dissipativity requirements now apply to $q$ (a degree of freedom) instead of $p$ (the posterior target).
- Sufficient conditions have been established on $q$ for convergence detection and control.



# Software Development

To try out these algorithms (in Python, Matlab and R), visit `Stein-Thinning.org`



# Broader Context: Optimisation over $\mathcal{P}(\Theta)$

Going beyond optimisation in $\Theta$, we can consider optimisation in $\mathcal{P}(\Theta)$:

$$D_{\mathcal{H}(k_P),P}(Q) := \sup_{\|f\|_{\mathcal{H}(k_P)} \leq 1} |\mathbb{E}_{\vartheta \sim Q}[f(\vartheta)]|$$

- **Variational Inference:** Ranganath et al. [2016], Hu et al. [2018], Fisher et al. [2021], ...

$$\min_{Q \in \mathcal{Q}} D_{\mathcal{H}(k_P),P}(Q), \qquad \text{(e.g.) } \mathcal{Q} = \{T_\# Q_0 : T \text{ a neural network}\}$$

  Avoids the requirement in VI that $T$ be a diffeomorphism (i.e. no need for normalising flows!).

- **Gradient Flow:** Korba et al. [2021]

$$\frac{\partial Q_t}{\partial t} + \mathrm{div}(Q_t v_{Q_t}) = 0, \qquad v_{Q_t} = -\nabla_{W_2} \mathcal{F}(Q_t), \qquad \mathcal{F}(Q) = \frac{1}{2} D_{\mathcal{H}(k_P),P}(Q)^2$$

  *not the same as SVGD [see Liu, 2017].

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# Broader Context: Sampling with Stein Discrepancies

For any Stein characterisation $(\mathcal{A}, \mathcal{F})$ we can consider an associated Stein discrepancy [Gorham and Mackey, 2015]:

$$D_{\mathcal{H}(k_P),P}(Q) := \sup_{f \in \mathcal{F}} |\mathbb{E}_{\vartheta \sim Q}[f(\vartheta)]|$$

- **Beyond Euclidean State Spaces:** Riemannian manifolds [Barp et al., 2022, Le et al., 2020], discrete spaces [Xu and Reinert, 2021], ...
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**The interaction between the sampling algorithms we have seen and the choice of Stein Discrepancy is not well-understood.**

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# Broader Context: Alternatives to Direct Minimisation of Stein Discrepancy

- **Stein Variational Gradient Descent:** Liu and Wang [2016], Liu [2017], Liu and Zhu [2018], Detommaso et al. [2018], ...
- **MCMC with Stein Control Variates:** Assaraf and Caffarel [1999], Mira et al. [2013], CJO et al. [2017], Belomestny et al. [2017], South et al. [2022], ...

$$\text{Given a QoI } f, \text{ seek } (u, c) \text{ such that } c + \frac{\nabla \cdot (p \nabla u)}{p} = f. \qquad \text{Then } c = \mathbb{E}_{\vartheta \sim P}[f(\vartheta)].$$

In practice, an approximate solution $u$ gives rise to a control variate $v = \nabla \cdot (p \nabla u)/p$ for use in MCMC.

For more, please see the recent review paper of Anastasiou et al. [2022].

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## Thank you for your attention!

### Collaborators:

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