On a new orthonormal basis for RBF native spaces and its fast computation

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Torino: June 11, 2014

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Outline

1. Data: $\Omega \subset \mathbb{R}^n$, $X \subset \Omega$, test function f
   - $X = \{x_1, \dots, x_N\} \subset \Omega$
   - $f_1, \dots, f_N$, where $f_i = f(x_i)$

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2. Approximation setting: kernel K_ε, $\mathcal{N}_K(\Omega)$, $\mathcal{N}_K(X) \subset \mathcal{N}_K(\Omega)$
   - kernel $K = K_\varepsilon$, positive definite and radial
   - native space $\mathcal{N}_K(\Omega)$ (where K is the reproducing kernel)
   - finite subspace $\mathcal{N}_K(X) = \mathrm{span}\{K(\cdot, x) : x \in X\} \subset \mathcal{N}_K(\Omega)$

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Aim

Find $s_f \in \mathcal{N}_K(X)$ s.t. $s_f \approx f$

Problem: the standard basis of translates (data-dependent) of $\mathcal{N}_K(X)$ is unstable and not flexible

Question 1

Is it possible to find a "better" basis $\mathcal{U}$ of $\mathcal{N}_K(X)$?

Question 2

How to embed information about K and Ω in the basis $\mathcal{U}$?

Question 3

Can we extract $\mathcal{U}' \subset \mathcal{U}$ s.t. s_f' is as good as s_f?

The “natural” basis

The “natural” (data-independent) basis for Hilbert spaces (Mercer’s theorem,1909)

Let K be a continuous, positive definite kernel on a bounded $\Omega \subset \mathbb{R}^n$. Then K has an eigenfunction expansion with non-negative coefficients, the eigenvalues, s.t.

$$K(x,y) = \sum_{j=0}^{\infty} \lambda_j \varphi_j(x)\varphi_j(y), \quad \forall\, x, y \in \Omega\,.$$

Moreover,

$$\lambda_j \varphi_j(x) = \int_\Omega K(x,y)\varphi_j(y)dy := \mathcal{T}[\varphi_j](x)\,, \; \forall x \in \Omega, \; j \geq 0$$

$$\begin{array}{lcl}
\{\varphi_j\}_{j>0} & & \textit{orthonormal} \in \mathcal{N}_K(\Omega) \\
\{\varphi_j\}_{j>0} & & \textit{orthogonal} \in L_2(\Omega), \; \|\varphi_j\|^2_{L_2(\Omega)} = \lambda_j \stackrel{\infty}{\longrightarrow} 0, \\
\sum_{j>0} \lambda_j & = & K(0,0)\,|\Omega|, \quad \text{(the operator is of trace-class)}
\end{array}$$

Notice: to find the functions φ_i explicitely it is not

[Fasshauer,McCourt 201

Change of basis

Notation

Letting $\Omega \subset \mathbb{R}^n$ and $X = \{x_1, \ldots, x_N\} \subset \Omega$

- $\mathcal{T}_X = \{K(\cdot, x_i),\ x_i \in X\}$: the standard basis of translates;
- $\mathcal{U} = \{u_i \in \mathcal{N}_K(\Omega),\ i = 1, \ldots, N\}$: another basis s.t.

$$\mathrm{span}(\mathcal{U}) = \mathrm{span}(\mathcal{T}_X) := \mathcal{N}_K(\Omega)\,.$$

- At $x \in \Omega$, $\mathcal{T}_X$ and $\mathcal{U}$ can be expressed as the row vectors

$$T(x) = [K(x, x_1), \ldots, K(x, x_N)] \in \mathbb{R}^N$$
$$U(x) = [u_1(x), \ldots, u_N(x)] \in \mathbb{R}^N\,.$$

- we need also the scalar products

$$(f, g)^2_{L_2(\Omega)} := \int_\Omega f(x)g(x)dx \approx \sum_{j=1}^{N} w_j f(x_j)g(x_j) =: (f, g)^2_{\ell_2^w(X)}\,.$$

Some useful results [Pazouki,Schaback 2011]

Change of basis

Let $A_{ij} = K(x_i, x_j) \in \mathbb{R}^{N\times N}$. Any basis $\mathcal{U}$ arises from a factorization $A = V_{\mathcal{U}} \cdot C_{\mathcal{U}}{}^{-1}$, where $V_{\mathcal{U}} = (u_j(x_i))_{1\leqslant i,j\leqslant N}$ and $C_{\mathcal{U}}$ is the matrix of change of basis s.t. $U(x) = T(x) \cdot C_{\mathcal{U}}$.

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Some consequences of this factorization

1. The interpolant $P_{f,X}$ at x can be written as

$$P_{f,X}(x) = \sum_{j=1}^{N} \Lambda_j(f) u_j(x) = U(x)\Lambda(f), \quad \forall x \in \Omega$$

   where $\Lambda(f) = [\Lambda_1(f), \ldots, \Lambda_N(f)]^T \in \mathbb{R}^N$ is a column vector of values of linear functionals defined by

$$\Lambda(f) = C_{\mathcal{U}}{}^{-1} \cdot A^{-1} \cdot f_X = V_{\mathcal{U}}{}^{-1} \cdot f_X\,,$$

   where f_X is the column vector given by

2. If $\mathcal{U}$ is a $\mathcal{N}_\kappa(\Omega)$-orthonormal basis, we get the stability estimate

$$\left|P_{f,X}(x)\right| \leqslant \sqrt{K(0,0)}\,\|f\|_K \quad \forall x \in \Omega\,. \tag{1}$$

In particular, for fixed $x \in \Omega$ and $f \in \mathcal{N}_K$ the values $\|U(x)\|_2$ and $\|\Lambda(f)\|_2$, are the same for all $\mathcal{N}_\kappa(\Omega)$-orthonormal bases independently on X

$$\|U(x)\|_2 \leqslant \sqrt{K(0,0)}, \quad \|\Lambda(f)\|_2 \leqslant \|f\|_K\,. \tag{2}$$

Other results [Pazouki,Schaback 2011]

Change of basis

- Each $\mathcal{N}_\kappa(\Omega)$-orthonormal basis $\mathcal{U}$ arises from an orthornormal decomposition $A = B^T \cdot B$ with $B = C_{\mathcal{U}}{}^{-1},\ V_{\mathcal{U}} = B^T = (C_{\mathcal{U}}{}^{-1})^T$.
- Each $\ell_2(X)$-orthonormal basis $\mathcal{U}$ arises from a decomposition $A = Q \cdot B$ with $Q = V_{\mathcal{U}}$, $Q^T Q = I$, $B = C_{\mathcal{U}}{}^{-1} = Q^T A$.

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Notice: the best bases in terms of stability are the $\mathcal{N}_\kappa(\Omega)$-orthonormal ones!

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Q1: It is possible to find a “better” basis? Yes, we can!

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Q2: How to embed information on K and Ω in $\mathcal{U}$?

Symmetric Nyström method [Atkinson,Han 2001]

The main idea for the construction of our basis is to discretize the "natural" basis introduced in Mercer's theorem.
To this aim, consider on Ω a cubature rule $(X, \mathcal{W})$, that is a set of distinct points $X = \{x_j\}_{j=1}^N \subset \Omega$ and a set of positive weights $\mathcal{W} = \{w_j\}_{j=1}^N$, $N \in \mathbb{N}$, such that

$$\int_\Omega f(y)dy \approx \sum_{j=1}^N f(x_j)w_j \quad \forall f \in \mathcal{N}_K(\Omega)\,. \tag{3}$$

WSVD Basis

Main idea: II

Thus, the operator $\mathcal{T}_K$ can be evaluated on X as

$$\lambda_j \varphi_j(x_i) = \int_\Omega K(x_i, y)\varphi_j(y)dy \quad i = 1, \ldots, N, \ \forall j > 0,$$

and then discretized using the cubature rule by

$$\lambda_j \varphi_j(x_i) \approx \sum_{h=1}^{N} K(x_i, x_h)\varphi_j(x_h)w_h \quad i, j = 1, \ldots, N. \tag{4}$$

Letting $W = \mathrm{diag}(w_j)$, it suffices to solve the following discrete eigenvalue problem in order to find the approximation of the eigenvalues and eigenfunctions (evaluated on X) of $\mathcal{T}_K[f]$:

$$\lambda v = (A \cdot W)v \tag{5}$$

WSVD basis

Main idea: III

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A solution is to rewrite (4) using the fact that the weights are positive as

$$\lambda_j(\sqrt{w_i}\varphi_j(x_i)) = \sum_{h=1}^{N}(\sqrt{w_i}\Phi(x_i, x_h)\sqrt{w_h})(\sqrt{w_h}\varphi_j(x_h)) \quad \forall i, j = 1, \ldots, N, \tag{6}$$

and then to consider the corresponding scaled eigenvalue problem

$$\lambda\left(\sqrt{W}\cdot v\right) = \left(\sqrt{W}\cdot A\cdot\sqrt{W}\right)\left(\sqrt{W}\cdot v\right)$$

which is equivalent to the previous one, now involving the symmetric and positive definite matrix $A_W := \sqrt{W}\cdot A\cdot\sqrt{W}$.

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$\{\lambda_j, \varphi_j\}_{j>0}$ are then approximated by eigenvalues/eigenvectors of $A_W := \sqrt{W} \cdot A \cdot \sqrt{W}$. This matrix is normal, then a *singular value decomposition* of A_W is a unitary diagonalization.

Definition:

A *weighted SVD basis* $\mathcal{U}$ is a basis for $\mathcal{N}_\kappa(X)$ s.t.

$$V_{\mathcal{U}} = \sqrt{W^{-1}} \cdot Q \cdot \Sigma, \quad C_{\mathcal{U}} = \sqrt{W} \cdot Q \cdot \Sigma^{-1}$$

since $A = V_{\mathcal{U}} C_{\mathcal{U}}{}^{-1}$, then $A_W = Q \cdot \Sigma^2 \cdot Q^T$ is the SVD .

Here $\Sigma_{jj} = \sigma_j, \ j = 1, \dots, N$ and $\sigma_1^2 \geq \dots \geq \sigma_N^2 > 0$ are the singular values of A_W.

WSVD Basis

Properties

This basis is in fact an approximation of the “natural” one (provided $w_i > 0$, $\sum_{i=1}^{N} w_i = |\Omega|$)

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Properties of the new basis $\mathcal{U}$ (cf. [De Marchi-Santin 2013])

- $u_j(x) = \dfrac{1}{\sigma_j^2} \displaystyle\sum_{i=1}^{N} w_i u_j(x_i) K(x, x_i) \approx \dfrac{1}{\sigma_j^2} \mathcal{T}_K[u_j](x)$, $\forall\ 1 \leqslant j \leqslant N,\ \forall x \in \Omega$;
- $\mathcal{N}_K(\Omega)$-orthonormal
- $\ell_2^w(X)$-orthogonal, $\|u_j\|^2_{\ell_2^w(X)} = \sigma_j^2 \quad \forall u_j \in \mathcal{U}$
- $\displaystyle\sum_{j=1}^{N} \sigma_j^2 = K(0,0)\, |\Omega|$

WSVD Basis

Approximation

Interpolant: $s_f(x) = \sum_{j=1}^{N} (f, u_j)_K u_j(x) \quad \forall x \in \Omega$

WDLS: $s_f^M := \operatorname{argmin} \left\{ \|f - g\|_{\ell_2^w(X)} : g \in \operatorname{span}\{u_1, \ldots, u_M\} \right\}$

Weighted Discrete Least Squares as truncation:

Let $f \in \mathcal{N}_K(\Omega)$, $1 \leqslant M \leqslant N$. Then $\forall x \in \Omega$

$$s_f^M(x) = \sum_{j=1}^{M} \frac{(f, u_j)_{\ell_2^w(X)}}{(u_j, u_j)_{\ell_2^w(X)}} u_j(x) = \sum_{j=1}^{M} \frac{(f, u_j)_{\ell_2^w(X)}}{\sigma_j^2} u_j(x) = \sum_{j=1}^{M} (f, u_j)_K u_j(x)$$

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Q3: Can we extract $\mathcal{U}' \subset \mathcal{U}$ s.t. s_f' is as good as s_f? Yes we can: take $\mathcal{U}' = \{u_1, \ldots, u_M\}$.

If we define the pseudo-cardinal functions as $\tilde{\ell}_i = s^M_{\ell_i}$, we get

$$s^M_f(x) = \sum_{i=1}^{N} f(x_i)\tilde{\ell}_i(x), \quad \tilde{\ell}_i(x) = \sum_{j=1}^{M} \frac{u_j(x_i)}{\sigma_j^2} u_j(x).$$

Generalized Power Function and Lebesgue constant:

If $f \in \mathcal{N}_K(\Omega)$, $\left|f(x) - s^M_f(x)\right| \leqslant P^{(M)}_{K,X}(x)\|f\|_{\mathcal{N}_K(\Omega)}$ $\forall x \in \Omega$, where

$$\left[P^{(M)}_{K,X}(x)\right]^2 = K(0,0) - \sum_{j=1}^{M}[u_j(x)]^2.$$

Moreover, $\|s^M_f\|_\infty \leqslant \tilde{\Lambda}_X \|f\|_X$.

How can we extract $\mathcal{U}' \subset \mathcal{U}$ s.t. s_f' is as good as s_f? Idea.

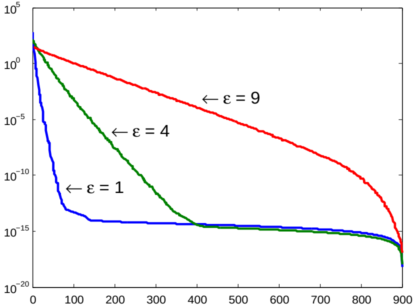

Figure: Gaussian kernel, σ_j^2 on equispaced points of the square

- recall that $\|u_j\|_{\ell_2^w(X)} = \sigma_j^2 \to 0$
- we can choose M s.t. $\sigma_{M+1}^2 < \mathrm{tol}$
- we don't need u_j, $j > M$

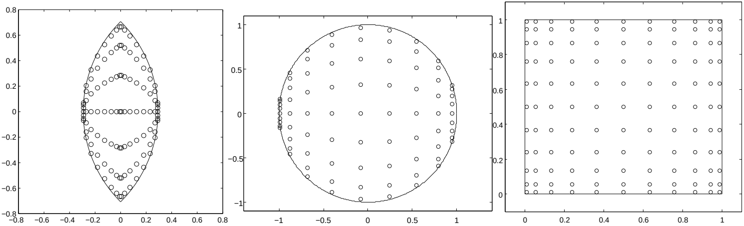

Figure: The domains used in the numerical experiments with an example of the corresponding sample points.
From left to right: the lens Ω_1 (trigonometric-gaussian points), the disk Ω_2 (trigonometric-gaussian points) and the square Ω_3 (product Gauss-Legendre points).

	$\varepsilon = 1$	$\varepsilon = 4$	$\varepsilon = 9$
Gaussian	100	340	500
IMQ	180	580	580
Matern3	460	560	580

Table: Optimal M for different kernels and shape parameter that correspond to the indexes such that the weighted least-squares approximant s_f^M provides the best approximation of the function $f(x, y) = \cos(20(x + y))$ on the disk with center $C = (1/2, 1/2)$ and radius $R = 1/2$

WSVD Basis

An Example: III

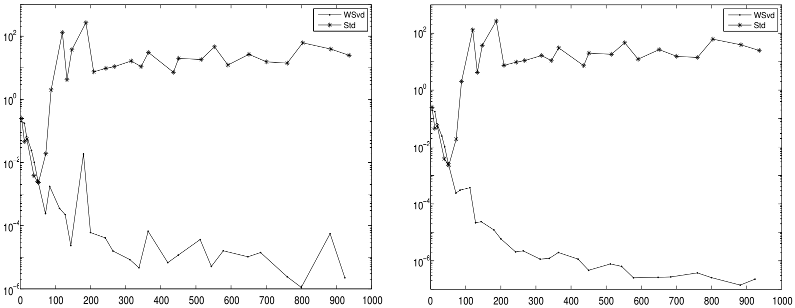

Figure: Franke's test function, *lens*, IMQ Kernel, $\varepsilon = 1$ and RMSE. Left: complete basis. Right: $\sigma^2_{M+1} < 10^{-17}$.

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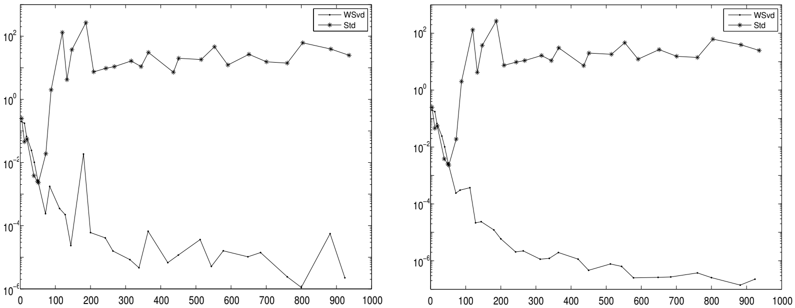

Figure: Franke's test function, *lens*, IMQ Kernel, $\varepsilon = 1$ and RMSE.
Left: complete basis. Right: $\sigma^2_{M+1} < 10^{-17}$.

Problem: We have to compute the whole basis before truncation!
Solution: Krylov methods.

Consider $A_{ij} = K(x_i, x_j)$ (which is symmetric), $b_i = f(x_i)$, $1 \leqslant i, j \leqslant N$

- define the Krylov subspace $\mathcal{K}_M(A, b) = \mathrm{span}\{b, Ab, \ldots, A^{M-1}b\}$, $M \ll N$.
- compute an o.n. basis $\{\phi_1, \ldots, \phi_M\}$ of $\mathcal{K}_M(A, b)$ and form $\Phi_M = [\phi_1, \ldots, \phi_M],\ N \times M$
- define the (tridiagonal) matrix $H_M = \Phi_M^T A \Phi_M$ which represents the projection of A into $\mathcal{K}_M(A, b)$

Arnoldi iteration gives $A\Phi_M = \Phi_{M+1}\overline{H}_M$ where $\overline{H}_M = \begin{bmatrix} H_M \\ h_{M+1,M} e_M^T \end{bmatrix}$ is $(M+1) \times M$. In practice $h_{M+1,M} \approx 0$ so that $\mathcal{K}_{M+1}(A, b) = \mathcal{K}_M(A, b)$.

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Consider a SVD $\overline{H}_M = U_M \Sigma_M^2 V_M^T$, where $U_M \in \mathbb{R}^{(M+1)\times(M+1)}$, $V_M \in \mathbb{R}^{M\times M}$, $\Sigma_M^2 = \left[\tilde{\Sigma}_M^2, 0\right]^T$ and $\tilde{\Sigma}_M^2 = \mathrm{diag}(\sigma_{M,1}^2, \ldots, \sigma_{M,M}^2)$.

Approximate SVD (Novati-Russo 2013:)

Let $\overline{U}_M = \Phi_{M+1} U_M$, $\overline{V}_M = \Phi_M V_M$, then

- $A\overline{V}_M = \overline{U}_M \Sigma_M^2$, $A\overline{U}_M = \overline{V}_M (\Sigma_M^2)^T$
- the first M singular values of A are well approx. by $\sigma_{M,j}^2$
- If $M = N$, in exact arithmetic the triplet $\left(\Phi_{M+1}\tilde{U}_M, \tilde{\Sigma}_M, \Phi_M V_M\right)$ is a SVD of A, where $\tilde{U}_M$ is U_M without the last column.

Recall:

- $A\Phi_M = \Phi_{M+1}\overline{H}_M$
- $\overline{H}_M = U_M \Sigma_M^2 V_M^T$
- $\Sigma_M^2 = \left[\tilde{\Sigma}_M^2, 0\right]^T$
- $\tilde{U}_M$ is U_M without the last column.

Definition:

The sub-basis $\mathcal{U}_M$ is a set $\{u_1, \ldots, u_M\} \subset \mathcal{N}_\kappa(X)$ defined by

$$V_{\mathcal{U}} = \Phi_{M+1}\tilde{U}_M\tilde{\Sigma}_M, \quad C_{\mathcal{U}} = \Phi_M V_M \tilde{\Sigma}_M^{-1}.$$

Properties [De Marchi, Santin 2014]:

The sub-basis $\mathcal{U}_M$ has the following properties for each $1 \leqslant M \leqslant N$:

1. it is $\ell_2(X)$-orthogonal with $\|u_j\|_{\ell_2(X)} = \sigma^2_{M,j}$ $1 \leqslant j \leqslant M$
2. it is near-orthonormal in $\mathcal{N}_\kappa(\Omega)$
3. if $M = N$ it is the SVD basis $\mathcal{U}$ $(\Phi_M = I)$

About point 2: it means that $(u_i, u_j) = \delta_{ij} + r_{ij}^{(M)}$ where $(R^{(M)})_{ij} := r_{ij}^{(M)}$ is a rank one matrix for $1 \leqslant M \leqslant N$, and $r_{ij}^{(M)} = 0$ if $M = N$;

Using this basis we get $\forall f \in \mathcal{N}_K(\Omega)$

$$s_f'(x) = \sum_{j=1}^{M} \frac{(f, u_j)_{\ell_2(X)}}{\sigma_{M,j}^2} u_j(x) = \sum_{j=1}^{M} (f, u_j)_K u_j(x) \quad \forall x \in \Omega$$

(and $P_{K,X}^{(M)}(x)$, $\tilde{\Lambda}_X$ as before)

Numerical Results

Stopping rule: I

Fix $\tau > 0$

$$\left(\overline{H}_M\right)_{M+1,M} \approx \sigma^2_{M,j} < \tau$$

or a better choice is the following

$$\left|\sum_{j=1}^{M} (\overline{H}_M)_{jj} - N\right| < \tau, \tag{7}$$

that works for functions lying in the native space of the kernel.

Numerical Results

Stopping rule: II

The decay of the residual described in (7) compared to the corresponding RMSE goes as in the Figure below with $\tau = 1.e - 15$

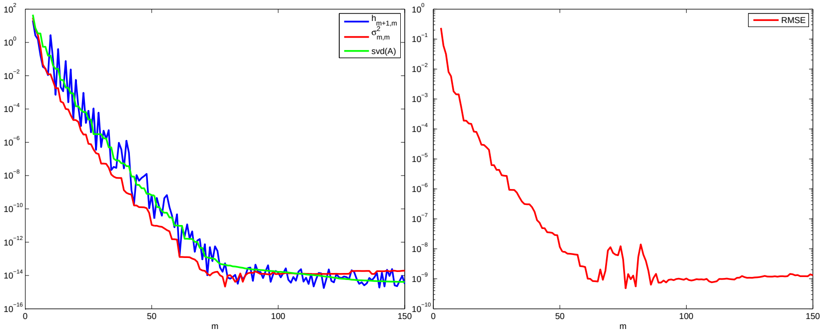

Figure: Gaussian kernel, $\varepsilon = 1$, square $[-1,1]^2$, $N = 200$ e.s. points, $f \in \mathcal{N}_K(\Omega)$, with $f(x) = K(x,y1) + 2K(x,y2) - 2K(x,y3) + 3K(x,y4)$, $y1 = (0,-1.2)$, $y2 = (-0.4, 0.5)$, $y3 = (-0.4, 1.1)$

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For each N we compute the optimal M using the new algorithm with tolerance $\tau = 1e - 14$.

N	121	225	361	529	729	961	1225	1521
optimal M	100	110	113	114	114	115	115	116
RMSE new	5.0e-08	3.4e-10	1.0e-10	6.7e-11	6.4e-11	5.5e-11	4.7e-11	3.4e-11
RMSE WSVD	5.0e-08	3.3e-09	1.3e-09	1.1e-09	1.1e-09	8.3e-10	7.8e-10	7.9e-10
Time new	1.7e-01	3.4e-01	6.1e-01	1.0e+00	1.6e+00	2.6e+00	3.7e+00	6.5e+00
Time WSVD	3.3e-01	7.2e-01	1.5e+00	4.2e+00	1.0e+01	2.5e+01	5.5e+01	1.1e+02

Table: Comparison between the WSVD basis and the new basis. Computational time in seconds and corresponding RMSE, restricted to $n = 49, \ldots, 1600$ equally spaced points.

Approximated Power function and Lebesgue function

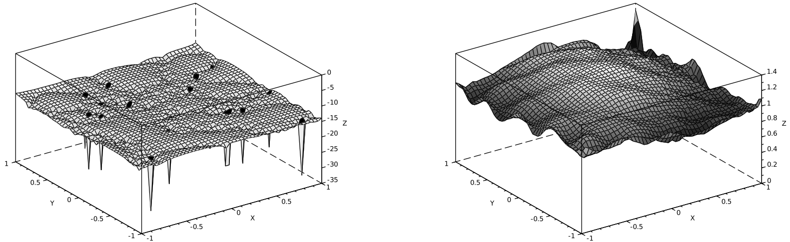

Figure: Approximated power function (left, logarithmic plot) and approximated Lebesgue function (right) Ω_1

Numerical Results

Another example

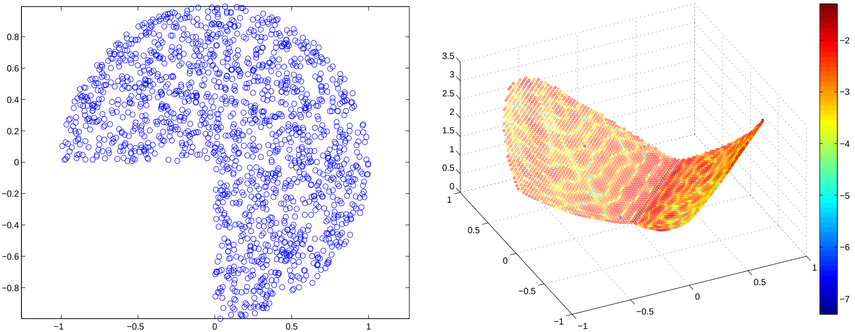

Figure: IMQ kernel, $\varepsilon = 1$, cutted-disk, $N = 1600$ random points, $M = 260$, $f(x, y) = exp(|x - y|) - 1$

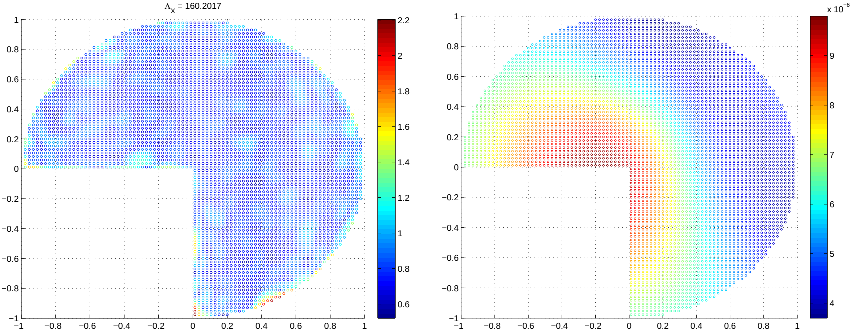

Figure: IMQ kernel, $\varepsilon = 1$, cutted-disk, $N = 1600$ random points, $M = 260$, $f(x, y) = exp(|x - y|) - 1$. Left: Lebesgue function. Right: power function

Further work

More analysis has to be done

- a better stopping rule
- understand the decay rate of $P_{K,X}^{(M)}$
- understand the growing rate of $\tilde{\Lambda}_X$
- understand how X, ε influence s_f'

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- understand the decay rate of $P^{(M)}_{K,X}$
- understand the growing rate of $\tilde{\Lambda}_X$
- understand how X, ε influence s'_f

Thank you for your attention!

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