New developments on rational RBF

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Outline

1. From RBF to Rational RBF (RRBF)
2. Eigen-rational interpolant
3. Numerical experiments
   - Lebesgue functions and constants
   - Errors
   - Landmark-based Image registration
4. Progetto GNCS 2016-17
From RBF to Rational RBF (RRBF) 
work with A. Martinez and E. Perracchione
Notations

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

2. Approximation setting:
   - $\phi(\varepsilon \cdot)$: Conditionally Positive Definite (CPD) of order $\ell$ or Strictly Positive Definite (SPD) and radial ($\varepsilon$, shape parameter)
     
     | name                      | $\phi$                          | $\ell$ |
     |----------------------------|---------------------------------|--------|
     | Gaussian $C^\infty$ (GA)   | $e^{-\varepsilon^2 r^2}$        | 0      |
     | Generalized Multiquadrics $C^\infty$ (GM) | $(1 + r^2 / \varepsilon^2)^{3/2}$ | 2      |

   - globally supported:

   - locally supported:
     
     | name                      | $\phi$                          | $\ell$ |
     |----------------------------|---------------------------------|--------|
     | Wendland $C^2$ (W2)        | $(1 - \varepsilon r)^4 (4\varepsilon r + 1)$ | 0      |
     | Buhmann $C^2$ (B2)         | $2r^4 \log r - 7/2r^4 + 16/3r^3 - 2r^2 + 1/6$ | 0      |
## Notations

1. **Data:** \( \Omega \subset \mathbb{R}^d, \ X \subset \Omega, \) test function \( f \)
   \[ X_N = \{x_1, \ldots, x_N\} \subset \Omega, \ f = \{f_1, \ldots, f_N\}, \text{ where } f_i = f(x_i) \]

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- kernel notation \( K_\varepsilon(\cdot, \cdot) \)
- native space \( \mathcal{N}_K(\Omega) \) (where \( K \) is the reproducing kernel)
- finite subspace \( \mathcal{N}_K(X_N) = \text{span}\{K(\cdot, x) : x \in X_N\} \subset \mathcal{N}_K(\Omega) \)
RBF Interpolation

Given $\Omega$, $X_N$, $f$, $K$

**Aim**

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

[Hardy and Gofert 1975] used multiquadrics $K(x, y) = \sqrt{1 + \epsilon^2 \|x - y\|^2}$.

Rescaled interpolant: $\hat{P}_f(x) = P_f(x) P_g(x) = \sum_{k=1}^{N} \alpha_k K(x, x_k) \sum_{k=1}^{N} \beta_k K(x, x_k)$

where $P_g$ is the kernel interpolant of $g(x) = 1$, $\forall x \in \Omega$.

Localized Rescaled and exactness on constants in [Deparis et al 2014]. In [DeM et al 2017] it is shown that it is a Shepard’s PU method.

Linear convergence of localized rescaled interpolants [DeM and Wendland, draft 2017]
RBF Interpolation

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- Classical interpolant: $P_f(x) = \sum_{k=1}^{N} \alpha_k K(x, x_k), \quad x \in \Omega, \ x_k \in X_N.$

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- **Classical 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
  
  $K(x, y) = \sqrt{1 + \epsilon^2 \|x - y\|^2}$.

- **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 interpolant of $g(x) = 1, \ \forall x \in \Omega$. Localized Rescaled and exactness on constants in [Deparis et al 2014]. In [DeM et al 2017] it is shown that it is a **Shepard’s PU method**. Linear convergence of localized rescaled interpolants [DeM and Wendland, draft 2017]
Rational RBF

\[ R(x) = \frac{R^{(1)}(x)}{R^{(2)}(x)} = \frac{\sum_{k=1}^{N} \alpha_k K(x, x_k)}{\sum_{k=1}^{N} \beta_k K(x, x_k)} \]

[Jackbsson et al. 2009, Sarra and Bai 2017]

\[ \Rightarrow \text{RRBFs well approximate data with steep gradients or discontinuities [rational with PU+VSK in DeM et al. 2017].} \]
Rational RBF
Learning from rational functions, \( d = 1 \)

- polynomial case.

\[
\begin{align*}
\quad r(x) &= \frac{p_1(x)}{p_2(x)} = \frac{a_m x^m + \cdots + a_0 x^0}{x^n + b_{n-1} x^{n-1} \cdots + b_0}.
\end{align*}
\]

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

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

Learning from rational functions, $d = 1$

- **polynomial case.**

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

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

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

- **RBF case.** 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 $R^{(2)}(x) \neq 0$, for all $x \in \Omega$. 
Rational RBF
Find the coefficients: I

[Jackobsson et al 2009] proved the well-posedness of the interpolation on $X_N$ via

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

(2)
Rational RBF

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Letting $\xi = (\alpha^T, \beta^T) \in \mathbb{R}^{2N}$ and $B$ the $N \times 2N$ matrix

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

The system $B\xi = 0$ can be written as $(A - DA)(\xi) = 0$ with $D = \text{diag}(f_1, \ldots, f_N)$, and $A_{i,j} = K(x_i, x_j)$. ...
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Non trivial solution

Following [GolubReinsch1975] non-trivial solutions exist by asking $\|\xi\|_2 = 1$ i.e. solving the problem $\min_{\xi \in \mathbb{R}^N, \|\xi\|_2 = 1} \|B\xi\|_2.$
Rational RBF

Find the coefficients: II

Obs: (Since $R^{(1)}(x_i) = f_i R^{(2)}(x_i)$, $i = 1, \ldots, N$)

Find $\mathbf{q} = (R^{(2)}(x_1), \ldots, R^{(2)}(x_N))^T$ and, as $\mathbf{p} = D\mathbf{q}$, then

$\mathbf{p} = (R^{(1)}(x_1), \ldots, R^{(1)}(x_N))^T$. 
Rational RBF

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

$$A\alpha = p, \quad A\beta = q.$$  \hspace{1cm} (3)
Rational RBF

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- Existence & Uniqueness of (3): $K$ is SPD

Using the native space norms the above problem is equivalent

Problem 1

$$\min_{R^{(1)}, R^{(2)} \in N_K, \ 1/\|f\|_2^2 \|p\|_2^2 + \|q\|_2^2 = 1, \ R^{(1)}(x_k) = f_k R^{(2)}(x_k)} \left( \frac{1}{\|f\|_2^2} \|R^{(1)}\|_{N_K}^2 + \|R^{(2)}\|_{N_K}^2 \right).$$  \hspace{1cm} (4)
Rational RBF

Find the coefficients: III

\[ \|R^{(1)}\|^{2}_{N_{K}} = \alpha^{T} A \alpha, \quad \text{and} \quad \|R^{(2)}\|^{2}_{N_{K}} = \beta^{T} A \beta. \]

Then, from (3) and symmetry of \( A \)

\[ \|R^{(1)}\|^{2}_{N_{K}} = p^{T} A^{-1} p, \quad \text{and} \quad \|R^{(2)}\|^{2}_{N_{K}} = q^{T} A^{-1} q. \]

Therefore, the Problem 1 reduces to solve

**Problem 2**

\[
\min_{q \in \mathbb{R}^{N}, \frac{1}{\|f\|^{2}_{2}} \|Dq\|^{2}_{2} + \|q\|^{2}_{2} = 1} \left( \frac{1}{\|f\|^{2}_{2}} q^{T} D^{T} A^{-1} D q + q^{T} A^{-1} q \right).
\]
[Jackbsson 2009] show that this is equivalent to solve the following generalized eigenvalue problem

**Problem 3**

\[ \Sigma q = \lambda \Theta q, \]

with

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

where \( I_N \) is the identity matrix.
[Jackbsson 2009] show that this is equivalent to solve the following generalized eigenvalue problem

**Problem 3**

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\[ \Sigma = \frac{1}{\|f\|_2^2} D^T A^{-1} D + A^{-1}, \quad \text{and} \quad \Theta = \frac{1}{\|f\|_2^2} D^T D + l_N, \]

where \( l_N \) is the identity matrix.

\( \Rightarrow \) \( q \) is the eigenvector associated to the smallest eigenvalue!
The new eigen-rational interpolant
work with M. Buhmann and E. Perracchione
New class of rational RBF

\[ \hat{P}_f(x) = \frac{\sum_{i=1}^{N} \alpha_i K(x, x_i) + \sum_{m=1}^{L} \gamma_m p_m(x)}{\sum_{k=1}^{N} \beta_k \bar{K}(x, x_k)} := \frac{P_g(x)}{P_h(x)} \]  

(5)

Ratio of a CPD $K$ of order $\ell$ and an associate PD $\bar{K}$ .... $\Rightarrow$ two kernel matrices, $\Phi_K$ and $\Phi_{\bar{K}}$. 

Obs: 1. Once we know the function values $P_h(x_i) = h_i, i = 1, \ldots, N$, we can construct $P_g$, i.e. it interpolates $g = (f_1 h_1, \ldots, f_N h_N)^T$. Hence $\hat{P}_f$ interpolates the given function values at the nodes $X_N$.

2. If $K$ is PD, we fix $\bar{K} = K$ so that we deal with the same kernel matrix for both numerator and denominator.
New class of rational RBF

\[ \hat{P}_f(x) = \frac{\sum_{i=1}^{N} \alpha_i K(x, x_i) + \sum_{m=1}^{L} \gamma_m p_m(x)}{\sum_{k=1}^{N} \beta_k \bar{K}(x, x_k)} := \frac{P_g(x)}{P_h(x)} \] (5)

Ratio of a CPD \( K \) of order \( \ell \) and an associate PD \( \bar{K} \) .... \( \Rightarrow \) two kernel matrices, \( \Phi_K \) and \( \Phi_{\bar{K}} \).

Obs:

1. Once we know the function values \( P_h(x_i) = h_i, i = 1, \ldots, N \), we can construct \( P_g \), i.e. it interpolates \( g = (f_1 h_1, \ldots, f_N h_N)^T \). Hence \( \hat{P}_f \) interpolates the given function values \( f \) at the nodes \( X_N \).

2. If \( K \) is PD, we fix \( \bar{K} = K \) so that we deal with the same kernel matrix for both numerator and denominator.
When $P_h(\mathbf{x}) \neq 0$, $\forall \mathbf{x} \in \Omega$?

**Theorem (Perron1907)**

All positive square matrices have a positive eigenvalue with corresponding eigenvector with all components positive (called Perron eigenpair).

**Theorem (Perron1907)**

All positive square matrices possess exactly one Perron eigenpair and the corresponding eigenvalue has the largest modulus.
dividing the interpolant (2) by the eigenvector associated to the largest eigenvalue of $\Phi_{\bar{K}}$ makes computations more accurate and hopefully more stable.

1 hence, the coefficients $\beta = (\beta_1, \ldots, \beta_N)^T$ are the components of the eigenvector associate to the eigenvalue

$$\max \tilde{\beta}^T \Phi_{\bar{K}} \tilde{\beta}, \quad \|\tilde{\beta}\|_2 = 1$$

2 This enables us to give an eigen-rational RBF expansion, independent of the function values of the approximant and depending only on the kernel $K$ (and its associate $\tilde{K}$) and $X_N$
Algorithmic issues

Assume $K$ is CPD of order $\ell$ and $\bar{K}$ the associate PD kernel.

1. Compute $\beta$ and so the values $P_h(x_i) = h_i, \ i = 1, \ldots, N$ where $h$ is defined by using the matrix $\Phi_{\bar{K}}$ (that depends on $X_N$ and $\phi$) and not on the function values.

2. Determine $\hat{P}_f$ in (5) with the function values $g = fh$ and $\mathbf{0}$ (of length $L$) instead of $(g, \mathbf{0})^T$. 
Cardinal functions: I

\[ \hat{P}_f = \sum_{j=1}^{N} \alpha_j \frac{K(x, x_j)}{\sum_{i=1}^{N} \beta_i K(x, x_i)} = \sum_{j=1}^{N} \alpha_j \frac{h_j K(x, x_j)}{\sum_{i=1}^{N} \beta_i K(x, x_i) \sum_{i=1}^{N} \beta_i K(x_j, x_i)}, \]

since \( h_j = \sum_{i=1}^{N} \beta_i K(x_j, x_i). \) Then

\[ \hat{P}_f = \sum_{j=1}^{N} \tilde{\alpha}_j \frac{K(x, x_j)}{\sum_{i=1}^{N} \beta_i K(x, x_i) \sum_{i=1}^{N} \beta_i \Phi(x_j, x_i)} =: \sum_{j=1}^{N} \tilde{\alpha}_j K_R(x, x_j). \]

Since \( P_h \) is not vanishing, the function

\[ K_R(x, y) = \frac{1}{P_h(x)} \frac{1}{P_h(y)} K(x, y), \]

is strictly positive definite [DeMIS17].

Obs:

The same argument applies when \( K \) is only CPD of order \( \ell \) giving \( K_R \) CPD of order \( \ell \).
Proposition (BDeMP18)

Suppose $K$ is CPD of order $\ell$ in $\mathbb{R}^d$, $\bar{K}$ is the associated PD kernel. Suppose $X_N \subset \Omega$ is $(\ell - 1)$-unisolvent, then there exist $N$ functions $\hat{u}_k$ so that the interpolant is

$$\hat{P}_f(x) = \sum_{j=1}^{N} f_j \hat{u}_j(x).$$
Proposition (BDeMP18)

Suppose $K$ is CPD of order $\ell$ in $\mathbb{R}^d$, $\check{K}$ is the associated PD kernel. Suppose $X_N \subset \Omega$ is $(\ell - 1)$-unisolvent, then there exist $N$ functions $\hat{u}_k$ so that the interpolant is

$$\hat{P}_f(x) = \sum_{j=1}^{N} f_j \hat{u}_j(x).$$

If $K = \check{K}$ is PD, the $\hat{u}_k$, $k = 1, \ldots, N$, form a partition of unity [DeMIS, AT15 (2017)].

Stability bound

$$\left| \sum_{i=1}^{N} f(x_i) \hat{u}_i(x) \right| \leq \left( \sum_{i=1}^{N} |\hat{u}_i(x)| \right) \|f\|_\infty =: \hat{\lambda}_N(x) \|f\|_\infty \leq \hat{\Lambda}_N \|f\|_\infty,$$

where $\Lambda_N$ the Lebesgue constant

$$\hat{\lambda}_N := \max_{x \in \Omega} \hat{\lambda}_N(x).$$
Error bound

**Proposition (BDeMP18)**

Let $\Omega \subseteq \mathbb{R}^d$ be open. Suppose $K \in C(\Omega \times \Omega)$ be CDP of order $\ell$ and $\bar{K}$ the associate PD kernel. Assume that $X_N \subset \Omega$ is $(\ell - 1)$-unisolvent. Then, for $x \in \Omega$, the pointwise error

$$|f(x) - \hat{P}_f(x)| \leq \frac{1}{|P_h(x)|} \left( \mathcal{P}_{\bar{K},x_N}(x)|h|_{N_{\bar{K}}(\Omega)}|f(x)| + \mathcal{P}_{K,x_N}(x)|g|_{N_K(\Omega)} \right).$$

with $\mathcal{P}_{K,x_N}$ the **power function** for the kernel $K$ and point set $X_N$ and $|\cdot|_{N_K(\Omega)}$ the semi-norm.

$\implies$ Similar bounds are derived using the **fill-distance**, $h_{x_N,\Omega}$. 
Numerical tests:

rational eigen-basis vs the standard one
Numerical tests: Lebesgue constants I

<table>
<thead>
<tr>
<th>$K$</th>
<th>$\Lambda_N (\varepsilon = 0.5)$</th>
<th>$\Lambda_N (\varepsilon = 3)$</th>
<th>$\hat{\Lambda}_N (\varepsilon = 0.5)$</th>
<th>$\hat{\Lambda}_N (\varepsilon = 3)$</th>
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<td>GM</td>
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<td>2.73</td>
<td>7.90</td>
</tr>
<tr>
<td>B2</td>
<td>30.6</td>
<td>–</td>
<td>29.1</td>
<td>–</td>
</tr>
</tbody>
</table>

Table: Lebesgue constants $\Lambda_N$ and $\hat{\Lambda}_N$ for classical and eigen-rational interpolants, respectively. They are computed on $N = 10$ equally spaced points on $\Omega = [-1, 1]$. Note: Buhmann’s function is independent of the shape parameter.
Numerical tests: Lebesgue functions (1d)

Figure: Top: 10 Halton points, GM kernel with $\varepsilon = 0.5$ (left) and $\varepsilon = 3$ (right). Bottom: 10 Chebyshev points, GA kernel with $\varepsilon = 0.5$ (left) and $\varepsilon = 3$ (right).
Numerical tests: Lebesgue functions (2d)

**Figure:** Top: Lebesgue functions computed via the W6 kernel with $\varepsilon = 0.5$ for standard (left) and eigen-rational (right) interpolants. Bottom: Lebesgue functions computed via the B2 kernel for standard (left) and eigen-rational (right) interpolants.
Error and max-abs error comparison

\[ f_1(x_1) = \text{sinc}(x_1), \quad x_1 \in [-1, 1] \]

**Figure:** Error estimates \( \hat{E} \) and \( E \) via LOOCV of max. abs. errors \( \hat{A} \) and \( A \) for eigen-rational and classical interpolants, respectively. Here we consider \( f_1 \) on 81 Chebyshev points on \( \Omega = [-1, 1] \) via GM (left) and GA (right) kernels.
\[ f_2(x_1) = \frac{x_1^8}{\tan(1 + x_1^2) + 0.5}, \quad x_1 \in [-1, 1] \]

**Figure:** Error estimates \( \hat{E} \) and \( E \) via LOOCV of max. abs. errors \( \hat{A} \) and \( A \) for eigen-rational and classical interpolants, respectively. Result are computed with \( f_2 \) and 81 Random points on \( \Omega = [-1, 1] \) via W6 (left) and M6 (right) kernels.
Image registration: landmarks [CDeR2018, C et al 2015]

Figure: (Above) 21 landmarks are plotted with squares on the source image (left) and with dots on the target image (left). (Below) The registered image via eigen-rational interpolants computed with the W2 (left) and M2 (right) kernels and shape parameter $\varepsilon = 0.1$. 

![Figure showing image registration landmarks and registered images with different kernels and parameter values](image-url)
Image registration: mean error comparison

\[ M = \left( \frac{\sum_{s \in S} \| s - F(s) \|_2^2}{\#S} \right)^{1/2}. \]

**Figure:** Mean errors \( M \) (standard) and \( \hat{M} \) (rational), varying the shape parameter.
Breve resoconto del progetto GNCS 2016-17
Alcuni dati

1. Finanziamento richiesto/ricevuto: 9.0K/7.8K euro
2. Partecipanti: 15 strutturati, 9 non strutturati;
3. Quote individuali: circa 300 euro
4. Organizzati dai componenti i seguenti meetings: Bernried17, MATAA17 (Torino), CMMSE (Cadiz), DRWA17 (Canazei), SMART17 (Gaeta), AMTA17 (Palermo).
5. Pubblicazioni relative al progetto: CAA Padova + Verona (22+13), Milano (3), Torino (10+2), Firenze (4+1), Potenza (9+2), Cosenza (4+?), Reggio Calabria (4), Palermo (5).
RITA (Rete ITaliana di Approssimazione): sito

https://sites.google.com/site/italianapproximationnetwork/
Some references


M. Buhmann, S. De Marchi, E. Perracchione : Analysis of a new class of rational RBF expansions, darft, 2018

grazie per la vostra attenzione!
thanks for your attention!