# 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





### From RBF to Rational RBF (RRBF) work with A. Martinez and E. Perracchione



### Notations

**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:
  - φ(ε·): Conditionally Positive Definite (CPD) of order ℓ or Strictly Positive Definite (SPD) and radial (ε, shape parameter)

 	name		$\phi$	l
globally supported:	Gaussian $C^{\infty}$ (GA)	(.	$e^{-\epsilon^2 r^2}$	0
	Generalized Multiquadrics C (Givi)	(	$1 + 1^{-}/\varepsilon^{-}$	2
locally supported:				
name	φ	l		
Wendland $C^2$ (W2)	$(1-\varepsilon r)^4_+ (4\varepsilon r+1)$	0		
Buhmann $C^2$ (B2) $2r$	$r^{4}\log r - 7/2r^{4} + 16/3r^{3} - 2r^{2} + 1/6$	0		



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erne	el notation $K_{\varepsilon}(\cdot, \cdot)$			
native	e space $\mathcal{N}_{\kappa}(\Omega)$ (w	here K is the reproducion	ng kernel)	

■ finite subspace  $N_{\kappa}(X_N) = \operatorname{span}\{K(\cdot, x) : x \in X_N\} \subset N_{\kappa}(\Omega)$ 



# **RBF** Interpolation

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

### Aim

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



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



# **RBF** Interpolation

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



definition

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

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

 $\implies$  RRBFs well approximate data with steep gradients or discontinuites [rational with PU+VSK in DeM et al. 2017].



#### Learning from rational functions, d = 1

polynomial case.

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

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

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



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■ RBF case. Let  $X_m = \{x_k, \dots, x_{k+m-1}\}, X_n = \{x_j, \dots, x_{j+n-1}\} \subset X_N$  be non empty, such that  $m + n \le N$ 

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

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



#### Find the coefficients: I

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

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

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

The system  $B\boldsymbol{\xi} = \mathbf{0}$  can be written as  $(A - DA)(\boldsymbol{\xi}) = \mathbf{0}$  with  $D = \text{diag}(f_1, \dots, f_N)$ , 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  $\min_{\xi \in \mathbb{R}^N, \|\xi\|_2 = 1} \|B\xi\|_2$ .



Find the coefficients: II

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

find 
$$\mathbf{q} = (R^{(2)}(x_1), \dots, R^{(2)}(x_N))^T$$
 and, as  $\mathbf{p} = D\mathbf{q}$ , then  
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If p, q are given then the rational interpolant is known by solving

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# **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  

$$\min_{\substack{R^{(1)}, R^{(2)} \in \mathcal{N}_{K}, \\ 1/\|\mathbf{f}\|_{2}^{2}\|\mathbf{p}\|_{2}^{2}+\|\mathbf{q}\|_{2}^{2}=1, \\ R^{(1)}(\mathbf{x}_{k})=f_{k}R^{(2)}(\mathbf{x}_{k}).}} \left(\frac{1}{\|\mathbf{f}\|_{2}^{2}}\|R^{(1)}\|_{\mathcal{N}_{K}}^{2}+\|R^{(2)}\|_{\mathcal{N}_{K}}^{2}\right). \tag{4}$$



Find the coefficients: III

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

Then, from (3) and symmetry of A

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

Therefore, the Problem 1 reduces to solve

### Problem 2

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



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

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

where  $I_N$  is the identity matrix.



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where  $I_N$  is the identity matrix.

 $\hookrightarrow$  q is the eigenvector associated to the smallest eigenvalue!  $\leftarrow$ 

# The new eigen-rational interpolant work with M. Buhmann and E. Perracchione



## New class of rational RBF

$$\hat{P}_{f}(\boldsymbol{x}) = \frac{\sum_{i=1}^{N} \alpha_{i} K(\boldsymbol{x}, \boldsymbol{x}_{i}) + \sum_{m=1}^{L} \gamma_{m} p_{m}(\boldsymbol{x})}{\sum_{k=1}^{N} \beta_{k} \bar{K}(\boldsymbol{x}, \boldsymbol{x}_{k})} := \frac{P_{g}(\boldsymbol{x})}{P_{h}(\boldsymbol{x})}$$
(5)

Ratio of a CPD *K* of order  $\ell$  and an associate PD  $\overline{K} \dots \Longrightarrow$  two kernel matrices,  $\Phi_K$  and  $\Phi_{\overline{K}}$ .



## New class of rational RBF

$$\hat{P}_{f}(\boldsymbol{x}) = \frac{\sum_{i=1}^{N} \alpha_{i} \mathcal{K}(\boldsymbol{x}, \boldsymbol{x}_{i}) + \sum_{m=1}^{L} \gamma_{m} \mathcal{P}_{m}(\boldsymbol{x})}{\sum_{k=1}^{N} \beta_{k} \bar{\mathcal{K}}(\boldsymbol{x}, \boldsymbol{x}_{k})} := \frac{P_{g}(\boldsymbol{x})}{P_{h}(\boldsymbol{x})}$$
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Ratio of a CPD *K* of order  $\ell$  and an associate PD  $\overline{K} \dots \Longrightarrow$  two kernel matrices,  $\Phi_K$  and  $\Phi_{\overline{K}}$ .

### Obs:

- Once we know the function values P<sub>h</sub>(x<sub>i</sub>) = h<sub>i</sub>, i = 1,..., N, we can construct P<sub>g</sub>, i.e. it interpolates g = (f<sub>1</sub>h<sub>1</sub>,..., f<sub>N</sub>h<sub>N</sub>)<sup>T</sup>. Hence P̂<sub>f</sub> interpolates the given function values f at the nodes X<sub>N</sub>.
- **2** If K is PD, we fix  $\overline{K} = K$  so that we deal with the same kernel matrix for both numerator and denominator.



# The rational interpolant is well-defined

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  $\Phi_{\vec{k}}$  makes computations more accurate and hopefully more stable.

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

$$\max_{\|\vec{\beta}\|_{2}=1} \tilde{\boldsymbol{\beta}}^{\mathsf{T}} \Phi_{\bar{K}} \tilde{\boldsymbol{\beta}}, \tag{6}$$

**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  $\overline{K}$ ) and  $\mathbf{X}_N$ 



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

- **1** Compute  $\beta$  and so the values  $P_h(\mathbf{x}_i) = h_i$ , i = 1, ..., N where h is defined by using the matrix  $\Phi_{\overline{K}}$  (that depends on  $\mathbf{X}_N$  and  $\phi$ ) and not on the function values.
- Determine \$\hat{P}\_f\$ in (5) with the function values \$\mathbf{g} = \mathbf{fh}\$ and \$\mathbf{0}\$ (of length L) instead of \$(\mathbf{g}, \mathbf{0})^T\$.



### Cardinal functions: I

$$\hat{P}_{f} = \sum_{j=1}^{N} \alpha_{j} \frac{K(\boldsymbol{x}, \boldsymbol{x}_{j})}{\sum_{i=1}^{N} \beta_{i} K(\boldsymbol{x}, \boldsymbol{x}_{i})} = \sum_{j=1}^{N} \alpha_{j} \frac{h_{j} K(\boldsymbol{x}, \boldsymbol{x}_{j})}{\sum_{i=1}^{N} \beta_{i} K(\boldsymbol{x}, \boldsymbol{x}_{i}) \sum_{i=1}^{N} \beta_{i} K(\boldsymbol{x}_{j}, \boldsymbol{x}_{i})},$$

since  $h_j = \sum_{i=1}^N \beta_i K(\mathbf{x}_j, \mathbf{x}_i)$ . Then

$$\hat{P}_f = \sum_{j=1}^N \tilde{\alpha}_j \frac{\mathcal{K}(\mathbf{x}, \mathbf{x}_j)}{\sum_{i=1}^N \beta_i \mathcal{K}(\mathbf{x}, \mathbf{x}_i) \sum_{i=1}^N \beta_i \Phi(\mathbf{x}_j, \mathbf{x}_i)} =: \sum_{j=1}^N \tilde{\alpha}_j \mathcal{K}_R(\mathbf{x}, \mathbf{x}_j).$$

Since  $P_h$  is not vanishing, the function

$$K_{R}(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{P_{h}(\boldsymbol{x})} \frac{1}{P_{h}(\boldsymbol{y})} K(\boldsymbol{x}, \boldsymbol{y}),$$

is strictly positive definite [DeMIS17].

### Obs:

The same argument applies when K is only CPD of order  $\ell$  giving K<sub>R</sub> CPD of order  $\ell$ .



### Proposition (BDeMP18)

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

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



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$$\hat{\mathsf{P}}_{f}(\boldsymbol{x}) = \sum_{j=1}^{N} f_{j}\hat{u}_{j}(\boldsymbol{x}).$$

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

⇒ Stability bound

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

where  $\Lambda_N$  the Lebesgue constant

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

### Proposition (BDeMP18)

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

$$|f(\boldsymbol{x}) - \hat{P}_{f}(\boldsymbol{x})| \leq \frac{1}{|P_{h}(\boldsymbol{x})|} \bigg( \mathcal{P}_{\bar{K}, \boldsymbol{X}_{N}}(\boldsymbol{x}) |h|_{\mathcal{N}_{\bar{K}}(\Omega)} |f(\boldsymbol{x})| + \mathcal{P}_{K, \boldsymbol{X}_{N}}(\boldsymbol{x}) |g|_{\mathcal{N}_{K}(\Omega)} \bigg).$$

with  $\mathcal{P}_{K,\mathbf{X}_N}$  the power function for the kernel *K* and point set  $\mathbf{X}_N$  and  $|\cdot|_{\mathcal{N}_K(\Omega)}$  the semi-norm.

 $\implies$  Similar bounds are derived using the fill-distance,  $h_{\mathbf{X}_{N},\Omega}$ .

### Numerical tests: rational eigen-basis vs the standard one



К	$\Lambda_N \ (\varepsilon = 0.5)$	$\Lambda_N \ (\varepsilon = 3)$	$\hat{\Lambda}_N (\varepsilon = 0.5)$	$\hat{\Lambda}_N \ (\varepsilon = 3)$
GM	4.98	8.69	5.14	9.13
GA	9.81	2.58	12.6	3.59
M6	10.6	2.20	11.1	2.60
W6	2.10	9.58	2.73	7.90
B2	30.6	-	29.1	-

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

$$f_1(x_1) = \operatorname{sinc}(x_1), \ x_1 \in [-1, 1]$$



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  $\varepsilon = 0.1$ .



#### Image registration: mean error comparison

$$M = \left(\frac{\sum_{\boldsymbol{s}\in\mathcal{S}} \|\boldsymbol{s} - \boldsymbol{F}(\boldsymbol{s})\|_2^2}{\#\mathcal{S}}\right)^{1/2}$$

.



Figure: Mean errors *M* (standard) and  $\hat{M}$  (rational), varying the shape parameter.

### Breve resoconto del progetto GNCS 2016-17



- 1 Finanziamento richiesto/ricevuto: 9.0K/7.8K euro
- 2 Partecipanti: 15 strutturati, 9 non strutturati;
- 3 Quote individuali: circa 300 euro
- Organizzati dai componenti i seguenti meetings: Bernried17, MATAA17 (Torino), CMMSE (Cadiz), DRWA17 (Canazei), SMART17(Gaeta), AMTA17 (Palermo).
- 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

**RITA** 



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





### Some references

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grazie per la vostra attenzione! thanks for your attention!

