Fast and stable rational RBF-based Partition of Unity interpolation[1]

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SMART 2017 - Gaeta
September 18, 2017

DIPARTIMENTO MATEMATICA

[1] joint work with A. Martinez (Padova) and E. Perracchione (Padova)

Outline

From RBF to Rational RBF (RRBF)

RBF Approximation

Notation

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

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2. Approximation setting: kernel K_ε, $\mathcal{N}_K(\Omega)$, $\mathcal{N}_K(X_N) \subset \mathcal{N}_K(\Omega)$
   - kernel $K = K_\varepsilon$, Strictly Positive Definite (SPD) and radial
     Examples:
     - globally supported: $K_\varepsilon(x, y) = e^{-(\varepsilon\|x-y\|)^2}$ (*gaussian*),
     - locally supported: $K_\varepsilon(x, y) = (1 - \varepsilon^2\|x - y\|^2)_+^4 [4\varepsilon^2\|x - y\|^2 + 1]$ ($C^2(\mathbb{R}^2)$ *Wendland*)
   - native space $\mathcal{N}_K(\Omega)$ (where K is the reproducing kernel)
   - finite subspace $\mathcal{N}_K(X_N) = \mathrm{span}\{K(\cdot, x) : x \in X_N\} \subset \mathcal{N}_K(\Omega)$

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Aim

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

RBF Interpolation

Given $\Omega, X_N, \mathbf{f}$

- Interpolant: $P_f(x) = \sum_{k=1}^{N} \alpha_k K(x, x_k), \quad x \in \Omega,\ x_k \in X_N$. [Hardy and Gofert 1975] used multiquadrics $K(x, y) = \sqrt{1 + \epsilon^2 \|x - y\|^2}$.

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- Rescaled interpolant: $\hat{P}_f(x) = \frac{P_f(x)}{P_g(x)} = \frac{\sum_{k=1}^{N} \alpha_k K(x, x_k)}{\sum_{k=1}^{N} \beta_k K(x, x_k)}$ where P_g is the kernel based interpolant of $g(x) = 1, \; \forall x \in \Omega$ [Deparis at al 2014, DeM et al 2017]. Shepard's PU method.

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- Rational interpolant: $R(x) = \frac{R^{(1)}(x)}{R^{(2)}(x)} = \frac{\sum_{k=1}^{N} \alpha_k K(x, x_k)}{\sum_{k=1}^{N} \beta_k K(x, x_k)}$ [Jackbsson et al. 2009, Sarra and Bai 2017].

Rational RBF

General framework

- polynomial case $d = 1$.

$$r(x) = \frac{p_1(x)}{p_2(x)} = \frac{a_m x^m + \dots + a_0 x^0}{x^n + b_{n-1} x^{n-1} \dots + b_0}.$$

$M = m + n + 1$ unknowns (Padé approximation). If $N > M$ to get the coefficients we may solve the LS problem

$$\min_{p_1 \in \Pi^1_m, p_2 \in \Pi^1_n} \left(\sum_{k=1}^{N} \left| f(x_k) - r(x_k) \right|^2 \right).$$

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$$\min_{p_1 \in \Pi_m^1, p_2 \in \Pi_n^1} \left(\sum_{k=1}^{N} \left| f(x_k) - r(x_k) \right|^2 \right).$$

- Let $X_m = \{x_k, \ldots, x_{k+m-1}\}, X_n = \{x_j, \ldots, x_{j+n-1}\} \subset X_N$ be non empty, such that $m + n \leq N$

$$R(x) = \frac{R^{(1)}(x)}{R^{(2)}(x)} = \frac{\sum_{i_1=k}^{k+m-1} \alpha_{i_1} K(x, x_{i_1})}{\sum_{i_2=j}^{j+n-1} \beta_{i_2} K(x, x_{i_2})}, \quad (1)$$

provided $R^{(2)}(x) \neq 0, x \in \Omega$.

Rational RBF

Posedness

In the case $m + n = N$, asking $R(x_i) = f_i$,

$$\boxed{R^{(1)}(x_i) - R^{(2)}(x_i) f_i = 0 \Longrightarrow \quad B\xi = 0}$$

with $\xi = (\alpha, \beta)$ and $B = B_1 + B_2$.

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Example

Given X_N and $\mathbf{f}$. Let $X_m \cap X_n \neq \emptyset$, with $m+n=N$. Suppose that $f_i = a$, $i=1,\ldots,N$, $a \in \mathbb{R}$, then the system $B\xi = \mathbf{0}$ admits infinite solutions.

Example

Example

$N = 26, m = n = 13, \Omega = [0,1], f_i = 1$ (Left) or f be piecewise constant (Right) .

Following [GolubReinsch1975] non-trivial solution by asking $\|\xi\|_2 = 1$ i.e. solving constrained problem $\min\limits_{\xi \in \mathbb{R}^N, \|\xi\|_2 = 1} \|B\xi\|_2$.

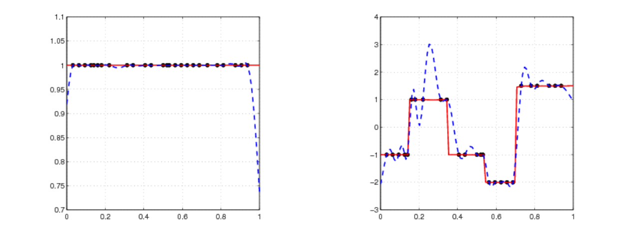

Figure : The black dots represent the set of scattered data, the red solid line and the blue dotted one are the curves reconstructed via the rational RBF and classical RBF approximation, by the Gaussian kernel.

Rational RBF

Find the coefficients: I

[Jackobsson et al 2009] proved the well-posedness of

$$R(x) = \frac{R^{(1)}(x)}{R^{(2)}(x)} = \frac{\sum_{i=1}^{N} \alpha_i K(x, x_i)}{\sum_{k=1}^{N} \beta_k K(x, x_k)},$$

B is now a sum of two squared blocks of order N i.e. B is $N \times 2N$

$$B = \begin{pmatrix} K(x_1, x_1) & \cdots & K(x_1, x_N) & -f_1\, K(x_1, x_1) & \cdots & -f_1\, K(x_1, x_N) \\ \vdots & & \vdots & & & \vdots \\ K(x_N, x_1) & \cdots & K(x_N, x_N) & -f_N\, K(x_N, x_1) & \cdots & -f_N\, K(x_N, x_N) \end{pmatrix}.$$

The system $B\xi = \mathbf{0}$ can be written as $(A - DA)(\xi) = \mathbf{0}$ with $D = \mathtt{diag}(f_1, \ldots, f_N)$, and $A_{i,j} = K(x_i, x_j)$. But underdetermined!

Rational RBF

Find the coefficients: II

- Since $R^{(1)}(x_i) = f_i R^{(2)}(x_i)$, find $\mathbf{q} = (R^{(2)}(x_1), \ldots, R^{(2)}(x_N))^T$ and then get $\mathbf{p} = (R^{(1)}(x_i), ..., R^{(1)}(x_N))^T$ as $\mathbf{p} = D\mathbf{q}$.

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- If **p, q** are given then the rational interpolant is known by solving

$$A\alpha = \mathbf{p}, \quad A\beta = \mathbf{q}\,. \tag{2}$$

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- Existence+Uniqueness of (2) since K is SPD

Using the native space norms the above problem is equivalent

Problem 1

$$\min_{\substack{R^{(1)},R^{(2)}\in\mathcal{N}_K,\\ 1/\|\mathbf{f}\|_2^2\|\boldsymbol{p}\|_2^2+\|\boldsymbol{q}\|_2^2=1,\\ R^{(1)}(x_k)=f_k R^{(2)}(x_k).}} \left(\frac{1}{\|\boldsymbol{f}\|_2^2} \|R^{(1)}\|_{\mathcal{N}_K}^2 + \|R^{(2)}\|_{\mathcal{N}_K}^2 \right). \tag{3}$$

Rational RBF

Find the coefficients: III

$$\|R^{(1)}\|_{\mathcal{N}_K}^2 = \alpha^T A \alpha, \quad \text{and} \quad \|R^{(2)}\|_{\mathcal{N}_K}^2 = \boldsymbol{\beta}^T A \boldsymbol{\beta}.$$

Then, from (2) and symmetry of A

$$\|R^{(1)}\|_{\mathcal{N}_K}^2 = \boldsymbol{p}^T A^{-1} \boldsymbol{p}, \quad \text{and} \quad \|R^{(2)}\|_{\mathcal{N}_K}^2 = \boldsymbol{q}^T A^{-1} \boldsymbol{q}.$$

Therefore, the **Problem 1** reduces to solve

Problem 2

$$\min_{\substack{\boldsymbol{q} \in \mathbb{R}^N, \\ 1/\|\boldsymbol{f}\|_2^2 \|D\boldsymbol{q}\|_2^2 + \|\boldsymbol{q}\|_2^2 = 1.}} \left(\frac{1}{\|\boldsymbol{f}\|_2^2} \boldsymbol{q}^T D^T A^{-1} D \boldsymbol{q} + \boldsymbol{q}^T A^{-1} \boldsymbol{q} \right).$$

Rational RBF

Find the coefficients: IV

[Jackbsson 2009] show that this is equivalent to solve the following generalized eigenvalue problem

Problem 3

$$\Sigma \boldsymbol{q} = \lambda \Theta \boldsymbol{q},$$

with

$$\Sigma = \frac{1}{||\boldsymbol{f}||_2^2} D^T A^{-1} D + A^{-1}, \quad \text{and} \quad \Theta = \frac{1}{||\boldsymbol{f}||_2^2} D^T D + I_N,$$

where I_N is the identity matrix.

Partion of Unity, VSK, Computational issues

RRBF- PU interpolation

- $\Omega = \cup_{j=1}^{s} \Omega_i$ (can overlap): that is, each $x \in \Omega$ belongs to a limited number of subdomains, say $s_0 < s$.
- Then we consider, W_j non-negative fnct on Ω_j, s.t. $\sum_{j=1}^{s} W_j = 1$ is a partition of unity .

RRBF-PU interpolant

$$I(x) = \sum_{j=1}^{s} R_j(x) W_j(x), \quad \forall\, x \in \Omega \tag{4}$$

where R_j is a RRBF interpolant on Ω_j i.e.

$$R_j(x) = \frac{R_j^{(1)}(x)}{R_j^{(2)}(x)} = \frac{\sum_{i=1}^{N_j} \alpha_i^j K(x, x_i^j)}{\sum_{k=1}^{N_j} \beta_k^j K(x, x_k^j)},$$

$N_j = |\Omega_j|$, $x_k^j \in X_{N_j}$, $k = 1, \ldots, N_j$.

RRBF-PU interpolation

- The RRBF interpolant is constructed as the global one solving Problem 3 on Ω_j .
- The RRBF interpolants can suffer of instability problems, especially for $\epsilon \to 0$ like the classical one.

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(Some) Stability issues

Optimal shape parameter (Trial&Error, Cross Validation), stable bases (RBF-QR, HS-SVD, WSVD) [Fornberg et al 2011, Fasshauer Mc Court 2012, DeM Santin 2013], Optimal shape parameters for PUM [Cavoretto et al. 2016], Rescaled RBF [Deparis 2015, DeM et al 2017], Variably Scaled Kernels [Bozzini et al. 2015].

(Some) Computational issues

Fast WSVD bases [DeM Santin 2015], Fast algorithm for shape and radius parameters [Cavoretto et al. 2016], Explicit formulas for the optimal shape parameters 1d [Bos et al 2017].

Our approach: RRBF-PU via VSK

Definition

Let $\psi : \mathbb{R}^d \to (0, \infty)$ be a given scale function. A Variably Scaled Kernel (VSK) K_ψ on $\mathbb{R}^d$ is

$$K_\psi(x, y) := \mathcal{K}((x, \psi(x)), (y, \psi(y))), \quad \forall x, y \in \mathbb{R}^d.$$

where $\mathcal{K}$ is a kernel on $\mathbb{R}^{d+1}$.

Definition

Given $\mathcal{X}_N$ and the scale functions $\psi_j : \mathbb{R}^d \to (0, \infty)$, $j = 1, \ldots, s$, the RVSK-PU is

$$\mathcal{I}_\psi(x) = \sum_{j=1}^{d} R_{\psi_j}(x)\, W_j(x), \quad x \in \Omega, \tag{5}$$

with $R_{\psi_j}(x)$ the RVSK-PU on Ω_j.

OBS: when Φ is radial

$(A_{\psi_j})_{ik} = \Phi(\|x_i^j - x_k^j\|^2 + (\psi_j(x_i^j) - \psi_j(x_k^j))^2), \quad i, k = 1, \ldots, N_j$

Computational steps

- PU construction: $\Omega = \cup_{i=1}^{s} \Omega_i$. We choose Ω_j as d-dimensional balls of radius δ and $s \propto N$. [Fassahuer2007] suggests

$$s = \left\lfloor \frac{\sqrt[d]{N}}{2^d} \right\rfloor, \quad \delta > \delta_0 = \sqrt[d]{1/s}\,.$$

- Choice of VSK scaling functions $\psi_j,\ j = 1, \ldots, s$.
- To compute the local rational fit, by solving on each Ω_j the eigenvalue Problem 3, we use the Deflated Augumented Conjugate Gradient (DACG) [Bergamaschi et al 2002].
- Construction of the RVSK-PU by finding $\mathbf{q}_{\psi_j}$ and $\mathbf{p}_{\psi_j}$ (solving two smaller linear systems (2)).
- Use then the PU weights to get the global rational VSK interpolant $\mathcal{I}_{\psi}$.

Numerical experiments

Globally supported RBFs

$d = 2$, $f_1(x_1, x_2) = (\tan(x_2 - x_1) + 1)/(\tan 9 + 1)$, circular patches and
$\psi_j^{(1)}(x_1, x_2) = 0.5 + \sqrt{9 - [(x_1 - \tilde{x}_{1j})^2 + (x_2 - \tilde{x}_{2j})^2]}$,

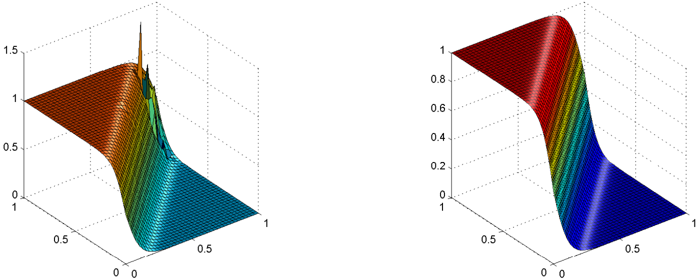

Figure : The approximate surface f_1 obtained with the SRBF-PU (left) and RVSK-PU (right) methods with $N = 1089$ Halton data. Results are computed using the Gaussian C^∞ kernel as local approximant.

Globally supported RBFs

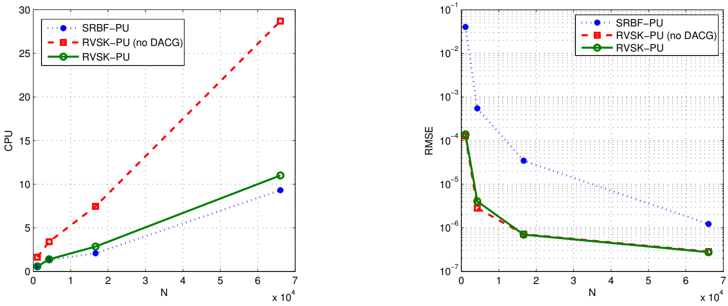

Figure : Left: the number of points N versus the CPU times for the SRBF-PU, RVSK-PU and RVSK-PU (no DACG), i.e. the RVSK-PU computed with the IRLM (Implicit Restarted Lanczos) method. Right: the number of points N versus the logarithmic scale of the RMSE for the SRBF-PU, RVSK-PU and RVSK-PU (no DACG).

Globally supported RBFs

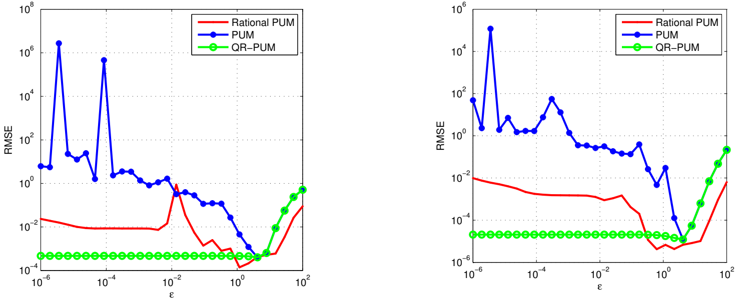

Figure : Comparison of RMSEs vs shape parameters for the SRBF-PUM, RRBF-PUM and RBF-QR+PUM methods on f_1 on two sets of Halton points, with Gaussian kernel

Compactly supported RBFs

$f_3(x_1, x_2) = \sin(3x_1^2 + 6x_2^2) - \sin(2x_1^2 + 4x_2 - 0.5)$. Noisy Halton data (0.01 noise), $s = 16$ subdivisions, $\delta = \delta_0$.

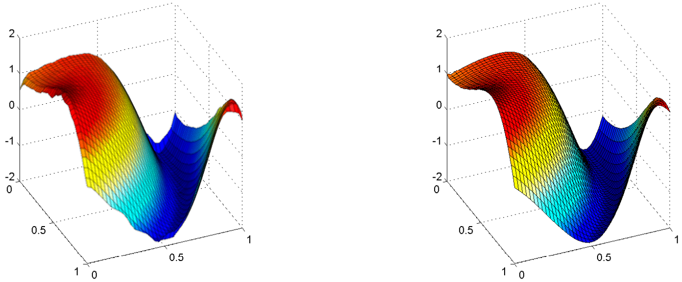

Figure : The approximate surface f_3 obtained with the SRBF-PU (left) and RVSK-PU (right) methods with $N = 1089$ noisy Halton data. Results are computed using the Wendland's C^2 function as local approximant. The shape parameter equal to 6.

Compactly supported RBFs

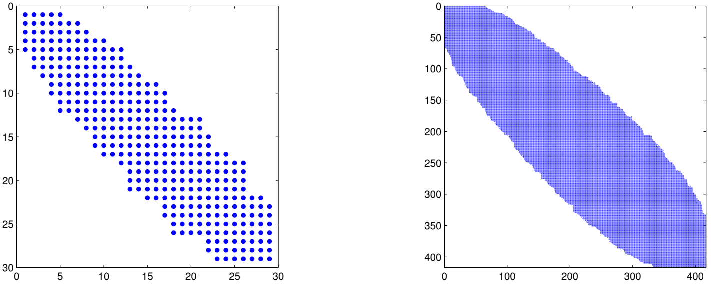

Figure : Typical sparsity pattern of the local interpolation matrices obtained via the RVSK-PU method with 289 (left) and 4225 (right) noisy Halton data. C^2 Wendland's kernel.

Future work

- Cardinal functions and barycentric form of the rational interpolant.
- Error estimates, native spaces.
- Applications and extensions.

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grazie per la vostra attenzione!

thanks for your attention!