Postprocessing Pseudospectral and Radial Basis Function Approximation Methods

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Talk Outline

- Global High Order Approximation Methods
  - Polynomial (Pseudospectral)
  - Radial Basis Function (RBF)
- The Gibbs Phenomenon
- Postprocessing Methods
- The Matlab Postprocessing Toolbox* (MPT)

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Global HOAMS

\[ I_N f(x) = \sum_k a_k \phi_k(x) \]

- \( I_N f(x_i) = f(x_i) \) at \( N + 1 \) interpolation cites \( x_i \)

- **Interpolation** - \( f(x) \) is a known function (at least at the interpolation cites)

- **collocation and pseudospectral** - global interpolation based methods for solving differential equations for an unknown function \( f(x) \)
Basis Functions

- **Polynomial** - structured grids/domains
  - Periodic - Fourier (Trigonometric)
    \[ \phi_k(x) = e^{i k \pi x}, \quad x_k = -1 + \frac{2}{N} \]
  - Non-periodic - Chebyshev (or Legendre)
    \[ \phi_k(x) = \cos(k \arccos(x)), \quad x_k = -\cos(\frac{k\pi}{N}) \]

- **RBFs** - scattered centers in complex domains
  \[ \phi_k(r = \|x - x_k\|_2, \varepsilon) = \sqrt{1 + \varepsilon^2 r^2} \]
Grids/Domains
Grids/Domains
RBFs

- Simple, Grid/Geometry free, Spectrally accurate.
- Extend trivially to any number of spatial dimensions.
- Ill-conditioning, Efficient implementation, Stability for time-dependent PDE problems.
- “small” $\varepsilon \Rightarrow$ better accuracy, worse conditioning of the system matrix.
- Uncertainty relation: The error and the condition number cannot both be kept small.
- $\nexists$ a formula to specify the optimal value of $\varepsilon$.
- Computation with the “optimal” $\varepsilon$ is often not possible with standard algorithms.
- In the limiting case $\varepsilon \rightarrow 0$ the RBF interpolant is a polynomial interpolant in 1d.
- RBF methods - generalized spectral methods
Spectral Accuracy

- Spectral
  - \( O(N^{-m}) \) (for every \( m \)) - infinitely differentiable
  - \( O(c^N) \), \( 0 < c < 1 \) - analytic
- RBF
  \[ O\left(e^{-\frac{K(\varepsilon)}{h}}\right) \]

where the fill distance

\[ h_{\Xi} = \sup_{\xi \in \Xi} \min_{\xi_j \in \Xi} ||\xi - \xi_j||. \]

and \( K(\varepsilon) \) is a constant that depends on the value of the shape parameter.
Spectral Accuracy
Gibbs Phenomenon
RBF vs. Pseudospectral Gibbs

From top to bottom, $N = 39, 79, 159$. Left: MQ RBF. Right: Chebyshev.
Pseudospectral events

- Fourier (1822)
- Wilbraham (1848)
- Gibbs (1898)
- Fejer (1900) - 1st order spectral filter
- Lanczos (1938) - application to ODEs
- Cooley and Tukey (1965) - FFT
- Kreiss and Oliger (1972) - Fourier spectral collocation
- Orzag (1972) - coined term pseudospectral
- Gottlieb and Orzag (1977) - theory
Pseudospectral events

- Gottlieb and Tadmor - (1984) physical space filters
- Vandeven (1991) - spectral filters
- Gottlieb, et. al (1992) - Gegenbauer reprojection
- Gelb and Tadmor (1999) - edge detection
- Shizgal and Jung (2003) - inverse reprojection
- Gelb and Tanner (2006) - Freud reprojection
- Sarra (2006) - DTV filtering
RBF events

- Hardy (1971) - MQ RBF for scattered interpolation
- Franke (1979) - survey of scattered methods
- Micchelli (1986) - RBF system matrix invertible
- Kansa (1990) - RBF methods for PDEs
- Madych and Nelson (1992) - spectral convergence
- Driscoll and Fornberg (2002) - connection to Lagrange interpolant
- Sarra (2006) - DTV filtering
- Bresten, Gottlieb, Higgs, and Jung (2008) - Gegenbauer reprojection
Postprocessing Methods

- Spectral filtering
- Rational Reconstruction (*)
- Reprojection Methods *
  - Gegenbauer *
  - Freud *
- Inverse Polynomial Reprojection *
- Digital Total Variation Filtering
- Hybrid Method

* Requires edge detection.
Matlab Postprocessing Toolbox

- collection of Matlab functions
- edge detection and postprocessing algorithms
- Fourier and Chebyshev
- one and two space dimensions
- applications, algorithm benchmarking, and educational purposes
- graphical user interface

http://www.scottssarra.org/mpt/mpt.html
The function is defined as:

\[ f(x) = \chi_{[-0.5, 0.5]} \cdot \sin[\cos(x)] \]
Spectral Filter

\[ \mathcal{F}_N f(x) = \sum_k \sigma(k/N) a_k \phi_k(x) \]

- **Exponential Filter**
  \[ \sigma_1(\omega) = e^{-\ln \varepsilon_m \omega^\rho} \]

- **Erfc-Log filter**
  \[ \sigma_2(\omega) = \frac{1}{2} \text{erfc} \left( 2\sqrt{\rho} \left| \omega \right| - 1/2 \right) \sqrt{\frac{-\ln \left( 1 - 4 \left| \omega \right| - 1/2 \right)^2}{4 \left| \omega \right| - 1/2}} \left( 2\sqrt{\rho} \left| \omega \right| - 1/2 \right) \]

- **Vandeven filter**
  \[ \sigma_3(\omega) = 1 - \frac{(2\rho - 1)!}{(\rho - 1)!} \int_0^{\left| \omega \right|} t^{\rho - 1} (1 - t)^{\rho - 1} dt \]
\[ |f(x) - \mathcal{F}_N(x)| \leq \frac{K}{d(x)^{\rho-1}N^{\rho-1}} \]

- discontinuity at \( x_0 \), \( d(x) = x - x_0 \)
- \( \rho \) sufficiently large, \( d(x) \) not too small, error goes to zero faster than any finite power of \( 1/N \), i.e. spectral accuracy is recovered.
- If \( d(x) = \mathcal{O}(1/N) \) then the error estimate is \( \mathcal{O}(1) \).
- extends easily to higher dimensions
Vandeven Filtered $\rho = 4$ Fourier approximation and error.
Rational Reconstruction

\[ R_{K,M} = \frac{P_K}{Q_M} = \frac{\sum_{k=0}^{K} p_k \phi_k(x)}{\sum_{m=0}^{M} q_m \phi_m(x)} \]

determined by imposing the orthogonality relations

\[ \langle Qu - P, \phi \rangle = 0, \quad \forall \phi \in \mathbb{P}_N \]

a (ill-conditioned) linear system must be solved

may incorporate edge detection

can be applied “slice by slice” in higher dimensions

high numbered spectral coefficients may contain significant noise and should not be used

lacks theoretical support - works mysteriously
Rational Reconstruction Example

Chebyshev Rational Reconstruction.
Reprojection Methods

In each of the $i$ smooth subintervals $[a, b]$ the function is projected or reprojected as

$$ f^i_P(x) = \sum_{\ell=0}^{m_i} g^i_{\ell} \Psi[\xi(x)] $$

1. $\xi(x)$ takes $x \in [a, b]$ to $\xi \in [-1, 1]$ and $x(\xi)$ is the inverse map
2. the reprojection basis $\Psi_{\ell}(x)$, orthogonal polynomials on $[-1, 1]$ wrt a weight $w(x)$
3. weighted inner product

$$ (\Psi_k(\xi), \Psi_{\ell}(\xi))_w = \int_{-1}^{1} \Psi_k(\xi)\Psi_{\ell}(\xi)w(\xi)d\xi = \gamma_{\ell}\delta_{k\ell} $$

- The reprojection coefficients $g^i_{\ell}$ are evaluated via a Gaussian quadrature formula.
- $\gamma_{\ell}$ is a normalization factor
Reprojection Methods

Exact Reprojection Coefficients (projection)

\[ g^i_\ell = \frac{1}{\gamma_\ell^\lambda} \int_{1}^{-1} w(\xi) \Psi^\lambda_\ell(\xi) f [x(\xi)] d\xi \]

Approximate Reprojection Coefficients (reprojection)

\[ \hat{g}^i_\ell = \frac{1}{\gamma_\ell^\lambda} \int_{1}^{-1} w(\xi) \Psi^\lambda_\ell(\xi) I_N f [x(\xi)] d\xi \]
Gegenbauer or Ultraspherical polynomials as the reprojection basis

\( w(x) = (1 - x^2)^{\lambda-1/2} \)

not known in closed form - calculated via a three term recurrence relationship

accurate edge detection critical

function dependent parameters \( \lambda \) and \( m \)

noise
Fourier Gegenbauer Reprojection.
Edges located at $x = -0.48$ and $x = 0.5$
Chebyshev spectral viscosity and GRP postprocessed Euler density solution at time $t = 0.4$. 
Freud Reprojection

- $\Psi^\lambda_\ell$, Freud polynomials
- $w(x) = e^{-cx^2}$
- $c = \ln \epsilon_M$ where $\epsilon_M$ is machine epsilon
- not known in closed form - calculated via a three term recurrence relationship; weights not known - quadrature or Stieltjes procedure
- accurate edge detection critical
- $\lambda = \text{round} \left( \sqrt{N(b-a)/2} - 2\sqrt{2} \right)$
- $m_i = N(b-a)/8$ (with earlier truncation possible)
Freud Reprojection Example

Fourier Freud Reprojection.
reprojection methods are referred to as direct methods as they compute the reprojection coefficients directly from the spectral expansion coefficients $a_k$ (or function values)

inverse methods compute the reprojection coefficients by solving a (ill-conditioned) linear system of equations, $Wg = a$

yield a unique reconstruction using any polynomial reconstruction basis functions

needs the exact value of the function being approximated at equally spaced grid points in order to calculate the spectral expansion coefficients $a \Rightarrow$ useless in PDE problems

accurate edge detection critical
IPRM postprocessed Fourier approximation.
DTV Filtering

- Originated in Image Processing
- Formulates a minimization problem which leads to a nonlinear Euler-Lagrange PDE to be solved
- Works with point values in physical space and not with the spectral expansion coefficients
- Built in edge detection
- Computationally efficient
- No claim of restoring spectral accuracy

DTV Filtering

- Neighborhood of a node $\alpha$: $N_\alpha = \{ \beta \in \Omega \mid \beta \sim \alpha \}$
- Graph variational problem - minimize the fitted TV energy

$$E^{TV}_\lambda(u) = \sum_{\alpha \in \Omega} |\nabla_\alpha u|_a + \frac{\lambda}{2} \sum_{\alpha \in \Omega} (u_\alpha - u^0_\alpha)^2$$

- unique solution - the solution of the nonlinear restoration equation

$$\sum_{\beta \sim \alpha} (u_\alpha - u_\beta) \left( \frac{1}{|\nabla_\alpha u|_a} + \frac{1}{|\nabla_\beta u|_a} \right) + \lambda (u_\alpha - u^0_\alpha) = 0$$

- $u^0$ - spectral approximation containing the Gibbs oscillations
- $\lambda$ the user specified fitting parameter
- regularized location variation (strength function) at node $\alpha$

$$|\nabla_\alpha u|_a = \left[ \sum_{\beta \in N_\alpha} (u_\beta - u_\alpha)^2 + a^2 \right]^{1/2}.$$
Solving the Restoration Equation

- linearized Jacobi iteration
- time marching with a preconditioned restoration equation

\[ \frac{du_\alpha}{dt} = \sum_{\beta \sim \alpha} (u_\alpha - u_\beta) \left( 1 + \frac{\left| \nabla_\alpha u \right|}{\left| \nabla_\beta u \right|} \right) + \lambda \left| \nabla_\alpha u \right| (u_\alpha - u_\alpha^0). \]

- about 100 time steps are required to approach a steady state
- stronger oscillations - small fitting parameter \((< 10)\)
- weaker oscillations - larger value of the fitting parameter
DTV postprocessed Fourier Approximation.
In 2d there is more than one way to define $N_\alpha$:

1. $N^4_\alpha = \{\alpha_{i,j+1}, \alpha_{i+1,j}, \alpha_{i,j-1}, \alpha_{i-1,j}\}$

2. $N^8_\alpha = \{\alpha_{i,j+1}, \alpha_{i+1,j+1}, \alpha_{i+1,j}, \alpha_{i+1,j-1}, \alpha_{i,j-1}, \alpha_{i-1,j-1}, \alpha_{i-1,j}, \alpha_{i-1,j+1}\}$. 
DTV postprocessed Fourier Approximation of

\[ f(x) = \begin{cases} 
1 & x^2 + y^2 \leq \frac{1}{4} \\
0 & \text{otherwise}
\end{cases} \]
Hybrid

Edge detection free postprocessing

- DTV filtering near discontinuities
- Spectral filtering away from discontinuities
- Normalized DTV strength function

\[ S = \frac{|\nabla_{\alpha} u|_a}{\max |\nabla_{\alpha} u|_a} \]

determine which is applied

- If \( S[f(x)] < S_{\text{max}} \) the spectral filter is applied at \( x \).

Hybrid, Shepp-Logan phantom slice

Left: hybrid postprocessed. Right: DTV normalized strength function.
Left: Hybrid error. Middle: spectral filter error. Right: DTV filter error.
Hybrid, Shepp-Logan phantom

Left: exact phantom. Right: Fourier approximation.
Hybrid, Shepp-Logan phantom

Left: hybrid postprocessed. Right: DTV application area (red), spectral filter (blue).
Hybrid, Shepp-Logan phantom zoom
Chebyshev Pseudospectral
Chebyshev Spectral Viscosity
Left: $N = 79$ MQ RBF, Right: DTV postprocessed $N = 79$. 
$N = 1126$ scattered points on a complexly shaped domain.
2d Neighborhoods $N_\alpha$
2d RBF DTV example
RBF-Gegenbauer example

![Graph showing f(x) and |error|](image-url)
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