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)

This work was partially supported by NSF grant DMS-0609747

Global HOAMS

$$\mathcal{I}_N f(x) = \sum_k a_k \, \phi_k(x)$$

- $\mathcal{I}_N f(x_i) = f(x_i)$ 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)

$$\phi_k(x) = e^{ik\pi x}, \quad x_k = -1 + \frac{2}{N}$$

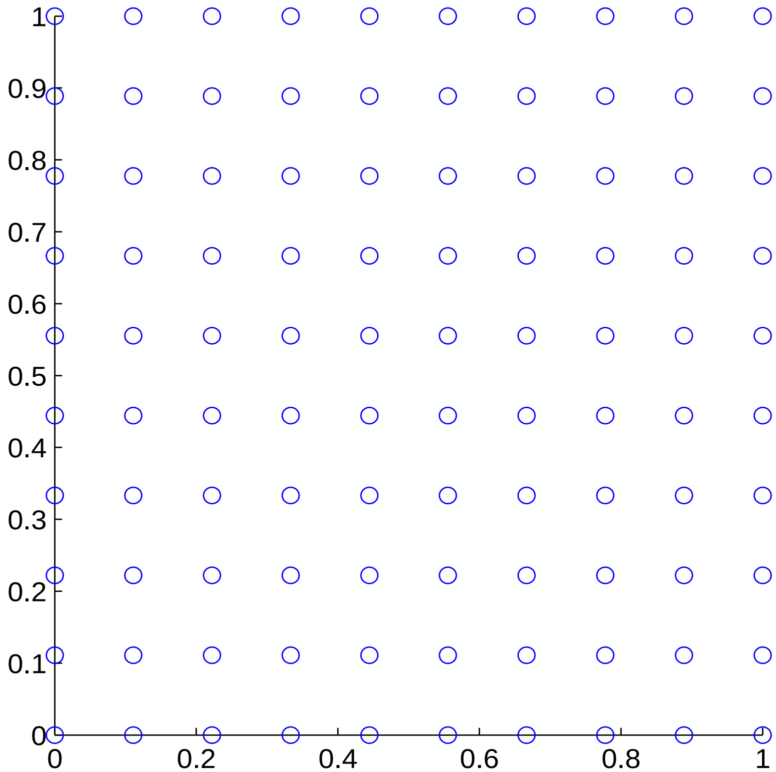
  - Non-periodic - Chebyshev (or Legendre)

$$\phi_k(x) = \cos(k \arccos{(x)}), \quad x_k = -\cos{(k\pi/N)}$$

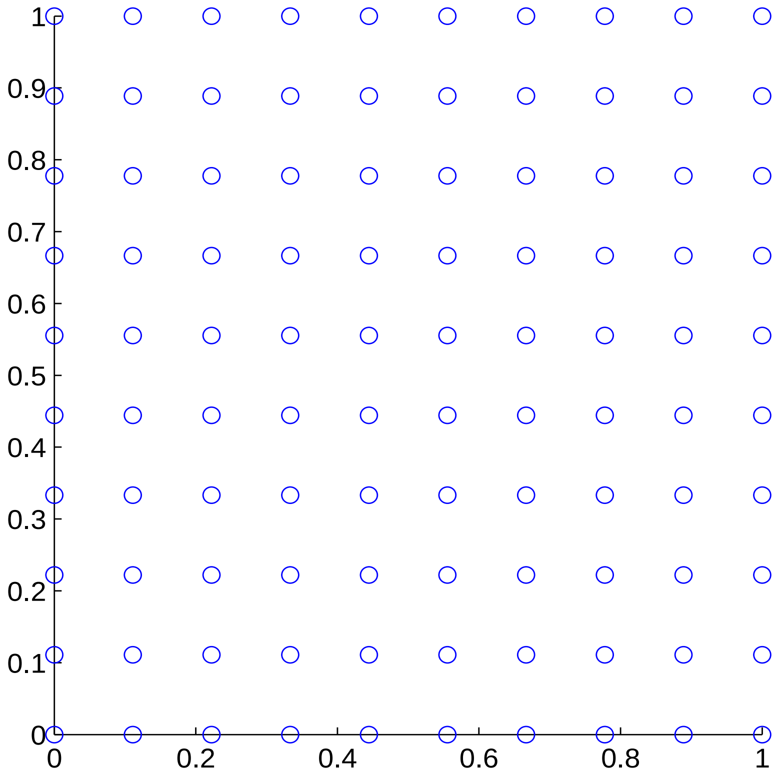
- RBFs: scattered centers in complex domains

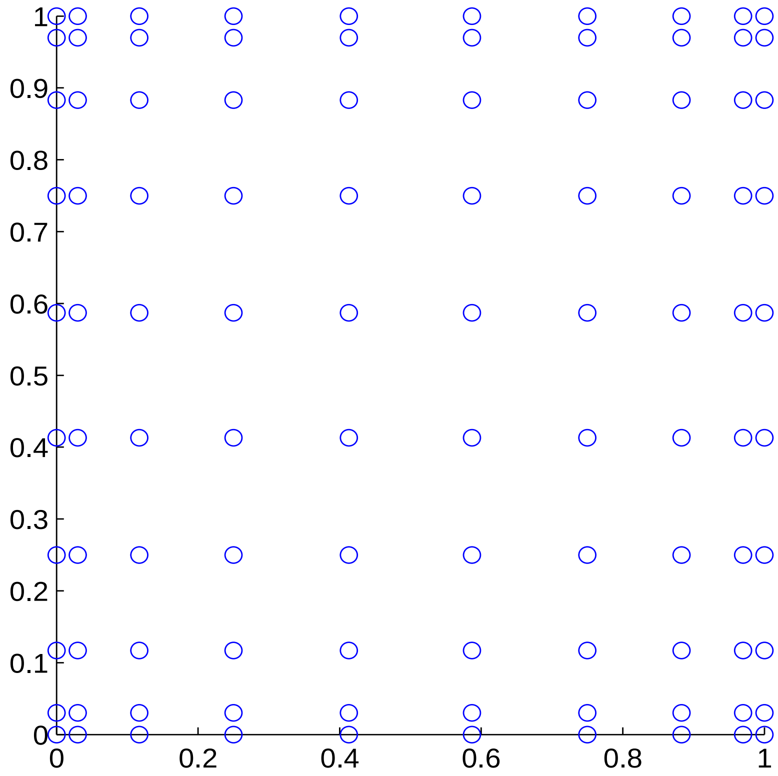
$$\phi_k(r = \left\|x - x_k\right\|_2, \varepsilon) = \sqrt{1 + \varepsilon^2 r^2}$$

Grids/Domains

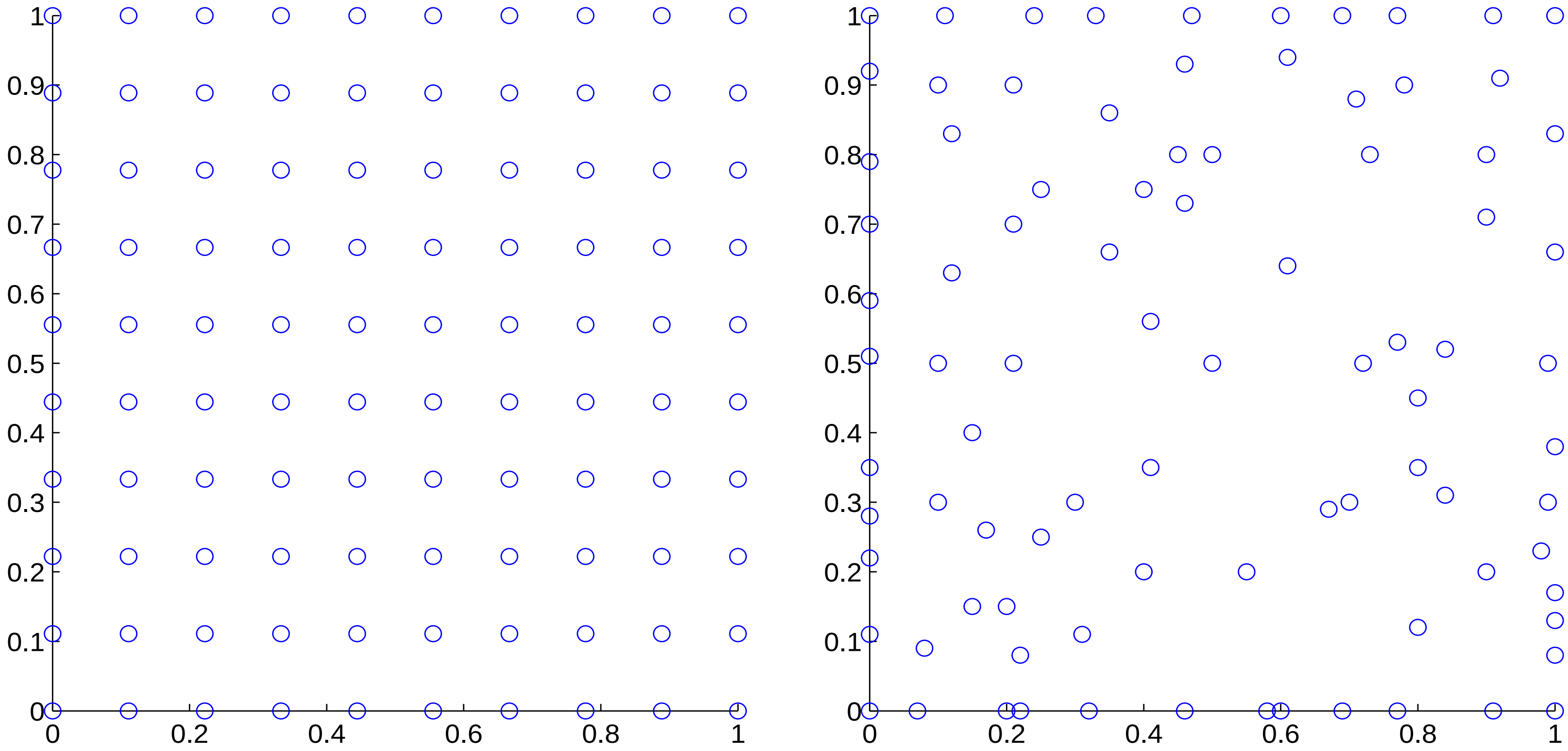


Grids/Domains

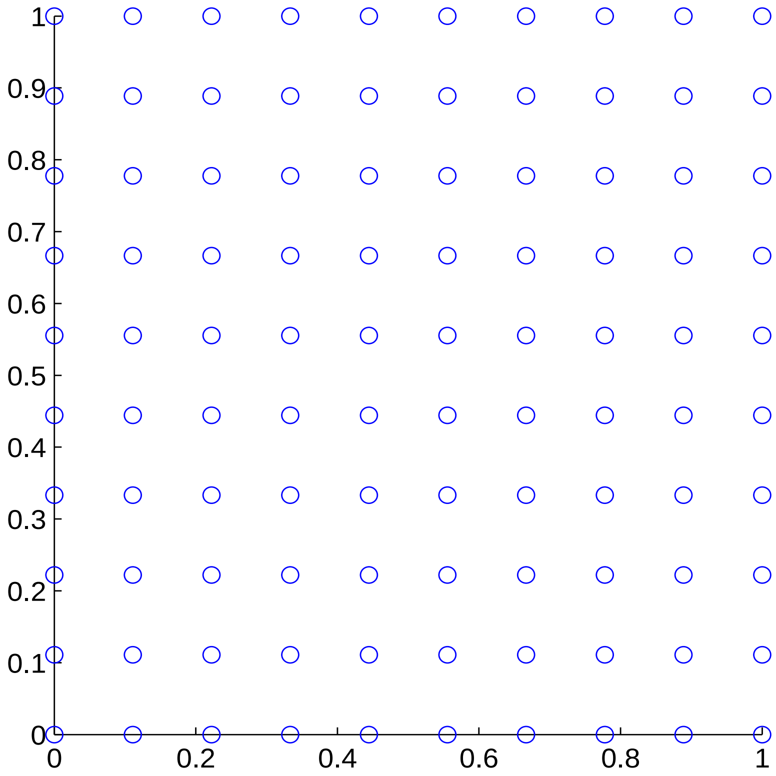


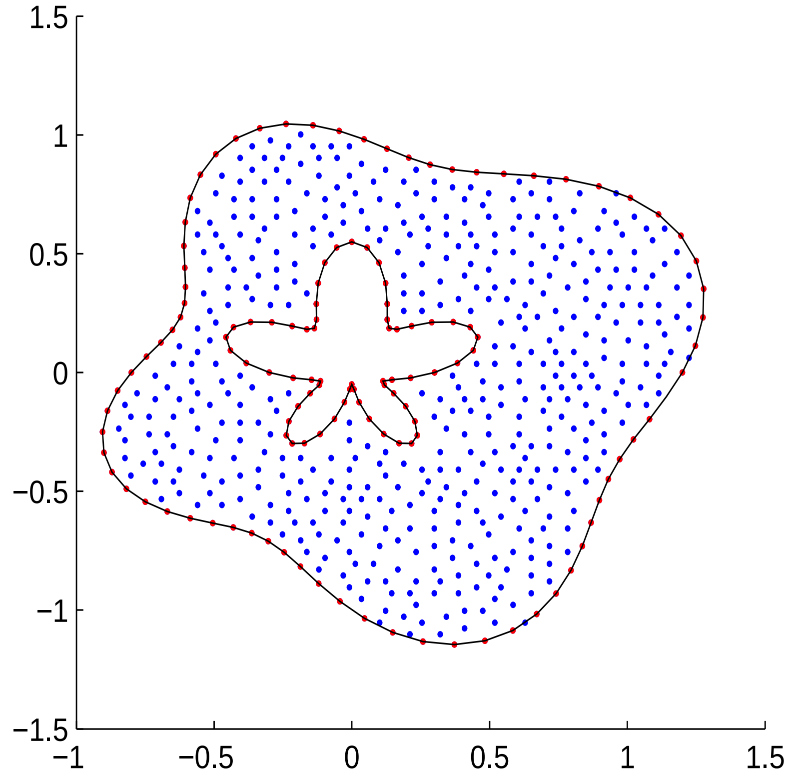


Grids/Domains



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 ε.
- Computation with the "optimal" ε is often not possible with standard algorithms.
- In the limiting case $\varepsilon \longrightarrow 0$ the RBF interpolant is a polynomial interpolant in 1d.
- RBF methods - generalized spectral methods

Spectral Accuracy

- Spectral
  - $\mathcal{O}\left(N^{-m}\right)$ (for every m) - infinitely differentiable
  - $\mathcal{O}\left(c^{N}\right)$, $0 < c < 1$ - analytic
- RBF

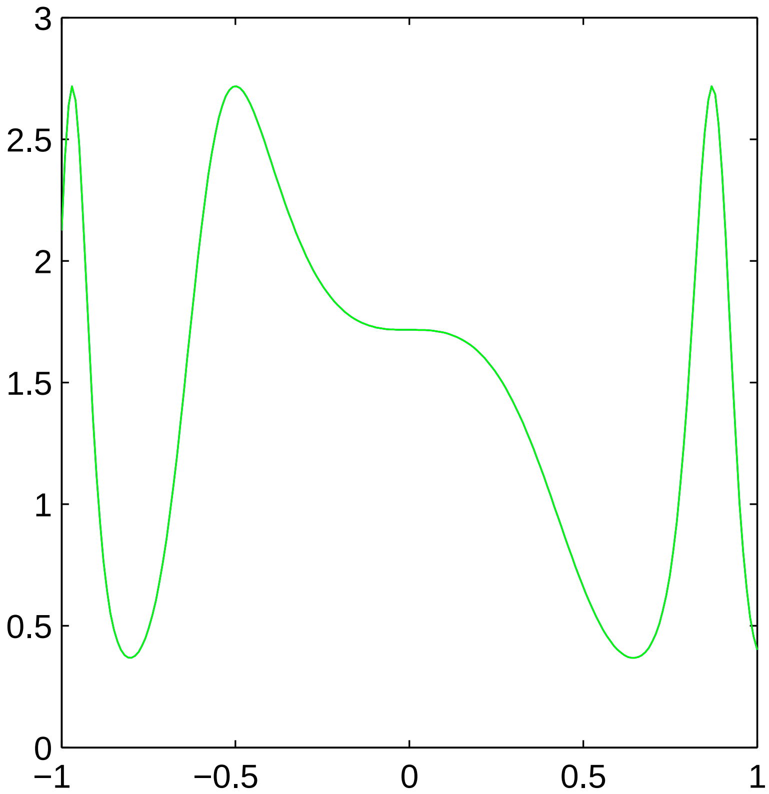
$$\mathcal{O}\left(e^{\frac{-K(\varepsilon)}{h}}\right)$$

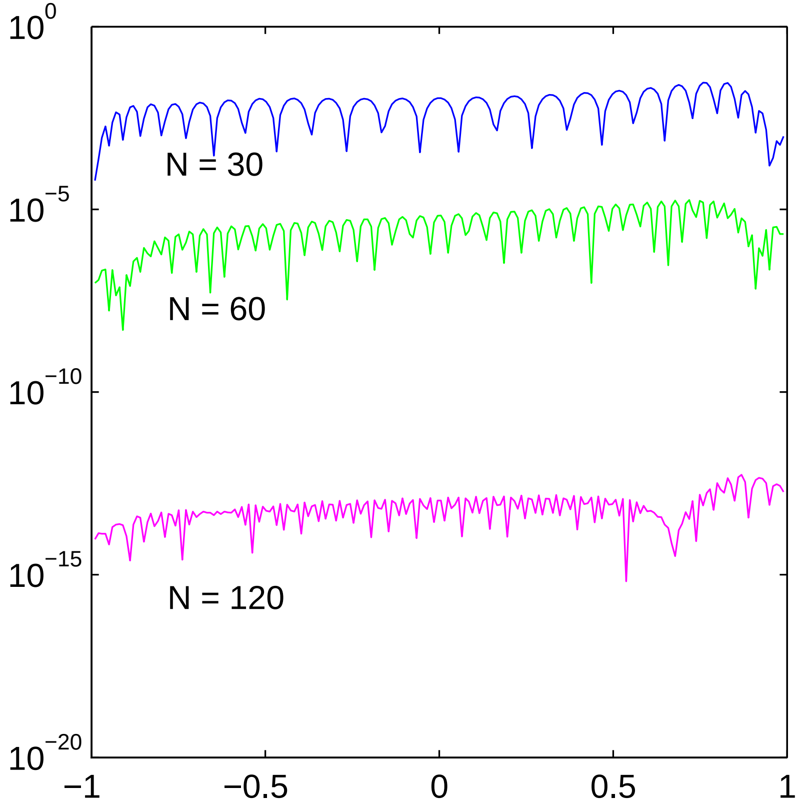
where the *fill distance*

(1) $$h_{\Xi} = \sup_{\xi \in \Xi} \min_{\xi_j \in \Xi} \left\| \xi - \xi_j \right\| .$$

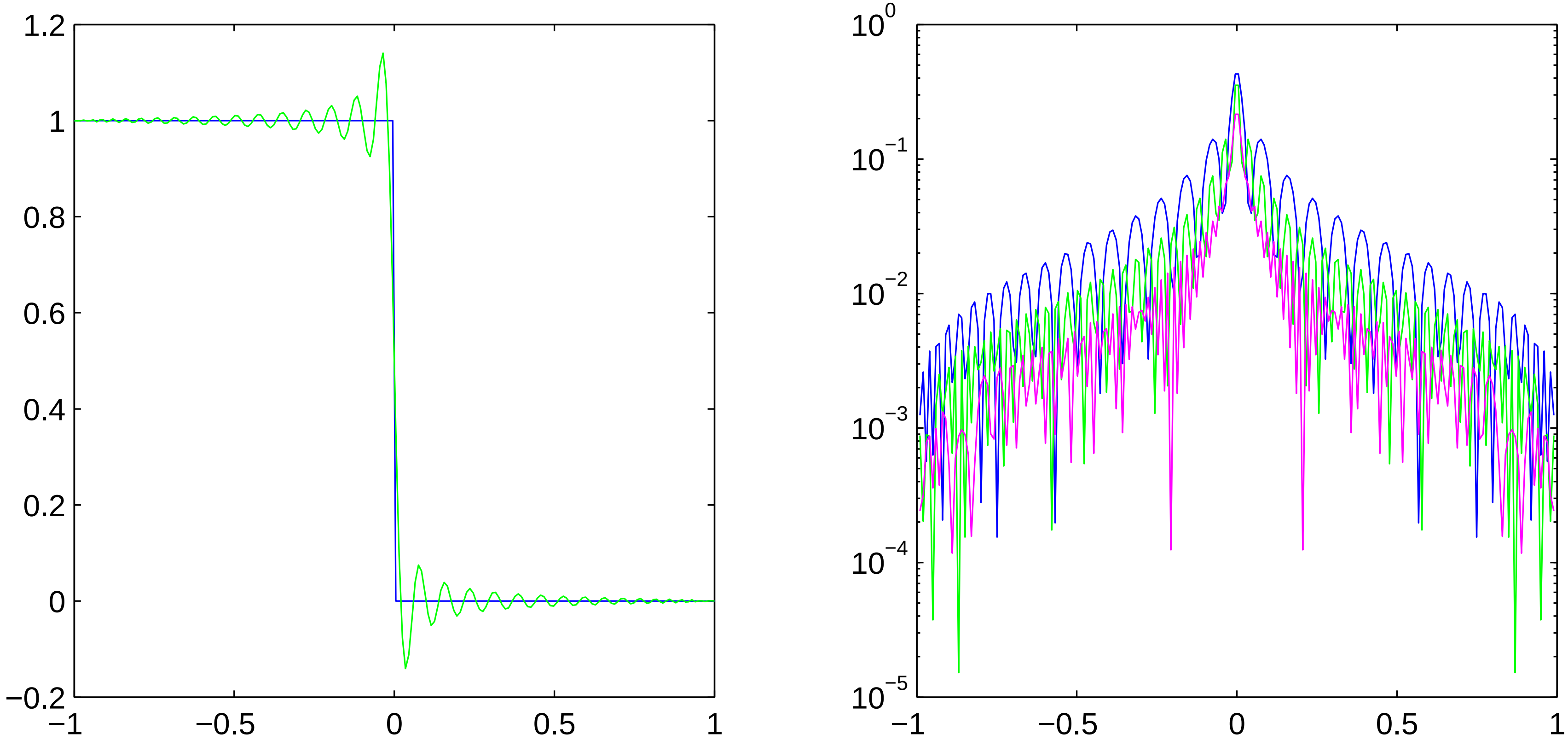
and $K(\varepsilon)$ is a constant that depends on the value of the shape parameter.

Spectral Accuracy

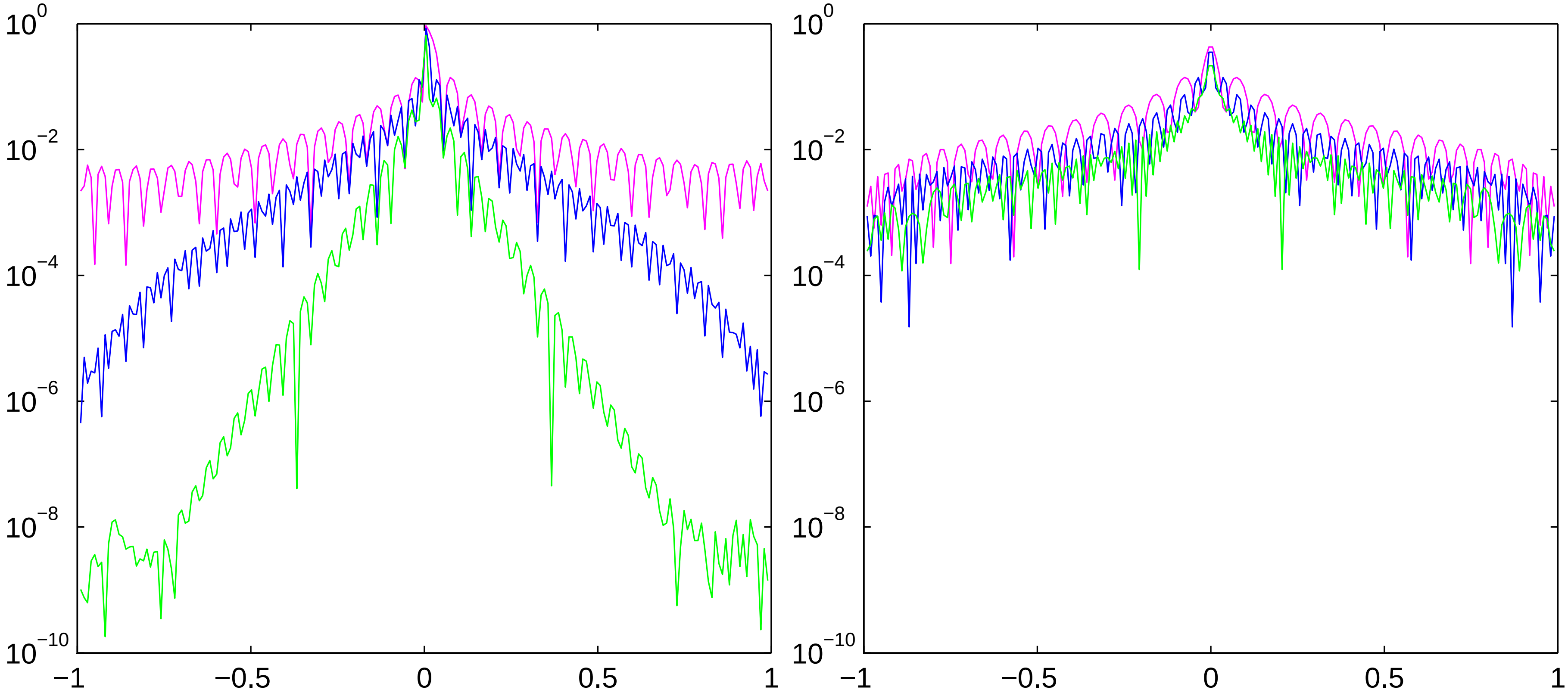




Gibbs Phenomenon



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

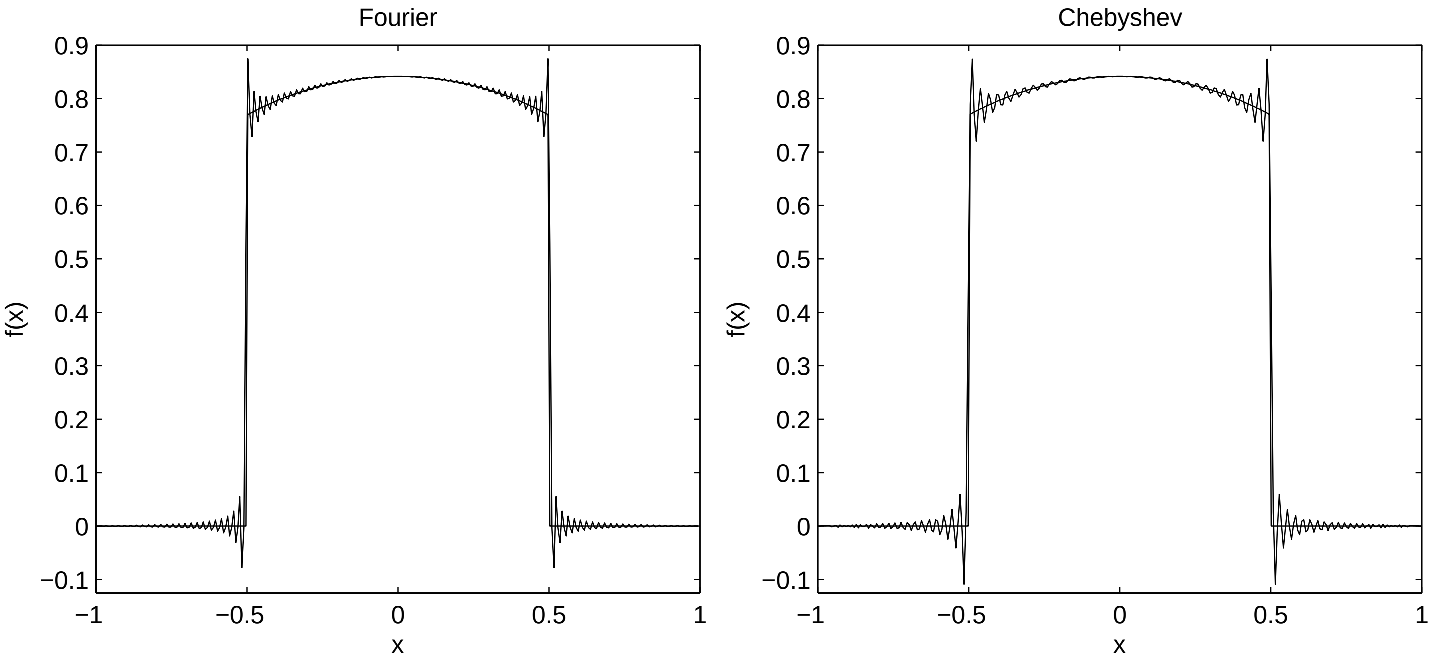
- Spectral filtering
- Rational Reconstruction $(*)$
- Reprojection Methods $*$
  - Gegenbauer $*$
  - Freud $*$
- Inverse Polynomial Reprojection $*$
- Digital Total Variation Filtering
- Hybrid Method

$*$ 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.scottsarra.org/mpt/mpt.html`

Test Function



$$f(x) = \chi_{[-0.5,0.5]} * \sin[\cos(x)]$$

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

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

- Vandeven filter

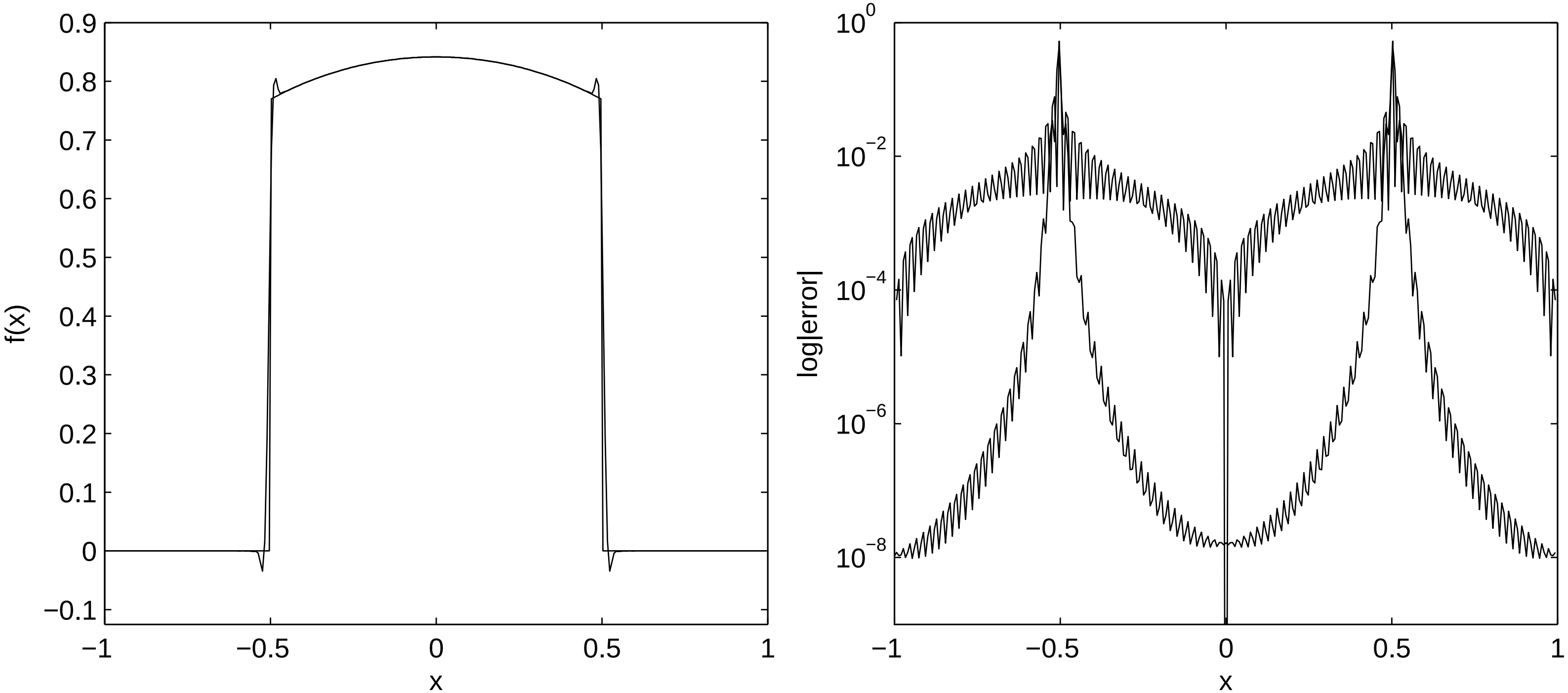
$$\sigma_3(\omega) = 1 - \frac{(2\rho - 1)!}{(p-1)!}\int_0^{|\omega|} t^{\rho-1}(1-t)^{\rho-1}\,dt$$

Spectral Filter

$$|f(x) - \mathcal{F}_N(x)| \leq \frac{K}{d(x)^{\rho-1} N^{\rho-1}}$$

- discontinuity at x_0, $d(x) = x - x_0$
- ρ 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

Spectral Filter Example



Vandeven Filtered $\rho = 4$ Fourier approximation and error.

Rational Reconstruction

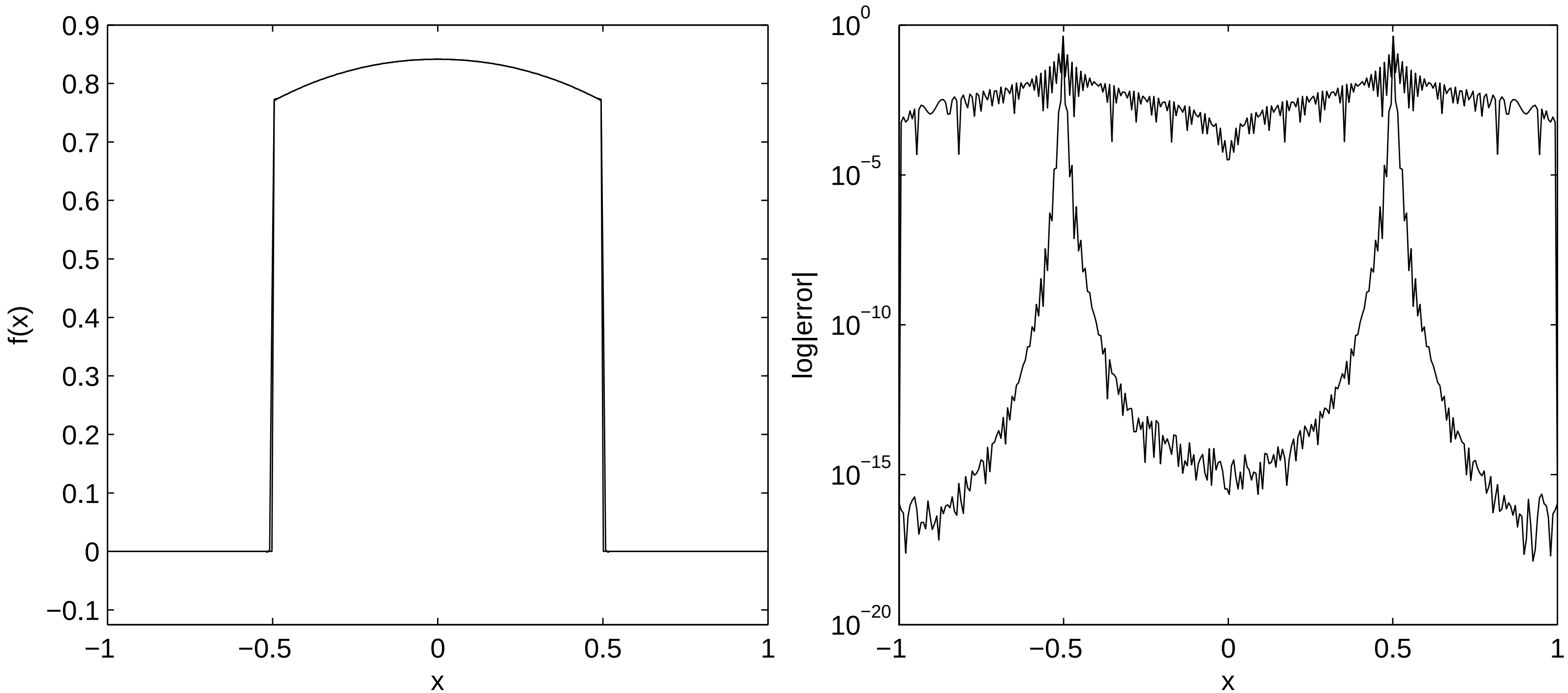
$$R_{K,M} = \frac{P_K}{Q_M} = \frac{\sum_{k=0}^{K} p_k \phi_k(x)}{\sum_{m=0}^{M} q_m \phi_m(x)}$$

- determined by imposing the orthogonality relations

$$\langle Qu - P, \phi \rangle = 0, \qquad \forall \phi \in \mathbb{P}_N$$

- 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

$$f_P^i(x) = \sum_{\ell=0}^{m_i} g_\ell^i \Psi_\ell[\xi(x)]$$

- $\xi(x)$ takes $x \in [a, b]$ to $\xi \in [-1, 1]$ and $x(\xi)$ is the inverse map
- the reprojection basis $\Psi_\ell(x)$, orthogonal polynomials on $[-1, 1]$ wrt a weight $w(x)$
- 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_ℓ^i are evaluated via a Gaussian quadrature formula.
- γ_ℓ is a normalization factor

Reprojection Methods

Exact Reprojection Coefficients (projection)

$$g_\ell^i = \frac{1}{\gamma_\ell^\lambda} \int_1^{-1} w(\xi)\Psi_\ell^\lambda(\xi) f[x(\xi)]d\xi$$

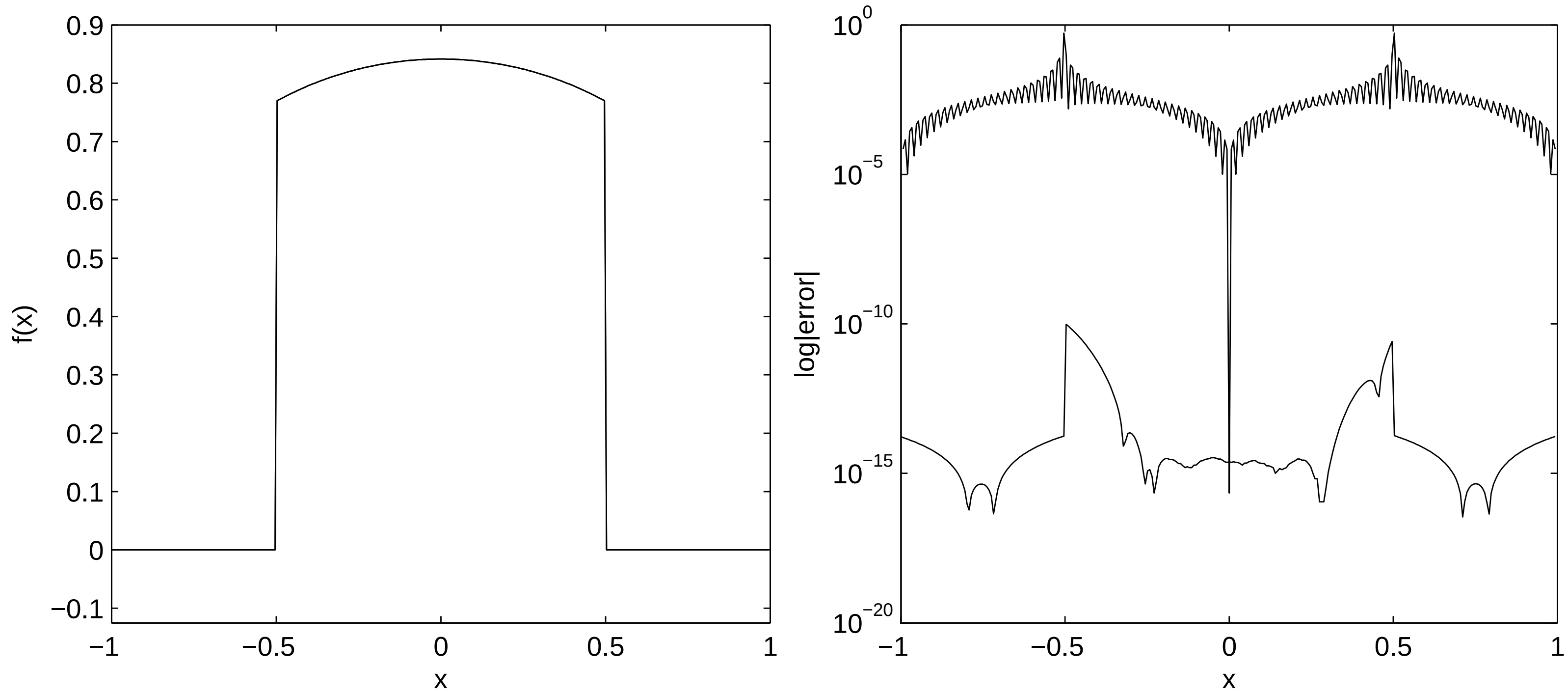
Approximate Reprojection Coefficients (reprojection)

$$\hat{g}_\ell^i = \frac{1}{\gamma_\ell^\lambda} \int_1^{-1} w(\xi)\Psi_\ell^\lambda(\xi) \mathcal{I}_N f[x(\xi)]d\xi$$

Gegenbauer Reprojection

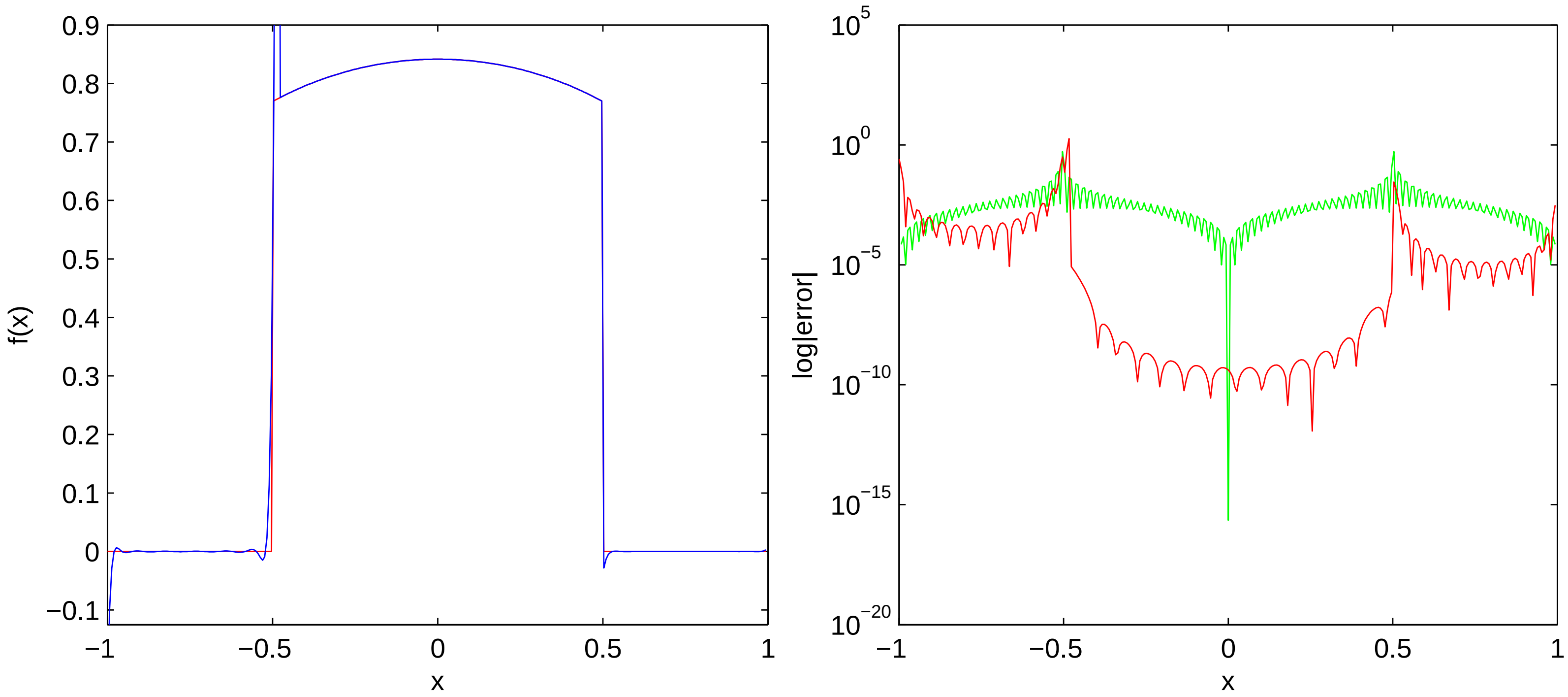
- Ψ_ℓ^λ Gegenbauer or Ultraspherical polynomials as the reprojection basis
- $w(x) = (1 - x^2)^{\lambda - 1/2}$
- not known in closed form - calculated via a three term recurrence relationship
- accurate edge detection critical
- function dependent parameters λ and m
- noise

Gegenbauer Reprojection Example



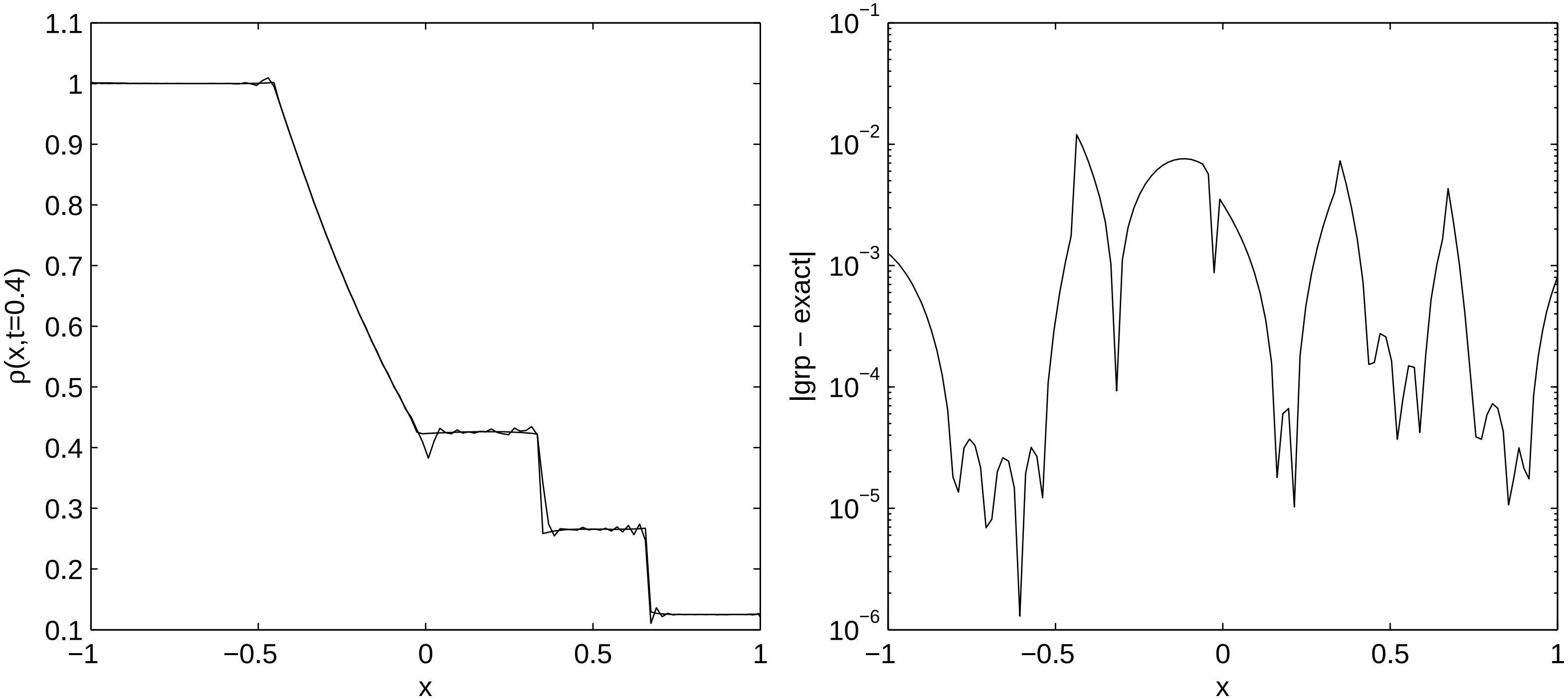
Fourier Gegenbauer Reprojection.

GRP - inaccurate edge detection



Edges located at $x = -0.48$ and $x = 0.5$

Gegenbauer Reprojection Example

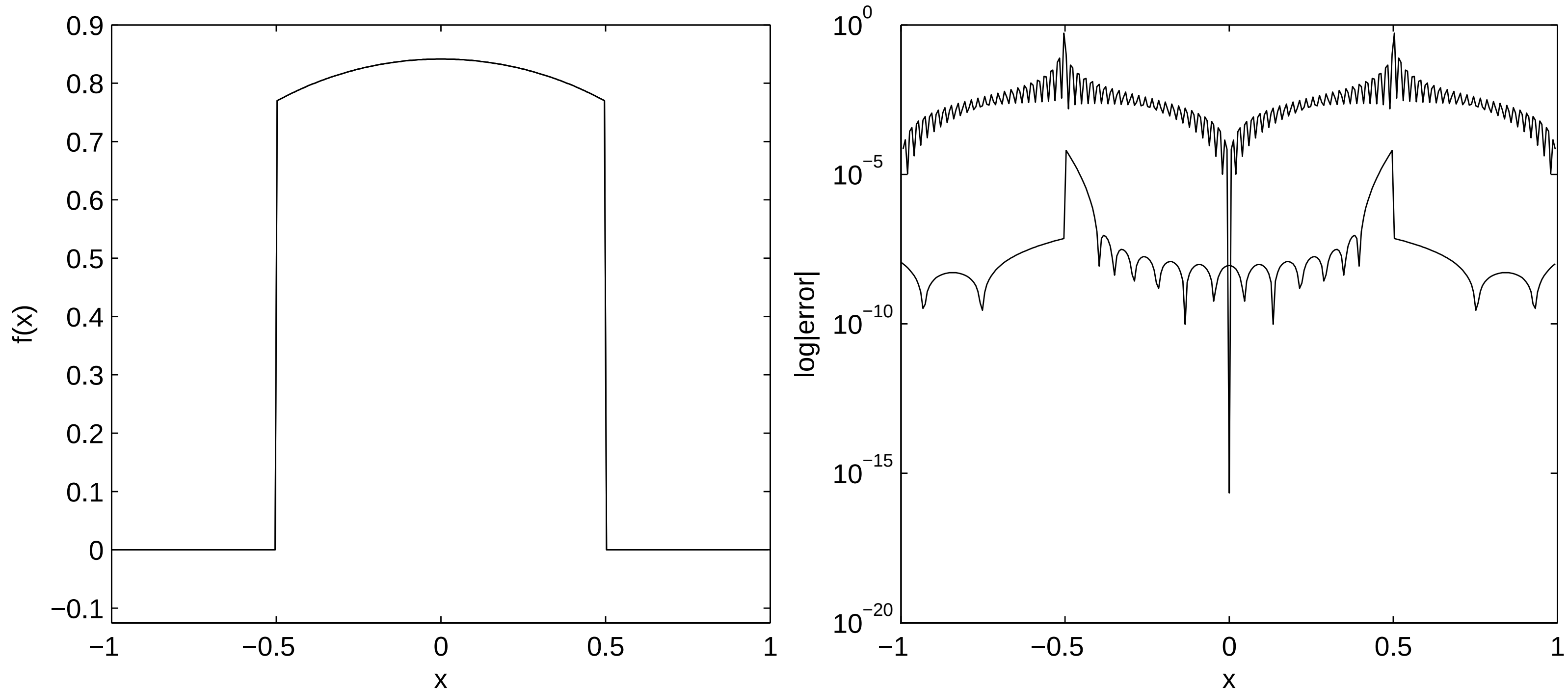


Chebyshev spectral viscosity and GRP postprocessed Euler density solution at time t = 0.4.

Freud Reprojection

- Ψ_ℓ^λ, Freud polynomials
- $w(x) = e^{-cx^{2\lambda}}$
- $c = \ln \epsilon_M$ where ϵ_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
- $\lambda =$ round $\left(\sqrt{N(b-a)/2} - 2\sqrt{(2)}\right)$
- $m_i = N(b-a)/8$ (with earlier truncation possible)

Freud Reprojection Example

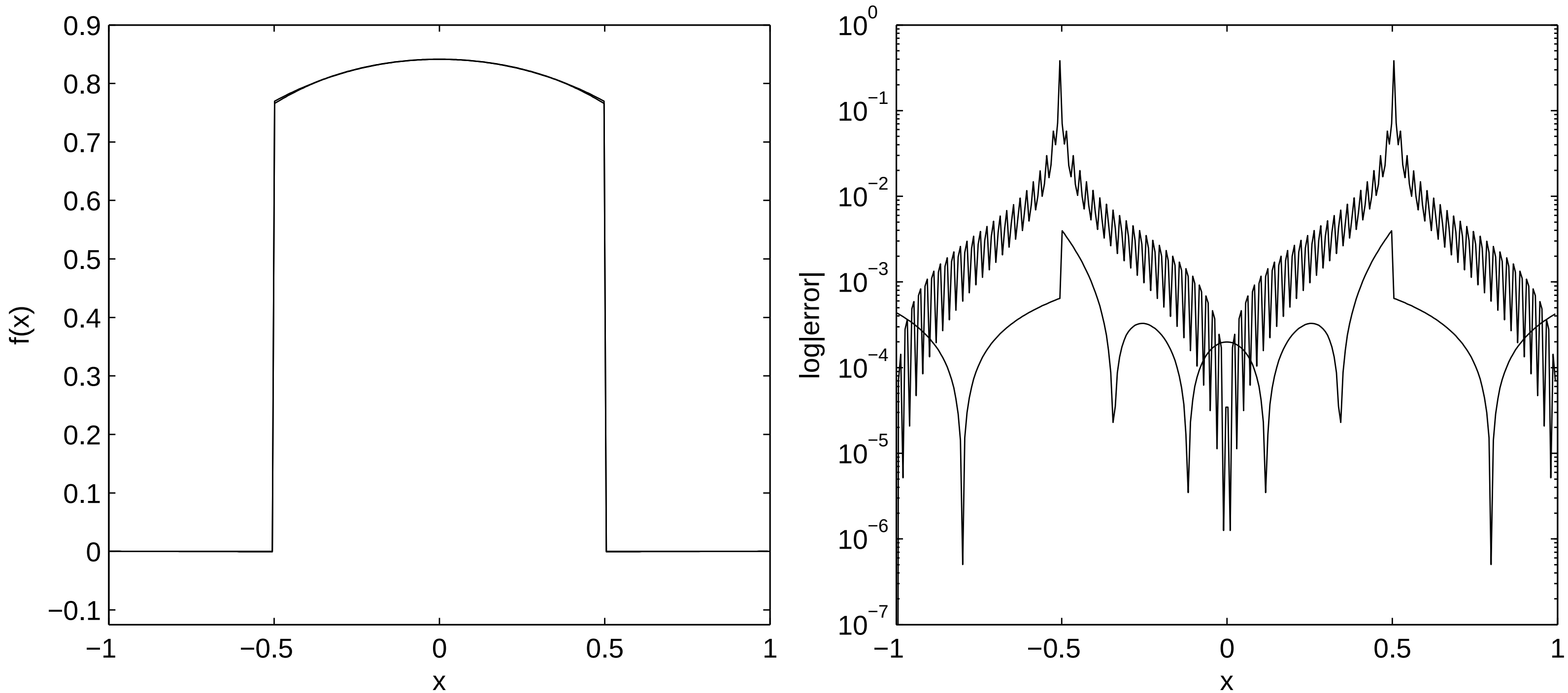


Fourier Freud Reprojection.

Inverse Polynomial 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

Inverse Polynomial Reprojection Example



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
- *Digital Total Variation Filtering as Postprocessing for Pseudospectral Methods for Conservation Laws*. Numerical Algorithms, vol. 41, p. 17-33, 2006.

DTV Filtering

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

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

- unique solution - the solution of the nonlinear restoration equation

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

- u^0 - spectral approximation containing the Gibbs oscillations
- λ the user specified fitting parameter
- regularized location variation (strength function) at node α

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

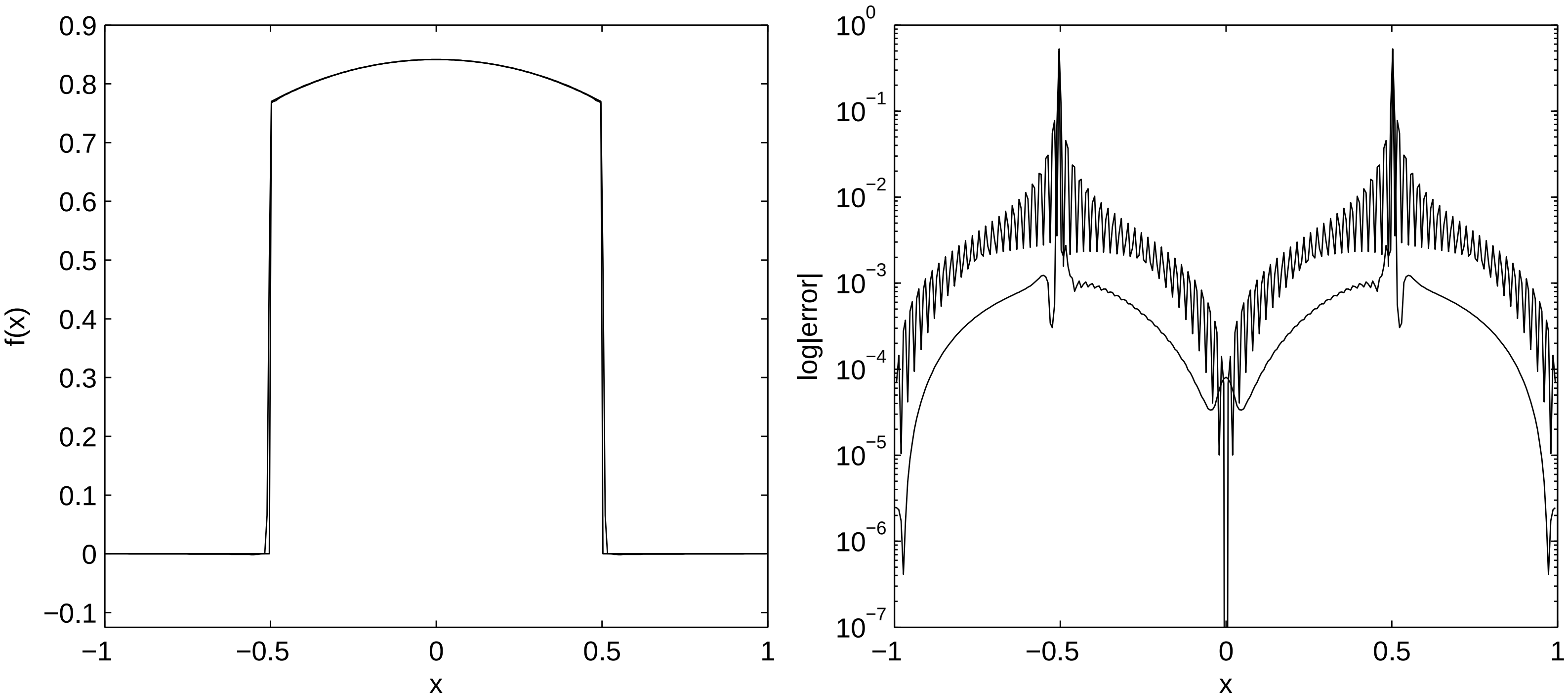
Solving the Restoration Equation

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

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

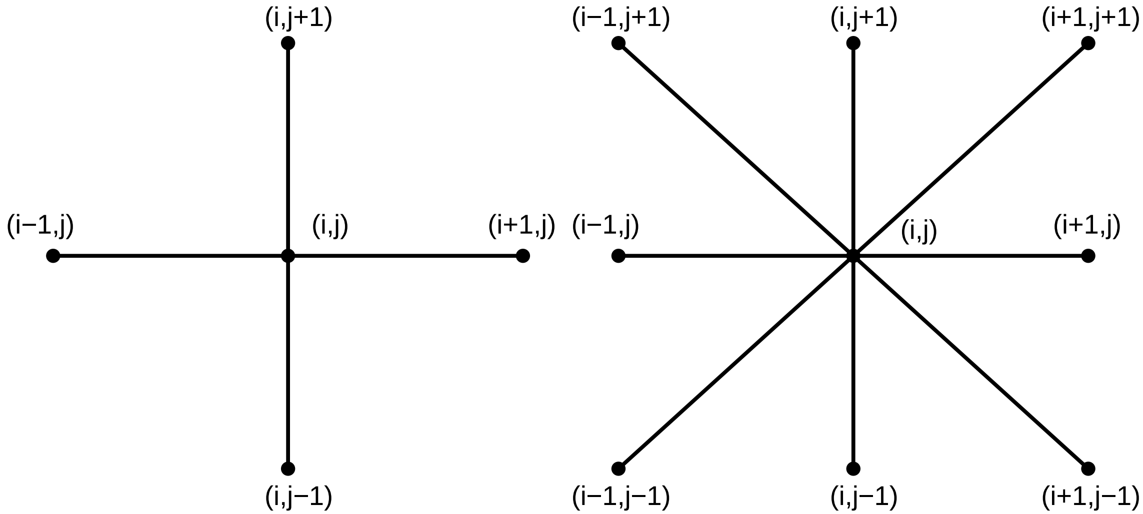
- about 100 time steps are required to approach a steady state
- stronger oscillations - small fitting parameter (< 10)
- weaker oscillations - larger value of the fitting parameter

DTV Filtering example



DTV postprocessed Fourier Approximation.

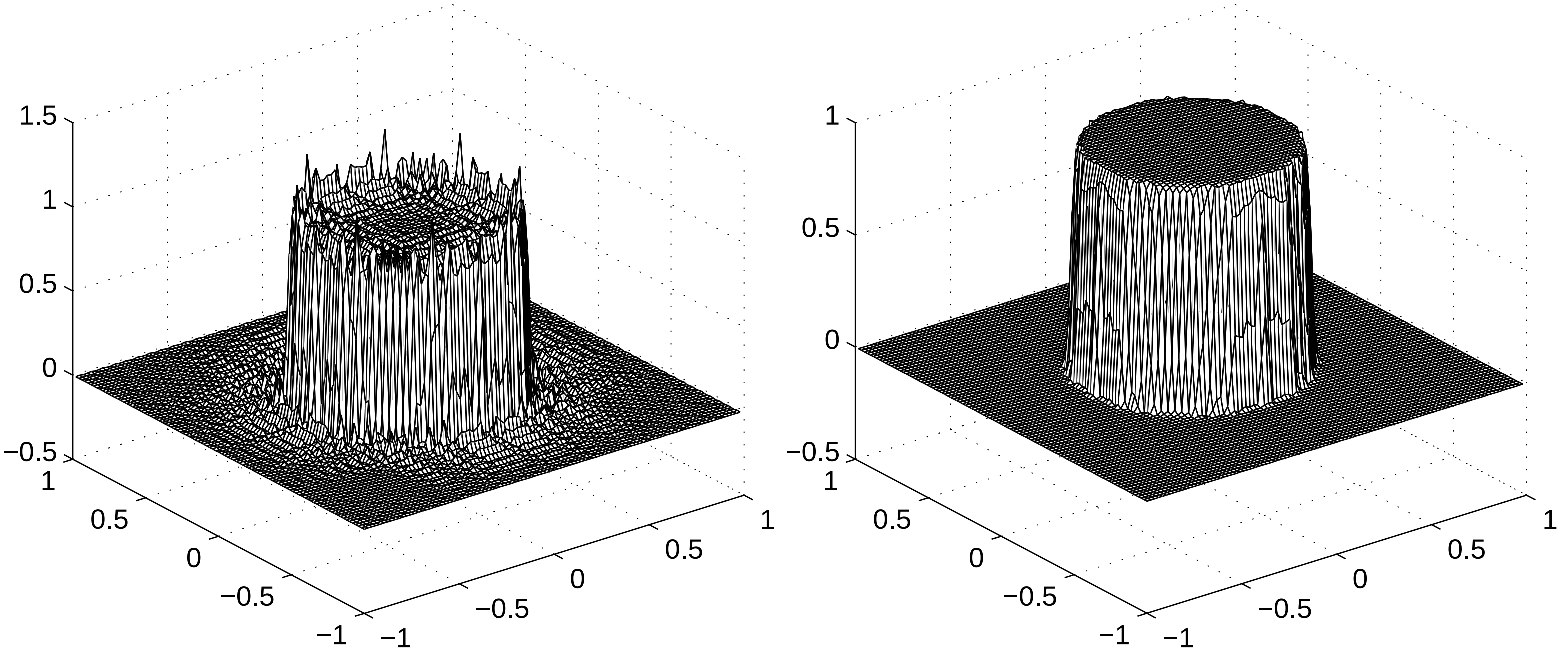
DTV Filtering - 2d



In 2d there is more than one way to define N_α:

1. $N_\alpha^4 = \{\alpha_{i,j+1}, \alpha_{i+1,j}, \alpha_{i,j-1}, \alpha_{i-1,j}\}$
2. $N_\alpha^8 = \{\alpha_{i,j+1}, \alpha_{i+1,j+1}, \alpha_{i+1,j}, \alpha_{i+1,j-1}, \alpha_{i,j-1}, \alpha_{i-1,j-1}, \alpha_{i-1,j}, \alpha_{i-1,j+1}\}$.

DTV Filtering - 2d example



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

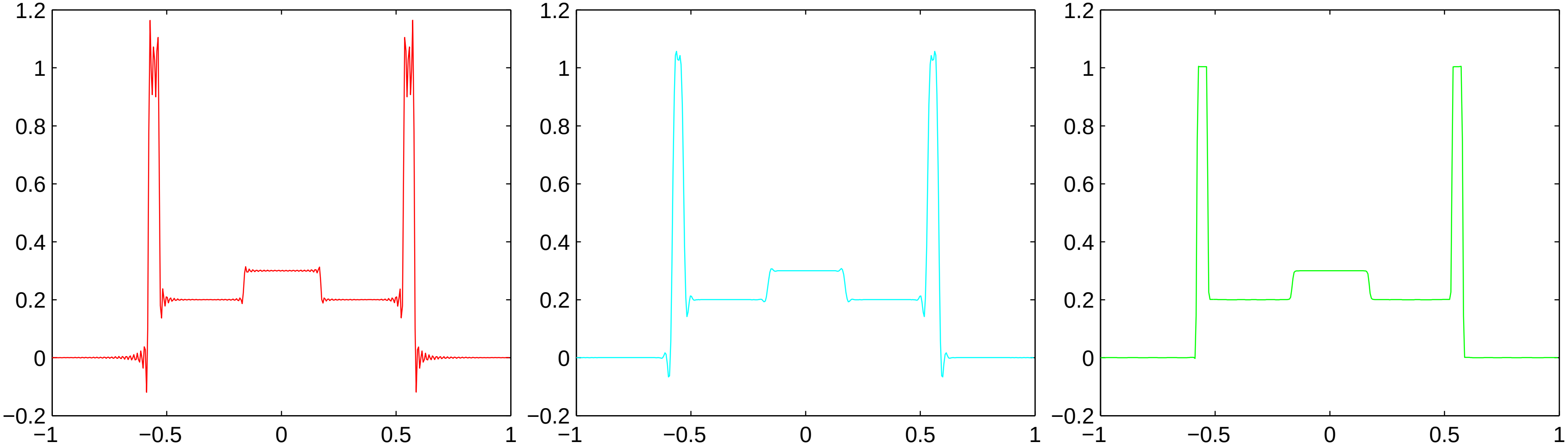
- DTV filtering near discontinuities
- Spectral filtering away from discontinuities
- normalized DTV strength function

$$\mathcal{S} = \frac{|\nabla_\alpha u|_a}{\max |\nabla_\alpha u|_a}$$

  determine which is applied

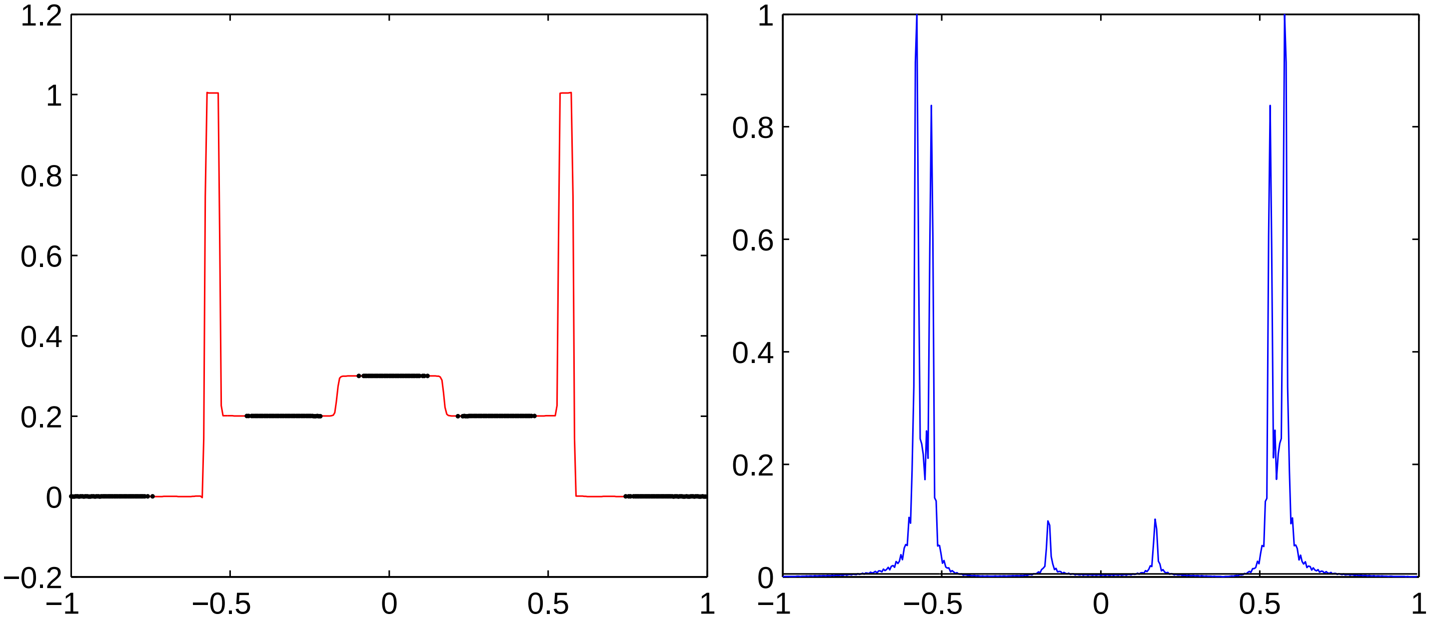
- If $\mathcal{S}[f(x)] < \mathcal{S}_{\max}$ the spectral filter is applied at x.
- *Edge Detection Free Postprocessing for Pseudospectral Approximations*. To appear in the Journal of Scientific Computing, 2009.

Hybrid, Shepp-Logan phantom slice



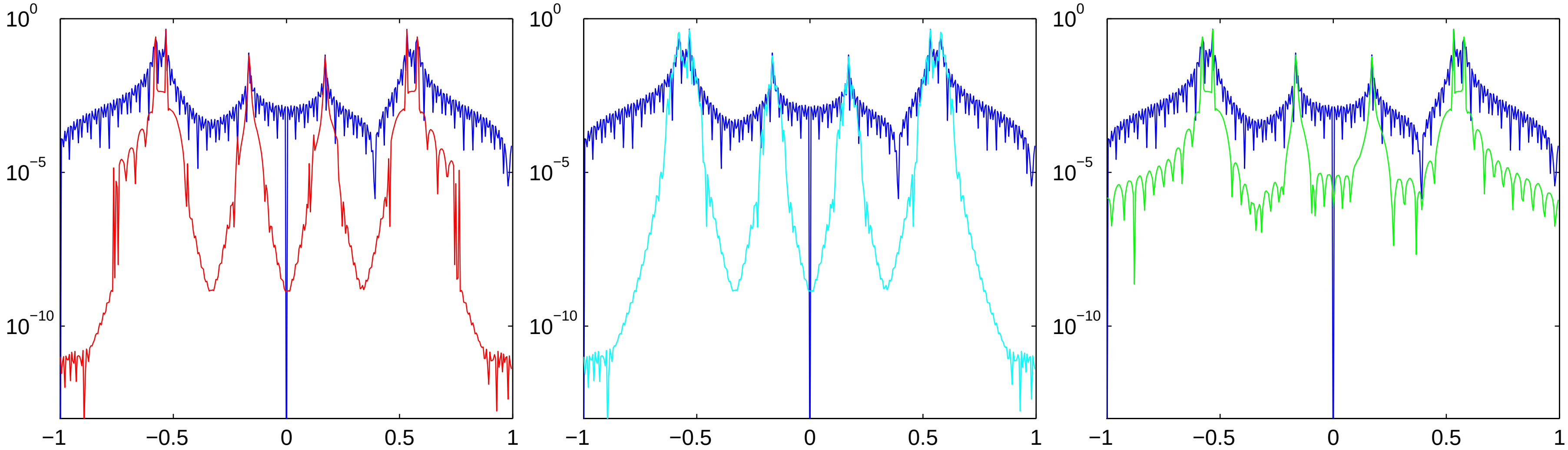
Left: Fourier approximation. Middle: weak spectral filter.
Right: DTV filtered.

Hybrid, Shepp-Logan phantom slice



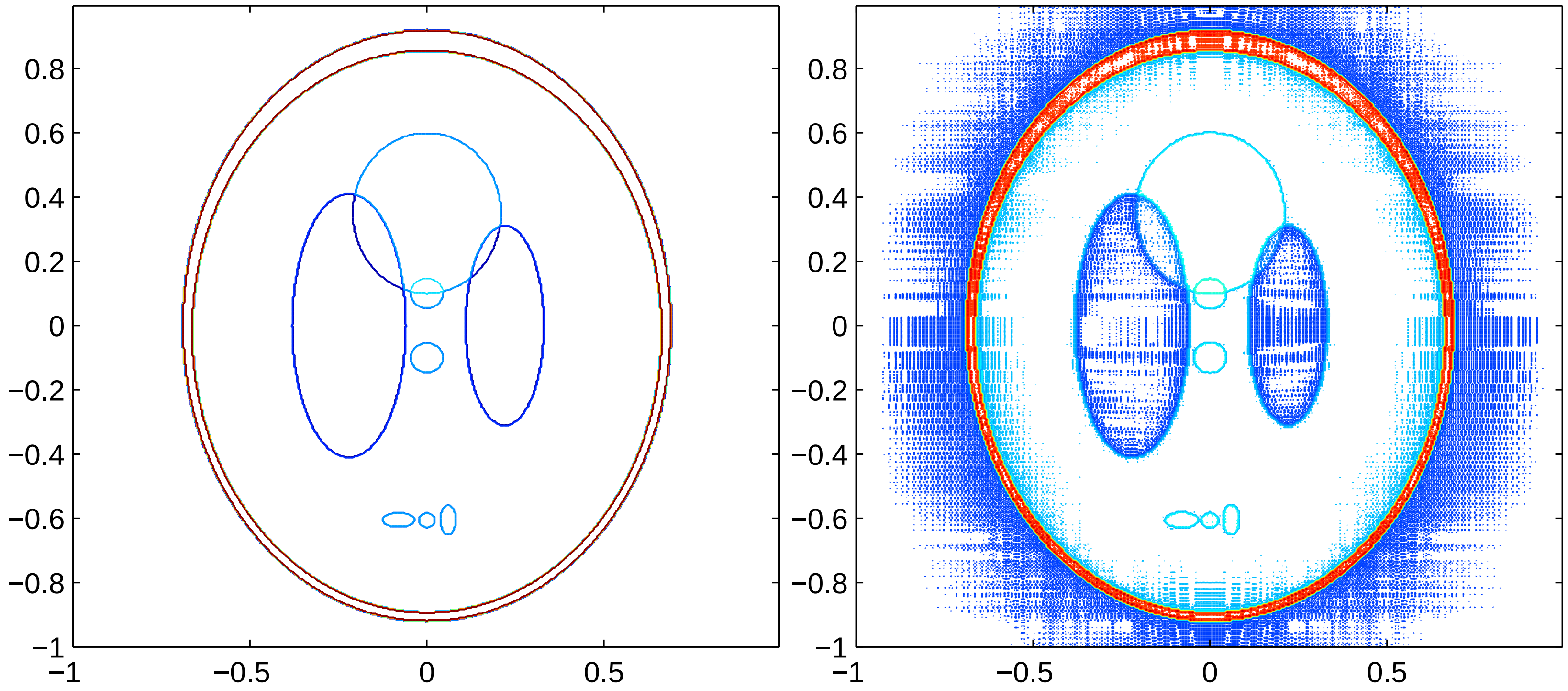
Left: hybrid postprocessed. Right: DTV normalized strength function.

Hybrid, Shepp-Logan phantom slice



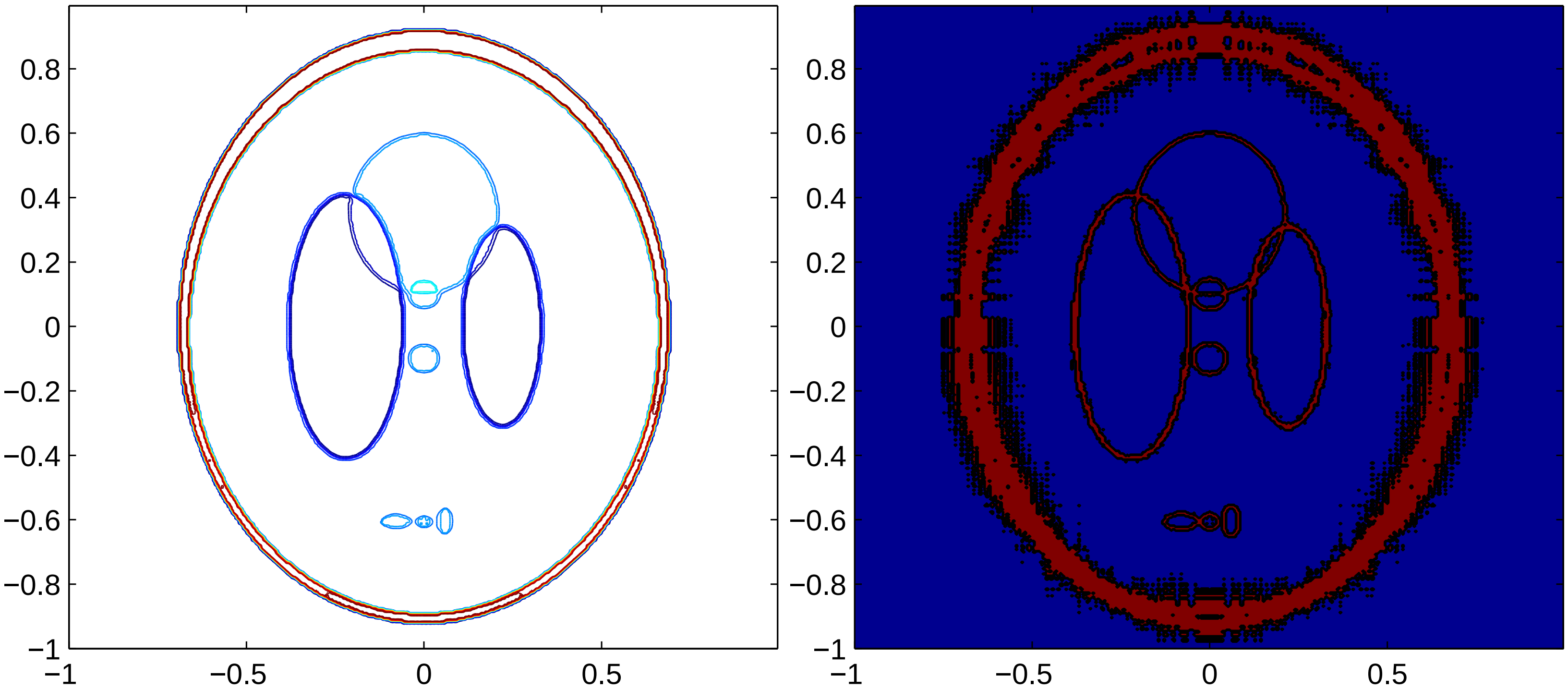
Left: Hybrid error. Middle: spectral filter error. Right: DTV filter error.

Hybrid, Shepp-Logan phantom



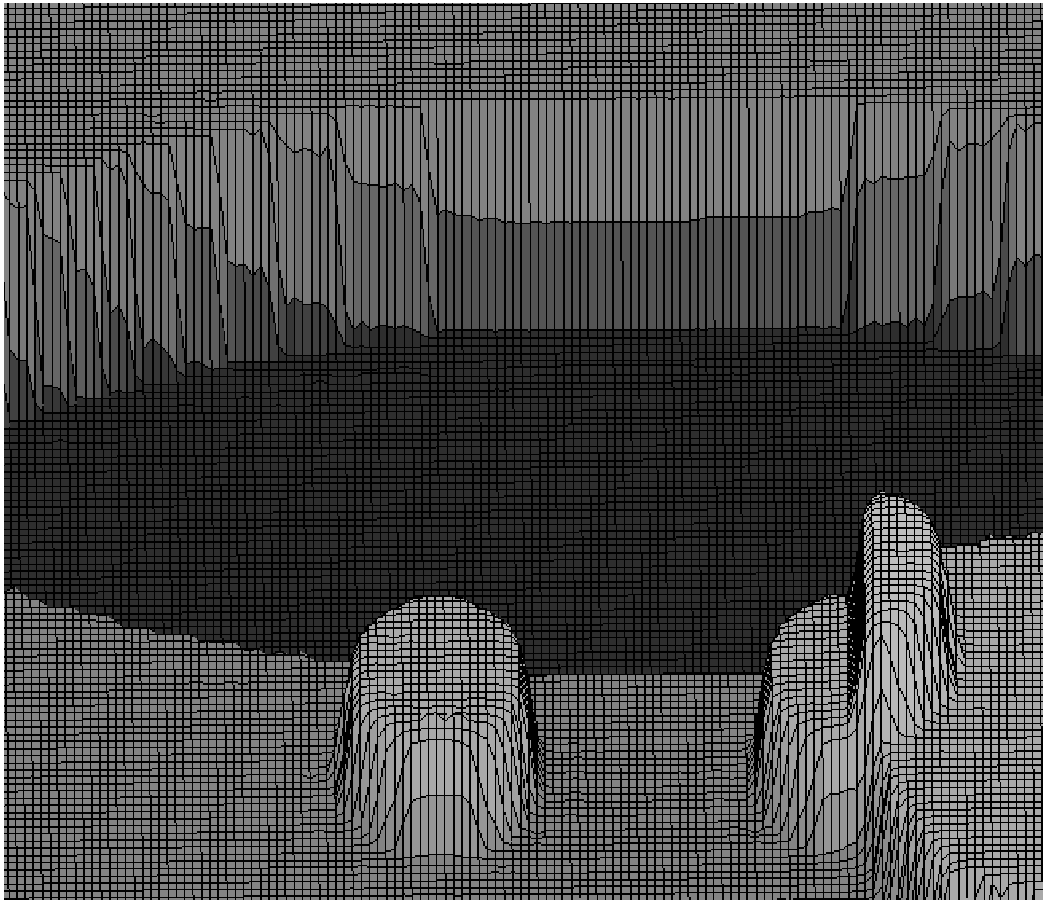
Left: exact phantom. Right: Fourier approximation.

Hybrid, Shepp-Logan phantom

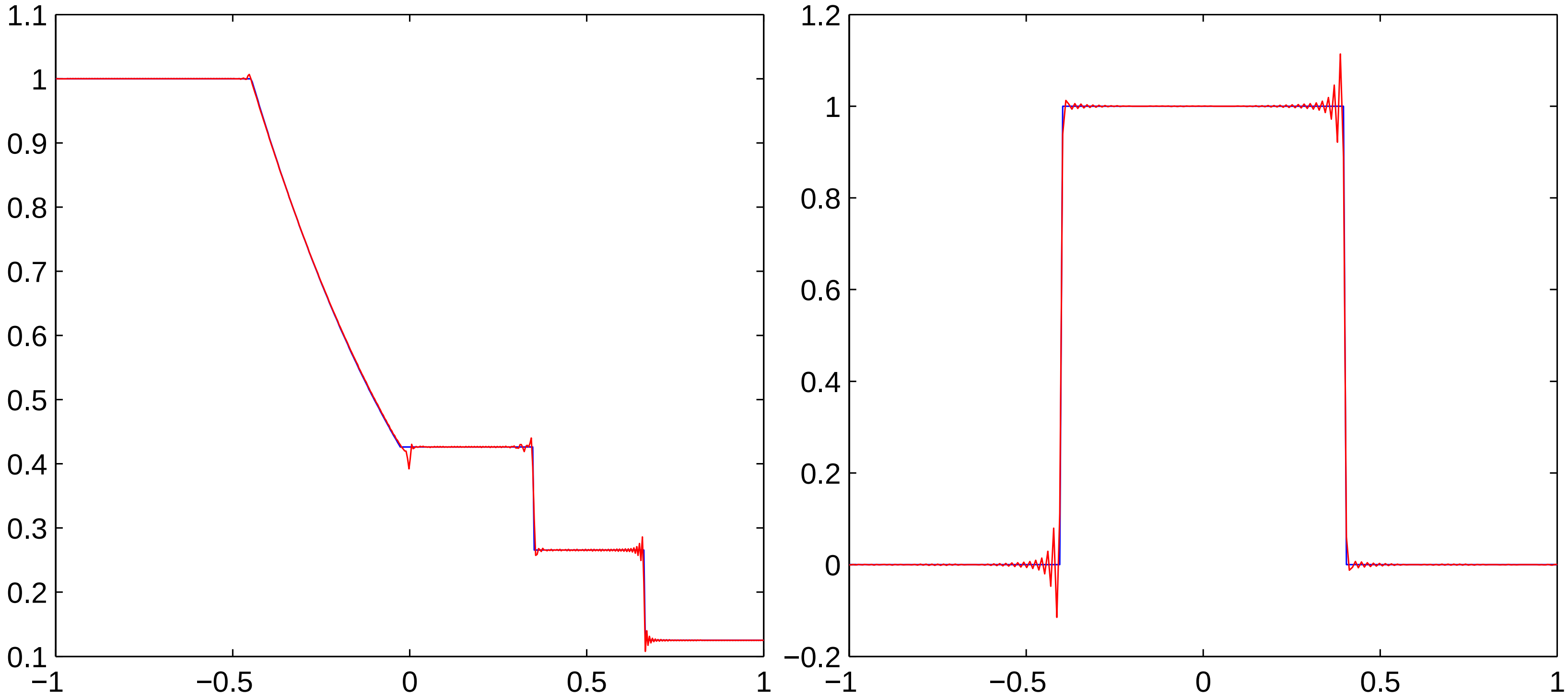


Left: hybrid postprocessed. Right: DTV application area (red), spectral filter (blue).

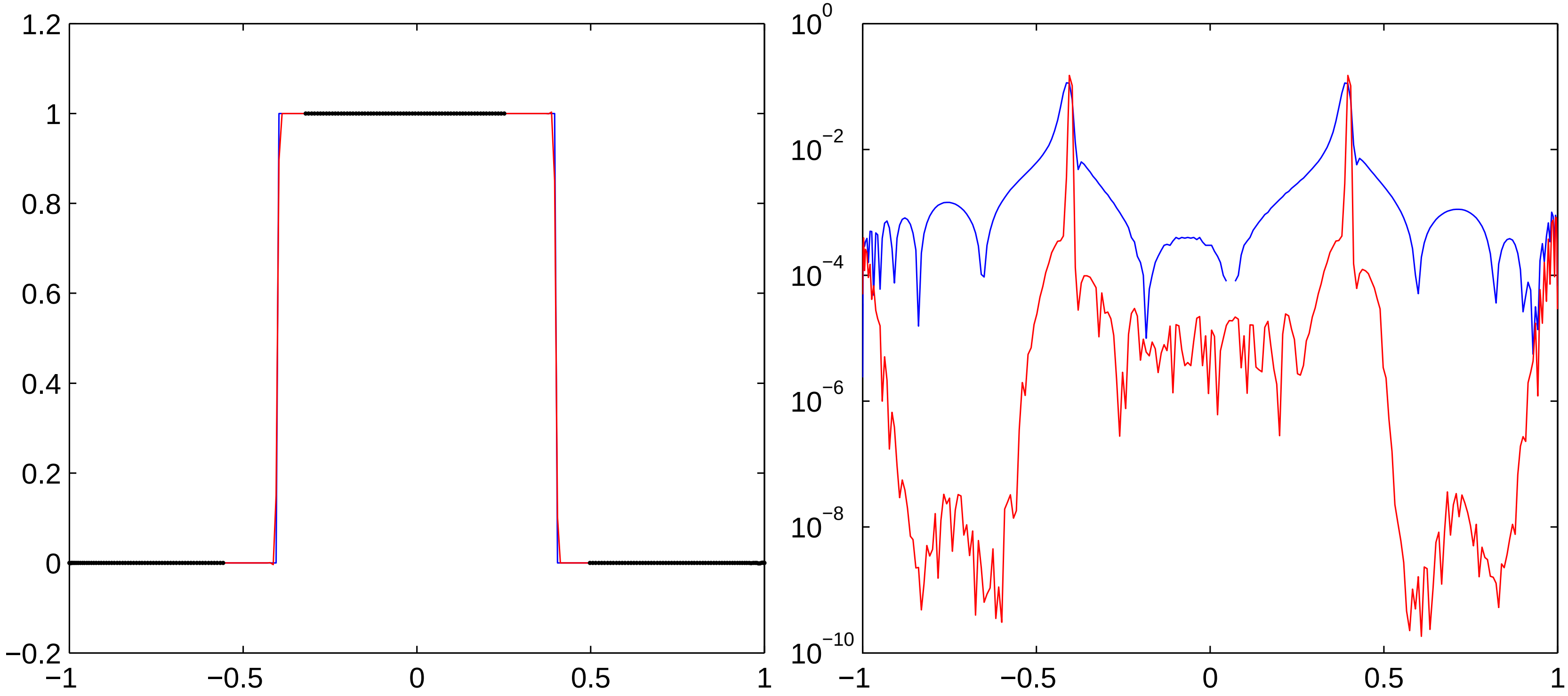
Hybrid, Shepp-Logan phantom zoom



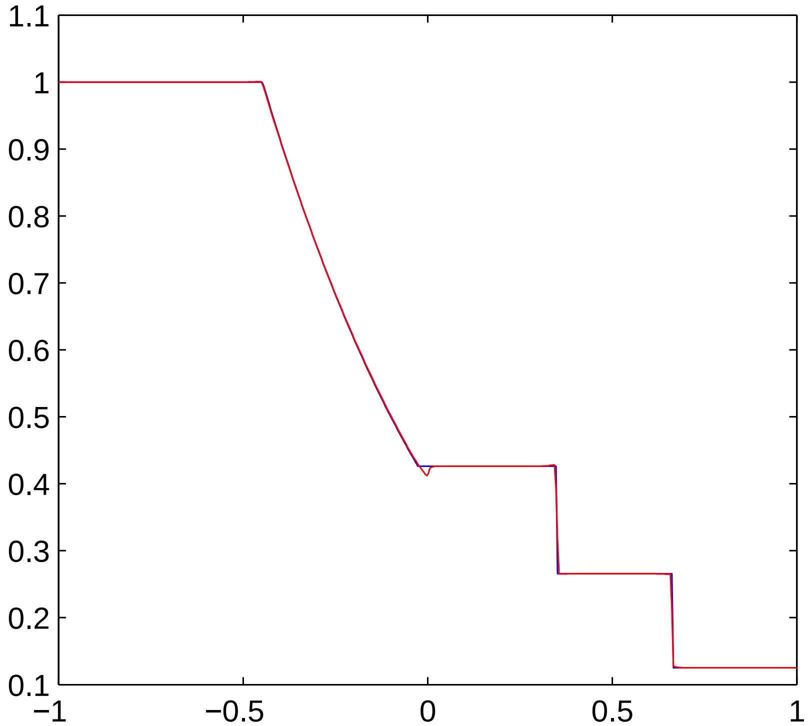
Chebyshev Pseudospectral

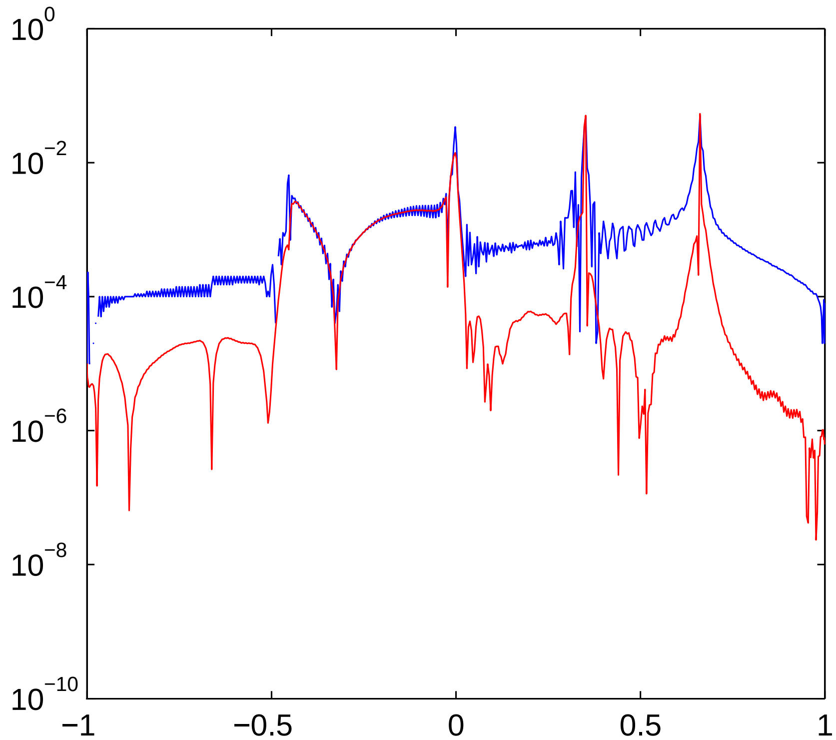


Chebyshev Pseudospectral



Chebyshev Spectral Viscosity

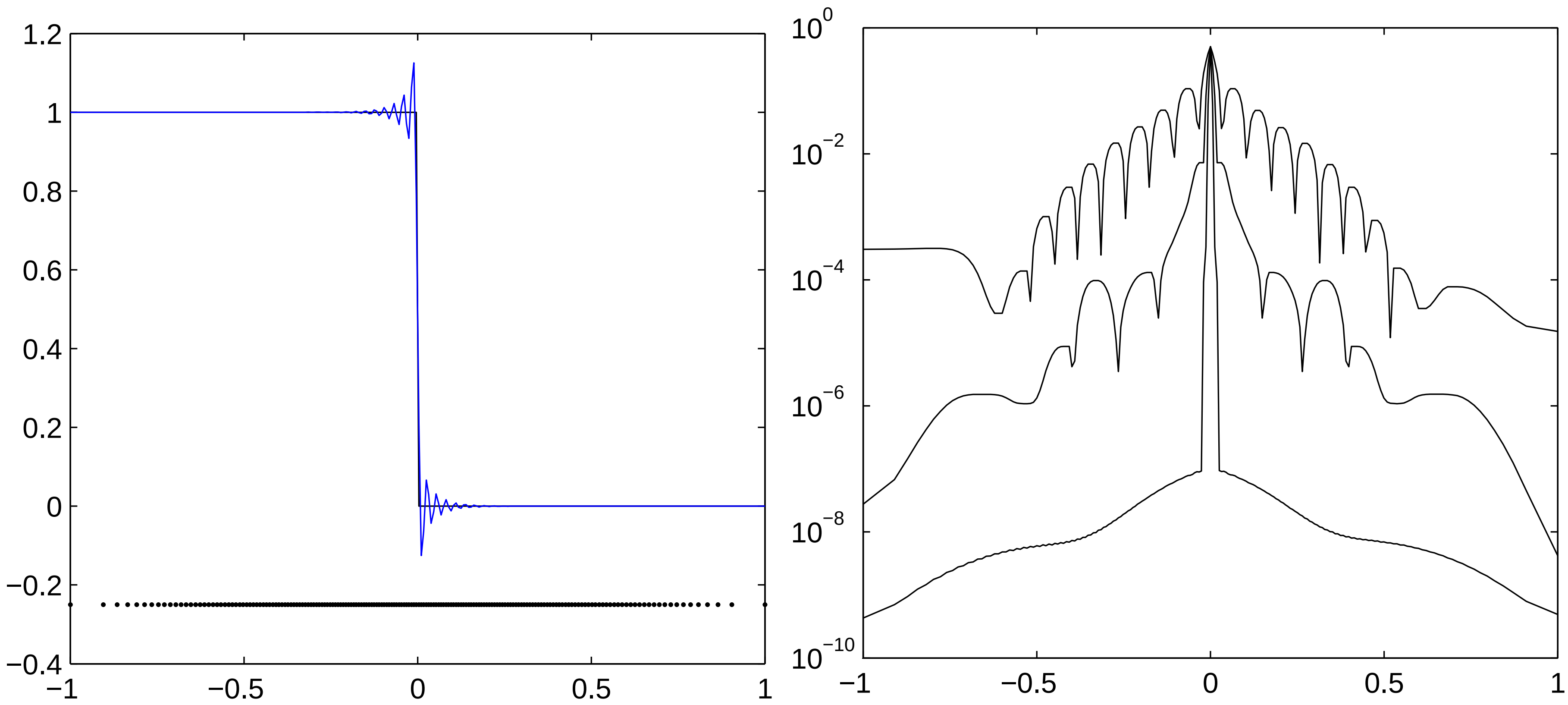




DTV Filter - RBF

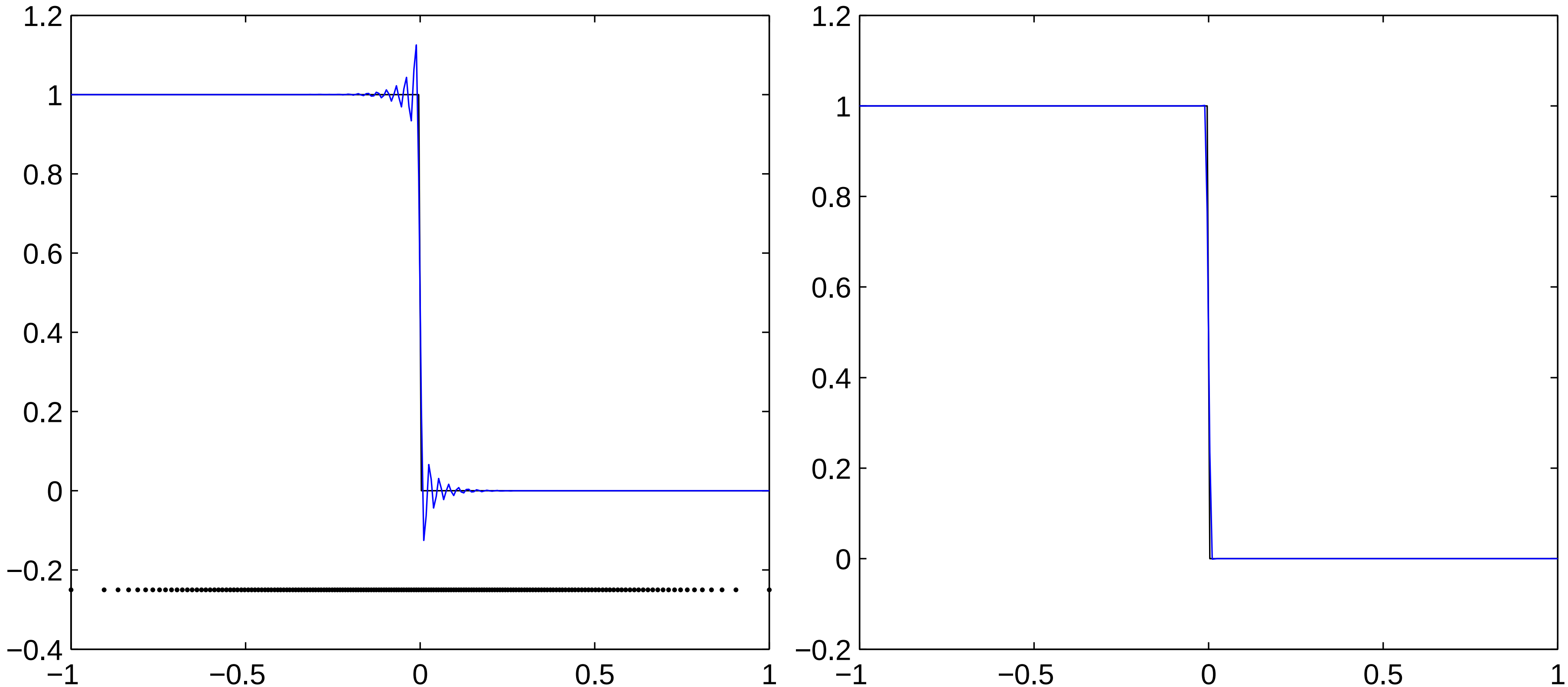
Digital Total Variation Filtering as postprocessing for Radial Basis Function Approximation Methods. Computers and Mathematics with Applications, vol. 52, p. 1119-1130, Sept. 2006.

RBF DTV example



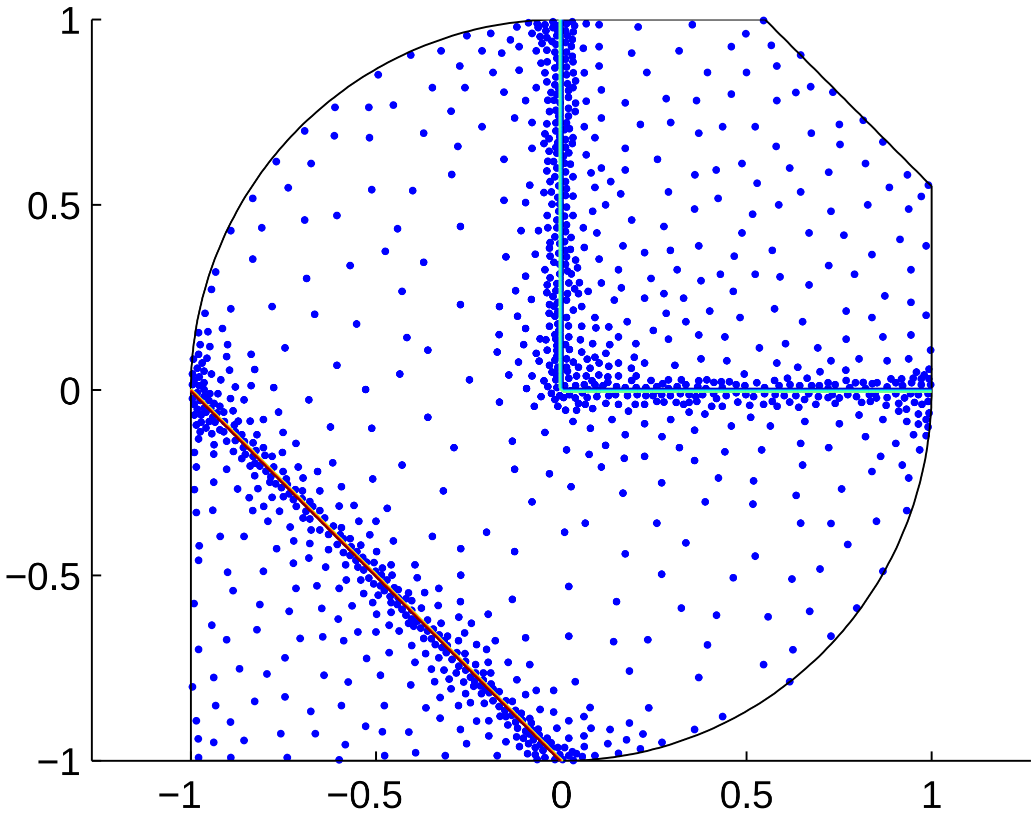
Left: $N = 79$ MQ RBF, Right: DTV postprocessed convergence $N = 39, 79, 159$.

RBF DTV example



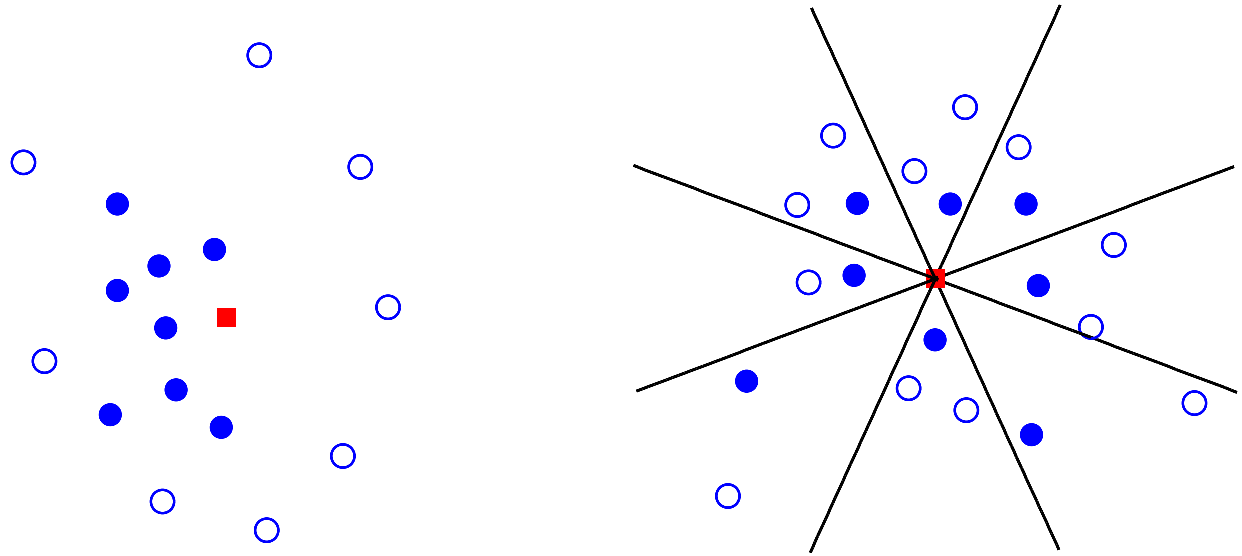
Left: $N = 79$ MQ RBF, Right: DTV postprocessed $N = 79$.

2d Complex Domain - Scattered Data

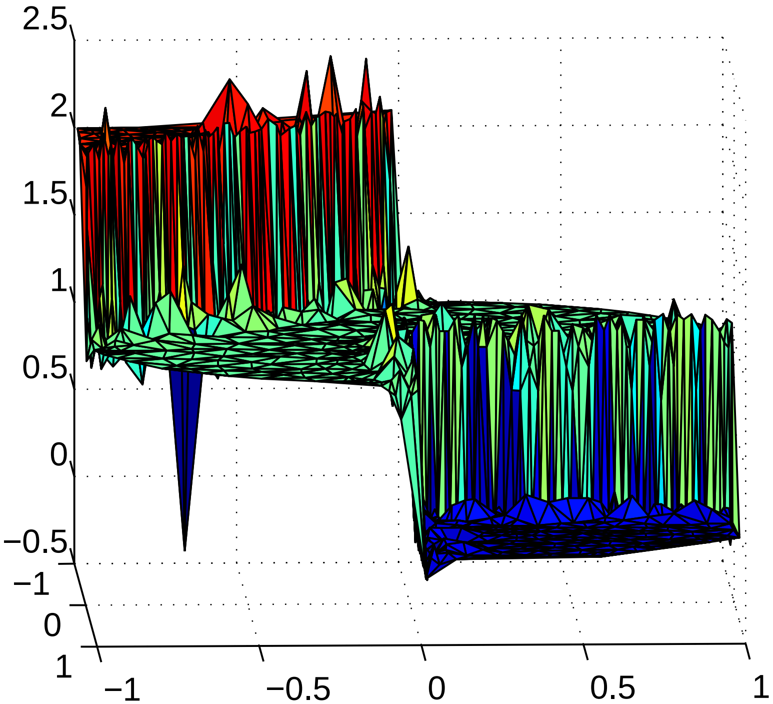


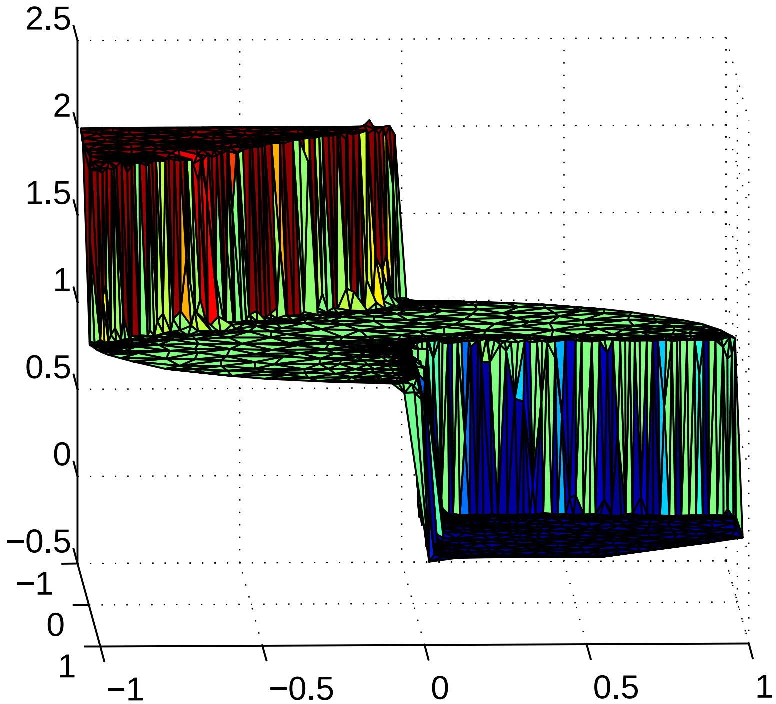
$N = 1126$ scattered points on a complexly shaped domain.

2d Neighborhoods N_α

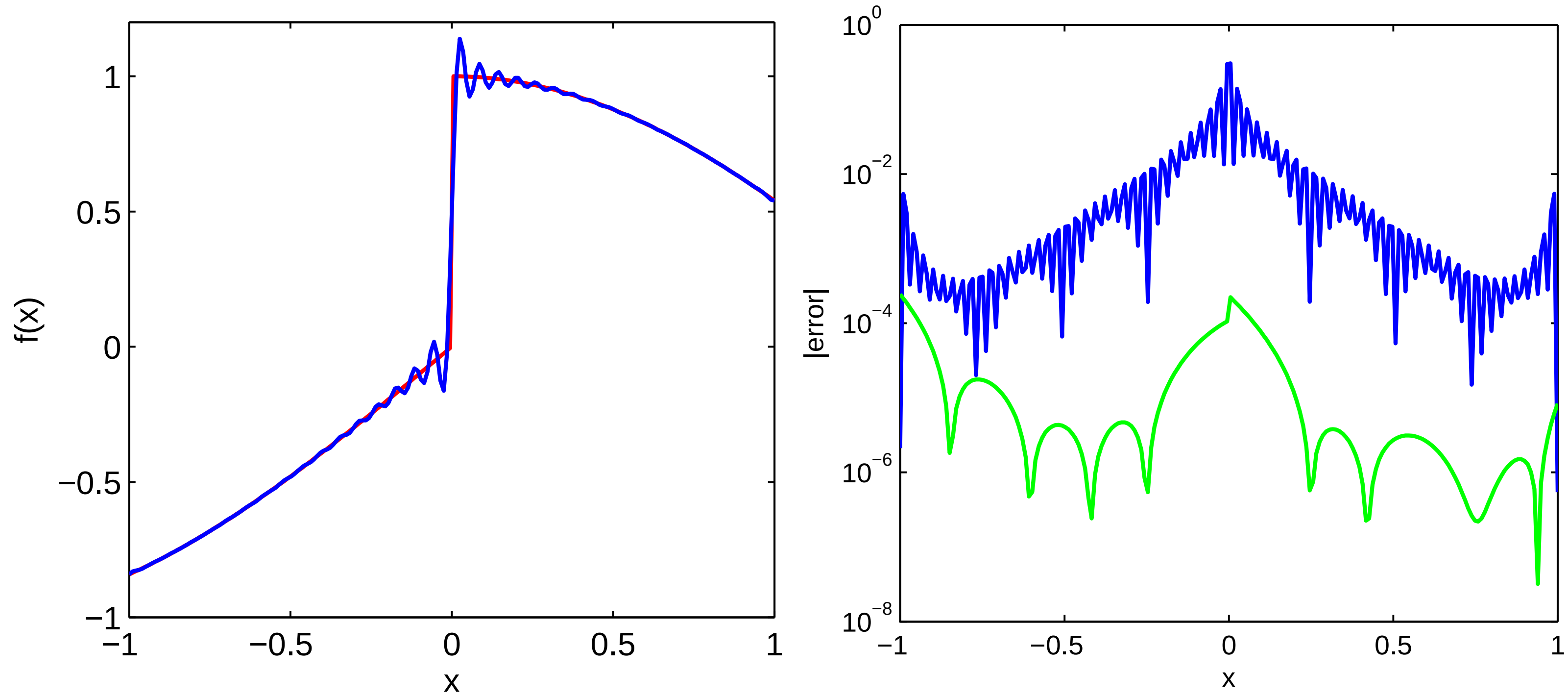


2d RBF DTV example





RBF-Gegenbauer example



Summary

method	edge detection	parameters	spectral accuracy	large $\kappa(A)$	noise
spectral filter		ρ	$\sim$		$\surd$
DTV		λ			$\surd$
Padé	$\sim$	M, N_c		$\surd$	$\surd$
GRP	$\surd$	λ, m_i	$\surd$		$\surd$
FRP	$\surd$		$\surd$		$\surd$
IPRM	$\surd$	m_i	$\surd$	$\surd$	