Consistency Estimates for gFD Methods and Selection of Sets of Influence

Oleg Davydov

University of Giessen, Germany

Localized Kernel-Based Meshless Methods for PDEs

ICERM / Brown University

7–11 August 2017

Outline

Generalized Finite Difference Methods

- Model problem: Poisson equation with Dirichlet boundary

$$\Delta u = f \ \text{ on } \Omega, \qquad u|_{\partial\Omega} = g.$$

- Localized numerical differentiation ($\Xi \subset \overline{\Omega}$, $\Xi_i \subset \Xi$ small):

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

- Find a discrete approximate solution $\hat{u}$ defined on Ξ s.t.

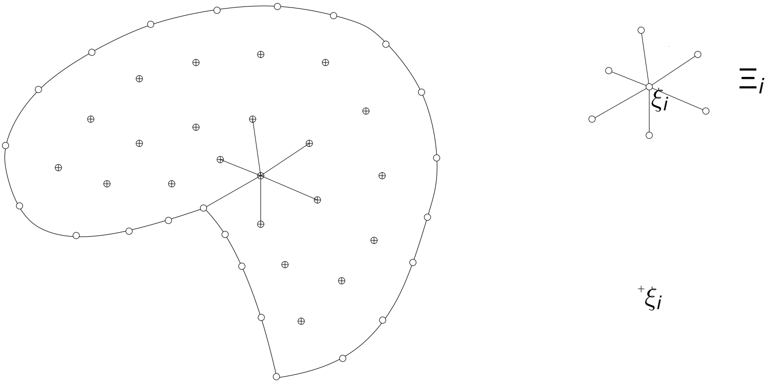
$$\sum_{\xi_j \in \Xi_i} w_{i,j} \hat{u}(\xi_j) = f(\xi_i) \ \text{ for } \xi_i \in \Xi \setminus \partial\Omega$$

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

Sparse system matrix $[w_{i,j}]_{\xi_i,\xi_j \in \Xi \setminus \partial\Omega}$.

Generalized Finite Difference Methods

Sets of influence: Select Ξ_i for each $\xi_i \in \Xi \setminus \partial\Xi$



Ξ_i is the 'star' or 'set of influence' of ξ_i

Generalized Finite Difference Methods

"Consistency and Stability $\Longrightarrow$ Convergence":

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

$S := \|[w_{i,j}]^{-1}_{\xi_i,\xi_j \in \Xi \setminus \partial\Omega}\|$ – stability constant

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

respectively a matrix norm, $\|\cdot\|_\infty$ or $\|\cdot\|_2$

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

Outline

1. Generalized Finite Difference Methods
2. Error of Polynomial and Kernel Numerical Differentiation
   - Numerical Differentiation
   - Polynomial Formulas
   - Kernel-Based Formulas
   - Least Squares Formulas
3. Selection of Sets of Influence
4. Conclusion

Numerical Differentiation

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 values $Df(\mathbf{z})$ at arbitrary points $\mathbf{z}$, where D is a linear differential operator

$$Df(\mathbf{z}) = \sum_{\alpha \in \mathbb{Z}_+^d,\, |\alpha| \le k} a_\alpha(\mathbf{z}) \partial^\alpha f(\mathbf{z})$$

k is the order of D, $\quad |\alpha| := \alpha_1 + \cdots + \alpha_d, \quad a_\alpha(\mathbf{z}) \in \mathbb{R}$.

Numerical Differentiation

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 $p = \phi\,\mathbf{a} = \phi A f|_{\mathbf{X}}$,

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

- This leads to a numerical differentiation formula

$$Df(\mathbf{z}) \approx \sum_{j=1}^{N} w_j\, f(\mathbf{x}_j), \quad \mathbf{w}\text{: a weight vector.}$$

Numerical Differentiation

Exactness approach

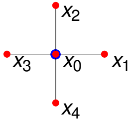
- Require exactness of the numerical differentiation formula for all elements of a space $\mathcal{P}$:

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

  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.)

- Example: five point star (exact for Π_4^2)



$$\Delta u(x_0) \approx \frac{1}{h^2}\big(u(x_1)+u(x_2)+u(x_3)+u(x_4) - 4u(x_0)\big)$$

Exactness approach

- A classical method for computing weights $\mathbf{w} \perp_D \Pi_q^d$ is truncation of Taylor expansion of local error $f - p$ near $\mathbf{z}$ (as in the Finite Difference Method).
- Instead, we can look at

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

  as an underdetermined linear system w.r.t. $\mathbf{w}$, and pick solutions with desired properties.
- Similar to quadrature rules (Gauss formulas), there are special point sets that admit weights with particularly high exactness order for a given N (five point star).

Numerical Differentiation

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, Minimal numerical differentiation formulas, preprint. `arXiv:1611.05001`
- O. Davydov and R. Schaback, Optimal stencils in Sobolev spaces, preprint. `arXiv:1611.04750`

Outline

Polynomial Formulas: General Error Bound

Theorem

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

Polynomial Formulas: General Error Bound

Theorem

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

Proof: Let $R(\mathbf{x}) := f(\mathbf{x}) - T_{q,\mathbf{z}} f(\mathbf{x})$ be the remainder of the Taylor polynomial or order q. Recall the integral representation

$$R(\mathbf{x}) = q \sum_{|\alpha|=q} \frac{(\mathbf{x}-\mathbf{z})^\alpha}{\alpha!} \int_0^1 (1-t)^{q-1} \partial^\alpha f(\mathbf{z} + t(\mathbf{x}-\mathbf{z}))\, dt.$$

Since $q > k$, it follows that $DR(\mathbf{z}) = 0$.

Polynomial Formulas: General Error Bound

Thus, we have for $\quad R(\mathbf{x}) := f(\mathbf{x}) - T_{q,\mathbf{z}}f(\mathbf{x})$: $DR(\mathbf{z}) = 0$,

$$R(\mathbf{x}) = q \sum_{|\alpha|=q} \frac{(\mathbf{x}-\mathbf{z})^\alpha}{\alpha!} \int_0^1 (1-t)^{q-1} \partial^\alpha f(\mathbf{z} + t(\mathbf{x}-\mathbf{z}))\, dt.$$

Hence

$$\begin{aligned}
|R(\mathbf{x}_j)| &\le \sum_{|\alpha|=q} \frac{|(\mathbf{x}_j-\mathbf{z})^\alpha|}{\alpha!} \|\partial^\alpha f\|_{C(\Omega)} \\
&\le \Big(\sum_{|\alpha|=q} \frac{(\mathbf{x}_j-\mathbf{z})^{2\alpha}}{\alpha!} \sum_{|\alpha|=q} \frac{\|\partial^\alpha f\|^2_{C(\Omega)}}{\alpha!} \Big)^{1/2} \\
&= \|\mathbf{x}_j - \mathbf{z}\|_2^q \underbrace{\Big(\frac{1}{q!} \sum_{|\alpha|=q} \frac{1}{\alpha!} \|\partial^\alpha f\|^2_{C(\Omega)} \Big)^{1/2}}_{=|f|_{\infty,q,\Omega}}
\end{aligned}$$

Polynomial Formulas: General Error Bound

With $\quad R(\mathbf{x}) := f(\mathbf{x}) - T_{q,\mathbf{z}} f(\mathbf{x}), \quad DR(\mathbf{z}) = 0 \quad$ and

$$|R(\mathbf{x}_j)| \le \|\mathbf{x}_j - \mathbf{z}\|_2^q \, |f|_{\infty,q,\Omega},$$

polynomial exactness implies

$$\begin{aligned} \Big|Df(\mathbf{z}) - \sum_{j=1}^N w_j\, f(\mathbf{x}_j)\Big| &= \Big|DR(\mathbf{z}) - \sum_{j=1}^N w_j\, R(\mathbf{x}_j)\Big| \\ &\le \sum_{j=1}^N |w_j R(\mathbf{x}_j)| \\ &= |f|_{\infty,q,\Omega} \sum_{j=1}^N |w_j| \|\mathbf{x}_j - \mathbf{z}\|_2^q. \quad \square \end{aligned}$$

Polynomial Formulas: General Error Bound

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

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

- Gives in particular an error bound in terms of Lebesgue (stability) constant $\|\mathbf{w}\|_1 := \sum_{j=1}^{N} |w_j|$:

$$Df(\mathbf{z}) - \sum_{j=1}^{N} w_j f(\mathbf{x}_j)| \leq |f|_{\infty,q,\Omega} \|\mathbf{w}\|_1 h_{\mathbf{z},\mathbf{X}}^q,$$

where

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

is the radius of the set of influence.

- Applicable in particular to polyharmonic formulas.

Polynomial Formulas: General Error Bound

If **w** is exact for polynomials of order $q > k$ (the order of D), then

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

- The best bound is obtained if $\displaystyle\sum_{j=1}^{N} |w_j| \|\mathbf{x}_j - \mathbf{z}\|_2^q$ is minimized over all weights **w** satisfying the exactness condition $Dp(\mathbf{z}) = \sum_{j=1}^{N} w_j\, p(\mathbf{x}_j)$, $\forall p \in \Pi_q^d$. $(\mathbf{w} \perp_D \Pi_q^d)$
  We call them $\|\cdot\|_{1,q}$-minimal weights.

Polynomial Formulas: $\|\cdot\|_{1,\mu}$-minimal weights

An $\|\cdot\|_{1,\mu}$-minimal ($\mu \geq 0$) weight vector $\mathbf{w}^*$ satisfies

$$\sum_{j=1}^{N} |w_j^*| \|\mathbf{x}_j - \mathbf{z}\|_2^{\mu} = \inf_{\substack{\mathbf{w} \in \mathbb{R}^N \\ \mathbf{w} \perp_D \Pi_q^d}} \sum_{j=1}^{N} |w_j| \|\mathbf{x}_j - \mathbf{z}\|_2^{\mu}.$$

Polynomial Formulas: $\|\cdot\|_{1,\mu}$-minimal weights

An $\|\cdot\|_{1,\mu}$-minimal ($\mu \geq 0$) weight vector $\mathbf{w}^*$ satisfies

$$\sum_{j=1}^{N} |w_j^*| \|\mathbf{x}_j - \mathbf{z}\|_2^{\mu} = \inf_{\substack{\mathbf{w} \in \mathbb{R}^N \\ \mathbf{w} \perp_D \Pi_q^d}} \sum_{j=1}^{N} |w_j| \|\mathbf{x}_j - \mathbf{z}\|_2^{\mu}.$$

- $\|\cdot\|_{1,\mu}$-minimal weights can be found by linear programming (e.g. simplex algorithm if N is small).

Polynomial Formulas: $\|\cdot\|_{1,\mu}$-minimal weights

An $\|\cdot\|_{1,\mu}$-minimal ($\mu \geq 0$) weight vector $\mathbf{w}^*$ satisfies

$$\sum_{j=1}^{N} |w_j^*| \|\mathbf{x}_j - \mathbf{z}\|_2^{\mu} = \inf_{\substack{\mathbf{w}\in\mathbb{R}^N \\ \mathbf{w}\perp_D \Pi_q^d}} \sum_{j=1}^{N} |w_j| \|\mathbf{x}_j - \mathbf{z}\|_2^{\mu}.$$

- $\|\cdot\|_{1,\mu}$-minimal weights can be found by linear programming (e.g. simplex algorithm if N is small).
- $\mu = 0$: formulas with optimal stability constant $\sum_{j=1}^{N} |w_j^*|$

Polynomial Formulas: $\|\cdot\|_{1,\mu}$-minimal weights

An $\|\cdot\|_{1,\mu}$-minimal ($\mu \geq 0$) weight vector $\mathbf{w}^*$ satisfies

$$\sum_{j=1}^{N} |w_j^*| \|\mathbf{x}_j - \mathbf{z}\|_2^{\mu} = \inf_{\substack{\mathbf{w}\in\mathbb{R}^N \\ \mathbf{w}\perp_D \Pi_q^d}} \sum_{j=1}^{N} |w_j| \|\mathbf{x}_j - \mathbf{z}\|_2^{\mu}.$$

- $\|\cdot\|_{1,\mu}$-minimal weights can be found by linear programming (e.g. simplex algorithm if N is small).
- $\mu = 0$: formulas with optimal stability constant $\sum_{j=1}^{N} |w_j^*|$
- Our error bound suggests the choice $\mu = q$.

Polynomial Formulas: $\|\cdot\|_{1,\mu}$-minimal weights

An $\|\cdot\|_{1,\mu}$-minimal ($\mu \geq 0$) weight vector $\mathbf{w}^*$ satisfies

$$\sum_{j=1}^{N} |w_j^*| \|\mathbf{x}_j - \mathbf{z}\|_2^{\mu} = \inf_{\substack{\mathbf{w}\in\mathbb{R}^N \\ \mathbf{w}\perp_D \Pi_q^d}} \sum_{j=1}^{N} |w_j| \|\mathbf{x}_j - \mathbf{z}\|_2^{\mu}.$$

- $\|\cdot\|_{1,\mu}$-minimal weights can be found by linear programming (e.g. simplex algorithm if N is small).
- $\mu = 0$: formulas with optimal stability constant $\sum_{j=1}^{N} |w_j^*|$
- Our error bound suggests the choice $\mu = q$.
- $\mathbf{w}^*$ is sparse in the sense that the number of nonzero w_j's does not exceed $\dim \Pi_q^d$.

Polynomial Formulas: $\|\cdot\|_{1,\mu}$-minimal weights

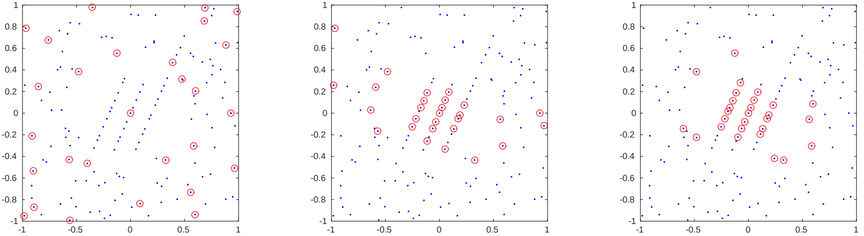
An $\|\cdot\|_{1,\mu}$-minimal ($\mu \geq 0$) weight vector $\mathbf{w}^*$ satisfies

$$\sum_{j=1}^{N} |w_j^*| \|\mathbf{x}_j - \mathbf{z}\|_2^{\mu} = \inf_{\substack{\mathbf{w} \in \mathbb{R}^N \\ \mathbf{w} \perp_D \Pi_q^d}} \sum_{j=1}^{N} |w_j| \|\mathbf{x}_j - \mathbf{z}\|_2^{\mu}.$$

- $\|\cdot\|_{1,\mu}$-minimal weights can be found by linear programming (e.g. simplex algorithm if N is small).
- $\mu = 0$: formulas with optimal stability constant $\sum_{j=1}^{N} |w_j^*|$
- Our error bound suggests the choice $\mu = q$.
- $\mathbf{w}^*$ 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 $q \leq 4$.

Polynomial Formulas: $\|\cdot\|_{1,\mu}$-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.

Polynomial Formulas: $\|\cdot\|_{1,\mu}$-minimal weights

Scalability

- $\|\cdot\|_{1,\mu}$-minimal formulas are scalable in the sence that the weight vector $\mathbf{w}$ can be computed by scaling $\mathbf{z}, \mathbf{X}$ into $\mathbf{0}, \mathbf{Y}$ in the unit circle by $\mathbf{y}_j = h_{\mathbf{z},\mathbf{X}}^{-1}(x_j - \mathbf{z})$, obtaining weight vector $\mathbf{v}$ for the mapped differential operator, and scaling back by $w_j = h_{\mathbf{z},\mathbf{X}}^{-k} v_j$.
- This allows for stable computation of this formulas for any small radius $h_{\mathbf{z},\mathbf{X}}$ by upscaling preconditioning.
- Any scalable differentiation formulas admit error bounds of the type $Ch_{\mathbf{z},\mathbf{X}}^{s-k}$ for sufficiently smooth functions f, where C depends on the Lebesque constant of the upscaled formula $\mathbf{v}$.

Polynomial Formulas: Growth Function

Duality:

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

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

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

- A special case of Fenchel's duality theorem, but can be also proved directly by using extension of linear functionals.
- We call $\rho_{q,D}(\mathbf{z}, \mathbf{X})$ the growth function.
- More general, for any seminorm $\|\cdot\|$ on $\mathbb{R}^N$,

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

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

Polynomial Formulas: Growth Function

Theorem

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

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

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

Polynomial Formulas: Growth Function

Default behavior of growth function

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

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

- 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 $\boxed{\rho_{q,D}(\mathbf{z},\mathbf{X}) \le C h_{\mathbf{z},\mathbf{X}}^{q-k},}$

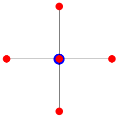
so that we get an error bound of order $h_{\mathbf{z},\mathbf{X}}^{q-k}$:

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

- $\mathbf{X}$ does not have to a norming set. Example: five point star.

Polynomial Formulas: Growth Function

Example: Five point stencil for Laplace operator Δ in 2D



$$\Delta u(\mathbf{z}) \approx \textstyle\sum_{i=1}^5 w_i u(\mathbf{x}_i),$$
$$\{\mathbf{x}_1, \dots, \mathbf{x}_5\} = \mathbf{X}^h = \{\mathbf{z}, \mathbf{z} \pm (h,0), \mathbf{z} \pm (0,h)\} \subset \Omega^h$$

- The classical FD formula with weights $w_2 = w_3 = w_4 = w_5 = 1/h^2$, $w_1 = -4/h^2$ is exact for Π_4^2.
- It is the only formula on $\mathbf{X}^h$ with this exactness order, hence it is $\|\cdot\|_{1,4}$-minimal.
- It is easy to show that $\rho_{4,\Delta}(\mathbf{z}, \mathbf{X}) = 4h^2$
- Hence,

$$|\Delta f(\mathbf{z}) - \sum_{i=1}^5 w_i u(\mathbf{x}_i)| \le 4h^2 \|f\|_{\infty,4,\Omega^h},$$

similar to classical error estimates for the five point stencil.

Polynomial Formulas: Growth Function

A lower bound for well separated centers

Theorem

Given $\mathbf{z}$ and $\mathbf{X}$, let $\gamma \geq 1$ be such that

$$\|\mathbf{x}_j - \mathbf{z}\|_2 \leq \gamma \operatorname{dist}(\mathbf{x}_j, \mathbf{X} \setminus \{\mathbf{x}_j\}), \quad j = 1, \ldots, N.$$

For any $\mathbf{w}$ and $q > k$ there exists a function $f \in C^\infty(\mathbb{R}^d)$ s. t.

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

where C depends only on q, k, N, d and γ.

In particular, if $\mathbf{w}$ is exact for polynomials of order q, then

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

Outline

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

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

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)

Kernel-Based Formulas

Optimal Recovery

- $r_{\mathbf{X},K,f}$ depends linearly on the data $f_j = f(\mathbf{x}_j)$,

$$r_{\mathbf{X},K,f}(\mathbf{z}) = \sum_{j=1}^{N} w_j^* f(\mathbf{x}_j), \qquad w_j^* \in \mathbb{R}, \quad j = 1, \ldots, N.$$

($w_j^* = w_j^*(\mathbf{z})$ depends on the evaluation point $\mathbf{z} \in \mathbb{R}^d$)

- The weights $\mathbf{w}^* = \{w_j^*\}_{j=1}^N$ provide optimal recovery of $f(\mathbf{z})$ for f in the native space $\mathcal{F}_K$ associated with K, i.e.,

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

$\mathbf{w} \perp \Pi_s^d$: exactness for polynomials in Π_s^d (empty if $s = 0$).

Kernel-Based Formulas

"Native Space" $\mathcal{F}_K$

- If K is positive definite, then $\mathcal{F}_K$ is just the reproducing kernel Hilbert space associated with K; in the c.p.d. case a generalization of it (a semi-Hilbert space).
- In the translation-invariant case $K(\mathbf{x},\mathbf{y}) = \Phi(\mathbf{x}-\mathbf{y})$ on $\mathbb{R}^d$,

$$\mathcal{F}_K = \{f \in L_2(\mathbb{R}^d) \ : \ \|f\|_{\mathcal{F}_K} := \left\| \hat{f}/\sqrt{\widehat{\Phi}} \right\|_{L_2(\mathbb{R}^d)} < \infty\}.$$

- Matérn kernel $K(\mathbf{x},\mathbf{y}) = \mathcal{K}_\nu(\|\mathbf{x}-\mathbf{y}\|)\|\mathbf{x}-\mathbf{y}\|^\nu$:

$$\widehat{\Phi}(\omega) = c_{\nu,d}(1+\|\omega\|^2)^{-\nu-d/2} \Longrightarrow \|f\|_{\mathcal{F}_K} = c_{\nu,d}\|f\|_{H^{\nu+d/2}(\mathbb{R}^d)}$$

(Sobolev space)

- Polyharmonics: $\|f\|_{\mathcal{F}_K}$ equlivalent to Sobolev seminorm
- C^∞ kernels: spaces of infinitely differentiable functions

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

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

Kernel-Based Formulas: Optimal recovery

- Kernel-based weights $\mathbf{w}^* = \{w_j^*\}_{j=1}^N$ provide optimal recovery of $Df(\mathbf{z})$ from $f(\mathbf{x}_j)$, $j = 1, \ldots, N$, 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 native space of K

$\mathbf{w} \perp_D \Pi_s^d$: exactness of numerical differentiation for polynomials in Π_s^d,

Kernel-Based Formulas: Optimal recovery

- 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 native space of K
$\mathbf{w} \perp_D \Pi_s^d$: exactness of numerical differentiation for polynomials in 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

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

Kernel-Based Formulas: Optimal recovery

- Optimal recovery error

$$P_{\mathbf{X}}(\mathbf{z}) := \sup_{\|f\|_{\mathcal{F}_K} \leq 1} \left| Df(\mathbf{z}) - \sum_{j=1}^{N} w_j^* f(\mathbf{x}_j) \right|$$

is called power function and can be evaluated as

$$P_{\mathbf{X}}(\mathbf{z}) = \sqrt{\epsilon_{\mathbf{w}^*}^{\mathbf{x}} \epsilon_{\mathbf{w}^*}^{\mathbf{y}} K(\mathbf{x}, \mathbf{y})}, \quad \epsilon_{\mathbf{w}} f := Df(\mathbf{z}) - \sum_{j=1}^{N} w_j f(\mathbf{x}_j)$$

$\Rightarrow$ can be used to optimize the choice of the local set **X**.

Kernel-Based Formulas: Error Bounds

Theorem

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

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

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

$$\rho_{q,D}(\mathbf{z}, \mathbf{X}) \quad \text{is the growth function,}$$

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

Kernel-Based Formulas: Error Bounds

Theorem

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

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

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

$$\rho_{q,D}(\mathbf{z}, \mathbf{X}) \quad \text{is the growth function,}$$

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

- To compare with the optimal error bound of polynomial approximation: $|Df(\mathbf{z}) - \sum_{j=1}^{N} w_j f(x_j)| \leq \rho_{q,D}(\mathbf{z}, \mathbf{X}) |f|_{\infty,q,\Omega}$.

Kernel-Based Formulas: Error Bounds

Theorem

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

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

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

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

Kernel-Based Formulas: Error Bounds

Theorem

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

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

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

$$\rho_{q,D}(\mathbf{z},\mathbf{X}) \quad \text{is the growth function,}$$

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

- Growth function $\rho_{q,D}(\mathbf{z},\mathbf{X})$ can be evaluated on repeated patterns, to get estimates without unknown constants.
- E.g., $\rho_{4,\Delta}(\mathbf{z},\mathbf{X}) = 4h^2$ for the five point star, leading to the estimate $|\Delta f(\mathbf{z}) - \Delta r_{\mathbf{X}^h,K,f}(\mathbf{z})| \leq 4h^2 C_{K,4} \|f\|_{\mathcal{F}_K}$ if the kernel K is sufficiently smooth.

Polyharmonic formulas with $\phi(r) = r^\nu \{\log r\}$ and $s \geq \lfloor \nu/2 \rfloor + 1$

- If $m := (\nu + d)/2$ is integer and $s \geq m$, they provide optimal recovery in Beppo-Levi space $BL_m(\mathbb{R}^d)$, the semi-Hilbert space generated by m-th order Sobolev seminorm, among all formulas with polynomial exactness order s, and admit error bounds of the type $C_1 h_{\mathbf{z},\mathbf{X}}^{\nu/2-k}$ for $f \in BL_m(\mathbb{R}^d)$.

Kernel-Based Formulas: Polyharmonic Formulas

Polyharmonic formulas with $\phi(r) = r^\nu\{\log r\}$ and $s \geq \lfloor \nu/2 \rfloor + 1$

- If $m := (\nu + d)/2$ is integer and $s \geq m$, they provide optimal recovery in Beppo-Levi space $BL_m(\mathbb{R}^d)$, the semi-Hilbert space generated by m-th order Sobolev seminorm, among all formulas with polynomial exactness order s, and admit error bounds of the type $C_1 h_{\mathbf{z},\mathbf{X}}^{\nu/2-k}$ for $f \in BL_m(\mathbb{R}^d)$.
- They are scalable and can therefore be stably computed by upscaling preconditioning for any small radius $h_{\mathbf{z},\mathbf{X}}$. The constant C_1 depends on the power function of the 'upscaled' formula $\mathbf{v}$.

Kernel-Based Formulas: Polyharmonic Formulas

Polyharmonic formulas with $\phi(r) = r^\nu\{\log r\}$ and $s \geq \lfloor \nu/2 \rfloor + 1$

- If $m := (\nu + d)/2$ is integer and $s \geq m$, they provide optimal recovery in Beppo-Levi space $BL_m(\mathbb{R}^d)$, the semi-Hilbert space generated by m-th order Sobolev seminorm, among all formulas with polynomial exactness order s, and admit error bounds of the type $C_1 h_{\mathbf{z},\mathbf{X}}^{\nu/2-k}$ for $f \in BL_m(\mathbb{R}^d)$.
- They are scalable and can therefore be stably computed by upscaling preconditioning for any small radius $h_{\mathbf{z},\mathbf{X}}$. The constant C_1 depends on the power function of the 'upscaled' formula **v**.
- As any scalable differentiation formulas of exactness order s, they also admit error bounds of the type $C_2 h_{\mathbf{z},\mathbf{X}}^{s-k}$ for sufficiently smooth f, where C_2 depends on on the Lebesgue constant of **v**.

Kernel-Based Formulas: Polyharmonic Formulas

Polyharmonic formulas with $\phi(r) = r^\nu\{\log r\}$ and $s \geq \lfloor \nu/2 \rfloor + 1$

- If $m := (\nu + d)/2$ is integer and $s \geq m$, they provide optimal recovery in Beppo-Levi space $BL_m(\mathbb{R}^d)$, the semi-Hilbert space generated by m-th order Sobolev seminorm, among all formulas with polynomial exactness order s, and admit error bounds of the type $C_1 h_{\mathbf{z},\mathbf{X}}^{\nu/2-k}$ for $f \in BL_m(\mathbb{R}^d)$.
- They are scalable and can therefore be stably computed by upscaling preconditioning for any small radius $h_{\mathbf{z},\mathbf{X}}$. The constant C_1 depends on the power function of the 'upscaled' formula **v**.
- As any scalable differentiation formulas of exactness order s, they also admit error bounds of the type $C_2 h_{\mathbf{z},\mathbf{X}}^{s-k}$ for sufficiently smooth f, where C_2 depends on on the Lebesgue constant of **v**.
- Robust kernel-based estimates are however not applicable.

Outline

Least Squares Formulas

Discrete Least Squares

Let $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ be unisolvent for $\Pi_q^d \quad (N \geq \dim \Pi_q^d)$.
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: $L_{\mathbf{X},q}^{\boldsymbol{\theta}} p = p$ for all $p \in \Pi_q^d$
- Num. differentiation: $Df(\mathbf{z}) \approx DL_{\mathbf{X},q}^{\boldsymbol{\theta}} f(\mathbf{z}) = \sum_{j=1}^N w_j^{2,\boldsymbol{\theta}} f(\mathbf{x}_j)$
- The weights $w_j^{2,\boldsymbol{\theta}}$ are scalable.

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

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

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

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

with a generalized growth function.

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

$$\rho_{q,D}(\mathbf{z},\mathbf{X},2) = \|\mathbf{w}^{2,q}\|_{2,q} := \Big(\sum_{j=1}^{N}(w_j^{2,q})^2\|\mathbf{x}_j - \mathbf{z}\|_2^{2q}\Big)^{1/2}$$

Least Squares Formulas

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

We have

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

Least Squares Formulas

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

We have

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

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

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

  which is only by factor $\sqrt{N}$ worse than the error bound for the $\|\cdot\|_{1,q}$-minimal formula.

Least Squares Formulas

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

We have

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

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

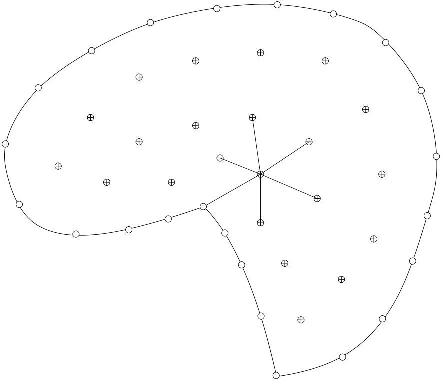
$$|Df(\mathbf{z}) - DL^q_{\mathbf{X},q}f(\mathbf{z})| \le \sqrt{N}\,\rho_{q,D}(\mathbf{z},\mathbf{X})\,|f|_{\infty,q,\Omega},$$

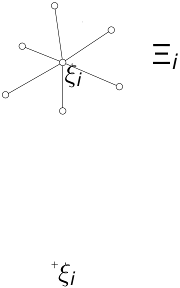
  which is only by factor $\sqrt{N}$ worse than the error bound for the $\|\cdot\|_{1,q}$-minimal formula.
- We can estimate $\rho_{q,D}(\mathbf{z},\mathbf{X})$ with the help of $\rho_{q,D}(\mathbf{z},\mathbf{X},2)$, which is cheaper to compute by quadratic minimization or orthogonal decompositions instead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

Outline

Selection of Sets of Influence

Sets of influence: Select Ξ_i for each $\xi_i \in \Xi \setminus \partial\Xi$

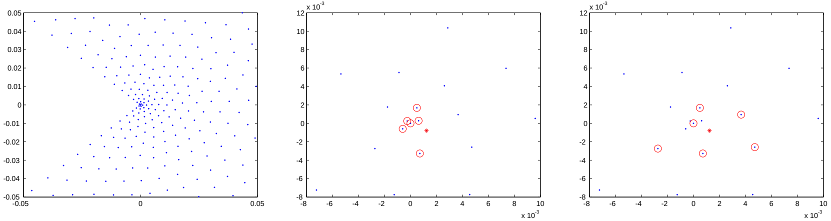




Ξ_i is the 'star' or 'set of influence' of ξ_i

Selection of Sets of Influence

- Selection is non-trivial on non-uniform points, especially near domain's boundary

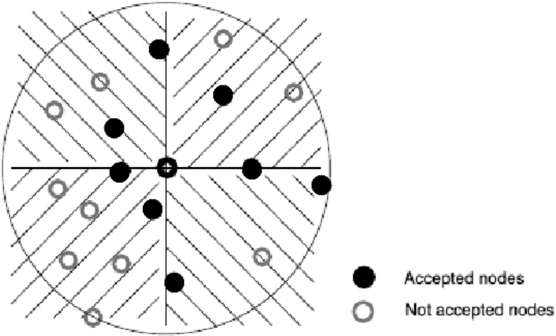


(a) adaptive points (b) 6 nearest points (c) better selection

Points in (a) are obtained by DistMesh (Persson & Strang, 2004) using a theoretically justified (Wahlbin, 1991) density function.

Geometric selection for Laplacian

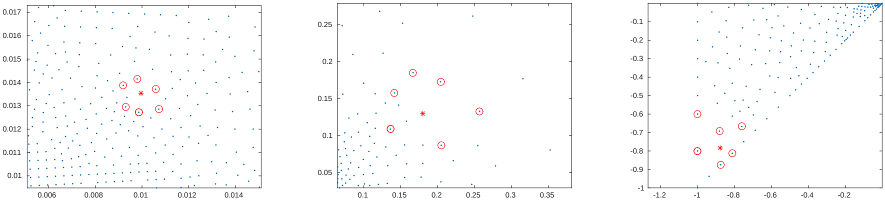
- Choose points in a rather uniform way around ξ_i.
- Four quadrant criterium (Liszka & Orkisz, 1980)



(Image from Lyszka, Duarte & Tworzydlo, 1996)

Selection of Sets of Influence: Geometric Selection

- Choose $n = 6$ points around ξ_i as close as possible to the vertices of an equilateral hexagon (D. & Dang, 2011; Dang, D. & Hoang, 2017): discrete optimization



- successful for low order methods ($\mathcal{O}(h^2)$ for Poisson eq.) ($n = 6$ gives a fair comparison to linear FEM where the rows of the system matrix have 7 nonzeros on average)
- too complicated to extend to higher order gFD methods

Selection of Sets of Influence

Selection via polynomial formulas

- For a given approximation order smaller sets of influence are preferred since they lead to sparser system matrices

Selection of Sets of Influence

Selection via polynomial formulas

- For a given approximation order smaller sets of influence are preferred since they lead to sparser system matrices
- This makes a case for $\|\cdot\|_{1,\mu}$-minimal formulas

Selection via polynomial formulas

- For a given approximation order smaller sets of influence are preferred since they lead to sparser system matrices
- This makes a case for $\|\cdot\|_{1,\mu}$-minimal formulas
- It is possible to employ $\|\cdot\|_{1,\mu}$-minimal formulas just as a method to select sets of influence, and compute the more robust kernel-based weights on these sets
(Bayona, Moscoso & Kindelan, 2011: for Seibold's positive minimal formulas)

Selection of Sets of Influence

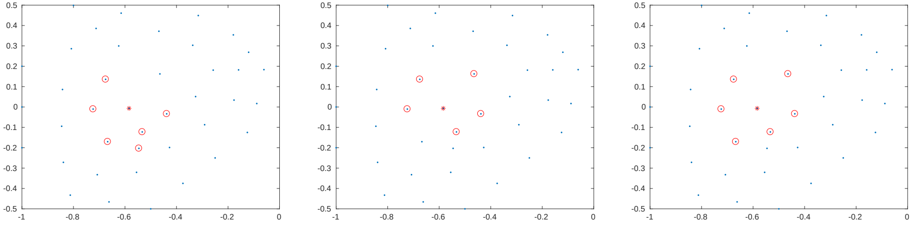
Selection via polynomial formulas

- For a given approximation order smaller sets of influence are preferred since they lead to sparser system matrices
- This makes a case for $\|\cdot\|_{1,\mu}$-minimal formulas
- It is possible to employ $\|\cdot\|_{1,\mu}$-minimal formulas just as a method to select sets of influence, and compute the more robust kernel-based weights on these sets
(Bayona, Moscoso & Kindelan, 2011: for Seibold's positive minimal formulas)
- New idea: least squares thresholding

Selection of Sets of Influence: LS Thresholding

Least squares thresholding: Compute a least squares numerical differentiation formula, and pick the positions of n largest weights.

- Example: compare (a) 6 nearest points, (b) 6 positions of nonzero $\|\cdot\|_{1,3}$-minimal weights of exactness order 3, (c) positions of $n = 6$ largest weights of a least squares formula of exactness order 3.

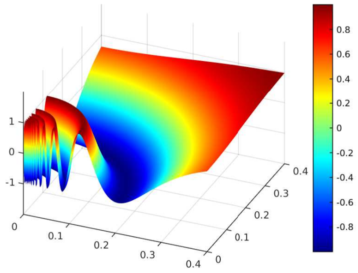


(a) 6 nearest points   (b) $\|\cdot\|_{1,3}$-minimal   (c) LS thresholding

Test Problem

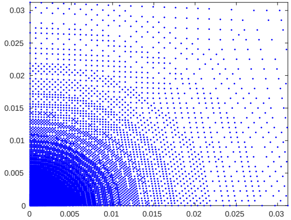
Dirichlet problem for the Helmholz equation $-\Delta u - \frac{1}{(\alpha+r)^4} u = f$, $r = \sqrt{x^2 + y^2}$ in the domain $\Omega = (0,1)^2$. RHS and the boundary conditions chosen such that the exact solution is $\sin(\frac{1}{\alpha+r})$, where $\alpha = \frac{1}{50\pi}$.

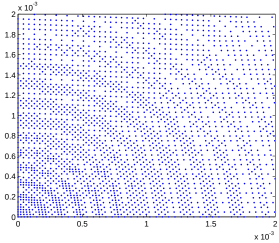
Exact solution:



Selection of Sets of Influence: LS Thresholding

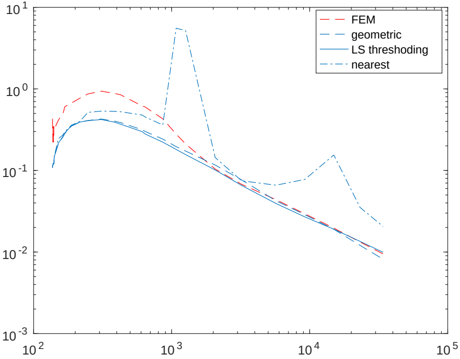
Adaptive nodes from a FEM triangulation by PDE Toolbox





Selection of Sets of Influence: LS Thresholding

RMS Errors of FEM and RBF-FD solutions with Gauss-QR and different selection methods for 6 neighbors



X-axis: number of interior nodes
Y-axis: RMS error

Outline

Conclusion

- Polynomial and kernel-based numerical differentiation share similar error bounds that split into factors responsible for the smoothness of the data (e.g. Sobolev norm) and for the geometry of the nodes (Lebesque constant, growth function).
- Growth function can be efficiently estimated by least squares methods. It may be useful for node generation and selection of sets of influence with prescribed consistency orders of generalized finite difference methods.
- Sparse sets of influence can be found with the help of $\|\cdot\|_{1,\mu}$-minimal polynomial formulas, and more efficiently by least squares thresholding.