Kernel Based Finite Difference Methods

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Building bridges: connections and challenges in modern approaches to numerical partial differential equations

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Outline

1. Kernel Methods
2. Adaptive Centres for Elliptic Equations
3. Conclusion

Outline

1. Kernel Methods
   - Kernel-based interpolation
   - Numerical differentiation
   - Kernel-based methods for PDEs
   - Generalized finite differences

2. Adaptive Centres for Elliptic Equations
   - Pointwise discretisation of Poisson equation
   - Numerical differentiation stencils on irregular centres
   - Stencil support selection
   - Adaptive meshless refinement of centres

3. Conclusion

Kernel-based interpolation

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

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

Kernel-based interpolation

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 $1/\sqrt{1 + r^2}$
- $(1 - r)_+^8(32r^3 + 25r^2 + 8r + 1)$ (for $d \leq 3$) (C^6 compactly supported Wendland function)
- Matérn kernel $\mathcal{K}_\nu(r)r^\nu$, $\nu > 0$
  ($\mathcal{K}_\nu(r)$ modified Bessel function of second kind)

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$s \ge 2$:
- thin plate spline $r^2 \log r$

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

Optimal Recovery

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

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

($w_j^* = w_j^*(\mathbf{z})$ 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 reproducing kernel Hilbert 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, e.g. $s = 0$ or 1.

Kernel-based interpolation

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

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

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

- Wendland kernels: $\|f\|_{\mathcal{F}_K}$ equlivalent to a Sobolev norm
- Thin plate spline: $\|f\|_{\mathcal{F}_K}$ equlivalent to a Sobolev seminorm
- C^∞ kernels: spaces of infinitely differentiable functions

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Further Info

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- Standard tool for spatial data fitting in Geosciences (kriging interpolation)
- Error bounds known under various assumptions on f. For example, order h^k if f is in the Sobolev space $W_p^k(\Omega)$, where h is the fill distance of the centres in Ω,

$$h = \max_{\mathbf{x}\in\Omega} \min_{1\leq i\leq N} \|\mathbf{x} - \mathbf{x}_i\|_2.$$

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- Spectral error bounds if both K and f are analytic functions
- However: Dense linear systems to find coefficients.
- Extensive literature, recent books: Buhmann; Wendland; Fasshauer.

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Numerical differentiation

Let D be a linear differential operator of order k. Given $\mathbf{z} \in \mathbb{R}^d$, a numerical differentiation formula

$$Df(\mathbf{z}) \approx \sum_{j=1}^{N} w_j f(\mathbf{x}_j)$$

is defined by the set of centres $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{R}^d$ and the weight vector $\mathbf{w} \in \mathbb{R}^N$.

- Formulas on grids are used in the finite difference method.
- Irregular $\mathbf{X} \implies$ generalized finite difference methods.

Numerical differentiation

Definition

A numerical differentiation formula for an operator D of order k is said to be polynomially consistent of order $m \geq 1$ if it is exact for any polynomial p of (total) order $m+k$:

$$Dp(\mathbf{z}) = \sum_{j=1}^{N} w_j\, p(\mathbf{x}_j) \text{ for all } p \in \Pi^d_{m+k}.$$

- A classical way to work out polynomially consistent formulas on grids is via truncation of Taylor expansion.
- On an irregular set $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ such formulas may be obtained by applying D to the least squares polynomial fit, or by numerically solving the consistency equations.

Numerical differentiation

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

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

- Polynomial consistency order is just s.
- The weights w_j^* can be calculated by solving the system

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

Numerical differentiation

- The 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 $f \in \mathcal{F}_K$,

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

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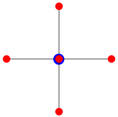
- In particular, the optimal formula does not need to be exact for any polynomials.
- Whenever centres $\mathbf{x}_1, \dots, \mathbf{x}_N$ admit a good formula $Df(\mathbf{z}) \approx \sum_{j=1}^N w_j f(x_j)$, the kernel-based formula will also perfom well.

Numerical differentiation

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



- $\Delta u(\zeta) \approx \sum_{i=1}^{5} w_i u(\xi_i)$
- $\Xi = \{\zeta, \zeta \pm (h,0), \zeta \pm (0,h)\} = \{\xi_1, \dots, \xi_5\}$

- By symmetry, $w_2 = w_3 = w_4 = w_5 =: w$
- For RBF interpolant with a constant term, $w_1 + 4w = 0$
- By substituting $w = -w_1/4$, arrive at

$$w_1 \Big(2\phi(h) - \frac{5}{4}\phi(0) - \frac{\phi(2h) + 2\phi(\sqrt{2}h)}{4} \Big) = \Delta\Phi(h) - \Delta\Phi(0)$$

- For scaled Gaussian $\phi(r) = e^{-(\varepsilon r)^2}$, $w_1 = -\frac{4}{h^2} + \mathcal{O}(\varepsilon^2 h^2)$ (same consistency order as the classical five point stencil)

Error bound for kernel-based formulas
(K is cpd of order s, D of order k)

Theorem [D. & Schaback, preprint]

Let $q \geq \max\{s, k+1\}$. Assume that

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

where $\Omega \supset \{\mathbf{z}\} \cup \mathbf{X}$ is star-shaped w.r.t. $\mathbf{z}$. Then

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

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$$\rho_{q,D}(\mathbf{z}, \mathbf{X}) := \sup\left\{Dp(\mathbf{z}) : p \in \Pi_q^d,\ |p(\mathbf{x}_i)| \leq \|\mathbf{x}_i - \mathbf{z}\|_2^q,\ i = 1, \ldots, N\right\}$$ is a polynomial growth function,

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$$\rho_{q,D}(\mathbf{z},\mathbf{X}) := \sup\Big\{ Dp(\mathbf{z}) : p \in \Pi_q^d,\ |p(\mathbf{x}_i)| \leq \|\mathbf{x}_i - \mathbf{z}\|_2^q, \; i = 1,\dots,N \Big\}$$ is a polynomial growth function,

$$M_{K,q} := \frac{1}{q!}\Big(\sum_{|\alpha|,|\beta|=q} \binom{q}{\alpha}\binom{q}{\beta} \max_{\mathbf{x},\mathbf{y}\in\Omega} |\partial^{\alpha,\beta} K(\mathbf{x},\mathbf{y})|^2 \Big)^{1/4}$$

Numerical differentiation

Discussion

$$|Df(\mathbf{z}) - Dr_{\mathbf{X},K,f}(\mathbf{z})| \le \min_{q \ge k+1} \left\{ \rho_{q,D}(\mathbf{z}, \mathbf{X}) M_{K,q} \right\} \|f\|_{\mathcal{F}_K},$$

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- Example. 5 point stencil: $\mathbf{X}^h = \mathbf{z} + \{(0,0), (0, \pm h), (\pm h, 0)\}$. Then $q \ge 3$, $\rho_{3,\Delta}(\mathbf{z}, \mathbf{X}) = 4h$, $\rho_{4,\Delta}(\mathbf{z}, \mathbf{X}) = 4h^2$, $\rho_{5,\Delta}(\mathbf{z}, \mathbf{X}) = \infty$. Hence consistency order 2:

$$|\Delta f(\mathbf{z}) - \Delta r_{\mathbf{X}^h,K,f}(\mathbf{z})| \le 4h^2 M_{K,4} \|f\|_{\mathcal{F}_K}$$

as soon as $\partial^{\alpha,\beta} K(\mathbf{x}, \mathbf{y}) \in C(\Omega \times \Omega), \ |\alpha|, |\beta| \le 4$. Also:

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  as soon as $\partial^{\alpha,\beta} K(\mathbf{x},\mathbf{y}) \in C(\Omega \times \Omega),\ |\alpha|,|\beta| \le 4$. Also:

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- If K is C^∞ and $\mathbf{X}$ big enough $\Longrightarrow$ spectral estimates

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Kernel-based methods for PDEs

- RBF numerical differentiation in explicit methods for time dependent problems (e.g. Iske & Sonar, 1996; Fuselier & Wright, 2013)
- Collocation of $\sum_{i=1}^{n} a_i K(\cdot, \mathbf{x}_i)$ (Kansa, 1990). "Symmetric" collocation (Fasshauer, 1997; Franke & Schaback, 1998; Schaback, 2014): spectral convergence, optimal recovery. However: dense system matrices
- Weak form methods: Compactly supported kernels $K(\cdot, \mathbf{x}_i)$ as shape functions (Wendland, 1999). Problems: high bandwidth of system matrices; the need for the integration of non-polynomial functions on unusual domains; difficulties to impose essential boundary conditions.

Kernel-based methods for PDEs

- Pseudospectral methods (Fasshauer, 2005; Fornberg et al)

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

Generate numerical differentiation formulas ($\Xi \subset \overline{\Omega}$)

$$\Delta u(\xi_i) \approx \sum_{j=1}^{N} w_{i,j} u(\xi_j) \quad \text{for all } \xi_i \in \Xi \setminus \partial\Omega$$

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

$$\sum_{j=1}^{N} w_{i,j} \hat{u}(\xi_j) = f(\xi_i) \text{ for } \xi_i \in \Xi \setminus \partial\Omega$$

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

Good results for small problems. Dense system matrix.

Kernel-based methods for PDEs

- Generalized finite differences

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

Localized numerical differentiation ($\Xi \subset \overline{\Omega}$):

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

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Sparse system matrix $\{w_{i,j}\}$.

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Generalized finite differences

Pro

- efficient numerics of sparse linear systems
- meshless
- no integration
- very flexible, easily made locally adaptive:
  - location of centres (irregularity, movement)
  - size of “stencils" Ξ_i (local approximation order)
  - choice of kernels (to reflect local variations in smoothness)
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Contra

- strong form method
- lack of theory (at least we now understand numerical differentiation error)
- sophisticated algorithms needed to handle so many parameters.

Generalized finite differences

History

- Polynomial stencils: obtained from polynomial interpolation or least squares.

  Jensen, 1972; Liszka & Orkisz, 1980; Kuhnert, 1999; Schönauer & Adolph, 2001; Benito, Urena, Gavete & Alvares, 2003; Perazzo, Löhner & Perez-Poro, 2008; Seibold, 2008; . . .

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History

- Polynomial stencils: obtained from polynomial interpolation or least squares.

  Jensen, 1972; Liszka & Orkisz, 1980; Kuhnert, 1999; Schönauer & Adolph, 2001; Benito, Urena, Gavete & Alvares, 2003; Perazzo, Löhner & Perez-Poro, 2008; Seibold, 2008; . . .

- Kernel stencils attract growing attention since 2003.

  Early papers: Lee, Liu & Fan, 2003; Shu, Ding & Yeo, 2003; Tolstykh & Shirobokov, 2003; Wright & Fornberg, 2006; Sarler & Vertnik, 2006

Generalized finite differences

Current research topics

- PDEs on surfaces (Fornberg; Wright; Flyer; Larsson; Lehto,...)

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- Adaptive centres for elliptic equations (D. & Oahn; Phu, D. & Oahn)
- Adaptive scaling parameter

Outline

1 Kernel Methods
- Kernel-based interpolation
- Numerical differentiation
- Kernel-based methods for PDEs
- Generalized finite differences

2 Adaptive Centres for Elliptic Equations
- Pointwise discretisation of Poisson equation
- Numerical differentiation stencils on irregular centres
- Stencil support selection
- Adaptive meshless refinement of centres

3 Conclusion

Pointwise discretisation of Poisson equation

Dirichlet problem for the Poisson equation

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

$\Omega \subset \mathbb{R}^d$: bounded domain

f, g: given functions

Discretised problem: find $\hat{u}$ such that

$$\sum_{\xi \in \Xi_\zeta} w_{\zeta,\xi} \hat{u}(\xi) = \sum_{\theta \in \Theta_\zeta} \sigma_{\zeta,\theta} f(\theta), \quad \zeta \in \Xi \setminus \partial\Xi$$
$$\hat{u}(\xi) = g(\xi), \quad \xi \in \partial\Xi$$

- $\Xi \subset \overline{\Omega}$: 'discretisation centres'
- $\Theta \subset \Omega$: 'collocation centres'

$\hat{u}$ defined on Ξ

$\partial\Xi := \Xi \cap \partial\Omega$

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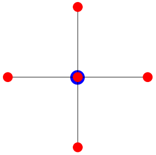
Classical finite differences



- $\Theta_\zeta = \{\zeta\}$, $\sigma_{\zeta,\zeta} = 1$
- Five point stencil: $\Xi_\zeta = \{\zeta, \zeta \pm (h,0), \zeta \pm (0,h)\}$; $w_{\zeta,\zeta} = -4/h^2$ and $w_{\zeta,\xi} = 1/h^2$ for $\xi \in \Xi_\zeta \setminus \{\zeta\}$

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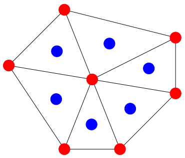
Linear triangle finite elements with midpoint rule quadrature



- Θ_ζ: barycentres of the triangles T_θ attached to ζ, $\sigma_{\zeta,\theta} = \text{area}(T_\theta)/3$
- Ξ_ζ: ζ and the vertices of the triangles T_θ, $\theta \in \Theta_\zeta$
- $w_{\zeta,\xi} = -\int_\Omega \nabla\phi_\xi \nabla\phi_\zeta, \quad \xi \in \Xi_\zeta; \quad \phi_\xi$: hat functions

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Generalised finite differences

- For each $\zeta \in \Xi \setminus \partial\Xi$, choose Θ_ζ, $\{\sigma_{\zeta,\theta},\ \theta \in \Theta_\zeta\}$ and Ξ_ζ
- Find the stencil coefficients $\{w_{\zeta,\xi},\ \xi \in \Xi_\zeta\}$ from a numerical differentiation formula

$$\sum_{\theta\in\Theta_\zeta} \sigma_{\zeta,\theta}\Delta u(\theta) \approx \sum_{\xi\in\Xi_\zeta} w_{\zeta,\xi} u(\xi)$$

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Numerical differentiation stencils on irregular centres

Low order RBF stencils (D. & Oanh, 2011)

- Look for stencils of small support, typically Ξ_ζ consisting of ζ and up to 6 nearby points.
    - Sparse matrices
    - Expect h^2 approximation order for $\|\hat{u} - u_{|\Xi}\|$ as with linear finite elements

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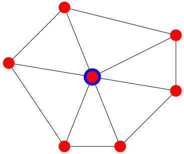
- Single point stencil (FD like)



$$\Theta_\zeta = \{\zeta\},\ \sigma_{\zeta,\zeta} = 1$$

$$\Delta u(\zeta) \approx \sum_{\xi \in \Xi_\zeta} w_{\zeta,\xi} u(\xi)$$

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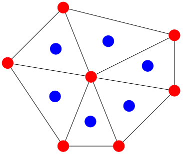
  - Expect h^2 approximation order for $\|\hat{u} - u_{|\Xi}\|$ as with linear finite elements
- Given ζ and Ξ_ζ, select the collocation centres Θ_ζ and weights $\sigma_{\zeta,\theta}$. Then find the stencil coefficients $w_{\zeta,\xi}$ by RBF numerical differentiation.
- Multipoint stencil (FEM like)



Θ_ζ: barycentres θ_i of the triangles T_i formed by ζ, ξ_i, ξ_{i+1}, $\sigma_{\zeta,\theta_i} = \text{area}(T_i)/3$

$$\sum_{\theta \in \Theta_\zeta} \sigma_{\zeta,\theta} \Delta u(\theta) \approx \sum_{\xi \in \Xi_\zeta} w_{\zeta,\xi} u(\xi)$$

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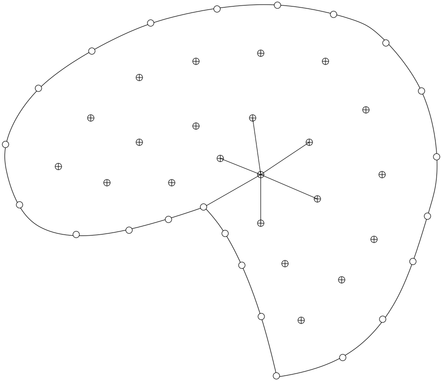
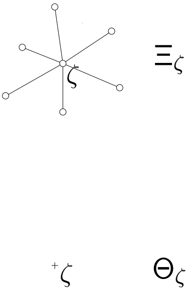
Stencil support selection

Need to select Ξ_ζ for each $\zeta \in \Xi \setminus \partial\Xi$





Ξ_ζ is ‘stencil support’ or ‘set of influence’

Stencil support selection

Test problem to compare various algorithms

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

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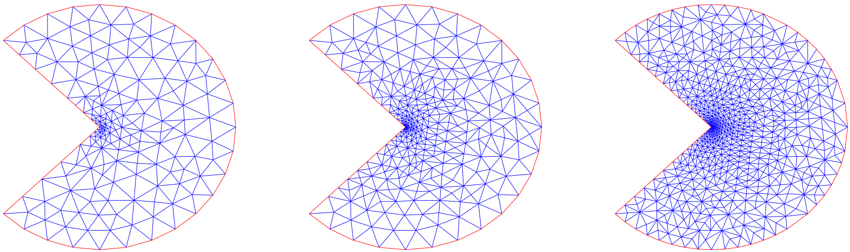
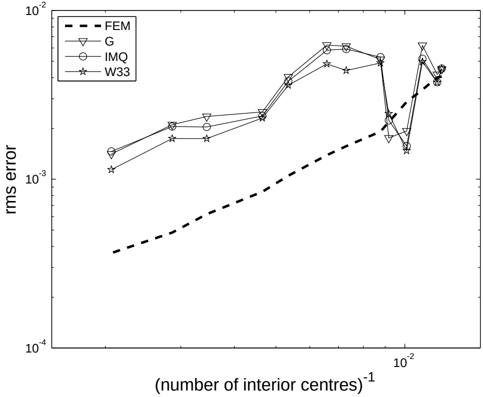
- Adaptive centres generated by PDE Toolbox (MATLAB)



Stencil support selection

Using FEM stencil supports Ξ_ζ (ζ and vertices connected to ζ in the triangulation): rms error $\left(\frac{1}{N}\sum_{\xi\in\Xi\setminus\partial\Xi}|u(\xi)-\hat{u}(\xi)|^2\right)^{1/2}$ for RBF-FD with single point stencil



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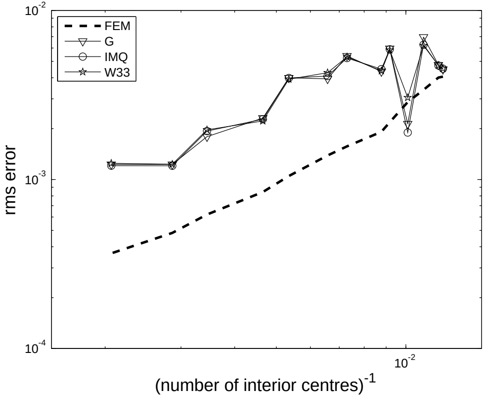
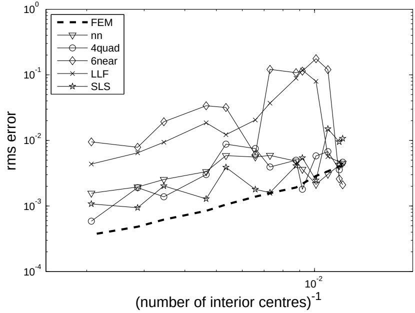
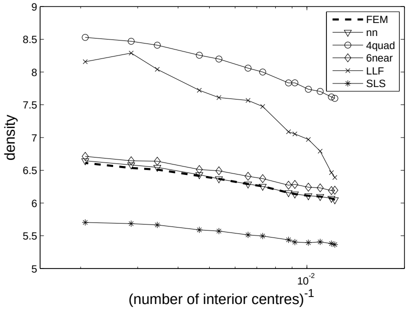


Stencil support selection

Further stencil support selection algorithms

6near: six nearest neighbours; nn: natural neighbours;
4quad: four quadrants criterium; LLF: Lee, Liu & Fun, 2003;
SLS: Shen, Lv, Shen, 2009

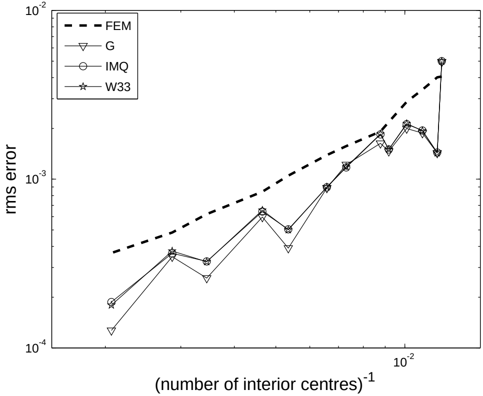




density: average size of Ξ_ζ

Stencil support selection

Our stencil support selection (D. & Oanh, 2011)
for RBF-FD with single point stencil



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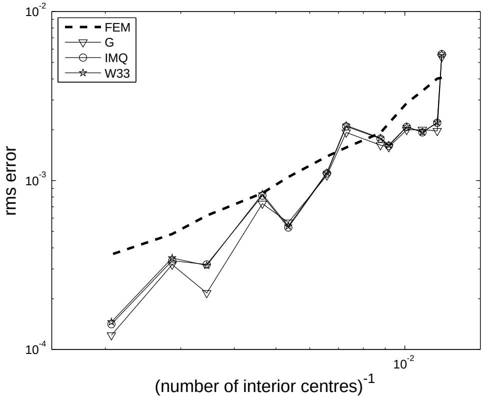

Stencil support selection

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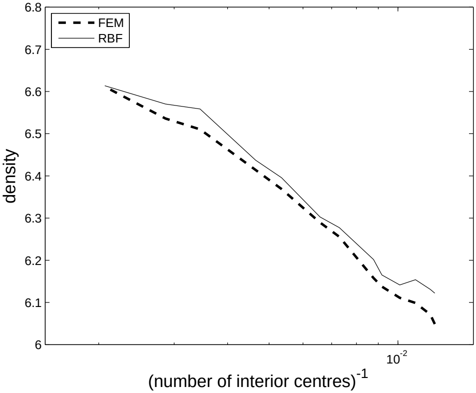
System matrix density



Stencil support selection

Algorithm

- For $\Xi_\zeta = \{\zeta, \xi_1, \dots, \xi_k\}$ define
$$\mu := \sum_{i=1}^{k} \alpha_i^2, \quad \underline{\alpha} := \min\{\alpha_1, \dots, \alpha_k\}, \quad \overline{\alpha} := \max\{\alpha_1, \dots, \alpha_k\}$$
where α_i denotes the angle between the rays $\zeta\xi_i$, $\zeta\xi_{i+1}$ (ξ_i counterclockwise).

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- The whole procedure is meshless.

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

$\gamma \in (0,1]$ is a user specified tolerance ($\gamma = 0.3$ in our tests).

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- Considered for polynomial stencils: Benito, Urena, Gavete & Alvares, 2003; Perazzo, Löhner & Perez-Poro, 2008

Adaptive meshless refinement of centres

Algorithm (D. & Oanh, 2011)

- Define local separation

$$\mathrm{sep}_\zeta(\Xi) := \frac{1}{4}\sum_{i=1}^{4} \mathrm{dist}(\xi_i, \Xi \setminus \{\xi_i\}), \qquad \zeta \notin \Xi,$$

where $\xi_1, \dots, \xi_4$ are the four closest points in Ξ to ζ.

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- Loop over marked edges $\xi\zeta$, inserting a new centre $\xi' = (\zeta + \xi)/2$ only if

$$\mathrm{dist}(\xi', \Xi) \geq \mu\, \mathrm{sep}_{\xi'}(\Xi).$$

  μ is another tolerance, we take $\mu = 0.7$.

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  μ is another tolerance, we take $\mu = 0.7$.

- Boundary is also refined if $\xi \in \partial\Xi$.

Adaptive meshless refinement of centres

Algorithm (D. & Oanh, 2011)

- Define local separation

$$\mathrm{sep}_\zeta(\Xi) := \frac{1}{4}\sum_{i=1}^{4} \mathrm{dist}(\xi_i, \Xi \setminus \{\xi_i\}), \qquad \zeta \notin \Xi,$$

  where $\xi_1, \dots, \xi_4$ are the four closest points in Ξ to ζ.

- Loop over marked edges $\xi\zeta$, inserting a new centre $\xi' = (\zeta + \xi)/2$ only if

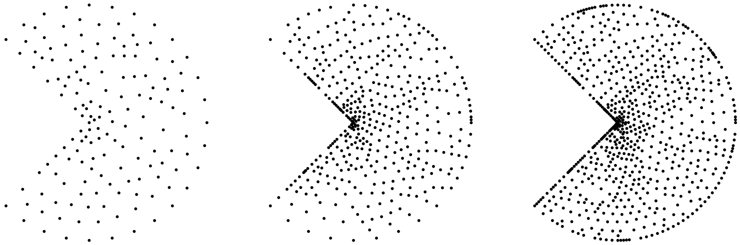
$$\mathrm{dist}(\xi', \Xi) \geq \mu\, \mathrm{sep}_{\xi'}(\Xi).$$

  μ is another tolerance, we take $\mu = 0.7$.

- Boundary is also refined if $\xi \in \partial\Xi$.
- Postprocessing to refine excessively long edges.
  Repeat with $\mu = 0.9\mu$ if no new centres have been created.

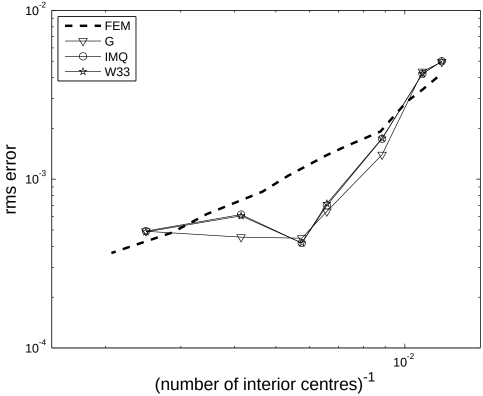
Adaptive meshless refinement of centres

Adaptive centres generated by the above meshless method

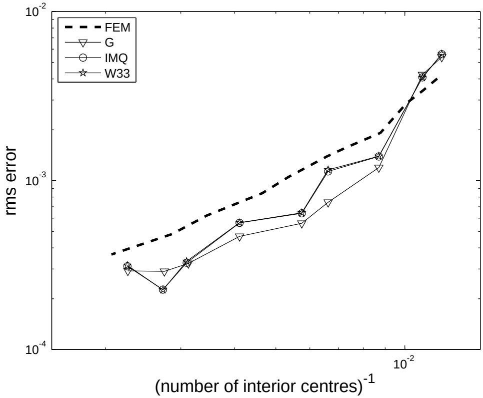


Adaptive meshless refinement of centres

Meshless refinement and stencil support selection:
RBF-FD with single point stencil



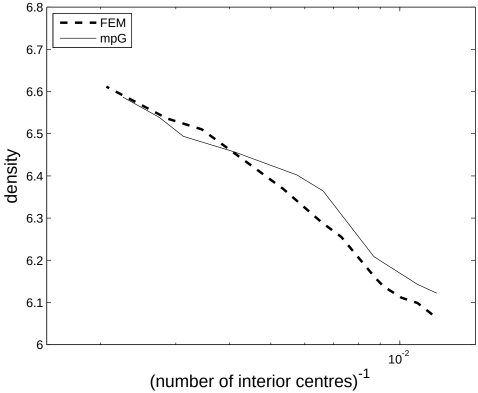
Meshless refinement and stencil support selection:
RBF-FD with multipoint stencil



Adaptive meshless refinement of centres

Meshless refinement and stencil support selection:

System matrix density



Adaptive meshless refinement of centres

Recent improvements [Phu, D., Oanh, in preparation]

- Improved stencil support selection (more effective optimisation)

Adaptive meshless refinement of centres

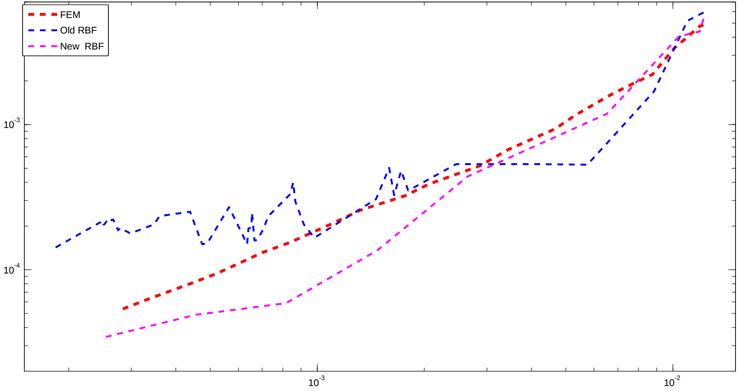
Recent improvements [Phu, D., Oanh, in preparation]

- Improved stencil support selection (more effective optimisation)
- Improved refinement (in addition to $\xi' = (\zeta + \xi)/2$ add up to 2 more points on the direction perpendicular to the edge $\zeta\xi$; the ”postprocessing" is not needed anymore)

Adaptive meshless refinement of centres

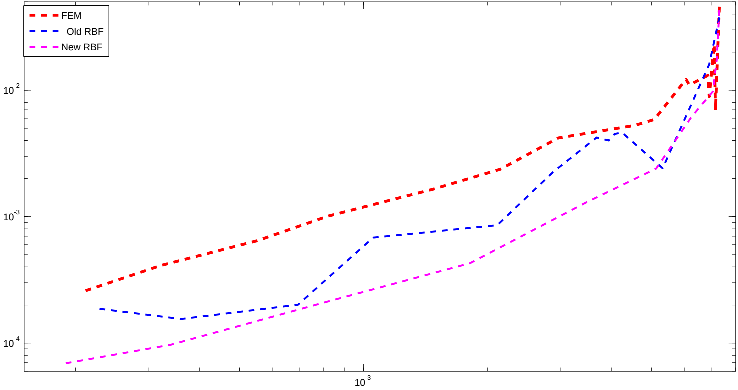
Numerical results for single point stencils [Phu, D. & Oanh]

- The above test problem (rms error vs. $(\#\text{centres})^{-1}$)



Adaptive meshless refinement of centres

- Dirichlet problem for the Laplace equation $\Delta u = 0$ in the domain $\Omega = (0.01, 1.01)^2$ with boundary conditions chosen such that the exact solution is $u(x, y) = \log(x^2 + y^2)$.

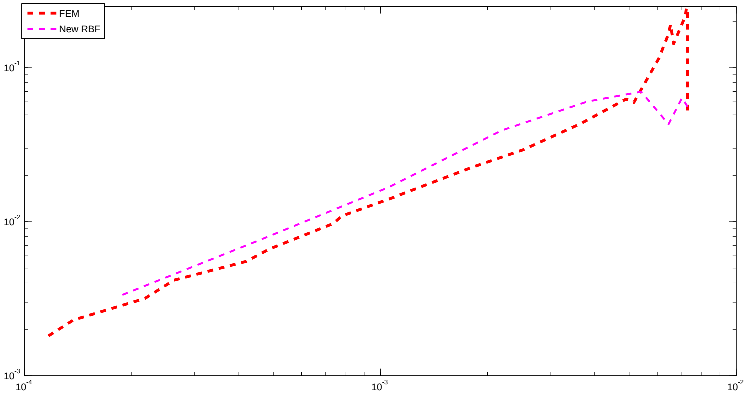


(rms error vs. $(\#\text{centres})^{-1}$)

Adaptive meshless refinement of centres

- Dirichlet problem for the Helmholz equation

$-\Delta u - \frac{1}{(\alpha+r)^4} = f$, $r = \sqrt{x^2 + y^2}$ 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 $\alpha = \frac{1}{10\pi}$.

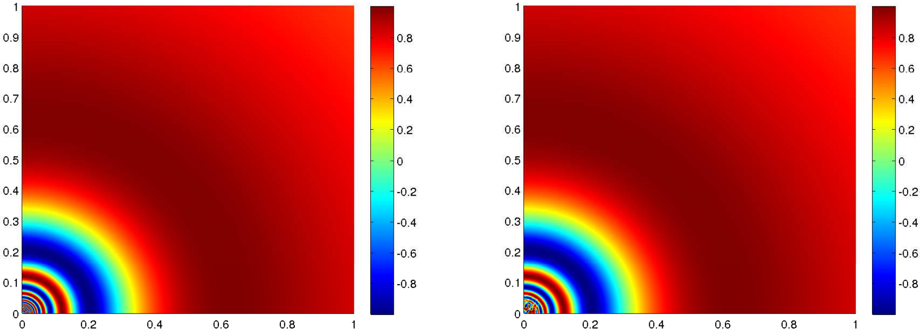


Adaptive meshless refinement of centres

- The same Helmholz problem $-\Delta u - \frac{1}{(\alpha+r)^4} = f$ with exact solution $\sin(\frac{1}{\alpha+r})$, where $\alpha = \frac{1}{50\pi}$.

Exact solution

RBF-FD (5782 centres)



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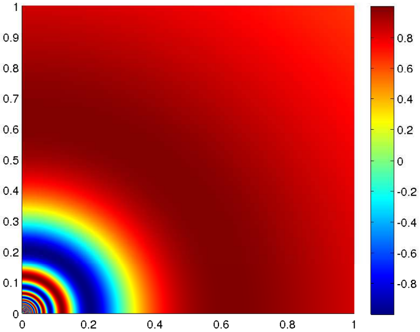
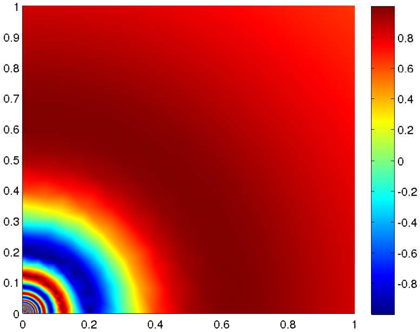


FEM (5937 centres)



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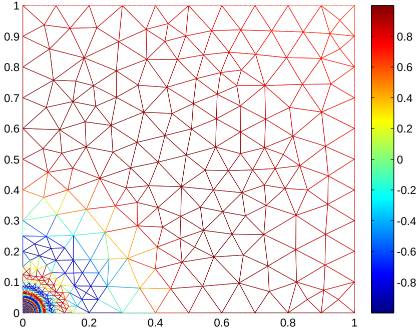
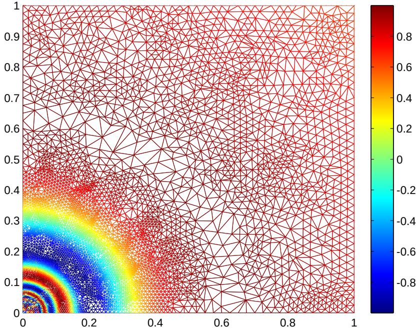
- The same Helmholz problem $-\Delta u - \frac{1}{(\alpha+r)^4} = f$ with exact solution $\sin(\frac{1}{\alpha+r})$, where $\alpha = \frac{1}{50\pi}$.

FEM centres



RBF centres



Outline

1. Kernel Methods
   - Kernel-based interpolation
   - Numerical differentiation
   - Kernel-based methods for PDEs
   - Generalized finite differences
2. Adaptive Centres for Elliptic Equations
   - Pointwise discretisation of Poisson equation
   - Numerical differentiation stencils on irregular centres
   - Stencil support selection
   - Adaptive meshless refinement of centres
3. Conclusion

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Conclusion

- Kernel-FD methods lead to sparse system matrices, unlike the more traditional kernel-based methods
- Efficiency of a strong form based, meshless method
- Numerical differentiation error estimates [D.& Schaback] give conditions for consistency of the discretization
- Good opportunities for adaptive algorithms
- Competitive with FEM in our numerical tests