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SFB F68
Tomography Across the Scales

Technische Universität Berlin


Fast and Accurate Approximation of High-Dimensional Radial Kernels via Slicing

Michael Quellmalz | TU Berlin | Chemnitz Summer School and Workshop on Applied Analysis, 22 September 2025
Joint work with Johannes Hertrich, Tim Jahn, Nicolaj Rux and Gabriele Steidl

The Problem

- **Given:** Points $x_n, y_m \in \mathbb{R}^d$ and coefficients $w_n \in \mathbb{R}$ for $n = 1, ..., N$, $m = 1, ..., M$
- **Radial kernel** $K: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$

$$K(x, y) = F(\|x - y\|)$$

  with basis function $F: \mathbb{R}_{\geq 0} \to \mathbb{R}$

- **We want:** Kernel sums

$$s_m = \sum_{n=1}^{N} w_n F(\|x_n - y_m\|) \qquad \forall\, m = 1, ..., M \tag{1}$$

Examples	$F(\|x\|)$
Gauss	$\exp(-\frac{\|x\|^2}{2\sigma^2})$
Matérn	$\frac{2^{1-\nu}}{\Gamma(\nu)}(\frac{\sqrt{2\nu}}{\beta}\|x\|)^\nu K_\nu(\frac{\sqrt{2\nu}}{\beta}\|x\|)$
Laplace	$\exp(-\alpha\|x\|)$
Riesz	$-\|x\|^r$

- **Goal:** Improve computational complexity $\mathcal{O}(MN)$

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Approach 1: Fast Fourier Summation

[Kunis Potts 2006] [Potts Steidl Nieslony 2004]

- Fourier expansion of the kernel with degree $N_{\text{ft}} \in \mathbb{N}$

$$F(\|x\|) \approx \sum_{k \in \{-N_{\text{ft}}, \dots, N_{\text{ft}}\}^d} c_k \mathrm{e}^{2\pi \mathrm{i} \langle x, k \rangle}$$

- Insert to (1)

$$s_m = \sum_{n=1}^{N} w_n F(\|x_n - y_m\|) \approx \sum_{n=1}^{N} w_n \sum_{k \in \{-N_{\text{ft}}, \dots, N_{\text{ft}}\}^d} c_k \mathrm{e}^{2\pi \mathrm{i} \langle x_n - y_m, k \rangle}$$

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1. Inner sum $\hat{w}_k$ is **non-equispaced fast Fourier transform (NFFT)** of w
2. Outer sum s_m is NFFT of $c_k \hat{w}_k$ $\rightsquigarrow$ Complexity $\mathcal{O}(N + M + N_{\text{ft}}^d \log N_{\text{ft}})$

☺ Efficient for $d \in \{1, 2, 3\}$

😐 Becomes unfeasible for larger d

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Approach 2: Random Fourier features (RFF)

[Rahimi Recht 2007]

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- Assumption: $F(\|\cdot\|)$ positive definite on $\mathbb{R}^d$ and $F(0) = 1$
- By **Bochner's theorem**, $F(\|\cdot\|)$ is the Fourier transform of a probability measure $\mu \in \mathcal{P}(\mathbb{R}^d)$
- Draw iid samples $v_1, \ldots, v_P$ from μ

$$F(\|x\|) = \int_{\mathbb{R}^d} \mathrm{e}^{-2\pi\mathrm{i}\langle x, v\rangle} \,\mathrm{d}\mu(v) \approx \frac{1}{P}\sum_{p=1}^{P} \mathrm{e}^{2\pi\mathrm{i}\langle x, v_p\rangle}$$

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☺ Complexity $\rightsquigarrow \mathcal{O}(P(N+M))$

☺ Simple to implement

😐 Error bound $\mathbb{E}[\|F - \tilde{F}\|_\infty] \in \mathcal{O}(1/\sqrt{P})$ [Sutherland Schneider 2015]

☹ Only for positive definite functions

Kernel	positive definite
Gaussian	☑
Matérn	☑
Laplacian	☑
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Approach 3: Slicing Summation

[Hertrich 2024]

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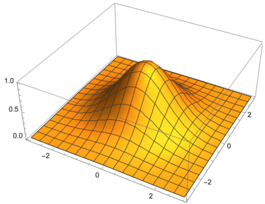
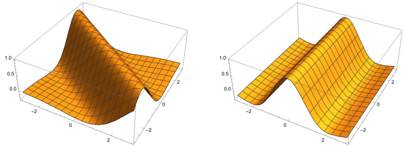
- Idea: Construct $f\colon \mathbb{R} \to \mathbb{R}$ s.t.

$$F(\|x\|) = \int_{\mathbb{S}^{d-1}} f(\langle x, \xi \rangle)\, \mathrm{d}\xi \qquad \forall\, x \in \mathbb{R}^d$$

(Integral normalized to 1)



radial function $F(\|x\|)$
(Gaussian)



$x \mapsto f(\langle x, \xi \rangle)$ for 2 different ξ

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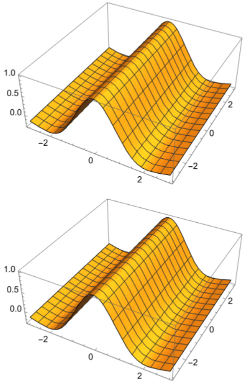

Top: Approximation of F
Bottom: $x \mapsto f(\langle x, \xi \rangle)$

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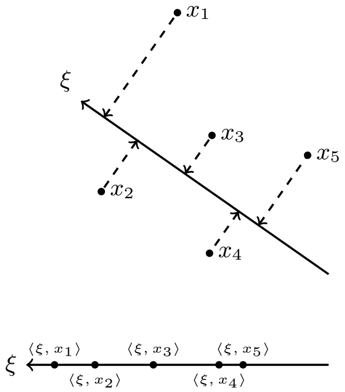
- Insert into the sum (1)

$$s_m = \sum_{n=1}^{N} w_n \int_{\mathbb{S}^{d-1}} f(\langle x_n, \xi \rangle - \langle y_m, \xi \rangle)\,\mathrm{d}\xi$$

Sample $\xi_p \sim \mathcal{U}_{\mathbb{S}^{d-1}}$ (uniform measure on the sphere)

$$\approx \frac{1}{P} \sum_{p=1}^{P} \underbrace{\sum_{n=1}^{N} w_n f(\langle x_n, \xi_p \rangle - \langle y_m, \xi_p \rangle)}_{\text{1D kernel sum}}$$

- P one-dimensional sums $\rightsquigarrow \mathcal{O}(P(N + M + N_{\mathrm{ft}} \log N_{\mathrm{ft}}))$



Projection of points $x_n \in \mathbb{R}^2$ to the line in direction ξ

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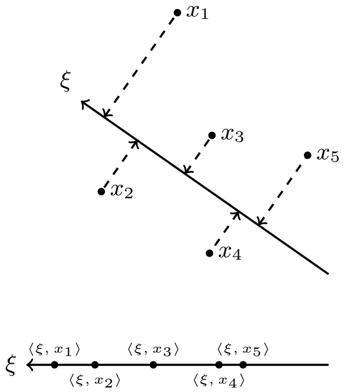

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The Slicing Transform

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Goal: Construct "sliced kernel function" $f\colon \mathbb{R} \to \mathbb{R}$ s.t.

$$F(\|x\|) = \int_{\mathbb{S}^{d-1}} f(\langle x, \xi \rangle)\,\mathrm{d}\xi \qquad \forall\, x \in \mathbb{R}^d$$

Theorem ($f \mapsto F$) [Hertrich 2024] [Rubin 2003]

For $d \geq 2$, a pair (F, f) of basis functions in $L^\infty_{\mathrm{loc}}(\mathbb{R}_{\geq 0})$ fulfills this relation if and only if F is the **generalized Riemann–Liouville fractional integral**

$$F(t) = \frac{2\Gamma(\frac{d}{2})}{\sqrt{\pi}\Gamma(\frac{d-1}{2})} \int_0^1 f(ts)(1-s^2)^{\frac{d-3}{2}}\,\mathrm{d}s.$$

Theorem (Smoothness of F) [Rux Q. Steidl 2025]

For $d \in \mathbb{N}$ with $d \geq 3$, let $f \in L^1_{\mathrm{loc}}([0,\infty))$ for odd d and $f \in L^p_{\mathrm{loc}}([0,\infty))$ with $p > 2$ for even d. Then F is $\lfloor \frac{(d-2)}{2} \rfloor$-times continuously differentiable on $(0, \infty)$.

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Inversion $F \mapsto f$ "Dimension Walk in Fourier Space"

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- **Rotation operator** $\mathcal{R}_d$ maps $F\colon [0,\infty) \to \mathbb{R}$ to the radial function

$$\mathcal{R}_d F(x) := F(\|x\|), \qquad x \in \mathbb{R}^d$$

- **Spherical averaging operator** maps $\Phi\colon \mathbb{R}^d \to \mathbb{R}$ to

$$\mathcal{A}_d \Phi(r) := \int_{\mathbb{S}^{d-1}} \Phi(r\,\xi)\,\mathrm{d}\xi, \qquad r \in \mathbb{R}$$

- **Multiplication operator**

$$\mathcal{M}_d F(r) := F(|r|)|r|^{d-1}, \quad r \in \mathbb{R}$$

Theorem (Inversion for L^1 functions) [Rux Q. Steidl 2025]

Let $d \geq 2$ and $F\colon [0,\infty) \to \mathbb{R}$ with $\mathcal{R}_d F, \mathcal{F}_d(\mathcal{R}_d F) \in L^1(\mathbb{R}^d)$. Then

$$f = \frac{|\mathbb{S}^{d-1}|}{2}(\mathcal{F}_1 \circ \mathcal{M}_d \circ \mathcal{A}_d \circ \mathcal{F}_d \circ \mathcal{R}_d)[F].$$

Theorem (Inversion via tempered distributions) [Rux Q. Steidl 2025]

Let $f \in C(\mathbb{R})$ is slowly increasing and even, it can be recovered via

$$f = (\mathcal{F}_1 \circ \mathcal{R}_d^{\star} \circ \mathcal{F}_d^{-1})[\mathcal{R}_d F]. \qquad (\star)$$

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Let $d \geq 2$ and $F\colon [0,\infty) \to \mathbb{R}$ with $\mathcal{R}_d F, \mathcal{F}_d(\mathcal{R}_d F) \in L^1(\mathbb{R}^d)$. Then

$$f = \frac{|\mathbb{S}^{d-1}|}{2}(\mathcal{F}_1 \circ \mathcal{M}_d \circ \mathcal{A}_d \circ \mathcal{F}_d \circ \mathcal{R}_d)[F].$$

Theorem (Inversion via tempered distributions) [Rux Q. Steidl 2025]

Let $f \in C(\mathbb{R})$ is slowly increasing and even, it can be recovered via

$$f = (\mathcal{F}_1 \circ \mathcal{R}_d^{\star} \circ \mathcal{F}_d^{-1})[\mathcal{R}_d F]. \qquad (\star)$$

Inversion $F \mapsto f$ "Dimension Walk in Fourier Space"

- **Rotation operator** $\mathcal{R}_d$ maps $F\colon [0,\infty) \to \mathbb{R}$ to the radial function

$$\mathcal{R}_d F(x) \coloneqq F(\|x\|), \qquad x \in \mathbb{R}^d$$

- **Spherical averaging operator** maps $\Phi\colon \mathbb{R}^d \to \mathbb{R}$ to

$$\mathcal{A}_d \Phi(r) \coloneqq \int_{\mathbb{S}^{d-1}} \Phi(r\,\xi)\,\mathrm{d}\xi, \qquad r \in \mathbb{R}$$

- **Multiplication operator**

$$\mathcal{M}_d F(r) \coloneqq F(|r|)|r|^{d-1}, \quad r \in \mathbb{R}$$

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Example: Gauss Kernel

Gauss kernel	$F(t) = \exp\left(-\frac{t^2}{2}\right)$
Radial function	$\mathcal{R}_d F(x) = \exp\left(-\frac{\|x\|^2}{2}\right)$
Fourier transform	$\mathcal{F}_d^{-1}\mathcal{R}_d F(x) = (2\pi)^{d/2}\exp(-2\pi^2\|x\|^2)$
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Sliced kernel	$f(t) = \mathcal{F}_1\mathcal{M}_d\mathcal{A}_d\mathcal{F}_d^{-1}\mathcal{R}_d F(t) = {}_1F_1\left(\frac{d}{2}, \frac{1}{2}, -\frac{t^2}{2}\right)$ (confluent hypergeometric function)

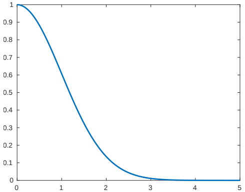

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Figure: Gauss kernel F and the corresponding sliced kernel f for $d = 10$

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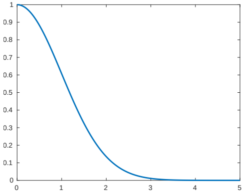

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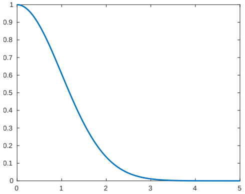

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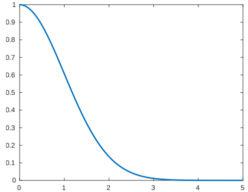

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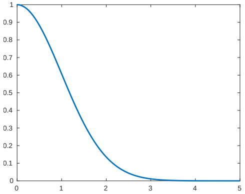

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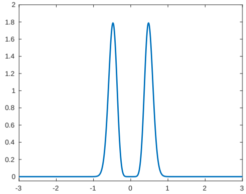

$\mathcal{M}_d\rho = \mathcal{F}_1 f$

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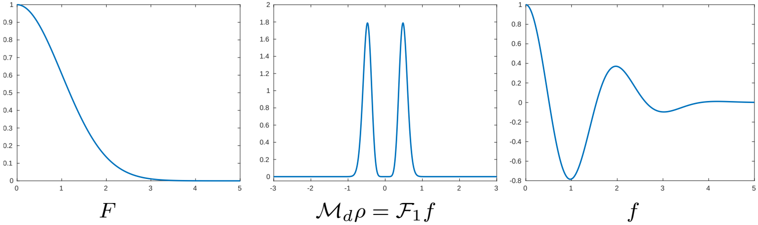

Figure: Gauss kernel F and the corresponding sliced kernel f for $d = 10$

Known Kernel Pairs (F, f)

Kernel	$F(x)$	$\mathcal{F}_d^{-1}[F(\\|\cdot\\|)](\\|\omega\\|)$	$f(x)$	$\mathcal{F}_1^{-1}[f](\lvert\omega\rvert)$
Gauss	$\exp(-\frac{x^2}{2\sigma^2})$	$(2\pi\sigma^2)^{d/2}\exp(-2\pi^2\sigma^2\omega^2)$	${}_1F_1(\frac{d}{2}; \frac{1}{2}; \frac{-x^2}{2\sigma^2})$	$\frac{\pi\sigma\exp(-2\pi^2\sigma^2\omega^2)(2\pi^2\sigma^2\omega^2)^{(d-1)/2}}{2\Gamma(\frac{d}{2})}$
Laplace	$\exp(-\alpha x)$	$\frac{\Gamma(\frac{d+1}{2})2^d\pi^{\frac{d-1}{2}}}{\alpha^d}(1+\frac{4\pi^2\omega^2}{\alpha^2})^{-\frac{d+1}{2}}$	$\sum_{n=0}^{\infty}\frac{(-\alpha)^n\sqrt{\pi}\Gamma(\frac{n+d}{2})}{n!\Gamma(\frac{d}{2})\Gamma(\frac{n+1}{2})}x^n$	$\frac{\Gamma(\frac{d+1}{2})2^d\pi^{\frac{d-1}{2}}\lvert\omega\rvert^{d-1}}{\Gamma(\frac{d}{2})\alpha^d}(1+\frac{4\pi^2\omega^2}{\alpha^2})^{-\frac{d+1}{2}}$
Sliced Laplace	$\frac{I_{\frac{d-2}{2}}(-\alpha t)+\mathbf{L}_{\frac{d-2}{2}}(-\alpha t)}{(\alpha t)^{\frac{d-2}{2}}}$	$\frac{2^{\frac{4-d}{2}}\Gamma(\frac{d}{2})}{\pi^{(d+1)/2}\Gamma(\frac{d-1}{2})\lvert\omega\rvert^{d-1}}\frac{2\alpha}{\alpha^2+4\pi^2\omega^2}$	$\frac{2^{\frac{4-d}{2}}}{\sqrt{\pi}\Gamma(\frac{d-1}{2})}\exp(-\alpha x)$	$\frac{2^{\frac{d-4}{2}}}{\sqrt{\pi}\Gamma(\frac{d-1}{2})}\frac{2\alpha}{\alpha^2+4\pi^2\omega^2}$
Matérn	$\frac{2^{1-\nu}}{\Gamma(\nu)}(\frac{\sqrt{2\nu}}{\beta}x)^\nu K_\nu(\frac{\sqrt{2\nu}}{\beta}x)$	$\frac{\Gamma(\frac{2\nu+d}{2})2^{\frac{d}{2}}\pi^{\frac{d}{2}}\beta^d}{\Gamma(\nu)\nu^{\frac{d}{2}}}(1+\frac{2\pi^2\beta^2\omega^2}{\nu})^{-\frac{2\nu+d}{2}}$	[Hertrich 2024, Appx C]	$\frac{\Gamma(\frac{2\nu+d}{2})2^{\frac{d}{2}}\pi^d\beta^d\lvert\omega\rvert^{d-1}}{\Gamma(\frac{d}{2})\Gamma(\nu)\nu^{\frac{d}{2}}}(1+\frac{2\pi^2\beta^2\omega^2}{\nu})^{-\frac{2\nu+d}{2}}$
Riesz for $r > -1$	$-x^r$	not a function	$-\frac{\sqrt{\pi}\Gamma(\frac{d+r}{2})}{\Gamma(\frac{d}{2})\Gamma(\frac{r+1}{2})}x^r$	not a function
Thin Plate Spline	$x^2\log(x)$	not a function	$dx^2\log(x)+C_dx^2$, with $C_d=\frac{d}{2}\big(H_{\frac{d}{2}}-2+\log(4)\big)$	not a function

Table: Basis functions F for different kernels $K(x,y)=F(\\|x-y\\|)$ and corresponding basis functions f.

Numerical computation of f ➔ Next talk by Nico

Slicing Error for Random Directions

Theorem [Hertrich Jahn Q. 2025]

The mean squared error is

$$\mathbb{E}_{\xi_1,\ldots,\xi_P \sim \mathcal{U}_{\mathbb{S}^{d-1}}}\left[\left(\frac{1}{P}\sum_{p=1}^{P} f(\langle x, \xi_p\rangle - F(\|x\|)\right)^2\right] = \frac{\mathbb{V}_d[f](x)}{P}$$

with

Kernel	$\mathbb{V}_d[f](x)$
Any positive definite	$\leq F(0)^2 - F(\|x\|)^2$
Riesz $F(\|x\|) = -\|x\|^r$, $r > 0$	$\leq \left(\frac{\sqrt{\pi}\Gamma(r+\frac{1}{2})}{\Gamma(\frac{r+1}{2})^2} - 1\right) F(\|x\|)^2.$

- ☺ Error rate independent of dimension d
- 😐 Exact error rate $\sim 1/\sqrt{P}$ for $P \to \infty$

Quasi Monte Carlo (QMC) on the Sphere

Goal: Improve Error Rate $\mathcal{O}(1/\sqrt{P})$

Idea: Replace random points ξ_p by a quadrature rule on $\mathbb{S}^{d-1}$

Definition [Brauchart Saff Sloan Womersley 2014]

A **QMC Design** for the Sobolev space $H^s(\mathbb{S}^{d-1})$ is a sequence $\boldsymbol{\xi}^P = (\xi_1^P, ..., \xi_P^P) \in (\mathbb{S}^{d-1})^P$ s.t.

$$\sup_{\substack{g \in H^s(\mathbb{S}^{d-1}) \\ \|g\|_{H^s(\mathbb{S}^{d-1})} \leq 1}} \left| \int_{\mathbb{S}^{d-1}} g(\xi) \, \mathrm{d}\xi - \frac{1}{P} \sum_{p=1}^{P} g(\xi_p^P) \right| \leq \frac{c(s,d)}{P^{s/(d-1)}}.$$

Question: How smooth is our integrand $g_x : \mathbb{S}^{d-1} \to \mathbb{R}, \quad g_x(\xi) = f(\langle \xi, x \rangle)$?

Theorem [Hertrich Jahn Q. 2025]

We have $g_x \in H^s(\mathbb{S}^{d-1})$ for

Kernel	s
Gaussian	all $s \geq 0$
Matérn (smoothness ν)	$s < 2\nu + 1/2$
Laplacian	$s < 3/2$
neg. distance (energy / Riesz)	$s < 3/2$

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Technische Universität Berlin

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- ☺ Always exists with $P \sim t^{d-1}$ and is a QMC design for $s > \frac{d-1}{2}$
- ☺ Numerically known for $d = 3$ [Gräf Potts 2011] and $d = 4$ [Womersley 2018]
- ☹ Hard to compute for larger d

Distance points: Maximize

$$\mathcal{E}(\boldsymbol{\xi}^P) = \sum_{p,q=1}^{P} \|\xi_p^P - \xi_q^P\|$$

- ☺ Is a QMC design for $s = \frac{d+1}{2}$ [Brauchart Saff Sloan Womersley 2014]
- ☺ Worst case error rate: $\mathcal{O}(1/P^{\frac{d}{2(d-1)}})$
  For $d = 3$: $\mathcal{O}(1/P^{3/4})$

(Computable) QMC Designs

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Spherical t-designs: $\boldsymbol{\xi}^P = (\xi_1^P, ..., \xi_P^P) \in \mathbb{S}^d$ with

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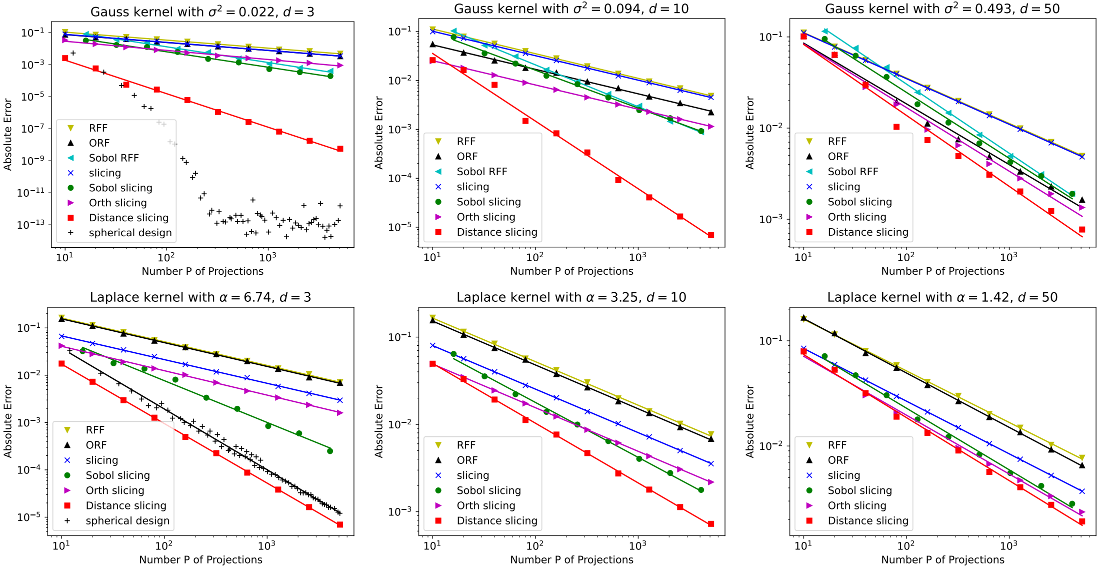
Slicing Directions ξ_p:

- Random directions
- Orthogonal directions
- Distance QMC Design

Compared Methods:

- Random Fourier features (RFF)
- Orthogonal Random Features (ORF) [Yu Suresh Choromanski Holtmann-Rice Kumar 2016]
- QMC-Random Fourier Features (Sobol RFF) for Gauss kernel [Avron Sindhwani Yang Mahoney 2016]

Slicing Error $\left|F(\|x\|) - \frac{1}{P}\sum_{p=1}^{P} f(\langle x, \xi_p\rangle)\right|$



Estimated Convergence Rates

Gauss kernel

Dimension	RFF-based			Slicing-based			
	RFF	Sobol	ORF	Slicing	Sobol	Orth	Distance
$d = 3$	0.50	0.98	0.50	0.50	0.96	0.57	**2.10**
$d = 10$	0.50	0.86	0.50	0.50	0.78	0.50	**1.38**
$d = 50$	0.50	0.76	0.67	0.50	0.72	0.70	**0.78**

Laplace kernel

Dimension	RFF-based		Slicing-based				
	RFF	ORF	Slicing	Sobol	Orth	Distance	spherical design
$d = 3$	0.50	0.50	0.50	0.88	0.52	1.26	**1.28**
$d = 10$	0.50	0.50	0.50	0.63	0.50	**0.68**	-
$d = 50$	0.49	0.52	0.50	0.59	0.56	**0.60**	-

Table: Estimated convergence rates r computed by fitting a regression line P^{-r} in the loglog plot. Larger r corresponds to faster convergence. The kernel parameters are determined via the median rule with scaling factor 1.

GPU Times for Slicing Summation

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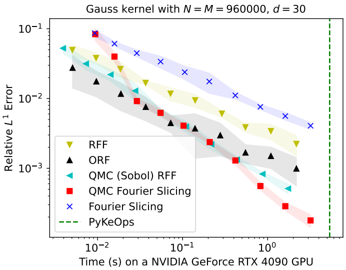
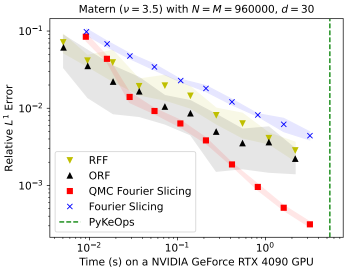
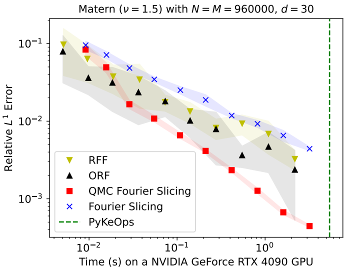
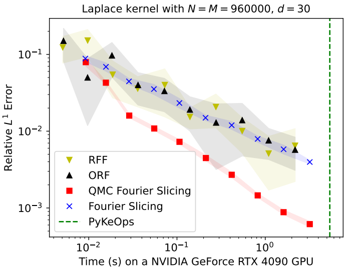
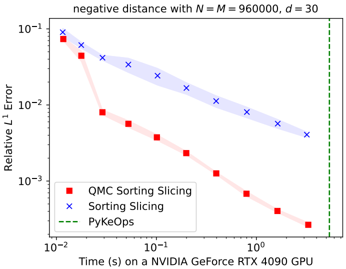


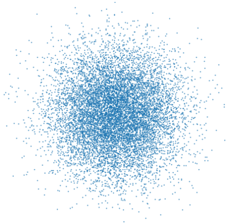




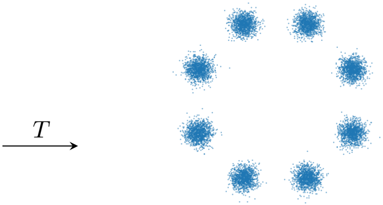




Application for MMD Flows in Generative Modeling



Latent distribution μ



Data distribution ν

- Given: Samples $y_1, \dots, y_M$ from a target probability measure ν
- Goal: Approximate ν
- Common Approach: Learn T such that $\nu \approx T_\# \mu = \mu \circ T^{-1}$ for a simple latent distribution μ

Examples: Generative Adversarial Nets (GANs), (Generalized) Normalizing Flows, etc.

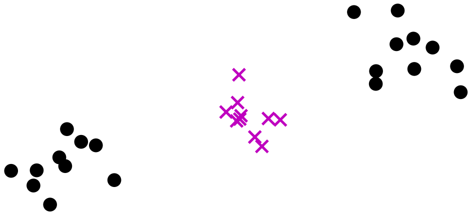
[Goodfellow et al. 2014] [Rezenede Mohamed 2015] [Hagemann Hertrich Steidl 2023]

Motivational Example

- Given: $\boldsymbol{y} = (y_1, \ldots, y_M) \in (\mathbb{R}^d)^M$
- Find: $\boldsymbol{x} = (x_1, \ldots, x_N) \in (\mathbb{R}^d)^N$ that "well approximate" $\boldsymbol{y}$

$$\min G_{\boldsymbol{y}}(\boldsymbol{x}) := \underbrace{-\frac{1}{2N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \|x_i - x_j\|}_{\text{repulsion}} + \underbrace{\frac{1}{MN} \sum_{i=1}^{N} \sum_{m=1}^{M} \|x_i - y_m\|}_{\text{attraction}}$$

- Gradient flow $\dot{\boldsymbol{x}}(t) = -\nabla G_{\boldsymbol{y}}(\boldsymbol{x}(t)),\ t > 0$, with $\boldsymbol{x}(0) = \boldsymbol{x}$



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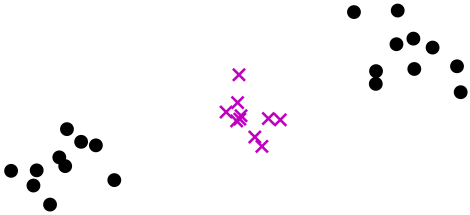

Maximum Mean Discrepancy (MMD)

[Szekely 2002] [Gretton Borgwardt et al. 2006]

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- $\mathcal{P}_2(\mathbb{R}^d)$ space of probability measures μ with $\int_{\mathbb{R}^d} \|x\|^2 \,\mathrm{d}\mu(x) < \infty$
- $K\colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ symmetric, positive definite kernel
- **Maximum mean discrepancy** (MMD) $\mathcal{D}_K\colon \mathcal{P}_2(\mathbb{R}^d) \times \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$

$$\mathcal{D}_K(\mu,\nu)^2 = \frac{1}{2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} K \,\mathrm{d}\mu\,\mathrm{d}\mu - \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} K\,\mathrm{d}\nu\,\mathrm{d}\mu + \frac{1}{2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} K\,\mathrm{d}\nu\,\mathrm{d}\nu$$

- If K is a so-called "characteristic" kernels, $\mathcal{D}_K$ is a metric on $\mathcal{P}_2(\mathbb{R}^d)$

- Fix target ν: $G(\mu) := \mathcal{D}_K(\mu,\nu)^2$
- **Wasserstein gradient flow**: "Analogue of gradient flow in $\mathcal{P}_2(\mathbb{R}^d)$ with Wasserstein distance"
  [Ambrosio Gigli Savaré 2008] [Arbel Korba Salim Gretton 2019]

- For $\mu = \frac{1}{N}\sum_{i=1}^N \delta_{x_i}$, $\nu = \frac{1}{M}\sum_{j=1}^M \delta_{y_j}$:

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- **Fast computation via Slicing!**

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What Kernels to use for MMD?

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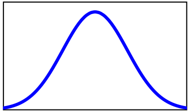
Gauss

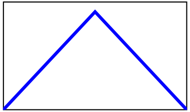
- ☺ Positive definite, characteristic kernel
- ☺ Defines a Wasserstein gradient flow
- ☹ Convergence depends heavily on a good parameter choice σ



$$F(t) = \mathrm{e}^{-\frac{t^2}{2\sigma^2}}$$

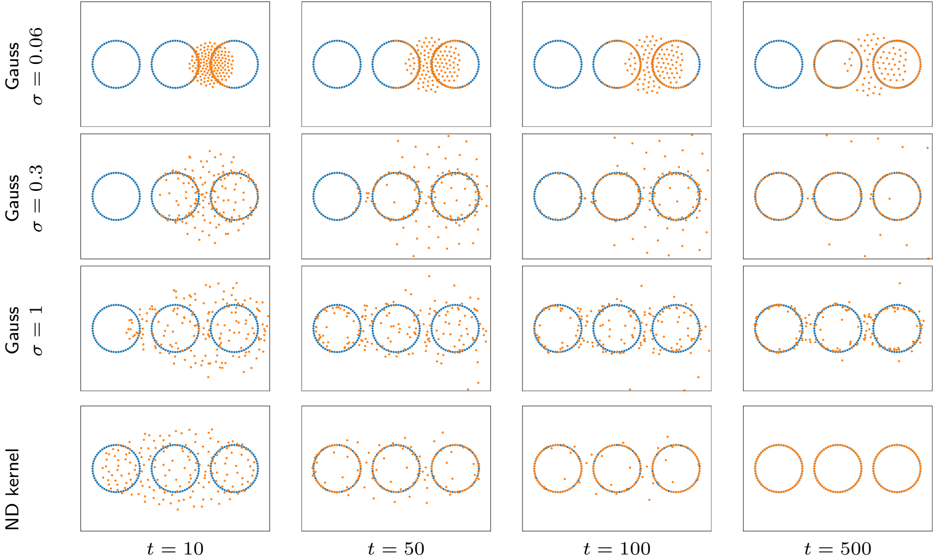
Negative Distance (ND)

- ☹ Not positive definite
- ☹ Not differentiable
- 😐 Wasserstein gradient flow of discrete measures can become continuous [Hertrich Gräf Beinert Steidl 2024]
- ☺ Often good numerical results
- ☺ Scale-independent, no parameter necessary



$$F(t) = -|t|$$

MMD Flows for Gauss and ND



Blue: target ν
Orange: Flow γ_t

Smooth Negative Distance (SND) Kernel

Goal: Smoothen the ND kernel $-\|x\|$ to retain the numeric behavior, and get theoretical properties

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Idea 1: Convolution of ND kernel function $\mathbb{R} \ni t \mapsto -|t|$ with a B–Spline M_n

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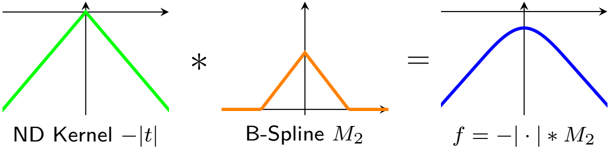

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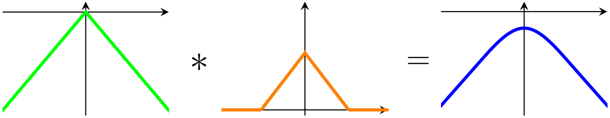


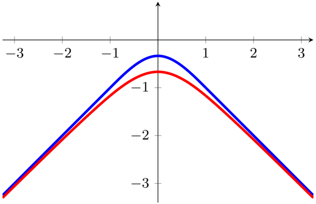
ND Kernel $-|t|$ B-Spline M_2 $f = -|\cdot| * M_2$

Idea 2 (Up-Slicing): Apply the slicing transform $\mathcal{I}_d$ to f

Theorem [Rux Q. Steidl 2025]

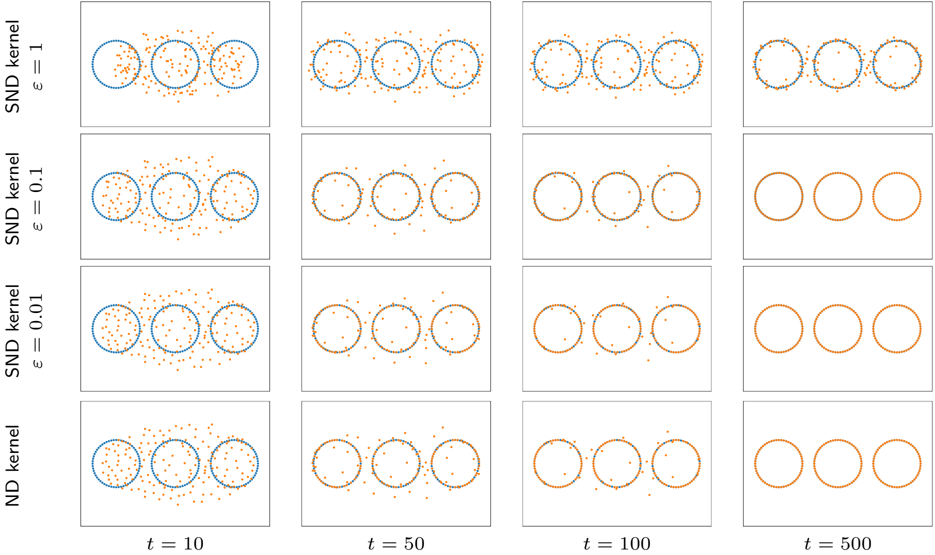
The kernel $K(x, y) = F(\|x - y\|) - F(\|x\|) - F(\|y\|)$ with $F := \mathcal{I}_d[|\cdot| * M_n]$ is positive definite on $\mathbb{R}^d$ and characteristic. There exists a Wasserstein gradient flow of the MMD functional G. It holds

$$v_t = -\int_{\mathbb{R}^d} \nabla_x F(\|x - y\|) \, \mathrm{d}(\gamma_t - \nu)(y).$$



Blue: $f = -|\cdot| * M_2$
Red: SND kernel $F = 2\mathcal{I}_3[f]$

Smooth Negative Distance (SND) Kernel



MMD flow with step size 0.01. Our SND kernel with small ε is as good as the ND kernel and better than the Gaussian.

MMD Flows on MNIST

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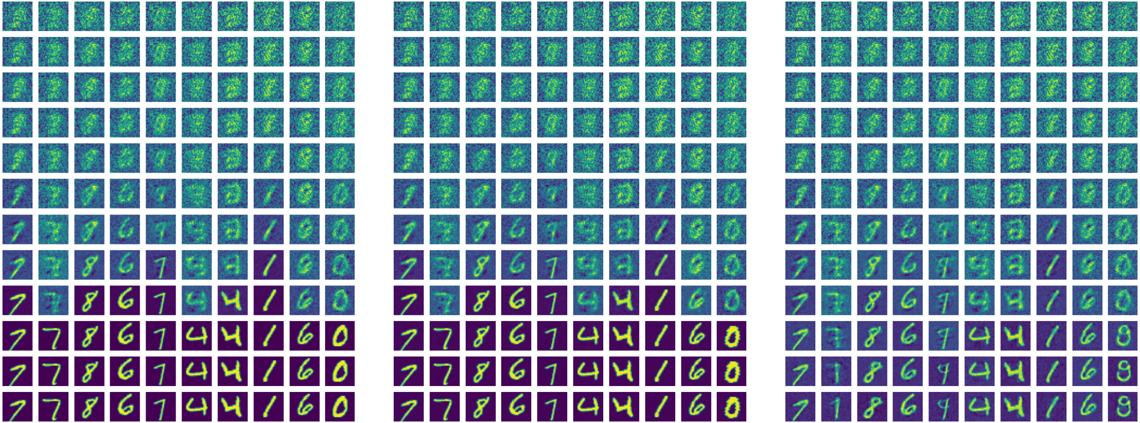

(a) ND (b) SND ($\varepsilon = 0.01$). (c) SND ($\varepsilon = 0.1$).

Figure: MMD flow for MNIST target ν with different kernels. Initial distribution is uniform random. Each row shows the first 10 images $x_n \in \mathbb{R}^{28\times 28}$, the ℓ-th row corresponds to the iteration $k = 2^{3+\ell}$, $\ell = 1, \dots, 12$.

Conclusions

- Slicing is applicable for many kernels, including the Riesz kernel
- Proven error rate $\mathcal{O}(1/\sqrt{P})$ for iid directions on the sphere
- Better rates via QMC designs (but they require some precomputation)
- SND kernel retains desired numerical properties of the ND, but comes with well-defined gradient and theoretical convergence guarantees of the corresponding gradient flow

References

J Hertrich, T Jahn, M Quellmalz. Fast Summation of Radial Kernels via QMC Slicing. *ICLR* 2025.

N Rux, M Quellmalz, G Steidl. Slicing of Radial Functions: a Dimension Walk in the Fourier Space. *Sampling Theory, Signal Processing, and Data Analysis* 23(6), 2025.

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Thank you for your attention!