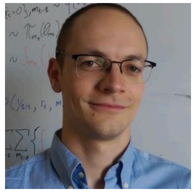
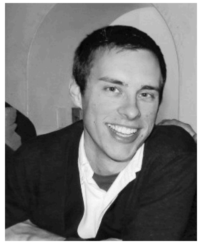
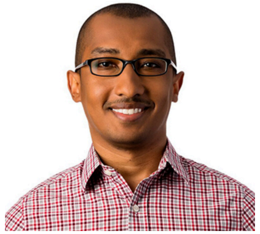
Stein's method as a computational tool



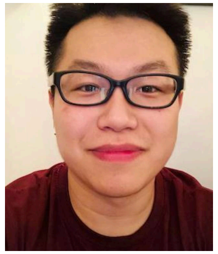











[+ many more who don't fit on slide…]

Dr François-Xavier Briol
Department of Statistical Science
University College London

A summary of this course

Statistical Science
2023, Vol. 38, No. 1, 120–139
https://doi.org/10.1214/22-STS863

Stein’s Method Meets Computational Statistics: A Review of Some Recent Developments

Andreas Anastasiou, Alessandro Barp, François-Xavier Briol, Bruno Ebner, Robert E. Gaunt, Fatemeh Ghaderinezhad, Jackson Gorham, Arthur Gretton, Christophe Ley, Qiang Liu, Lester Mackey, Chris J. Oates, Gesine Reinert and Yvik Swan

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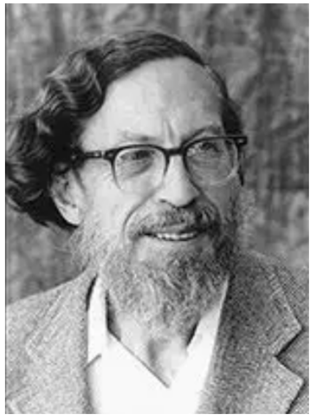
We started with two authors back in 2018 then things got out of hands….

The birth of Stein's method (1972)

A BOUND FOR THE ERROR IN THE NORMAL APPROXIMATION TO THE DISTRIBUTION OF A SUM OF DEPENDENT RANDOM VARIABLES

CHARLES STEIN
STANFORD UNIVERSITY



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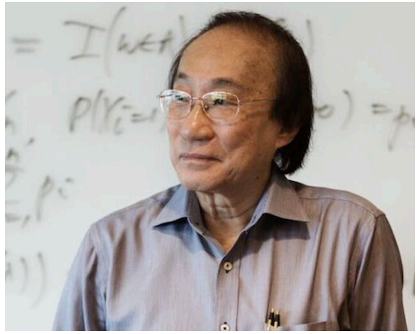

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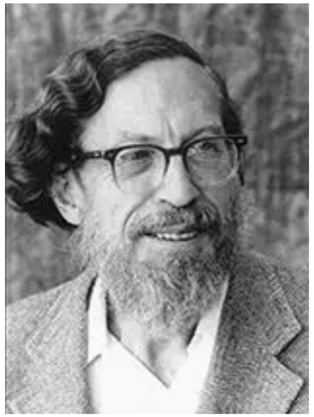

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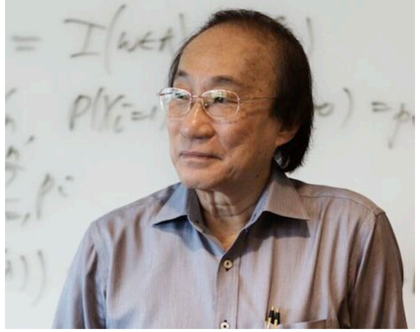

Prof. Louis Chen (NUS)

<u>1972-2015:</u> most of the focus is on probability theory of theoretical statistics.

Stein goes computational (2015-…)

arXiv 2014 - JRSSB 2017

J. R. Statist. Soc. B (2017)
79, *Part* 3, *pp.* 695–718

Control functionals for Monte Carlo integration

Chris J. Oates,
University of Technology Sydney, Australia

Mark Girolami
University of Warwick, Coventry, and Alan Turing Institute, London, UK

and Nicolas Chopin
Centre de Recherche en Economie et Statistique and Ecole Nationale de la Statistique et de l'Administration Economique, Paris, France

NeurIPS 2015

Measuring Sample Quality with Stein's Method

Jackson Gorham
Department of Statistics
Stanford University

Lester Mackey
Department of Statistics
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We will now discuss why Stein characterisations are so useful…

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ICML 2016

A Kernel Test of Goodness of Fit

Kacper Chwialkowski* KACPER.CHWIALKOWSKI@GMAIL.COM
Heiko Strathmann* HEIKO.STRATHMANN@GMAIL.COM
Arthur Gretton ARTHUR.GRETTON@GMAIL.COM
Gatsby Unit, University College London, United Kingdom

ICML 2016

A Kernelized Stein Discrepancy for Goodness-of-fit Tests

Qiang Liu QLIU@CS.DARTMOUTH.EDU
Computer Science, Dartmouth College, NH, 03755

Jason D. Lee JASONDLEE88@EECS.BERKELEY.EDU
Michael Jordan JORDAN@CS.BERKELEY.EDU
Department of Electrical Engineering and Computer Science University of California, Berkeley, CA 94709

We will now discuss why Stein characterisations are so useful…

Some exciting new algorithms!

Stein's Method

Some exciting new algorithms!

Hypothesis testing

Stein's Method

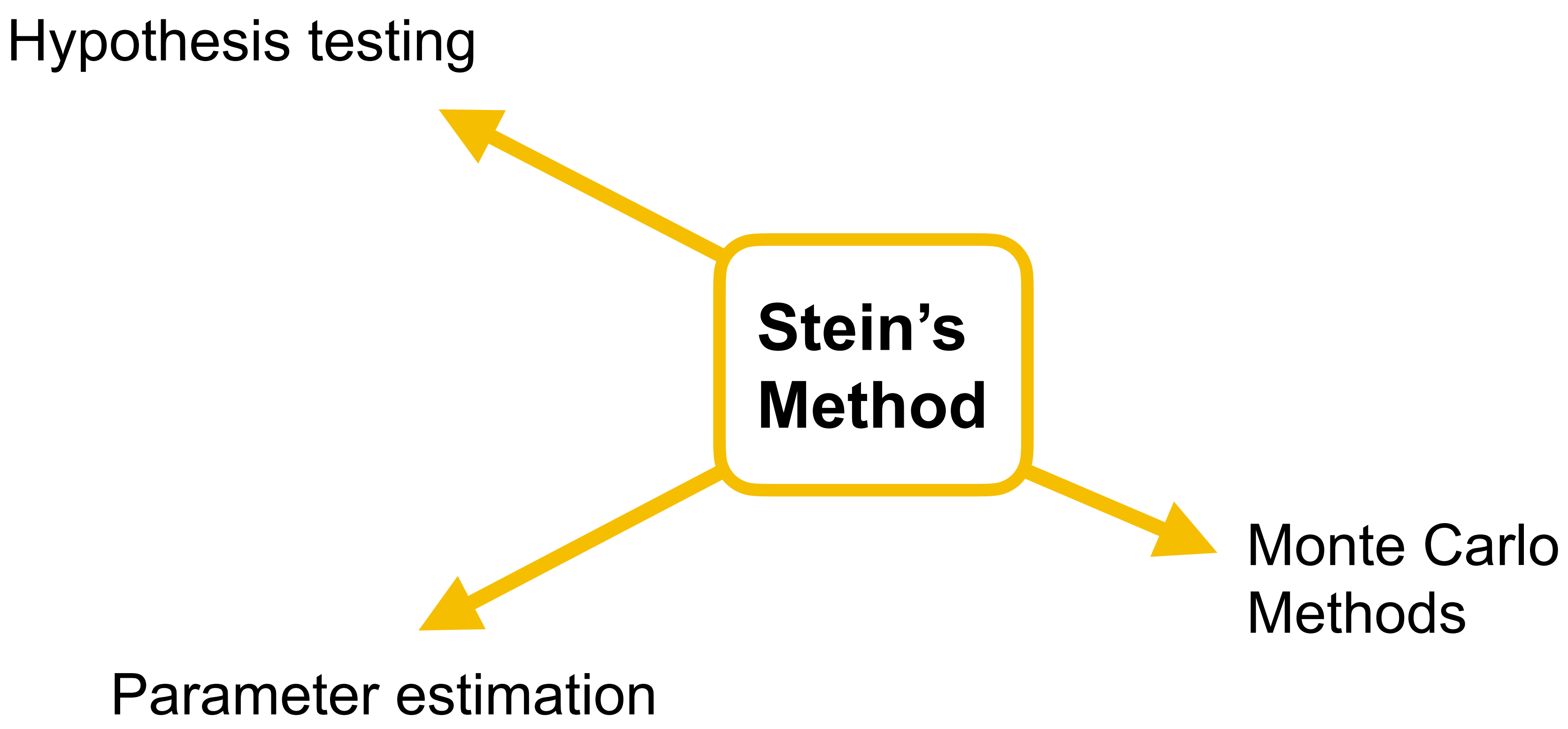
Some exciting new algorithms!

Hypothesis testing

Stein's Method

Monte Carlo Methods

Some exciting new algorithms!



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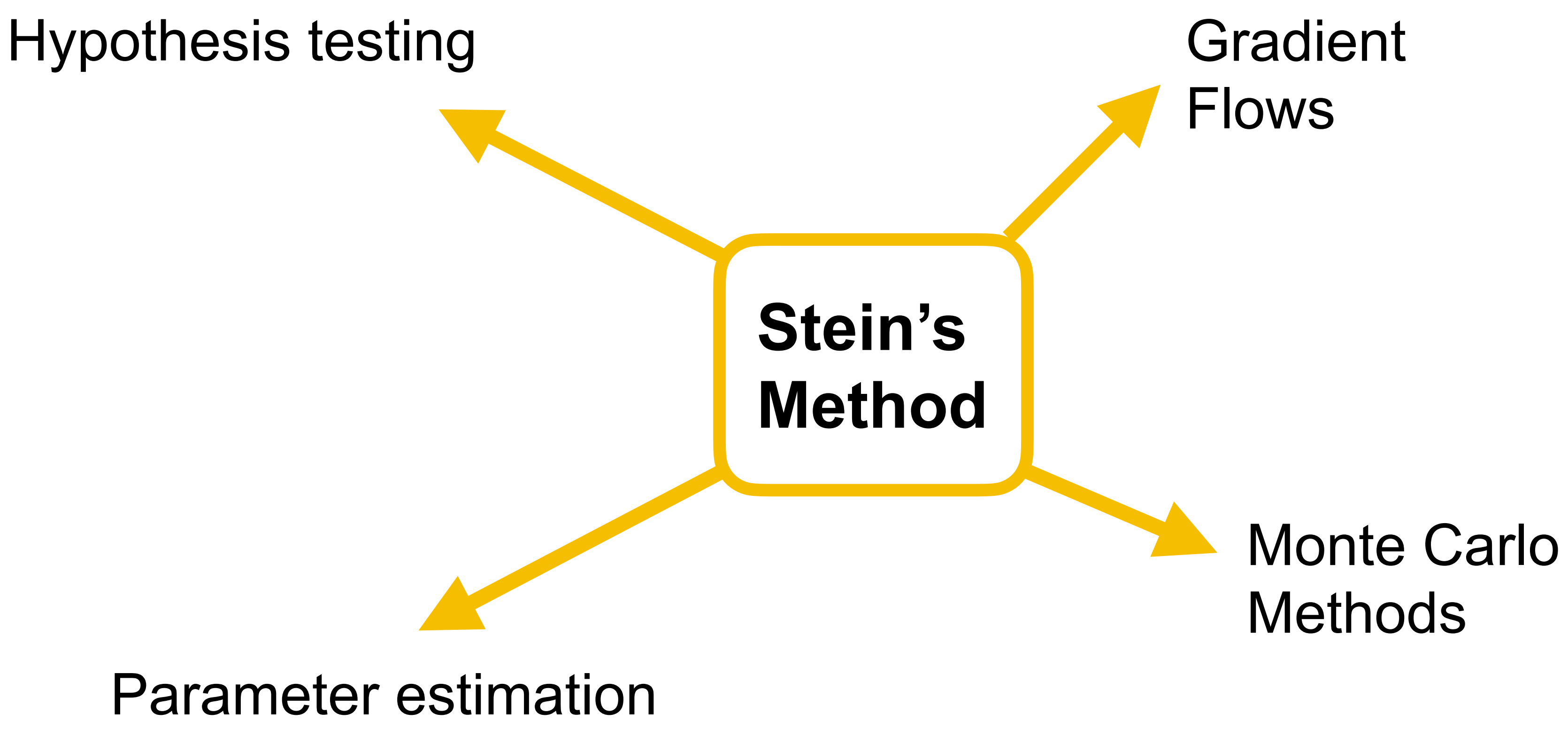

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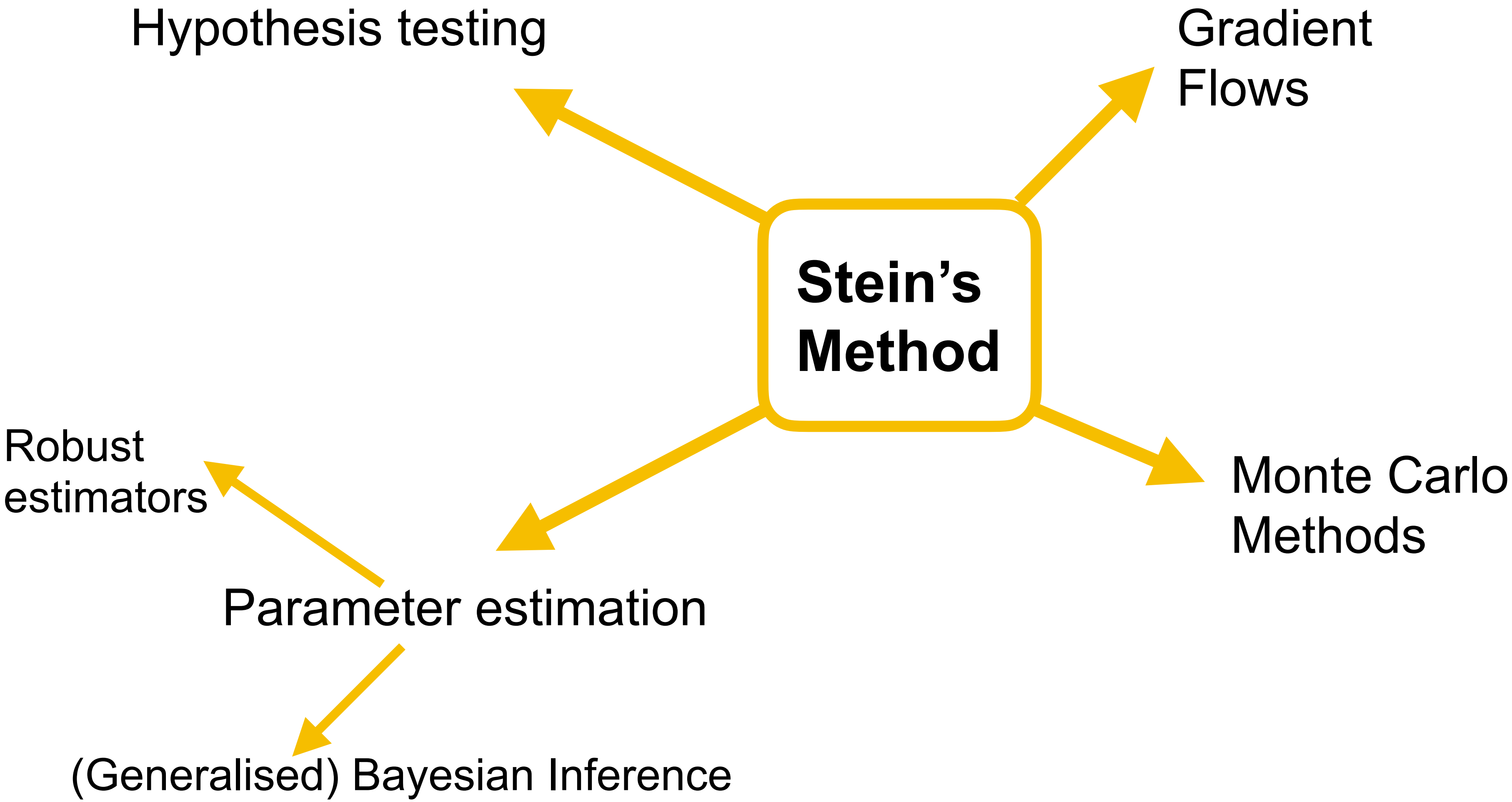

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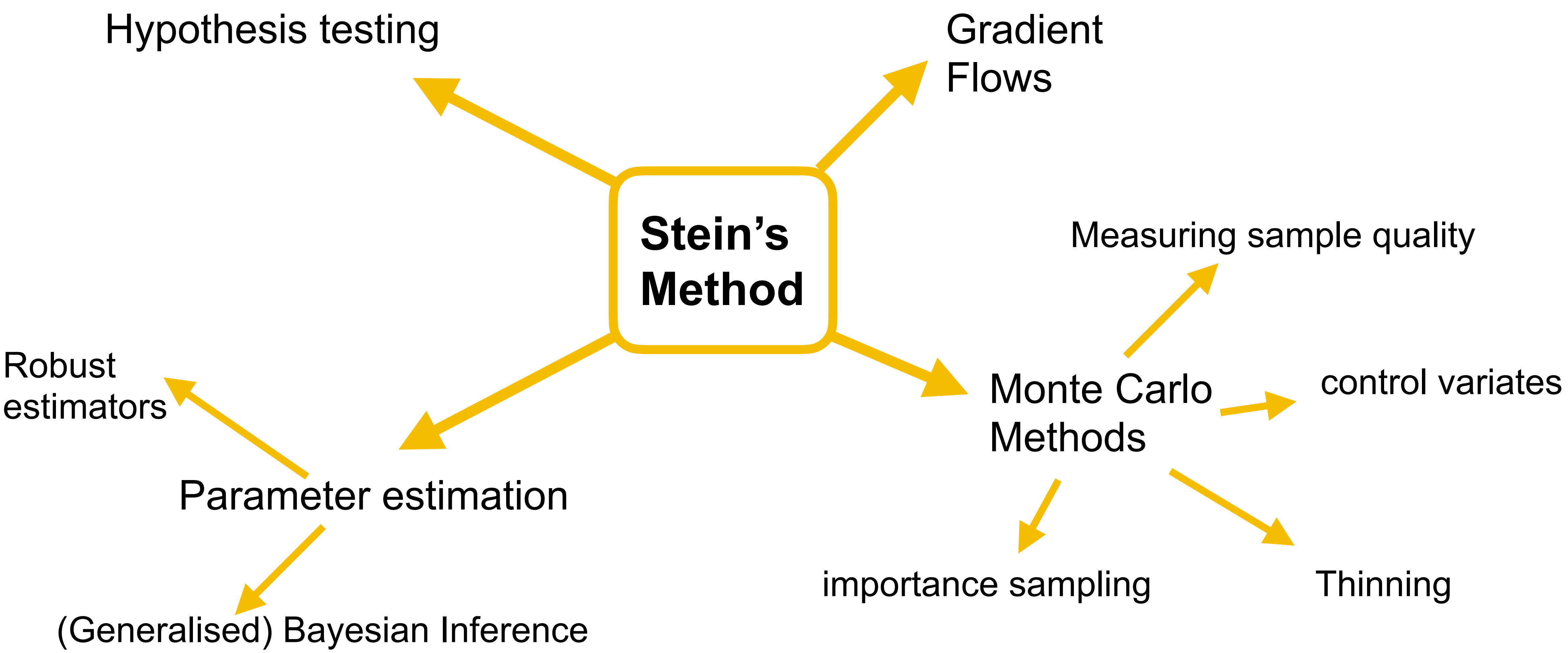

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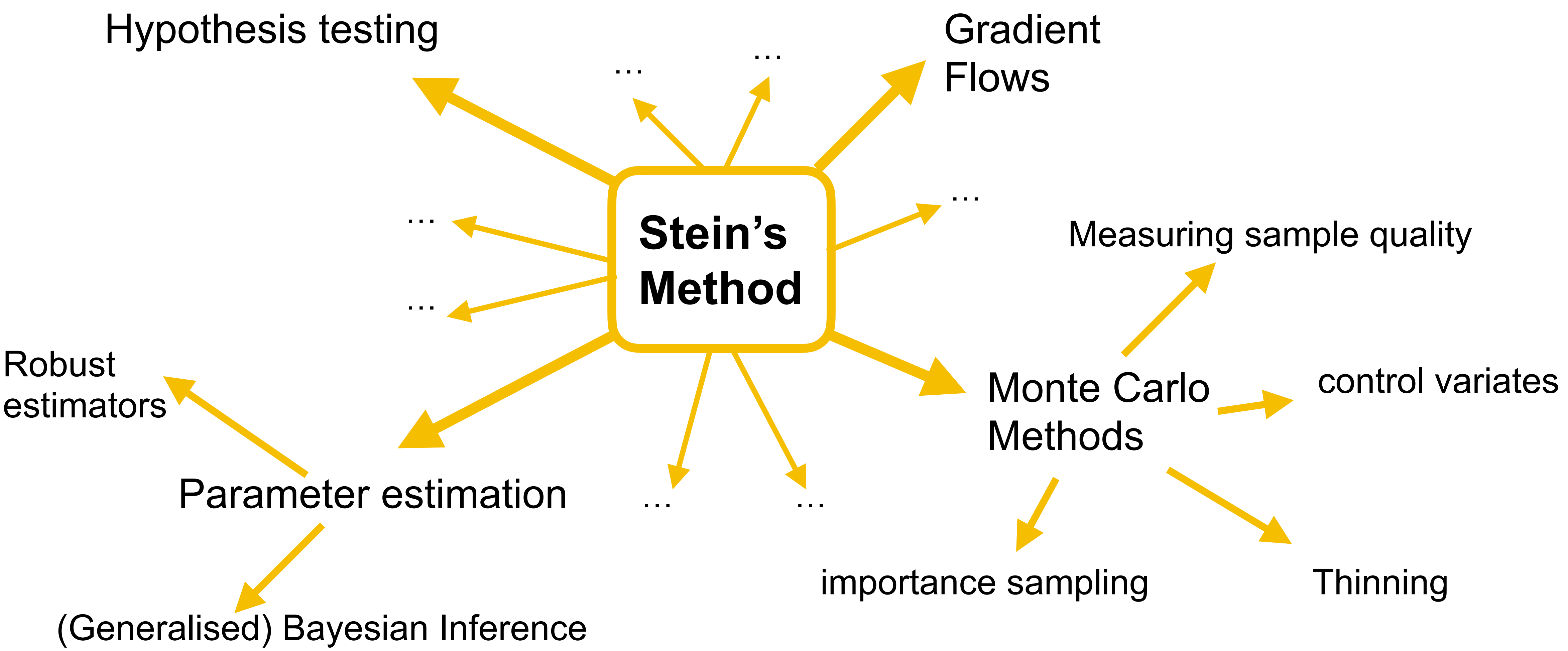

Outline

- What is Stein's method, and why should you care…
- Computational tools based on Stein's method.
- Some nice (new) algorithms!

Stein’s method as a computational tool

Stein characterisations

Uncertainty through distributions

- Our job, as statisticians, is to help make sense of the world around us by collecting and analysis data, and making conclusions from this.
- This is hard as we typically only have limited data, and we therefore need to be careful in how we **represent and communicate uncertainty**!

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- In statistics, we typically represent uncertainty through **probability distributions**.

Some popular characterisations

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CF: $\varphi(t) = \mathbb{E}_{X \sim P}[\exp(itX)]$

…

Difference between characterisations

- **Q:** *“Why do we need so many ways of describing probability distributions?”*

Difference between characterisations

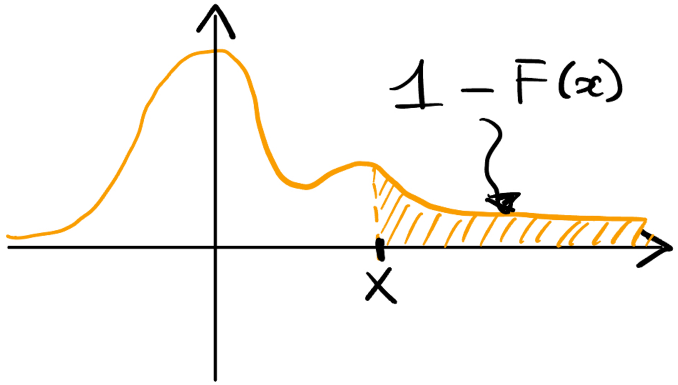
- **Q:** *"Why do we need so many ways of describing probability distributions?"*

- **A:** They each give us a **mathematical language** to work with probability distributions, and sometime expressing yourself in one language is easier than doing so with another.

Characterisations in probability theory

Characterisations in probability theory

- **Example 1:** Cumulative distribution functions are great for computing tail probabilities $P(X \geq x) = 1 - F(x)$, but really terrible for representing multivariate distributions!



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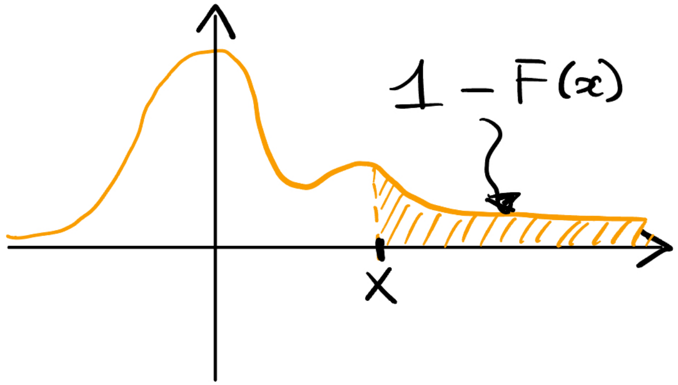

- **Example 2:** Characteristic functions are the expectation of a complex function and so not very interpretable, but their properties make the proof of the central limit theorem much easier!

$$\sqrt{n}\left(\frac{1}{n}\sum_{i=1}^{n} X_i - \mathbb{E}_{X\sim P}[X]\right) \to \mathcal{N}(0,\sigma^2)$$

Characterisations in statistics and machine learning

- **Example 1:** The moment generating function $M(t)$ is convenient for hypothesis testing or parameter estimation:

$$\mathbb{E}_{X\sim P}[X^n] = \left.\frac{d^n M(t)}{dt^n}\right|_{t=0}$$

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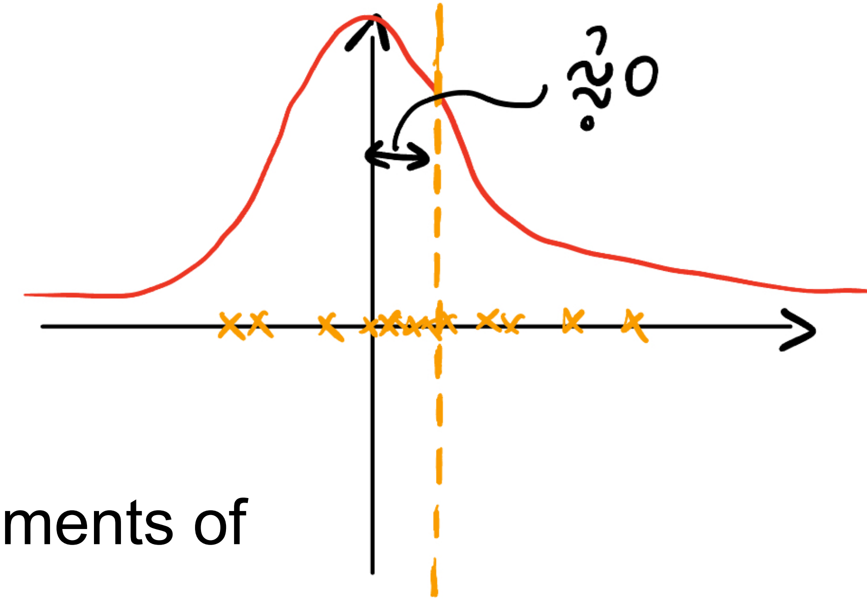

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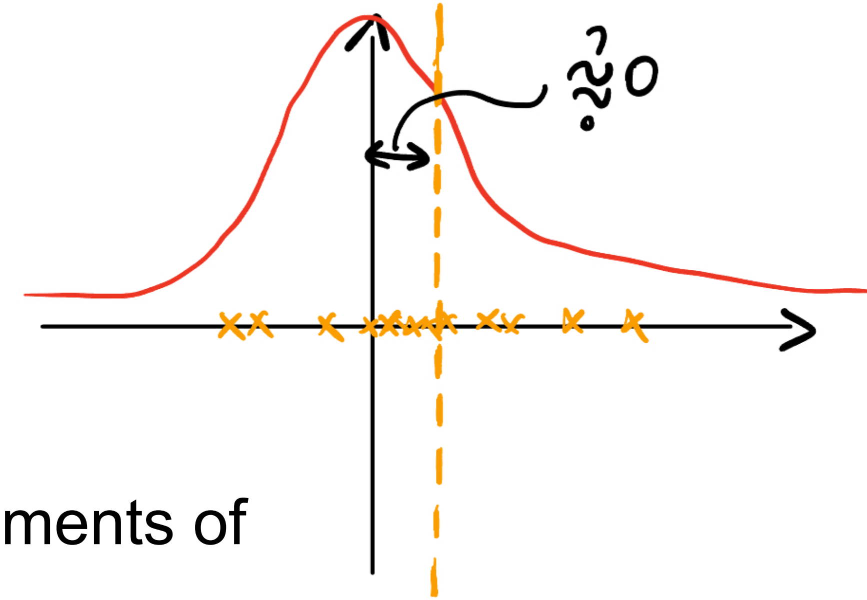

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- We will now see yet another characterisation….

Stein characterisation

- A **Stein characterisation** for P is a pair $(\mathcal{S}_P, \mathcal{G}_P)$ such that

$$Q = P \quad \Leftrightarrow \quad \mathbb{E}_{X\sim Q}[\mathcal{S}_P[g](X)] = 0 \quad \forall g \in \mathcal{G}_P$$

Stein characterisation

Stein operator

Stein class

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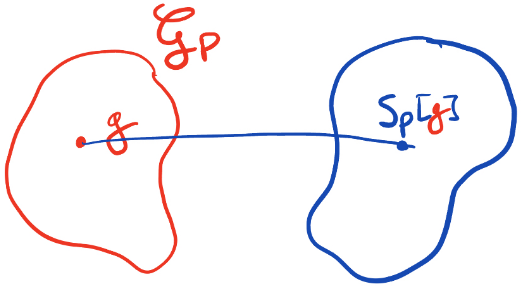

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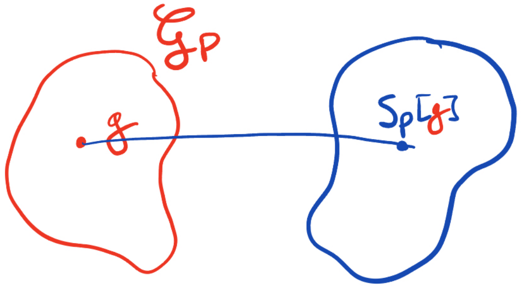

- In other words, you are now **representing** P **with an entire family of functions** with some peculiar property:

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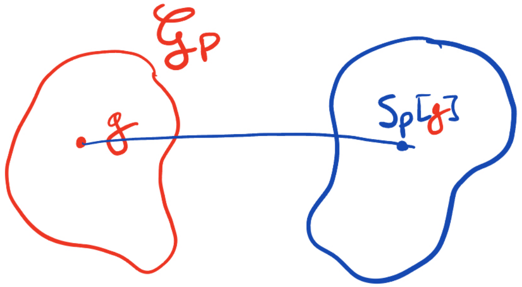

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- (At this point I want to clarify I am not a sadistic mathematician…. We will see why shortly, but first lets see some examples…)

Characterising a $\mathcal{N}(0, \sigma^2)$

- At some point in your BSc/MSc/PhD, you have probably come across the many characterisations of a Gaussian:

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{x^2}{2\sigma^2}\right)$$

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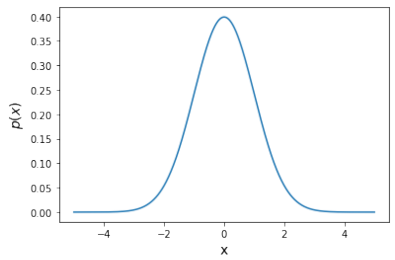
- We will now add a new one…

Stein characterisation for a $\mathcal{N}(0,\sigma^2)$



- Recall the general form of a Stein characterisation as a pair $(\mathcal{S}_P, \mathcal{G}_P)$:

$$Q = \mathcal{N}(0,\sigma^2) \quad \Leftrightarrow \quad \mathbb{E}_{X \sim Q}[\mathcal{S}_P[g](X)] = 0 \quad \forall g \in \mathcal{G}_P$$

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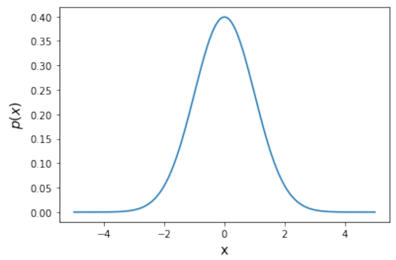

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$$Q = \mathcal{N}(0,\sigma^2) \quad \Leftrightarrow \quad \mathbb{E}_{X \sim Q}[\mathcal{S}_P[g](X)] = 0 \quad \forall g \in \mathcal{G}_P$$

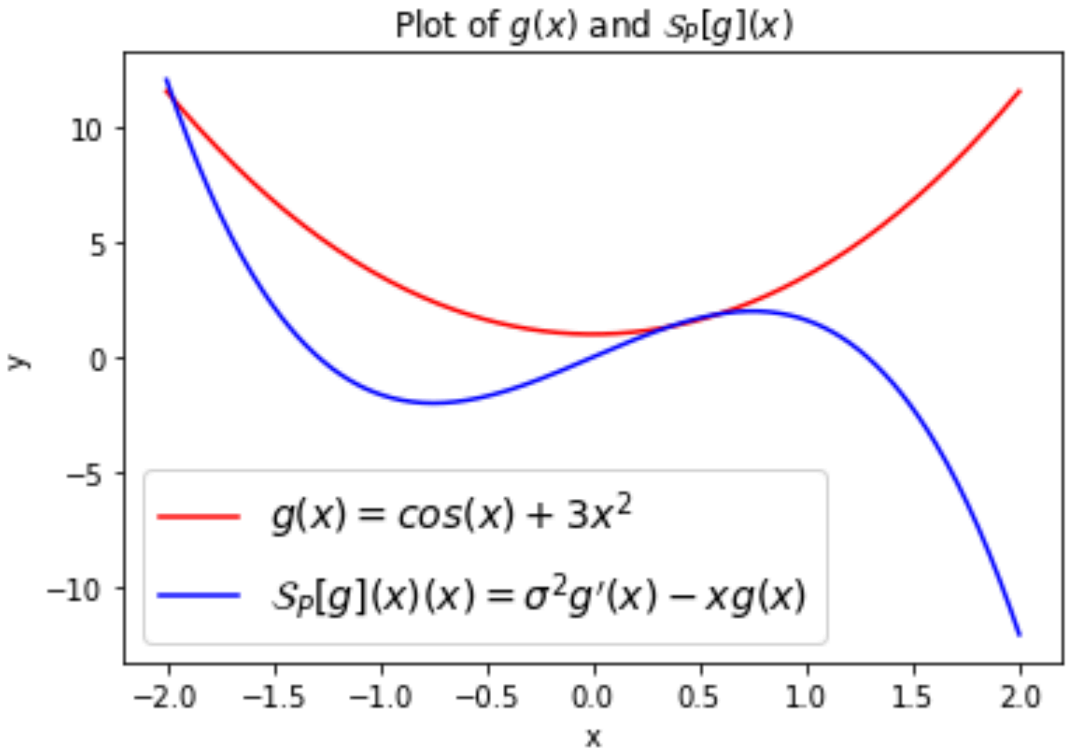
- For $P = \mathcal{N}(0,\sigma^2)$, one such pair is

$$\mathcal{G}_P := \left\{ g : \mathbb{R}^d \to \mathbb{R} \,|\, g \text{ almost diff. \& } \int |g'(x)| p(x) dx < \infty \right\}$$

$$\mathcal{S}_P[g](x) := \sigma^2 g'(x) - x g(x)$$

Illustration for a first function

$$P = \mathcal{N}(0,1)$$



$$\sigma^2 = 1, \quad n = 10^6,$$

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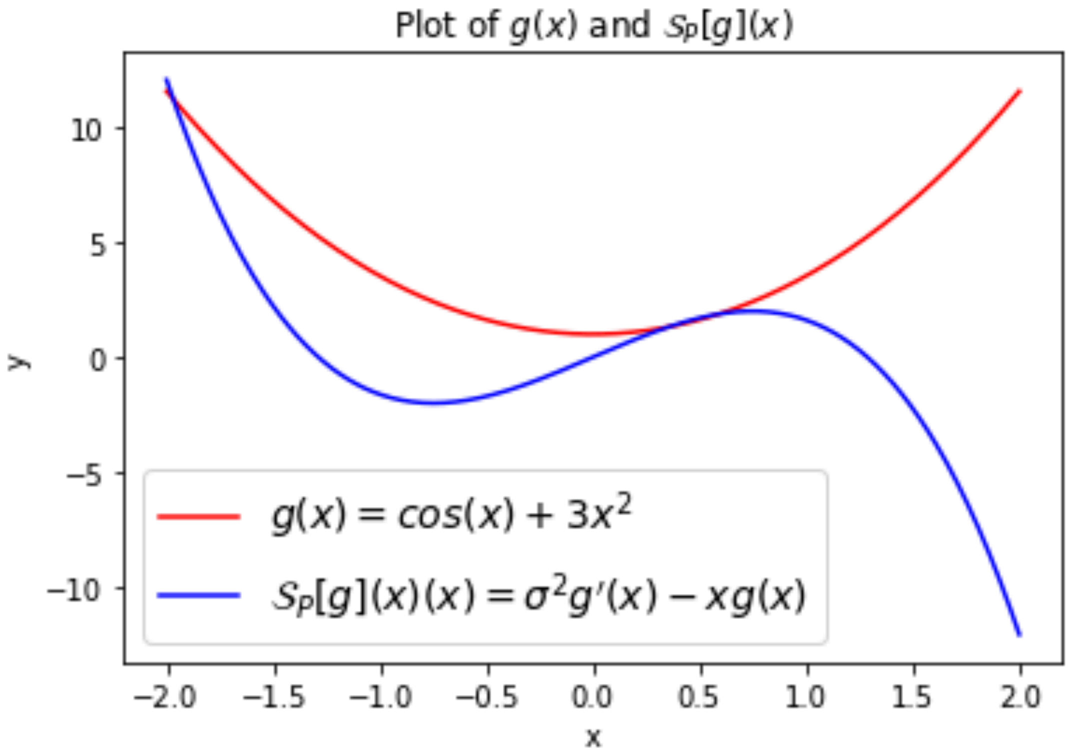

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Arbitrary function in $\mathcal{G}_P$.
Unknown mean…

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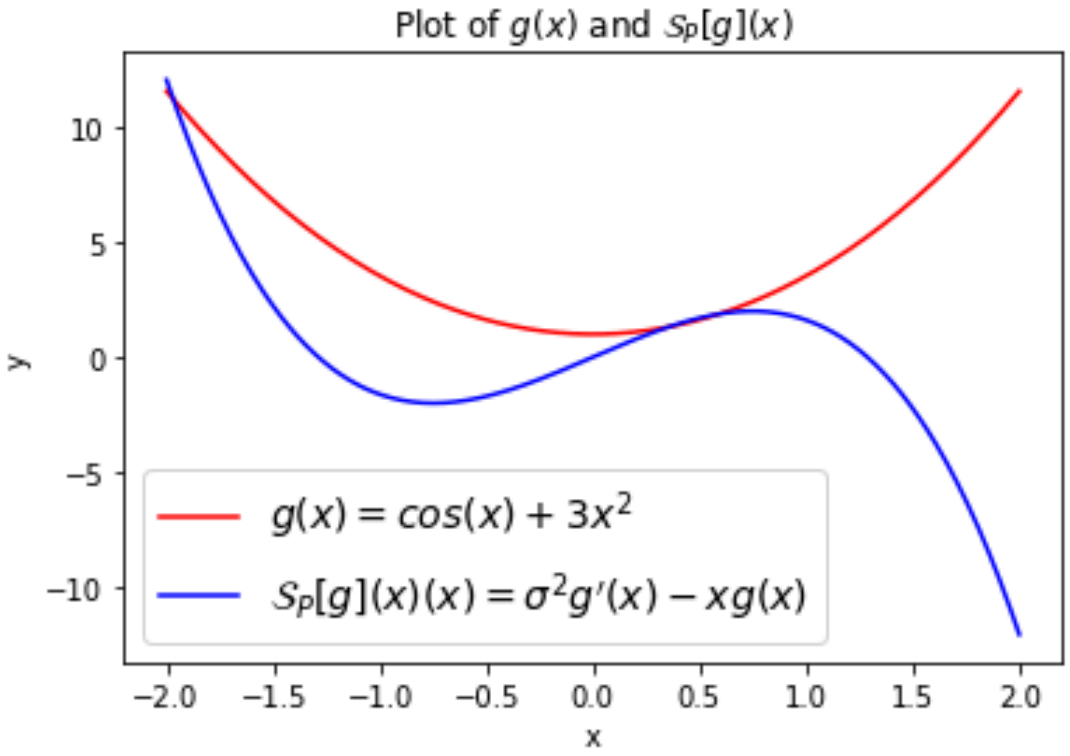

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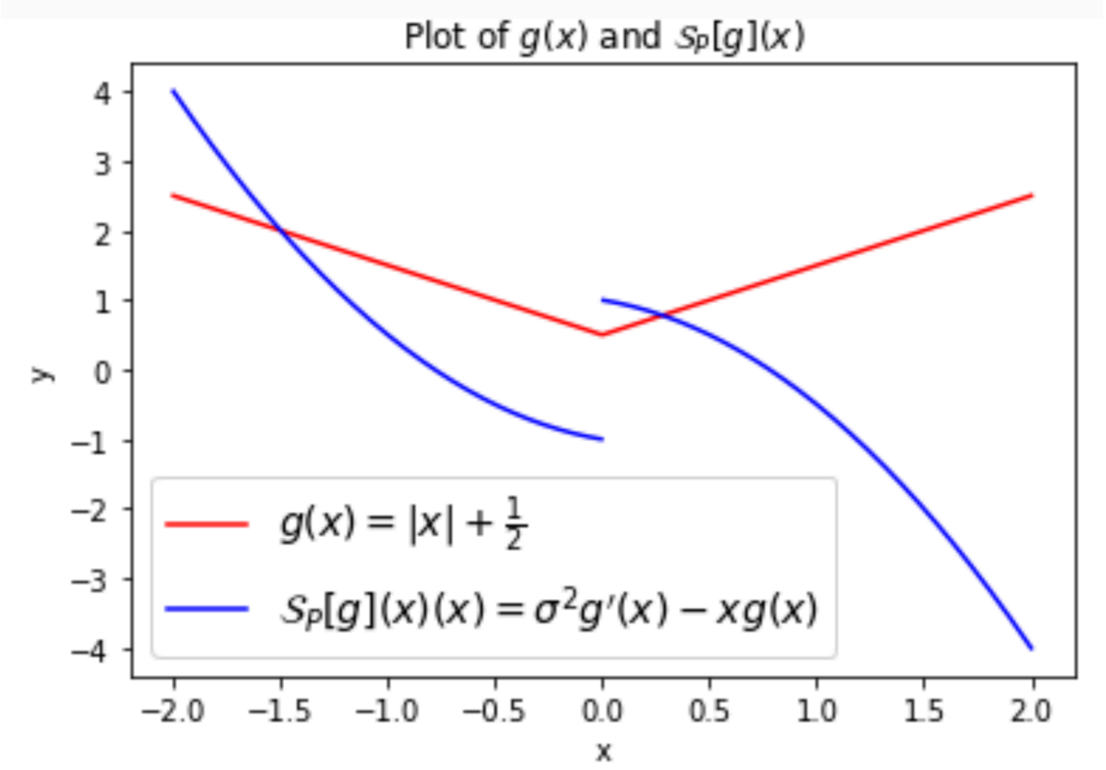
Arbitrary function in $\mathcal{G}_P$.
Unknown mean…

$$\frac{1}{n}\sum_{i=1}^n \mathcal{S}_P[g](x_i) \approx 0.007$$

Mean zero function!

Illustration for a second function

$$P = \mathcal{N}(0,1)$$



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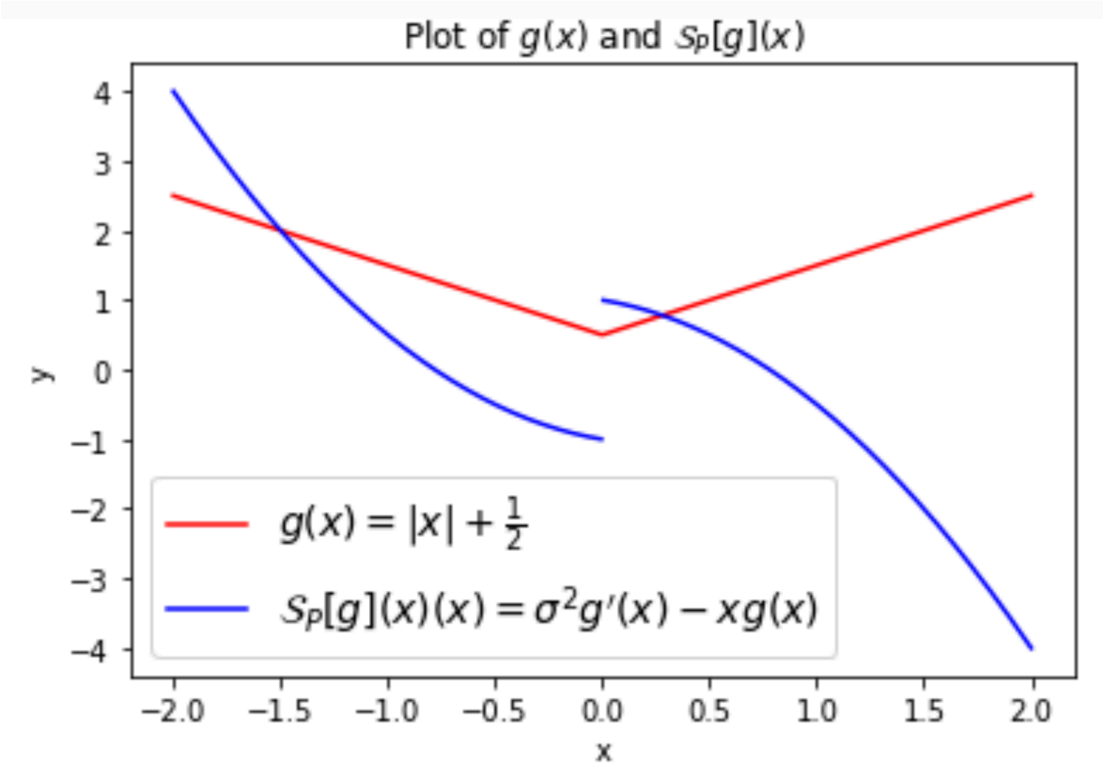

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$$\{x_i\}_{i=1}^n \sim P = \mathcal{N}(0,\sigma^2)$$

$$\frac{1}{n}\sum_{i=1}^n g(x_i) \approx 1.298$$

Arbitrary function in $\mathcal{G}_P$.
Unknown mean…

Illustration for a second function

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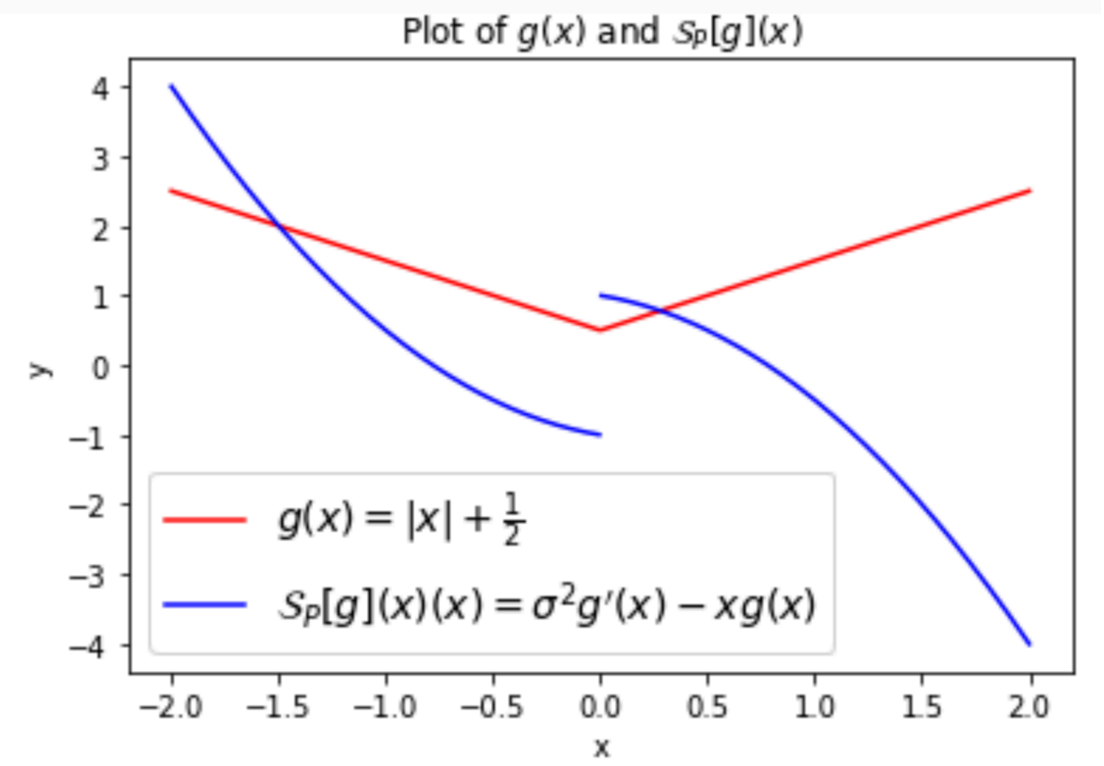

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Arbitrary function in $\mathcal{G}_P$.
Unknown mean…

$$\frac{1}{n}\sum_{i=1}^n \mathcal{S}_P[g](x_i) \approx 0.002$$

Mean zero function!

Illustration for a second function

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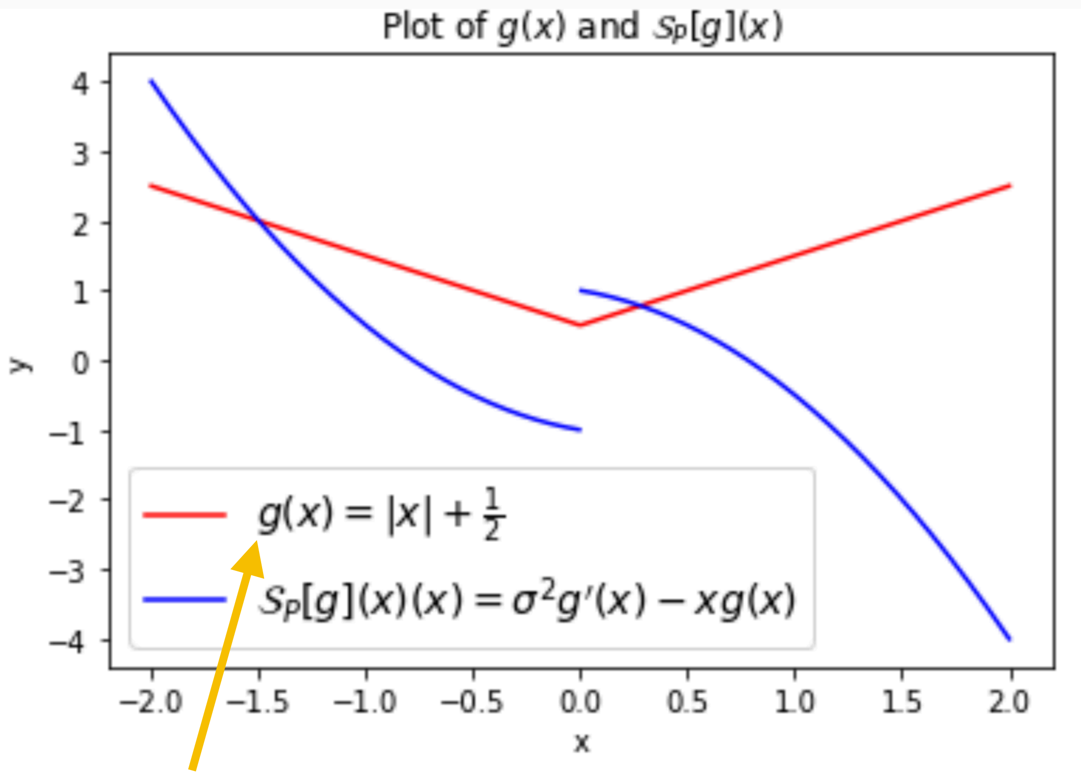

Not differentiable but almost differentiable…
We can make many many functions have mean zero!

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Unknown mean…

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Mean zero function!

Mean zero only against P though!

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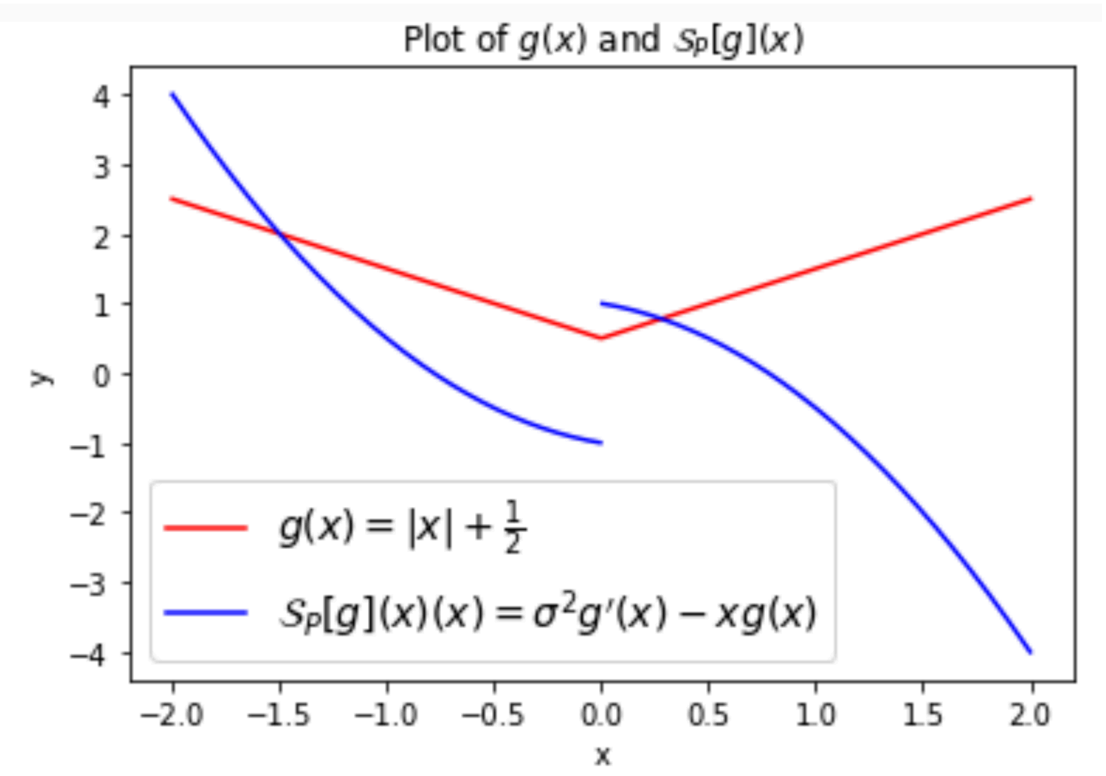

$$\{x_i\}_{i=1}^n \sim Q = \mathcal{N}(1,1) \neq P$$

$$\frac{1}{n}\sum_{i=1}^n \mathcal{S}_P[g](x_i) \boxed{\approx -1.661}$$

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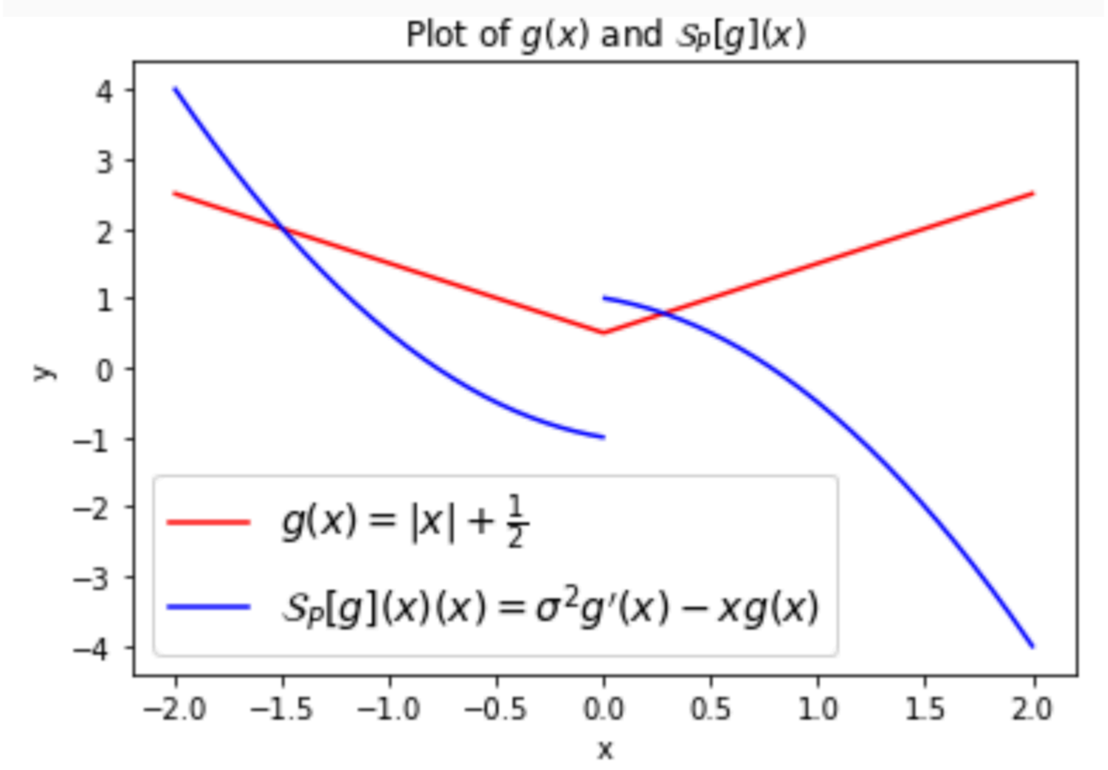

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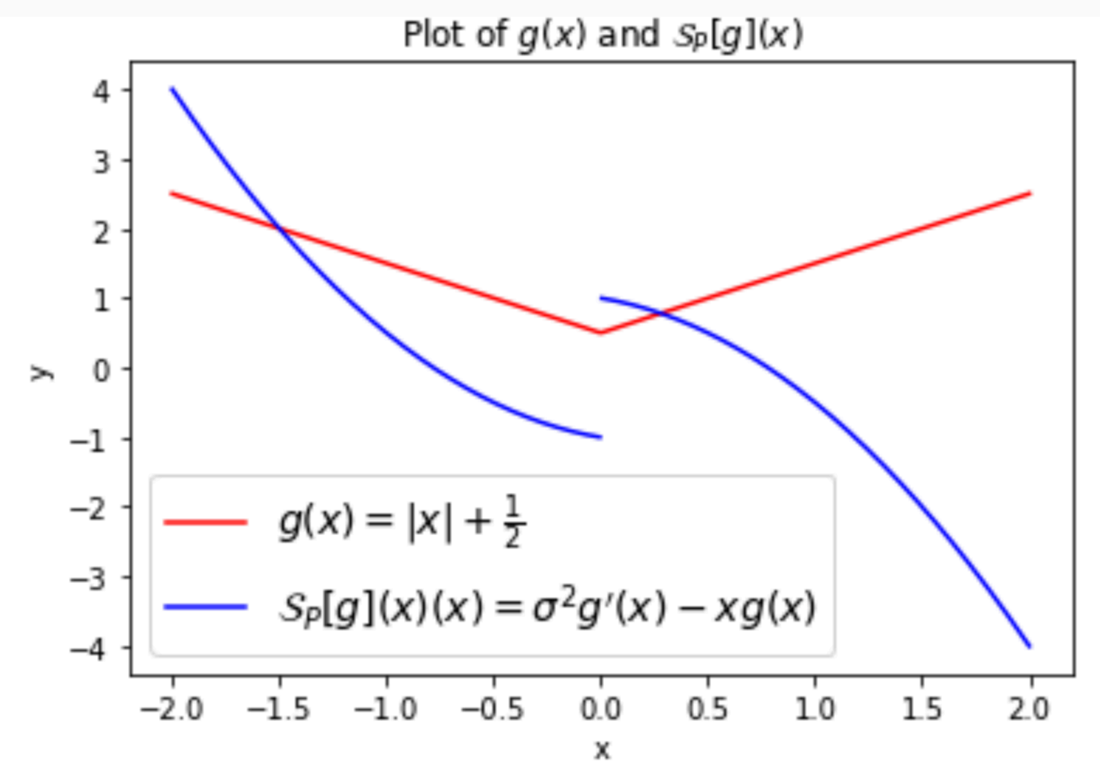

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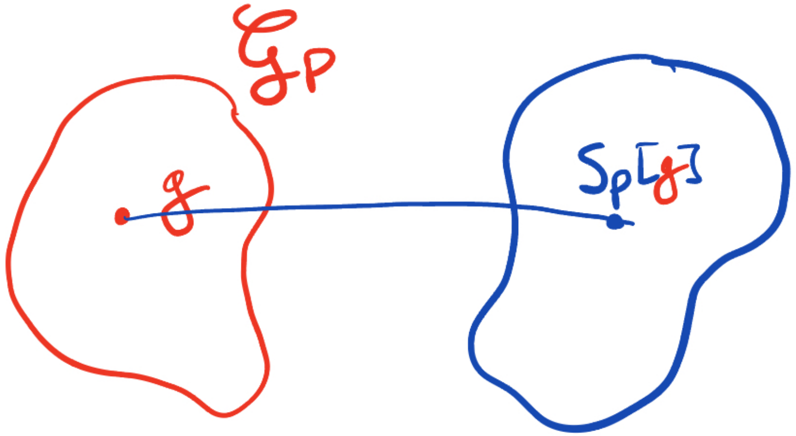
We have a characterisation!

Stein characterisation

- One last time to make sure you remember it, a **Stein characterisation** for P is a pair $(\mathcal{S}_P, \mathcal{G}_P)$ such that

$$Q = P \quad \Leftrightarrow \quad \mathbb{E}_{X \sim Q}[\mathcal{S}_P[g](X)] = 0 \quad \forall g \in \mathcal{G}_P$$



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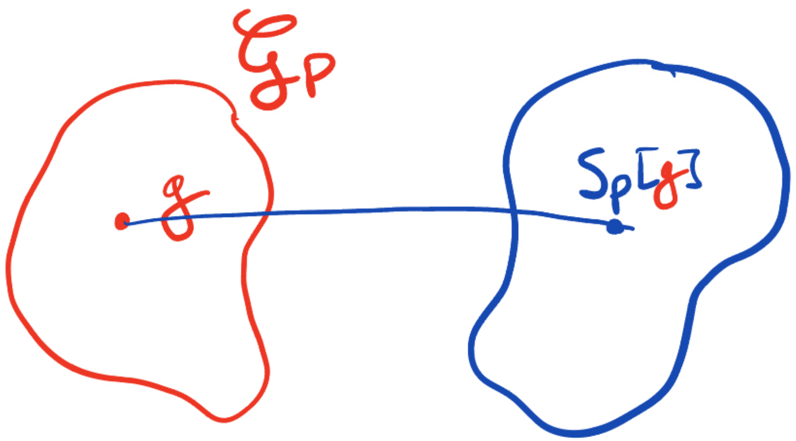
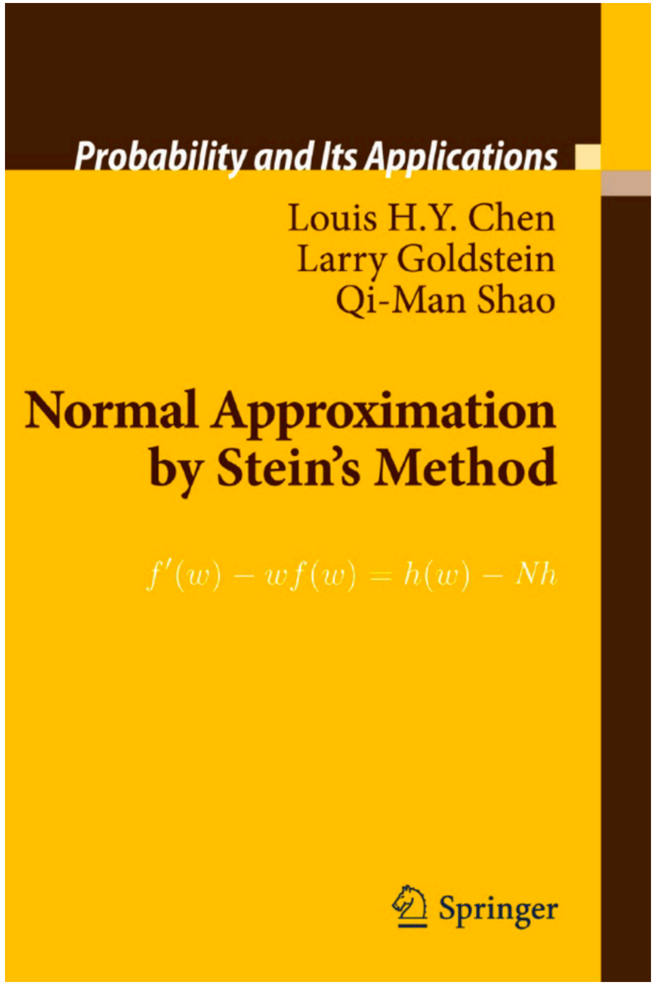
Any questions??



Stein characterisations are not unique!

- Some might be more computationally convenient than others.
- Some might be easier to manipulate…
- This book has 350+ pages on characterising Gaussian distributions in different ways, and how this can help for theory…



Stein characterisations for other distributions

Surveys

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[https://sites.google.com/site/steinsmethod]

Prof. Yvik Swan (ULB)

Stein’s method as a computational tool

Why Stein? Part I: Intractable integrals

Why Stein characterisations?

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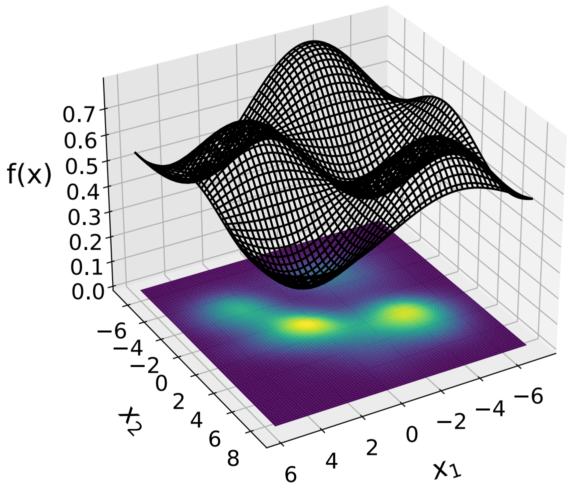
The key point is that **all of these functions have mean zero under a distribution of interest**, which is super useful from a computational viewpoint!

A key challenge in computational statistics

- Let $\mathcal{X} \subseteq \mathbb{R}^d$. One of the main computational challenges encountered in statistics and machine learning is to have to compute:

$$\mathbb{E}_{X \sim P}[f(X)] = \int_{\mathcal{X}} f(x)p(x)dx = ??$$



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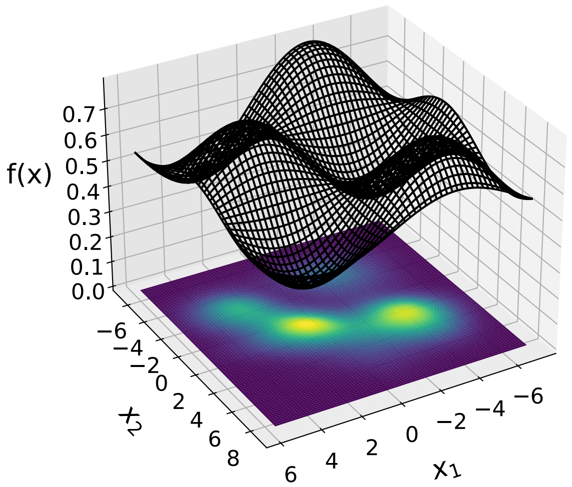

- This is a really **hard problem** when:
  - The problem is high-dimensional (i.e. d is large).
  - The function $f : \mathcal{X} \to \mathbb{R}$ is complicated and/or expensive.
  - The distribution P is complex/multi-modal and/or $p(x)$ cannot be evaluated point wise.

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1. **Marginalisation:** Our likelihood could be based on some unobserved variables (nuisance parameters) which need to be integrated out.

2. **Unnormalised likelihoods:** Sometimes we only have access to a likelihood up to a normalisation constant, which is the integral of the unnormalised part (e.g. graphical models, models on manifolds, deep exponential family models).

Why Stein characterisations: Intractable integrals

- Clearly if we have that f can be written as

$$f(x) = \mathcal{S}_P[g](x) + C \quad \text{for some } \mathcal{S}_P, g \in \mathcal{G}_P, C \in \mathbb{R}$$

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- The flexibility in $\mathcal{S}_P, g, C$ makes this not too unlikely!
- A key trick is therefore to replace our intractable integrals with integrals that we can compute exactly.

Stein’s method as a computational tool

Why Stein? Part II: Intractable densities

Why Stein characterisations: Complex probability distributions

- Our first motivation for Stein characterisations was for calculating intractable integrals.
- But equally important is the case where our distribution is not very tractable in the sense that we only know its unnormalised density:

$$p(x) = \frac{\tilde{p}(x)}{C}$$

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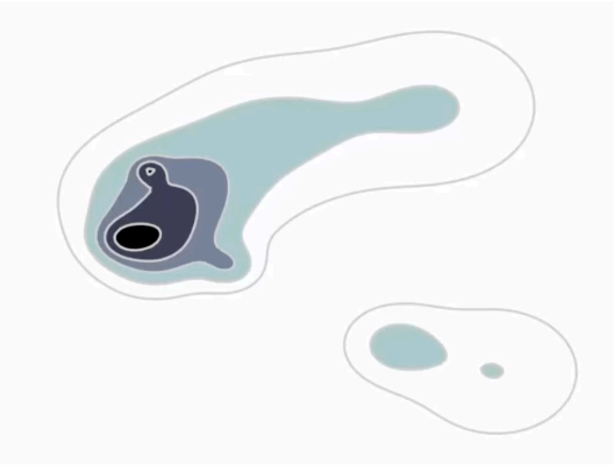

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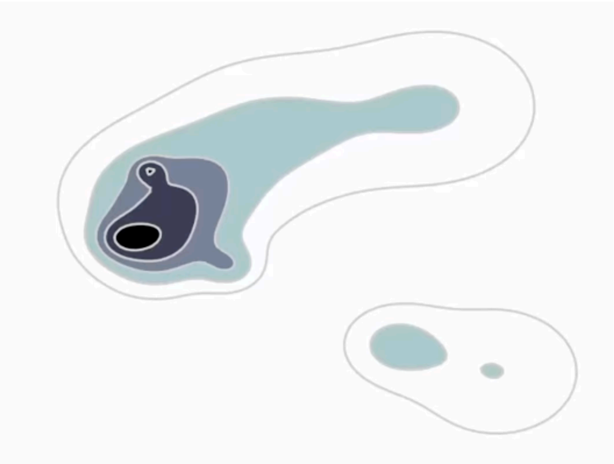

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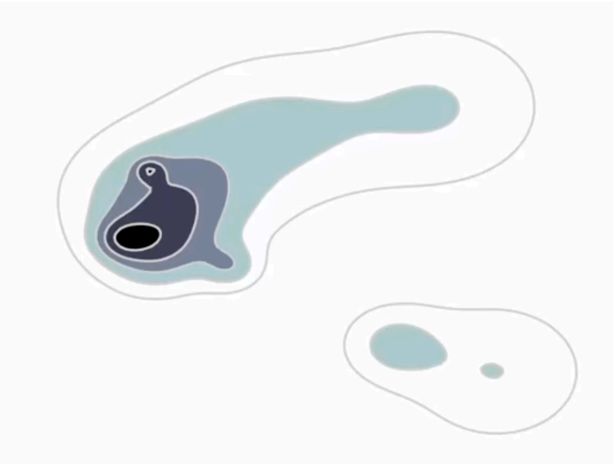

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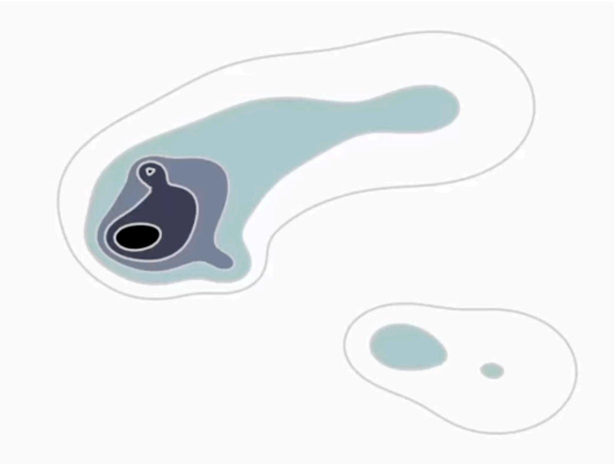

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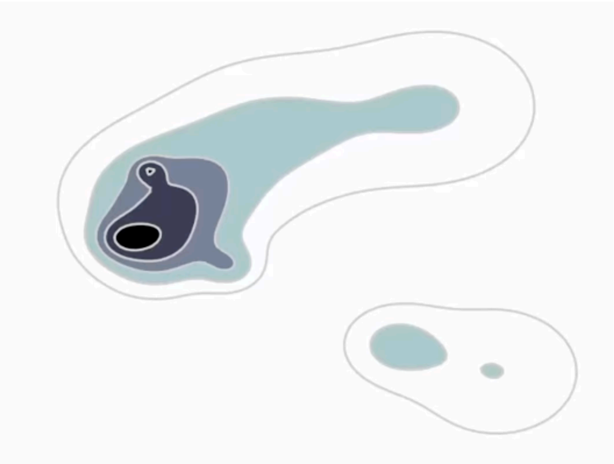

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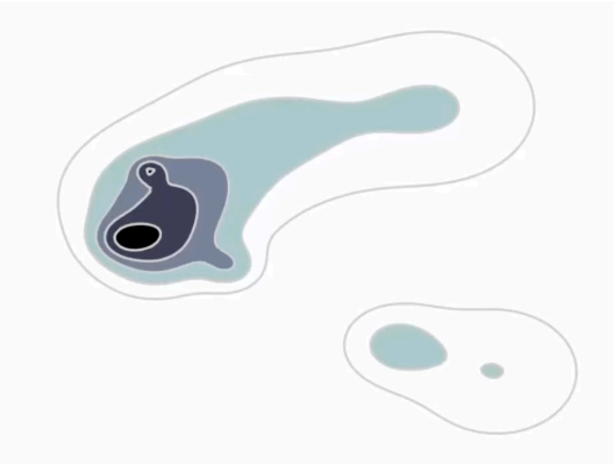

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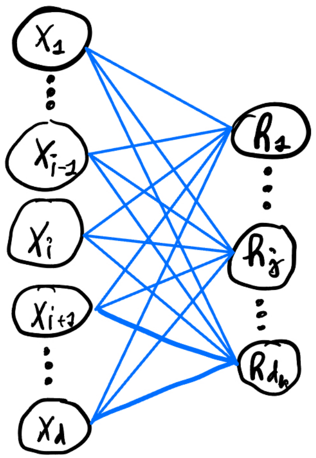

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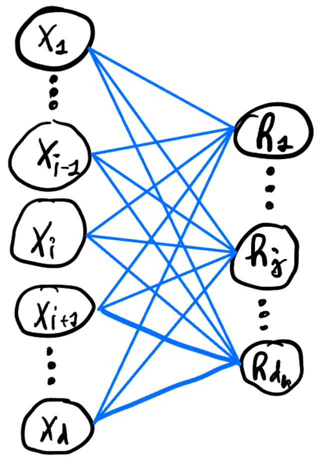

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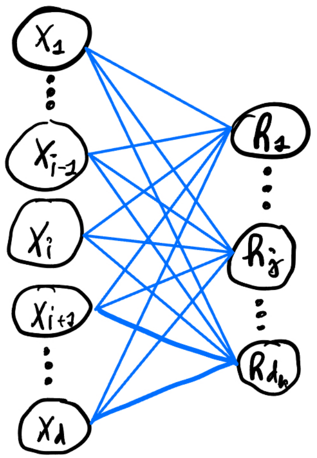

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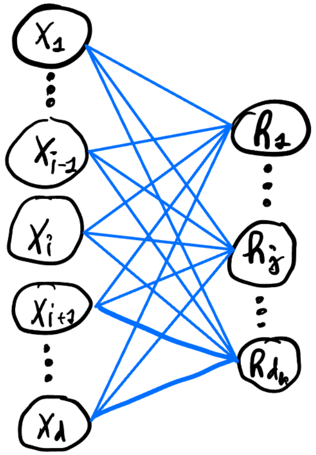

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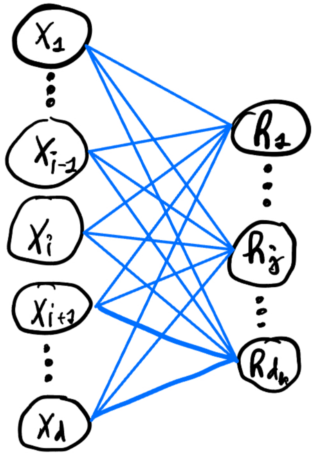

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Thankfully, this is another case where Stein characterisations shine!

The main reason is that $\mathcal{S}_P$ and $\mathcal{G}_P$ can be obtained without knowledge of normalisation constants (more on this shortly).

Stein’s method as a computational tool

The generator approach to Stein operators

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- Since this is hard, we will just follow what serious mathematicians have previously proposed…

The Langevin Stein operator

- Suppose g is a (sufficiently regular) vector-valued function $g : \mathbb{R}^d \to \mathbb{R}^d$. The **Langevin Stein operator** is given by:

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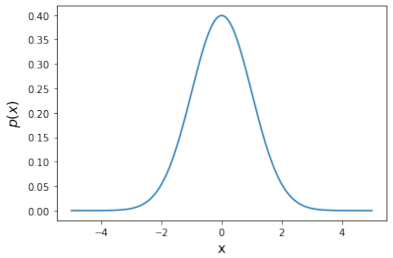
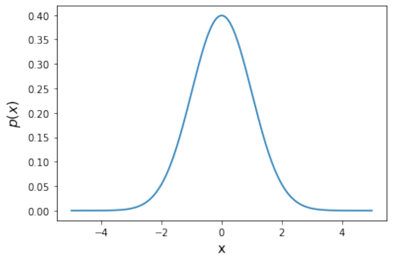
Recovering our operator for $N(0,\sigma^2)$



- Take $d = 1$ and $p(x) = \dfrac{1}{\sqrt{2\pi\sigma}} \exp\left(-\dfrac{x^2}{2\sigma^2}\right)$

Recovering our operator for $N(0,\sigma^2)$



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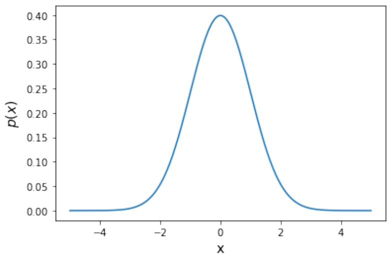

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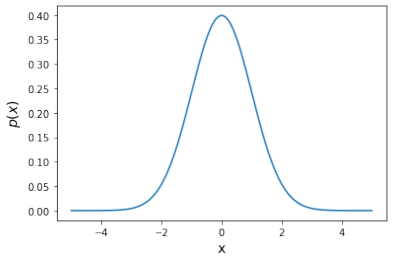

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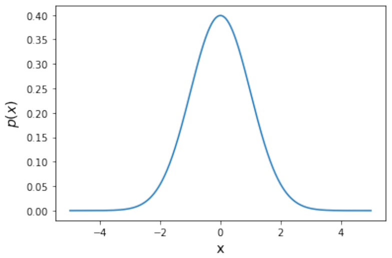

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→ i.e. $\mathcal{S}_P[g](x) = \sigma^2 \mathcal{T}[g](x)$!!

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Intractable!

$$= \nabla_x \log \tilde{p}(x) - \nabla_x \log C \quad = \boxed{\nabla_x \log \tilde{p}(x)}$$

Tractable!!

Operators based on the score

- The Langevin operator is therefore ideal for unnormalised densities:

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- It is however not the only Stein operator based on score functions (recall that Stein characterisations are not unique!).

The generator approach

Prof. A. Barbour
(U. Zurich)

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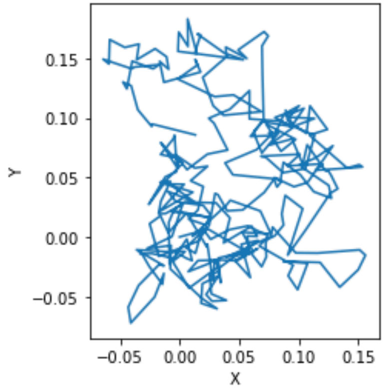

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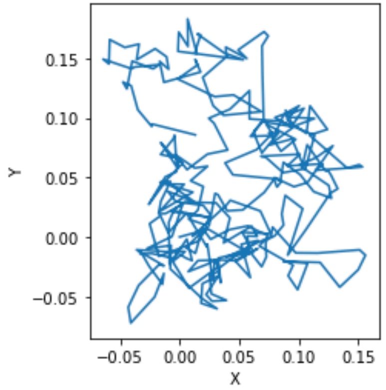

- One representation of a Markov chain is through its infinitesimal generator.

→ Infinitesimal generator = Stein operator

The diffusion Stein operator

- Suppose g is a (sufficiently regular) vector-valued function $g : \mathbb{R}^d \to \mathbb{R}^d$ and m is a (nice) matrix-valued function $m : \mathbb{R}^d \to \mathbb{R}^{d\times d}$. The **diffusion Stein operator** is given by:

$$\mathcal{T}_{\text{diff}}[g](x) := \langle m(x)^\top \nabla_x \log p(x), g(x)\rangle + \langle \nabla, m(x)g(x)\rangle$$

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- We recover the Langevin Stein operator when $m(x) = I_d$:

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- What should we do with our new tool?

Outline (updated)

- What is Stein's method, and why should you care…
- Computational tools based on Stein's method.
- Some nice (new) algorithms!

Stein’s method as a computational tool

Stein discrepancies

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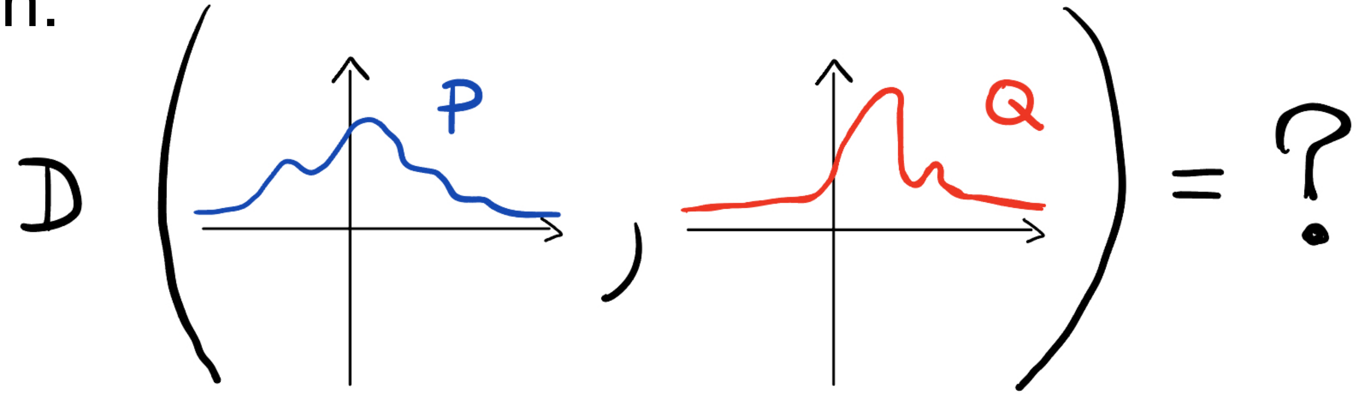

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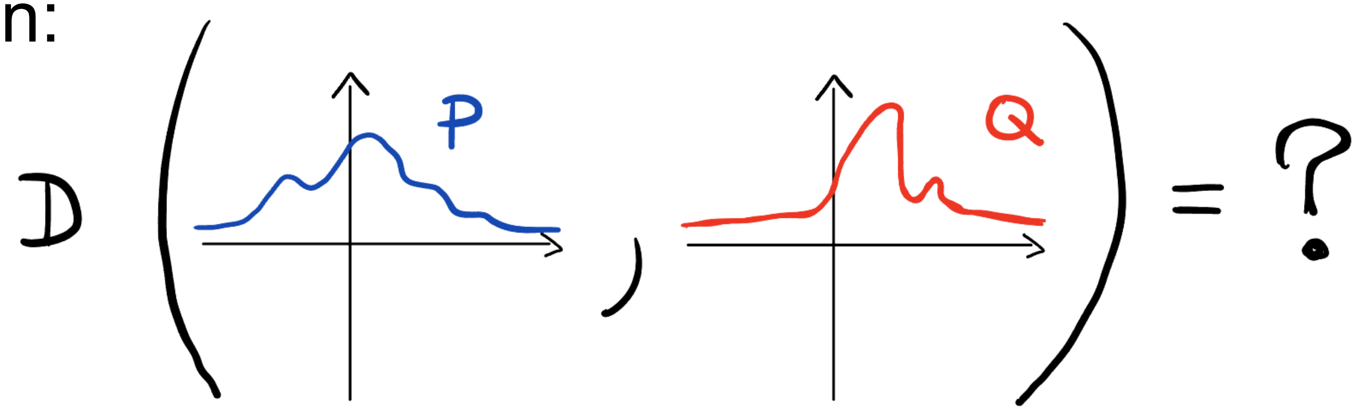
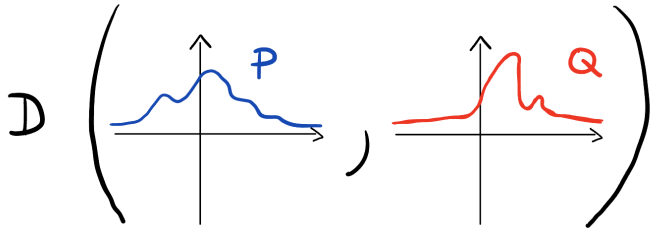


- One limitation of most existing discrepancies is stats/ML is that they are **not computable** for complex P, Q.

Integral probability metrics



- A very popular class of discrepancies in statistics and ML are **integral probability metrics (IPMs)**:

$$D(P, Q) = \sup_{h \in \mathcal{H}} |\, \mathbb{E}_{X \sim P}[h(X)] - \mathbb{E}_{X \sim Q}[h(X)] \,|$$

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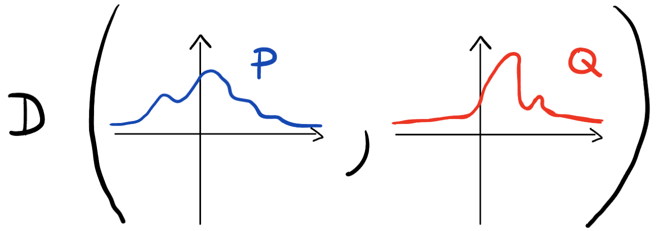

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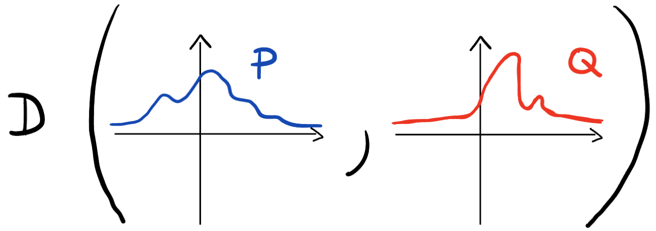

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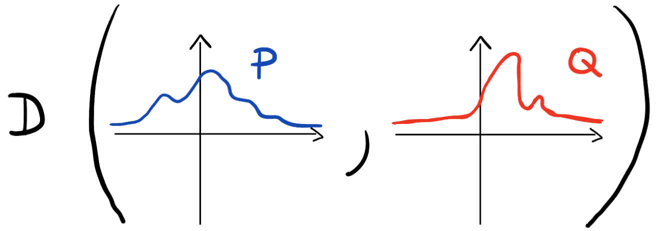

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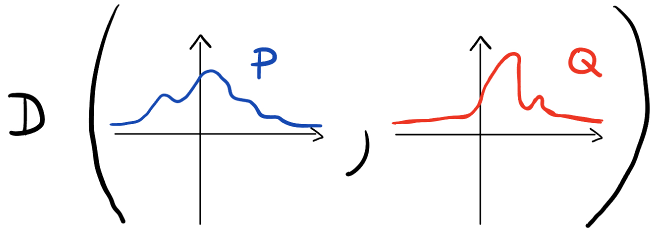

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Hard to compute!

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We use our key property that our functions integrate to zero under P

Stein discrepancy

- A **Stein discrepancy (SD)** is a measure of dissimilarity between P and Q:

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If we find that at least one $g \in \mathcal{G}$ such that $\mathbb{E}_{X \sim Q}[\mathcal{S}_P[g](X)] \neq 0$, then we know $Q \neq P$!

Stein discrepancy

$$\mathrm{SD}(P||Q) = \sup_{g \in \mathcal{G}} |\mathbb{E}_{X \sim Q}[\mathcal{S}_P[g](X)]|$$

- **Question 1:** What properties does this measure of dissimilarity have?
- **Question 2:** When can we actually compute this?
- **Question 3:** What can we use this measure of dissimilarity for?

Q1: What properties does this have?

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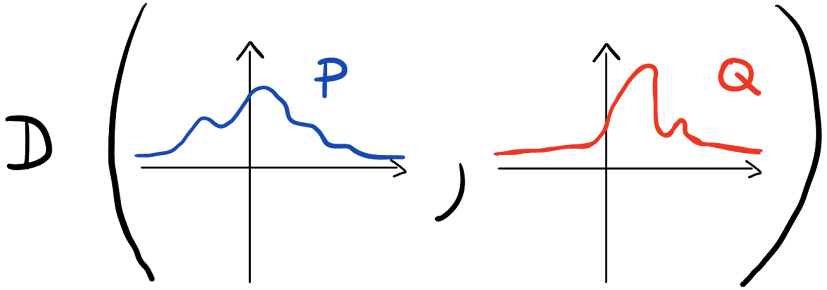
- The magnitude of $\mathrm{SD}(P\,||\,Q)$ tells us something about how far Q is from P.

Q2: When can we compute it?

$$\mathrm{SD}(P\,||\,Q) = \sup_{g \in \mathcal{G}} |\mathbb{E}_{X\sim Q}[\mathcal{S}_P[g](X)]|$$



= ??

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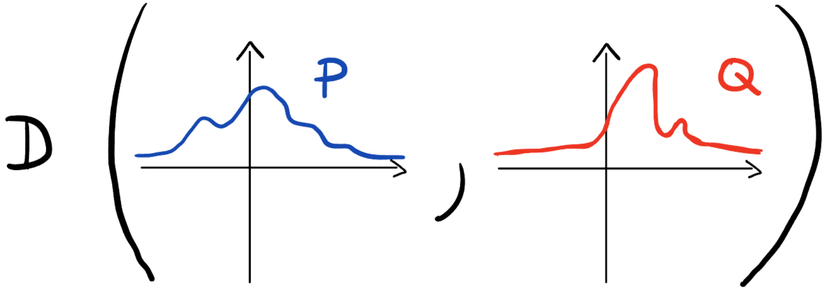

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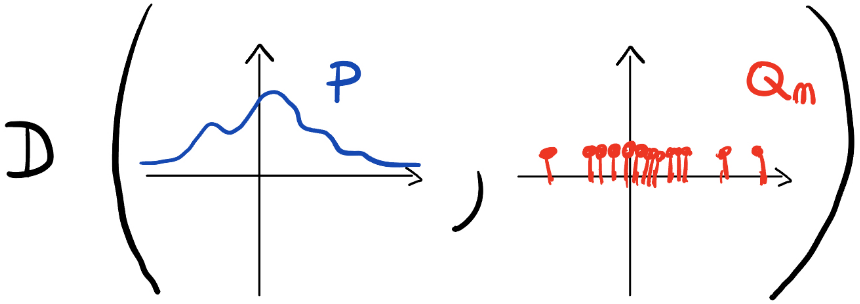

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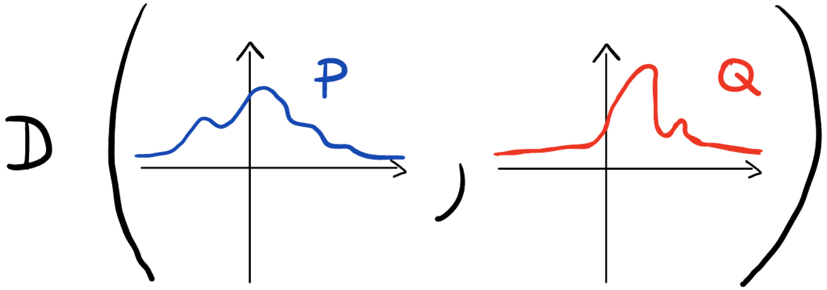

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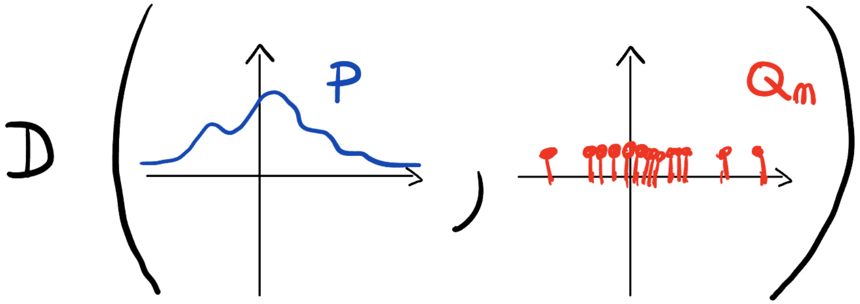

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Answer 1: Compare to an empirical measure/dataset! $Q_n = \frac{1}{n}\sum_{i=1}^{n} \delta_{x_i}$

Q2: When can we compute it?

$$\text{SD}\left(P \,\middle|\middle|\, \frac{1}{n}\sum_{i=1}^{n}\delta_{x_i}\right) = \sup_{g\in\mathcal{G}}\left|\frac{1}{n}\sum_{i=1}^{n}\mathcal{S}_P[g](X)\right|$$

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Goal: Choose $\mathcal{G}$ the largest possible such that SD is still tractable!

Example: SD for $N(0,\sigma^2)$

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The Stein class of almost differentiable functions is way too large for us to be able to find this supremum. Not so helpful as a computational tool….

Example 1: Graph-Stein discrepancies

$$\mathrm{GSD}(P \,||\, Q) = \sup_{g \in \mathcal{G}} \left\| \mathbb{E}_{X \sim P}[\mathcal{S}_P[g](X)] \right\|$$

$$\mathcal{G} = \left\{ g : \max \left(\|g(v)\|_\infty, \|\nabla g(v)\|_\infty, \frac{\|g(x) - g(y)\|_\infty}{\|x - y\|_1}, \frac{\|\nabla g(x) - \nabla g(y)\|_\infty}{\|x - y\|_1} \right) \leq 1, \right.$$
$$\left. \frac{\|g(x) - g(y) - \nabla g(x)(x-y)\|_\infty}{\frac{1}{2}\|x - y\|_1^2} \leq 1, \frac{\|g(x) - g(y) - \nabla g(y)(x-y)\|_\infty}{\frac{1}{2}\|x - y\|_1^2} \leq 1, \quad \forall x, y \in E, v \in \{x_i\}_{i=1}^n \right\}$$

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The class is small enough that we can find the maximum through linear programming!

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Example 2: Hyvarinen divergence

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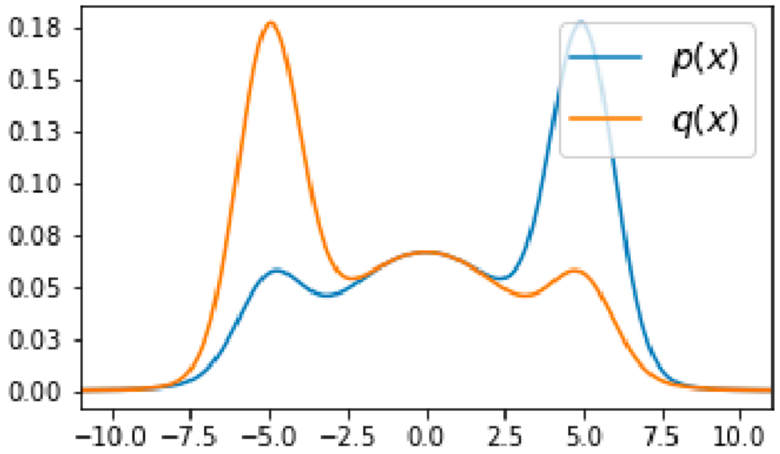

Cannot use this as we typically don't know the densities exactly….

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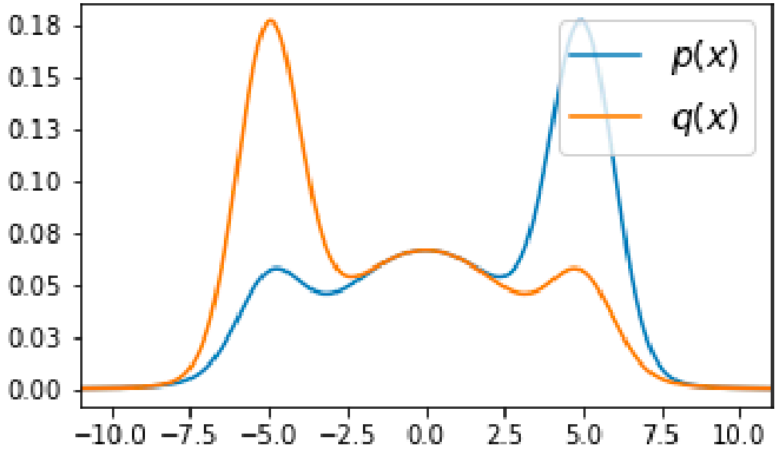

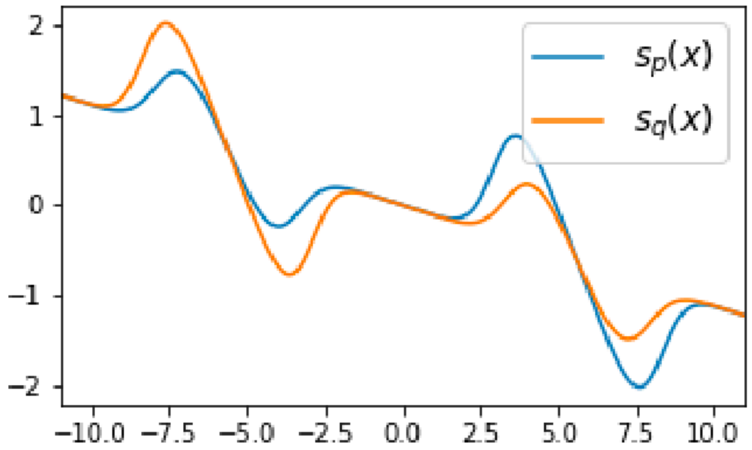

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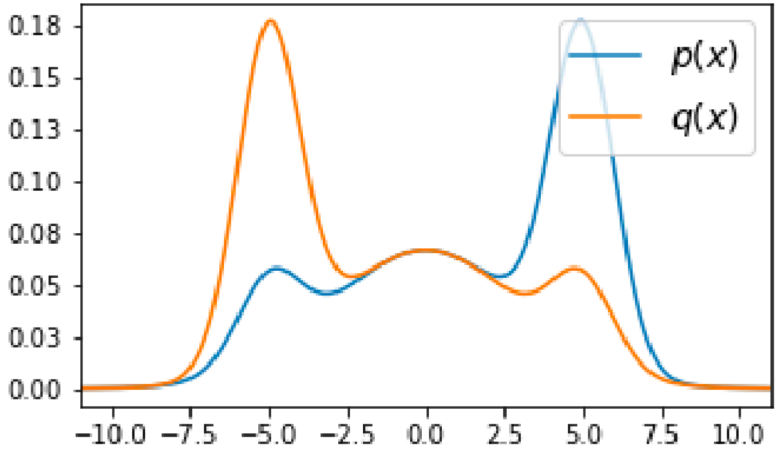

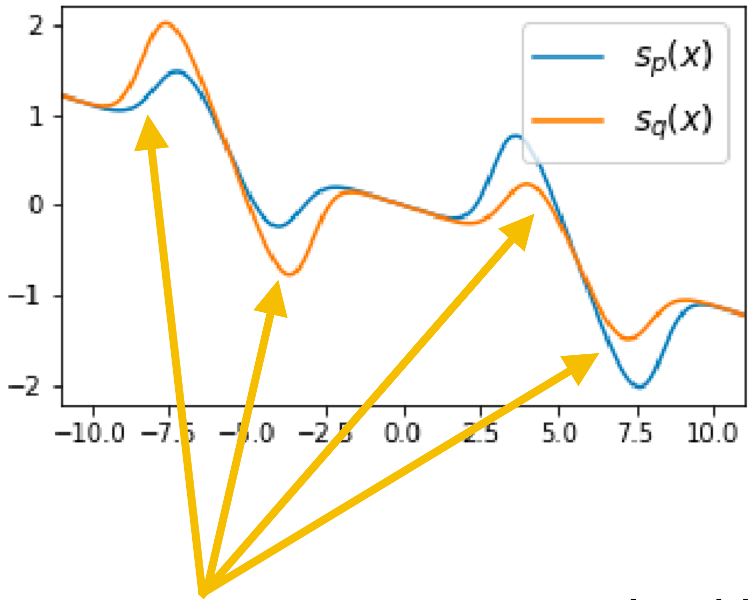

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- Sadly we usually do not have access to $\nabla \log q$ in most applications (typically Q is some unknown data-generating process).

- The only type of application where this can be used is for parameter estimation/generative modelling, since we can typically still evaluate the divergence up to some additive constant.

More on this shortly….

Example 3: Kernel Stein discrepancies

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$$\mathcal{G} = \left\{ g = (g_1, \ldots, g_d) \in \mathcal{H}_k : \|v\|_2 \leq 1 \text{ where } v_i = \|g_i\|_{\mathcal{H}_k} \right\}$$

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→ The most practical class as it can be evaluated in closed-form!

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Stein’s method as a computational tool

Kernel Stein discrepancies

Reproducing kernels

- A reproducing kernel is any symmetric and positive-semidefinite function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$.

   1. Symmetric means that for any $x, x' \in \mathcal{X}$, $k(x, x') = k(x', x)$.

   2. Positive semi-definite means that for any $x_1, \ldots, x_n$ and $n \in \mathbb{N}$, the Gram matrix $K \in \mathbb{R}^{n \times n}$ (where $K_{ij} = k(x_i, x_j)$) must be positive semidefinite.

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One way to think about kernel is as measuring the similarity between points!

Examples of kernels

- **Example 1:** Squared exponential (or Gaussian) kernel:

$$k(x, x') = \lambda \exp\left(-\frac{\|x - x'\|_2^2}{l}\right)$$

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- **Example 3:** Polynomial kernel

$$k(x, x') = \lambda(c + x^\top x')^p$$

Properties of kernels

- Many of the kernels we have seen so far only depend on x, x' through $||x - x'||$. They are therefore called **translation invariant.**

- They also all take the following form for some bounded $\phi : \mathcal{X} \to \mathbb{R}_+$, making them **radial**
$$k(x, x') = \lambda^2 \phi \left(-\frac{||x - x'||_2}{l^2} \right)$$

- All of these kernels are bounded, which is a super helpful property for most of what we will do.

Kernel hyperparameters

- The parameter λ is called the **amplitude,** whilst the parameter l is called the **lengthscale.**

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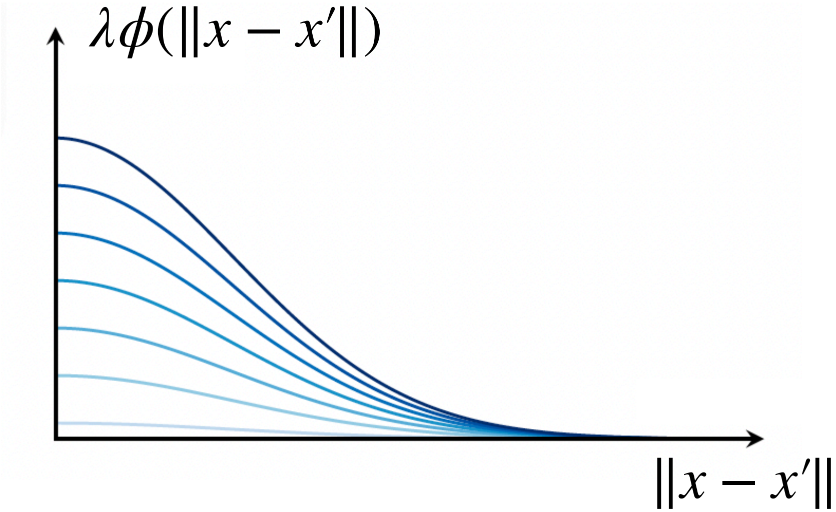
Varying amplitude parameter



[Garnett, 2023]

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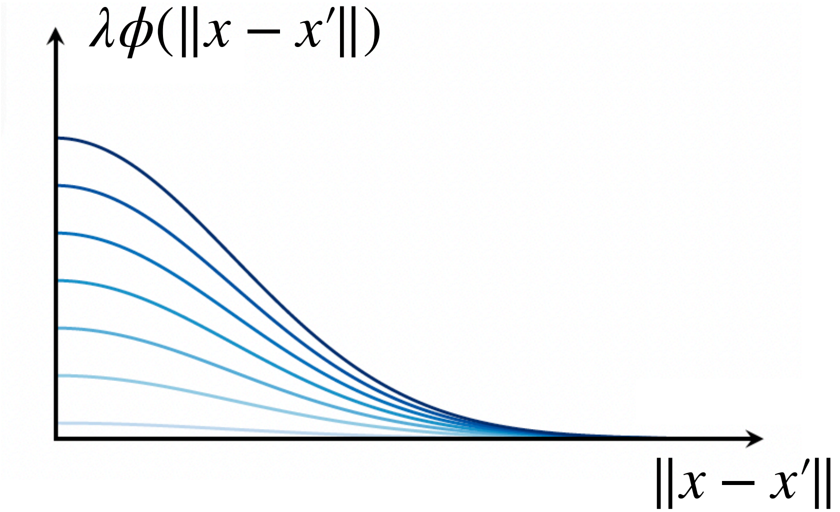
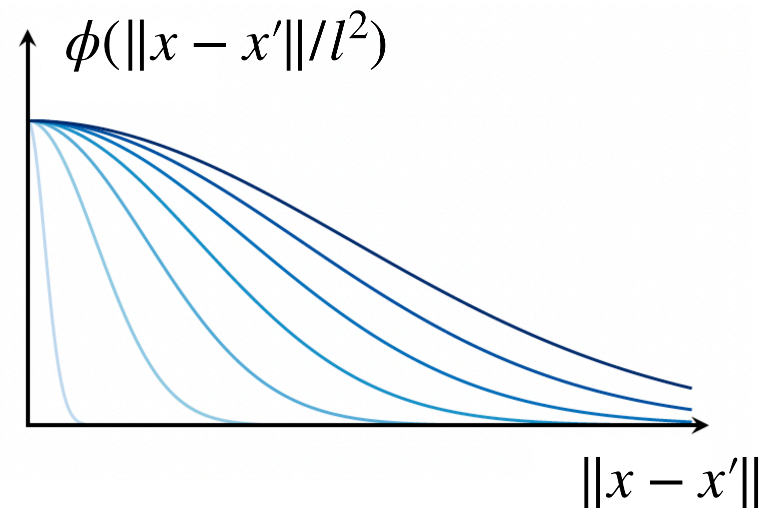


Varying lengthscale parameter



[Garnett, 2023]

Reproducing kernel Hilbert Spaces

- Let $\mathscr{H}_k$ be a Hilbert space of functions from $\mathscr{X}$ to $\mathbb{R}$ (i.e. a complete inner-product space).
- We say that $\mathscr{H}_k$ is an RKHS if and only if it has a reproducing kernel; ie. a kernel which satisfies:
    - $\forall x \in \mathscr{X}, k(\cdot, x) \in \mathscr{H}_k$
    - $\forall x \in \mathscr{X}, \forall f \in \mathscr{H}_k, \langle f, k(\cdot, x) \rangle_{\mathscr{H}_k} = f(x)$

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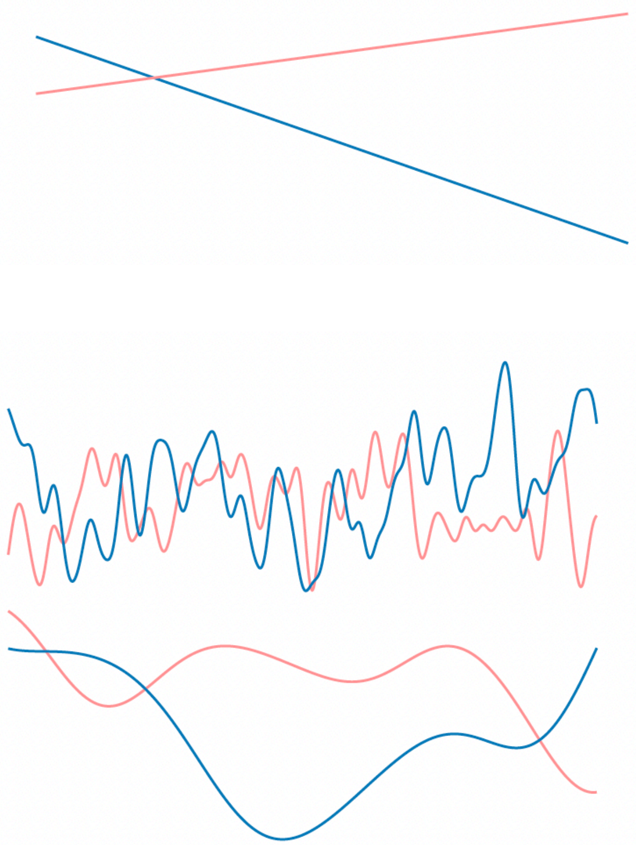
- **Intuition (not fully rigorous):** I like to think of RKHS functions as functions of the form:

$$f(x) = \sum_{i=1}^{n} w_i k(x, x_i)$$

Examples of RKHS

[Garnett, 2023]



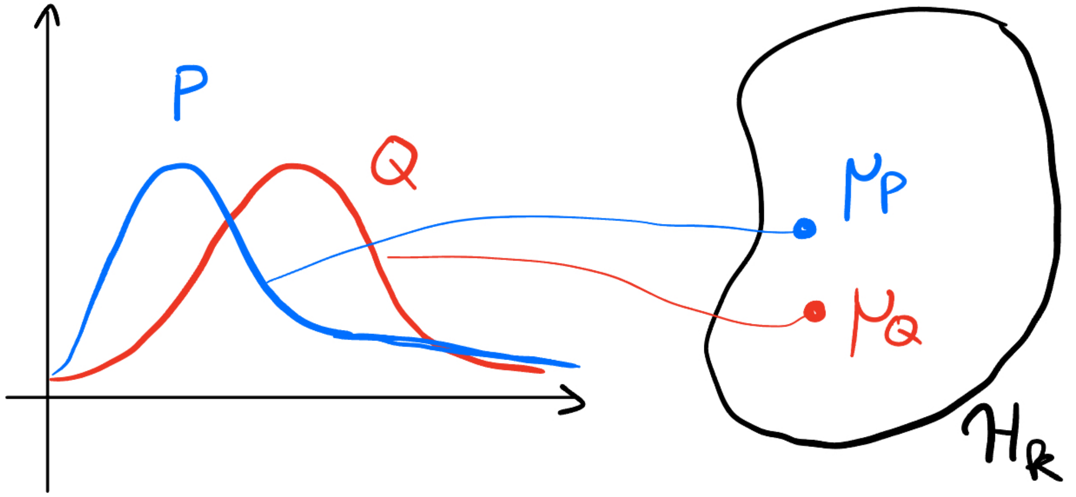
- **Example 1:** If we take an order-1 polynomial kernel, the RKHS is simply the space of straight lines!

- **Example 2:** If we take a Gaussian or inverse-multi quadric kernel, the RKHS is a space of infinitely smooth function!

Kernel mean embeddings

- Due to its nice properties, we may **want to represent probability distributions as functions** in an RKHS.
- This is achieved through the kernel mean embedding:

$$\mu_P(x) = \int k(x,y)p(y)dy$$



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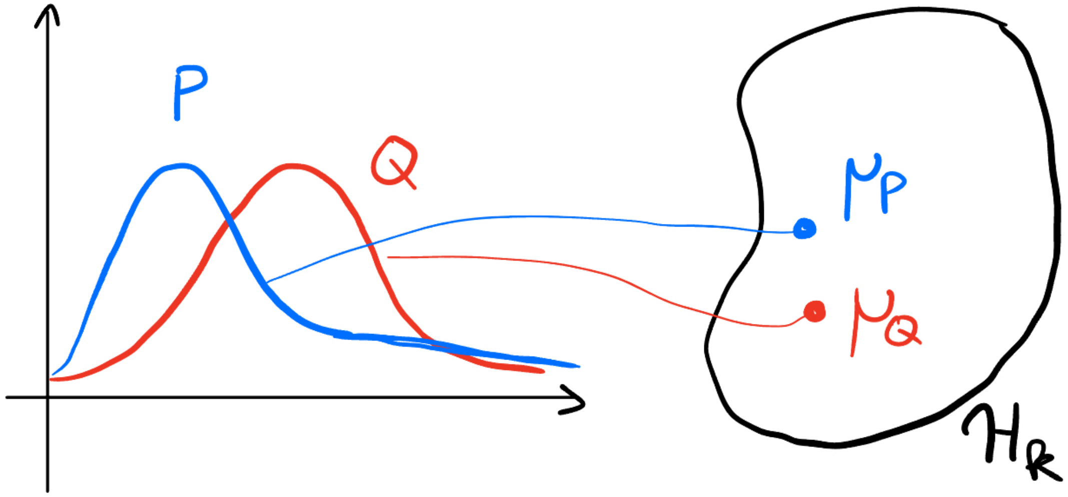
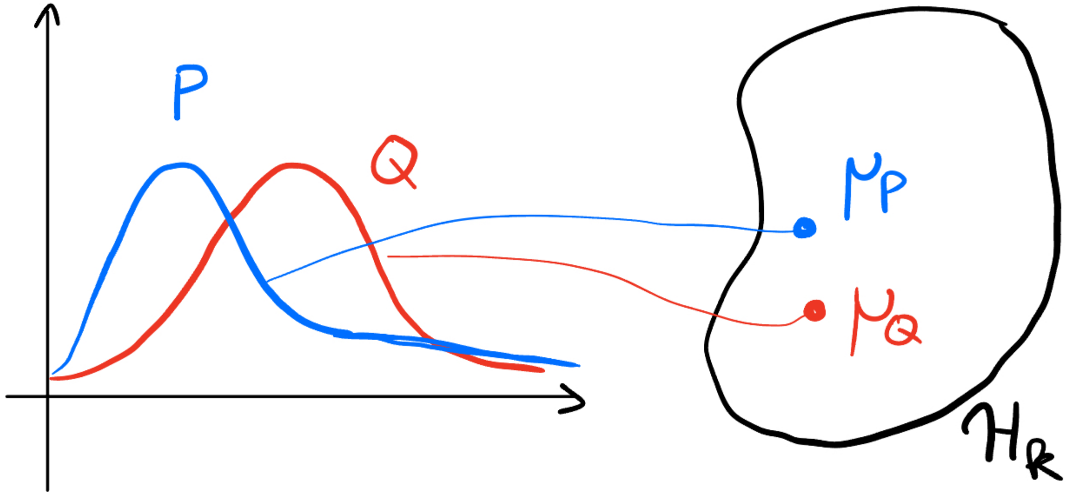


→ Working with functions is a lot easier than working with distributions… This is another convenient characterisation!!

Maximum mean discrepancy

- For example, we can just compare two distributions based on the distance between their kernel mean embeddings.
- This is called the **maximum mean discrepancy (MMD)**!

$$\text{MMD}(P\,||\,Q) = \|\mu_P - \mu_Q\|_{\mathscr{H}_k}$$



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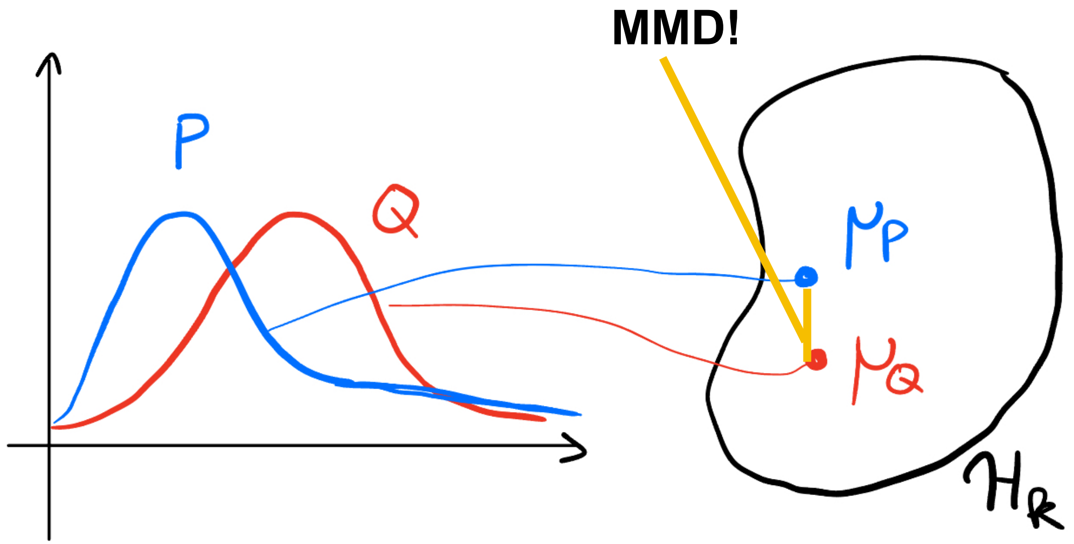

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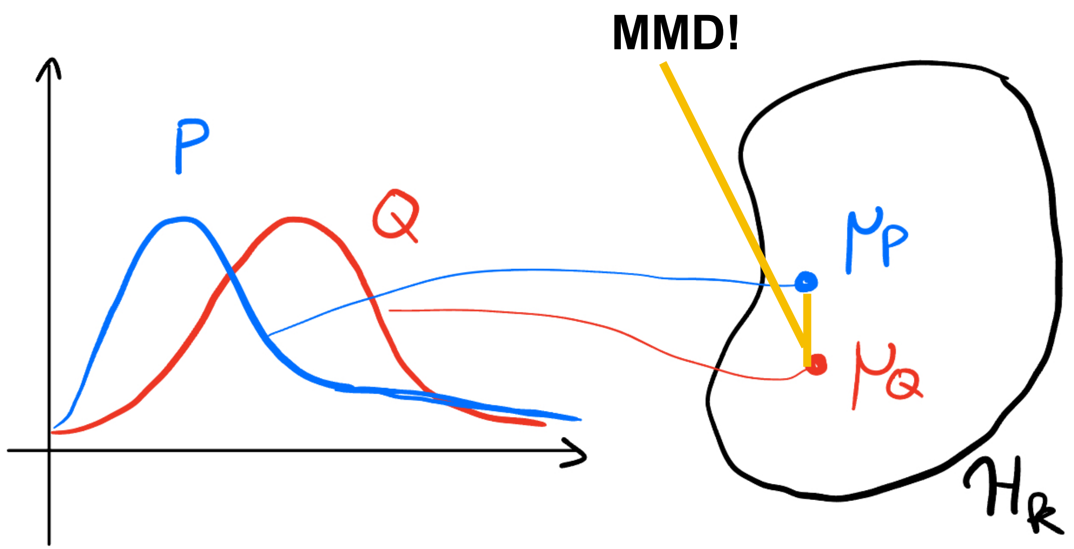

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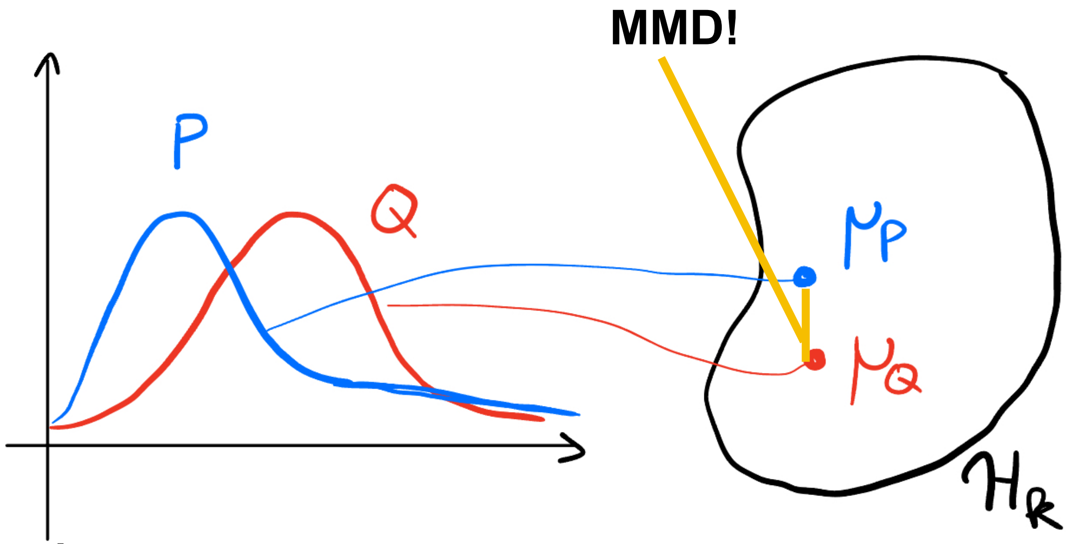

- This is actually an integral probability metric based on all functions of a fixed size in this RKHS!
- Of course we often can't compute the kernel mean embedding since it is an integral…

Stein RKHS

- We can use our favourite tool to make these embeddings tractable!
- Consider $g(x) = (g_1(x), \ldots, g_d(x))$ where each $g_i(x) \in \mathcal{H}_k$. Then:

$$h(x) = \mathcal{S}_P[g](x) \in \mathcal{H}_{k_p}$$

  where k_p is another reproducing kernel.

- All the functions in $\mathcal{H}_{k_p}$ have **mean zero under P by construction**, and therefore we definitely have that:

$$\mu_p(x) = \int k_p(x, y)p(y)dx = 0\,.$$

Kernel Stein discrepancies

$$\text{KSD}(P \,||\, Q) = \sup_{g \in \mathcal{G}} \|\mathbb{E}_{X \sim Q}[\mathcal{S}_P[g](X)]\|$$

- The Stein discrepancy with the RKHS $\mathcal{H}_k$ is equivalent to the the MMD with kernel k_p!

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Expression for the Langevin KSD

- The Stein discrepancy can be simplified to

$$\text{KSD}(P\,||\,Q_n) = \sqrt{\frac{1}{n^2}\sum_{i,j=1}^{n} k_P(x_i, x_j)}$$

$$k_P(x,x') = k(x,x')\langle \nabla_x \log p(x), \nabla_{x'} \log p(x')\rangle + \langle \nabla_x k(x,x'), \nabla_{x'} \log p(x')\rangle$$
$$+\langle \nabla_{x'} k(x,x'), \nabla_x \log p(x)\rangle + \text{Tr}(\nabla_x \nabla_{x'} k(x,x'))$$

- The function k_P is a **Stein reproducing kernel** (i.e. it is also a kernel!)

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→ Looks complicated but it's all straightforward to compute!

Kernel derivatives

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→ This is indeed straightforward to compute!

Computational complexity of the KSD

$$\text{KSD}(P\,||\,Q_n) = \sqrt{\frac{1}{n^2}\sum_{i,j=1}^{n} k_P(x_i, x_j)}$$

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- The computational complexity of each k_P evaluation is $O(d)$.

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$$k_P(x,x') = k(x,x')\langle \nabla_x \log p(x), \nabla_{x'} \log p(x')\rangle + \langle \nabla_x k(x,x'), \nabla_{x'} \log p(x')\rangle$$
$$+ \langle \nabla_{x'} k(x,x'), \nabla_x \log p(x)\rangle + \text{Tr}(\nabla_x \nabla_{x'} k(x,x'))$$

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→ Total cost is $O(n^2 d)$!

Scalable Stein discrepancies

- It is possible to bring down the cost to linear (rather than quadratic) in n through very accurate approximations (i.e. random features).
- When P is a posterior based on a lot of data points, the cost of each score function evaluation can be prohibitive. Approximations based on stochastic estimates of the score can be used in those cases.

Jitkrittum, W., Xu, W., Szabo, Z., Fukumizu, K., & Gretton, A. (2017). A linear-time kernel goodness-of-fit test. *NeurIPS*.

Huggins, J. H., & Mackey, L. (2018). Random feature Stein discrepancies. NeurIPS.

Gorham, J., Raj, A., & Mackey, L. (2020). Stochastic Stein discrepancies. NeurIPS.

U-statistic or V-statistic

- Interestingly, this is not the only way to approximate KSD$(P||Q)$:

$$\mathrm{KSD}(P||Q_n) = \sqrt{\frac{1}{n^2}\sum_{i,j=1}^{n} k_P(x_i, x_j)} \quad \longleftarrow \quad \text{V-statistic}$$

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U-statistic

- The U-statistic is unbiased but has higher variance, whereas the V-statistic is biased but has lower variance.

Outline (updated)

- What is Stein’s method, and why should you care…
- Computational tools based on Stein’s method.
- Some nice (new) algorithms!

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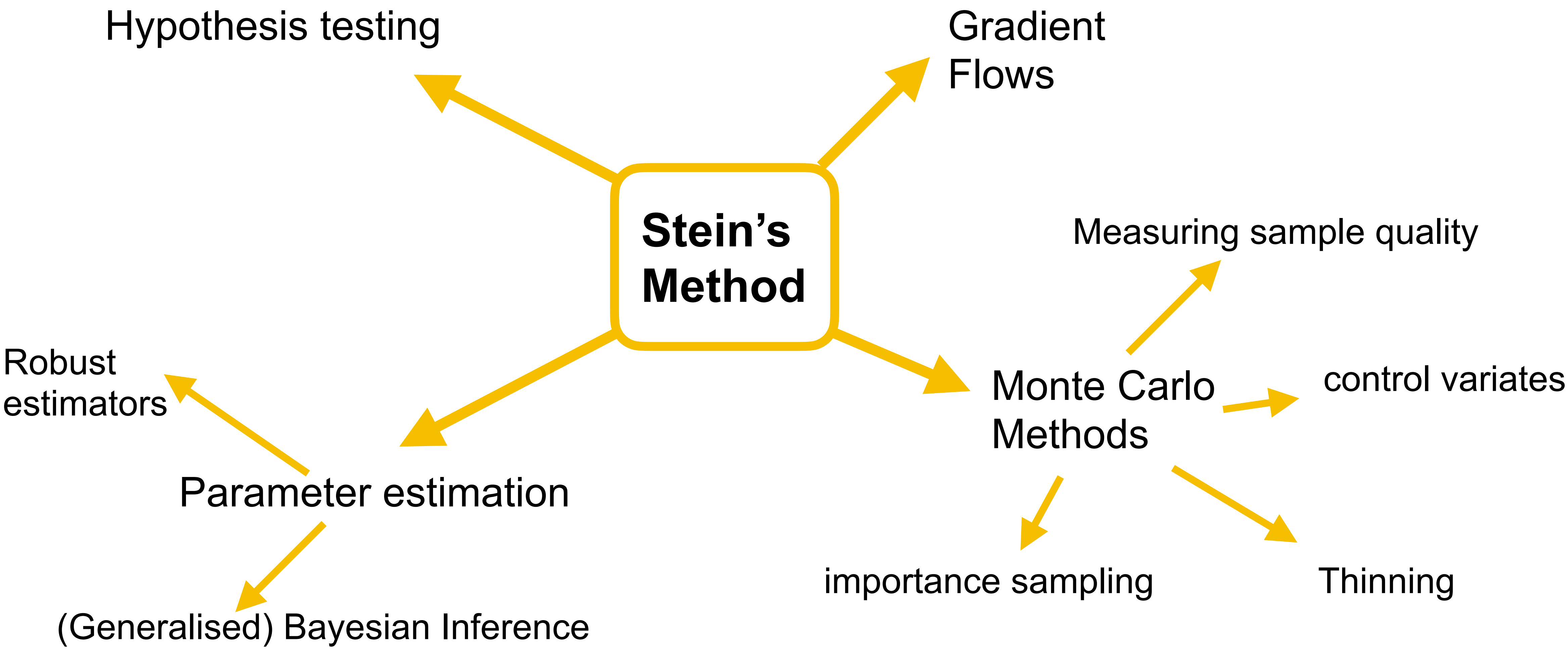
We now have an **amazing hammer** and we can use it to hit pretty much all the nails in computational statistics.

Our nails…



Hypothesis testing
Gradient Flows
Stein's Method
Measuring sample quality
Robust estimators
Monte Carlo Methods
control variates
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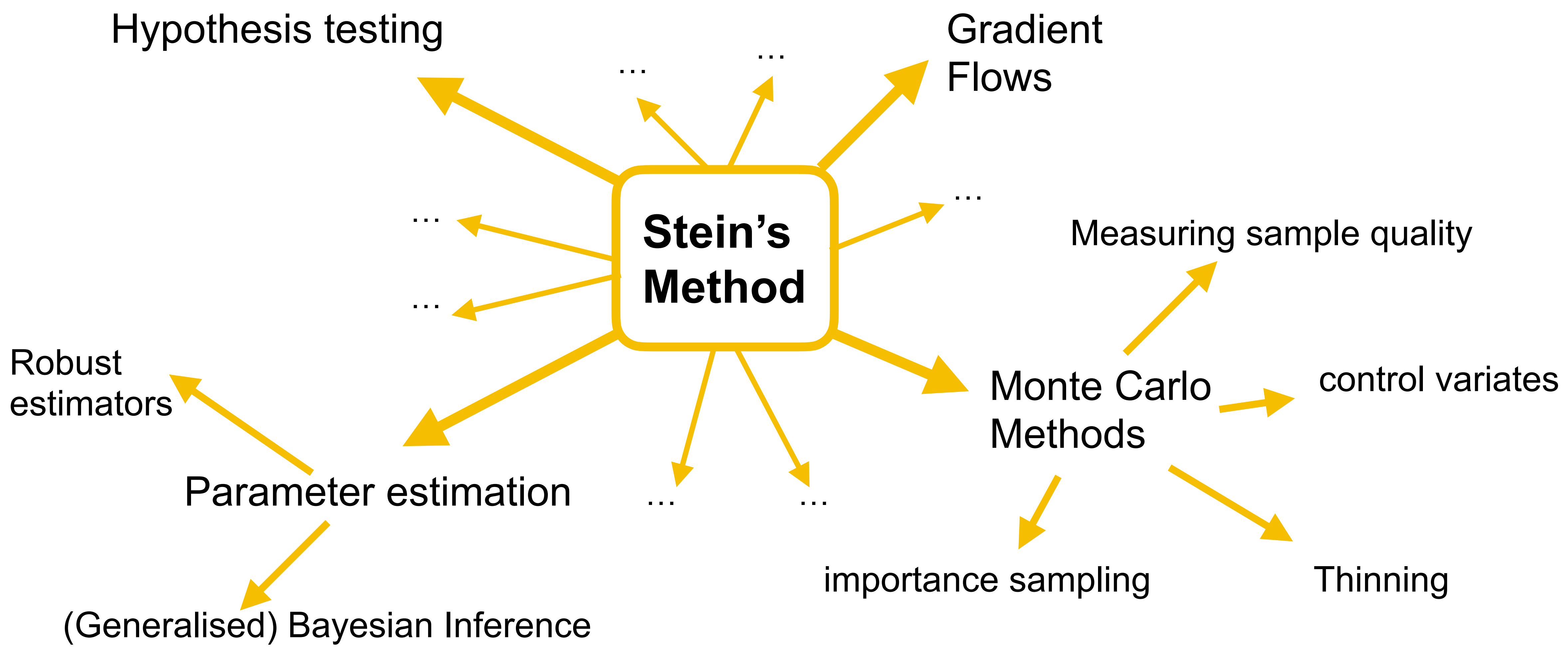
importance sampling
Thinning
(Generalised) Bayesian Inference

Our nails…



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- I will be biased towards topics on which I have myself worked…

Stein’s method as a computational tool

Hypothesis testing

Goodness-of-fit testing

- In goodness-of-fit testing, we want to answer questions such as:

"Do I have a good model for my observed data?"

"Are the distributional assumptions of my analysis reasonable"

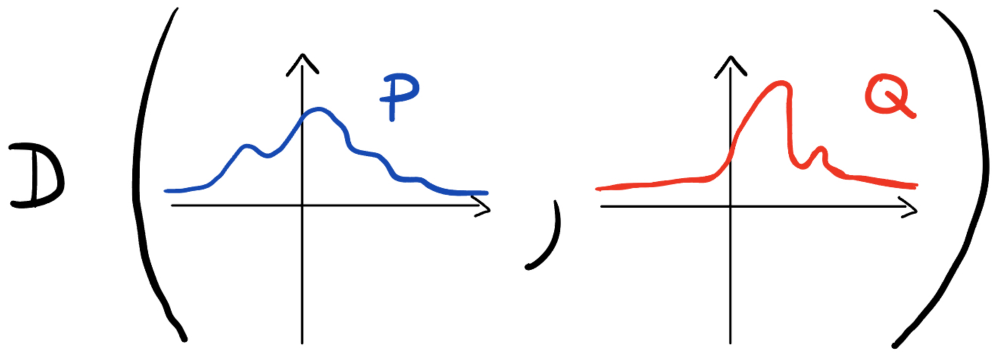
- Given a distribution P and some observed data $\{x_i\}_{i=1}^n \sim Q$, this is formalised as:

$$H_0 : P = Q$$
$$H_1 : P \neq Q$$

Testing with discrepancies

$$H_0 : P = Q$$
$$H_1 : P \neq Q$$

- Assume we have a "reasonable" notion of discrepancy/dissimilarity D. Then a good way to check whether H_0 holds is to compute:



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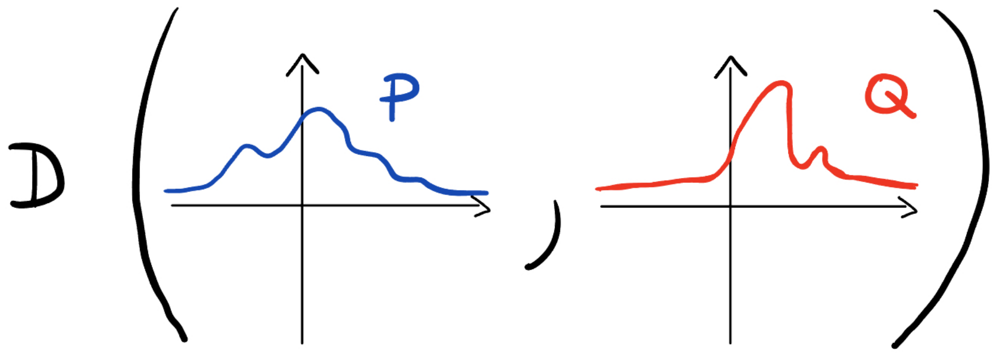

- If this is zero, we know that $P = Q$!
- If this is strictly greater than zero, we know that $P \neq Q$!

Existing work

- Most existing work focuses on very simple P; e.g. Gaussian, Poisson, etc..

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$D = L^\infty$ distance between CDFs → Kolmogorov-Smirnov test

D = weighted L^2 between CDFs → Anderson-Darling test

- The main reason that these consider only simple P is that the distance is otherwise infeasible to compute/estimate!

Goodness of fit testing with kernels

- Sadly most of these existing tests are very limited in the sense that you have to find a new test for every distribution P you care about….

Goodness of fit testing with kernels

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A Kernel Test of Goodness of Fit

Kacper Chwialkowski* KACPER.CHWIALKOWSKI@GMAIL.COM
Heiko Strathmann* HEIKO.STRATHMANN@GMAIL.COM
Arthur Gretton ARTHUR.GRETTON@GMAIL.COM
Gatsby Unit, University College London, United Kingdom

A Kernelized Stein Discrepancy for Goodness-of-fit Tests

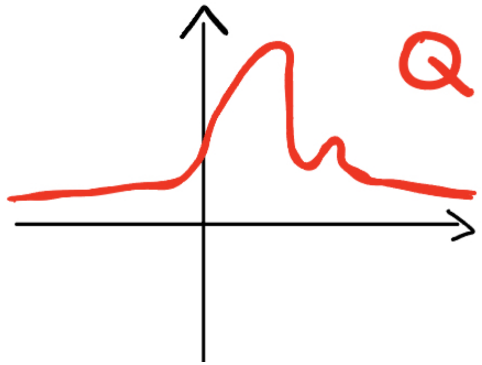
Qiang Liu QLIU@CS.DARTMOUTH.EDU
Computer Science, Dartmouth College, NH, 03755
Jason D. Lee JASONDLEE88@EECS.BERKELEY.EDU
Michael Jordan JORDAN@CS.BERKELEY.EDU
Department of Electrical Engineering and Computer Science University of California, Berkeley, CA 94709

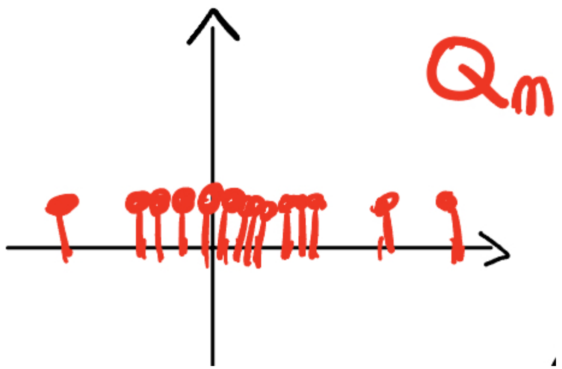
Idea: Let's use our hammer (the KSD) for goodness-of-fit testing!

Goodness-of-fit testing with KSD

$$H_0 : P = Q$$
$$H_1 : P \neq Q$$

- In practice we do not observe Q but only observe Q_n:





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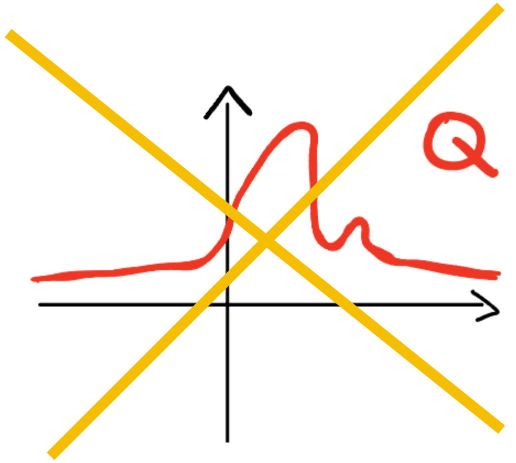

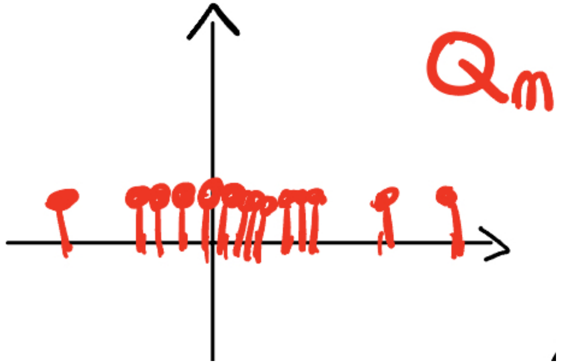

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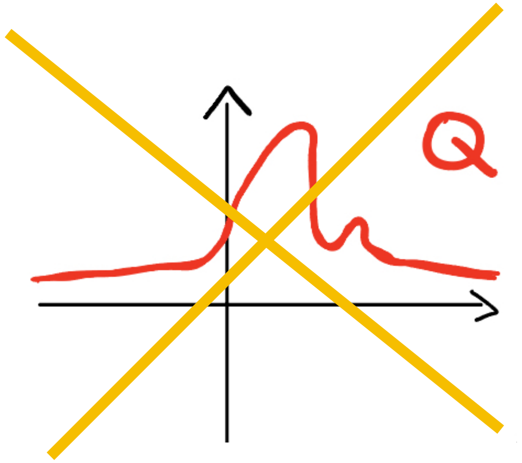

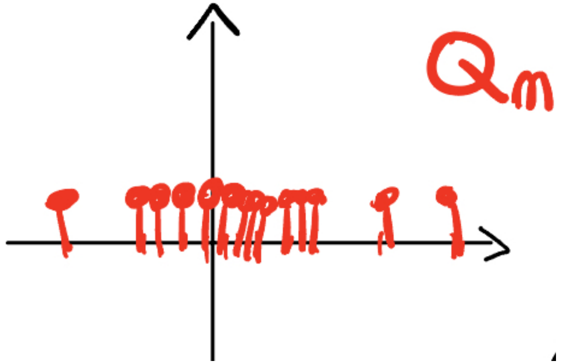

- We will therefore compute KSD$(P \,||\, Q_n)$ instead of KSD$(P \,||\, Q)$, which very conveniently turns out to be exactly what we can compute!

Accounting for finite data

$$H_0 : P = Q$$
$$H_1 : P \neq Q$$

- Since we are using Q_n instead of Q, we do not have that

$$\text{KSD}(P \,||\, Q_n) \neq 0 \qquad \Rightarrow \qquad P \neq Q$$

- We must account for the fact that **we have a finite amount of data** n.

Accounting for finite data

$$H_0 : P = Q$$
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$$\text{KSD}(P\,||\,Q_n) \neq 0 \qquad \Rightarrow \qquad P \neq Q$$

- We must account for the fact that **we have a finite amount of data** n.
- However, we would still expect that

$$\text{KSD}(P\,||\,Q_n) \approx 0 \qquad \Rightarrow \qquad P = Q$$
$$\text{KSD}(P\,||\,Q_n) \gg 0 \qquad \Rightarrow \qquad P \neq Q$$

Test statistic

$$H_0 : P = Q$$
$$H_1 : P \neq Q$$

- To construct this test, we will therefore choose:

$$\Delta = n\mathrm{KSD}(P\,||\,Q_n)^2$$

- If Δ is larger than we would expect under the null, we will reject the null hypothesis, and otherwise we will not reject.

- In practice the p-values will be computed using a Wild bootstrap algorithm which approximates the distribution of Δ under H_0:

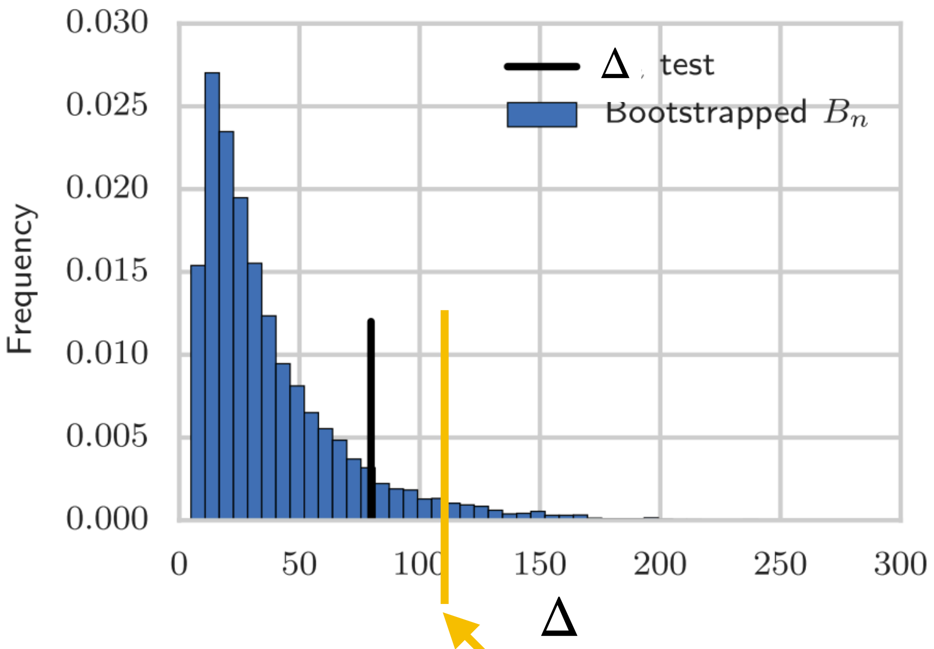
$$B = n \sum_{i,j=1}^{n} W_i W_j k_p(x_i, x_j) \qquad W_1, \ldots, W_n \sim \text{Rademacher}$$

Kernel goodness-of-fit in practice

$$H_0 : P = Q$$
$$H_1 : P \neq Q$$

- **Goodness-of-fit testing algorithm:**
  - Set level of the test to α (e.g. 0.05)
  - Calculate $\Delta = n\text{KSD}(P\,||\,Q_n)$.
  - Obtain c_α, the $(1-\alpha)$-quantile from the M bootstrap samples $B_1, \ldots, B_M$.
  - If $\Delta > c_\alpha$ then reject, otherwise do not reject.

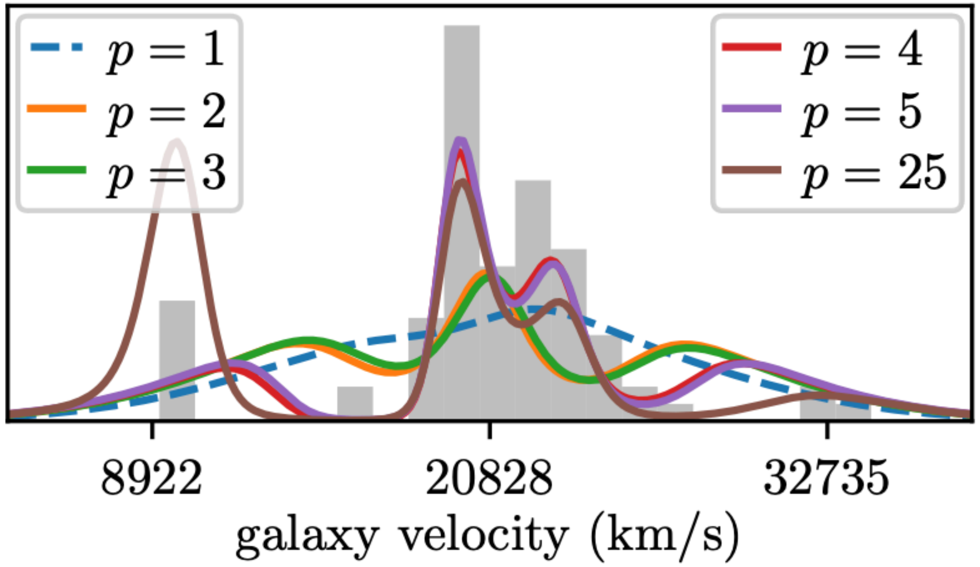
[Chwialkowski et al 2016 - slightly modified]



Quantile corresponding to our level

Composite goodness-of-fit

- Consider some parametric family of models: $\{P_\theta : \theta \in \Theta\}$



Key, O., Gretton, A., **Briol, F-X.** & Fernandez, T.. (2021). Composite goodness-of-fit tests with kernels. *arXiv:2111.10275 (under review).*

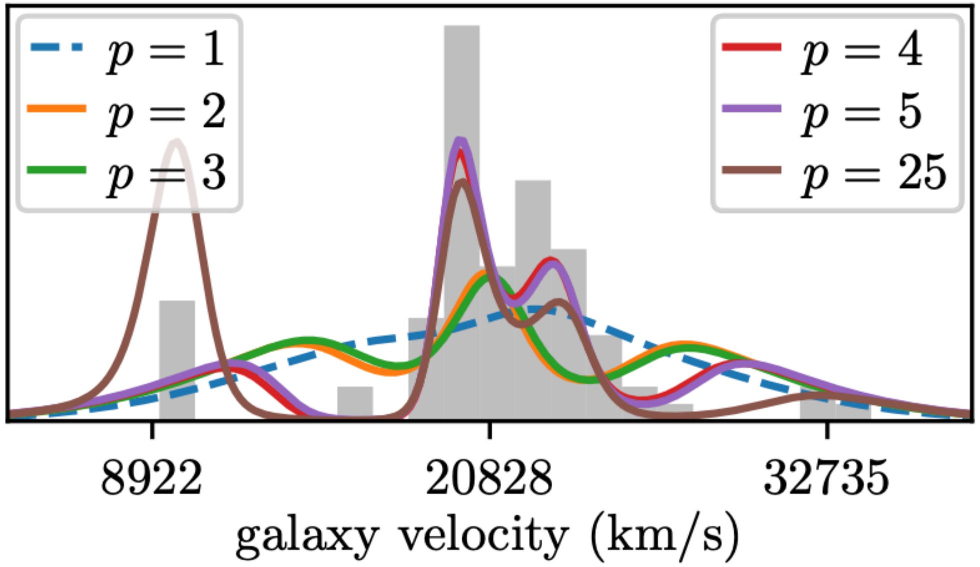
Composite goodness-of-fit

- Consider some parametric family of models: $\{P_\theta : \theta \in \Theta\}$

- An interesting question could be:

"Is my parametric model misspecified?"

$$H_0 : \exists \theta^* \text{ such that } P_{\theta^*} = Q$$
$$H_1 : \nexists \theta^* \text{ such that } P_{\theta^*} = Q$$



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Overview: goodness-of-fit with Stein

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“Are the distributional assumptions of my analysis reasonable”

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Stein characterisations allow us to design goodness-of-fit tests for a very wide variety of models so long as $\nabla_x \log p(x)$ is tractable!

Stein’s method as a computational tool

Parameter estimation and gen-Bayes

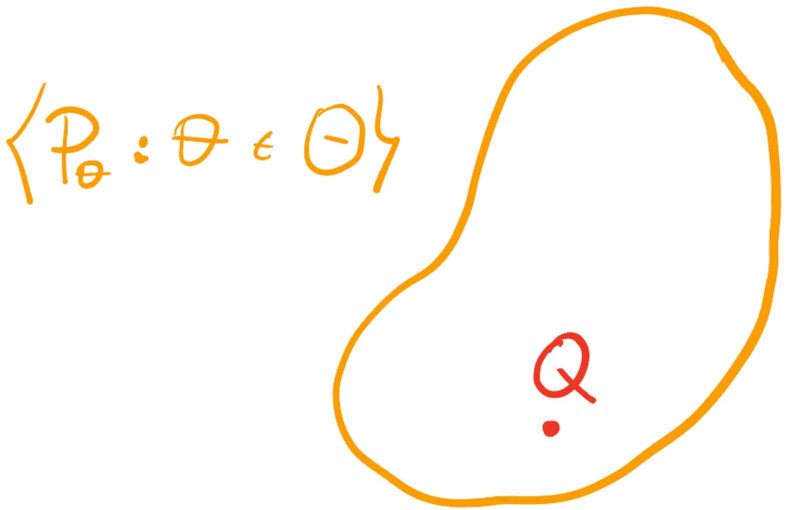
Minimum distance estimators

- In parameter estimation, we typically have a parametric family of distributions:

$$\{P_\theta : \theta \in \Theta\}$$

- Given some data $x_1, \ldots, x_n \sim Q$, we would like to find

$$\theta^* \text{ such that } P_{\theta^*} = Q$$



Why discrepancies?

- We already have plenty of good ways to estimate parameters, including maximum likelihood estimation and Bayes:

$$\arg\max_{\theta \in \Theta} \log\left(\prod_{i=1}^{n} p_\theta(x_i)\right) \qquad \pi(\theta \,|\, x_1, \ldots, x_n) \propto \prod_{i=1}^{n} p_\theta(x_i)\pi(\theta)$$

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- These are even known to be optimal in some ways, but….

“What if the model/likelihood is misspecified?”

“What if these approaches are computationally intractable?”

Minimum distance estimators

- A natural approach is to use a minimum distance estimator:

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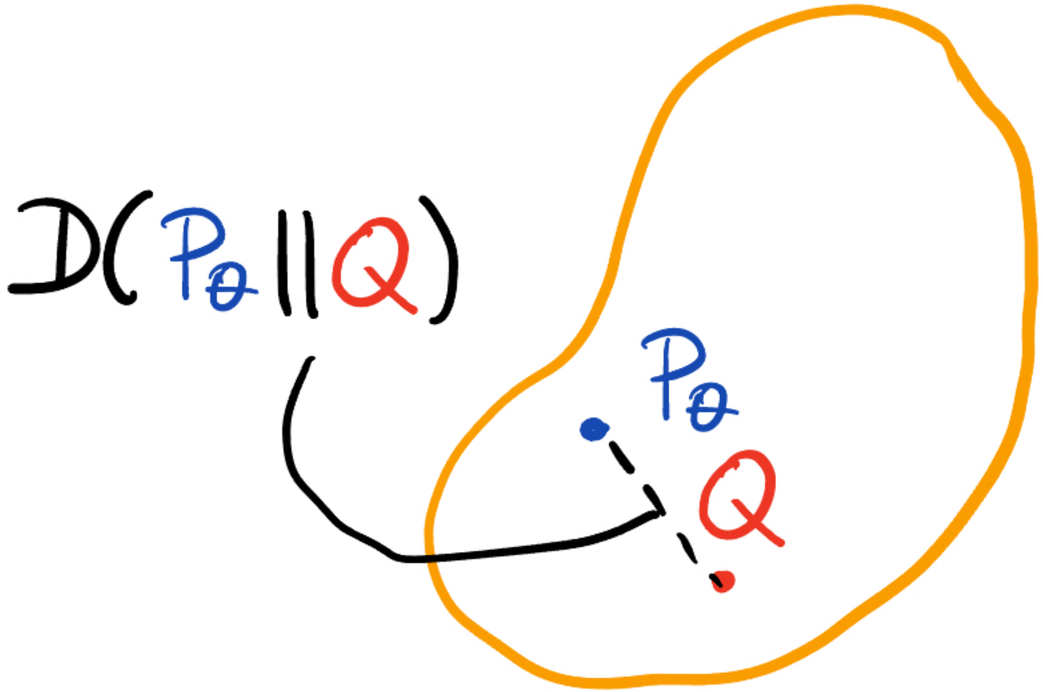
- We are simply asking for the model P_θ and the true data generating process Q to be the same, or as similar as possible.



Existing methods

- Of course, we do not have access to Q, but we have access to Q_n

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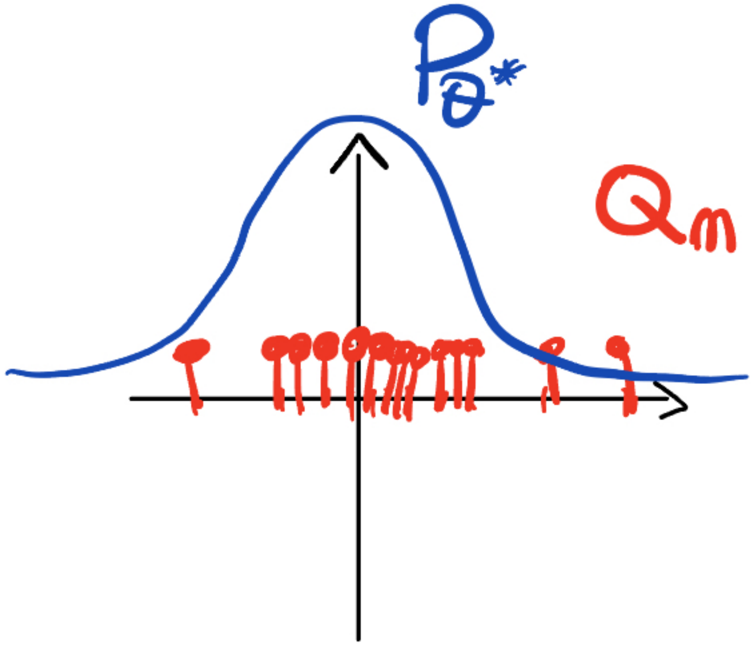
- **Examples:**

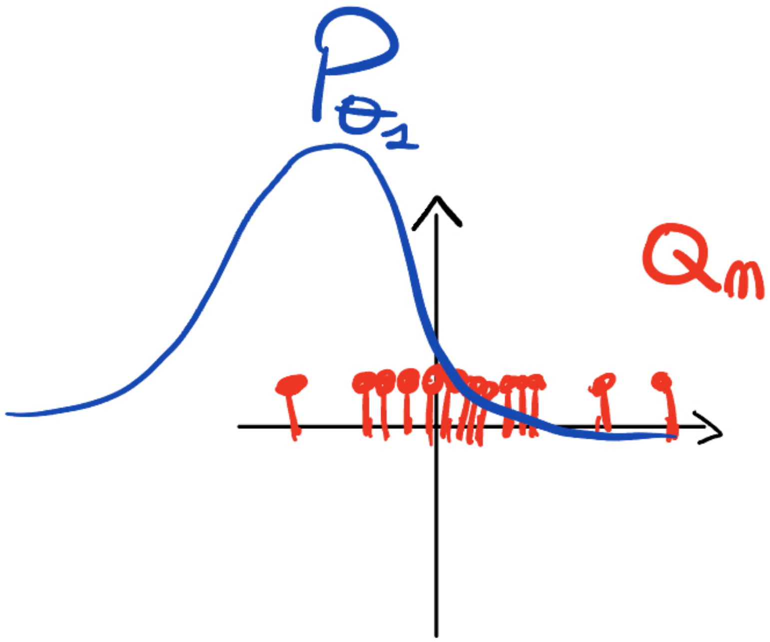
D compares moments $\longrightarrow$ Method of moments

D is KL divergence $\xrightarrow{\text{"morally"}}$ Maximum likelihood

A sketch of minimum distance estimation

$$\arg\min_{\theta \in \Theta} D(P_\theta \,||\, Q_n)$$





✓ $D(P_{\theta^*} \,||\, Q_n)$ is small

✗ $D(P_{\theta_1} \,||\, Q_n)$ is large

More on existing methods

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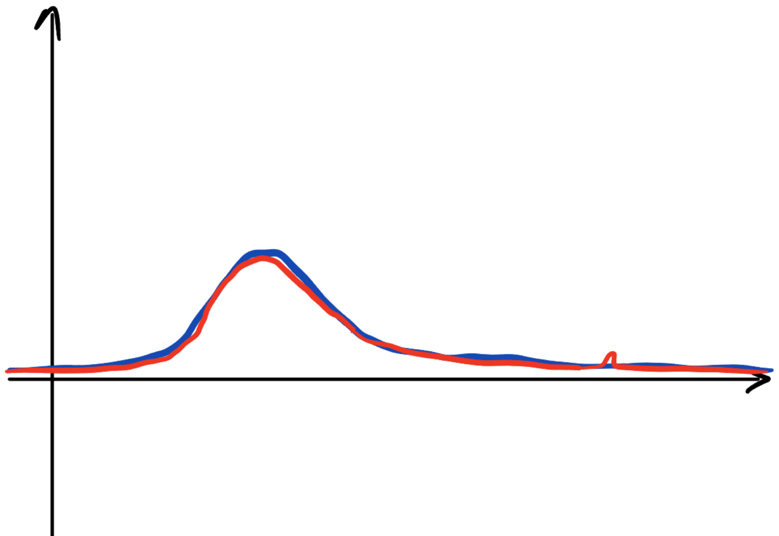

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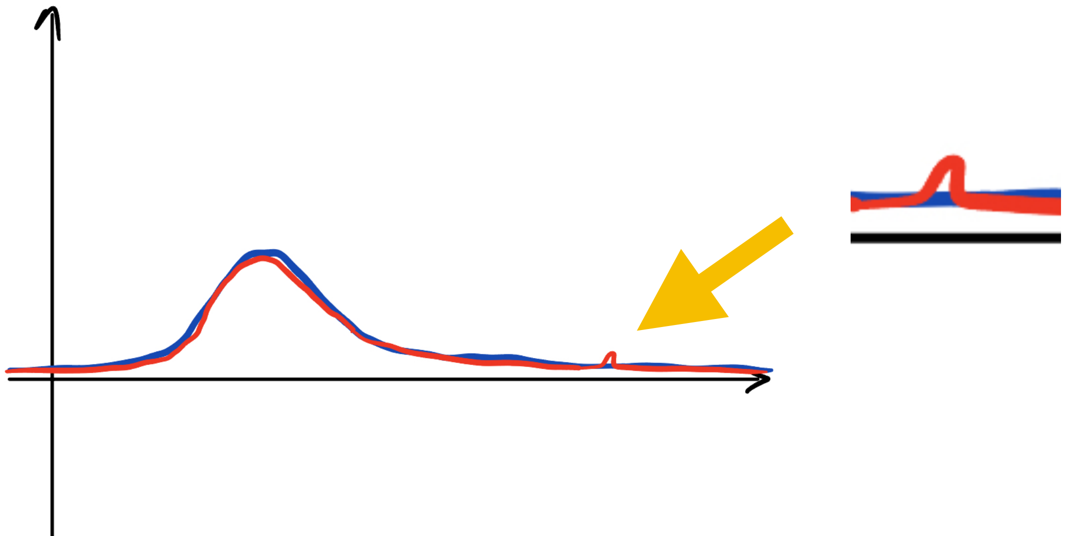

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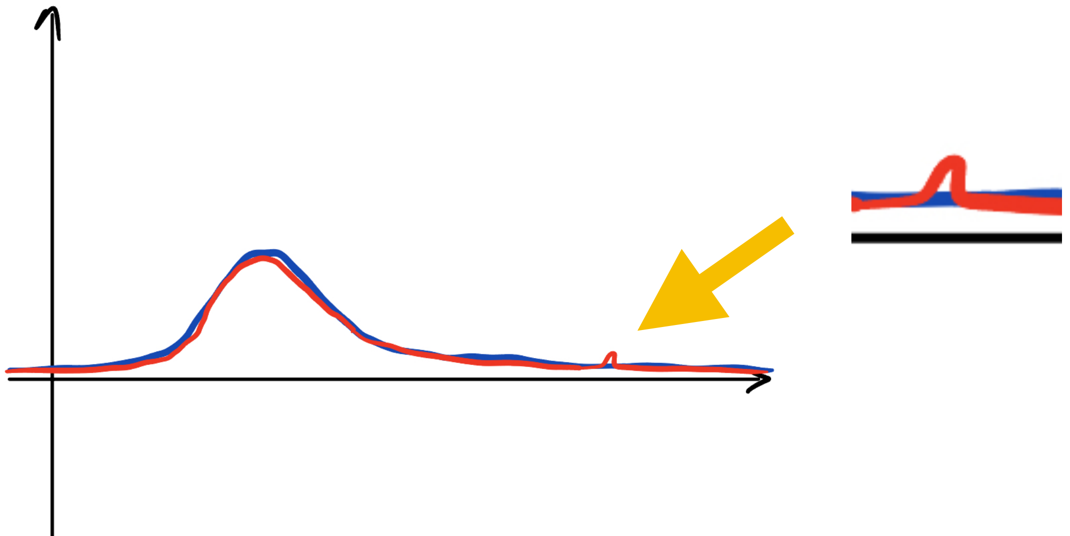
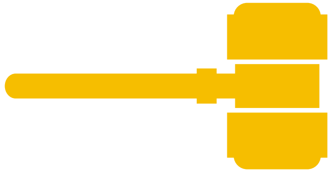


Answer: it depends on the discrepancy…

Minimum Stein discrepancy estimators

- We will come back to these properties later on. In the meantime…

- We can use our favourite hammer on this nail:



$$\arg\min_{\theta\in\Theta} \mathrm{SD}(P_\theta \,||\, Q_n)$$

Barp, A., Briol, F.-X., Duncan, A. B., Girolami, M., & Mackey, L. (2019). Minimum Stein discrepancy estimators. *NeurIPS*, 12964–12976.

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- **Examples:**
  - We recover score-matching with the Hyvarinen divergence.
  - For those that are old enough to know what this is, we can also recover minimum probability flow or contrastive divergence…

Barp, A., Briol, F.-X., Duncan, A. B., Girolami, M., & Mackey, L. (2019). Minimum Stein discrepancy estimators. *NeurIPS*, 12964–12976.

Generalised Bayesian Inference

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- Generalised Bayesian Inference proposes to use instead:

$$\pi(\theta \mid x_1, \ldots, x_n) \propto \exp\left(-L(\theta; x_1, \ldots, x_n)\right)\pi(\theta)$$

where $L(\theta; x_1, \ldots, x_n)$ is an empirical loss.

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Prior

Likelihood

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Generalised Posterior

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Prior

Loss

where $L(\theta; x_1, \ldots, x_n)$ is an empirical loss.

Generalised Bayesian Inference with Stein Discrepancies

- A natural choice of loss function is to pick a discrepancy:

$$\pi(\theta \,|\, x_1, \ldots, x_n) \propto \exp\left(-n\mathrm{SD}(P_\theta \,||\, Q_n)\right)\pi(\theta)$$

i.e. $L(\theta; x_1, \ldots, x_n) = n\mathrm{SD}(P_\theta, Q_n)$

Matsubara, T., Knoblauch, J., Briol, F.-X., & Oates, C. J. (2022). Robust generalised Bayesian inference for intractable likelihoods. *Journal of the Royal Statistical Society: Series B: (Statistical Methodology)*, *84*(3), 997–1022.

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i.e. $L(\theta; x_1, \ldots, x_n) = n\mathrm{SD}(P_\theta, Q_n)$

Intuition: Our generalised posterior will have more mass in regions where $\mathrm{SD}(P_\theta \,||\, Q_n)$ is small (or equivalently where $\exp(-n\mathrm{SD}(P_\theta \,||\, Q_n))$ is large). This will typically happen close to the minimum Stein discrepancy estimator

Matsubara, T., Knoblauch, J., Briol, F.-X., & Oates, C. J. (2022). Robust generalised Bayesian inference for intractable likelihoods. *Journal of the Royal Statistical Society: Series B: (Statistical Methodology)*, *84*(3), 997–1022.

Why Stein discrepancies?

- A very reasonable question at this point is:

“Why Stein discrepancies? Why not anything else?”

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  "Why Stein discrepancies? Why not anything else?"

- In turns out that they have two key properties:

  1. Their computational tractability makes them straightforward to apply even when dealing with somewhat complex models.
  2. The generator approach gives us a lot of flexibility in terms of which operator to use, and hence how the discrepancies encode similarity…

Weighted discrepancies

- One property we might want is "**outlier robustness**"; i.e. a small number of outliers do not impact our estimator/inference procedure.

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- This can be achieved by weighting our favourite discrepancies:

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$$\text{DKSD}^2(P\,||\,Q) := \mathbb{E}_{X,X'\sim Q}\left[k_p(X,X')\right] \longleftarrow \quad k(x,x') = w(x)\tilde{k}(x,x')w(x')$$

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- In particular, we can choose weights which decrease the impact of data far away from the modes of the distribution.

Robustness for KSD Bayes

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$$P_\theta = \mathcal{N}(\theta, 1) \qquad Q = (1-\epsilon)\mathcal{N}(\underbrace{\theta^*}_{=1}, 1) + \epsilon\mathcal{N}(10, 1)$$

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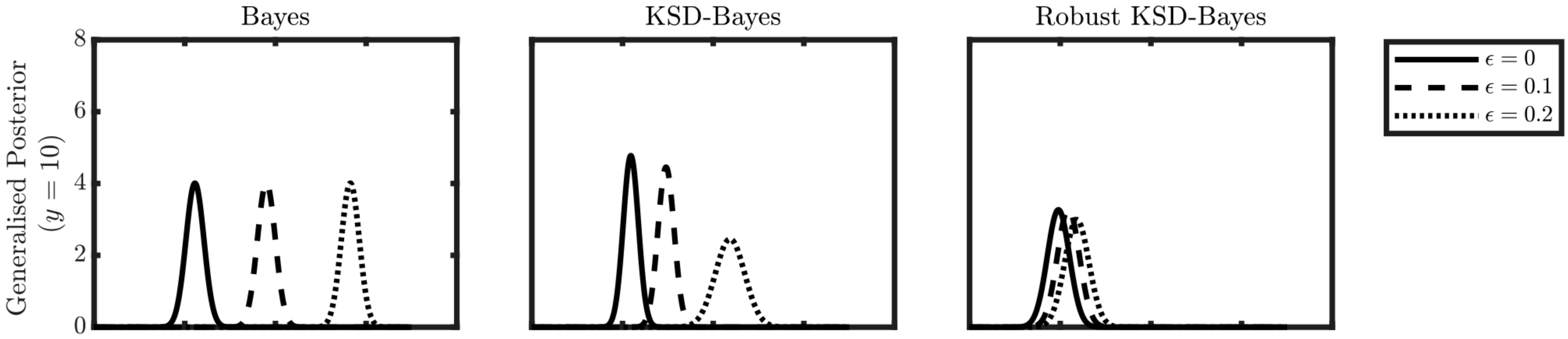

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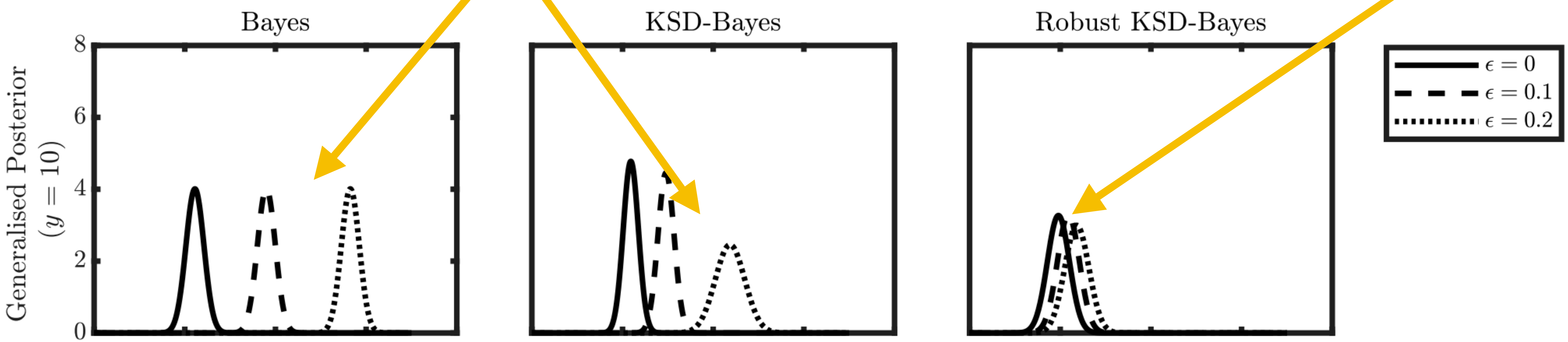
Not robust!

Robust!



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- The second property relates to computational tractability. We have already discussed the fact that some models have intractable likelihoods:

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→ Stein discrepancies remove only the worst constant (i.e. C_θ but not C)!

Stein discrepancies as quadratic forms

- Assume that you have a (natural) exponential family model:

$$p_\theta(x) \propto \exp(-T(x)^\top \theta + b(\theta) + h(x))$$

for some $T : \mathbb{R}^d \to \mathbb{R}^p$, $b : \mathbb{R}^p \to \mathbb{R}$ and $h : \mathbb{R}^d \to \mathbb{R}$.

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→ This works even when we do not know the normalisation constant!

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Gaussian!! **Gaussian** **Gaussian???**

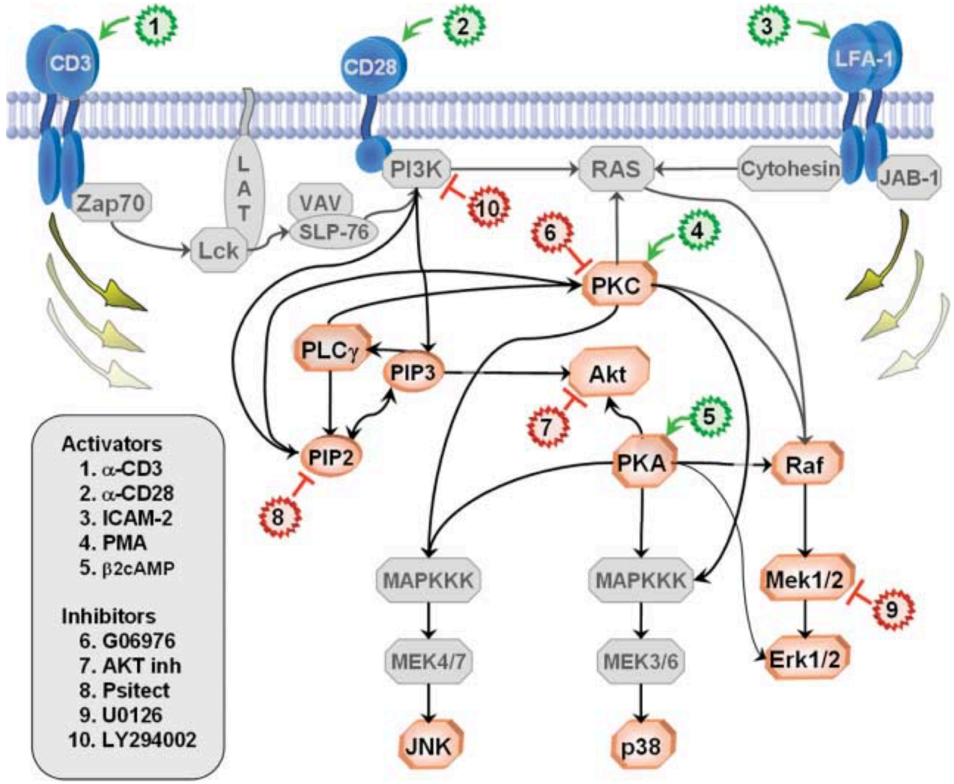
→ We get conjugacy for all natural exponential family models even when we do not know their normalisation constant!

Protein signalling networks

Parameters: $\theta_i \geq 0,\ \theta_{i,j} \geq 0$

$$p_\theta(x) \propto \exp\left(-\sum_{i=1}^{d} \theta_i \exp(x_i) - \sum_{i<j} \theta_{i,j} \exp(x_i)\exp(x_j)\right)$$

Strength of interactions
between proteins i and j



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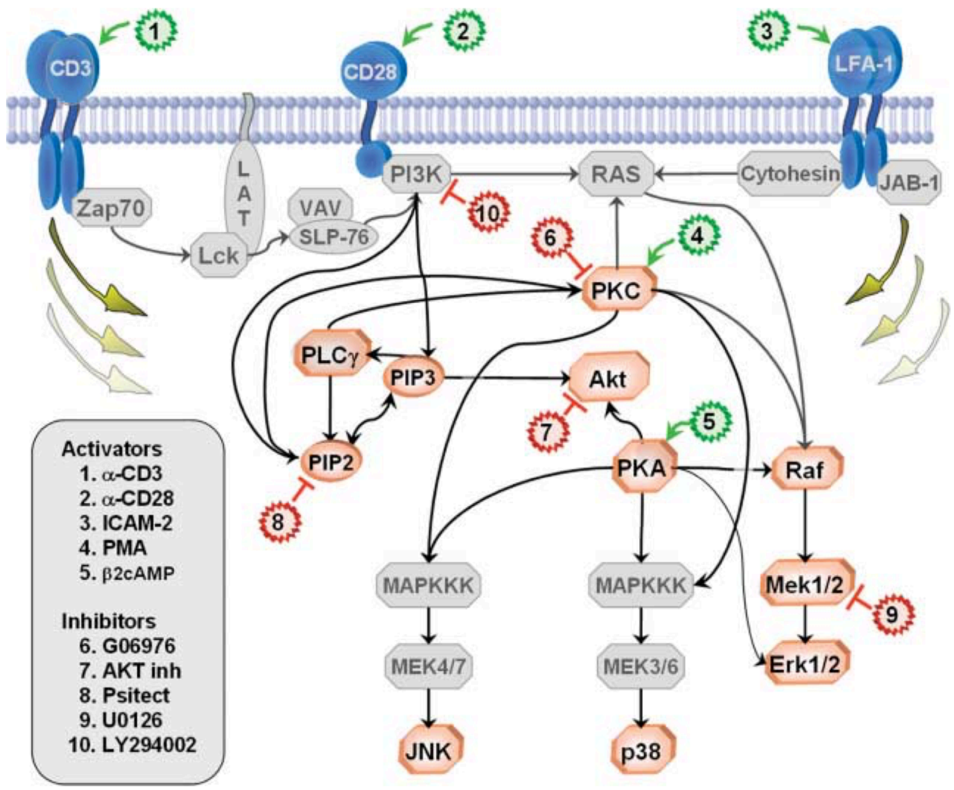

This is an exponential family, so we can have conjugate (and robust) gen-Bayes!

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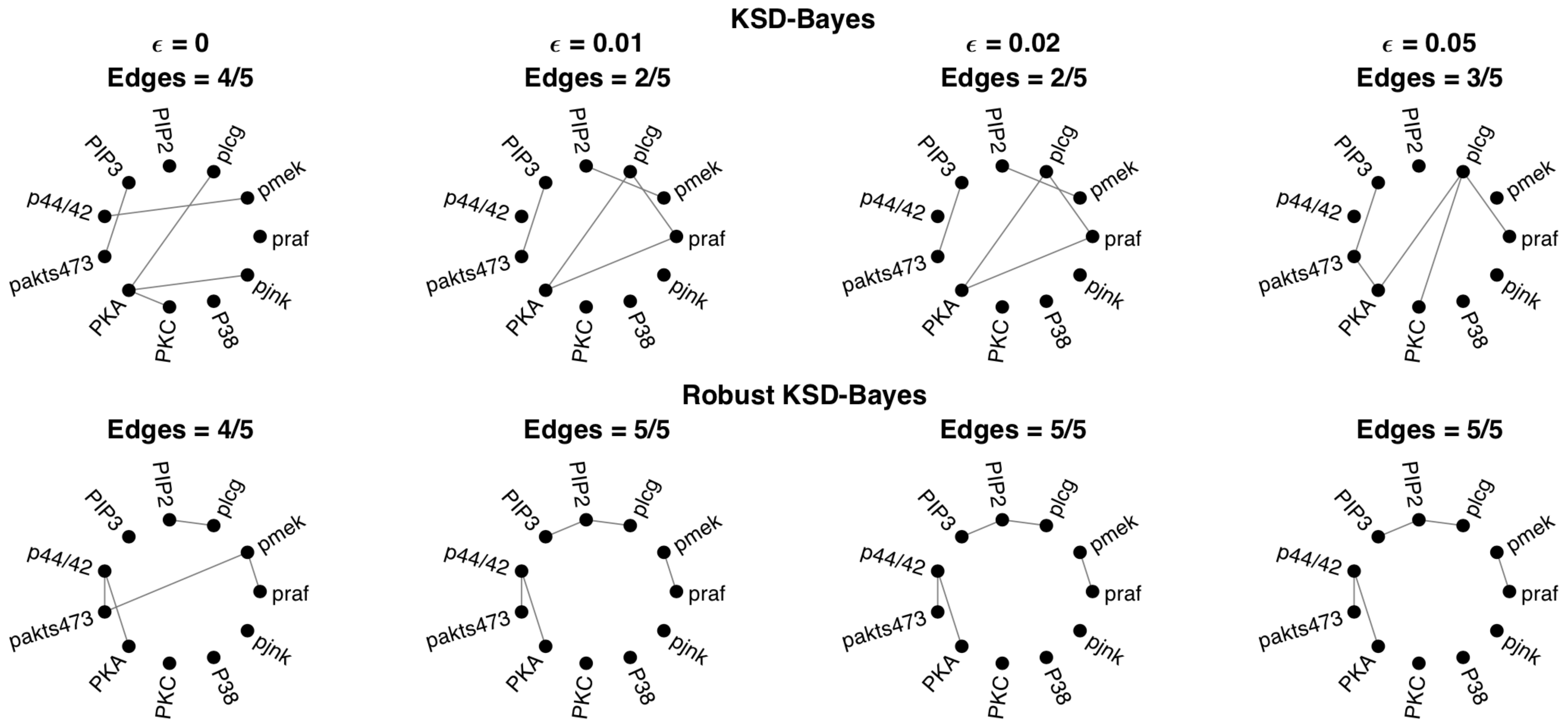

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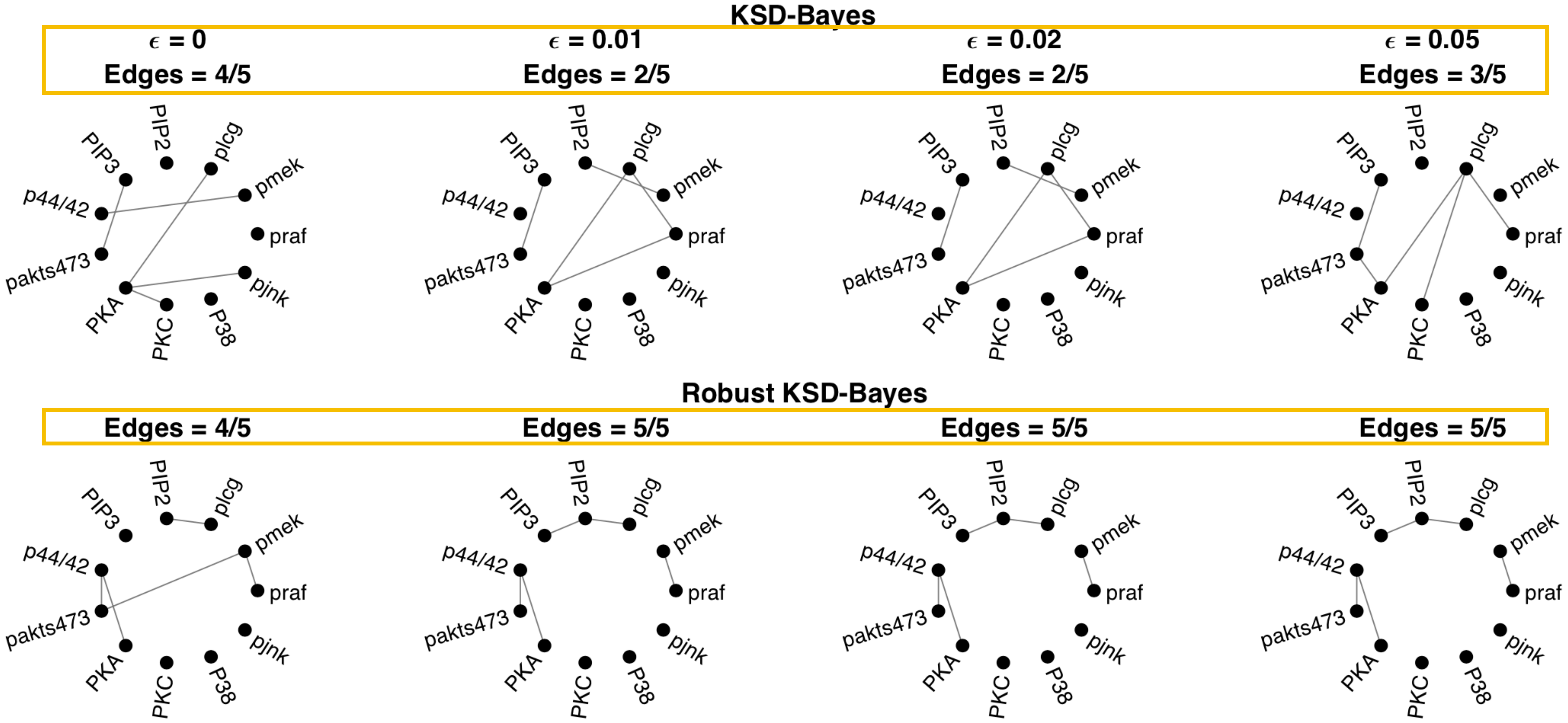

Ising model

Data space: $\mathcal{X} = \{0,1\}^d$, $n = 1000$

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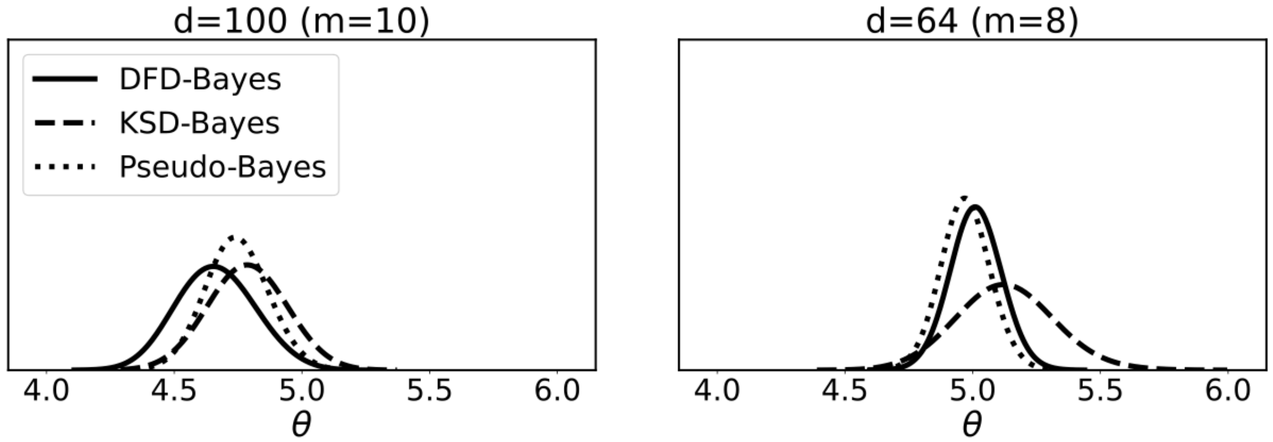

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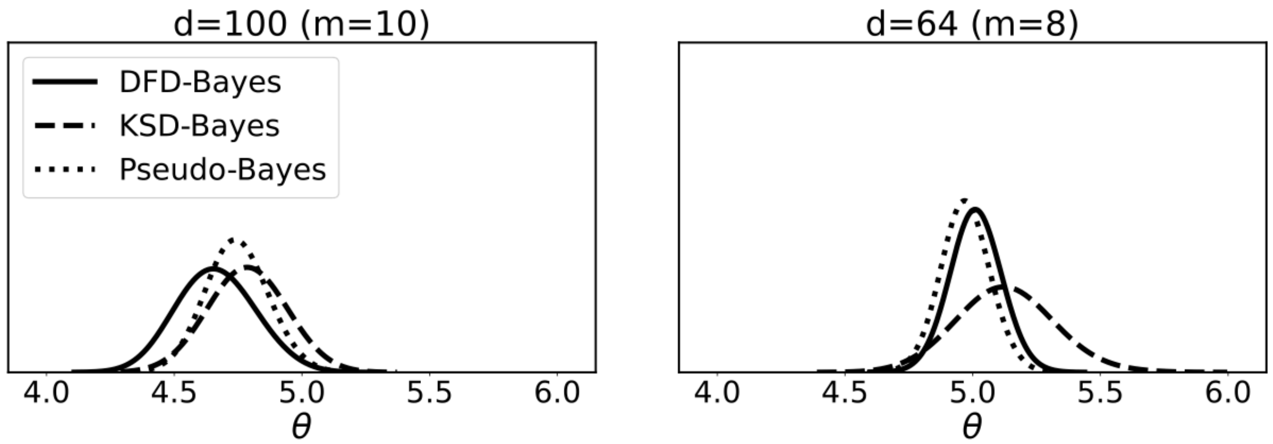

<u>Computational cost:</u>

Bayes: ???

DFD-Bayes: 540s

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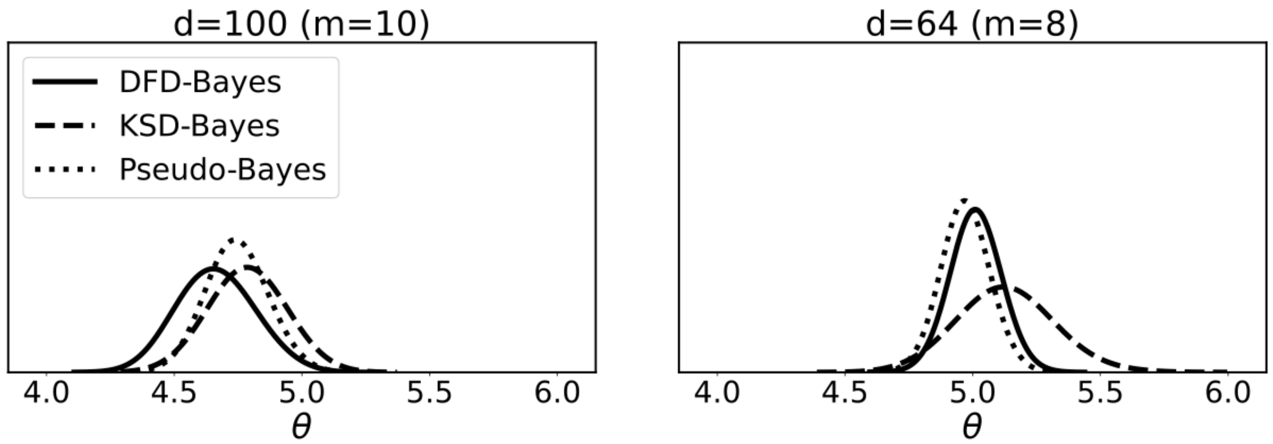

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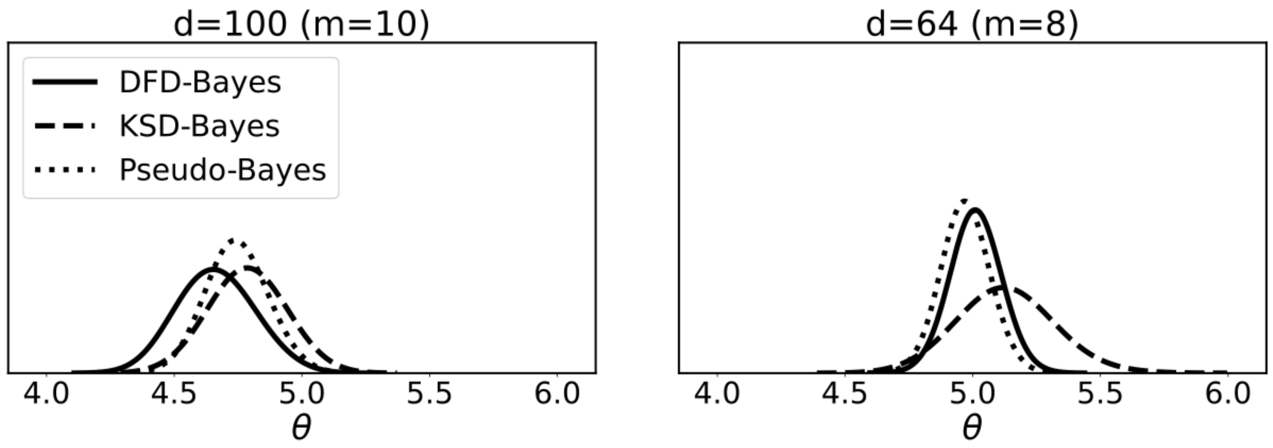

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Pseudo-Bayes uses the wrong model and so does not converge when we get more data…!

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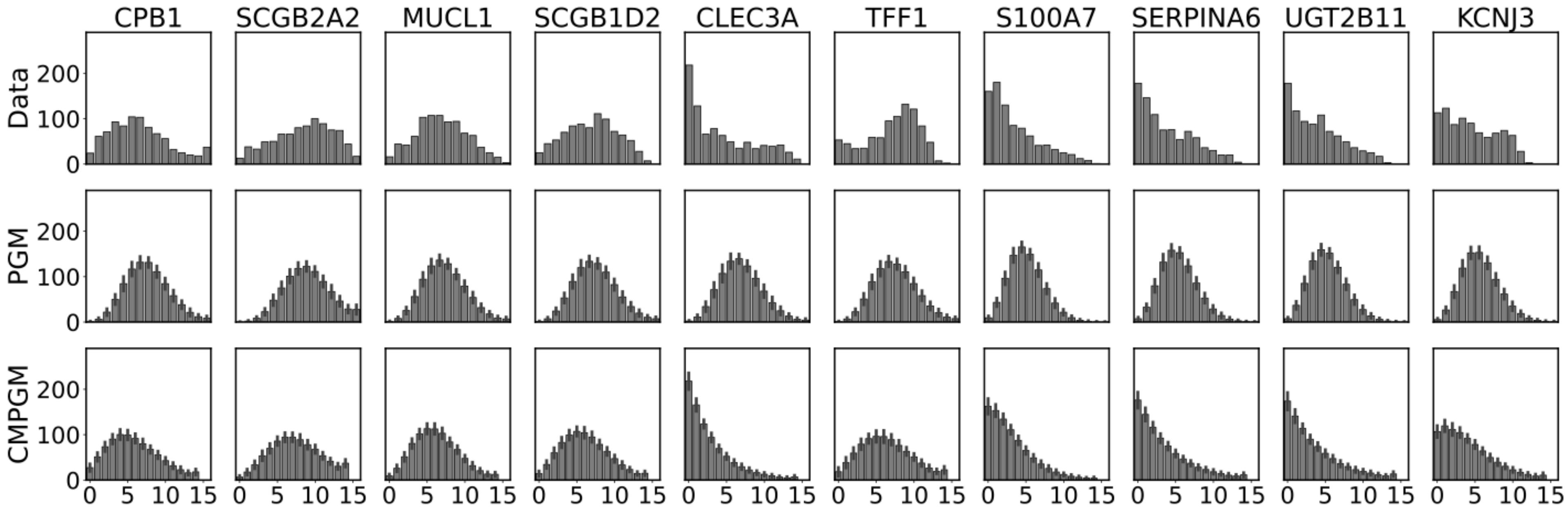
Conway-Maxwell Poisson graphical model

$$p_\theta(x) \propto \exp\left(\sum_{i=1}^{d}\theta_i x_i - \sum_{i=1}^{d}\sum_{j\in\mathcal{N}_i}\theta_{i,j}x_i x_j - \sum_{i=1}^{d}\log(x_i!)\right)$$

“Truth”

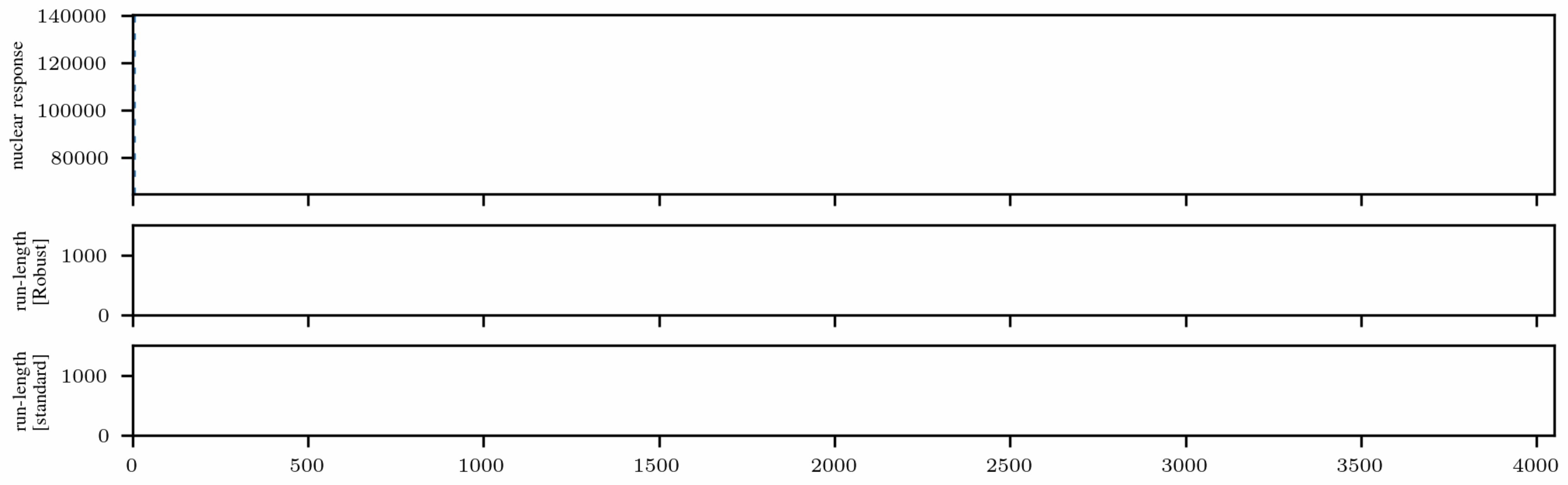
“Easy-ish”

“Very hard”



Bayesian online change-point detection

Conjugacy and robustness can be helpful for much simpler likelihoods…



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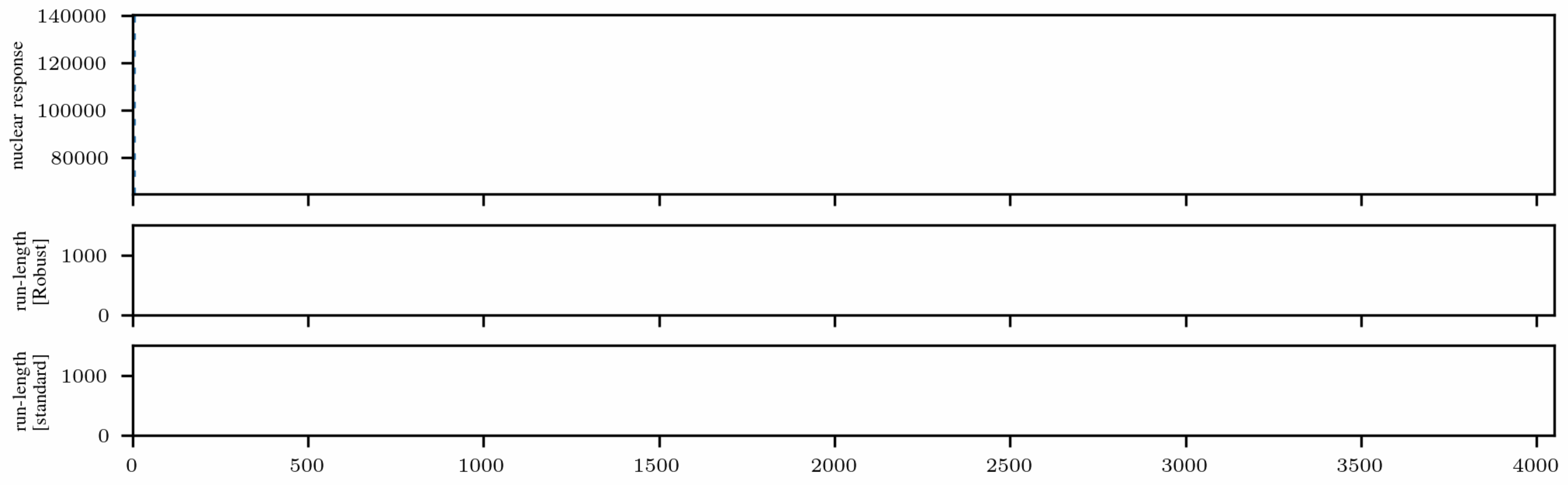

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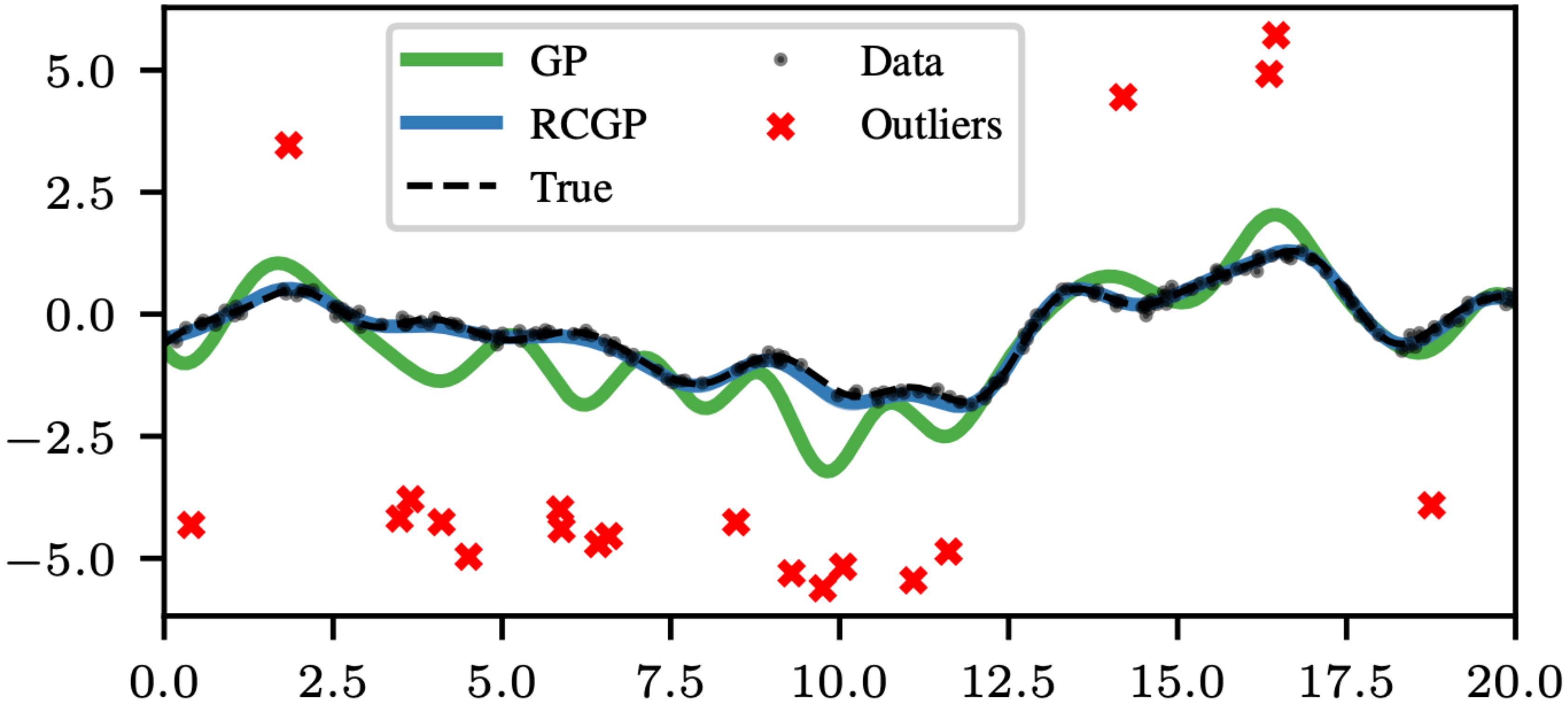
Robust Gaussian process regression



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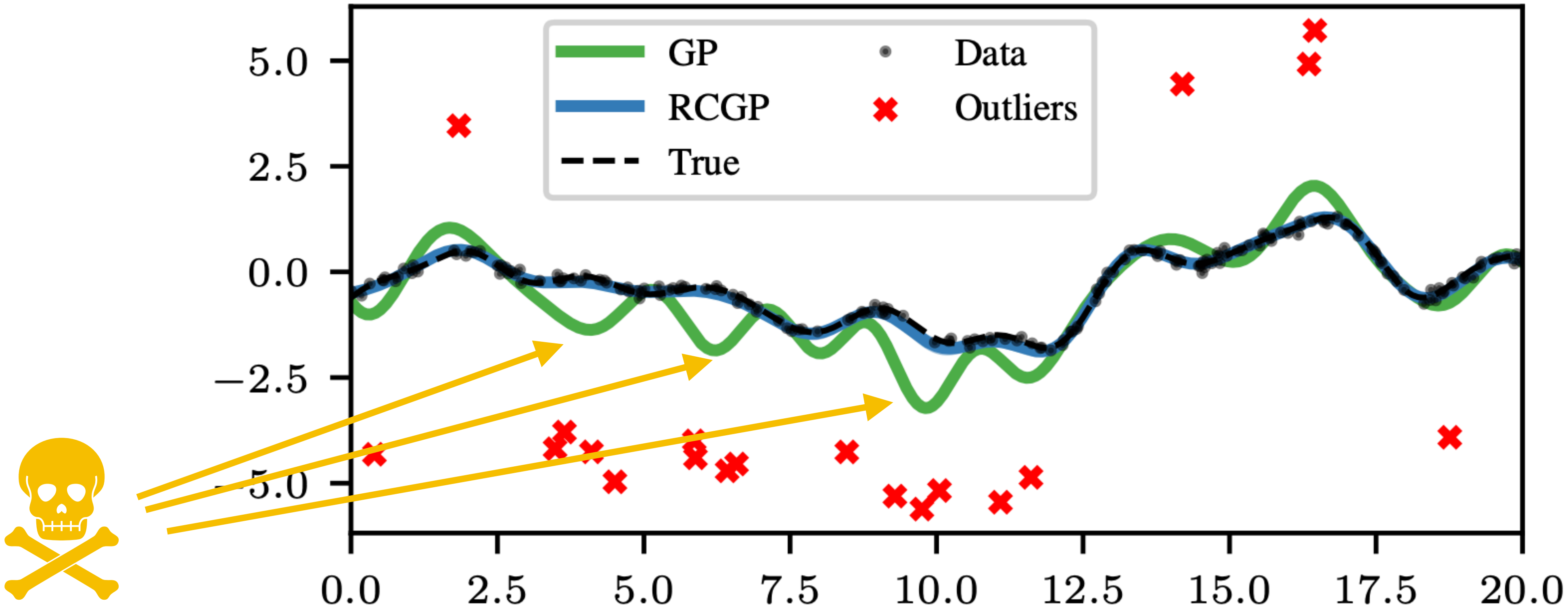

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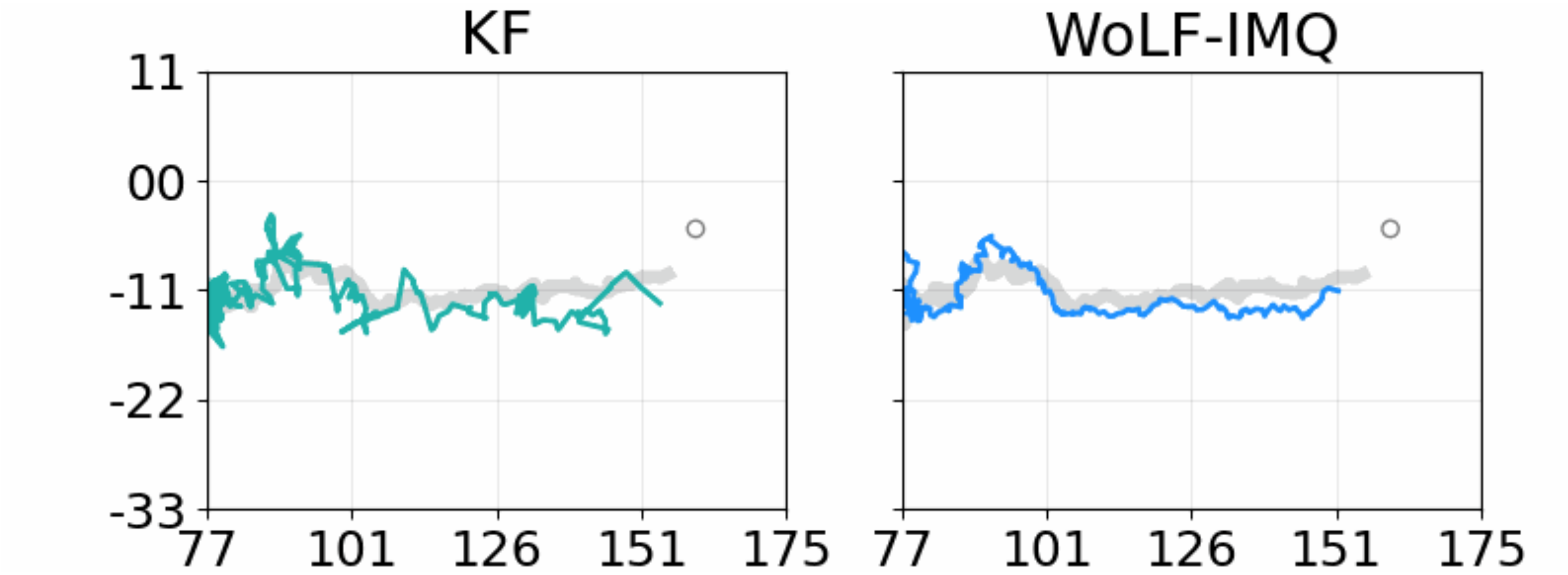

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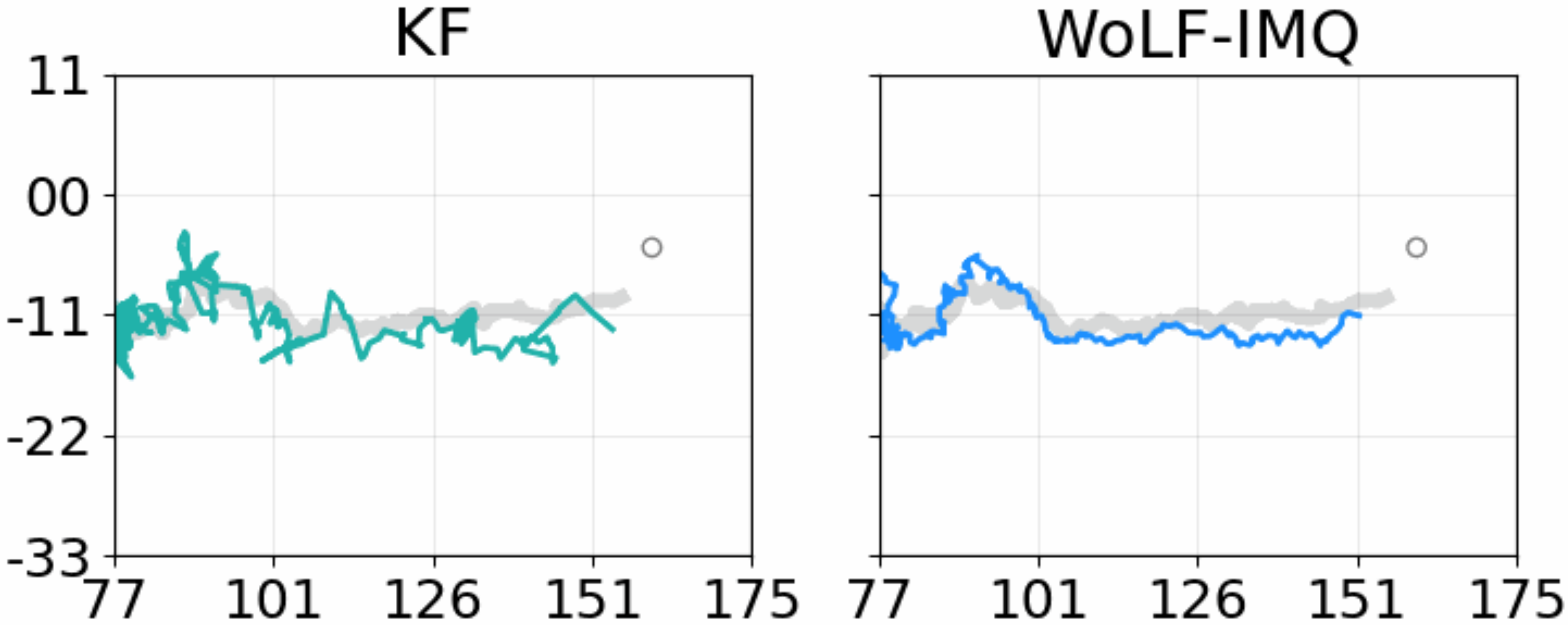

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Overview: parameter estimation and Bayes with Stein's method

- Parameter estimation is challenging in the following two setting: (i) model misspecification, (i) complex models leading to challenging computation.

- Stein discrepancies can tackle these issues due to their computational tractability and their flexibility!

Stein’s method as a computational tool

Measuring sample quality

Computational statistics with MCMC

- Suppose we are performing Bayesian inference and end up with some posterior distribution denoted P.

- The posterior is often intractable, and needs to be approximated through sampling. One such approach consists of running a Markov chain with invariant distribution P.

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- Ergodic theorems and central limit theorems can be used to **justify this approach asymptotically (i.e. as $n \to \infty$)**, but there are still many practical problems with this in practice…

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“Good MCMC”

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“Slow mixing”

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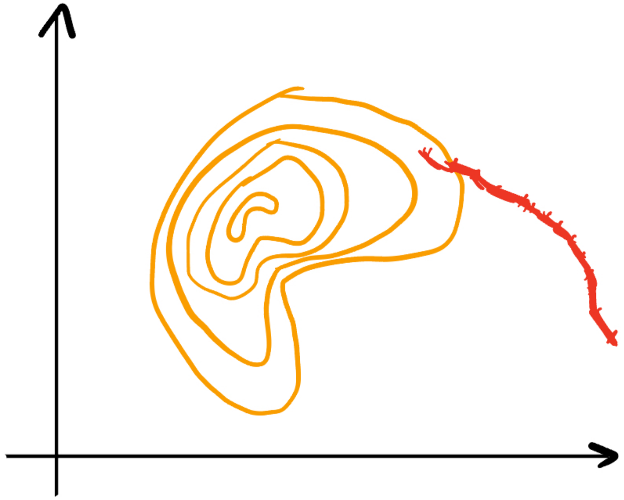

“Poor initialisation”

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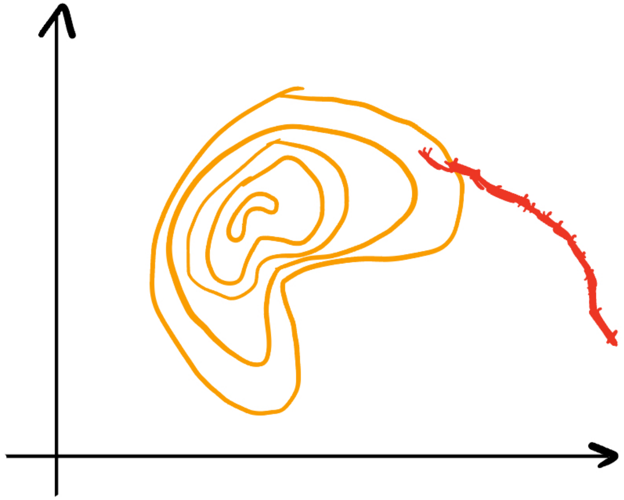

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The main problem is that we typically only see the red trajectory and not the orange contour lines…

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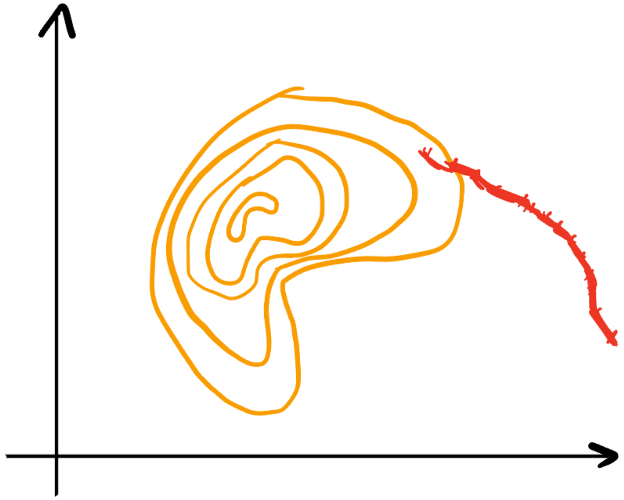

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<u>Question 1:</u> Do we have a good MCMC sampler?

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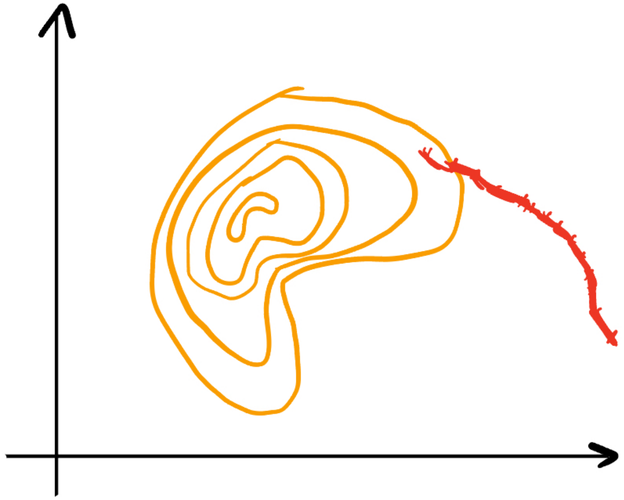

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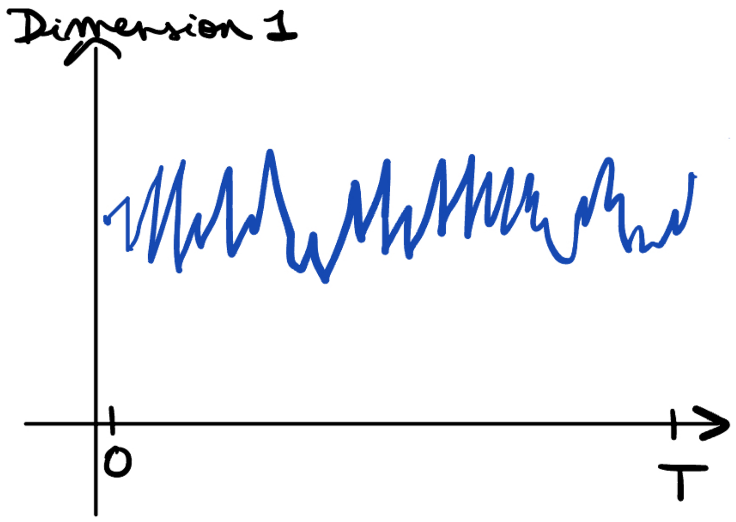
Question 1: *Do we have a good MCMC sampler?*

Question 2: *Have we run the MCMC sampler for long enough?*

Trace-plots for MCMC



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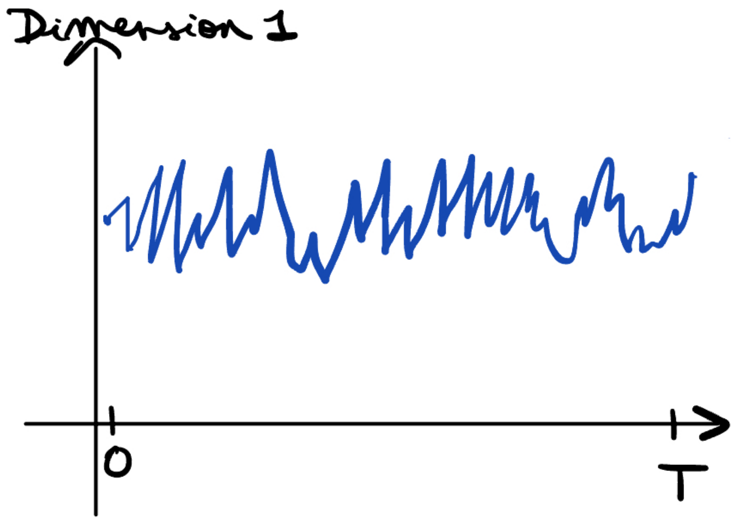

Visually seems to be mixing…
Now let me look at the other dimensions…

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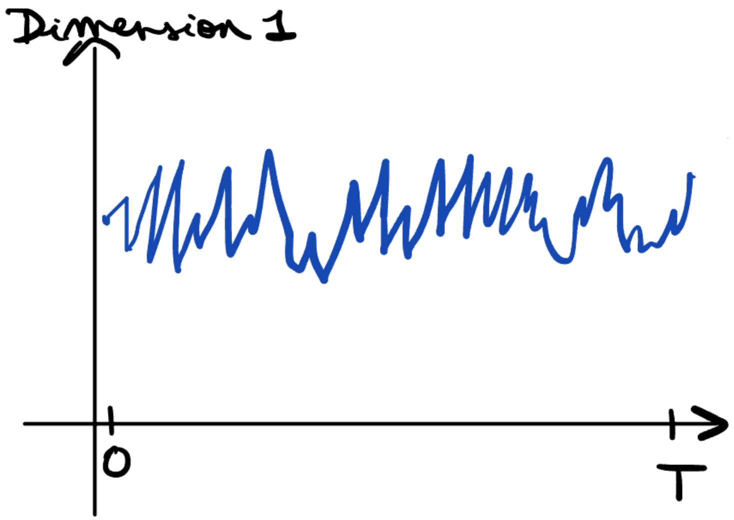

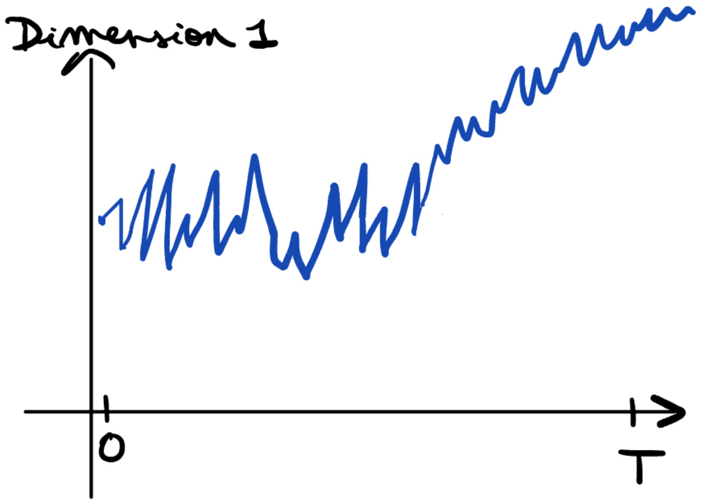

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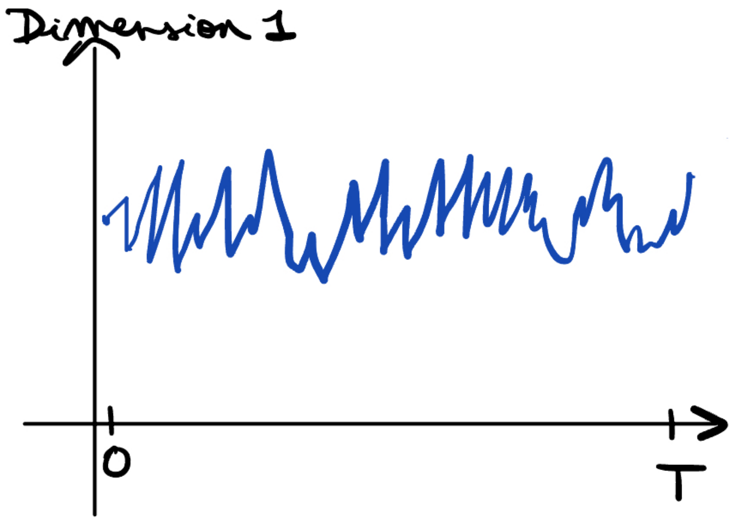

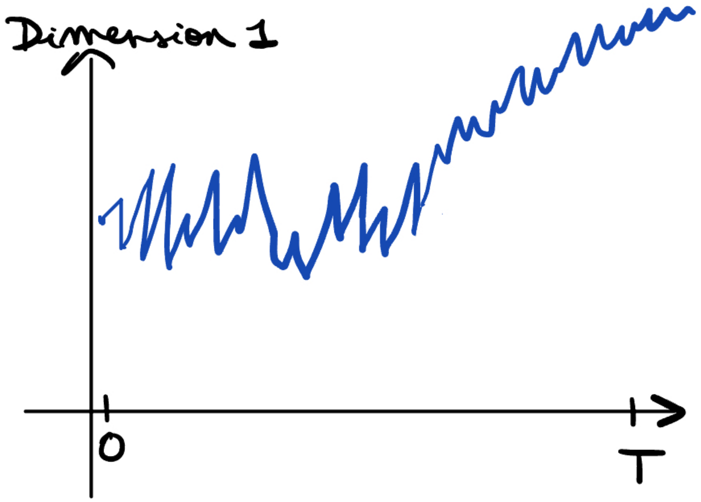

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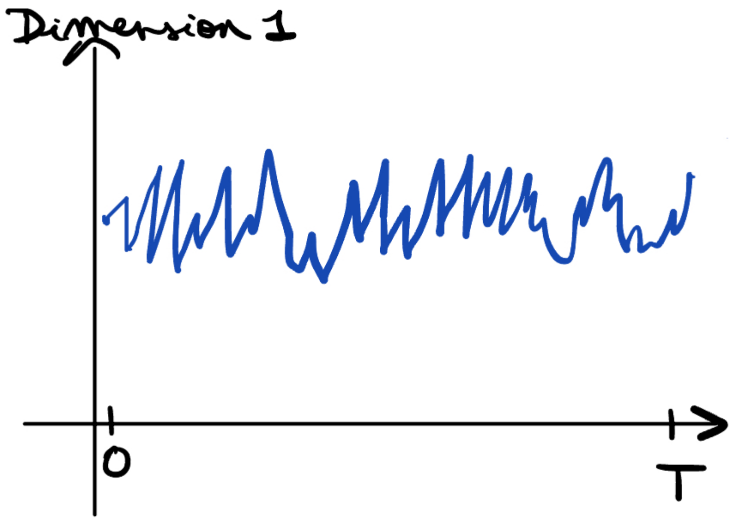

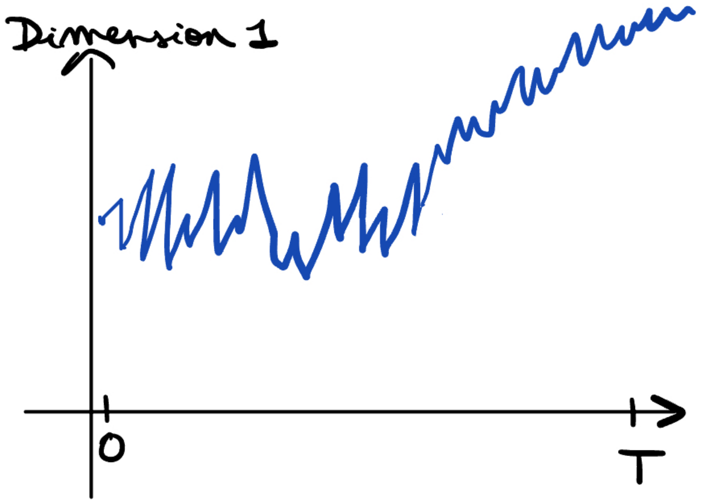

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This is really **not** a **scalable/rigorous** approach….

Other diagnostics for MCMC

- Another approach is to track the **effective sample size**:

$$\text{ESS} = \frac{n}{1 + \sum_{k=1}^{\infty} \rho_k}$$

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- **Potential issues:**
  - This is not always very reliable as a way of estimating how good our samples are as we need to estimate the autocorrelation.

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$$\text{ESS} = \frac{n}{1 + \sum_{k=1}^{\infty} \rho_k}$$

Number of MCMC samples

Autocorrelation at lag k

- **Potential issues:**
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  - Is not valid for stochastic gradient MCMC or any other approximate MCMC methods where we do not necessarily target the right P

Measuring sample quality

- A natural approach would be to look at some discrepancy:

$$\mathrm{D}(P \,||\, Q_n)$$

Target distribution

Particle approximation: $Q_n = \frac{1}{n}\sum_{i=1}^{n} \delta_{x_i}$

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✗ This is completely useless as a practical tool since we cannot compute it!

Measuring sample quality with SDs

$$\mathrm{SD}(P \,||\, Q_n) \to 0 \text{ ??}$$

Gorham, J., & Mackey, L. (2015). Measuring sample quality with Stein's method. *NeurIPS*, 226–234.

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Measuring sample quality with SDs

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- The graph Stein discrepancy and the KSD have been proposed for this task since they are both **computable!**

- The former essentially always controls weak convergence, whilst the latter does so under certain conditions of the kernel.

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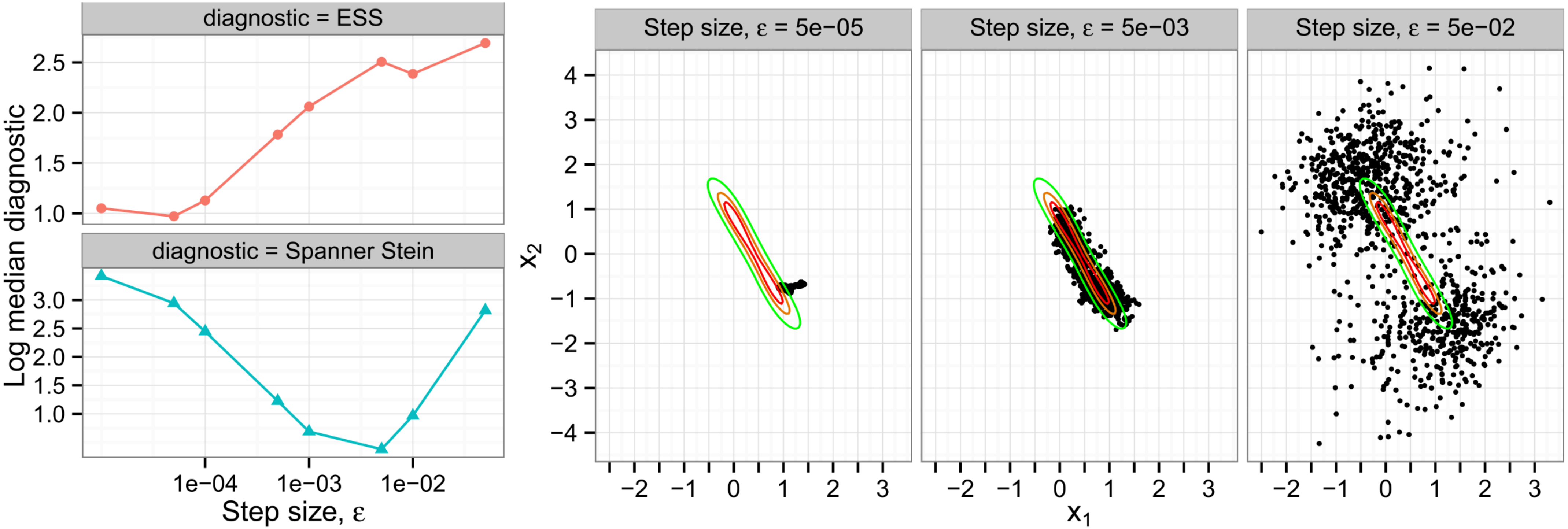
Example: Stochastic gradient langevin dynamics



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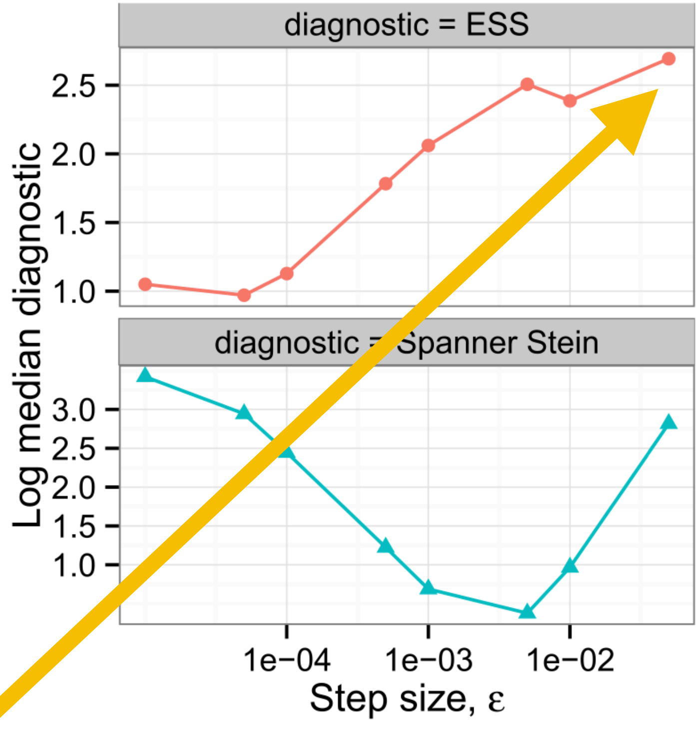

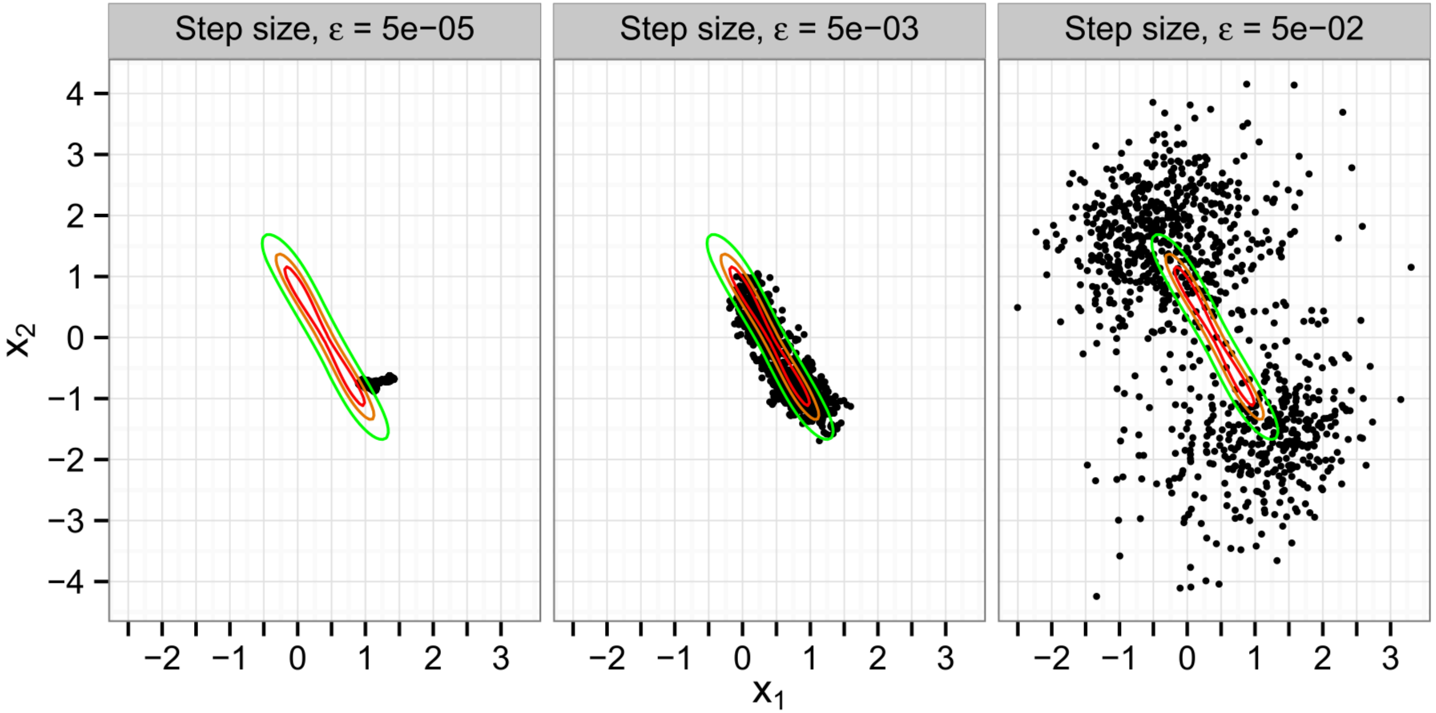

Identifies sampler which jumps around too much…

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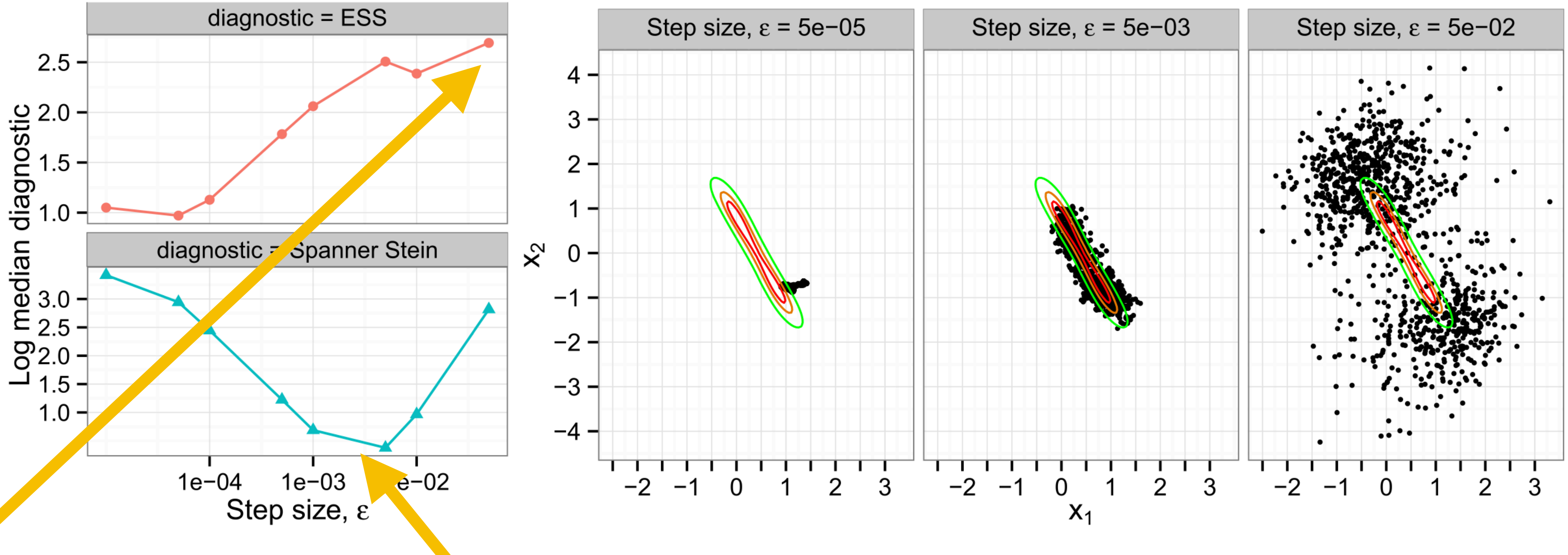

Identifies sampler which jumps around too much…

Correctly identifies good sampler!

Overview: measuring sample quality with Stein's method

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$$\mathrm{SD}(P\,||\,Q_n)$$

- This allows us to answer concretely many questions that were previously completely intractable from a computational viewpoint…!

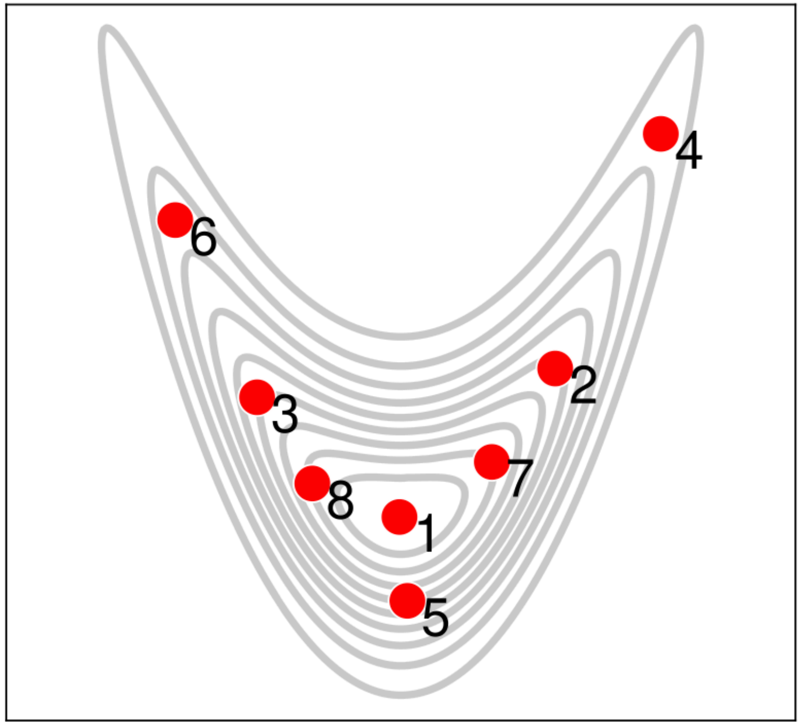
Stein’s method as a computational tool

Deterministic approximations of probability distributions

Deterministic approximations

- Suppose we have a target distribution P.
- We would like a very good approximation of the form:

$$P \approx \frac{1}{n}\sum_{i=1}^{n} \delta_{x_i}$$



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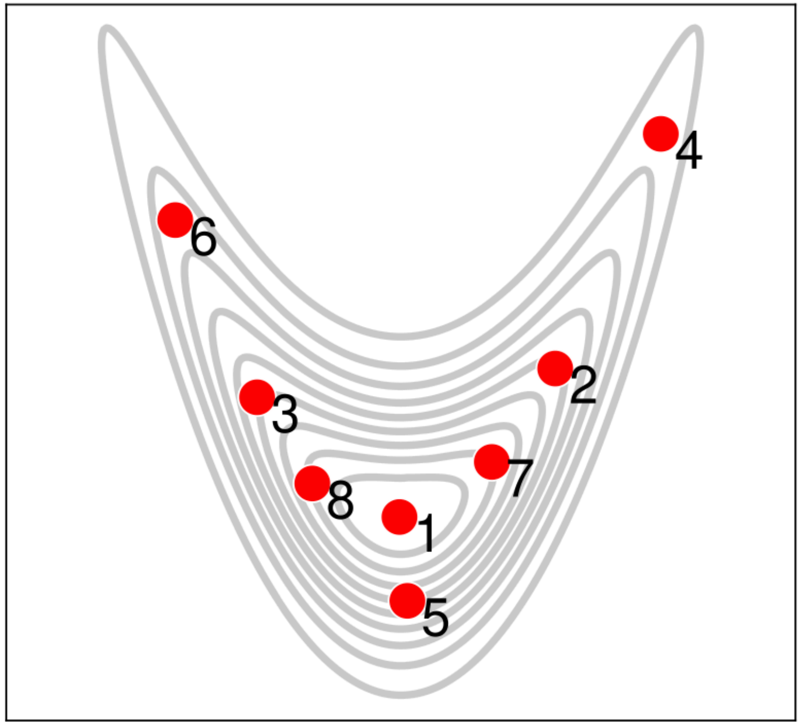
- The main question is:

"How should we pick the points $x_1, \ldots, x_n$?"



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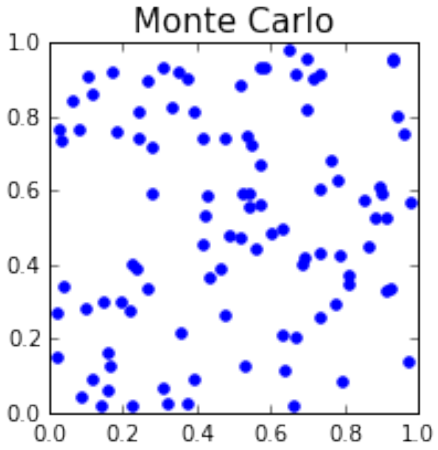

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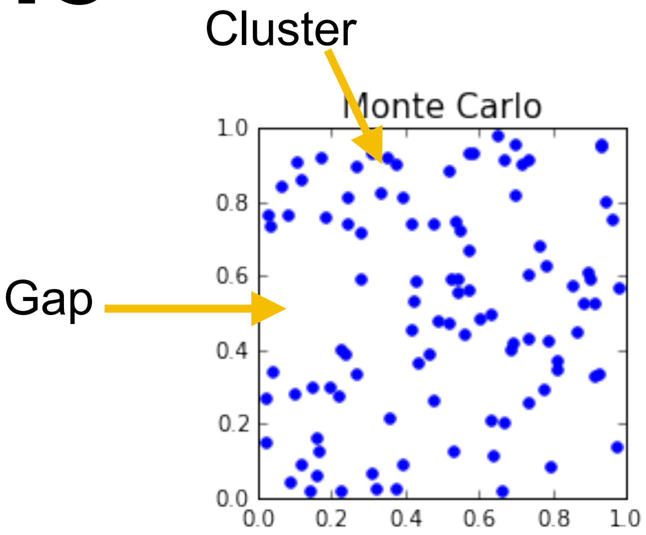

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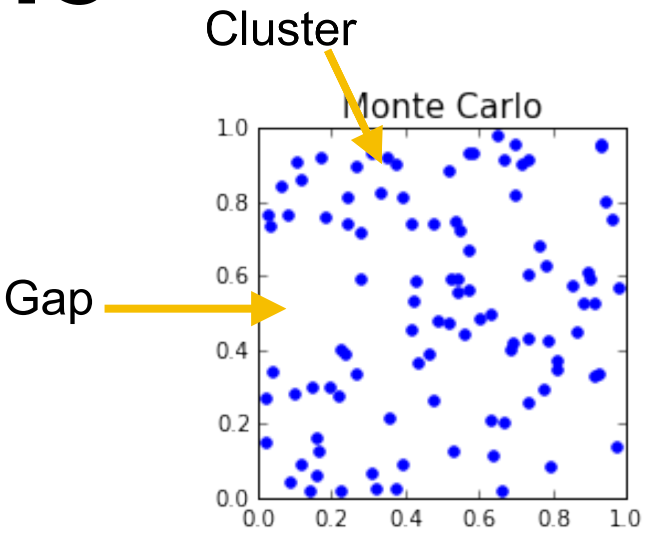
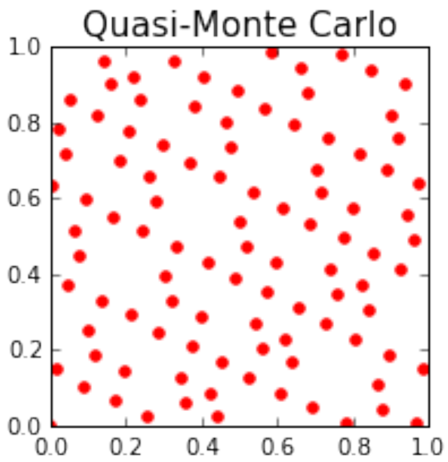
- Instead, a zoo of deterministic point sets or sequences have been proposed under the name **Quasi-Monte Carlo.**





High-level idea behind QMC

- QMC points aim to do the following:

$$D\left(P, \frac{1}{n}\sum_{i=1}^{n} \delta_{x_i}\right) \to 0 \qquad \text{at a “fast” rate as} \qquad n \to \infty$$

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- D is typically the **star discrepancy.**

The star discrepancy

- The **star discrepancy** is a function of a dataset which tells us how spread out these point are over the domain.

$$D_{\text{star}}\left(U([0,1]^d), \frac{1}{n}\sum_{i=1}^{n}\delta_{x_i}\right)$$

$$= \sup_{B=[0,B_1)\times\ldots\times[0,B_d)} \left| \frac{\text{\#points in } B}{n} - \text{Vol}(B) \right|$$

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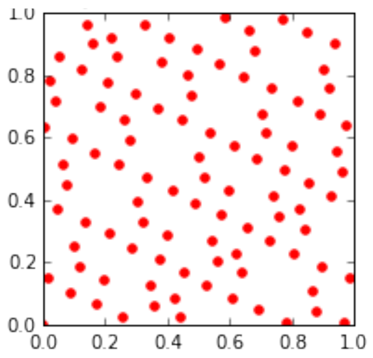

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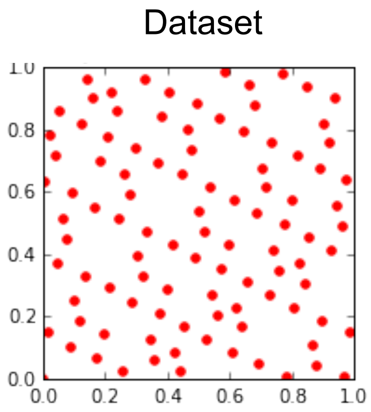

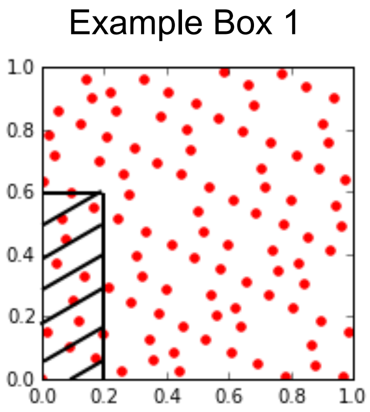

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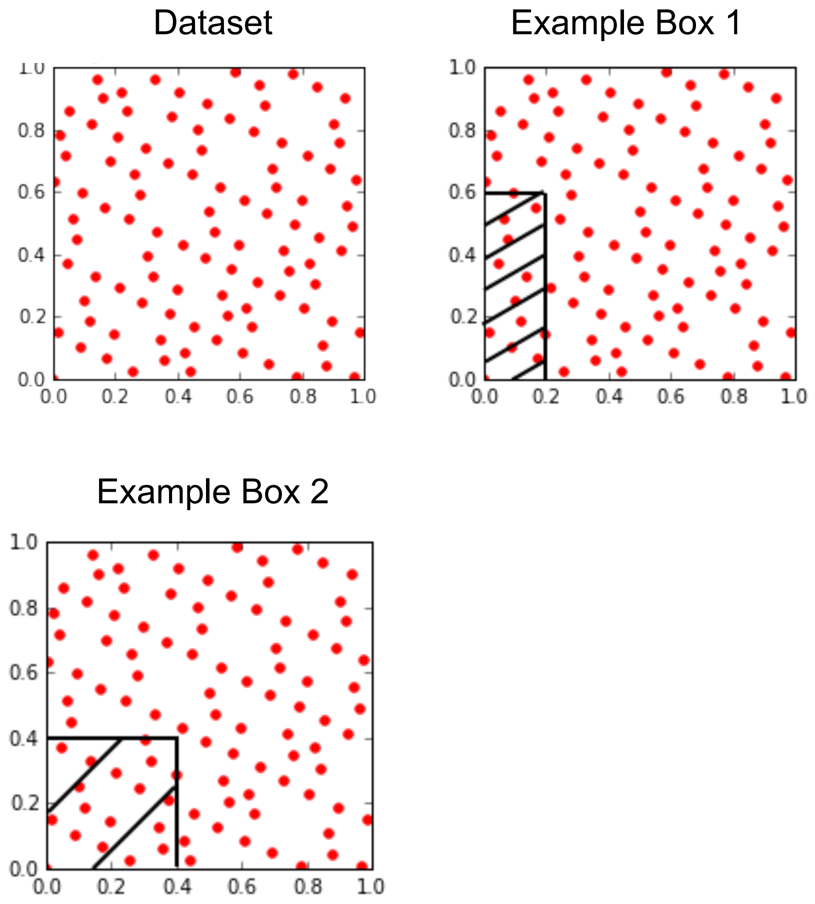

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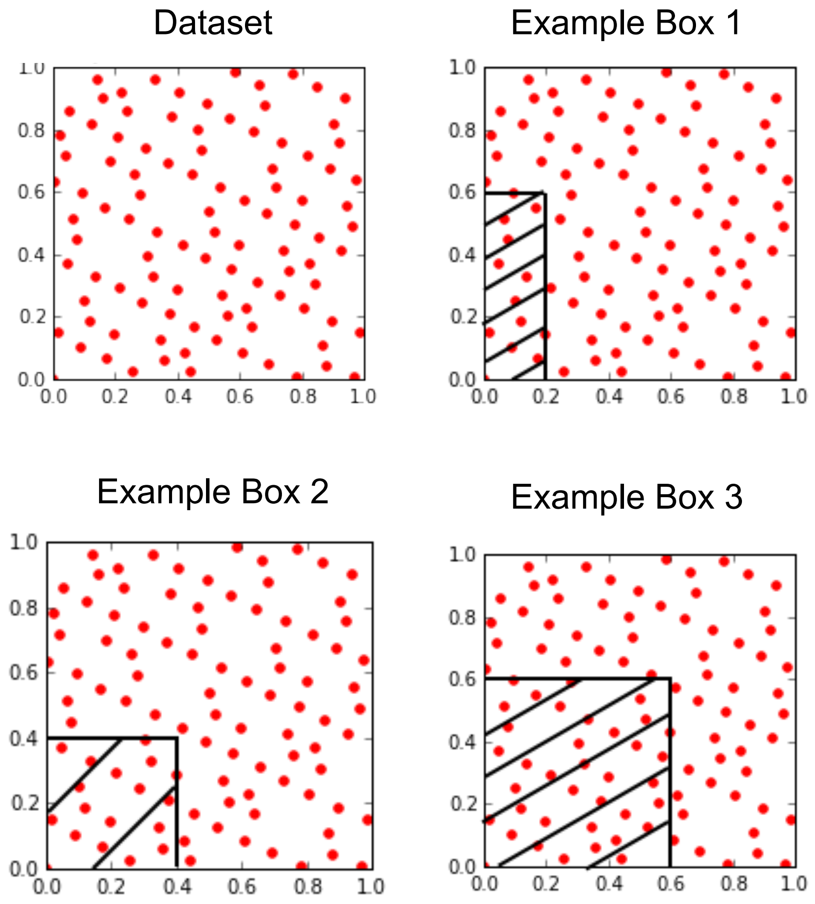

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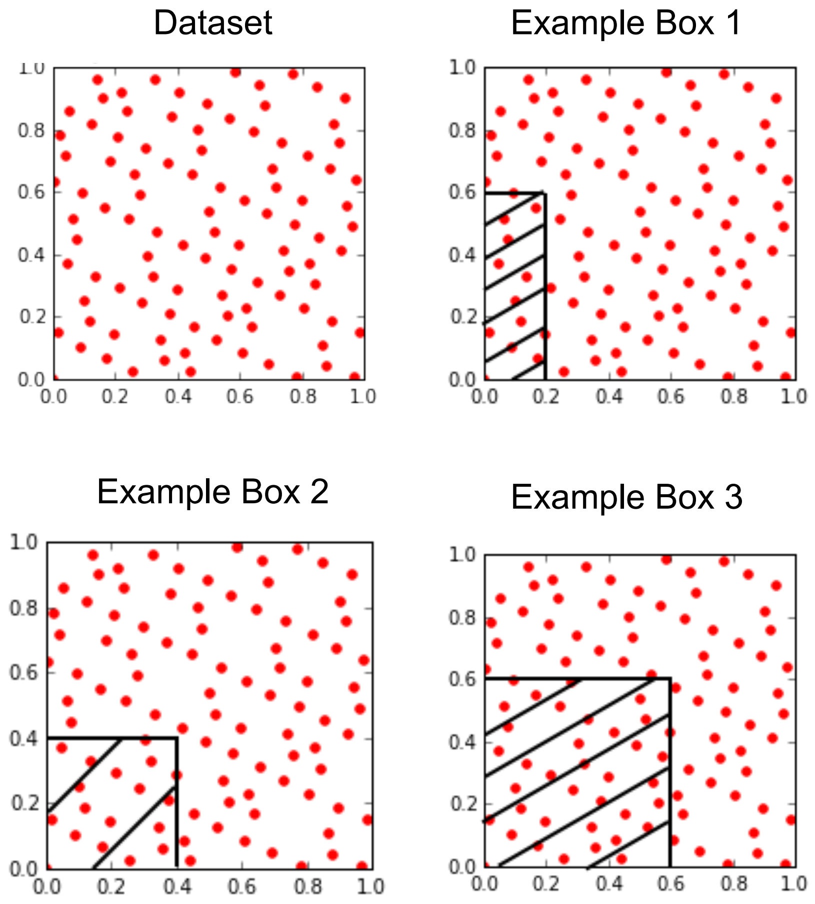

- It can also be thought of as a measure of dissimilarity between our dataset and a $U([0,1]^d)$!

Low-discrepancy sequences

- The star discrepancy is a convenient choice since we have that:

$$\left| \mathbb{E}_{X\sim P}[f(X)] - \frac{1}{n}\sum_{i=1}^{n} f(x_i) \right| \leq V(f) \times D_{\text{star}}\left(U([0,1]^d), \frac{1}{n}\sum_{i=1}^{n} \delta_{x_i} \right)$$

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Integration error

Complexity of the function

Star discrepancy

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→ A major limitation of this approach is that you can only approximate $P = \text{Unif}([0,1]^d)$!

Stein Points

- Choosing another discrepancy (i.e. our favourite hammer) can lead to more practical algorithms:

$$\arg \min_{x_1,\ldots,x_n \in \mathbb{R}^d} \mathrm{KSD}\left(P \,\middle|\middle|\, \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i} \right)$$

- This is still a very high-dimensional and non-convex optimisation problem, so we need to introduce some approximation….

Chen, W. Y., Mackey, L., Gorham, J., **Briol, F-X.**, & Oates, C. J. (2018). Stein points. *ICML*, 1320–1350.

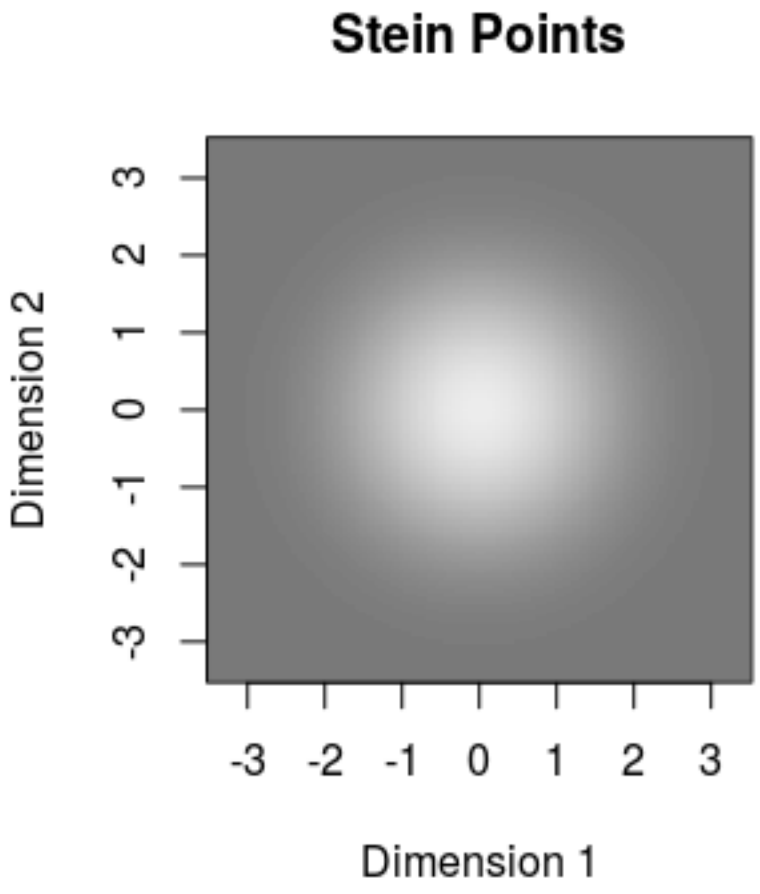
Chen, W. Y., Barp, A., **Briol, F-X**., Gorham, J., Girolami, M., Mackey, L., & Oates, C. J. (2019). Stein point Markov chain Monte Carlo. *ICML*, 1737–1767.

Greedy Stein Points

- We choose points one at a time to decrease the KSD the most.
- Thanks to the nice expression for the KSD, this simply becomes:

$$x_n \in \arg\min_{x \in \mathbb{R}^d} \text{KSD}\left(P \middle|\middle| \frac{1}{n}\sum_{i=1}^{n-1} \delta_{x_i} + \frac{1}{n}\delta_x\right)$$

$$= \arg\min_{x \in \mathbb{R}^d} \frac{k_P(x,x)}{2} + \sum_{i=1}^{n-1} k_P(x_i, x)$$



Example: 2d-Gaussian.

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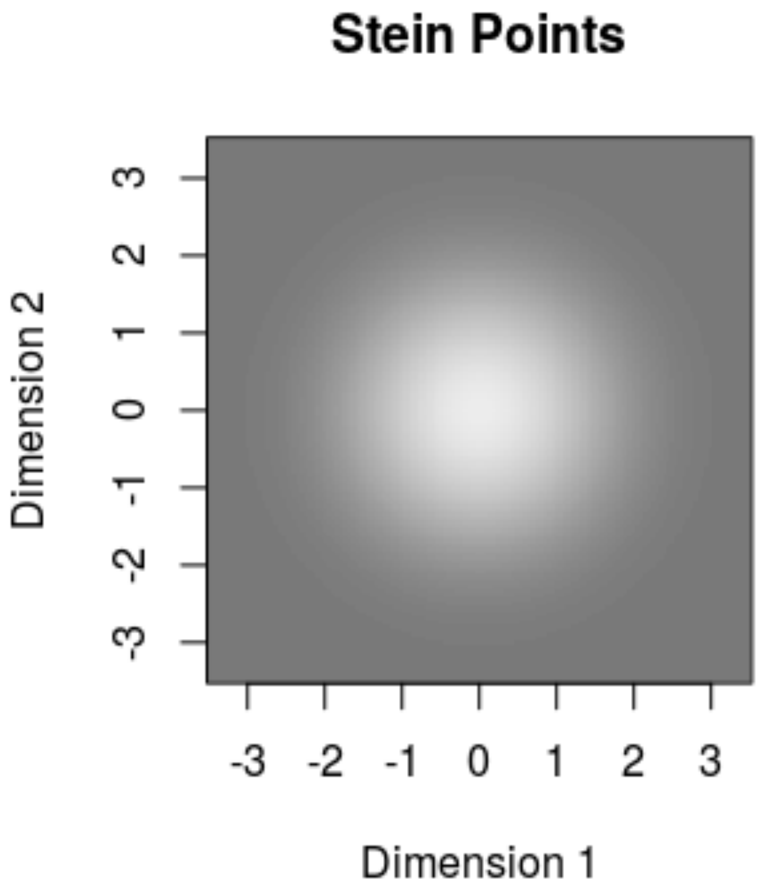

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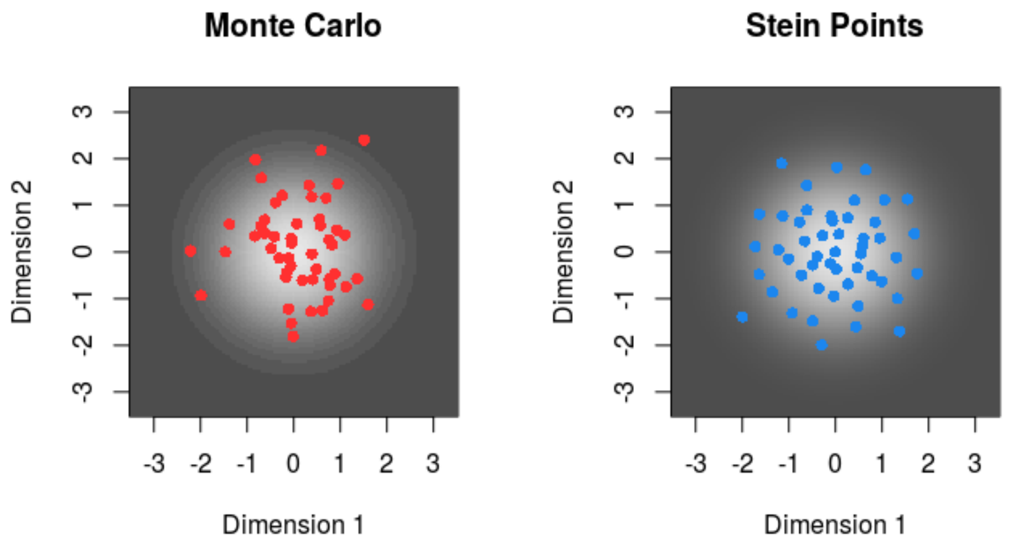
Greedy Stein Points on Gaussian



$$\mathbb{E}_{X\sim P}[f(X)] = ?$$

$$f(x) = \sin(x_1) + \sin(x_2) \qquad P = N(0, I_{2\times 2})$$

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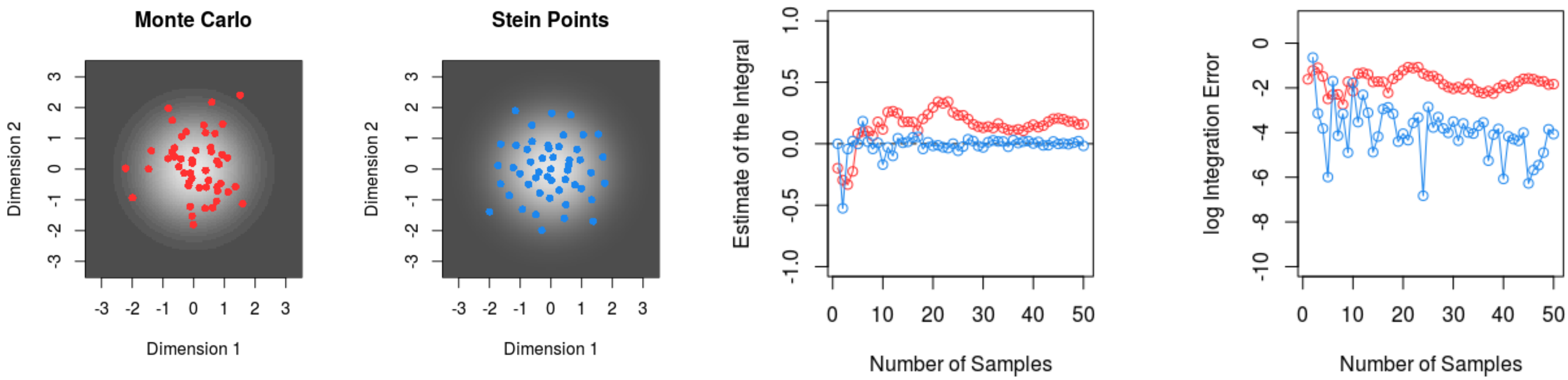

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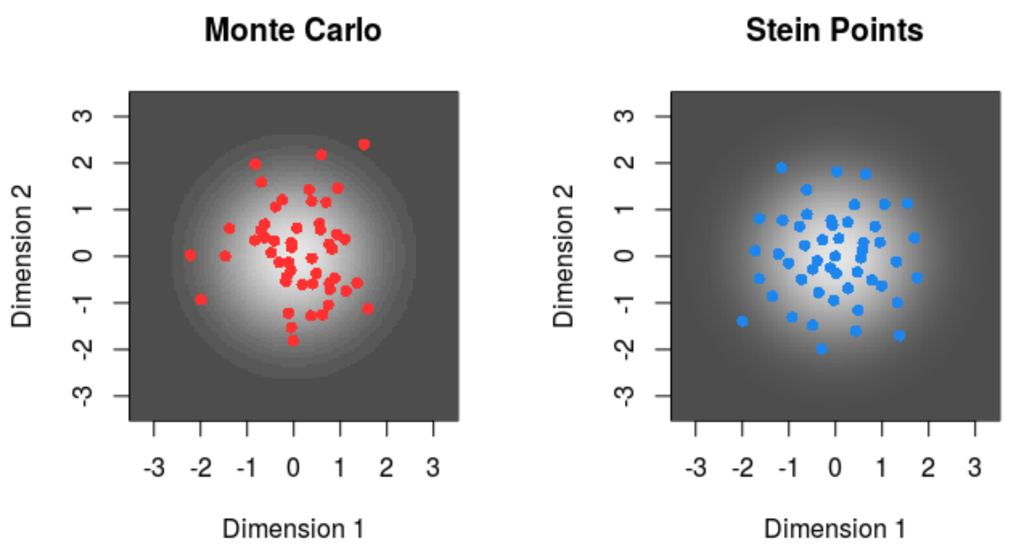

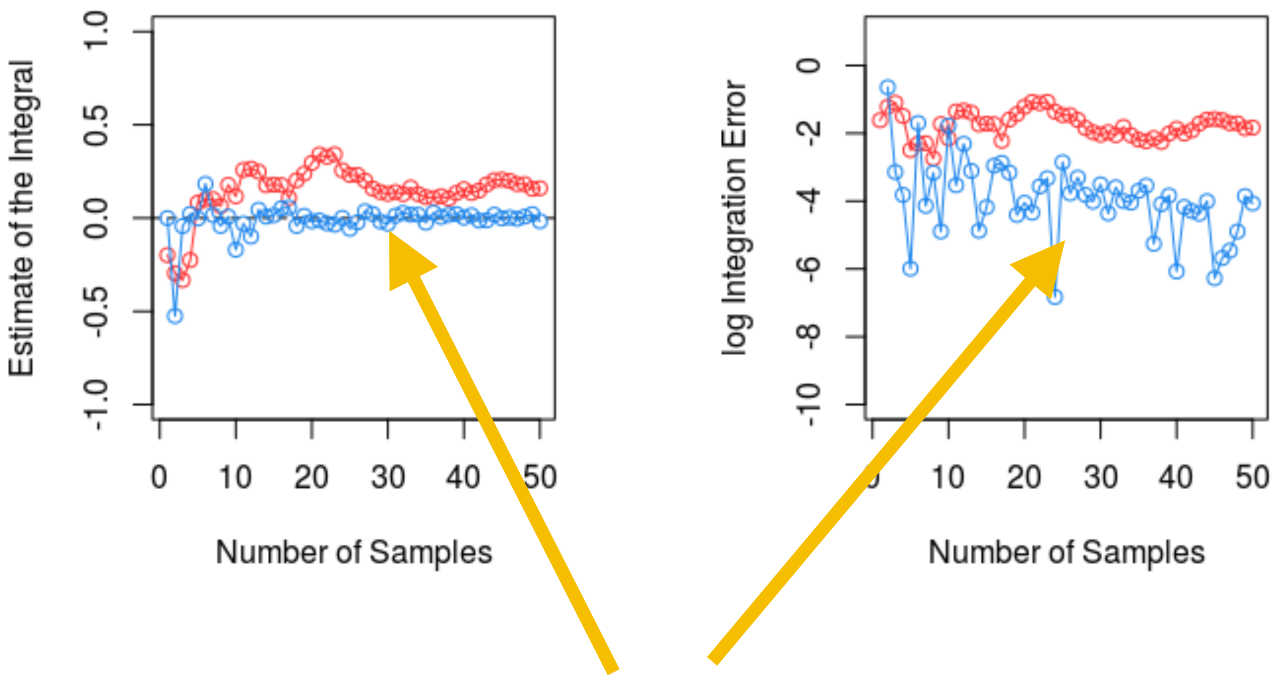

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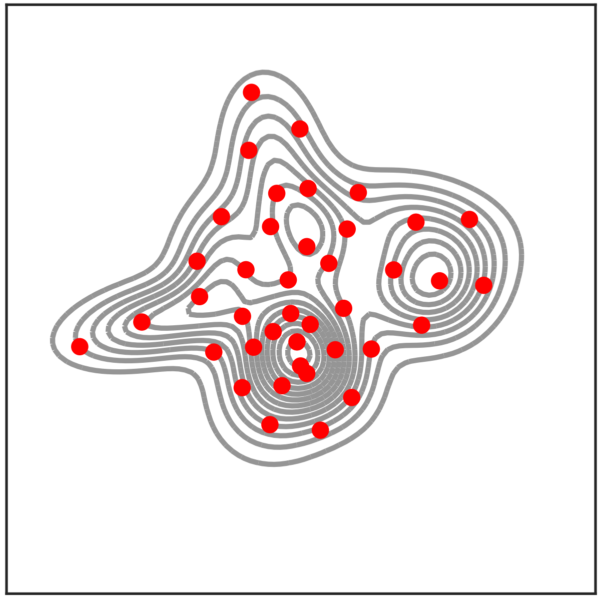
Convergence is much faster for Stein Points than Monte Carlo!

Stein Points for complex targets

- One of the main advantages of Stein points is that we can approximate any distribution P for which we have a suitable Stein characterisation!

- This includes complex probabilistic models, or Bayesian posterior distributions!



https://github.com/wilson-ye-chen/stein_points

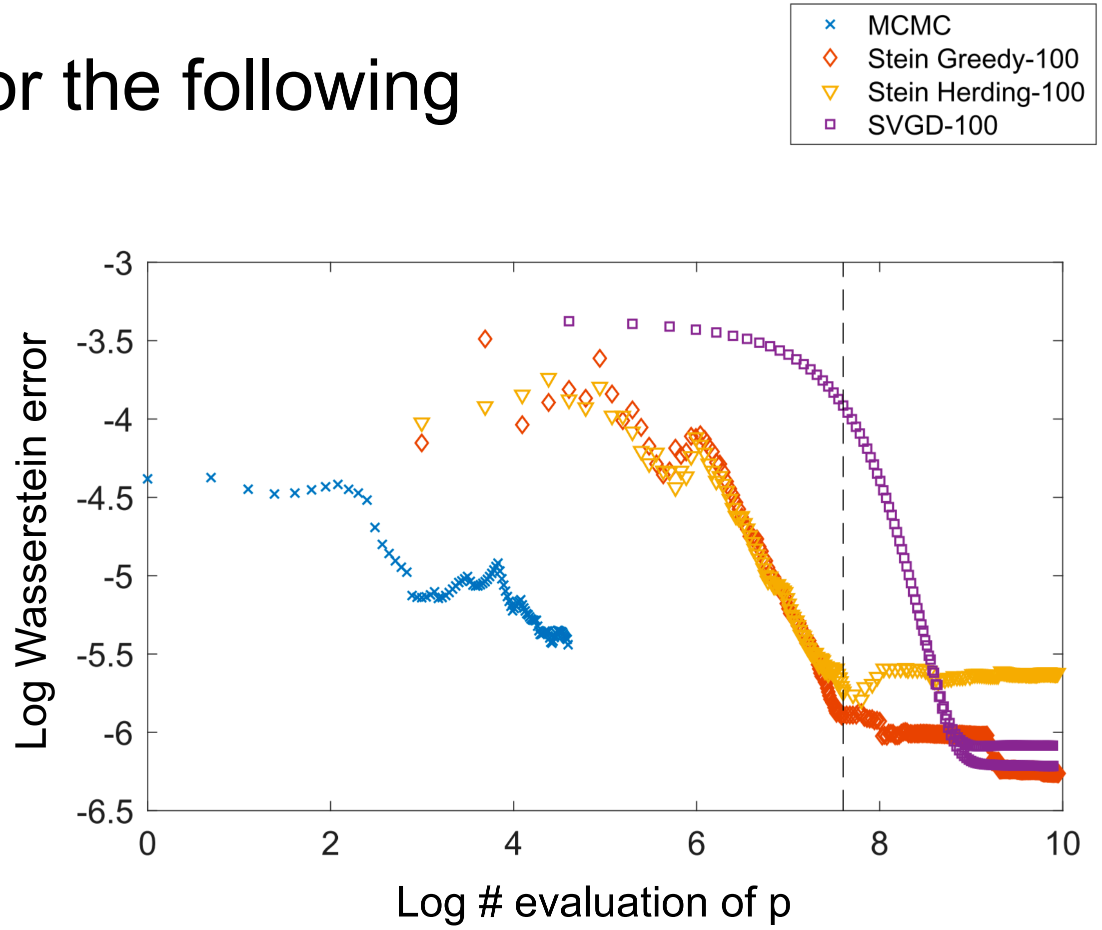
https://github.com/wilson-ye-chen/sp-mcmc

Example: IGARCH posterior

- Consider some Bayesian posterior for the following time-series model:

$$y_t = \sigma_t \epsilon_t, \quad \epsilon_t \sim N(0,1)$$

$$\sigma_t^2 = \boxed{\theta_1} + \boxed{\theta_2} y_{t-1}^2 + (1 - \boxed{\theta_2})\sigma_{t-1}^2$$



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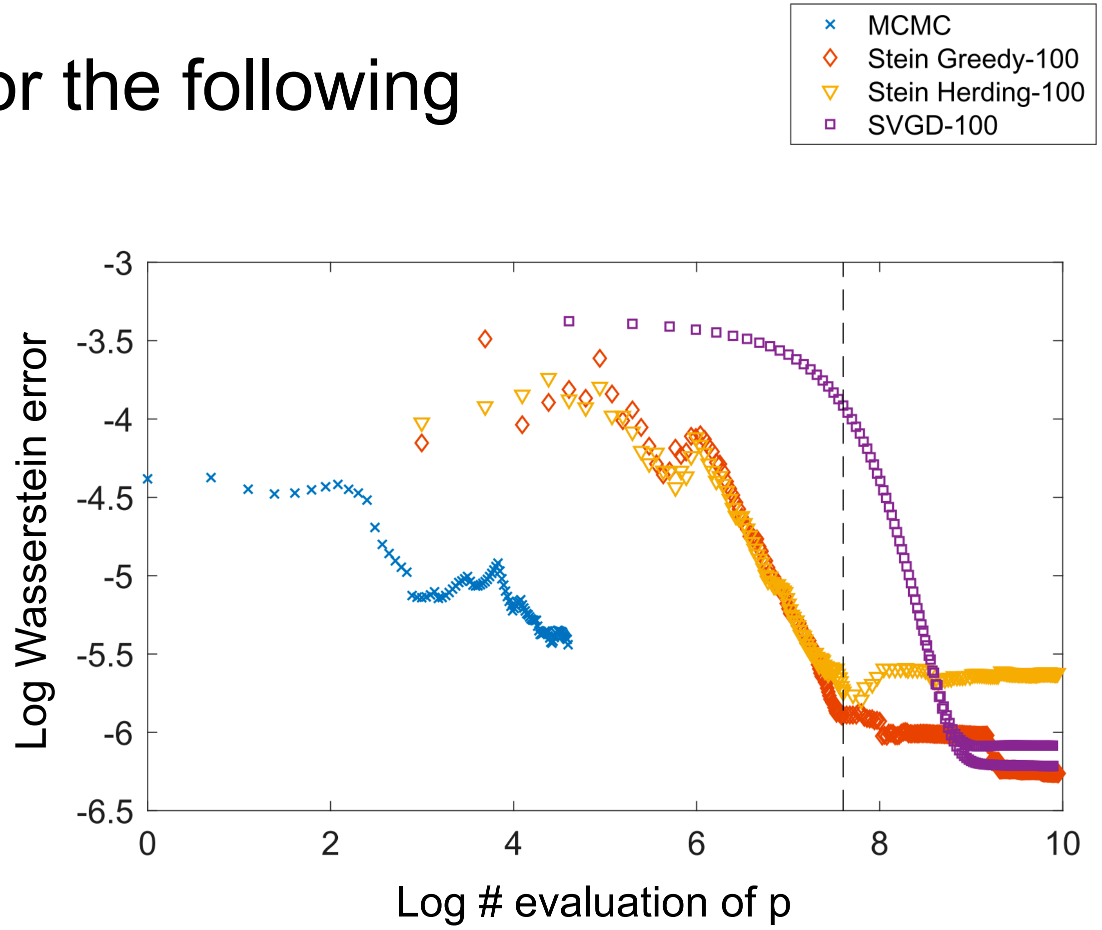
- Stein points give much smaller Wasserstein distance approximation than MCMC!



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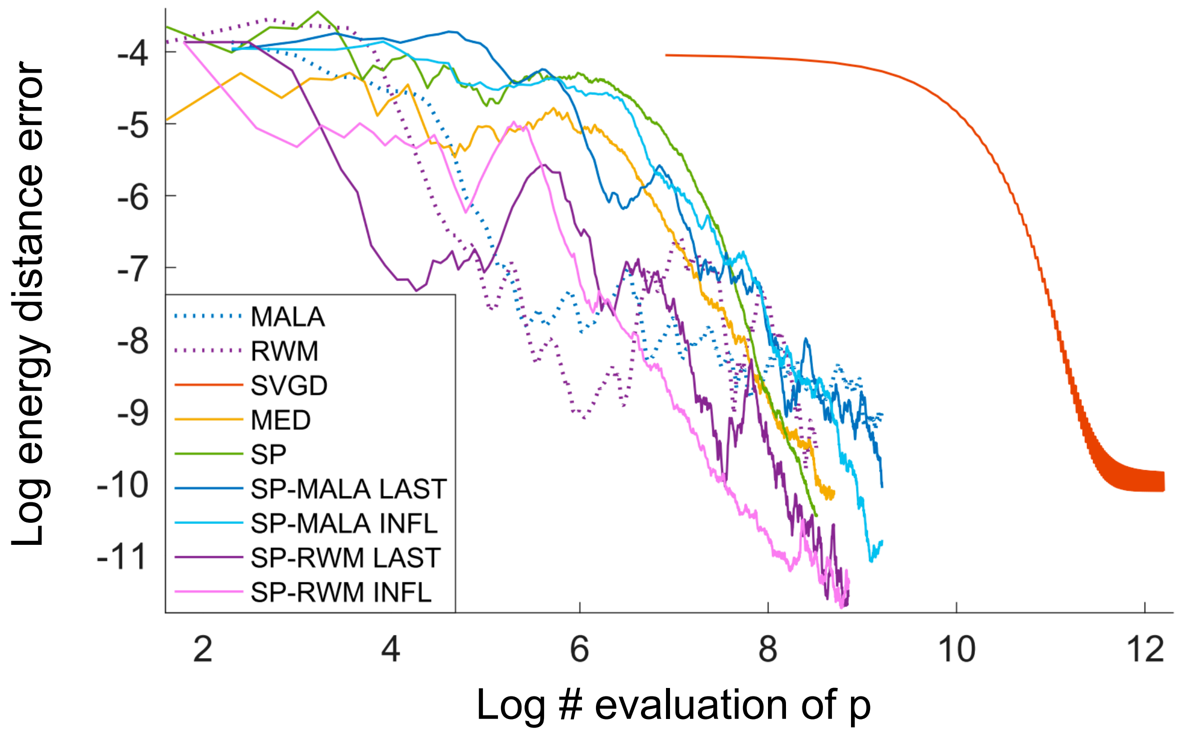

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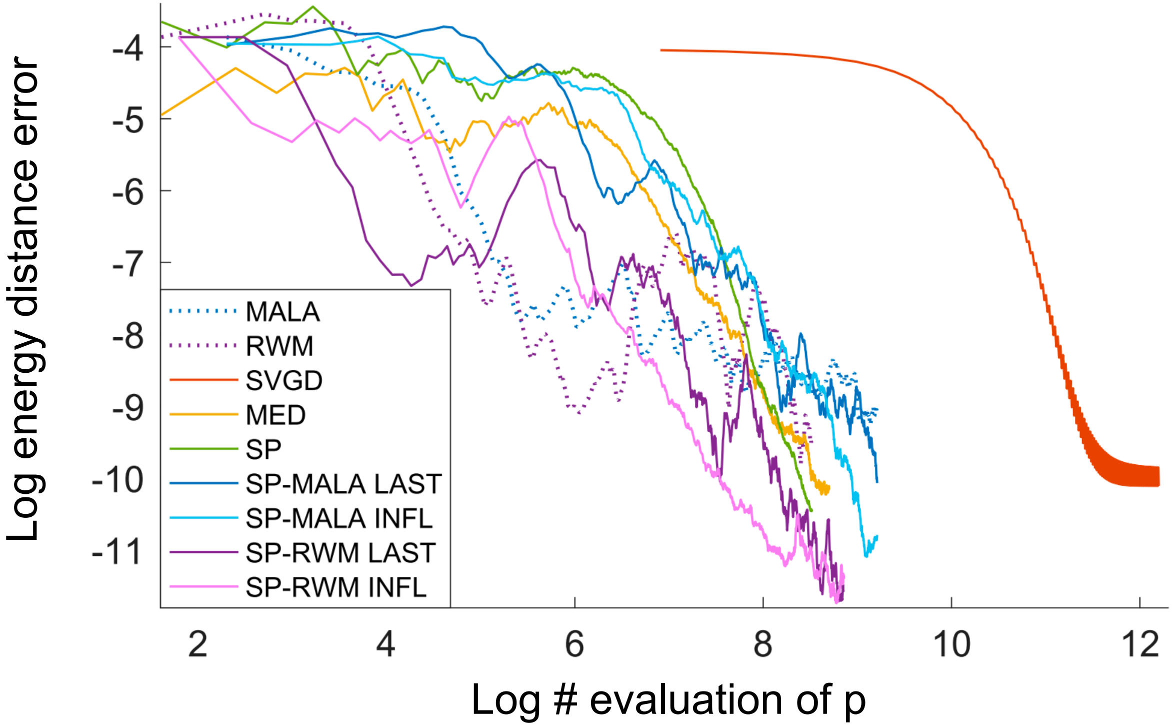
- Advanced versions of Stein Points can do much better…



Stein's method as a computational tool

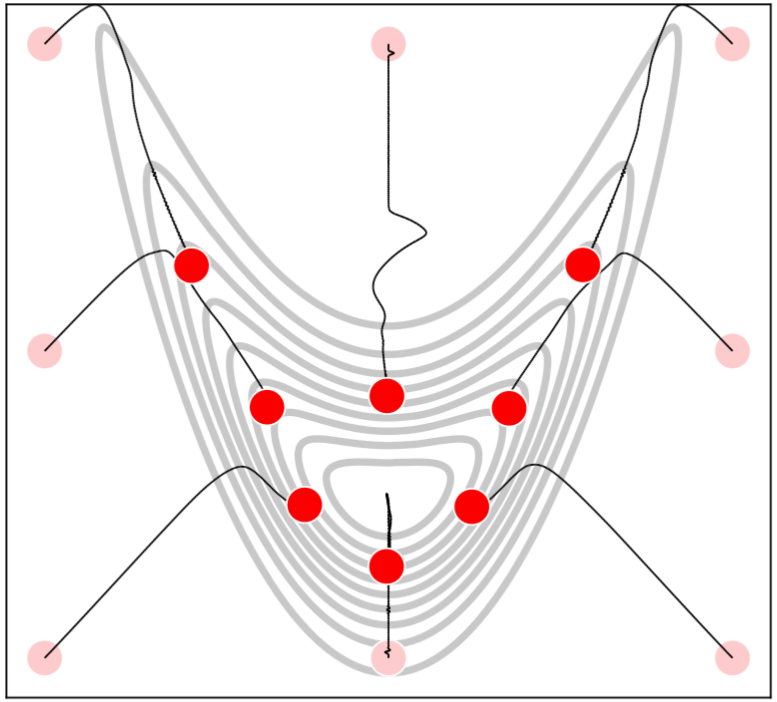
Stein Variational Gradient Descent

Particle-based approximations

Stein Variational Gradient Descent: A General Purpose Bayesian Inference Algorithm

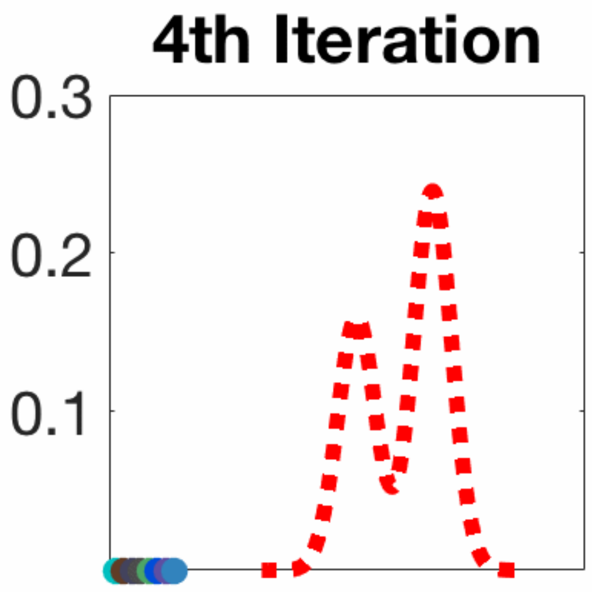
Qiang Liu **Dilin Wang**
Department of Computer Science
Dartmouth College

Stein Variational Gradient Descent



Particle-based approximations

- We are still interested in approximating some distribution P.
- This time, we start with some particles which we then move towards P.



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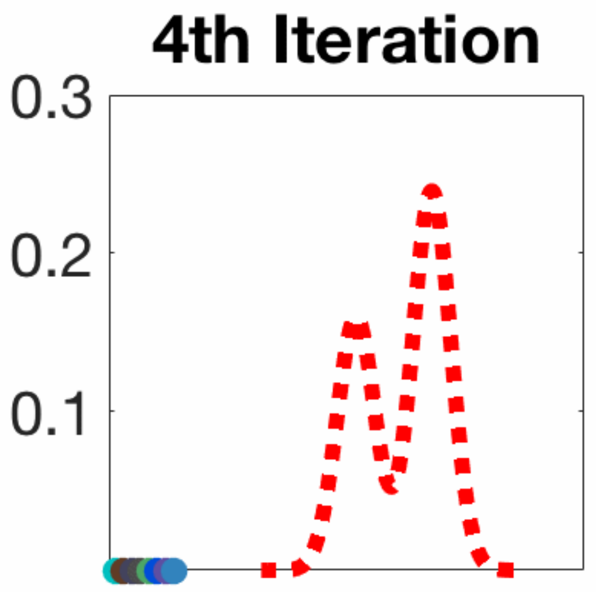

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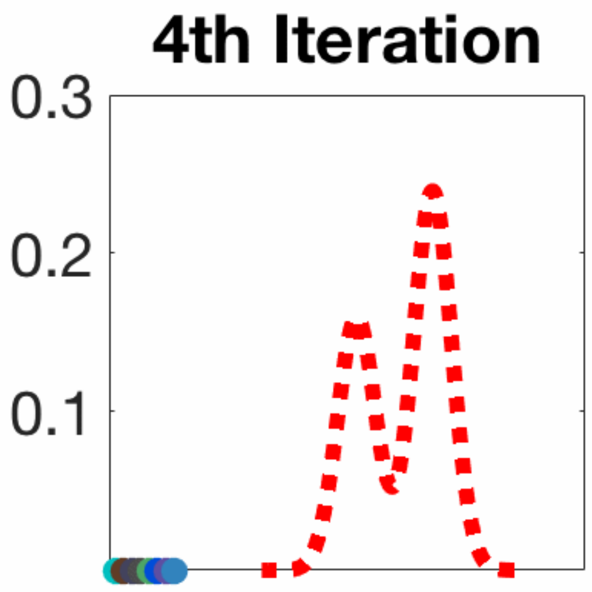

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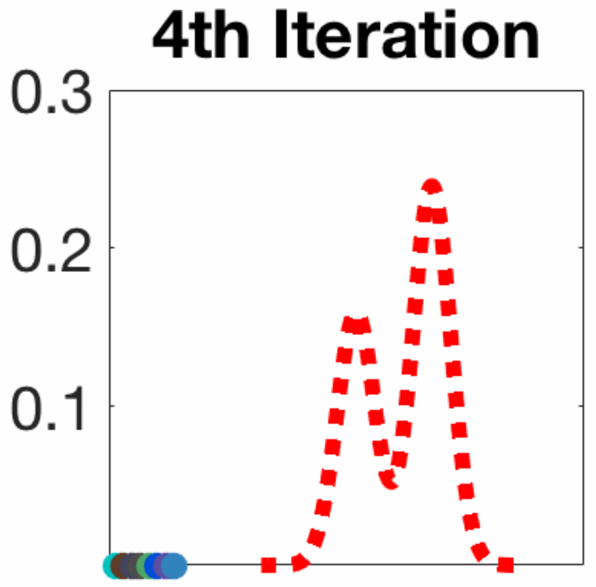
Current Position — Step-size — Direction of move



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SVGD as transport of measure

- The algorithm mostly relies on this identity:

$$\max_{g \in \mathcal{G}} \left\{ -\frac{d}{d\epsilon} \mathrm{KL}\left(\Phi^g_{\#} Q \,||\, P \right) \Big|_{\epsilon=0} \right\} = \mathrm{KSD}(P \,||\, Q)$$

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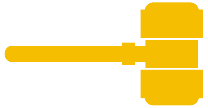

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- The best transport map is therefore the function:

$$g^*_{Q,P}(\cdot) \propto \mathbb{E}_{X \sim Q}[\nabla \log p(X) k(X, \cdot) + \nabla_x k(X, \cdot)]$$

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Stein variational gradient descent (SVGD)

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for every iteration $t = 1,2,\ldots,T$.

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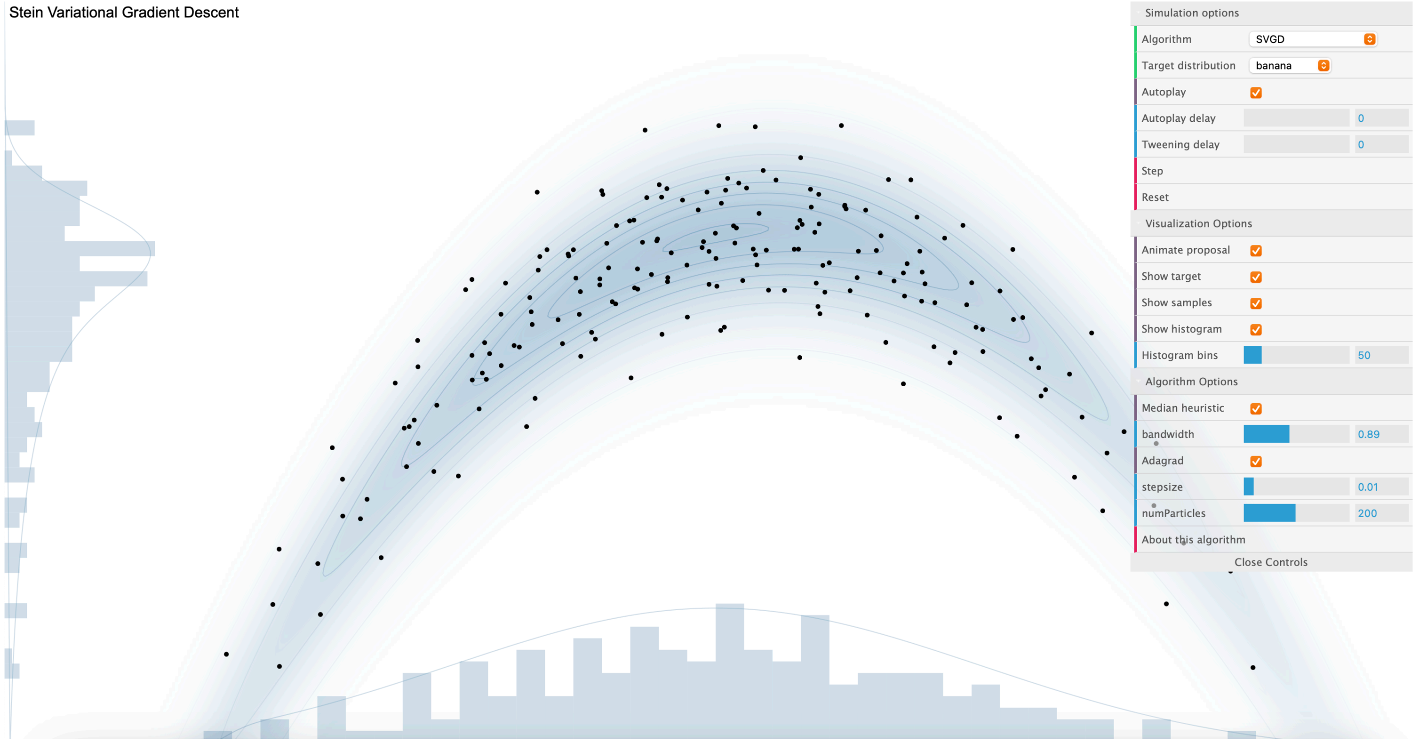
Pushes particles towards regions of high prob under P

Pushes particles away from one another ("repulsive force")

SVGD in practice



https://chi-feng.github.io/mcmc-demo/app.html?algorithm=SVGD

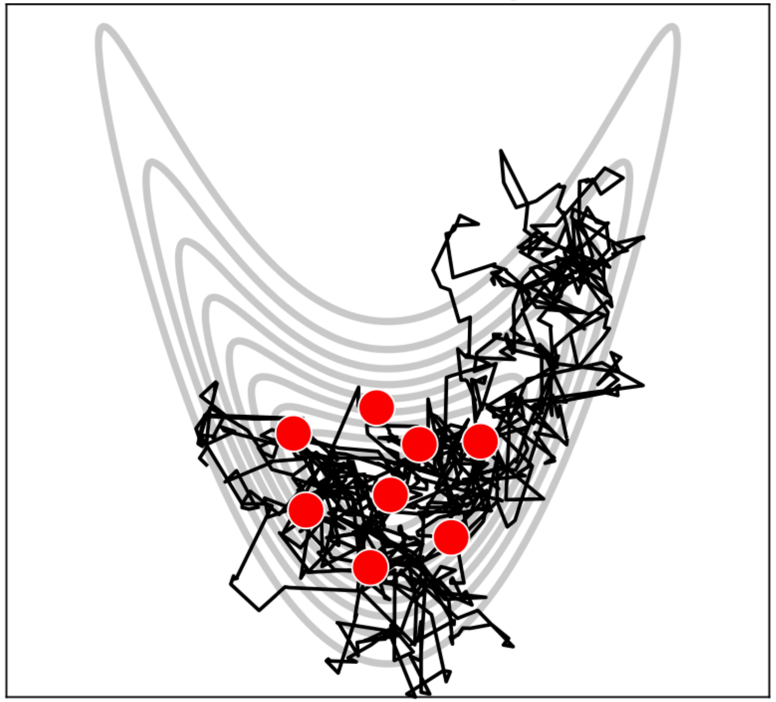
Stein’s method as a computational tool

Thinning MCMC

Thinning MCMC

- Suppose we would like to compute some predictive distribution:

$$p(y^* \mid x^*, x_1, \ldots, x_n, y_1, \ldots, y_n) = \int_\Theta p(y^* \mid x^*, \theta) p(\theta \mid x_1, \ldots, x_n, y_1, \ldots, y_n) d\theta$$



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Expensive likelihood

Posterior distribution
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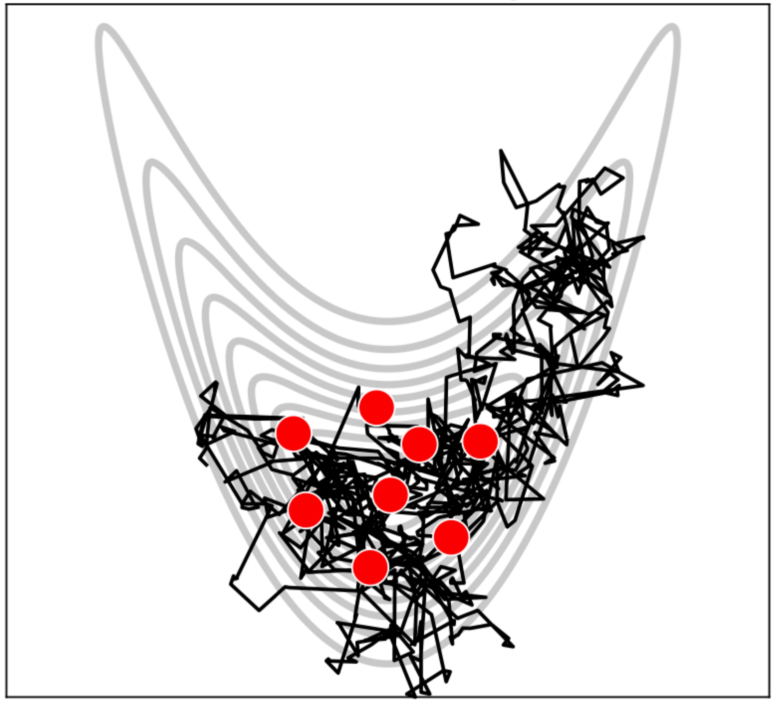

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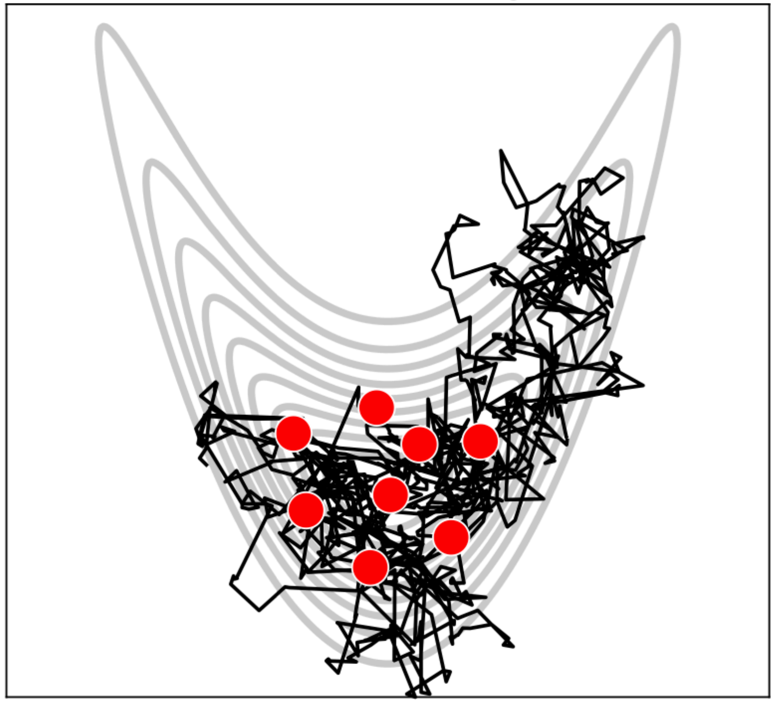

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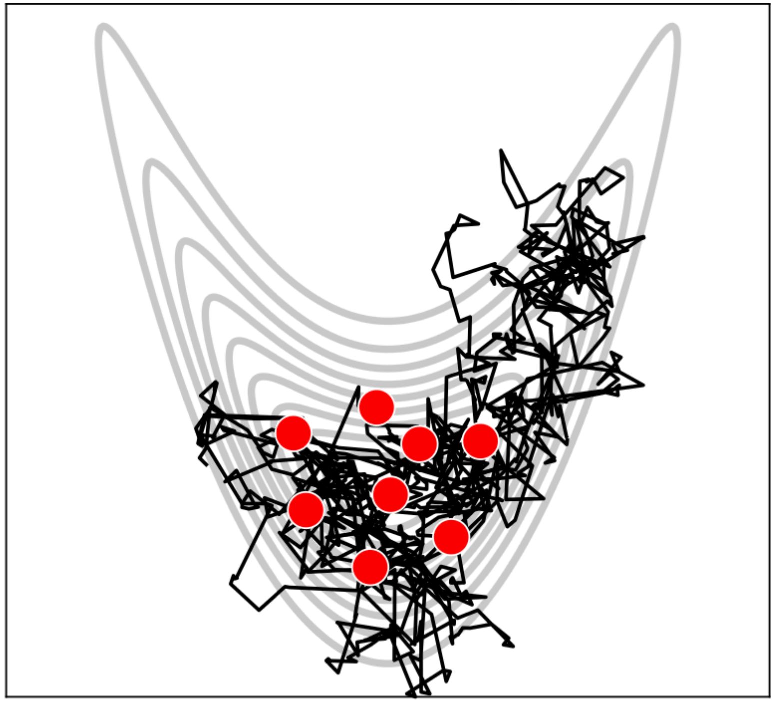

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- **Solution:** Thinning our MCMC sampler!

Thinning MCMC

- The simplest method is independent sub-sampling.
- …but the independence can be quite **wasteful** as we might end up with some very similar samples!

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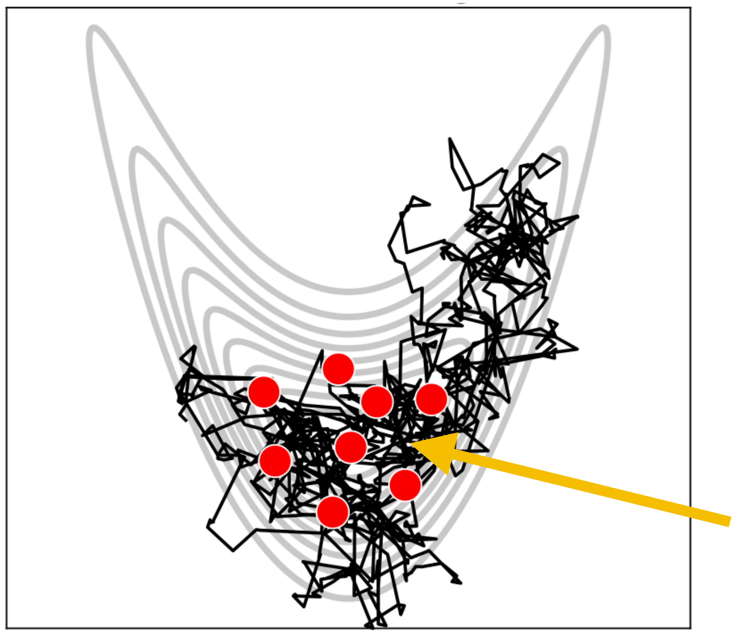

We ideally want an approximation where points are far from one another but concentrated in region of high probability mass…

Stein thinning

- Let's use our favourite hammer on this nail:

$$\arg \min_{\{x_i\}_{i=1}^n \subset \{y_i\}_{i=1}^N} \text{KSD}\left(P \middle|\middle| \frac{1}{n}\sum_{i=1}^{n} \delta_{x_i}\right)$$

Riabiz, M., Chen, W., Cockayne, J., Swietach, P., Niederer, S. A., Mackey, L., & Oates, C. J. (2022). Optimal thinning of MCMC output. *JRSSB*, *84*(4), 1059–1081.

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UCL

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Original approximation of P

- Similarly to Stein points, this is usually intractable so we select one point at a time.

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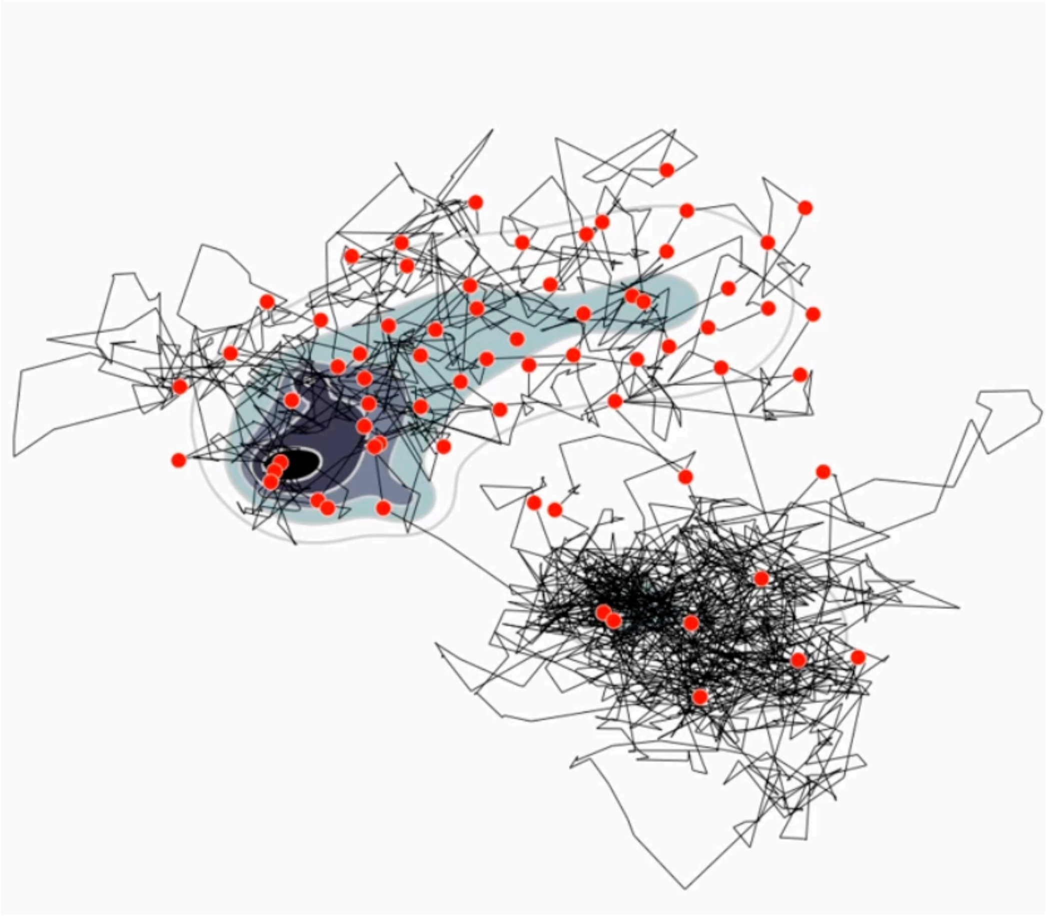
Stein thinning in practice



[https://en.wikipedia.org/wiki/File:Stein_Thinning_of_MCMC_output.webm]

Stein's method as a computational tool

Importance sampling

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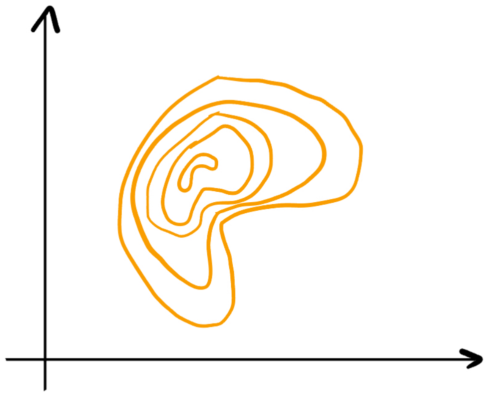

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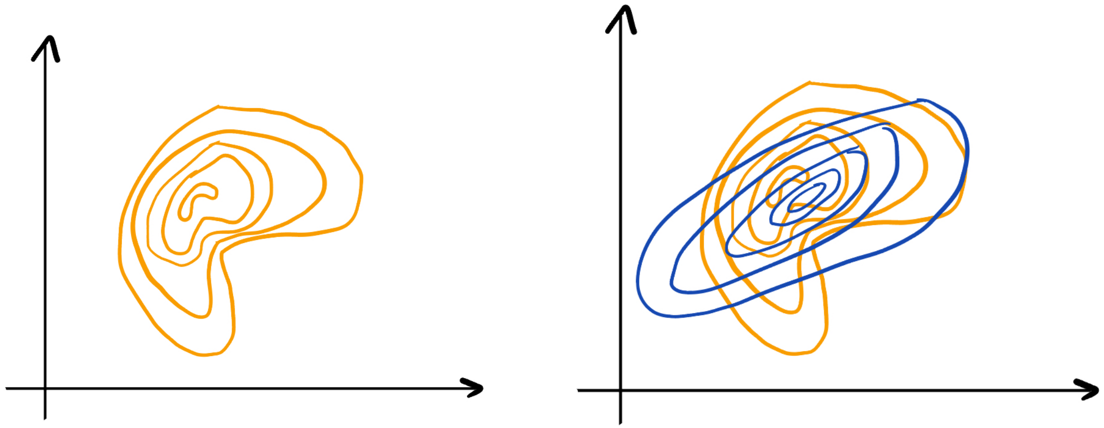

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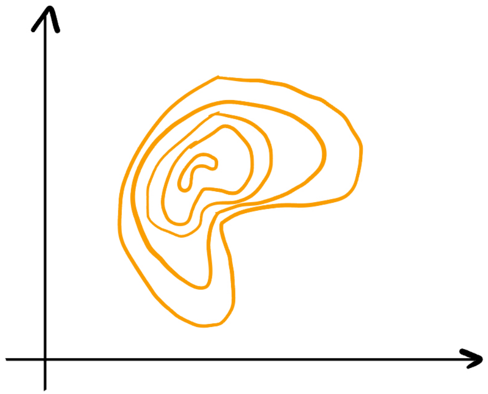

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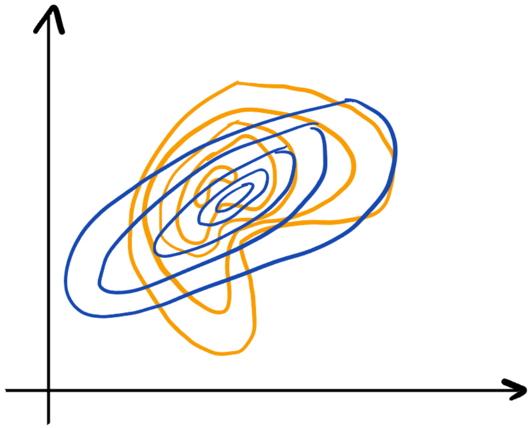

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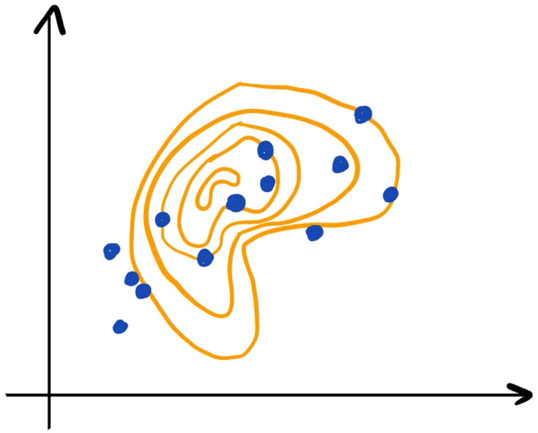

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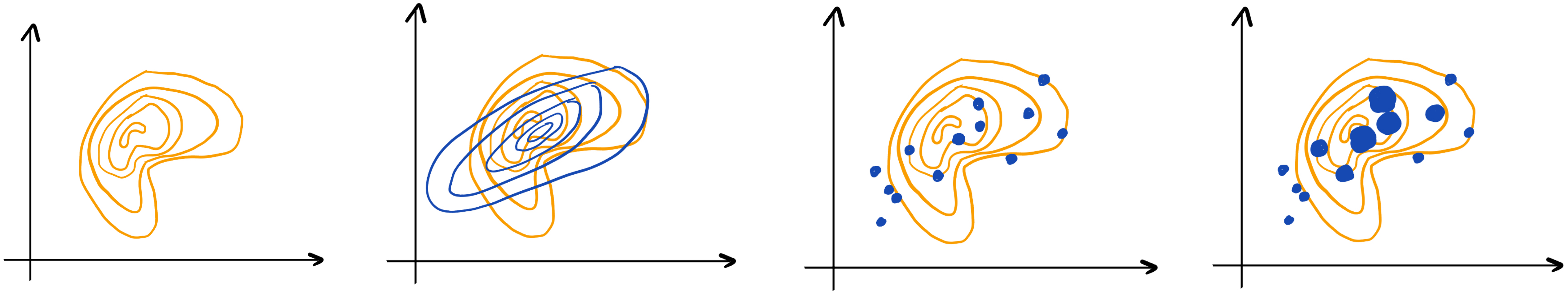

Target distribution P

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IIID realisations from importance distribution

Weighted samples from target distribution

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- To find the appropriate weights, we can use the following derivation:

$$\mathbb{E}_{X \sim P}[f(X)] = \int f(x)p(x)dx$$

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- **Question:** *“This choice of weights gives us good Monte Carlo estimators, but is it the best possible way to weight our samples?”*

Stein importance sampling

Stage 1: Sample $x_1, \ldots, x_n$ from some proposal P'

Stage 2: $$\arg \min_{w_1,\ldots,w_n \geq 0, \sum_{i=1}^n w_i = 1} \text{KSD}\left(P \,\Big|\Big|\, \sum_{i=1}^n w_i \delta_{x_i}\right)$$

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Gives a stable set of weights, and exact estimation for constant functions

- A standard approach for the proposal P' is to use a Markov chain which approximates the target P (or close enough).

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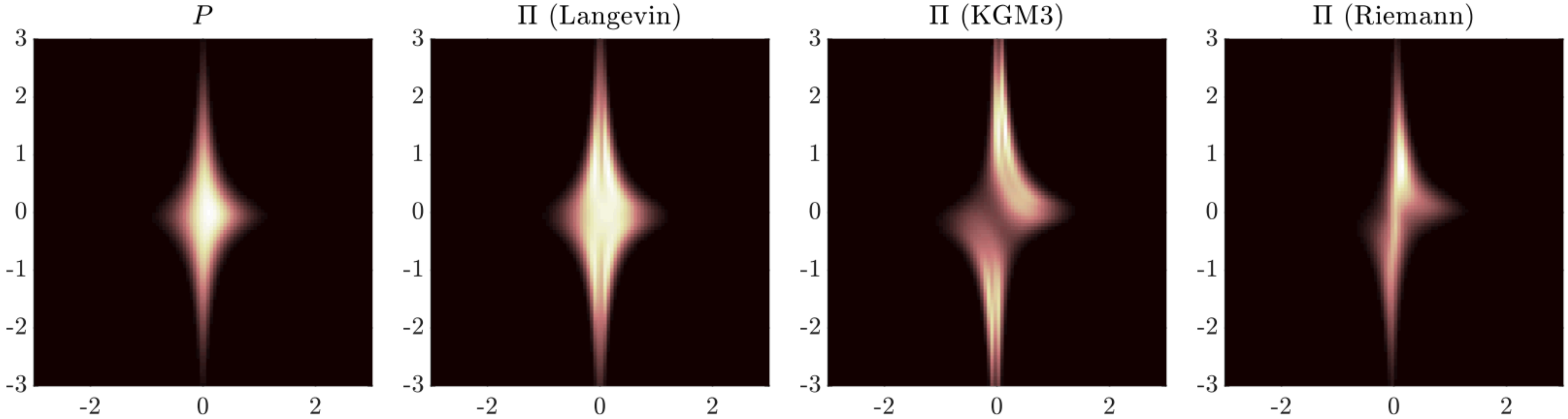
Stein importance sampling with different kernels



[Wang, 2023]

Overview: point set approximation with Stein's method

- We have seen many approaches (importance sampling, thinning, deterministic, gradient flows) to getting a good point set approximation of a target:

$$P \approx \sum_{i=1}^{n} w_i \delta_{x_i}$$

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→ Having a computable Stein discrepancy which can be used for most P's with unnormalised densities is a real asset here!

Stein’s method as a computational tool

Control variates for Monte Carlo

Monte Carlo methods

- We have already discussed extensively the need for good estimators of:

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- The above is for standard Monte Carlo, but similar results hold for MCMC, QMC, etc…

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- We therefore have a choice of estimator:

<u>Estimator 1</u>: Monte Carlo:

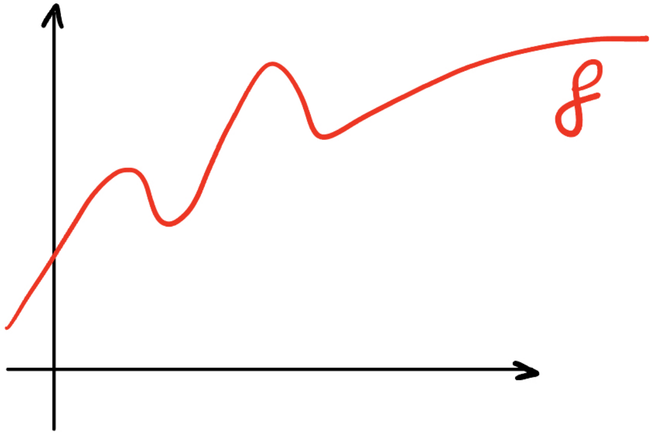
$$\mathbb{E}_{X\sim P}[f(X)] \approx \frac{1}{n}\sum_{i=1}^{n} f(x_i)$$

<u>Estimator 2</u>: Control Variate

$$\mathbb{E}_{X\sim P}[f(X)] \approx \frac{1}{n}\sum_{i=1}^{n} (f(x_i) - h(x_i)) + c$$

The control variate (CV)!

A sketch of control variate estimators



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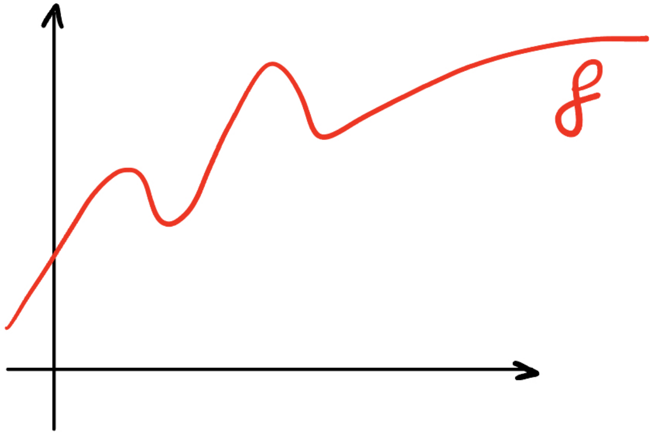

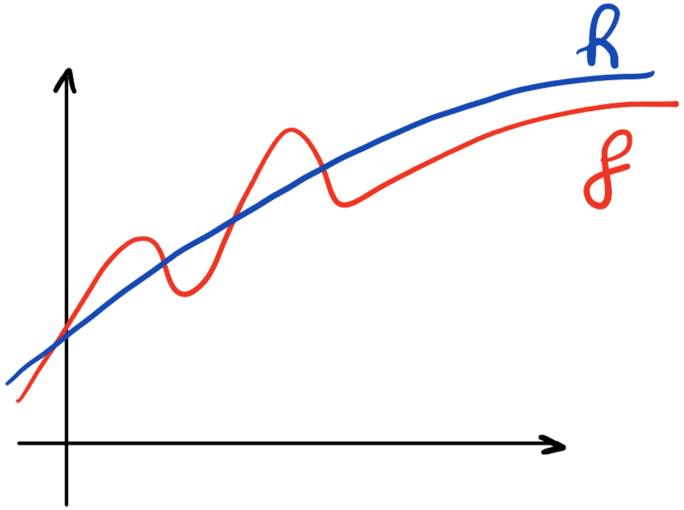

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Step 1: Find control variate h with known $\mathbb{E}_{X\sim P}[h(X)]$

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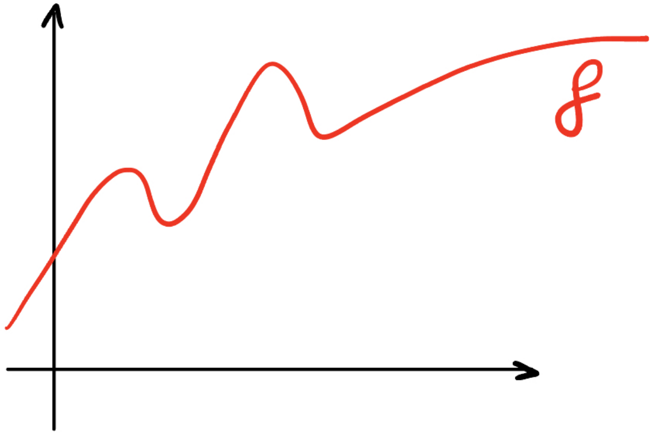

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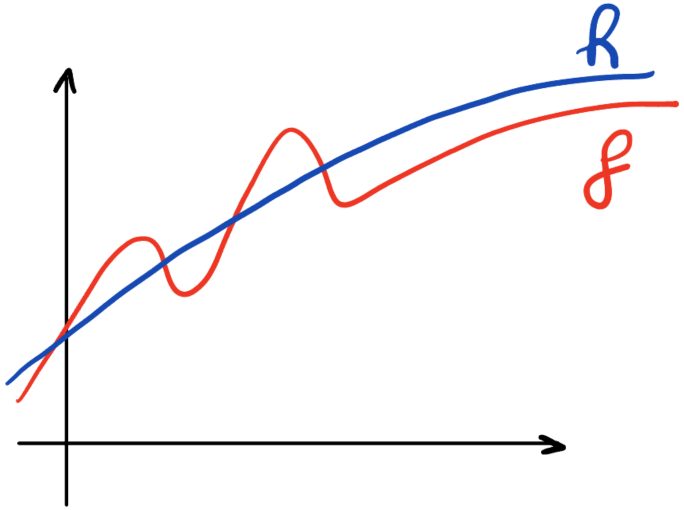

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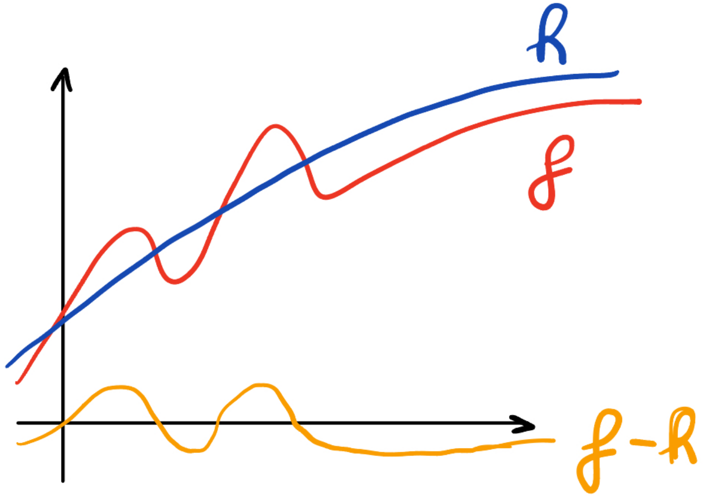

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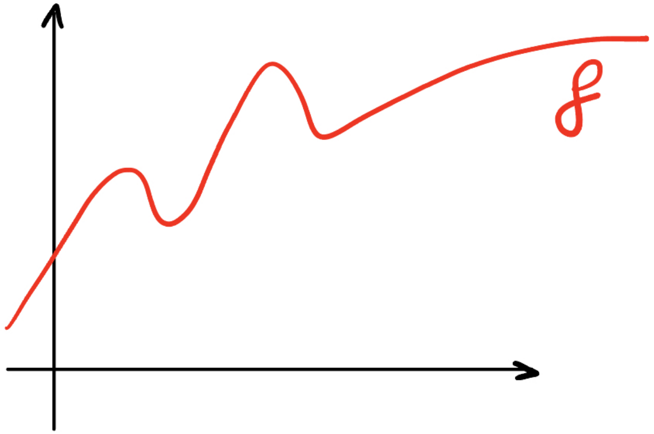

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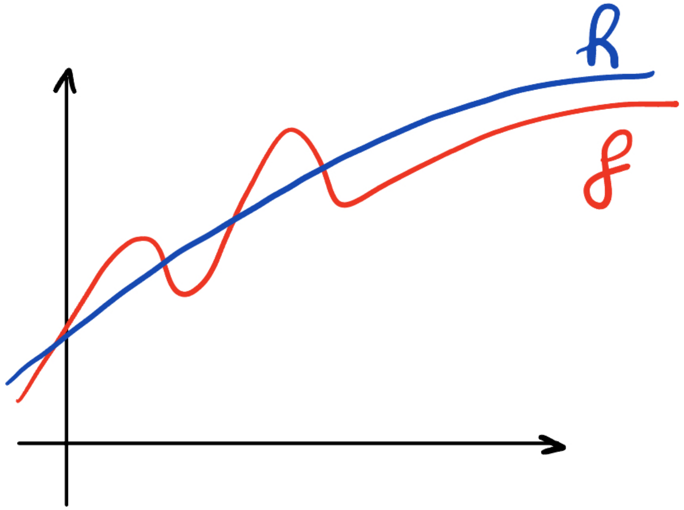

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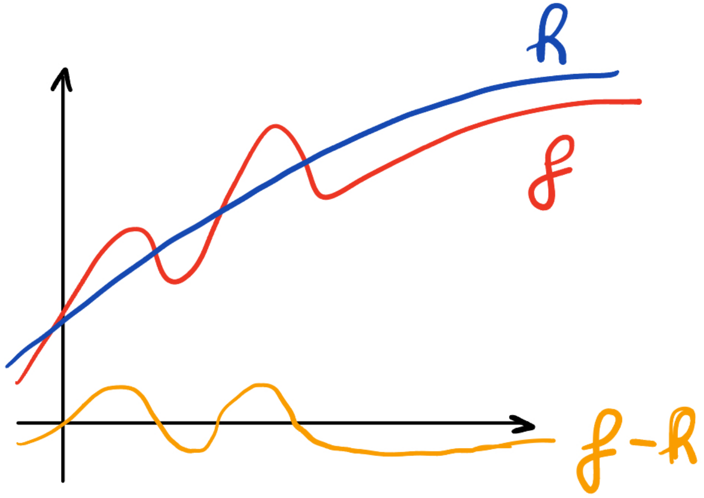

Step 2: Estimate $\mathbb{E}_{X\sim P}[f(X) - h(X)]$ with a Monte Carlo estimator

Turns out that if we choose h carefully, then the Monte Carlo estimator of $f - h$ will be much more accurate than the Monte Carlo estimator of f

Existing control variates

- Using the CLT, we see that the accuracy of control variate estimators depend on

$$\text{Var}[f - h]$$

- This leads to a few key questions:

"How do we guarantee that Var$[f - h] \ll$ *Var*$[f]$*?"*

"Can we choose h *to minimise Var*$[f - h]$*?"*

"How do we guarantee that we know the integral of h*?"*

Existing methods

- **Problem:** In general it is really hard to find a function $h : \mathbb{R}^d \to \mathbb{R}$ with known $E_{X \sim P}[h(X)]$.

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***Question:** What are we supposed to do when P is more complicated?*

Stein control variates

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- Initial work in Bayesian computation mostly used the equivalent of polynomial-based Stein control variates without realising they were using Stein!

Mira, A., Solgi, R., & Imparato, D. (2013). Zero variance Markov chain Monte Carlo for Bayesian estimators. *Statistics and Computing*, *23*(5), 653–662.

Papamarkou, T., Mira, A., & Girolami, M. (2014). Zero variance differential geometric Markov chain Monte Carlo algorithms. *Bayesian Analysis*, *9*(1), 97–128.

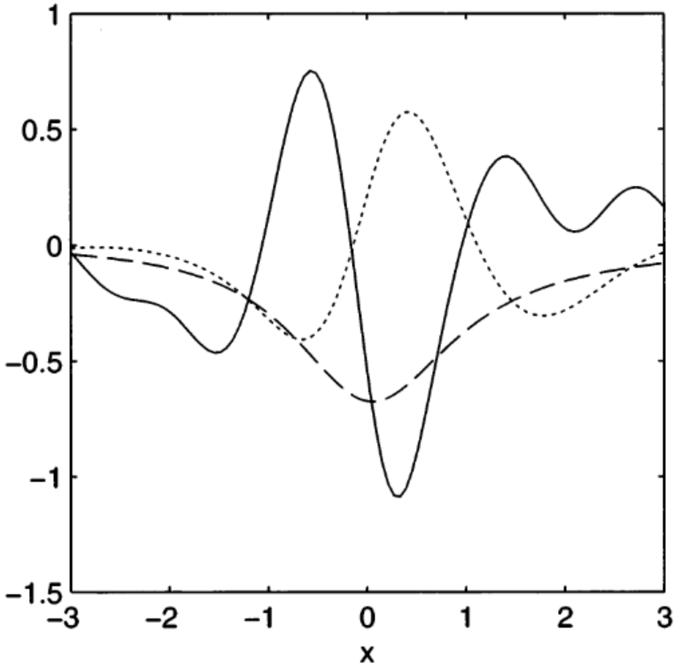
Elements of Stein RKHS

- Recall that we can take an RKHS $\mathscr{H}_k$ and create a new one by applying a Stein operator to functions in the space:

$$\mathcal{S}_P[g](x), \qquad g \in \mathscr{H}_k^d$$

- This leads to the RKHS with kernel k_P given by:

$$k_p(x, x') = \mathcal{S}_P^x \mathcal{S}_P^{x'}[k](x, x')$$



[Oates et al 2017, JRSSB]

Oates, C. J., Girolami, M., & Chopin, N. (2017). Control functionals for Monte Carlo integration. *Journal of the Royal Statistical Society B: Statistical Methodology*, *79*(3), 695–718.

Oates, C. J., Cockayne, J., Briol, F.-X., & Girolami, M. (2019). Convergence rates for a class of estimators based on Stein's identity. *Bernoulli*, *25*(2), 1141–1159.

South, L. F., Karvonen, T., Nemeth, C., Girolami, M., & Oates, C. J. (2022). Semi-exact control functionals from Sard's method. *Biometrika*, *109*, 351–367.

Stein Neural Networks

- We can also take our favourite (sufficiently smooth) neural network $g_\theta : \mathbb{R}^d \to \mathbb{R}^d$ and apply a Stein operator to the output.
- To use the language in this field, we can add a **“Stein layer”**.

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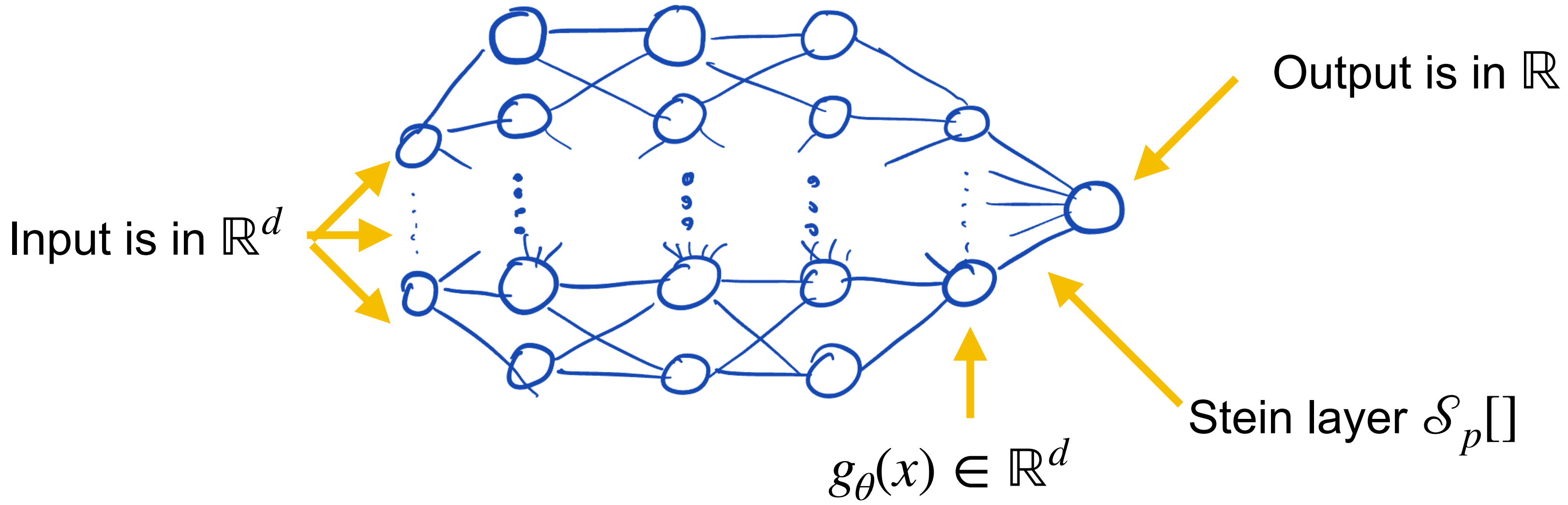

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Stein CVs as empirical risk minimisation

- Clearly a natural objective to choose our control variate is:

$$J(\theta) = \mathrm{Var}[f - h_\theta] = \mathrm{Var}[f - \mathcal{S}_P[g_\theta](x) - \theta_0]$$

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- We then choose our control variate as follows:

$$\hat{\theta}_m = \arg\min_{\theta\in\Theta} J_m(\theta) \longrightarrow h_{\hat{\theta}_m}(x)$$

Linear Stein CVs

- We note that Stein operators are usually **linear operators,** meaning that

$$\theta \mapsto h_\theta(x)$$

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- This is the case for polynomials or for kernels, but not for neural networks.

- The great advantage of linear Stein CVs is that $\theta \mapsto J_m(\theta)$ becomes a quadratic function in θ and **can hence be solved through a linear system** (we are essentially doing least squares)!

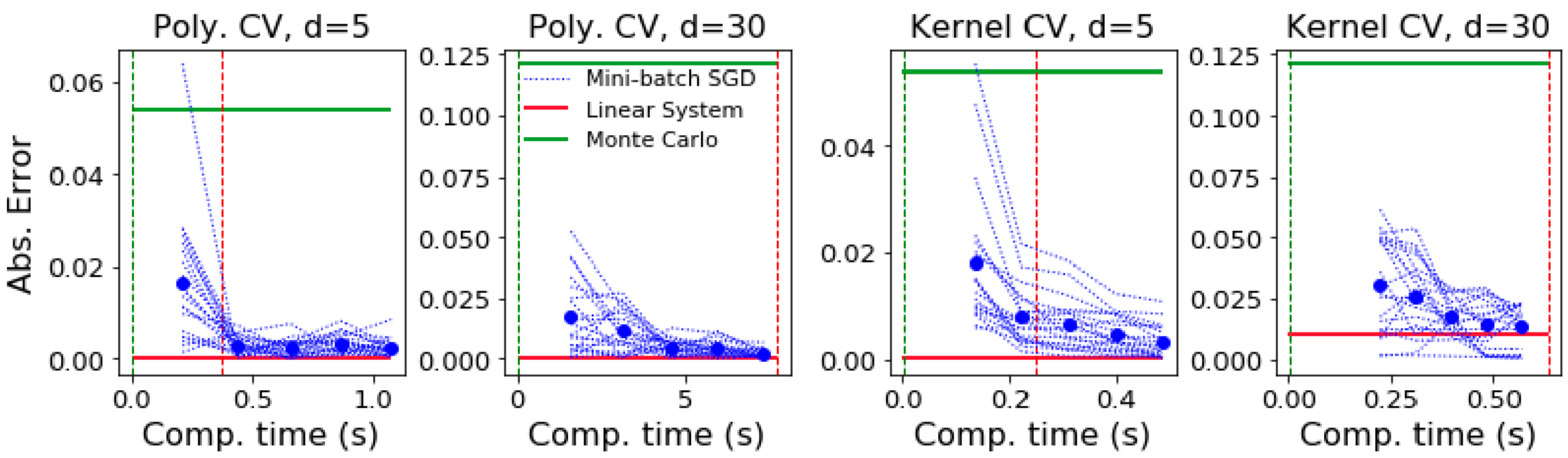
Stochastic optimisation for linear Stein CVs: a toy problem

- Of course another approach is to use gradient-based optimisation, such as stochastic gradient descent…

$$f(x) = x_1 + \ldots + x_d$$

$$P = \mathcal{N}(0, I_d)$$

Half of the samples were used for learning the CV, the other half for the estimator



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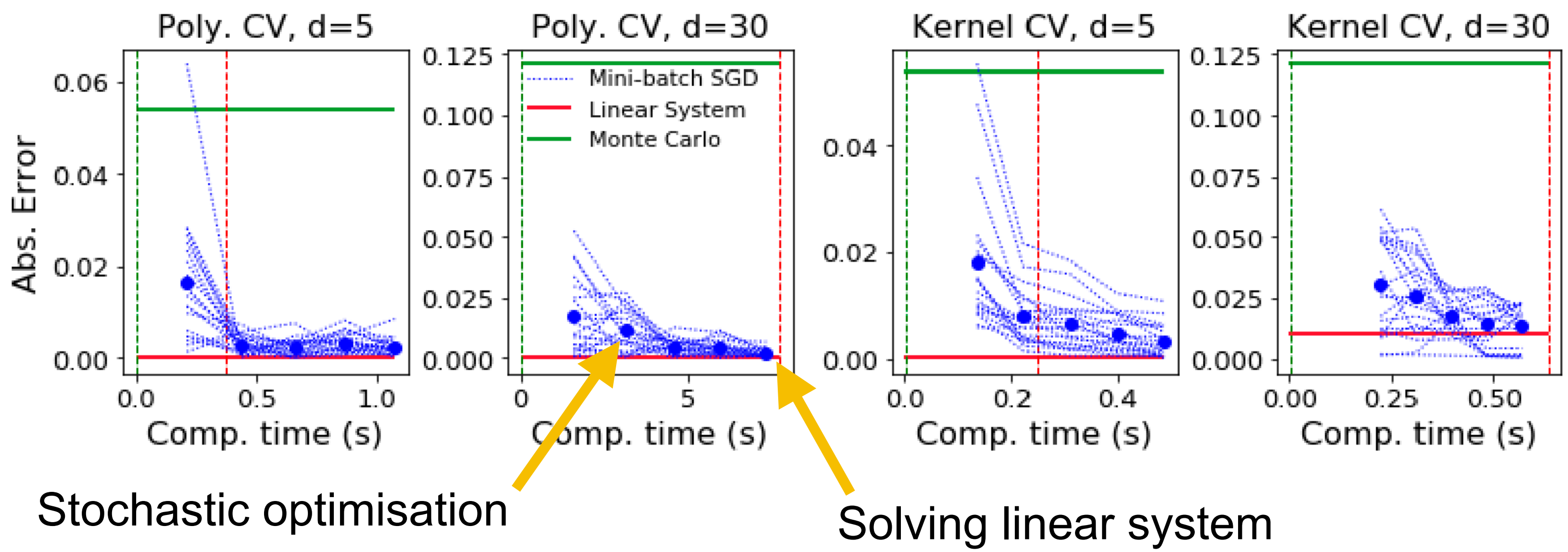

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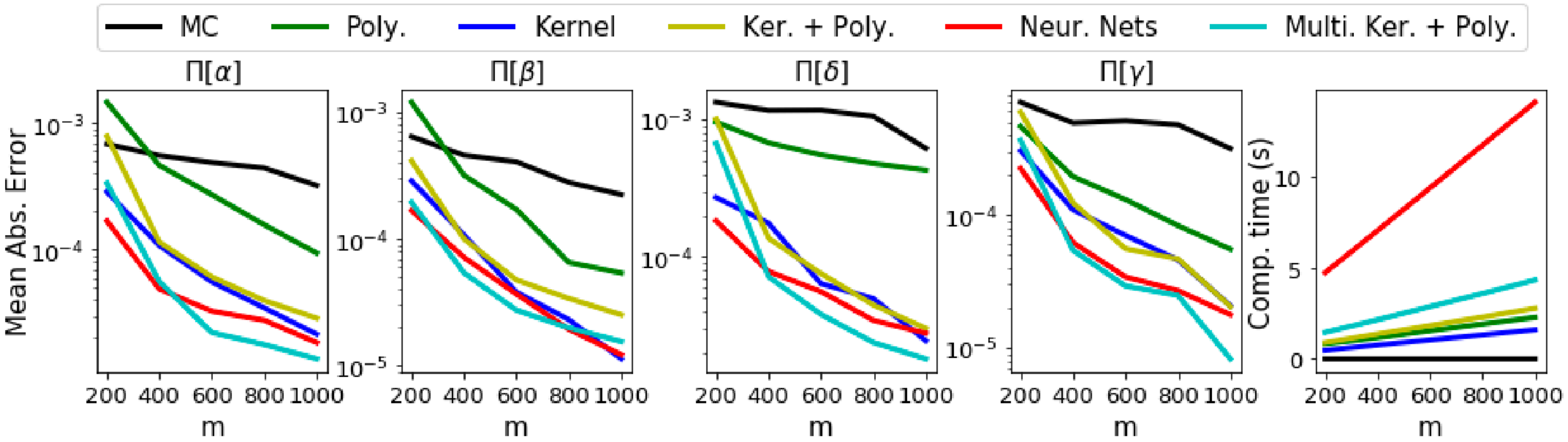
Posterior inference for ODE system



Computing expectations under the posterior for $(\alpha, \beta, \delta, \gamma)$ given some observations of the following Lotka-Volterra ODE system:

(Half of the samples were used for learning the CV, the other half for the estimator)

$$\dot{x} = \alpha x - \beta x y \qquad \dot{y} = \delta x y - \gamma y$$

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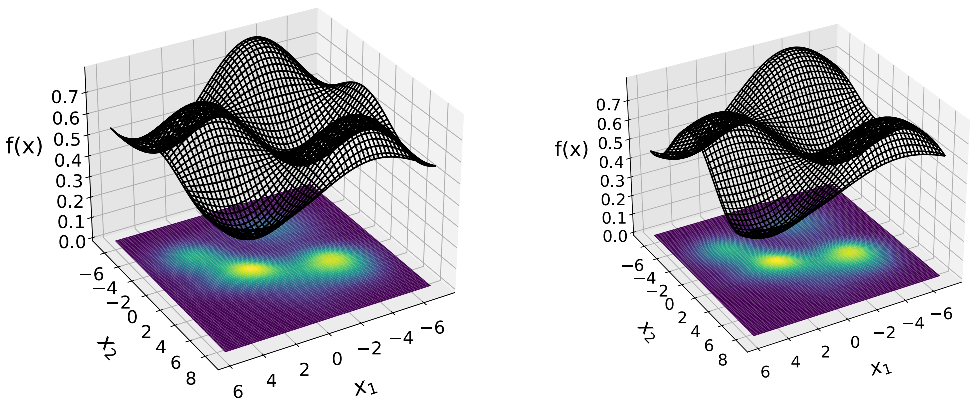
Multiple related integrals



- In some situations, we have to estimate several integrals either sequentially or simultaneously:

$$\mathbb{E}_{X\sim P_1}[f_1(X)], \ldots, \mathbb{E}_{X\sim P_T}[f_T(X)]$$

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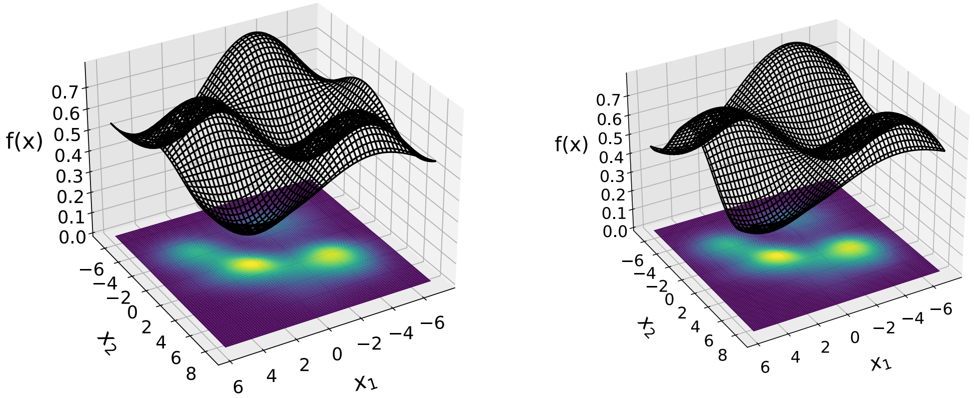

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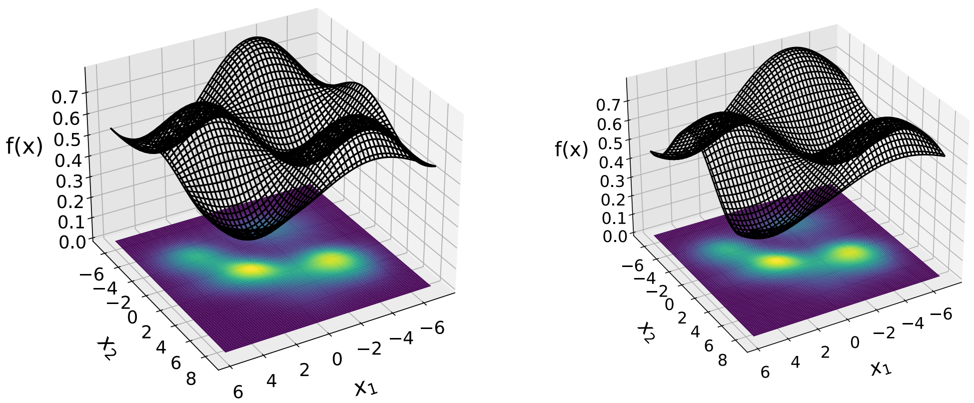

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- Thankfully Stein's method can be extended to vector-valued functions to create control variates suitable for tackling this task!

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Overview: numerical integration with Stein's method

- The accuracy of Monte Carlo methods can be significantly improved through control variates, but finding a good control variate can be very hard.

Overview: numerical integration with Stein’s method

- The accuracy of Monte Carlo methods can be significantly improved through control variates, but finding a good control variate can be very hard.

→ Stein’s method allows us to create very flexible classes of control variates for a very broad variety of applications!

Stein’s method as a computational tool

Beyond Euclidean domains

A computational tool beyond Euclidean spaces…

- Recall our favourite Stein operator:

$$\mathcal{T}[g](x) := \langle \nabla_x \log p(x), g(x) \rangle + \langle \nabla, g(x) \rangle$$

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None of the tools we have seen so far work….

Stein on bounded subsets of Euclidean space

- The defining property of the Langevin Stein operator is:

$$\mathbb{E}_{X \sim P}\left[\mathcal{T}[g](X)\right] = \int_{\mathbb{R}^d} \mathcal{T}[g](x)p(x)dx = 0$$

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- There are plenty of cases where our models/data does not have full support, but where $\mathcal{X} \subset \mathbb{R}^d$ and this is a **strict subset**.

Stein on bounded subsets of Euclidean space

- A straightforward solution in this case is to use a modified RKHS as the Stein space:

$$\tilde{k}(x, x') = \delta(x)k(x, x')\delta(x')$$

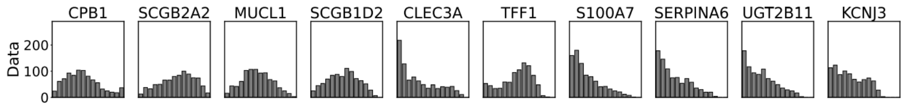
- Where we enforce that the kernel vanishes on the boundary:

$$\delta(x) = 0 \quad \text{for} \quad x \in \partial\mathcal{X}$$

Oates, C. J., Cockayne, J., Briol, F.-X., & Girolami, M. (2019). Convergence rates for a class of estimators based on Stein's identity. *Bernoulli*, *25*(2), 1141–1159.

Williams, D. J., & Liu, S. (2023). Approximate Stein Classes for truncated density estimation. *International Conference on Machine Learning*.

Stein on discrete spaces



[Matsubara et al., 2024+]

$$\mathcal{X} = \mathcal{S}_1 \times \ldots \times \mathcal{S}_d$$

$\mathcal{S}_i$ is a countable ordered set

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Yang, J., Liu, Q., Rao, V., & Neville, J. (2018). Goodness-of-fit testing for discrete distributions via Stein discrepancy. *ICML*.

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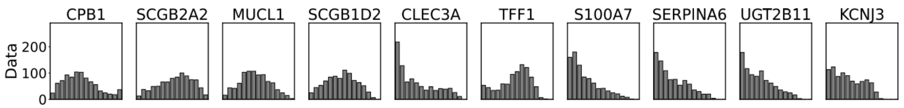
Stein on discrete spaces



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$$\nabla^- g(x) = \begin{bmatrix} g(x^{1-}) - g(x) \\ \cdots \\ g(x^{d-}) - g(x) \end{bmatrix} \qquad \nabla^+ g(x) = \begin{bmatrix} g(x^{1+}) - g(x) \\ \cdots \\ g(x^{d+}) - g(x) \end{bmatrix}$$

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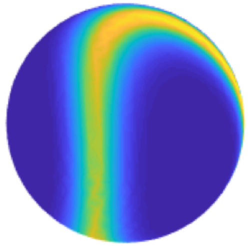
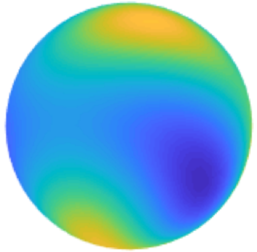
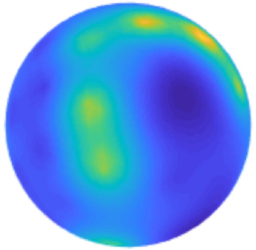
Stein on manifolds

[Barp et al., 2022]







- Sometimes we also want to consider data on manifolds (e.g. spheres, positive definite matrices, etc…)

Xu, W., & Matsuda, T. (2020). A Stein goodness-of-fit test for directional distributions. *AISTATS*.

Xu, W., & Matsuda, T. (2021). Interpretable Stein goodness-of-fit tests on Riemannian manifolds. *ICML*.

Barp, A., Oates, C. J., Porcu, E., & Girolami, M. (2022). A Riemannian–Stein kernel method. *Bernoulli*, *28*(4), 2181–2208.

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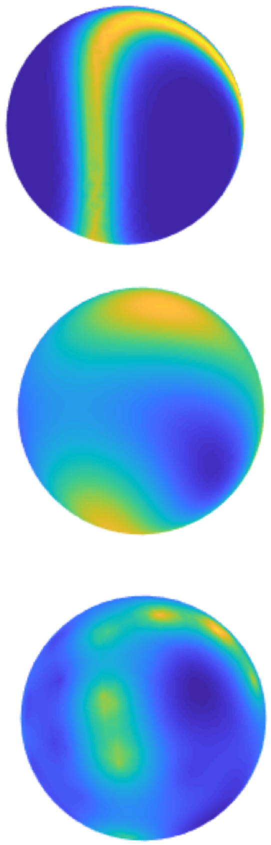

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- Once again the generator approach comes to the rescue: we just need a Markov process defined on this space….

- There are abundant choices available from physics and computational chemistry literatures!

Xu, W., & Matsuda, T. (2020). A Stein goodness-of-fit test for directional distributions. *AISTATS*.

Xu, W., & Matsuda, T. (2021). Interpretable Stein goodness-of-fit tests on Riemannian manifolds. *ICML*.

Barp, A., Oates, C. J., Porcu, E., & Girolami, M. (2022). A Riemannian–Stein kernel method. *Bernoulli*, *28*(4), 2181–2208.

Stein on function spaces

- $\mathscr{X}$ is a space of function (e.g. time series, spatial measurements, etc…).

Wynne, G., Kasprzak, M., & Duncan, A. B. (2024+). A spectral representation of kernel Stein discrepancy with application to goodness-of-fit tests for measures on infinite dimensional Hilbert spaces. *Bernoulli (to appear)*.

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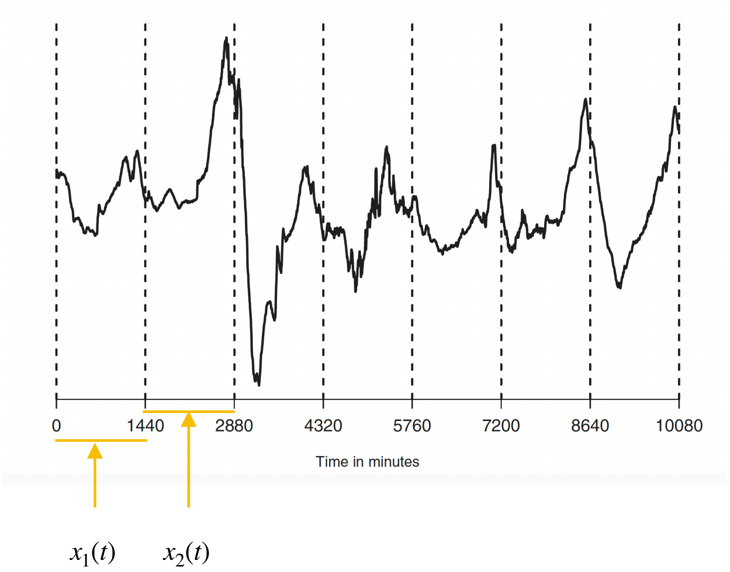
Magnetic field in Honolulu



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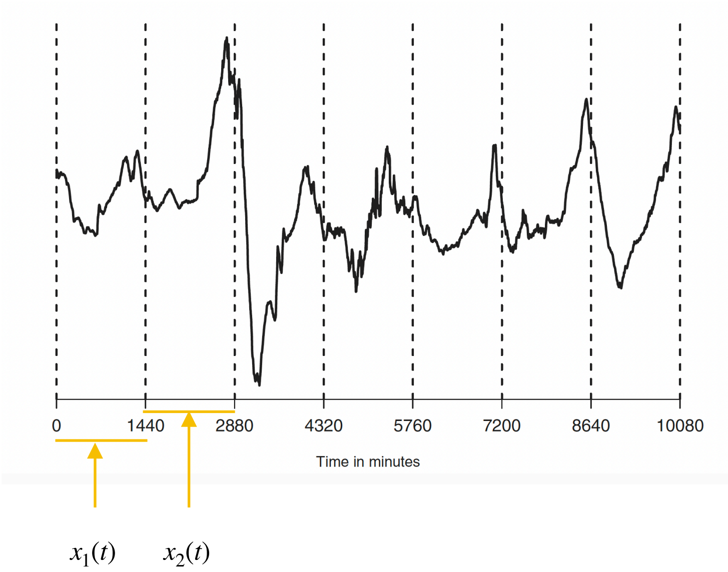
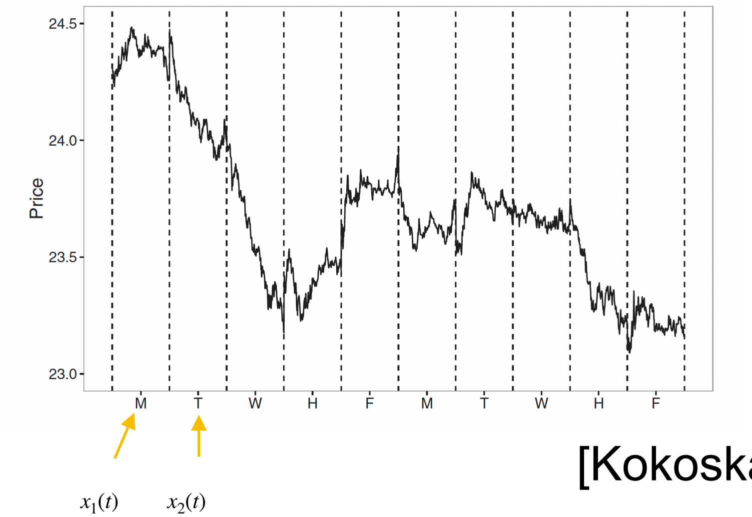


Microsoft stock price in May 2006



[Kokoska, 2017]

Wynne, G., Kasprzak, M., & Duncan, A. B. (2024+). A spectral representation of kernel Stein discrepancy with application to goodness-of-fit tests for measures on infinite dimensional Hilbert spaces. *Bernoulli (to appear)*.

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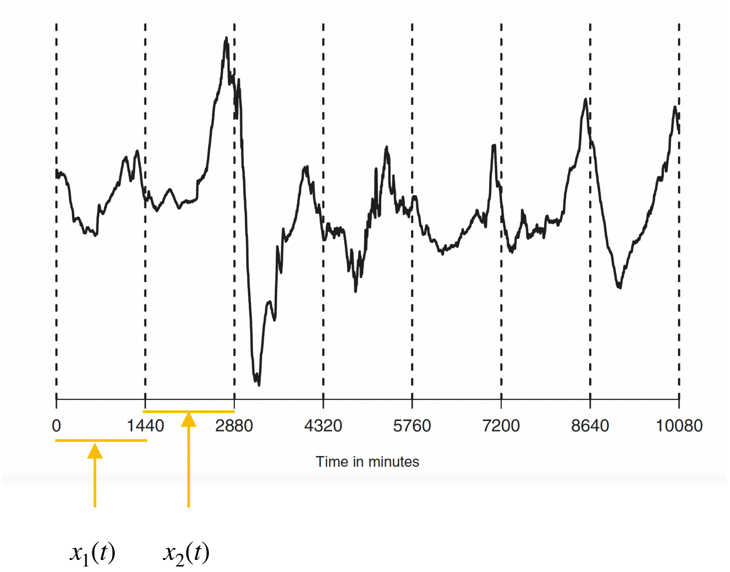

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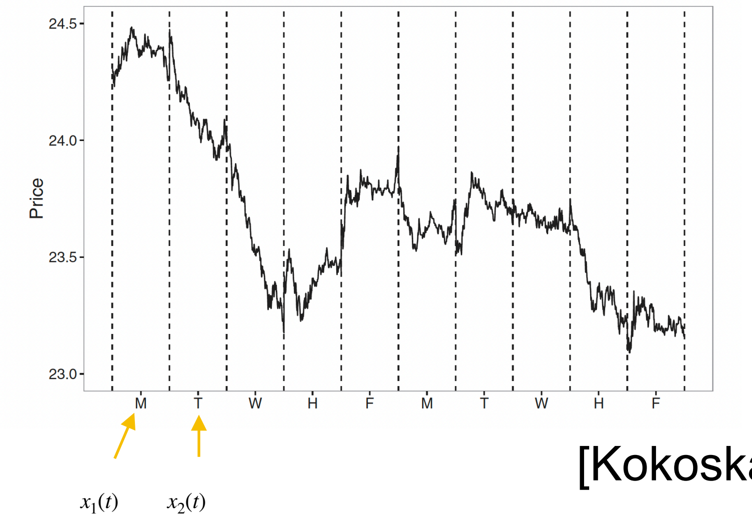


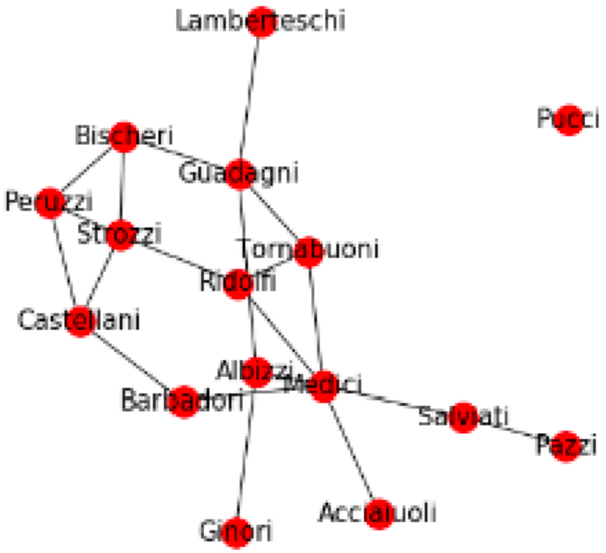
[Kokoska, 2017]

- Once again the generator approach comes to the rescue - we can use the generator of a Wiener process with a carefully selected kernel.

Wynne, G., Kasprzak, M., & Duncan, A. B. (2024+). A spectral representation of kernel Stein discrepancy with application to goodness-of-fit tests for measures on infinite dimensional Hilbert spaces. *Bernoulli (to appear)*.

Stein on graphs

- A lot less straightforward to write on a slide, but is based on the generator approach of Barbour…
- The exact operator is based on Glauber dynamics which allows you to simulate on the space of graphs.



[Xu & Reinert 2022]

Xu, W., & Reinert, G. (2021). A Stein goodness of fit test for exponential random graph models. *AISTATS*.

Xu, W., & Reinert, G. (2022). AgraSSt: Approximate graph Stein statistics for interpretable assessment of implicit graph generators. *NeurIPS*.

Stein's method as a computational tool

The end

Outline (updated)

- What is Stein’s method, and why should you care…
- Computational tools based on Stein’s method.
- Some nice (new) algorithms!

Conclusions/Take-Away

- Stein’s method gives us a new **characterisation of distributions** which is particularly **convenient from a computational viewpoint**!

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- Stein's method has now touched most areas in these fields…!

Conclusions/Take-Away

- Stein's method gives us a new **characterisation of distributions** which is particularly **convenient from a computational viewpoint**!
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