

Optimal Quantisation of Probability Measures Using Maximum Mean Discrepancy

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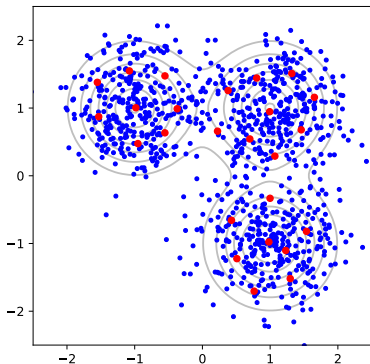
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CORE AIM

Aim: to 'optimally approximate' a probability measure P on \mathcal{X} by a discrete distribution $Q_m = \frac{1}{m} \sum_{i=1}^m \delta(X_i)$. Our starting point is a *discrete* set X_1, \dots, X_n of points in \mathcal{X} ($n \gg m$) that we aim to 'thin'.



BASIC PROBLEM SETUP

We have: a target distribution P , and a set of samples X_i – from the samples we form an empirical distribution Q_n :

$$P \qquad Q_n := \frac{1}{n} \sum_{i=1}^n \delta(X_i)$$

But: n is large and it is expensive to compute with all n samples.

Or: Q_n is not actually that good an approximation to P .

So: We choose $m \ll n$ and then try to find a **representative subset** of samples of size m that minimises

$$\text{“difference”} \left(P, \frac{1}{m} \sum_{i=1}^m \delta(X_i) \right) \quad \text{given } m; \quad \{X_i\}_{i=1}^m \subset \{X_i\}_{i=1}^n$$

We refer to this as **optimal quantisation**.

Our task will be to define some appropriate measure of "difference" to do this, and thereby to find an appropriate representative subset.

Note: We are concerned with (somehow) minimising:

$$\text{“difference”} \left(P, \frac{1}{m} \sum_{i=1}^m \delta(X_i) \right) \quad \text{given } m; \{X_i\}_{i=1}^m \subset \{X_i\}_{i=1}^n$$

This is not the same as:

- “diff.” $\left(\frac{1}{n} \sum_{i=1}^n \delta(X_i), \frac{1}{m} \sum_{i=1}^m \delta(X_i) \right); \{X_i\}_{i=1}^m \subset \{X_i\}_{i=1}^n$
- “diff.” $\left(P, \frac{1}{m} \sum_{i=1}^m \delta(X_i) \right); \{X_i\}_{i=1}^m \subset \mathcal{X}$

BASIC PROBLEM SETUP

$$\operatorname{argmin}_{\substack{S \subset \{1, \dots, n\} \\ |S|=m}} \text{MMD} \left(P, \frac{1}{m} \sum_{i=1}^m \delta(X_i) \right)$$

SOME RELATED APPROACHES

- Minimise Wasserstein distance [Graf & Luschgy 2007]
- Minimise 'power function' (worse-case interpolation error)
[de Marchi et al. 2005; Santin & Haasdonk 2017]
- Support points (minimise 'energy distance') [Mak & Joseph 2018]
- Minimise Stein discrepancy to optimally *weight* $\{X_i\}_{i=1}^n$
[Liu & Lee 2017]
- Minimum energy designs [Joseph 2015,2019]
- "Kernel herding" [Chen et al. 2010; Lacoste-Julien et al. 2015]
- "Stein points" [Chen et al. 2018]
- Stein Variational Gradient Descent [Liu & Wang 2019; Duncan et al. 2018]
- "Kernel Thinning" [Dwivedi & Mackey 2021]
- "Cube Thinning" [Chopin & Ducrocq 2021]

- Motivating examples
- Introduction to Maximum mean discrepancy (MMD)
- Algorithms for selecting points
- Some theory
- Heuristics

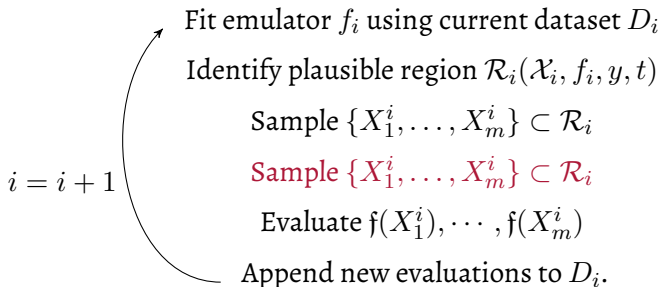
EXAMPLE 1: HISTORY MATCHING

Core idea: establish which inputs $x \in \mathcal{X}$ to a computer model $f(\cdot)$ could have generated a known output y .

- Construct a *surrogate* or *emulator* f trained on evaluations of f – use this to determine which x are compatible with y , while accounting for uncertainty introduced by the emulation.
- Fix a t , and say x is *plausible* if $\|\mathbb{C}[f(x)]^{-1/2}(\mathbb{E}[f(x)] - y)\| < t$.
- This defines a *plausible region*

$$\mathcal{R}(\mathcal{X}, f, y, t) = \{x \in \mathcal{X} : \|\mathbb{C}[f(x)]^{-1/2}\{\mathbb{E}[f(x)] - y\}\| < t\}$$

EXAMPLE 1: HISTORY MATCHING



EXAMPLE 1: HISTORY MATCHING

In practical settings \mathcal{R}_i can be very complicated – non-convex, highly curved boundaries, disconnected regions etc.

Checking whether a point x is in \mathcal{R}_i is easy. But characterising the entire region is very difficult.

Depending on which statistical model one uses for f , there might be different optimal ways of selecting the new points (Uniform sampling? Space-filling design? Sobol' sequence? ...)

Some of these may be difficult to do given the form of \mathcal{R}_i (Taking the intersection of an existing low-discrepancy set with \mathcal{R}_i ? Does this guarantee anything?)

EXAMPLE 1: HISTORY MATCHING

Many good reasons to use MMD instead:

- it doesn't care about the region \mathcal{R}_i being really complicated,
- it can 'correct' statistical inaccuracies caused by having to perform rejection sampling when first identifying \mathcal{R}_i ,
- theoretical guarantees in some settings:

If f is a Gaussian process (very common), a natural quantification of the uncertainty present is via the *maximum eigenvalue of its integrated covariance*

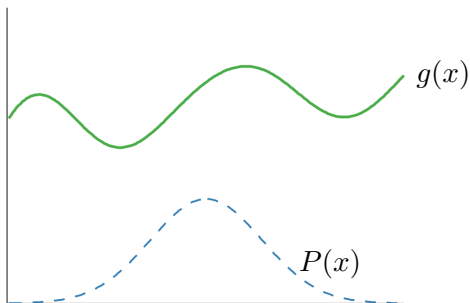
$$U(\Sigma, \mathcal{X}) = \lambda_{\max} \left\{ \iint_{\mathcal{X} \times \mathcal{X}} \Sigma(x, x') d\mathcal{U}(x) d\mathcal{U}(x') \right\},$$

and using MMD sampling we have $U(\Sigma, \mathcal{X}) = O(m^{-1})$.

EXAMPLE 2: BAYESIAN QUADRATURE

Let g be a function that we would like to integrate against P .

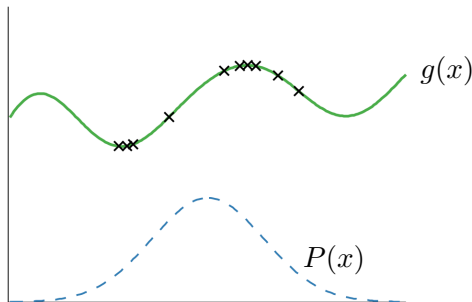
$$Z = \int g(x) dP(x)$$



EXAMPLE 2: BAYESIAN QUADRATURE

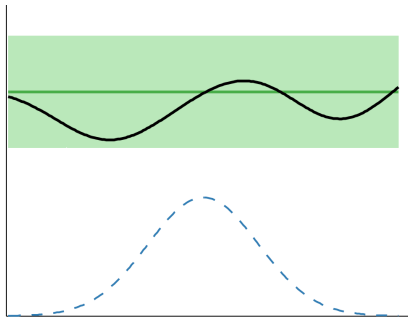
Let g be a function that we would like to integrate against P .

$$Z \approx \frac{1}{n} \sum_{i=1}^n g(X_i), \quad (X_i \sim P)$$



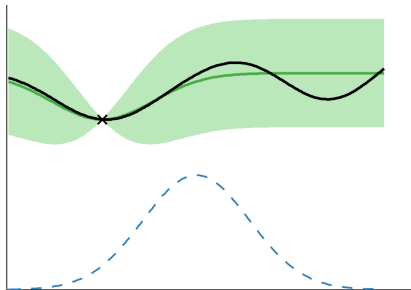
EXAMPLE 2: BAYESIAN QUADRATURE

Instead: Model $g(x)$ a priori as a **Gaussian process** with covariance k , then condition on 'data' $\mathcal{D} = \{g(X_i)\}_{i=1}^n$.



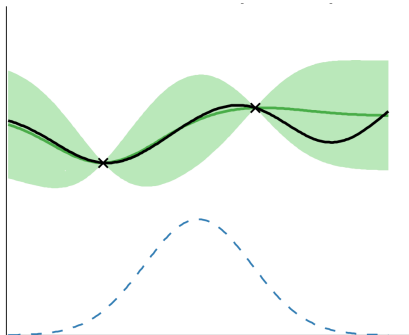
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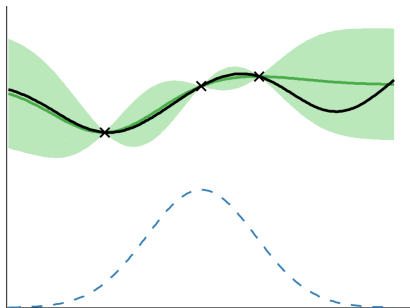
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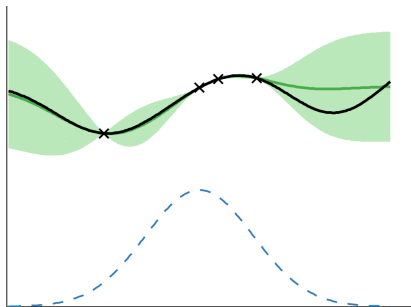
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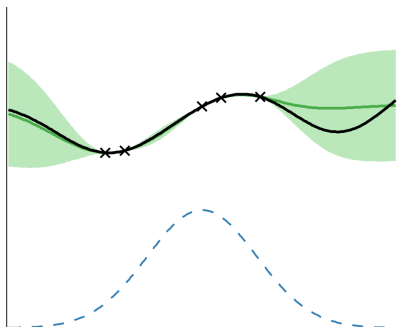
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EXAMPLE 2: BAYESIAN QUADRATURE

This gives a *probabilistic* approximation to Z – its (Gaussian) posterior distribution $p(Z|\mathcal{D})$.

$$\text{std}[Z|\mathcal{D}] = \min_{\substack{w_1, \dots, w_m \\ \in \mathbb{R}}} \text{MMD}_{P,k} \left(\sum_{i=1}^m w_i \delta(X_i) \right)$$

This is bounded above by $\text{MMD}_{P,k} \left(\frac{1}{m} \sum_{i=1}^m \delta(X_i) \right)$

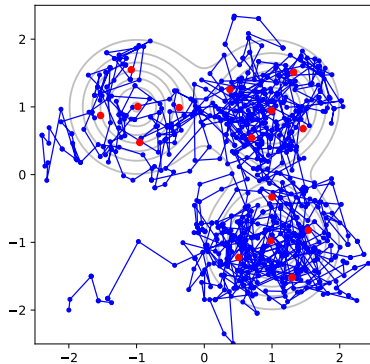
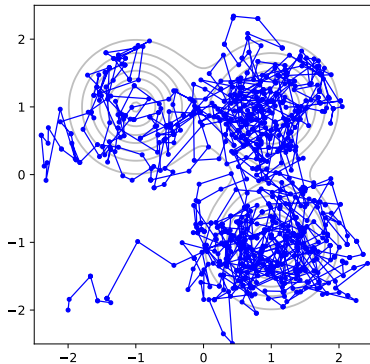
[Huszár & Duvenaud (2012), Briol et al. (2015)]

EXAMPLE 2: BAYESIAN QUADRATURE

It's quite common here that g is complicated and expensive to evaluate, but P is something straightforward like a Gaussian or uniform distribution (against which the integration of k required to calculate MMD is easy).

So MMD can be tractable and useful in this setting.

EXAMPLE 3: THINNING OF MCMC OUTPUT



See Marina's talk :)

Let \mathcal{X} be a measurable space,

- $\mathcal{P}(\mathcal{X})$ be the set of probability distributions on \mathcal{X} ,
- \mathcal{F} be some set of bounded real-valued functions on \mathcal{X} .

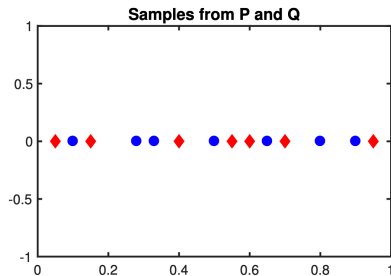
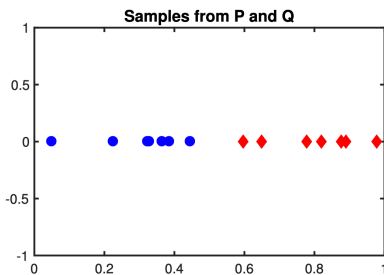
For $P, Q \in \mathcal{P}(\mathcal{X})$, a **discrepancy** is a quantity of the form

$$D_{\mathcal{F}}(P, Q) = \sup_{f \in \mathcal{F}} \left| \int f \, dP - \int f \, dQ \right|$$

(If $D_{\mathcal{F}}(P, Q) = 0$ implies $P = Q$ then \mathcal{F} is called *measure-determining*, and $D_{\mathcal{F}}$ is also called an **integral probability metric**.)

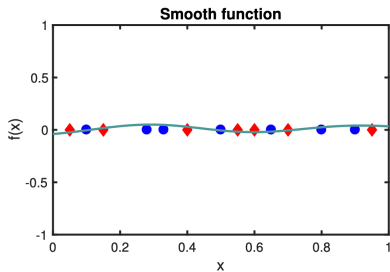
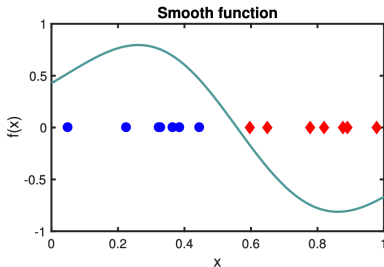
MAXIMUM MEAN DISCREPANCY – INTUITION

(Images borrowed/looted from Arthur Gretton)



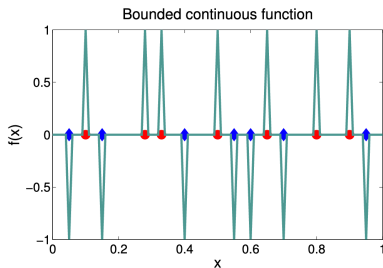
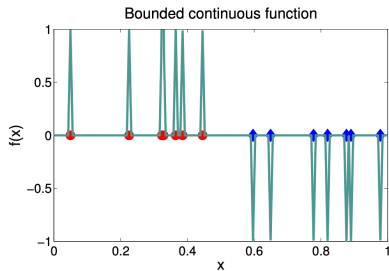
$$\left| \int f dP - \int f dQ \right|$$

MAXIMUM MEAN DISCREPANCY – INTUITION _____



$$\sup_{f \in \mathcal{F}_1} \left| \int f dP - \int f dQ \right|$$

MAXIMUM MEAN DISCREPANCY – INTUITION



$$\sup_{f \in \mathcal{F}_2} \left| \int f dP - \int f dQ \right|$$

Recall the general form of an integral probability metric:

$$D_{\mathcal{F}}(P, Q) = \sup_{f \in \mathcal{F}} \left| \int f \, dP - \int f \, dQ \right|$$

Choose a **kernel** k and consider its RKHS $\mathcal{H}(k)$.

(A kernel is a symmetric, positive definite function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$. k reproduces a Hilbert space $\mathcal{H}(k) : \mathcal{X} \rightarrow \mathbb{R}$ for which (i) for all $x \in \mathcal{X}$, $k(\cdot, x) \in \mathcal{H}(k)$, and (ii) for all $x \in \mathcal{X}$ and $f \in \mathcal{H}(k)$, $\langle k(\cdot, x), f \rangle_{\mathcal{H}(k)} = f(x)$.)

Let $\mathcal{B}(k) = \{f \in \mathcal{H}(k) : \langle f, f \rangle_{\mathcal{H}(k)} \leq 1\}$ be the unit ball in $\mathcal{H}(k)$.

Setting \mathcal{F} to be $\mathcal{B}(k)$ defines the **maximum mean discrepancy**.

Why this choice?

- Opportunity to easily enforce different degrees of smoothness through choice of the kernel k .
- If P and/or Q are empirical distributions, we can write $\mathcal{D}_{\mathcal{H}}(k)(P, Q)$ in closed form using only kernel evaluations.
- Furthermore in this setting $\mathcal{D}_{\mathcal{B}(k)}(P_n, Q_m)$ is a consistent estimator of $\mathcal{D}_{\mathcal{B}(k)}(P, Q)$ and the rate of convergence is *independent* of d .
- Since kernels can be defined on arbitrary domains \mathcal{X} , MMD can be used to measure distances between measures on eg. graphs, strings, etc., (not just \mathbb{R}^d).

Has been used for (amongst other things):

- Hypothesis testing [Fukumizu et al. 2008; Gretton et al. 2012; Doran et al. 2014, Chwialkowski and Gretton 2014]
- Density estimation [Song et al. 2007,2008; Sriperumbudur 2011]
- Clustering [Jegelka et al. 2009]
- Causal discovery [Sgouritsa et al. 2013; Chen et al. 2014; Schölkopf et al. 2015]
- Statistical model criticism [Lloyd & Ghahramani 2015; Kim et al. 2016]
- MCMC [Sejdinovic et al. 2014]
- ABC [Park et al. 2016]
- Training generative models [Li et al. 2015; Dziugaite et al. 2015]

MMD can be written *in closed form* (without the supremum).

$$D_{\mathcal{B}(k)}(P, Q)^2 = \iint k(x, y) dP(x) dP(y) \\ - 2 \iint k(x, y) dP(x) dQ(y) + \iint k(x, y) dQ(x) dQ(y)$$

With $Q = \frac{1}{m} \sum_{i=1}^m \delta(X_i)$, this becomes

$$\text{MMD}_{P,k}(Q)^2 = \frac{1}{m^2} \sum_{i,j=1}^m k(X_i, X_j) - \frac{2}{m} \sum_{i=1}^m \int k(X_i, x) dP(x) \\ + \iint k(x, y) dP(x) dP(y)$$

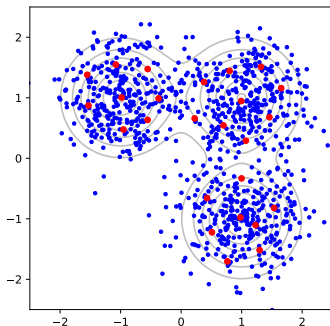
“But what about the integral with respect to P ?”

For general or unknown P is this not usually possible.

- In many useful cases, combinations of P and k are in fact tractable. (table below from [Briol et al. 2015])
- Otherwise consider using Kernel Stein Discrepancy instead.

\mathcal{X}	π	k	Reference
$[0, 1]^d$	Unif(\mathcal{X})	Wendland TP	Oates et al. (2016b)
$[0, 1]^d$	Unif(\mathcal{X})	Matérn Weighted TP	Sec. 5.4
$[0, 1]^d$	Unif(\mathcal{X})	Exponentiated Quadratic	Use of error function
\mathbb{R}^d	Mixt. of Gaussians	Exponentiated Quadratic	Kennedy (1998)
\mathbb{S}^d	Unif(\mathcal{X})	Gegenbauer	Sec. 5.5
Arbitrary	Unif(\mathcal{X}) / Mixt. of Gauss.	Trigonometric	Integration by parts
Arbitrary	Unif(\mathcal{X})	Splines	Wahba (1990)
Arbitrary	Known moments	Polynomial TP	Briol et al. (2015)
Arbitrary	Known $\partial \log \pi(\mathbf{x})$	Gradient-based Kernel	Oates et al. (2016a, 2017a)

BACK TO OUR PROBLEM



Given $m \ll n$, we'd like to find a minimiser of $\text{MMD}_{P,k}(Q)$ over size- m subsets of $\{X_1, \dots, X_n\}$.

$$\underset{\substack{S \subset \{1, \dots, n\} \\ |S|=m}}{\text{argmin}} \text{MMD}_{P,k} \left(\frac{1}{m} \sum_{i=1}^m \delta(X_i) \right)$$

Given a set of samples X_1, \dots, X_{i-1} that we use to form a measure $Q_{i-1} = \frac{1}{i-1} \sum_{j=1}^{i-1} \delta(X_j)$ that minimises $\text{MMD}_{P,k}(Q_{i-1})$ over all possible size $(i-1)$ subsets, we select for the next point X_i that which minimises $\text{MMD}_{P,k}(Q_i)$, where $Q_i = \frac{1}{i} \sum_{j=1}^i \delta(X_j)$.

Notation: The indices of the points we select will be written:

$$\pi(1), \pi(2), \dots, \pi(m) \quad , \quad \pi(\cdot) \in \{1, \dots, n\}$$

A SIMPLE SEQUENTIAL ALGORITHM

$$M_i = \frac{1}{i^2} \sum_{j,j'}^i k(X_j, X_{j'}) - \frac{2}{i} \sum_j^i \int k(X_j, y) dP(y) + \iint k(x, y) dP(x) dP(y)$$

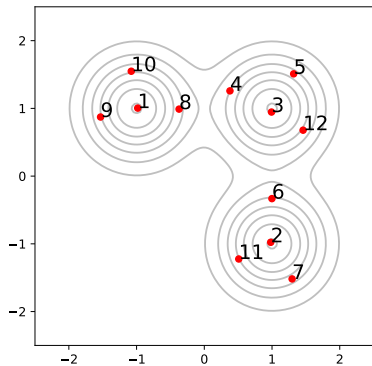
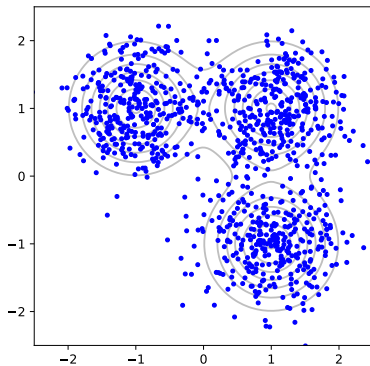
$$M_{i-1} = \frac{1}{(i-1)^2} \sum_{j,j'}^{i-1} k(X_j, X_{j'}) - \frac{2}{i-1} \sum_j^{i-1} \int k(X_j, y) dP(y) + \iint k(x, y) dP(x) dP(y)$$

$$\begin{aligned} M_i - M_{i-1} &= \left(\frac{1}{i^2} - \frac{1}{(i-1)^2} \right) \sum_{j,j'}^{i-1} k(X_j, X_{j'}) + \frac{2}{i^2} \sum_j^{i-1} k(X_j, X_i) + \frac{1}{i^2} k(X_i, X_i) \\ &\quad - \left(\frac{2}{i} - \frac{2}{i-1} \right) \sum_j^{i-1} \int k(X_j, y) dP(y) - \frac{2}{i} \int k(X_i, y) dP(y) \end{aligned}$$

A SIMPLE SEQUENTIAL ALGORITHM

$$\pi(i) \in \operatorname{argmin}_{j \in \{1, \dots, n\}} \left[\frac{1}{2} k(X_j, X_j) + \sum_{i'=1}^{i-1} k(X_{\pi(i')}, X_j) - i \int k(x, X_j) dP(x) \right]$$

A SIMPLE SEQUENTIAL ALGORITHM



A SIMPLE SEQUENTIAL ALGORITHM

Issues:

- This algorithm is **greedy**. (It scans through, and calculates with, all n points at each iteration).

This makes it (potentially) expensive.

- This algorithm is **myopic**. (It chooses the next point optimally, but this may not be the best long-term strategy).

This makes it (potentially) inaccurate.

What if we chose **more than one point** simultaneously?

- Greater statistical efficiency?
- Computationally favourable? (Or if not: acceptable overhead?)
- Can we implement it cleverly?

NON-MYOPIC ALGORITHM

Choose s points simultaneously. Write the index of the i 'th point within iteration j as $\pi(i, j)$, i.e. $\pi(i, \cdot) \in \{1, \dots, n\}^s$. Then pick:

index set of size s

$$\pi(i, \cdot) \in \operatorname{argmin}_{S \in \{1, \dots, n\}^s} \left[\frac{1}{2} \sum_{j, j' \in S} k(X_j, X_{j'}) + \sum_{i'=1}^{i-1} \sum_{j=1}^s \sum_{j' \in S} k(X_{\pi(i', j)}, X_{j'}) - is \sum_{j \in S} \int k(x, X_j) dP(x) \right]$$

We can rewrite this problem as an
integer quadratic programme (IQP),
and in doing so use state-of-the-art discrete optimisation codes.

INTEGER QUADRATIC PROGRAMMES

Let $v \in \{0, \dots, s\}^n : \sum_{j=1}^n v_j = s$ be a vector listing the number of copies of each sample that are selected at iteration i .

Algorithm chooses: $\{X_5, X_6, X_{10}, X_5, X_3\}$

$$v = \begin{pmatrix} X_1 & X_2 & X_3 & X_4 & X_5 & X_6 & X_7 & X_8 & X_9 & X_{10} \\ 0 & 0 & 1 & 0 & 2 & 1 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$(n = 10, s = 5)$$

INTEGER QUADRATIC PROGRAMMES

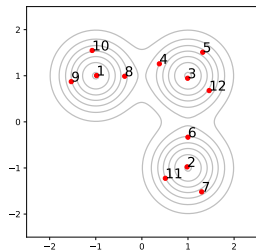
$$\operatorname{argmin}_{S \in \{1, \dots, n\}^s} \left[\frac{1}{2} \sum_{j, j' \in S} k(X_j, X_{j'}) + \sum_{i'=1}^{i-1} \sum_j \sum_{j' \in S} k(X_{\pi(i', j)}, X_{j'}) - is \sum_{j \in S} \int k(x, X_j) dP(x) \right]$$

$$\operatorname{argmin}_{v \in \mathbb{N}_0^s} \frac{1}{2} v^\top K v + c^i{}^\top v \quad \text{such that} \quad \mathbf{1}^\top v = s$$

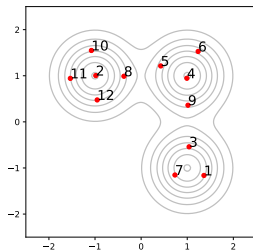
$$K_{j, j'} := k(X_j, X_{j'}), \quad \mathbf{1}_j := 1 \text{ for } j = 1, \dots, n,$$

$$c_j^i := \sum_{i'=1}^{i-1} \sum_{j'=1}^s k(X_{\pi(i', j')}, X_j) - is \int k(x, X_j) dP(x)$$

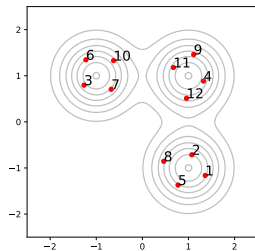
NON-MYOPIC SELECTION



1 point at a time

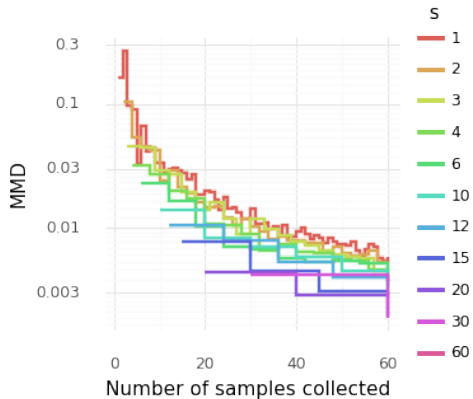
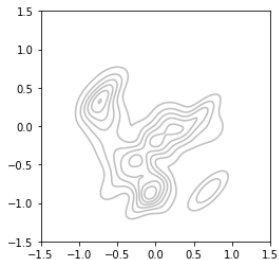


4 points at a time



12 points together

NON-MYOPIC SELECTION



Myopic algorithm is $O(nm^2)$, non-myopic algorithm is $O(n^s(ms)^2)$.

In both, the algorithm scans all n possible points at every iteration.

We can **mini-batch** the candidate set $\{X_1, \dots, X_n\}$ and retain $b \ll n$ at each iteration, then choose $s > 1$ samples from each batch of b .

This approach has complexity $O(b^s(ms)^2)$. In practice we find this makes it tractable in many settings.

THEOREMS

1:

Let $\{X_i\}_{i=1}^n \subset \mathcal{X}$ be **fixed**. Consider an index sequence π of length m and with selection size s . Then for all $m \geq 1$ there is a C such that

$$\begin{aligned} & \text{MMD}_{P,k} \left(\frac{1}{ms} \sum_{i=1}^m \sum_{j=1}^s \delta(X_{\pi(i,j)}) \right)^2 \\ & \leq \underbrace{\min_{\substack{1^\top w=1 \\ w_i \geq 0}} \text{MMD}_{P,k} \left(\sum_{i=1}^n w_i \delta(X_i) \right)^2}_{\text{optimal (weighted) quantisation} \\ & \quad \text{of } P \text{ achievable with the candidate set}} + C^2 \left(\frac{1 + \log m}{m} \right) \end{aligned}$$

2:

Let $\{X_i\}_{i=1}^n \subset \mathcal{X}$ be **independently sampled** from P . Consider an index sequence π of length m and with selection size s . Then for all $s \in \mathbb{N}$ and all $m, n \geq 1$, there are constants C, C', γ such that

$$\begin{aligned} \mathbb{E} \left[\text{MMD}_{P,k} \left(\frac{1}{ms} \sum_{i=1}^m \sum_{j=1}^s \delta(X_{\pi(i,j)}) \right)^2 \right] \\ \leq \frac{\log(C')}{n\gamma} + 2 \left(C^2 + \frac{\log(nC')}{\gamma} \right) \left(\frac{1 + \log m}{m} \right). \end{aligned}$$

3:

Consider a P -invariant, time-homogeneous, reversible **Markov chain** $\{X_i\}_{i \in \mathbb{N}} \subset \mathcal{X}$. Consider an index sequence π of length m and selection subset size s . Then there are constants C, C', C'', γ such that

$$\mathbb{E} \left[\text{MMD}_{P,k} \left(\frac{1}{ms} \sum_{i=1}^m \sum_{j=1}^s \delta(X_{\pi(i,j)}) \right)^2 \right] \leq \frac{\log(C')}{n\gamma} + \frac{C''}{n} + 2 \left(C^2 + \frac{\log(nC')}{\gamma} \right) \left(\frac{1 + \log m}{m} \right).$$

4:

Let each **mini-batch** $\{X_j^i\}_{j=1}^b \subset \mathcal{X}$ be independently sampled from μ . Consider an index sequence π of length m . Then $\forall m, n \geq 1$ there are constants C, C' such that

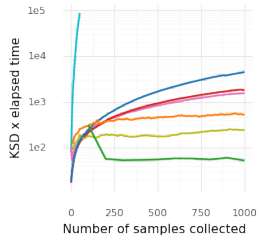
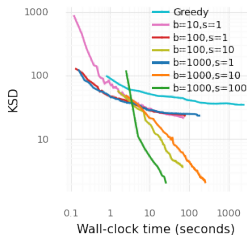
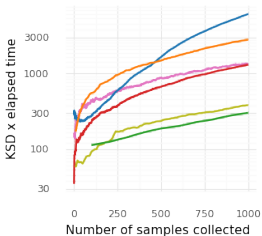
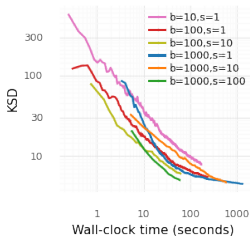
$$\mathbb{E} \left[\text{MMD}_{P,k} \left(\frac{1}{ms} \sum_{i=1}^m \sum_{j=1}^s \delta(X_{\pi(i,j)}^i) \right)^2 \right] \leq \frac{\log(C')}{b\gamma} + 2 \left(C^2 + \frac{\log(bC')}{\gamma} \right) \left(\frac{1 + \log m}{m} \right).$$

- Bounds are all **independent of s** . (Does not necessarily imply that $s = 1$ is optimal; indeed experiments show otherwise.)

What's missing:

- Mini-batch result in dependent sampling context. Seems achievable but technically involved.
- Different regimes of mini-batching. (ie. non-independent mini-batches). This seems harder.
- Output from non P -stationary Markov chains. (ie. chains that have not yet converged.)

EXPERIMENTS & HEURISTICS



*Optimal Quantisation of Probability Measures
Using Maximum Mean Discrepancy*
PMLR 130:1027–1035 / arXiv 2010.07064



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