Consistency Error of Meshless Finite Difference Methods

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Tight Frames and Approximation

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Outline

1. Meshless Finite Difference Methods
2. Consistency Error
3. Conclusion

Outline

Meshless methods for numerical PDEs

- Growing interest since 1990s in particular in the engineering literature.
- As the name suggests there is no mesh or grid (even 'unstructured'), just unconnected nodes spread out over the computational domain.
- Motivation: difficulties of mesh generation for complex geometries, and difficulties of the modification of a mesh when singularities or domain boundary move in time.
- Many versions with different backgrounds.

Meshless FDM

- Model problem: Poisson equation $\Delta u = f$ on Ω, $u|_{\partial\Omega} = g$.
- Distribute nodes $\{\xi_i\}_{i \in I} = \Xi \subset \overline{\Omega}$.
- Choose a small set of influence $\Xi_i \subset \Xi$ for each $\xi_i \in \Xi \setminus \partial\Omega$.
- Find the weights $w_{i,j}$ of a numerical differentiation formula:

$$\Delta u(\xi_i) \approx \sum_{\xi_j \in \Xi_i} w_{i,j} u(\xi_j) \quad \text{for each } \xi_i \in \Xi \setminus \partial\Omega.$$

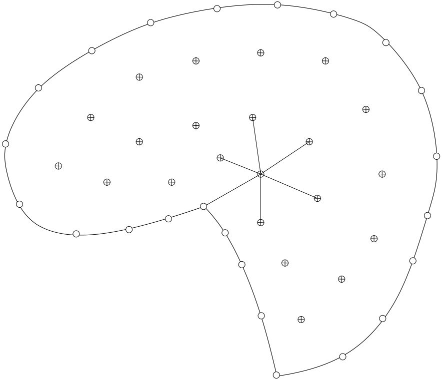
- Find a discrete approximate solution $\hat{u}$ defined on Ξ by solving sparse linear system with matrix $W = [w_{i,j}]_{\xi_i, \xi_j \in \Xi \setminus \partial\Omega}$

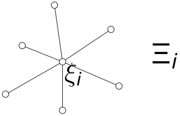
$$\sum_{\xi_j \in \Xi_i} w_{i,j} \hat{u}(\xi_j) = f(\xi_i) \;\; \text{for } \xi_i \in \Xi \setminus \partial\Omega$$

$$\hat{u}(\xi_i) = g(\xi_i) \;\; \text{for } \xi_i \in \partial\Omega.$$

Meshless Finite Difference Methods

Set Ξ of all nodes and a set of influence Ξ_i:





ξ_i

Meshless Finite Difference Methods

Classical FD method is a special case:

- Ξ is a tensor-product grid (or union of several grids)
- Ξ_i and $\{w_{i,j}\}_{j\in\Xi_i}$ are shifted and scaled versions of a single stencil
- The weights $w_{i,j}$ are in fact chosen such that numerical differentiation is exact for polynomials of certain degree:

$$\Delta u(\xi_i) = \sum_{\xi_j\in\Xi_i} w_{i,j} u(\xi_j) \quad \text{if } u \text{ is a polynomial of degree } n$$

Meshless Finite Difference Methods

Meshless FD vs. classical FD method:

- Ξ is arbitrary
- Ξ_i are chosen individually
- The weights $w_{i,j}$ are obtained by a method that ensures exactness of the formula for either
  - polynomials of certain degree, or
  - kernel sums:

$$\Delta u(\xi_i) = \sum_{\xi_j \in \Xi_i} w_{i,j} u(\xi_j) \quad \text{if} \;\; u = \sum_{\xi_j \in \Xi_i} a_j K(\cdot, \xi_j)$$

    where $K(x, y)$ is a positive definite kernel, or
  - kernel sums + polynomials
    (also for conditionally positive definite kernels)

Meshless Finite Difference Methods

Advantages of meshless finite difference methods

- genuinely meshless, no need to maintain any mesh
- efficient numerics of sparse linear systems
- no integration over complicated subdomains
- system matrix assembly amounts to
  (a) search for sets of influence, and
  (b) computation of numerical differentiation weights
- full flexibility for local adaptation to reflect local features: free to choose
  - location of nodes
  - local sets of influence Ξ_i
  - numerical differentiation formulae

Meshless Finite Difference Methods: Examples

Numerical Examples

Joint work with Dang Thi Oanh and Hoang Xuan Phu

- Oleg Davydov and Dang Thi Oanh, Adaptive meshless centres and RBF stencils for Poisson equation, J. Comput. Phys., 230 (2011), 287-304.
- Dang Thi Oanh, Oleg Davydov and Hoang Xuan Phu, Adaptive RBF-FD method for elliptic problems with point singularities in 2D, Appl. Math. Comput., 313 (2017), 474–497.

Meshless Finite Difference Methods: Examples

Low order mFD method competing with linear FEM

- Sets of influence of size $n_i = 7$ with "geometric selection"
- Gaussian kernel $K(\mathbf{x}, \mathbf{y}) = e^{-\epsilon^2 \|\mathbf{x}-\mathbf{y}\|_2^2}$ with small $\epsilon = 10^{-4}$ via Gauss-QR preconditioning by Fornberg, Larsson et al.
- Error indicator: $\varepsilon(\zeta, \xi)$ defined for all $\zeta \in \Xi$, $\xi \in \Xi_\zeta$.
  An 'edge' $\zeta\xi$ is marked for refinement if

$$\varepsilon(\zeta, \xi) \geq \bar{\varepsilon} := \gamma \max\{\varepsilon(\zeta, \xi) : \zeta \in \Xi, \xi \in \Xi_\zeta\}$$

  $\gamma \in (0, 1]$ is a tolerance ($\gamma = 0.5$ in all our tests).

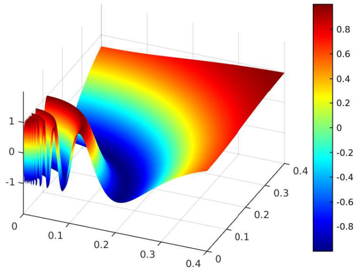
  - 2011: $\varepsilon(\zeta, \xi) = |\hat{u}(\zeta) - \hat{u}(\xi)|$
  - 2017: indicator of averaging type
    $\varepsilon(\zeta, \xi) = |(\hat{u}(\zeta) - \hat{u}(\xi)) - (\ell_\zeta(\zeta) - \ell_\zeta(\xi))|$, where ℓ_ζ is a linear polynomial least squares fit to data $\{(\xi, \hat{u}(\xi))\}_{\xi \in \Xi_\zeta}$ (motivated by Zienkiewicz-Zhu indicator in FEM).

Meshless Finite Difference Methods: Examples

Test Problem 1

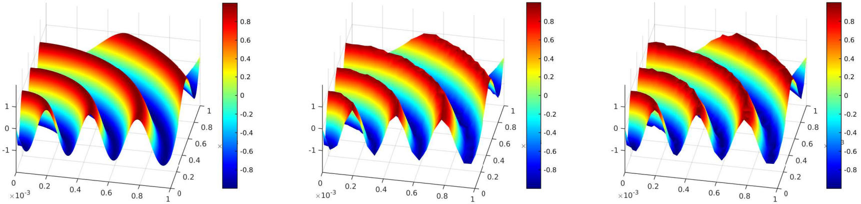
Dirichlet problem for the Helmholz equation $-\Delta u - \frac{1}{(\alpha+r)^4} u = f$, $r = \sqrt{x^2+y^2}$ in the domain $\Omega = (0,1)^2$. RHS and the boundary conditions chosen such that the exact solution is $\sin(\frac{1}{\alpha+r})$, where $\alpha = \frac{1}{50\pi}$.

Exact solution:



Meshless Finite Difference Methods: Examples

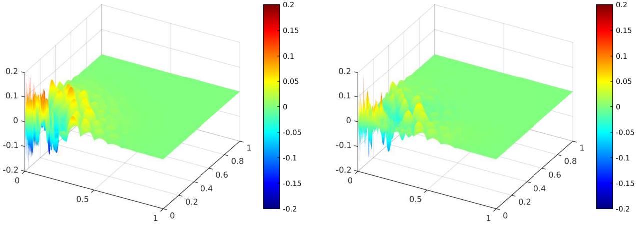
Zooms of the exact solution, FEM (with 9225 centers) and mFD (with 9775 centers)



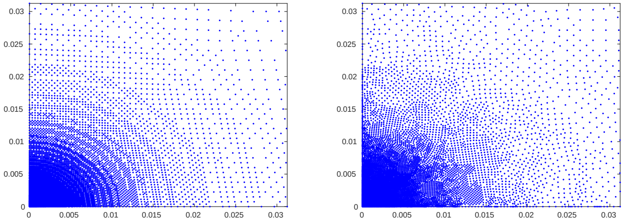
exact FEM mFD

Meshless Finite Difference Methods: Examples

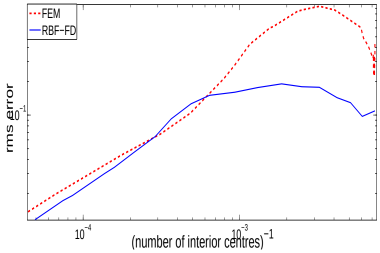
Error plots: FEM (left) vs. mFD (right)



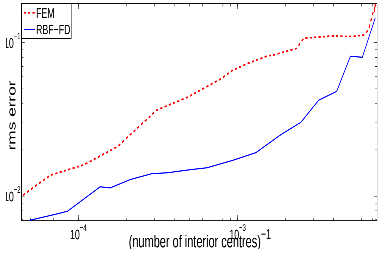
Centers (zoomed)



RMS Errors



(a) RMS errors on centers



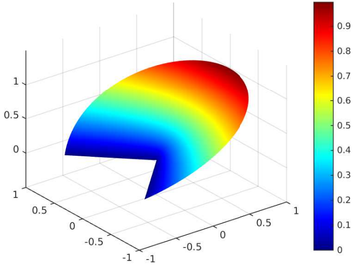
(b) RMS errors on a grid

X-axis: (the number of interior centers)$^{-1}$
Y-axis: RMS error

Meshless Finite Difference Methods: Examples

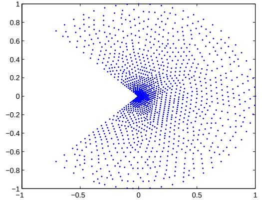
Test problem 2

- Laplace equation $\Delta u = 0$ in a circle sector $-3\pi/4 \le \psi \le 3\pi/4$
- Boundary conditions $g(r,\psi) = \cos(2\psi/3)$ along the arc, and $g(r,\psi) = 0$ along the straight lines
- Exact solution $u(r,\psi) = r^{2/3}\cos(2\psi/3)$

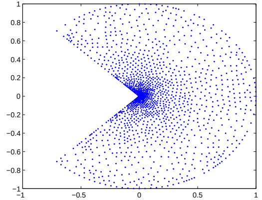


Meshless Finite Difference Methods: Examples

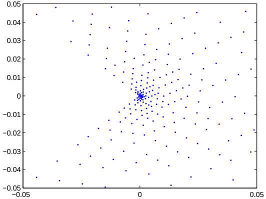
Adaptive centers by PDE Toolbox (MATLAB) and by mFD



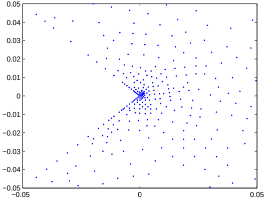
(a) FEM centers (1431)



(b) mFD centers (1444)



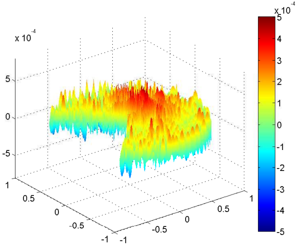
(c) FEM centers zoom



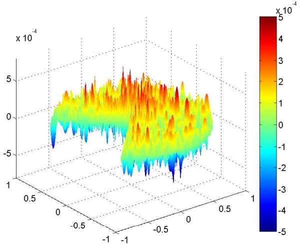
(d) mFD centers zoom

Meshless Finite Difference Methods: Examples

Error plots: $u - \hat{u}$
($\hat{u}$ obtained by piecewise linear w.r.t. Delaunay triangulation)

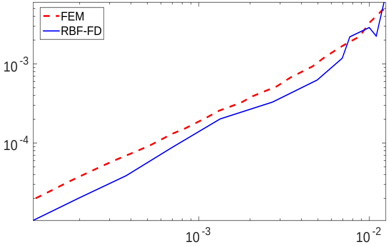


(a) FEM (1431 centers)

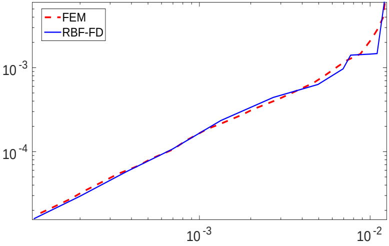


(b) mFD (1444 centers)

RMS Errors



(a) RMS errors on centers



(b) RMS errors on a grid

X-axis: (the number of interior centers)$^{-1}$
Y-axis: RMS error

Meshless Finite Difference Methods: Error Bounds

"Consistency and Stability $\Longrightarrow$ Convergence":

$$\underbrace{\|\hat{u} - u|_\Xi\|}_{\text{solution error}} \le S \underbrace{\Big\| \Big[\Delta u(\xi_i) - \sum_{\xi_j \in \Xi_i} w_{i,j} u(\xi_j) \Big]_{\xi_i \in \Xi \setminus \partial\Omega} \Big\|}_{\text{consistency error}}$$

$\|\cdot\|$ – a vector norm, e.g. $\|\cdot\|_\infty$ (max) or quadratic mean (rms), respectively a matrix norm, $\|\cdot\|_\infty$ or $\|\cdot\|_2$,

$S := \|[w_{i,j}]^{-1}_{\xi_i,\xi_j \in \Xi \setminus \partial\Omega}\|$ – stability constant (can be estimated once $w_{i,j}$ are known).

If S is bounded, then the convergence order for a sequence of discretisations Ξ_n is determined by the consistency error:

$$\Delta u(\xi_i) - \sum_{\xi_j \in \Xi_i} w_{i,j} u(\xi_j) \quad \text{(numerical differentiation error)}$$

Outline

Consistency Error

Joint work with Robert Schaback

- O. Davydov and R. Schaback, Error bounds for kernel-based numerical differentiation, Numer. Math., 132 (2016), 243-269.
- O. Davydov and R. Schaback, Optimal stencils in Sobolev spaces, to appear in IMA J. Numer. Anal. Preprint: arXiv:1611.04750
- O. Davydov and R. Schaback, Minimal numerical differentiation formulas, preprint. arXiv:1611.05001

Consistency Error

Numerical differentiation formulas

Given a finite set of points $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{R}^d$ and function values $f_j = f(\mathbf{x}_j)$, we want to approximate the value $Df(\mathbf{z})$ at a point $\mathbf{z}$ by a linear combination

$$Df(\mathbf{z}) \approx \sum_{i=1}^{N} w_i f(\mathbf{x}_i),$$

where D is a differential operator $Df(\mathbf{z}) = \sum_{\alpha \in \mathbb{Z}_+^d,\, |\alpha| \le k} a_\alpha(\mathbf{z}) \partial^\alpha f(\mathbf{z})$.

Consistency Error

Approximation approach

- $Df(\mathbf{z}) \approx Dp(\mathbf{z})$, where p is an approximation of f, e.g.,
  - least squares fit from a finite dimensional space $\mathcal{P}$
  - partition of unity interpolant
  - moving least squares fit
  - RBF / kernel interpolant
- If $p = \sum_{i=1}^{m} a_i \phi_i$ and the coefficients a_i depend linearly on $f(\mathbf{x}_j)$, i.e. $\mathbf{a} = Af|_{\mathbf{X}}$, then $p = \phi\,\mathbf{a} = \phi Af|_{\mathbf{X}}$,

$$Dp(\mathbf{z}) = \underbrace{D\phi(\mathbf{z})A}_{\mathbf{w}}\, f|_{\mathbf{X}} = \sum_{j=1}^{N} w_j\, f(\mathbf{x}_j).$$

Exactness approach

- Require exactness of the numerical differentiation formula for all elements of a space $\mathcal{P}$:

$$Dp(\mathbf{z}) = \sum_{j=1}^{N} w_j\, p(\mathbf{x}_j) \quad \text{for all } \ p \in \mathcal{P}.$$

  Notation: $\mathbf{w} \perp_D \mathcal{P}$.

- E.g., exactness for polynomials of certain order q: $\mathcal{P} = \Pi_q^d$, the space of polynomials of total degree $< q$ in d variables. (Polynomial numerical differentiation.)

Consistency Error: $\|\cdot\|_{1,\mu}$-minimal formulas

Theorem

If $\mathbf{w}$ is exact for polynomials of order $q > k$ (the order of D), then

$$|Df(\mathbf{z}) - \sum_{j=1}^{N} w_j f(\mathbf{x}_j)| \le |f|_{\infty,q,\Omega} \sum_{j=1}^{N} |w_j| \|\mathbf{x}_j - \mathbf{z}\|_2^q,$$

where $$|f|_{\infty,q,\Omega} := \Big(\frac{1}{q!} \sum_{|\alpha|=q} \frac{1}{\alpha!} \|\partial^\alpha f\|^2_{\infty,\Omega} \Big)^{1/2}.$$

- The best bound is obtained if $\sum_{j=1}^{N} |w_j| \|\mathbf{x}_j - \mathbf{z}\|_2^q$ is minimized over all weights $\mathbf{w}$ satisfying the exactness condition $Dp(\mathbf{z}) = \sum_{j=1}^{N} w_j\, p(\mathbf{x}_j)$, $\forall p \in \Pi_q^d$. ($\mathbf{w} \perp_D \Pi_q^d$)
- More general: minimize $\sum_{j=1}^{N} |w_j| \|\mathbf{x}_j - \mathbf{z}\|_2^\mu$, $\mu \ge 0$.

  We say that formula is $\|\cdot\|_{1,\mu}$-minimal.

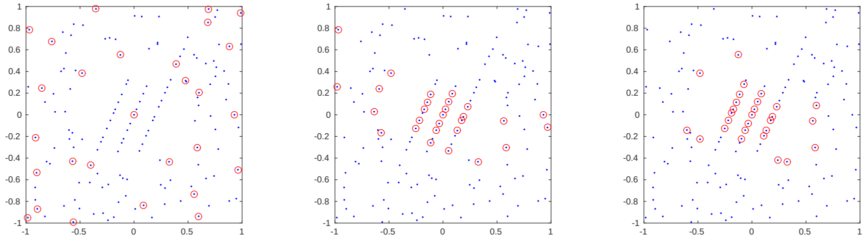
Consistency Error: $\|\cdot\|_{1,\mu}$-minimal formulas

Minimize $\sum_{j=1}^{N} |w_j| \|\mathbf{x}_j - \mathbf{z}\|_2^{\mu}$ subject to $\mathbf{w} \perp_D \Pi_q^d$.

- $\|\cdot\|_{1,\mu}$-minimal weights can be found by linear programming (e.g. simplex algorithm if N is small).
- $\mu = 0$: formulas with optimal stability constant $\sum_{j=1}^{N} |w_j|$
- $\mathbf{w}$ is sparse in the sense that the number of nonzero w_j's does not exceed $\dim \Pi_q^d$.
- Considered by Seibold (2006) for $D = \Delta$ under additional condition of "positivity" (which restricts exactness to $q \leq 4$).
- Our error bound suggests the choice $\mu = q$.

Consistency Error: $\|\cdot\|_{1,\mu}$-minimal weights

Influence of μ on the location of nonzero weights $w_j^* \neq 0$.



(a) $\mu = 0$ (b) $\mu = q = 7$ (c) $\mu = 15$

$\|\cdot\|_{1,\mu}$-minimal weights ($\mu = 0, 7, 15$) of exactness order $q = 7$ computed for the Laplacian at the origin from the data at 150 points. Locations of 28 points $\mathbf{x}_j$ for which $w_j^* \neq 0$ are shown.

- The set for $\mu = q = 7$ looks like most reasonable choice.

Consistency Error: Growth Function

Duality:

$$\inf_{\mathbf{w} \perp_D \Pi_q^d} \sum_{i=1}^{N} |w_i| \, \|\mathbf{x}_i - \mathbf{z}\|_2^q =$$

$$= \sup \left\{ Dp(\mathbf{z}) : p \in \Pi_q^d, \; |p(\mathbf{x}_i)| \le \|\mathbf{x}_i - \mathbf{z}\|_2^q, \; \forall i \right\}$$

$$=: \rho_{q,D}(\mathbf{z}, \mathbf{X}, 1)$$

- A special case of Fenchel's duality theorem, but can also be proved directly by using extension of linear functionals.
- More general, for any seminorm $\|\cdot\|$ on $\mathbb{R}^N$,

$$\inf_{\mathbf{w} \perp_D \Pi_q^d} \|\mathbf{w}\| = \sup \left\{ Dp(\mathbf{z}) : p \in \Pi_q^d, \; \|p|_{\mathbf{X}}\|^* \le 1 \right\}$$

$$=: \rho_{q,D}(\mathbf{z}, \mathbf{X}, \|\cdot\|).$$

- We call $\rho_{q,D}(\mathbf{z}, \mathbf{X}, \|\cdot\|)$ the growth function.

Consistency Error: Growth Function

Theorem

For any $\|\cdot\|_{1,q}$-minimal formula,

$$|Df(\mathbf{z}) - \sum_{j=1}^{N} w_j f(x_j)| \leq \rho_{q,D}(\mathbf{z}, \mathbf{X}, 1)|f|_{\infty,q,\Omega}.$$

- As we will see, similar estimates involving $\rho_{q,D}(\mathbf{z}, \mathbf{X}, 1)$ hold for kernel methods as well.

Consistency Error: Growth Function

Default behavior of growth function

$$\rho_{q,D}(\mathbf{z},\mathbf{X},1) := \sup\left\{|Dp(\mathbf{z})| : p \in \Pi_q^d,\ |p(\mathbf{x}_i)| \le \|\mathbf{x}_i - \mathbf{z}\|_2^q,\ \forall i\right\},$$

$$h_{\mathbf{z},\mathbf{X}} := \max_{1\le j\le N} \|\mathbf{z} - \mathbf{x}_j\|_2$$

- If $\mathbf{X}$ is a "good" set for Π_q^d ("norming set"), then

$$\max_{\|\mathbf{x}-\mathbf{z}\|_2 \le h_{\mathbf{z},\mathbf{X}}/2} |p(\mathbf{x})| \le C \max_i |p(\mathbf{x}_i)| \le C h_{\mathbf{z},\mathbf{X}}^q,$$

  hence $|Dp(\mathbf{z})| \le C h_{\mathbf{z},\mathbf{X}}^{q-k}$ and $\rho_{q,D}(\mathbf{z},\mathbf{X},1) \le C h_{\mathbf{z},\mathbf{X}}^{q-k}$,
  so that we get an error bound of order $h_{\mathbf{z},\mathbf{X}}^{q-k}$:

$$|Df(\mathbf{z}) - \sum_{j=1}^{N} w_j f(x_j)| \le C h_{\mathbf{z},\mathbf{X}}^{q-k} |f|_{\infty,q,\Omega}.$$

- This means mFD method on such formulas has consistency order $q-k$

Consistency Error: Least Squares Formulas

Discrete Least Squares

Let $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ be unisolvent for Π_q^d $\quad (N \geq \dim \Pi_q^d)$.
The weighted least squares polynomial $L_{\mathbf{X},q}^{\boldsymbol{\theta}} f \in \Pi_q^d$ is uniquely defined by the condition

$$\|(L_{\mathbf{X},q}^{\boldsymbol{\theta}} f - f)|_{\mathbf{X}}\|_{2,\boldsymbol{\theta}} = \min\left\{\|(p - f)|_{\mathbf{X}}\|_{2,\boldsymbol{\theta}} : p \in \Pi_q^d\right\},$$

where

$$\|\mathbf{v}\|_{2,\boldsymbol{\theta}} := \Big(\sum_{j=1}^N \theta_j v_j^2\Big)^{1/2}, \quad \boldsymbol{\theta} = [\theta_1, \dots, \theta_N]^T, \quad \theta_j > 0.$$

- Exact for polynomials: $\quad L_{\mathbf{X},q}^{\boldsymbol{\theta}} p = p$ for all $p \in \Pi_q^d$
- Num. differentiation: $\quad Df(\mathbf{z}) \approx DL_{\mathbf{X},q}^{\boldsymbol{\theta}} f(\mathbf{z}) = \sum_{j=1}^N w_j^{2,\boldsymbol{\theta}} f(\mathbf{x}_j)$

Consistency Error: Least Squares Formulas

Dual formulation

The weight vector $\mathbf{w}^{2,\boldsymbol{\theta}}$ of $\quad Df(\mathbf{z}) \approx DL^{\boldsymbol{\theta}}_{\mathbf{X},q} f(\mathbf{z}) = \sum_{j=1}^{N} w_j^{2,\boldsymbol{\theta}} f(\mathbf{x}_j)$

solves the quadratic minimization problem

$$\|\mathbf{w}^{2,\boldsymbol{\theta}}\|^2_{2,\boldsymbol{\theta}^{-1}} = \inf_{\substack{\mathbf{w}\in\mathbb{R}^N \\ \mathbf{w}\perp_D \Pi^d_q}} \|\mathbf{w}\|^2_{2,\boldsymbol{\theta}^{-1}},$$

where $\boldsymbol{\theta}^{-1} := [\theta_1^{-1}, \dots, \theta_N^{-1}]^T, \quad \|\mathbf{w}\|_{2,\boldsymbol{\theta}^{-1}} = \Big(\sum_{j=1}^{N} \frac{w_j^2}{\theta_j} \Big)^{1/2}.$

- It follows that

$$\|\mathbf{w}^{2,\boldsymbol{\theta}}\|_{2,\boldsymbol{\theta}^{-1}} = \sup \Big\{ Dp(\mathbf{z}) : p \in \Pi^d_q,\ \|p|_{\mathbf{X}}\|_{2,\boldsymbol{\theta}} \le 1 \Big\}$$
$$= \rho_{q,D}(\mathbf{z}, \mathbf{X}, \|\cdot\|_{2,\boldsymbol{\theta}^{-1}}).$$

Consistency Error: Least Squares Formulas

Theorem

$$|Df(\mathbf{z}) - DL^{\theta}_{\mathbf{X},q}f(\mathbf{z})| \le$$
$$\le \rho_{q,D}(\mathbf{z},\mathbf{X},\|\cdot\|_{2,\theta^{-1}})\Big(\sum_{j=1}^{N}\theta_j\|\mathbf{x}_j-\mathbf{z}\|_2^{2q}\Big)^{1/2}|f|_{\infty,q,\Omega}.$$

In particular, for $\theta_j = \|\mathbf{x}_j - \mathbf{z}\|_2^{-2q}$,

$$|Df(\mathbf{z}) - DL^{q}{}_{\mathbf{X},q}f(\mathbf{z})| \le \sqrt{N}\,\rho_{q,D}(\mathbf{z},\mathbf{X},2)\,|f|_{\infty,q,\Omega},$$

where

$$\rho_{q,D}(\mathbf{z},\mathbf{X},2) = \sup\Big\{|Dp(\mathbf{z})| : p\in\Pi^d_q,\ \sum_{j=1}^{N}\frac{|p(\mathbf{x}_j)|^2}{\|\mathbf{x}_j-\mathbf{z}\|_2^{2q}} \le 1,\ \forall i\Big\}$$

- $\rho_{q,D}(\mathbf{z},\mathbf{X},2) = \|\mathbf{w}^{2,q}\|_{2,q} = \Big(\sum_{j=1}^N (w_j^{2,q})^2\|\mathbf{x}_j-\mathbf{z}\|_2^{2q}\Big)^{1/2}$ can be computed a posteriori and used in degree adaptation algorithms similar to [D. & Zeilfelder, 2004]

Consistency Error: Least Squares Formulas

Inequalities between $\rho_{q,D}(\mathbf{z}, \mathbf{X}, 1)$ and $\rho_{q,D}(\mathbf{z}, \mathbf{X}, 2)$:

$$\rho_{q,D}(\mathbf{z}, \mathbf{X}, 2) \leq \rho_{q,D}(\mathbf{z}, \mathbf{X}, 1) \leq \sqrt{N}\rho_{q,D}(\mathbf{z}, \mathbf{X}, 2).$$

- This implies for the least squares formulas with $\theta_j = \|\mathbf{x}_j - \mathbf{z}\|_2^{-2q}$ an error bound in terms of $\rho_{q,D}(\mathbf{z}, \mathbf{X}, 1)$:

$$|Df(\mathbf{z}) - DL^q_{\mathbf{X},q}f(\mathbf{z})| \leq \sqrt{N}\,\rho_{q,D}(\mathbf{z}, \mathbf{X}, 1)\,|f|_{\infty,q,\Omega},$$

  which is only by factor $\sqrt{N}$ worse than the error bound for the $\|\cdot\|_{1,q}$-minimal formula.
- We can estimate $\rho_{q,D}(\mathbf{z}, \mathbf{X}, 1)$ with the help of $\rho_{q,D}(\mathbf{z}, \mathbf{X}, 2)$, which is cheaper to compute by quadratic minimization or orthogonal decompositions instead of ℓ_1 minimization.

Consistency Error: Least Squares Formulas

Comparison to earlier work

For non-weighted least squares ($\theta_j = 1$) we get

$$|Df(\mathbf{z}) - DL_{\mathbf{X},q}f(\mathbf{z})| \le \sqrt{N}\,\rho_{q,D}(\mathbf{z},\mathbf{X},\|\cdot\|_2)h^q_{\mathbf{z},\mathbf{X}}\,|f|_{\infty,q,\Omega}$$
$$\le \sqrt{N}\,\rho_{q,D}(\mathbf{z},\mathbf{X},\|\cdot\|_1)h^q_{\mathbf{z},\mathbf{X}}\,|f|_{\infty,q,\Omega}.$$

Hence, for $D = I$

$$\|f - L_{\mathbf{X},q}f\|_{L_\infty(\Omega)} \le \sqrt{N}\,\rho_{q,I}(\Omega,\mathbf{X},\|\cdot\|_1)\,\mathrm{diam}^q(\Omega)\,|f|_{\infty,q,\Omega},$$

where $\rho_{q,I}(\Omega,\mathbf{X},\|\cdot\|_1) := \sup_{\mathbf{z}\in\Omega} \rho_{q,I}(\mathbf{z},\mathbf{X},\|\cdot\|_1)$
$= \sup\left\{\|p\|_{L_\infty(\Omega)} : p \in \Pi^d_q,\ |p(\mathbf{x}_i)| \le 1,\ \forall i\right\}$

is the norming constant of $\mathbf{X}$ w.r.t. Π^d_q on Ω. Compare [D., 2002]:

$$\|f - L_{\mathbf{X},q}f\|_{L_\infty(\Omega)} \le \left(1 + \sqrt{N}\,\rho_{q,I}(\Omega,\mathbf{X},\|\cdot\|_1)\right) E(f,\Pi^d_q)_{L_\infty(\Omega)}.$$

Consistency Error: Kernel-Based Formulas

Let $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ be a symmetric kernel, conditionally positive definite (cpd) of order $s \geq 0$ on $\mathbb{R}^d$ (positive definite when $s = 0$). Π_s^d: polynomials of order s.

For a Π_s^d-unisolvent $\mathbf{X}$, the kernel interpolant $r_{\mathbf{X},K,f}$ in the form

$$r_{\mathbf{X},K,f} = \sum_{j=1}^{N} a_j K(\cdot, \mathbf{x}_j) + \sum_{j=1}^{M} b_j p_j, \quad a_j, b_j \in \mathbb{R}, \quad M = \dim(\Pi_s^d),$$

is uniquely determined from the positive definite linear system

$$\begin{aligned} r_{\mathbf{X},K,f}(\mathbf{x}_k) = \sum_{j=1}^{N} a_j K(\mathbf{x}_k, \mathbf{x}_j) + \sum_{j=1}^{M} b_j p_j(\mathbf{x}_k) &= f_k, \quad 1 \leq k \leq N, \\ \sum_{j=1}^{N} a_j \, p_i(\mathbf{x}_j) &= 0, \quad 1 \leq i \leq M. \end{aligned}$$

Consistency Error: Kernel-Based Formulas

Examples. $K(\mathbf{x}, \mathbf{y}) = \phi(\|\mathbf{x} - \mathbf{y}\|)$
($\phi : \mathbb{R}_+ \to \mathbb{R}$ is then a radial basis function (RBF))

$s \geq 0$: Any ϕ with positive Fourier transform of $\Phi(\mathbf{x}) = \phi(\|\mathbf{x}\|)$

- Gaussian $\phi(r) = e^{-r^2}$
- inverse quadric $1/(1 + r^2)$
- inverse multiquadric $1/\sqrt{1 + r^2}$
- Matérn kernel $\mathcal{K}_\nu(r)r^\nu$, $\nu > 0$
  ($\mathcal{K}_\nu(r)$ modified Bessel function of second kind)

$s \geq 1$:
- multiquadric $\sqrt{1 + r^2}$

$s \geq \lfloor \nu/2 \rfloor + 1$:
- polyharmonic / thin plate spline $r^\nu \{\log r\}$

$K(\varepsilon\mathbf{x}, \varepsilon\mathbf{y})$ are also cpd kernels ($\varepsilon > 0$: shape parameter)

Consistency Error: Kernel-Based Formulas

A kernel-based numerical differentiation formula is obtained by applying D to the kernel interpolant (approximation approach):

$$Df(\mathbf{z}) \approx Dr_{\mathbf{X},K,f}(\mathbf{z}) = \sum_{j=1}^{N} w_j^* \, f(\mathbf{x}_j).$$

The weights w_j^* can be calculated by solving the system

$$\begin{aligned}
\sum_{j=1}^{N} w_j^* K(\mathbf{x}_k, \mathbf{x}_j) \quad + \quad \sum_{j=1}^{M} c_j p_j(\mathbf{x}_k) \quad &= \quad [DK(\cdot, \mathbf{x}_k)](\mathbf{z}), \quad 1 \le k \le N, \\
\sum_{j=1}^{N} w_j^* p_i(\mathbf{x}_j) \quad + \quad 0 \quad &= \quad Dp_i(\mathbf{z}), \quad 1 \le i \le M.
\end{aligned}$$

Consistency Error: Kernel-Based Formulas

Kernel-based weights $\mathbf{w}^* = \{w_j^*\}_{j=1}^N$ provide optimal recovery of $Df(\mathbf{z})$ from $f(\mathbf{x}_j)$, $j = 1, \dots, N$, for $f \in \mathcal{F}_K$,

$$\inf_{\substack{\mathbf{w}\in\mathbb{R}^N \\ \mathbf{w}\perp_D \Pi_s^d}} \sup_{\|f\|_{\mathcal{F}_K}\le 1} \Big| Df(\mathbf{z}) - \sum_{j=1}^N w_j f(\mathbf{x}_j) \Big| = \sup_{\|f\|_{\mathcal{F}_K}\le 1} \Big| Df(\mathbf{z}) - \sum_{j=1}^N w_j^* f(\mathbf{x}_j) \Big|,$$

$\mathcal{F}_K$ is the RKHS or native space of K,
$\mathbf{w} \perp_D \Pi_s^d$: exactness of numerical differentiation for Π_s^d.

- For example, the formula obtained with Matérn kernel

$$K(\mathbf{x}, \mathbf{y}) = \mathcal{K}_\nu(\|\mathbf{x} - \mathbf{y}\|)\|\mathbf{x} - \mathbf{y}\|^\nu, \quad \nu > 0 \quad (s = 0),$$

gives the best possible estimate of $Df(\mathbf{z})$ if we only know that f belongs to the Sobolev space

$$\mathcal{F}_K = H^{\nu+d/2}(\mathbb{R}^d)$$

Consistency Error: Kernel-Based Formulas

Theorem

For any $q \geq \max\{s, k+1\}$,

$$|Df(\mathbf{z}) - Dr_{\mathbf{X},K,f}(\mathbf{z})| \leq \rho_{q,D}(\mathbf{z}, \mathbf{X}, 1) C_{K,q} \|f\|_{\mathcal{F}_K}, \qquad f \in \mathcal{F}_K,$$

as soon as $\partial^{\alpha,\beta} K(\mathbf{x}, \mathbf{y}) \in C(\Omega \times \Omega)$ for $|\alpha|, |\beta| \leq q$, where

$\rho_{q,D}(\mathbf{z}, \mathbf{X}, 1)$ is the $\|\cdot\|_{1,q}$-growth function,

$$C_{K,q} := \frac{1}{q!} \Big(\sum_{|\alpha|,|\beta|=q} \binom{q}{\alpha} \binom{q}{\beta} \|\partial^{\alpha,\beta} K\|^2_{C(\Omega\times\Omega)} \Big)^{1/4} < \infty.$$

- To compare with the above error bound of $\|\cdot\|_{1,q}$-formulas:
  $$|Df(\mathbf{z}) - \sum_{j=1}^{N} w_j f(x_j)| \leq \rho_{q,D}(\mathbf{z}, \mathbf{X}, 1) |f|_{\infty,q,\Omega}.$$
- Robustness: Prior knowledge of the approximation order attainable on **X** is not needed since estimate holds for all q.

Outline

Conclusion

- Meshless finite difference method can be based on polynomial or kernel numerical differentiation
- Numerical experiments suggest it is competitive with FEM
- Consistency estimates are available in terms of a growth function
- Good sets of nodes for these methods would possess small growth functions on influence sets (e.g. “weakly admissible” etc. sets are good for spectral type mFDM with global sets of influence)