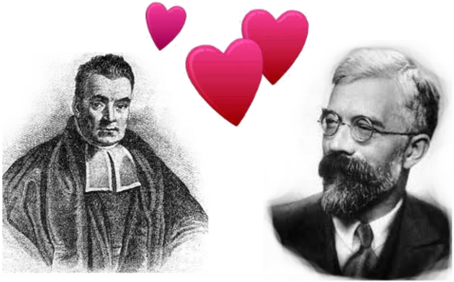
Deterministic Sampling Methods



David Duvenaud

Cambridge University
Computational and Biological Learning Lab

August 7, 2013

Outline

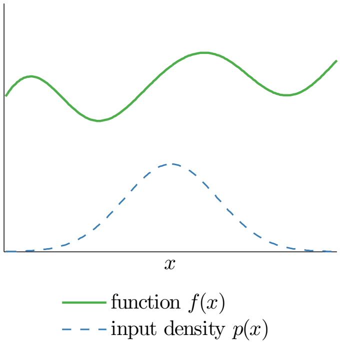
- Kernel Herding
- Bayesian Quadrature
- Unifying Results
- Demos

The Quadrature Problem

- We want to estimate an integral

$$Z = \int f(x)p(x)dx$$

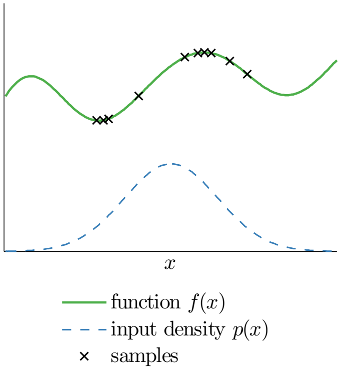
- Most computational problems in Bayesian inference correspond to integrals:
  - Expectations
  - Marginal distributions
  - Integrating out nuisance parameters
  - Normalization constants



Sampling Methods

- Monte Carlo methods:
  Sample from $p(x)$, take empirical mean:

$$\hat{Z} = \frac{1}{N} \sum_{i=1}^{N} f(x_i)$$



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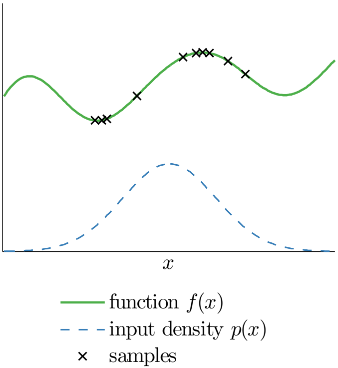

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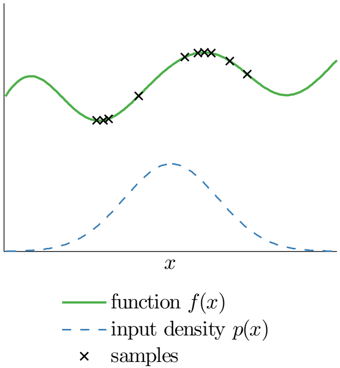

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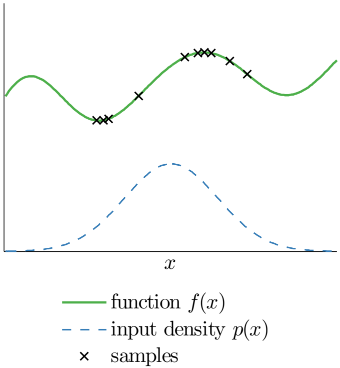

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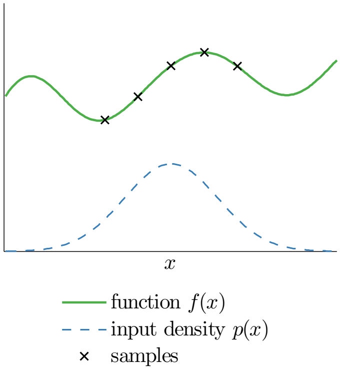
  - Often, nearby function values will be similar
- Quasi-Monte Carlo methods spread out samples to achieve faster convergence.



Kernel Herding [Welling et. al., 2009, Chen et. al., 2010]

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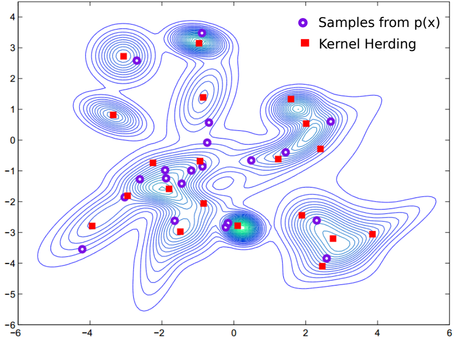
- A sequential procedure for choosing sample locations, depending on previous locations.
- Keeps estimate rule $\hat{Z} = \frac{1}{N} \sum_{i=1}^{N} f(x_i)$
- Almost $\mathcal{O}(1/N)$ convergence instead of $\mathcal{O}(1/\sqrt{N})$ typical of random sampling, by spreading out samples.



Kernel Herding Objective

KH was found to minimize Maximum Mean Discrepancy:

$$\mathrm{MMD}_{\mathcal{H}}(p,q) = \sup_{\substack{f \in \mathcal{H} \\ \|f\|_{\mathcal{H}}=1}} \left| \int f(x)p(x)dx - \int f(x)q(x)dx \right|$$

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In KH, $p(x)$ is true distribution, and $q(x)$ is a set of point masses at sample locations $\{x_1, \ldots, x_N\}$:

$$\epsilon_{KH}\left(\{x_1, \ldots, x_N\}\right) = \mathrm{MMD}_{\mathcal{H}}\left(p, \underbrace{\frac{1}{N}\sum_{n=1}^{N} \delta_{x_n}}_{q(x)} \right)$$

Kernel Herding

- Assuming function is in a Reproducing Kernel Hilbert Space defined by $k(\cdot, \cdot)$, MMD has closed form.

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- When sequentially minimizing MMD, new point is added at:

$$x_{N+1} = \underset{x \in \mathcal{X}}{\operatorname{argmax}} \left[2 \int k(x, x') p(x') dx' - \frac{1}{N+1} \sum_{m=1}^{N} k(x, x_m) \right]$$

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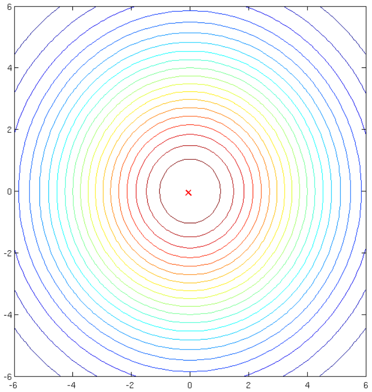

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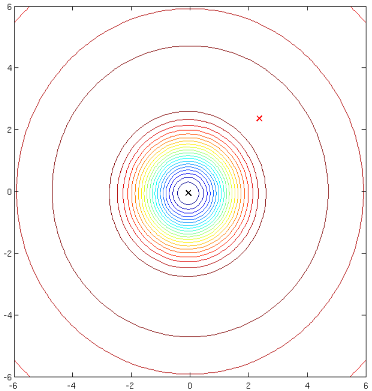

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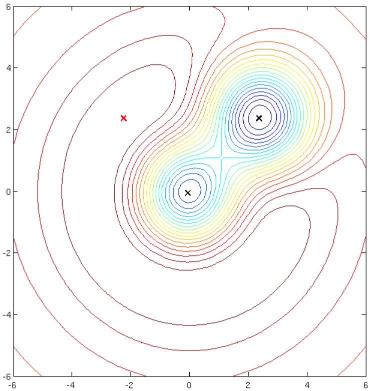

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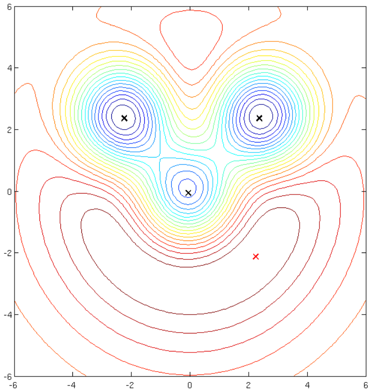

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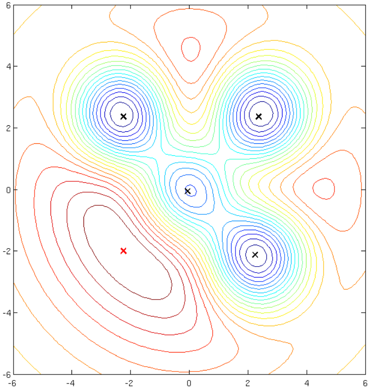

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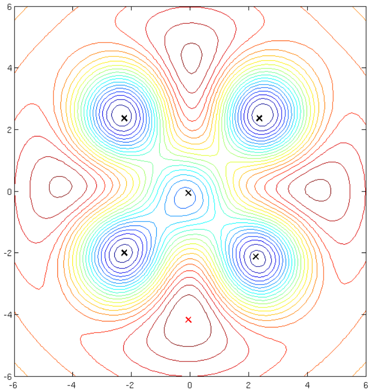

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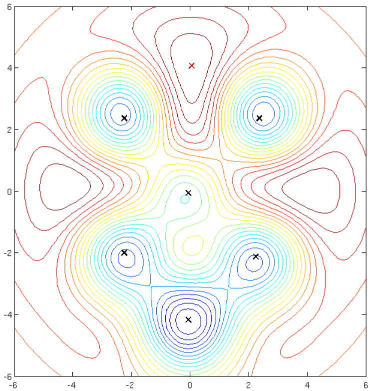

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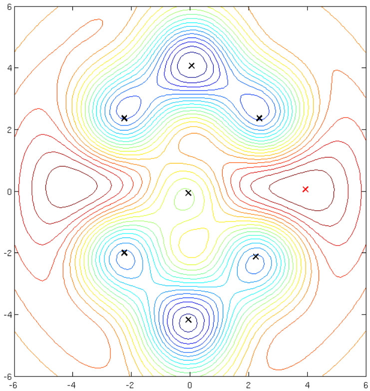

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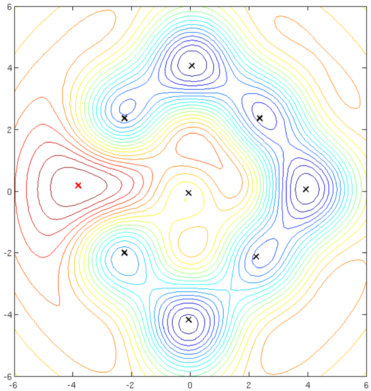

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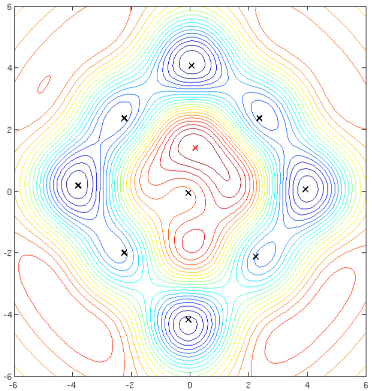

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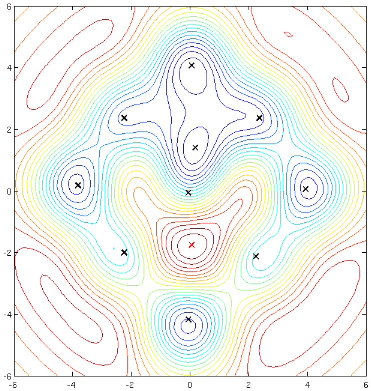

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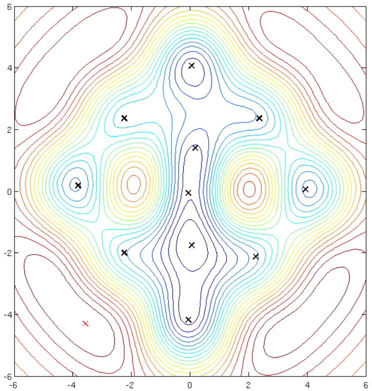

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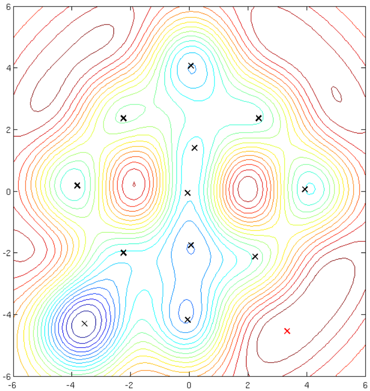

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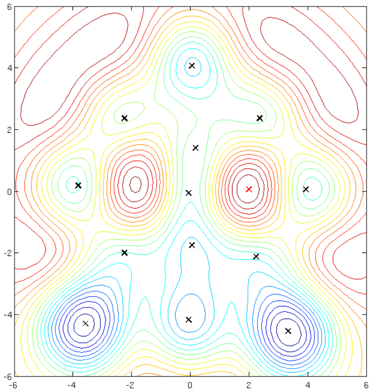

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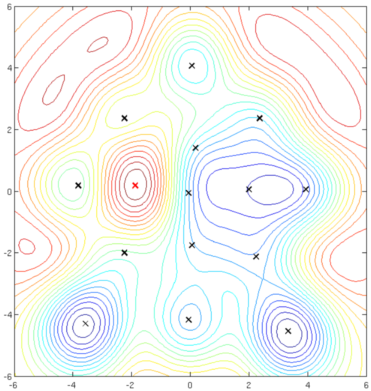

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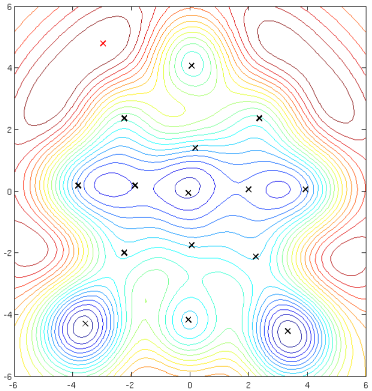

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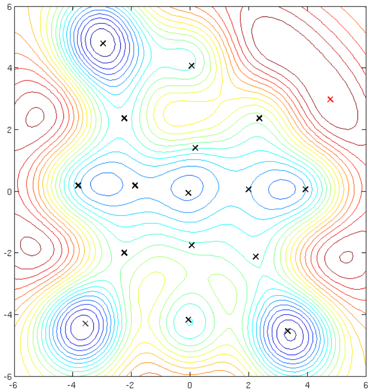

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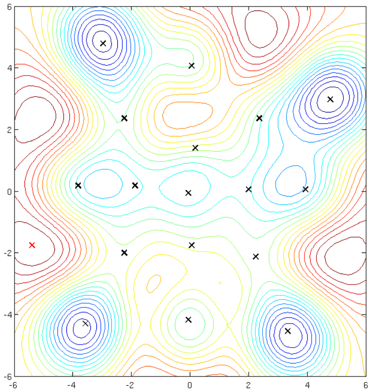

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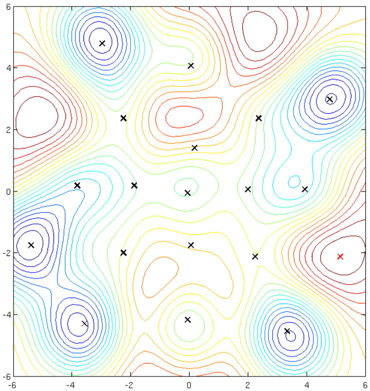

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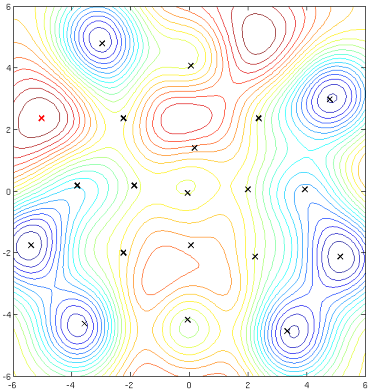

Kernel Herding Summary

- A sequential sampling method which minimizes a worst-case divergence, given that $f(x)$ belongs to a given RKHS.
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Can we reason about the optimal weighting strategy?

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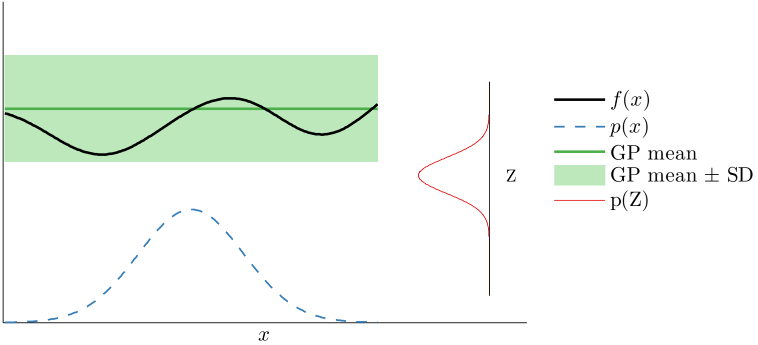

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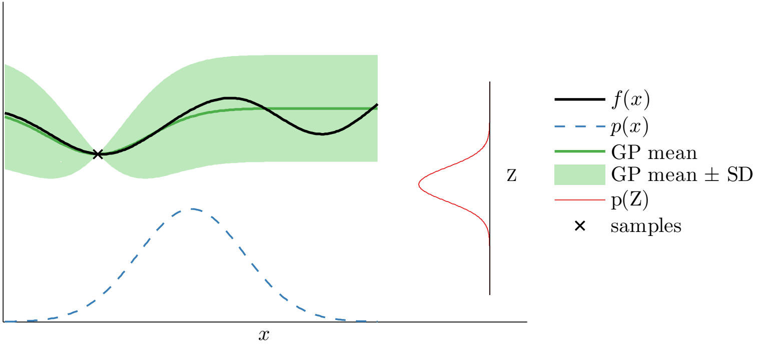

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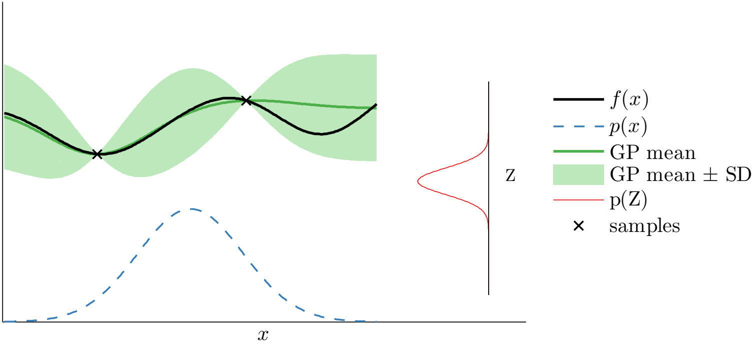

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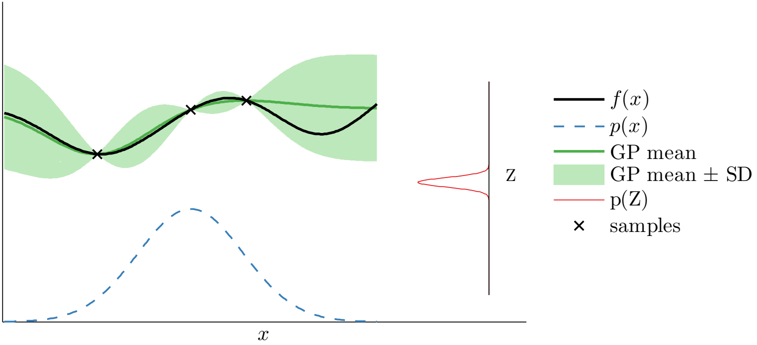

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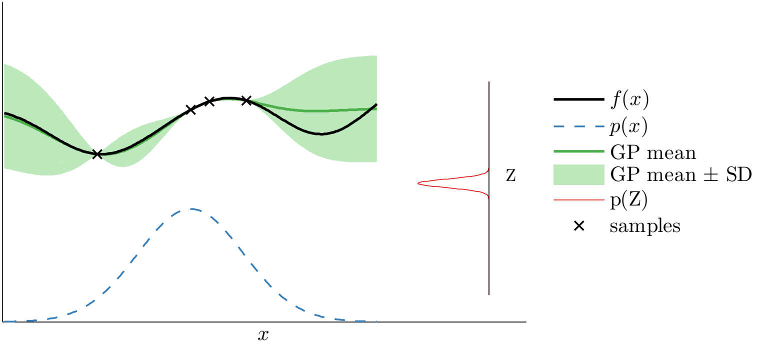

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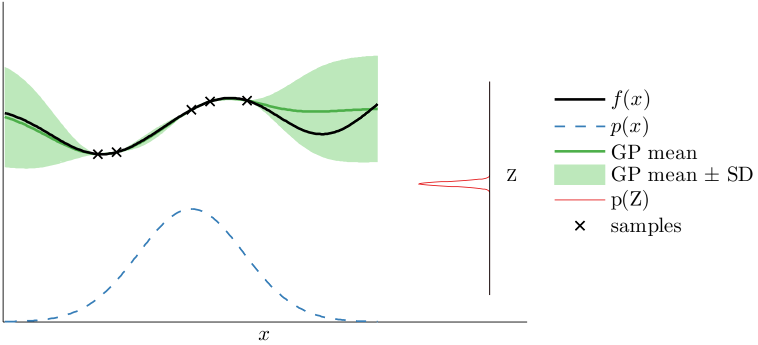

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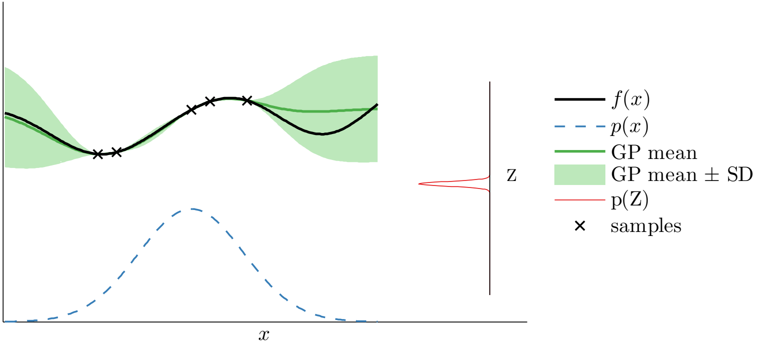

- Can choose samples however we want.

Bayesian Quadrature Estimator

Posterior over Z has mean linear in $f(x_s)$:

$$\mathbb{E}_{\text{GP}}\left[Z|f(x_s)\right] = \sum_{i=1}^{N} w_{BQ}^{(i)} f(x_i)$$

where

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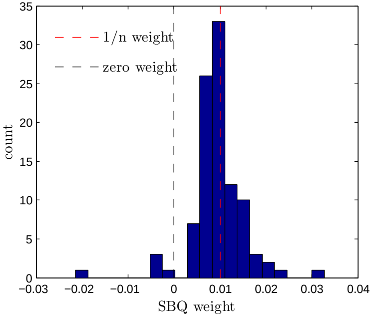

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- Natural to minimize the posterior variance of Z:

$$\mathbb{V}\left[Z|f(x_s)\right] = \int\int k(x, x')p(x)p(x')dxdx' - z^T K^{-1} z$$

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- Can choose samples sequentially: Sequential Bayesian Quadrature.

Relating Objectives

KH and BQ have completely different motivations:

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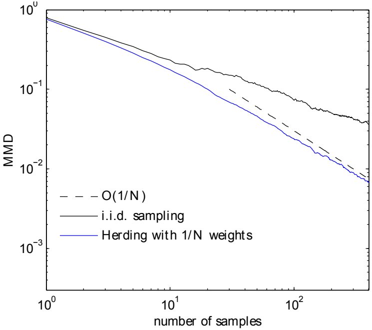
$\mathbb{V}\left[Z|f(x_s)\right]$ has two interpretations:

- Bayesian: posterior variance of Z under a GP prior.
- Frequentist: tight bound on estimation error of Z.

Rates of Convergence

What is rate of convergence of BQ?

Expected Variance / MMD



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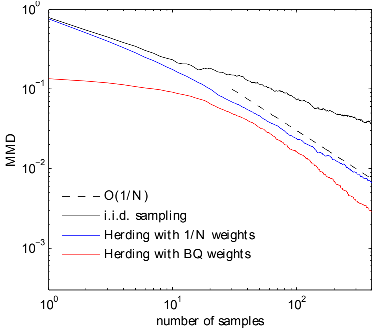

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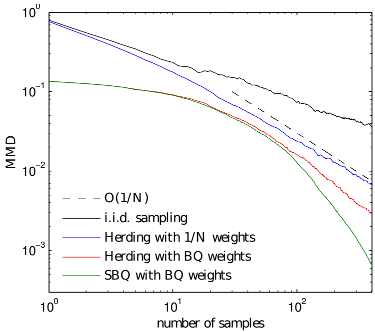

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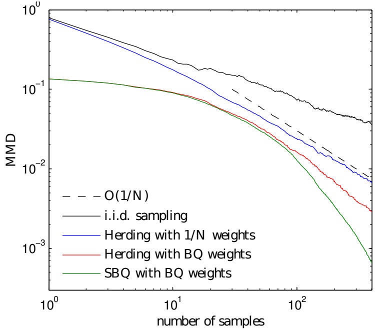

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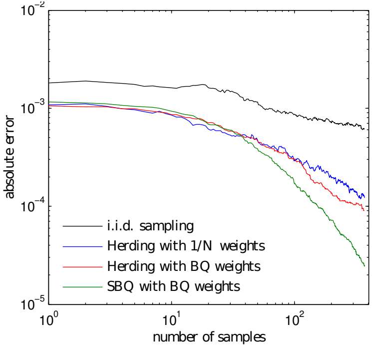

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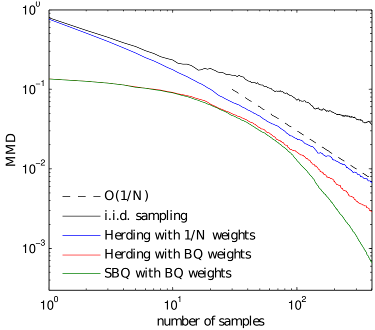

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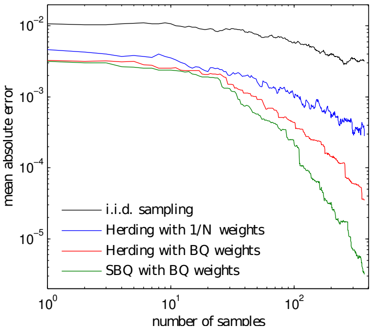

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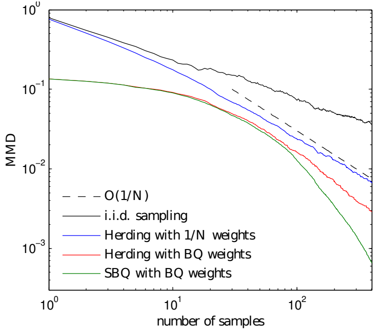
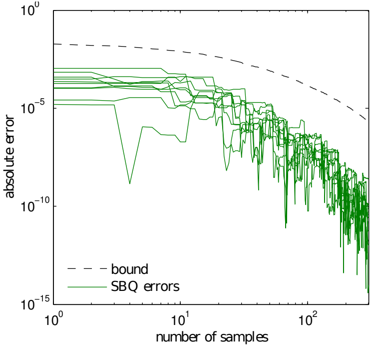


Bound on Bayesian Error



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- Joint work with Ferenc Huzsar