Monte Carlo integration with repulsive point processes

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https://statisfaction-blog.github.io/

Figure imposée

The goal is to approximate

$$\int f \,\mathrm{d}\mu \approx \sum_{i=1}^{N} w_i f(x_i).$$

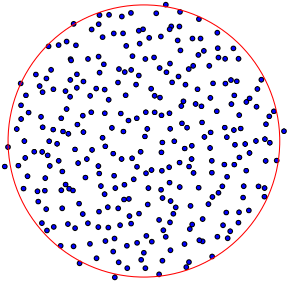
- How to choose the nodes x_i?
- How to choose the weights w_i?

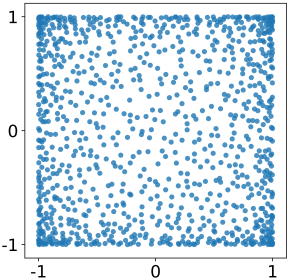
Monte Carlo integration (importance sampling, MCMC, etc.)

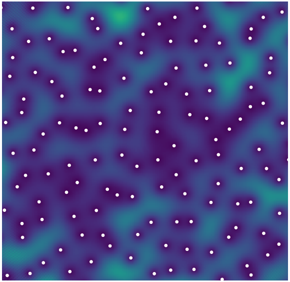
- Choose the nodes randomly, and the weights $w_i = w_i(x_1, \dots, x_N)$.
- Typical error is

$$\sqrt{\mathbb{E}\left[\int f \,\mathrm{d}\mu - \sum_{i=1}^{N} w_i f(x_i)\right]^2} \sim \frac{1}{\sqrt{N}}.$$

Prologue: Repulsive point processes







Go to CLT

Monte Carlo with DPPs

DPPs lead to tight rates in RKHSs

Repelled point processes

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Repelled point processes

Projection DPPs

- Let $(\varphi_k)_{k=0,\dots,N-1}$ be an orthonormal sequence in $L^2(\mu)$.
- Let $\mathrm{K}(x,y) = \sum_{k=0}^{N-1} \varphi_k(x)\varphi_k(y)$.

Definition (Hough, Krishnapur, Peres, and Virág, 2006)

$X = \{x_1, \dots, x_N\}$ is the DPP with kernel K and reference measure μ if

$$x_1, \dots, x_N \sim \frac{1}{N!} \det \Big[\mathrm{K}(x_i, x_\ell)\Big]_{i,\ell=1}^{N} \mathrm{d}\mu(x_1)\dots\mathrm{d}\mu(x_N).$$

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What projection DPP samples look like

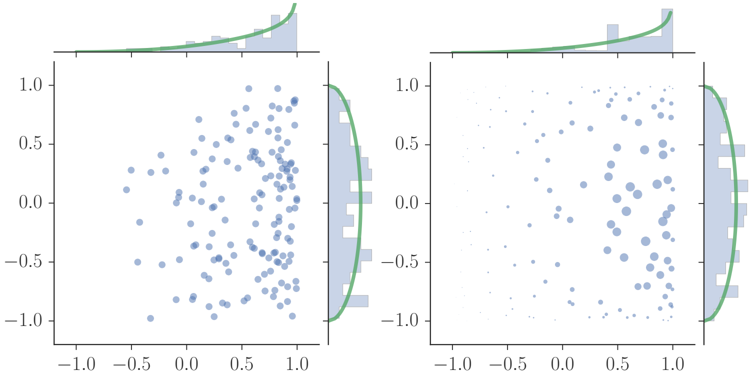

Figure: Left:i.i.d., Right: orthogonal polynomial ensemble (DPP)

Theorem (Bardenet and Hardy, 2020)

Let $\mu(\mathrm{d}x) = \omega(x)\mathrm{d}x$ with ω separable, $\mathscr{C}^1$, positive on the open set $(-1,1)^d$, and satisfying a technical regularity assumption. Let $\varepsilon > 0$. If $x_1, \dots, x_N$ stands for the associated multivariate OP Ensemble, then for every f $\mathscr{C}^1$ vanishing outside $[-1+\varepsilon, 1-\varepsilon]^d$,

$$\sqrt{N^{1+1/d}} \left(\sum_{i=1}^{N} \frac{f(x_i)}{\mathrm{K}(x_i, x_i)} - \int f(x)\mu(\mathrm{d}x) \right) \xrightarrow[N\to\infty]{law} \mathcal{N}(0, \Omega_{f,\omega}^2),$$

where

$$\Omega_{f,\omega}^2 = \frac{1}{2} \sum_{k_1,\dots,k_d=0}^{\infty} (k_1 + \cdots + k_d) \widehat{\left(\frac{f\omega}{\omega_{eq}^{\otimes d}} \right)} (k_1, \dots, k_d)^2,$$

and $\omega_{eq}^{\otimes d}(x) = \pi^{-d}(1-x^2)^{-1/2}$.

- With Thibaut Lemoine, we have a CLT with rate $\sqrt{N^{1+2/d}}$ (soon).

Theorem (Bardenet and Hardy, 2020)

Let $\mu(\mathrm{d}x) = \omega(x)\mathrm{d}x$ with ω $\mathscr{C}^1$ on $(-1,1)^d$. Consider a measure $q(x)\mathrm{d}x$ satisfying the assumptions of the previous theorem, let $K_N(x,y)$ be the corresponding kernel, and $x_1,\dots,x_N$ the associated multivariate OP Ensemble. Then, for every f as before,

$$\sqrt{N^{1+1/d}}\left(\sum_{i=1}^{N}\frac{f(x_i)}{\mathrm{K}(x_i,x_i)}\frac{\omega(x_i)}{q(x_i)} - \int f(x)\mu(\mathrm{d}x)\right) \xrightarrow[N\to\infty]{law} \mathcal{N}\left(0,\Omega_{f,\omega}^2\right),$$

where $\Omega_{f,\omega}^2$ is unchanged.

Plan

Monte Carlo with DPPs

DPPs lead to tight rates in RKHSs

Repelled point processes

RKHSs are spaces of smooth functions with a kernel

- Consider the RKHS $\mathcal{F}$ with kernel k, i.e. the completion of

$$\left\{ \sum_{i=1}^{M} \alpha_i k(x_i, \cdot), M \in \mathbb{N}, \alpha_1, \dots, \alpha_n \in \mathbb{R}, x_1, \dots, x_M \in \mathbb{R}^d \right\}.$$

for the inner product defined by $\langle k(x, \cdot), k(y, \cdot) \rangle_{\mathcal{F}} := k(x, y)$.

- For $f \in \mathcal{F}$ and $x \in \mathcal{X}$, $f(x) = \langle f, k(x, \cdot) \rangle$.

- Under general assumptions, $\mathcal{F} \subset L^2(\mathrm{d}\mu)$, is dense, there is an ON basis (e_n) of $L^2(\mathrm{d}\mu)$ and $\sigma_n \to 0$ such that, pointwise,

$$k(x, y) = \sum_{n \geqslant 1} \sigma_n e_n(x) e_n(y).$$

- In that case, $f \in \mathcal{F}$ if and only if $\sum_n \sigma_n^{-1} |\langle f, e_n \rangle|^2$ converges.

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- In that case, $f \in \mathcal{F}$ if and only if $\sum_n \sigma_n^{-1} |\langle f, e_n \rangle|^2$ converges.

- Let $f \in \mathcal{F}$, $g \in L^2(\mathrm{d}\mu)$ then

$$\left| \int fg\mathrm{d}\mu - \sum_{i=1}^{N} w_i f(x_i) \right| \leqslant \|f\|_{\mathcal{F}} \left\| \mu_g - \sum_{i=1}^{N} w_i k(x_i, .) \right\|_{\mathcal{F}}, \qquad (1)$$

where

$$\mu_g = \int g(x)k(x,.)\mathrm{d}\mu(x)$$

is the mean element of g.

- Once the nodes $x_1, \dots, x_N$ are known, minimizing the RHS of (1) in w boils down to inverting the $N \times N$ Gram matrix $((k(x_i, x_j)))$.

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Volume sampling and tight rates

Volume sampling

- Let $x_1, \dots, x_N \sim Z^{-1} \det[k(x_i, x_j)] \, \mathrm{d}\mu(x_1) \dots \mathrm{d}\mu(x_N)$
- Solve the linear program for the weights $w_1, \dots, w_N$.

Theorem (Belhadji, Bardenet, and Chainais, 2020)

Assume again $\sum_{n=1}^{N} |\langle g, e_n \rangle|^2 \leqslant 1$. *Then*

$$\mathbb{E} \left\| \mu_g - \sum_{i=1}^{N} w_i k(x_i, \cdot) \right\|_{\mathcal{F}}^2 \leqslant \sigma_N \left(1 + \beta_N\right),$$

where $\beta_N = \min_{M \in [2:N]} [(N - M + 1)\sigma_N]^{-1} \sum_{m \geqslant M} \sigma_m$.

- Pinkus, 2012 shows that $\inf_{\substack{Y \subset \mathcal{F} \\ \dim Y = N}} \sup_{\|g\|_{L^2(\mu)} \leqslant 1} \inf_{y \in Y} \|\mu_g - y\|_{\mathcal{F}}^2 = \sigma_{N+1}$.

Go to repelled PPs

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Go to repelled PPs

- For $f \in \mathcal{F} \subset L^2(\mu)$, we investigate guarantees on

$$\mathbb{E}\|f - \hat{f}\|^2_{L^2(\mu)}$$

in (Belhadji, Bardenet, and Chainais, 2023, *preprint*).

- In (Rouault, Bardenet, and Maida, 2024), we investigate the Coulomb gas with interaction potential k and confining potential V,

$$\mathrm{d}\mathbb{P}^V_{n,\beta_n}(X_n) = \frac{1}{Z^V_{n,\beta_n}} \mathrm{e}^{-\frac{\beta_n}{2n^2}\sum_{i\neq j} K(x_i,x_j) - \frac{\beta_n}{n}\sum_{i=1}^n V(x_i)} \mathrm{d}x_1 \ldots \mathrm{d}x_n,$$

In particular, we prove that for $\beta_n = n^2$ and $r \leqslant 1/\sqrt{n}$,

$$\mathbb{P}^V_{n,\beta_n}\left(\sup_{f\in B_{\mathcal{F}}} \left| \int f \mathrm{d}\mu_n - \int f \mathrm{d}\mu_V \right|^2 > r^2 \right) \leqslant \exp\left(-u_1 \beta_n r^2\right). \quad (2)$$

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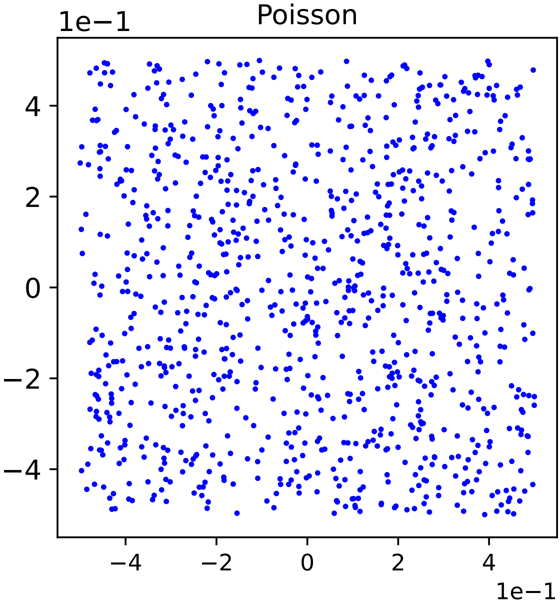
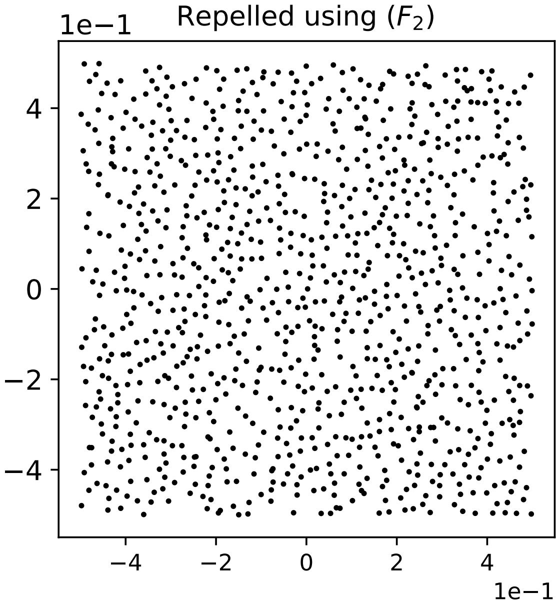

Poisson
1e−1
4
2
0
−2
−4
−4
−2
0
2
4
1e−1

The repelled Poisson point process



Coulomb repulsion leads to variance reduction

- Let $\mathcal{P} \subset \mathbb{R}^d$ be a homogeneous Poisson point process.
- For x in $\mathbb{R}^d$ and a collection C of points in $\mathbb{R}^d$, consider

$$F_C(x) = \sum_{y \in C, y \neq x} \frac{x - y}{\|x - y\|^d},$$

- Consider the repelled point process

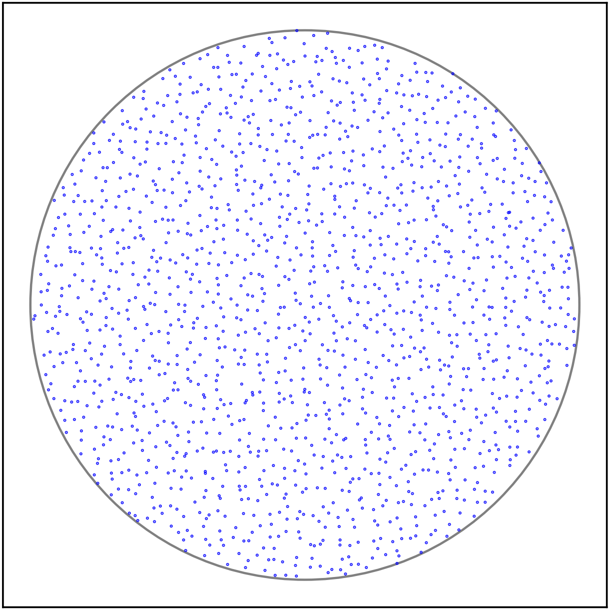
$$\Pi_\varepsilon \mathcal{P} \triangleq \{x + \varepsilon F_{\mathcal{P}}(x), \quad x \in \mathcal{P}\}.$$

Theorem (Hawat, Bardenet, and Lachièze-Rey, 2023)

- $\Pi_\varepsilon \mathcal{P}$ is well-defined and has the same intensity λ as $\mathcal{P}$.
- For f compactly supported in $S \subset \mathbb{R}^d$, there is an $\varepsilon > 0$ such that

$$\mathrm{Var}\left[\frac{1}{\lambda} \sum_{x \in S \cap \Pi_\varepsilon \mathcal{P}} f(x)\right] < \mathrm{Var}\left[\frac{1}{\lambda} \sum_{x \in S \cap \mathcal{P}} f(x)\right].$$

The repelled Ginibre point process[1]



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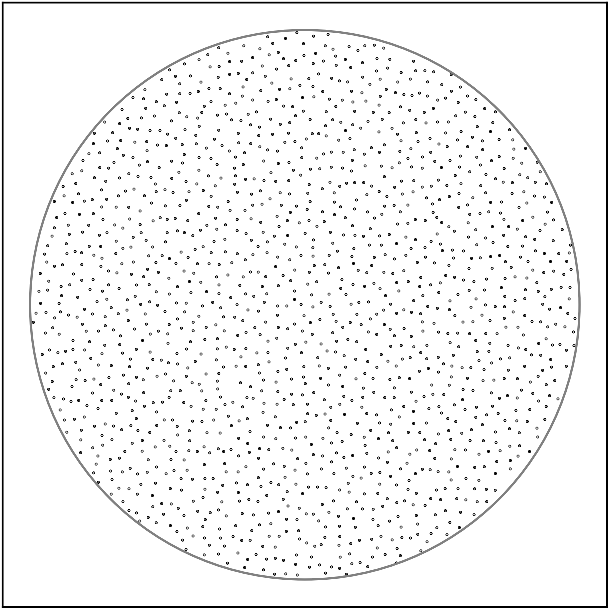

Wrapping up

- Volume sampling yields tight MSE bounds in RKHSs.[2][3][4]
- DPP sampling is an active research topic. Check out our Python toolbox DPPy.[5]
- Coulomb repulsion yields variance reduction at a lower cost, and is potentially widely applicable.[6]

Take-home message

- Repulsive point processes yield fast Monte Carlo integration.
- DPPs tie analytic assumptions with node design.
- PhD and postdoc applications welcome! remi.bardenet@gmail.com

[2] Belhadji, Bardenet, and Chainais, 2019.
[3] Belhadji, Bardenet, and Chainais, 2020.
[4] Belhadji, Bardenet, and Chainais, 2023.
[5] Gautier, Bardenet, Polito, and Valko, 2019, github.com/guilgautier/DPPy.
[6] Hawat, Bardenet, and Lachièze-Rey, 2023.

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