Kernel Based Finite Difference Methods

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Outline

1. Kernel Methods
2. Adaptive Centres for Elliptic Equations
3. Conclusion
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 $s = 0$). $\Pi^d_s$: polynomials of order $s$.

For a $\Pi^d_s$-unisolvent $X$, the kernel interpolant $r_{X,K,f}$ in the form

$$r_{X,K,f} = \sum_{j=1}^{N} a_j K(\cdot, x_j) + \sum_{j=1}^{M} b_j p_j, \quad a_j, b_j \in \mathbb{R}, \quad M = \text{dim}(\Pi^d_s),$$

is uniquely determined from the positive definite linear system

$$r_{X,K,f}(x_k) = \sum_{j=1}^{N} a_j K(x_k, x_j) + \sum_{j=1}^{M} b_j p_j(x_k) = f_k, \quad 1 \leq k \leq N,$$

$$\sum_{j=1}^{N} a_j p_i(x_j) = 0, \quad 1 \leq i \leq M.$$
Examples. \[ K(\mathbf{x}, \mathbf{y}) = \phi(\|\mathbf{x} - \mathbf{y}\|) \]
\[(\phi : \mathbb{R}_+ \to \mathbb{R} \text{ is then a radial basis function (RBF)})\]

\(s \geq 0:\) Any \(\phi\) 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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& \bullet \text{ inverse multiquadric } 1/\sqrt{1 + r^2} \\
& \bullet (1 - r)^\delta (32r^3 + 25r^2 + 8r + 1) \text{ (for } d \leq 3) \text{ (}C^6\text{ compactly supported Wendland function)} \\
& \bullet \text{ Matérn kernel } K_\nu(r)r^\nu, \nu > 0 \\
& \text{ (}K_\nu(r)\text{ modified Bessel function of second kind)}
\end{align*}
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\begin{align*}
s \geq 1: \ & \bullet \text{ multiquadric } \sqrt{1 + r^2} \\
s \geq 2: \ & \bullet \text{ thin plate spline } r^2 \log r
\end{align*}
\]
Kernel-based interpolation

Examples.

\[ K(x, y) = \phi(\|x - y\|) \]

(\( \phi : \mathbb{R}_+ \to \mathbb{R} \) is then a radial basis function (RBF))

\( s \geq 0: \) Any \( \phi \) with positive Fourier transform of \( \Phi(x) = \phi(\|x\|) \)

- Gaussian \( \phi(r) = e^{-r^2} \)
- inverse quadric \( 1 / (1 + r^2) \)
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\( s \geq 1: \) multiquadric \( \sqrt{1 + r^2} \)

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\( K(\varepsilon x, \varepsilon y) \) are also cpd kernels (\( \varepsilon > 0: \) shape parameter)
Kernel-based interpolation

Optimal Recovery

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

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

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

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

\[
\inf_{\mathbf{w} \in \mathbb{R}^N} \sup_{\|f\|_{\mathcal{F}_K} \leq 1} \left| f(\mathbf{z}) - \sum_{j=1}^{N} w_j f(\mathbf{x}_j) \right| = \sup_{\|f\|_{\mathcal{F}_K} \leq 1} \left| f(\mathbf{z}) - \sum_{j=1}^{N} w_j^* f(\mathbf{x}_j) \right|,
\]

\( \mathbf{w} \perp \Pi^d_s : \text{exactness for polynomials in } \Pi^d_s \), e.g. \( s = 0 \) or \( 1 \).
“Native Space" $\mathcal{F}_K$

- In the translation-invariant case $K(x, y) = \Phi(x - y)$ on $\mathbb{R}^d$,

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

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

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

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

Further Info

- Kernel-based interpolants exist with no restrictions on the location of the centres, in contrast to, say, polynomials.
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- Standard tool for **spatial data fitting** in Geosciences (kriging interpolation)
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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 $W^k_p(\Omega)$, where $h$ is the fill distance of the centres in $\Omega$,

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h = \max_{x \in \Omega} \min_{1 \leq i \leq N} \| x - x_i \|_2.
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- However: **Dense linear systems** to find coefficients.
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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**
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3 Conclusion
Let $D$ be a linear differential operator of order $k$. Given $z \in \mathbb{R}^d$, a numerical differentiation formula

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

is defined by the set of centres $X = \{x_1, \ldots, x_N\} \subset \mathbb{R}^d$ and the weight vector $w \in \mathbb{R}^N$.

- Formulas on grids are used in the finite difference method.
- Irregular $X \implies$ generalized finite difference methods.
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 $m + k$:

$$Dp(z) = \sum_{j=1}^{N} w_j p(x_j) \quad \text{for all } p \in \Pi_{m+k}^d.$$ 

- A classical way to work out polynomially consistent formulas **on grids** is via truncation of Taylor expansion.
- On an **irregular** set $X = \{x_1, \ldots, x_N\}$ 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:

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

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

  $$\sum_{j=1}^{N} w_j^* K(x_k, x_j) + \sum_{j=1}^{M} c_j p_j(x_k) = [DK(\cdot, x_k)](z), \quad 1 \leq k \leq N,$$

  $$\sum_{j=1}^{N} w_j^* p_i(x_j) + 0 = Dp_i(z), \quad 1 \leq i \leq M.$$
The weights \( w^*_j \) provide optimal recovery of \( Df(z) \) from \( f(x_j), j = 1, \ldots, N \), for \( f \in \mathcal{F}_K \),

\[
\inf_{w \in \mathbb{R}^N} \sup_{\|f\|_{\mathcal{F}_K} \leq 1} \left| Df(z) - \sum_{j=1}^{N} w_j f(x_j) \right| = \sup_{\|f\|_{\mathcal{F}_K} \leq 1} \left| Df(z) - \sum_{j=1}^{N} w^*_j f(x_j) \right|,
\]
The weights $\mathbf{w}^* = \{w_j^*\}_{j=1}^N$ provide optimal recovery of $Df(z)$ from $f(x_j)$, $j = 1, \ldots, N$, for $f \in \mathcal{F}_K$, i.e.,

$$
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$$

E.g. Matérn kernel-based formula with $s = 0$ gives the best possible estimate of $Df(z)$ if we only know that $f$ belongs to the respective Sobolev space.
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In particular, the optimal formula does not need to be exact for any polynomials.
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In particular, the optimal formula does not need to be exact for any polynomials.

Whenever centres $x_1, \ldots, x_N$ admit a good formula $Df(z) \approx \sum_{j=1}^N w_j f(x_j)$, the kernel-based formula will also perform well.
Example: Five point stencil for Laplace operator $\Delta$ in 2D

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

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

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

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

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

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

\[
|Df(z) - Dr_{x,K,f}(z)| \leq \rho_{q,D}(z, X) M_{K,q} \|f\|_{\mathcal{F}_K}, \quad f \in \mathcal{F}_K.
\]
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$$\rho_{q,D}(z, X) := \sup \{Dp(z) : p \in \Pi_{d, q}, \ |p(x_i)| \leq \|x_i - z\|_2^q, \quad i = 1, \ldots, N\}$$

is a polynomial growth function,
Numerical differentiation

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

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$$\rho_{q,D}(z, X) := \sup \left\{ Dp(z) : p \in \prod^q_{\mathbb{N}}, \ |p(x_i)| \leq \|x_i - z\|^q, \ i = 1, \ldots, N \right\} \text{ is a polynomial growth function,}$$

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

\[ |Df(z) - Dr_{x,K,f}(z)| \leq \min_{q \geq k+1} \left\{ \rho_{q,D}(z,X) M_{K,q} \right\} \|f\|_{\mathcal{F}_K}, \]

\[ \rho_{q,D}(z,X) := \sup \left\{ Dp(z) : p \in \Pi^d q, \ |p(x_i)| \leq \|x_i - z\|_2^q, \ \forall i \right\} \]
Numerical differentiation

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\[ \rho_{q,D}(z, X) := \sup \{ D\rho(z) : \rho \in \Pi_d^q, \ |\rho(x_i)| \leq \|x_i - z\|_2^q, \ \forall i \} \]

Example. 5 point stencil: \( X^h = z + \{(0, 0), (0, \pm h), (\pm h, 0)\} \).

Then \( q \geq 3, \rho_{3,\Delta}(z, X) = 4h, \rho_{4,\Delta}(z, X) = 4h^2, \rho_{5,\Delta}(z, X) = \infty \). Hence consistency order 2:

\[ |\Delta f(z) - \Delta r_{x^h,K,f}(z)| \leq 4h^2 M_{k,4} \| f \|_{\mathcal{F}_K} \]

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

\[ |\Delta f(z) - \Delta r_{x^h,K,f}(z)| \leq 4h M_{k,3} \| f \|_{\mathcal{F}_K} \]
Discussion

\[ |Df(z) - Dr_{x,K,f}(z)| \leq \min_{q \geq k+1} \{ \rho_{q,D}(z, X) M_{K,q} \} \|f\|_{\mathcal{F}_K}, \]

\[ \rho_{q,D}(z, X) := \sup \{ Dp(z) : p \in \Pi^d_q, |p(x_i)| \leq \|x_i - z\|_2^q, \forall i \} \]

- **Example.** 5 point stencil: \( X^h = z + \{(0, 0), (0, \pm h), (\pm h, 0)\} \).
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- If \( K \) is \( C^\infty \) and \( X \) big enough \( \implies \) spectral estimates
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3 Conclusion
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 \( \sum_{i=1}^{n} a_i K(\cdot, x_i) \) (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 \( K(\cdot, x_i) \) 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 \(\Xi\) s.t.

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

\[ \hat{u}(\xi_i) = g(\xi_i) \quad \text{for } \xi_i \in \partial \Omega \]

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” $\Xi_i$ (local approximation order)
  - choice of kernels (to reflect local variations in smoothness)
- **isogeometric**: bare centres $\xi_i$ fit into any geometry
Generalized finite differences

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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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- **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
Current research topics

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

- **PDEs on surfaces** (Fornberg; Wright; Flyer; Larsson; Lehto,...)
  - Kernels on a surface in $\mathbb{R}^3$ are easily obtained by restricting 3D kernels
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- **PDEs on surfaces** (Fornberg; Wright; Flyer; Larsson; Lehto,...)
  - Kernels on a surface in $\mathbb{R}^3$ are easily obtained by restricting 3D kernels
  - Optimal recovery properties hold
Current research topics

- **PDEs on surfaces** (Fornberg; Wright; Flyer; Larsson; Lehto,...)
  - Kernels on a surface in $\mathbb{R}^3$ are easily obtained by restricting 3D kernels
  - Optimal recovery properties hold
  - Any quasi-uniformly distributed centres (e.g. minimal energy points) can be used as replacement for grids
Generalized finite differences

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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**

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

**Discretised problem:** find \( \hat{u} \) such that

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

\[
\hat{u}(\xi) = g(\xi), \quad \xi \in \partial \Xi
\]

- \( \Xi \subset \overline{\Omega} \): ‘discretisation centres’
- \( \Theta \subset \Omega \): ‘collocation centres’

**Notes**

- \( \Omega \subset \mathbb{R}^d \): bounded domain
- \( f, g \): given functions
- \( \hat{u} \) defined on \( \Xi \)
- \( \partial \Xi := \Xi \cap \partial \Omega \)
- \( \Xi = \bigcup_{\zeta \in \Xi} \Xi_{\zeta} \)
- \( \Theta_{\zeta} \subset \Theta, \zeta \in \Xi \)
**Discretised problem:** find $\hat{u}$ such that

$$
\sum_{\xi \in \Xi} w_{\zeta,\xi} \hat{u}(\xi) = \sum_{\theta \in \Theta^\zeta} \sigma_{\zeta,\theta} f(\theta), \quad \zeta \in \Xi \setminus \partial \Xi
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$\hat{u}$ defined on $\Xi$

$$
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$$

$$
\Xi = \bigcup_{\zeta \in \Xi \setminus \partial \Xi} \Xi^\zeta
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$$
\Theta^\zeta \subset \Theta, \zeta \in \Xi
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Pointwise discretisation of Poisson equation

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

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

$$\hat{u}(\xi) = g(\xi), \quad \xi \in \partial \Xi$$

$\Xi \subset \overline{\Omega}$: ‘discretisation centres’

$\Theta \subset \Omega$: ‘collocation centres’

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 $\xi \in \Xi_{\zeta} \setminus \{\zeta\}$

$\hat{u}$ defined on $\Xi$

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

$\Xi = \bigcup_{\zeta \in \Xi \setminus \partial \Xi} \Xi_{\zeta}$

$\Theta_{\zeta} \subset \Theta$, $\zeta \in \Xi$
Discretised problem: find $\hat{u}$ such that

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

$$\hat{u}(\xi) = g(\xi), \quad \xi \in \partial \Xi$$

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

Linear triangle finite elements with midpoint rule quadrature

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

Discretised problem: find \( \hat{u} \) such that

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

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\hat{u}(\xi) = g(\xi), \quad \xi \in \partial \Xi
\]

- \( \Xi \subset \overline{\Omega} \): ‘discretisation centres’
- \( \Theta \subset \Omega \): ‘collocation centres’

Generalised finite differences

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

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

\( \hat{u} \) defined on \( \Xi \)

\( \partial \Xi := \Xi \cap \partial \Omega \)

\( \Xi = \bigcup_{\zeta \in \Xi \setminus \partial \Xi} \Xi_{\zeta} \)

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3 Conclusion
Numerical differentiation stencils on irregular centres

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

- Look for stencils of small support, typically $\Xi_\zeta$ consisting of $\zeta$ and up to 6 nearby points.
  - Sparse matrices
  - Expect $h^2$ approximation order for $\| \hat{u} - u_{|\Xi} \|$ as with linear finite elements
Low order RBF stencils (D. & Oanh, 2011)

- Look for **stencils of small support**, typically $\Xi$ consisting of $\zeta$ and up to 6 nearby points.
  - Sparse matrices
  - Expect $h^2$ approximation order for $\| \hat{u} - u_{\Xi} \|$ as with linear finite elements
- Given $\zeta$ and $\Xi$, select the collocation centres $\Theta_{\zeta}$ and weights $\sigma_{\zeta, \theta}$. Then find the stencil coefficients $w_{\zeta, \xi}$ by RBF numerical differentiation.
Numerical differentiation stencils on irregular centres

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

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  - Sparse matrices
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- Given $\zeta$ and $\Xi_\zeta$, select the collocation centres $\Theta_\zeta$ and weights $\sigma_{\zeta, \theta}$. Then find the stencil coefficients $w_{\zeta, \xi}$ by RBF numerical differentiation.

- **Single point stencil** (FD like)

  \[ \Theta_\zeta = \{\zeta\}, \quad \sigma_{\zeta, \zeta} = 1 \]

  \[ \Delta u(\zeta) \approx \sum_{\xi \in \Xi_\zeta} w_{\zeta, \xi} u(\xi) \]
Low order RBF stencils (D. & Oanh, 2011)

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

- Given $\zeta$ and $\Xi_\zeta$, select the collocation centres $\Theta_\zeta$ and weights $\sigma_{\zeta, \theta}$. Then find the stencil coefficients $w_{\zeta, \xi}$ by RBF numerical differentiation.

Multipoint stencil (FEM like)

$\Theta_\zeta$: barycentres $\theta_i$ of the triangles $T_i$ formed by $\zeta, \xi_i, \xi_{i+1}$, $\sigma_{\zeta, \theta_i} = \text{area}(T_i)/3$

$$\sum_{\theta \in \Theta_\zeta} \sigma_{\zeta, \theta} \Delta u(\theta) \approx \sum_{\xi \in \Xi_\zeta} w_{\zeta, \xi} u(\xi)$$
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3 Conclusion
Stencil support selection

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

$\Xi_\zeta$ is ‘stencil support’ or ‘set of influence’
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 $u(r, \psi) = r^{2/3} \cos(2\psi/3)$
Test problem to compare various algorithms

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- Exact solution $u(r, \psi) = r^{2/3} \cos(2\psi/3)$

- Adaptive centres generated by PDE Toolbox (MATLAB)
Stencil support selection

Using FEM stencil supports $\Xi_\zeta$ ($\zeta$ and vertices connected to $\zeta$ in the triangulation): 

$$\text{rms error } \left( \frac{1}{N} \sum_{\xi \in \Xi \setminus \partial \Xi} |u(\xi) - \hat{u}(\xi)|^2 \right)^{1/2}$$

for RBF-FD with single point stencil.
Stencil support selection

Using FEM stencil supports $\Xi_\zeta$ ($\zeta$ and vertices connected to $\zeta$ 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 multipoint stencil
Stencil support selection

Further stencil support selection algorithms


density: average size of $\Xi_\zeta$
Our stencil support selection (D. & Oanh, 2011) for RBF-FD with single point stencil
Our stencil support selection (D. & Oanh, 2011) for RBF-FD with multipoint stencil
Our stencil support selection (D. & Oanh, 2011)

System matrix density

![Graph showing system matrix density](image-url)

- **FEM**
- **RBF**

(number of interior centres)⁻¹

density
Stencil support selection

Algorithm

For $\Xi_\zeta = \{\zeta, \xi_1, \ldots, \xi_k\}$ define

$$\mu := \sum_{i=1}^{k} \alpha_i^2, \quad \underline{\alpha} := \min\{\alpha_1, \ldots, \alpha_k\}, \quad \overline{\alpha} := \max\{\alpha_1, \ldots, \alpha_k\}$$

where $\alpha_j$ denotes the angle between the rays $\zeta \xi_i, \zeta \xi_{i+1}$ ($\xi_i$ counterclockwise).
Stencil support selection

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- Start with six closests points $\xi_1, \ldots, \xi_6 \in \Xi \setminus \{\zeta\}$
Stencil support selection

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For $\Xi_\zeta = \{\zeta, \xi_1, \ldots, \xi_k\}$ define

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Start with six closest points $\xi_1, \ldots, \xi_6 \in \Xi \setminus \{\zeta\}$

Go over $\xi_7, \xi_8, \ldots, \xi_{30}$ replacing one of the points in $\Xi_\zeta \setminus \{\zeta\}$ if this makes $\mu$ smaller.

(Then the angles $\alpha_i$ are more uniformly distributed.)
Algorithm

• For \( \Xi_\zeta = \{\zeta, \xi_1, \ldots, \xi_k\} \) define

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(Then the angles \( \alpha_i \) are more uniformly distributed.)

• Terminate early if \( \overline{\alpha} \leq 3\alpha \). If this condition is never satisfied, remove ‘the worst point’ (the one next to \( \alpha_j = \alpha \)).
Stencil support selection

Algorithm

- For \( \Xi_\zeta = \{\zeta, \xi_1, \ldots, \xi_k\} \) define
  
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  where \( \alpha_i \) denotes the angle between the rays \( \zeta \xi_i, \zeta \xi_{i+1} \) (\( \xi_i \) counterclockwise).

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- Go over \( \xi_7, \xi_8, \ldots, \xi_{30} \) replacing one of the points in \( \Xi_\zeta \setminus \{\zeta\} \) if this makes \( \mu \) smaller.
  (Then the angles \( \alpha_i \) are more uniformly distributed.)

- Terminate early if \( \underline{\alpha} \leq 3\overline{\alpha} \). If this condition is never satisfied, remove ‘the worst point’ (the one next to \( \alpha_i = \underline{\alpha} \)).

- The whole procedure is meshless.
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3 Conclusion
Adaptive meshless refinement of centres

- Need a meshless method to generate the set of centres $\Xi$. 
Adaptive meshless refinement of centres

- Need a meshless method to generate the set of centres $\Xi$.
- Try obtaining it by adaptive refinement.
Adaptive meshless refinement of centres

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- Try obtaining it by adaptive refinement.
- Error indicator: $\varepsilon(\zeta, \xi) := |\hat{u}(\zeta) - \hat{u}(\xi)|$, $\zeta \in \Xi$, $\xi \in \Xi_\zeta$. 

Oleg Davydov
Kernel Based FD
Adaptive meshless refinement of centres

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- Try obtaining it by adaptive refinement.
- Error indicator: $\varepsilon(\zeta, \xi) := |\hat{u}(\zeta) - \hat{u}(\xi)|$, $\zeta \in \Xi$, $\xi \in \Xi_\zeta$.
- An ‘edge’ $\zeta \xi$ is marked for refinement if

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

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

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- Refine $\zeta \xi$ by inserting a new centre at $(\zeta + \xi)/2$
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$\gamma \in (0, 1]$ is a user specified tolerance ($\gamma = 0.3$ in our tests).

- Refine $\zeta\xi$ by inserting a new centre at $\frac{(\zeta + \xi)}{2}$

- **Problem**: This new point may be located very close to an existing centre $\xi' \in \Xi$, or to a new centre already created by the refinement of a different edge.
Adaptive meshless refinement of centres

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- Refine $\zeta\xi$ by inserting a new centre at $(\zeta + \xi)/2$
- Problem: This new point may be located very close to an existing centre $\xi' \in \Xi$, or to a new centre already created by the refinement of a different edge.
- 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

\[
\text{sep}_\zeta(\Xi) := \frac{1}{4} \sum_{i=1}^{4} \text{dist}(\xi_i, \Xi \setminus \{\xi_i\}), \quad \zeta \notin \Xi,
\]

where \(\xi_1, \ldots, \xi_4\) are the four closest points in \(\Xi\) to \(\zeta\).
Adaptive meshless refinement of centres

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- Define local separation

\[
\text{sep}_\zeta(\Xi) := \frac{1}{4} \sum_{i=1}^{4} \text{dist}(\xi_i, \Xi \setminus \{\xi_i\}), \quad \zeta \notin \Xi,
\]

where \(\xi_1, \ldots, \xi_4\) are the four closest points in \(\Xi\) to \(\zeta\).

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

\[
\text{dist}(\xi', \Xi) \geq \mu \text{sep}_{\xi'}(\Xi).
\]

\(\mu\) is another tolerance, we take \(\mu = 0.7\).
Adaptive meshless refinement of centres

**Algorithm (D. & Oanh, 2011)**

- Define **local separation**
  
  \[ \text{sep}_\zeta(\Xi) := \frac{1}{4} \sum_{i=1}^{4} \text{dist}(\xi_i, \Xi \setminus \{\xi_i\}), \quad \zeta \notin \Xi, \]

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- Boundary is also refined if \( \xi \in \partial \Xi \).
Adaptive meshless refinement of centres

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\(\mu\) 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 centres generated by the above meshless method
Adaptive meshless refinement of centres

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

![Graph showing RMS error vs. number of interior centres]
Adaptive meshless refinement of centres

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

![Graph showing the relationship between the number of interior centres and root mean square error for different methods (FEM, G, IMQ, W33)]
Adaptive meshless refinement of centres

Meshless refinement and stencil support selection:
System matrix density

![Graph showing system matrix density (number of interior centres)^{-1} vs. density)](image-url)
Adaptive meshless refinement of centres

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

- Improved stencil support selection (more effective optimisation)
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 \( u(x, y) = \log(x^2 + y^2) \).

\[ \begin{array}{c|c|c}
\text{Method} & \text{FEM} & \text{Old RBF} & \text{New RBF} \\
\hline
\text{rms error vs. } (\# \text{centres})^{-1} & \end{array} \]
Dirichlet problem for the Helmholtz equation
\[-\Delta u - \frac{1}{(\alpha+r)^4} = f, \ r = \sqrt{x^2 + y^2} \text{ in the domain } \Omega = (0, 1)^2.\]
RHS and the boundary conditions chosen such that the exact solution is \(\sin\left(\frac{1}{\alpha+r}\right)\), where \(\alpha = \frac{1}{10\pi}\).
Adaptive meshless refinement of centres

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

### Exact solution

### RBF-FD (5782 centres)
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**

![Exact solution graph](image1)

**FEM (5937 centres)**

![FEM graph](image2)
Adaptive meshless refinement of centres

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

FEM centres

RBF centres
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3 Conclusion
Kernel-FD methods lead to \textit{sparse system matrices}, unlike the more traditional kernel-based methods.
Kernel-FD methods lead to **sparse system matrices**, unlike the more traditional kernel-based methods

**Efficiency** of a strong form based, meshless method
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
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.