Kernel approximations using determinantal point processes

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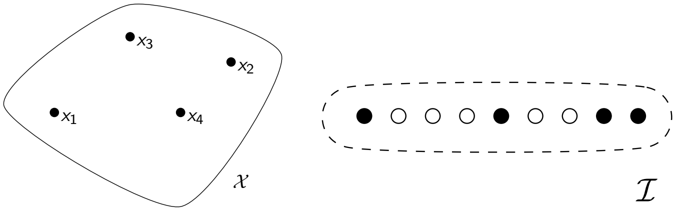
Outline

A **determinantal point process** (DPP) is a **distribution over subsets** of some set $\mathcal{X}, \mathcal{I}, \ldots$



Introduction

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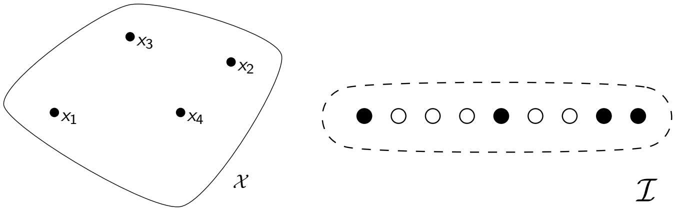
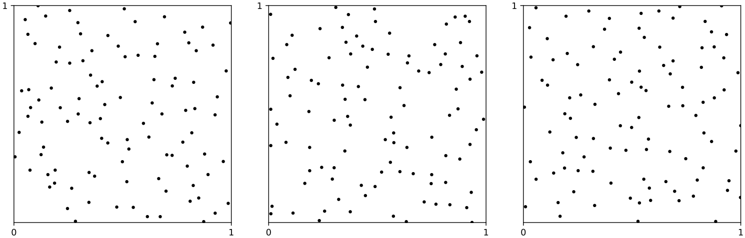


...with the **negative correlation** property:

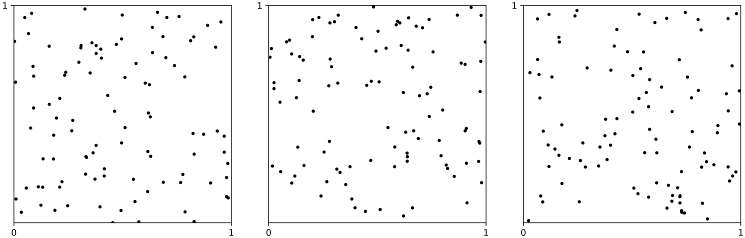
$$\forall B, B' \subset \mathcal{X}, \;\; B \cap B' = \emptyset \implies \mathbb{C}\mathrm{ov}(n_{\boldsymbol{x}}(B), n_{\boldsymbol{x}}(B')) \leq 0,$$

$$\text{where } n_{\boldsymbol{x}}(B) := |B \cap \boldsymbol{x}|$$

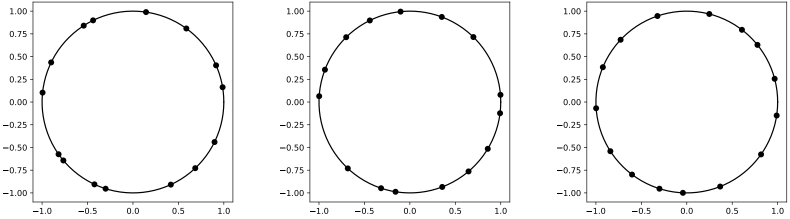
A DPP on $[0,1]^2$



i.i.d. particles on $[0,1]^2$



A DPP on the unit circle



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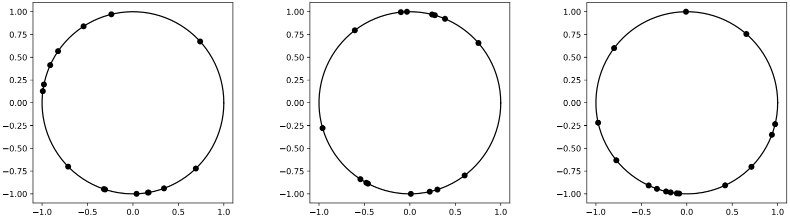

Introduction

DPPs were used as **tools of modelisation**

- models for (fermions in particle physics) [Macchi (1975)]
- eigenvalues of random matrices [Weyl (1946), Dyson (1962), Ginibre (1965)]
- statistical models (spatial statistics) [Lavancier et al. (2012)]

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they were also used as **tools of simulation**

- subset selection (feature selection, subsampling of nodes in graphs...)[Belhadji et al. (2018), Tremblay et al. (2017) ...]
- numerical integration [Bardenet and Hardy (2016)]

Kernel approximations

We study the quality of the kernel approximations

$$\mu \approx \sum_{i=1}^{N} w_i k(x_i, .),$$

where the $\boldsymbol{x} = \{x_1, \dots, x_N\}$ follows the distribution of a DPP and

- k is a kernel over a domain $\mathcal{X}$
- $\mu \in \mathcal{F}$ the RKHS associated to the kernel k

Assumption: the Mercer decomposition of the kernel k

$$k(x, y) = \sum_{m \in \mathbb{N}^*} \sigma_m e_m(x) e_m(y)$$

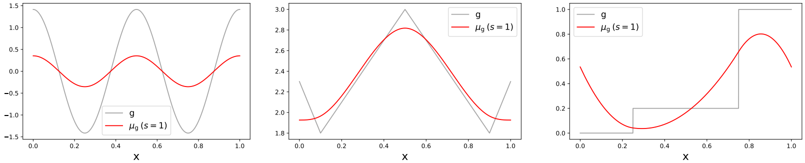
with $\sigma_1 \geq \sigma_2 \geq ... > 0$

Kernel approximations

Definition: an embedding of an element of $\mathbb{L}_2(\omega)$

Let $g \in \mathbb{L}_2(\omega)$, the *embedding* of g is defined by

$$\mu_g := \int_{\mathcal{X}} k(x,.)g(x)\mathrm{d}\omega(x).$$



In particular, we have

$$\forall f \in \mathcal{F}, \ \ \langle f, \mu_g \rangle_{\mathcal{F}} = \int_{\mathcal{X}} f(x)g(x)\mathrm{d}\omega(x).$$

Kernel approximations for the study of quadrature rules

For a given $f \in \mathcal{F}$ and $g \in \mathbb{L}_2(\omega)$, we have

$$\begin{aligned}\Big| \int_{\mathcal{X}} f(x)g(x)\mathrm{d}\omega(x) - \sum_{i \in [N]} w_i f(x_i) \Big| &= \big| \langle f, \mu_g - \sum_{i \in [N]} w_i k(x_i, .) \rangle_{\mathcal{F}} \big|, \\ &\leq \|f\|_{\mathcal{F}} \|\mu_g - \sum_{i \in [N]} w_i k(x_i, .)\|_{\mathcal{F}}.\end{aligned}$$

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$$\leq \|f\|_{\mathcal{F}} \|\mu_g - \sum_{i \in [N]} w_i k(x_i, .)\|_{\mathcal{F}}.$$

Definition: the worst integration error on the unit ball

$$\Big\| \mu_g - \sum_{i \in [N]} w_i k(x_i, .) \Big\|_{\mathcal{F}} = \sup_{\|f\|_{\mathcal{F}} \leq 1} \Big| \int_{\mathcal{X}} f(x)g(x)\mathrm{d}\omega(x) - \sum_{i \in [N]} w_i f(x_i) \Big|$$

The optimal kernel quadrature

$$x_1, \dots, x_N = \text{i.i.d.} \sim \omega \implies \mathbb{E}\|\mu_g - \sum_{i \in [N]} \frac{1}{N} k(x_i, .)\|_{\mathcal{F}}^2 = \mathcal{O}(1/N).$$

Can we improve on the rate $\mathcal{O}(1/N)$?

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Definition

Given a set of nodes $\boldsymbol{x} = \{x_1, \dots, x_N\}$ s.t. $\boldsymbol{K}(\boldsymbol{x})$ is non-singular, the **optimal kernel quadrature** is the couple $(\boldsymbol{x}, \hat{\boldsymbol{w}})$ such that

$$\left\| \mu_g - \sum_{i \in [N]} \hat{w}_i k(x_i, .) \right\|_{\mathcal{F}} = \min_{\boldsymbol{w} \in \mathbb{R}^N} \left\| \mu_g - \sum_{i \in [N]} w_i k(x_i, .) \right\|_{\mathcal{F}}$$

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In particular

$$\left\| \mu_g - \sum_{i \in [N]} \hat{w}_i k(x_i, .) \right\|_{\mathcal{F}} = \left\| \mu_g - \mathbf{\Pi}_{\mathcal{T}(\boldsymbol{x})} \mu_g \right\|_{\mathcal{F}},$$

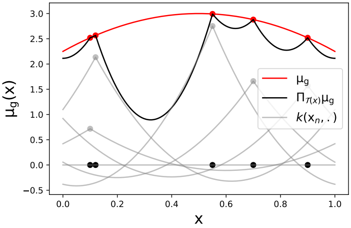
$\mathbf{\Pi}_{\mathcal{T}(\boldsymbol{x})}$: the orthogonal projection onto $\mathcal{T}(\boldsymbol{x}) = \mathrm{Span}(k(x_i, .))_{i \in [N]}$.

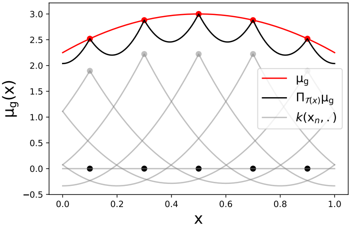
The optimal kernel quadrature

Kernel interpolation

The optimal mixture $\hat{\mu}_g := \sum_{i\in[N]} \hat{w}_i k(x_i, .)$ satisfies

$$\forall i \in [N],\ \hat{\mu}_g(x_i) = \mu_g(x_i).$$





How to choose the nodes in general?

The determinantal distributions

Definition

Let κ be a kernel s.t. $\int_{\mathcal{X}} \kappa(x,x)\mathrm{d}\omega(x) < +\infty$. The function

$$f_\kappa(x_1, \ldots, x_N) \propto \operatorname{Det} \boldsymbol{\kappa}(\boldsymbol{x})$$

is a p.d.f. on $\mathcal{X}^N$.

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We study two cases:

- Projection DPP:

$$\kappa(x,y) := \mathfrak{K}(x,y) = \sum_{n \in [N]} e_n(x) e_n(y)$$

- Continuous volume sampling (CVS):

$$\kappa(x,y) = k(x,y) = \sum_{m \in \mathbb{N}^*} \sigma_m e_m(x) e_m(y)$$

Main results

Theorem (Belhadji et al. (2019); Belhadji (2021))

Under the distribution of the Projection DPP, we have

$$\forall g \in \mathbb{L}_2(\omega), \ \mathbb{E}_{\mathrm{DPP}} \left\| \mu_g - \mathbf{\Pi}_{\mathcal{T}(\boldsymbol{x})} \mu_g \right\|_{\mathcal{F}}^2 = \mathcal{O}(r_{N+1}),$$

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Theorem (Belhadji et al. (2020))

Under the distribution of CVS, we have

$$\forall g \in \mathbb{L}_2(\omega),\ \ \mathbb{E}_{\mathrm{DPP}} \left\|\mu_g - \mathbf{\Pi}_{\mathcal{T}(\boldsymbol{x})}\mu_g\right\|_{\mathcal{F}}^2 = \mathcal{O}(\sigma_{N+1}).$$

Theorem: a lower bound (Pinkus (1985); Belhadji et al. (2020))

For any configuration $\boldsymbol{x} \in \mathcal{X}^N$ such that $\dim \mathcal{T}(\boldsymbol{x}) = N$,

$$\sup_{\|g\|_\omega \leq 1} \|\mu_g - \mathbf{\Pi}_{\mathcal{T}(\boldsymbol{x})}\mu_g\|_{\mathcal{F}}^2 \geq \sigma_{N+1}$$

$\mathcal{X}$	$\mathcal{F}$ or k	σ_{N+1}	(e_m)
$[0,1]$	Sobolev	$\mathcal{O}(N^{-2s})$	Fourier
$[0,1]^d$	Korobov	$\mathcal{O}(\log(N)^{2s(d-1)}N^{-2s})$	$\otimes$ of Fourier
$[0,1]^d$	Sobolev	$\mathcal{O}(N^{-2s/d})$	"Fourier"
$\mathbb{S}^d$	Dot product	"-"	Spherical Harmonics
$\mathbb{R}$	Gaussian	$\mathcal{O}(e^{-\alpha N})$	Hermite Polys.
$\mathbb{R}^d$	Gaussian	$\mathcal{O}(e^{-\alpha d N^{1/d}})$	$\otimes$ of Hermite Polys.
...	...	...	...

Numerical simulations: DPP vs uniform grid

$\mathcal{F}$ = Korobov space of order $s = 1$, $\mathcal{X} = [0,1]^2$
We report $\epsilon_m(N) = \mathbb{E}_\kappa \|\mu_{e_m} - \mathbf{\Pi}_{\mathcal{T}(\boldsymbol{x})}\mu_{e_m}\|_{\mathcal{F}}^2$
under DPP ($\kappa = \mathfrak{K}$).

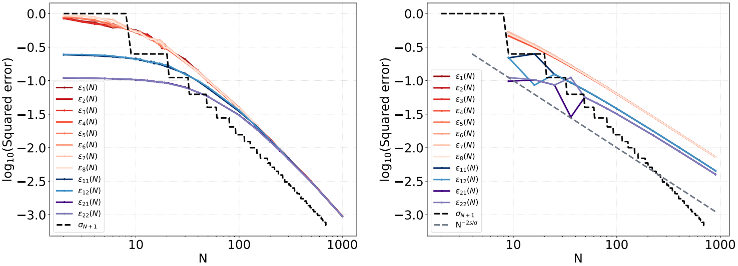


Figure: OKQ using DPPs (left) vs OKQ using the uniform grid (right)

Numerical simulations: the Gaussian space

$\mathcal{F}$ = the RKHS associated to the Gaussian kernel
We report $\epsilon_m(N) = \mathbb{E}_\kappa \|\mu_{e_m} - \mathbf{\Pi}_{\mathcal{T}(\boldsymbol{x})}\mu_{e_m}\|^2_{\mathcal{F}}$ for $m \in \{1, 15\}$
under DPP ($\kappa = \mathfrak{K}$).

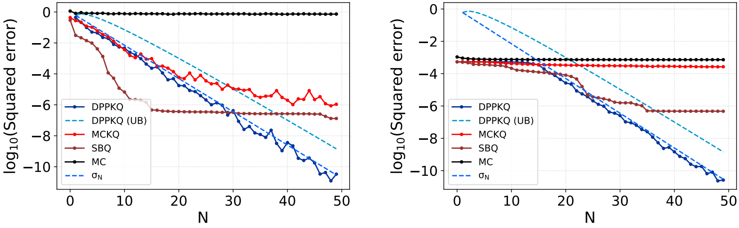
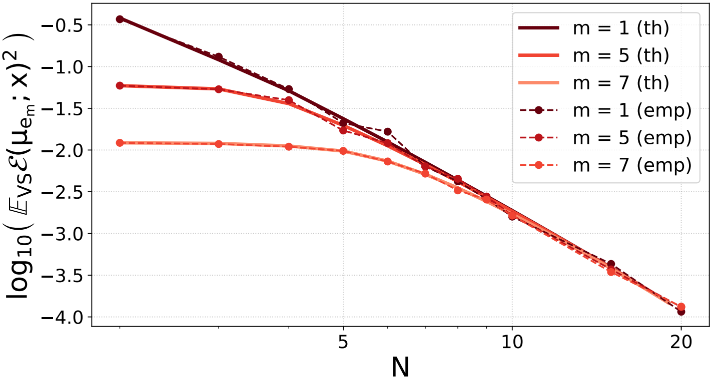


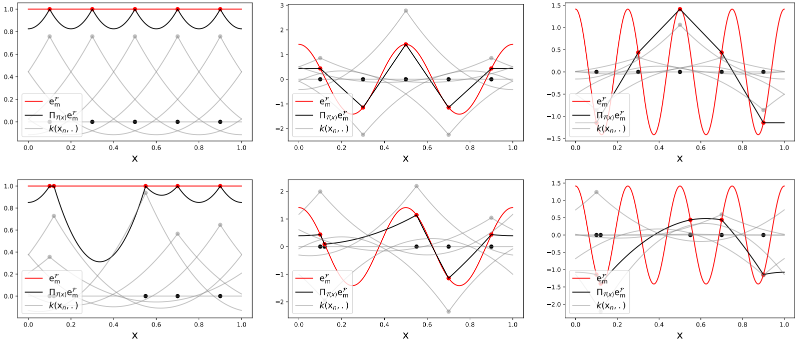
Figure: The squared interpolation error for e_1 (Left), vs e_{15} (Right).

$\mathcal{F} =$ the periodic Sobolev space of order $s = 2$, $\mathcal{X} = [0, 1]$
We report $\epsilon_m(N) = \mathbb{E}_\kappa \|\mu_{e_m} - \mathbf{\Pi}_{\mathcal{T}(\boldsymbol{x})}\mu_{e_m}\|^2_{\mathcal{F}}$ for $m \in \{1, 5, 7\}$
under CVS ($\kappa = k$).



An intuition

The reconstruction on the RKHS is governed by the reconstruction of the eigenfunctions e_m



A summary

Take Home Messages

- A general **theoretical analysis of kernel interpolation** for nodes sampled according to **the projection DPP or CVS**
- New **geometric intuitions** behind the use of **DPPs** for this task
- Empirical validation on different RKHSs: **the optimal rate of convergence $\mathcal{O}(\sigma_{N+1})$ is achieved**

Distribution	Theoretical rate	Empirical rate
P. DPP	$N^2\mathcal{O}(r_{N+1})$ [Belhadji et al. (2019)] $\mathcal{O}(r_{N+1})$ [Belhadji (2021)]	$\mathcal{O}(\sigma_{N+1})$ [Belhadji et al. (2019)]
CVS	$\mathcal{O}(\sigma_{N+1})$ [Belhadji et al. (2020)]	$\mathcal{O}(\sigma_{N+1})$ [Belhadji et al. (2020)]

Thank you for your attention!