Processing Discontinuous Spectral Data

To David Gottlieb with friendship and appreciation

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PROLOGUE 1984–2004

David Gottlieb and Eitan Tadmor, **Recovering pointwise values of discontinuous data within spectral accuracy,**

"Progress and Supercomputing in Computational Fluid Dynamics",
Proc. 1984 U.S.-Israel Workshop, Progress in Scientific Computing, v. 6 (E. M. Murman and S. S. Abarbanel, eds.), Birkhauser (1985), 357-375.

ABSTRACT. We show how *pointwise values* of a function, $f(x)$, can be accurately recovered either from its spectral or pseudospectral approximations, so that the accuracy depends *solely* on the *local* smoothness of f in the neighborhood of the point x. Most notably, given the equidistant function grid values, its intermediate point values are recovered within spectral accuracy, despite the possible presence of discontinuities scattered in the domain. (Recall that the usual spectral convergence rate decelerates to first order throughout the domain).

To this end we employ a highly oscillatory smoothing kernel in contrast to the more standard positive unit-mass mollifiers.

In particular, post-processing of a stable Fourier method applied to hyperbolic equations with discontinuous data recovers the exact solution modulo a spectrally small error. Numerical examples are presented.

2004: Manipulation of piecewise smooth data from its spectral information

OVERVIEW

Part I. Detection of edges from global moments

$\boxed{\text{Concentration Kernels}}$ – localization around edges

- Enhancement – separation of scales

⊙ Extensions: discrete and non-periodic data; noisy data; 2D data, ...

Part II. High resolution reconstruction.

$\boxed{\text{Adaptive Mollifiers}}$ – high order accurate 2-parameter kernels

- Normalization — high resolution near edges

⊙ Spectral Viscosity: spontaneous shock discontinuities




Different scales of smoothness: detection of edges

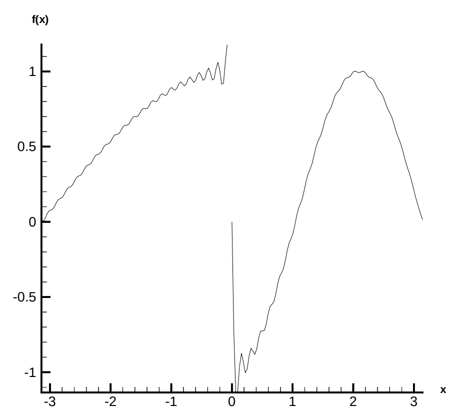
- Global moments: $\widehat{f}_k = \langle f, \phi_k \rangle$

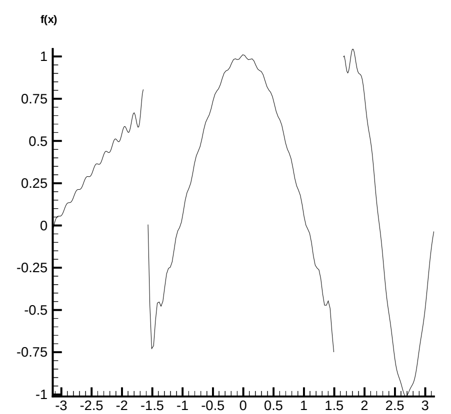
$$S_N[f](x) = \sum_{-N}^{N} \widehat{f}_k e^{ikx}, \qquad \phi_k \longleftrightarrow e^{ikx}$$

⊙ Smooth f's: spectral/exponential accuracy ...

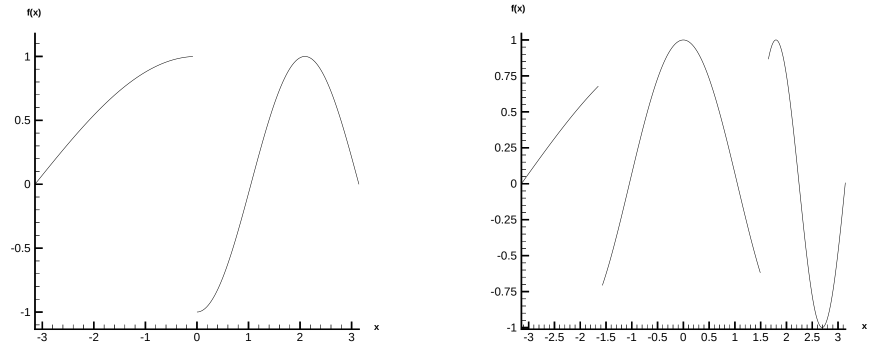
$$|S_N[f](x) - f(x)| \leq Const.e^{-\eta N}.$$

⊙ Piecewise smooth f's: Gibbs' phenomenon

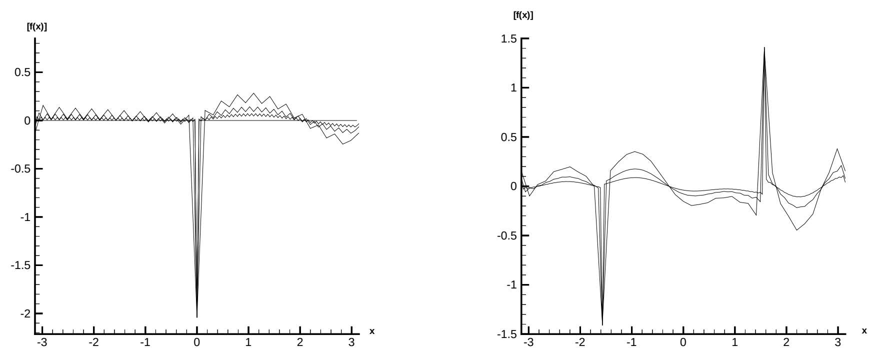




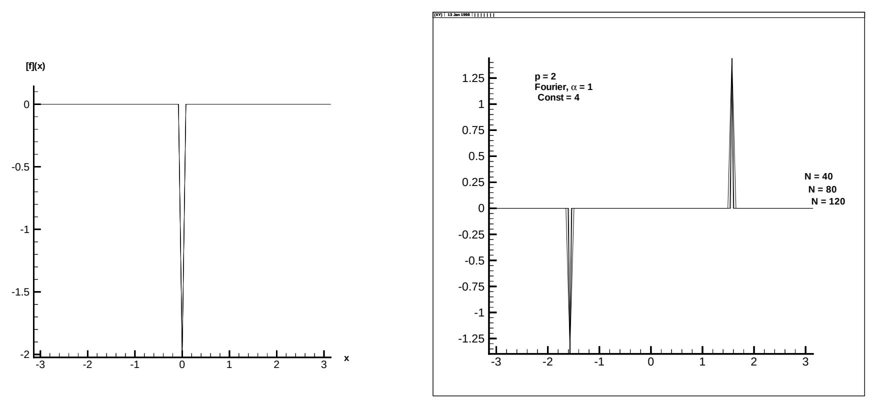
○ Spurious oscillations ('ringing'); first-order accuracy



~~Example~~ Reconstruction of discontinuous f's from their spectral data



Concentration near edges: concentration kernels $S_N^{\sigma}[f]$, w/$N = 20, 40, 80$ modes



Concentration kernels with enhancement

I. Concentration kernels

$$\boxed{S_N^\sigma[f] := \frac{1}{c_\sigma} \sum_{k=-N}^{N} sgn(k)\sigma\left(\frac{|k|}{N}\right)\widehat{f}_k e^{ikx}}$$

- Normalization: $c_\sigma = \dfrac{1}{\pi i}\displaystyle\int_0^1 \frac{\sigma(\theta)}{\theta} d\theta \quad \forall\sigma(\cdot) \in C^2(0,1)$

$$\boxed{S_N^\sigma[f] = [f](x) + \mathcal{O}(\varepsilon_N) \sim \begin{cases} \mathcal{O}(1), & x \sim singsupp[f] \\ \mathcal{O}(\varepsilon_N), & f(\cdot)_{|\sim x} \text{ smooth} \end{cases}}$$

- Detection of edges by separation of scales: $\varepsilon_N \sim \frac{1}{(N\mathrm{d}(\mathrm{x}))^s} \ll 1$

$\odot$ Concentration kernels: concentrate near $\mathcal{O}(1)$ edges

$$\boxed{K_N^\sigma(t) := -\frac{1}{c_\sigma} \sum_{|k|\leq N} \sigma\left(\frac{|k|}{N}\right) \sin kt}$$

$$S_N^\sigma[f] := K_N^\sigma * S_N f \equiv K_N^\sigma * f \sim [f](x)....$$

Concentration Kernels – the general framework

(i) Odd kernels: $K_N(-t) = -K_N(t)$

(ii) Normalized: $\int_{t\geq 0} K_N(t)dt \sim -1$

(iii) Admissibility condition:

$$\boxed{\left|\int tK_N(t)\varphi(t)dt\right| \leq Const.\varepsilon_N\|\varphi\|_{BV}}$$

<u>Main result</u>: (i), (ii) and (iii) imply for piecewise smooth f

$$\boxed{K_N(x) * f = [f](x) + \mathcal{O}(\varepsilon_N) \sim \begin{cases} [f](\xi) = \mathcal{O}(1) & x \in singsupp(f) \\ \mathcal{O}(\varepsilon_N) & f(\cdot)\ \ smooth \sim x \end{cases}}$$

- Detection of edges by separation of scales

Local vs global concentration kernels

odd, normalized and admissible:

(i) Local kernels:

$K_N(t) = \phi'_{\varepsilon_N}(t), \quad \phi_\varepsilon(t) = \frac{1}{\varepsilon_N}\phi(\frac{t}{\varepsilon_N}), \quad \phi \in C_0^1(-1,1)$

Admissibility – concentrates near the origin: $\int |tK_N(t)|dt \leq C\varepsilon_N$.

⊙ Haar and bi-orthogonal moments — localized kernels

(ii) Global kernels: $K_N^\sigma(t) = -\frac{1}{c_\sigma}\sum \sigma\Big(\frac{|k|}{N}\Big)\sin kt, \quad \sigma(\theta) \in C^2(0,1)$

Admissibility — 'heroic' cancelation of oscillations:

$$K_N(t) \sim \sigma(1)\frac{\cos(N+\frac{1}{2})t}{2\pi\sin(t/2)} + Const\frac{1}{Nt} + \dots$$

- Convergence rate: $\Big|S_N^\sigma[f](x) - [f](x)\Big| \leq Const.\Big(N\mathrm{d}(x)\Big)^{-s_\sigma} + \dots$

Concentration factors $\sigma(\theta_k)$: $\dfrac{1}{c_\sigma}\sum_k sgn(k)\sigma(\theta_k)\widehat{f}_k e^{ikx}$

$\odot$ 'Linear' (*Fejer*): $\boxed{\sigma(\theta_k) = \theta_k}$ $\quad \theta_k = \frac{|k|}{N}, \quad |k| \le N$

$$S_N^{\sigma=lin}[f](x) = \pi \sum \frac{ik}{N}\widehat{f}_k e^{ikx} = \frac{\pi}{N}\Big(S_N(f)\Big)' = [f](x) + \mathcal{O}\Big(\frac{1}{N\mathsf{d}(x)}\Big),$$

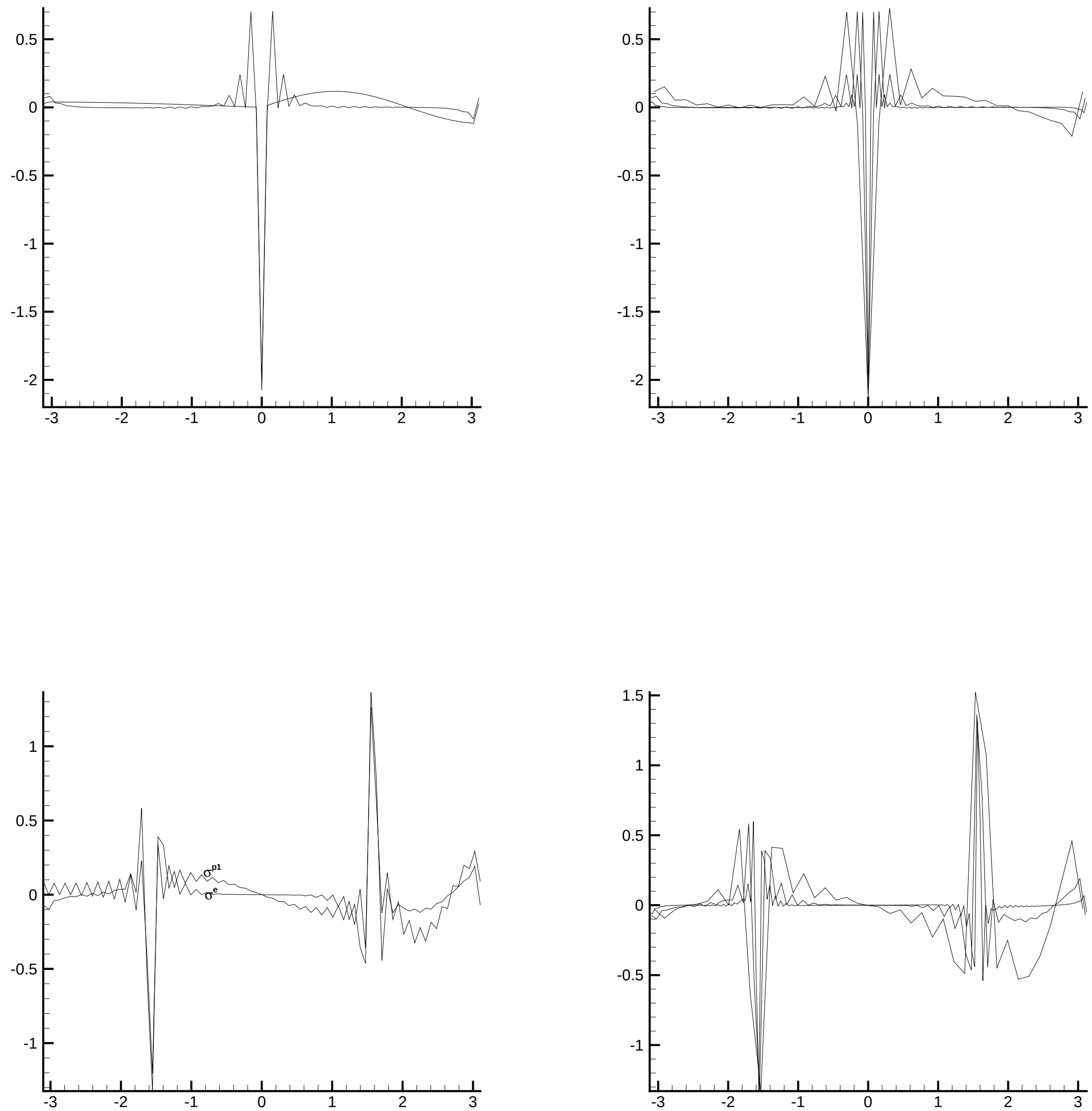
$\circ$ Adaptivity: dependence on $\mathsf{d}(x)$:= distance$(x, singsupp(f))$

$\odot$ 'Exponential' (*Gelb-ET.*): $\boxed{\sigma^{exp}(\theta_k) = \theta_k \cdot e^{\frac{c}{\theta_k(\theta_k-1)}}}$

$\circ$ optimal localization: $S_N^{\sigma=exp}[f](x) \sim [f](x) + \mathcal{O}\Big(e^{-Const\sqrt{N\mathsf{d}(x)}}\Big)$

- Extensions: ψdospectral data, Chebyshev, ...

$$\boxed{T_N^\sigma[f](x) = \frac{1}{c_\sigma}\sum_{k=-N}^{N} sgn(k)\sigma(\theta_k)\tilde{f}_k e^{ikx}, \quad \tilde{f}_k = \Delta x \sum f(x_\nu)e^{-ikx_\nu}}$$



Edge detection, $S_N^\sigma[f]$, using (*left*) — the exponential concentration factor $\sigma^{exp}(\theta) = 3exp(\frac{1}{6\theta(\theta-1)})$ vs. (*right*) — the linear $\sigma(\theta) = \theta$ with $N = 20, 40, 80$ modes.

Top: $f = f_a(x)$ and Bottom: $f = f_b(x)$.

Enhancement

- Enhance separation of scales: fix $r > 1$

$$\left(\sqrt{N} \times S_N^\sigma[f](x)\right)^r \sim \begin{cases} N^{-r/2} & x \in \text{ smooth regions} \\ N^{r/2}[f]^r(\xi) & \text{at jumps} \end{cases}$$

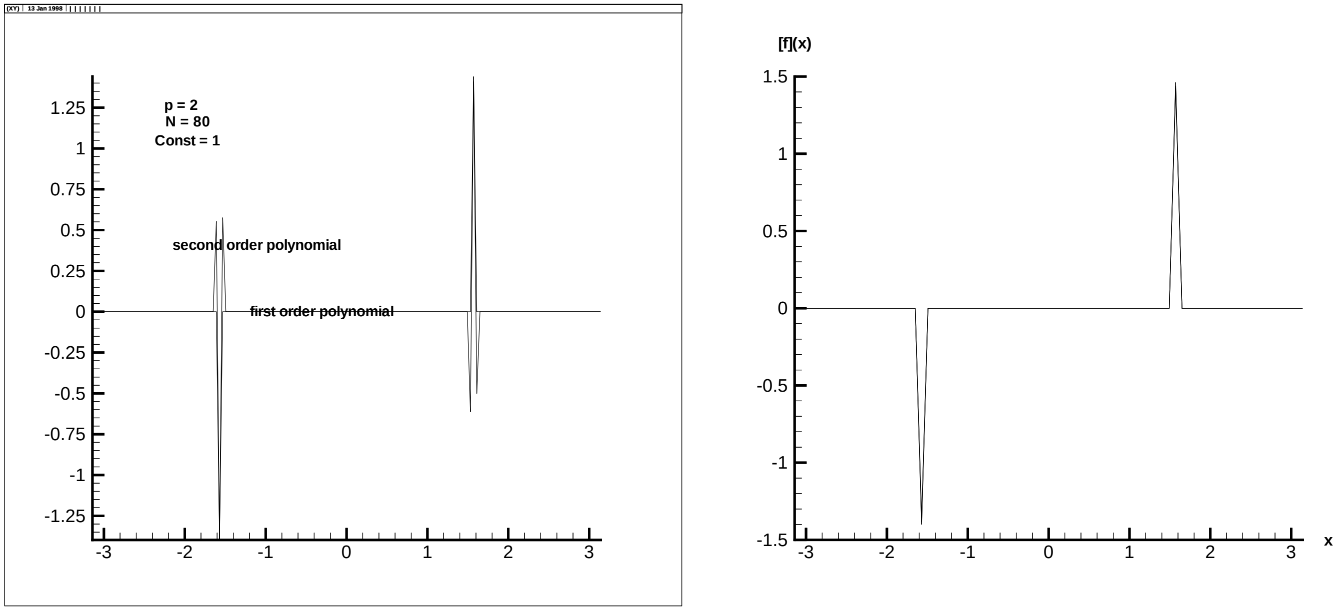
- Threshold for identifying an edge ———>>> $\boxed{J_{crit}}$

$$S_N^{\text{enhance}}[f](x) = \begin{cases} S_N^\sigma[f](x) & \text{if } \left|\sqrt{N} S_N^\sigma[f](x)\right|^r > J_{crit} \\ 0 & \text{otherwise} \end{cases}$$

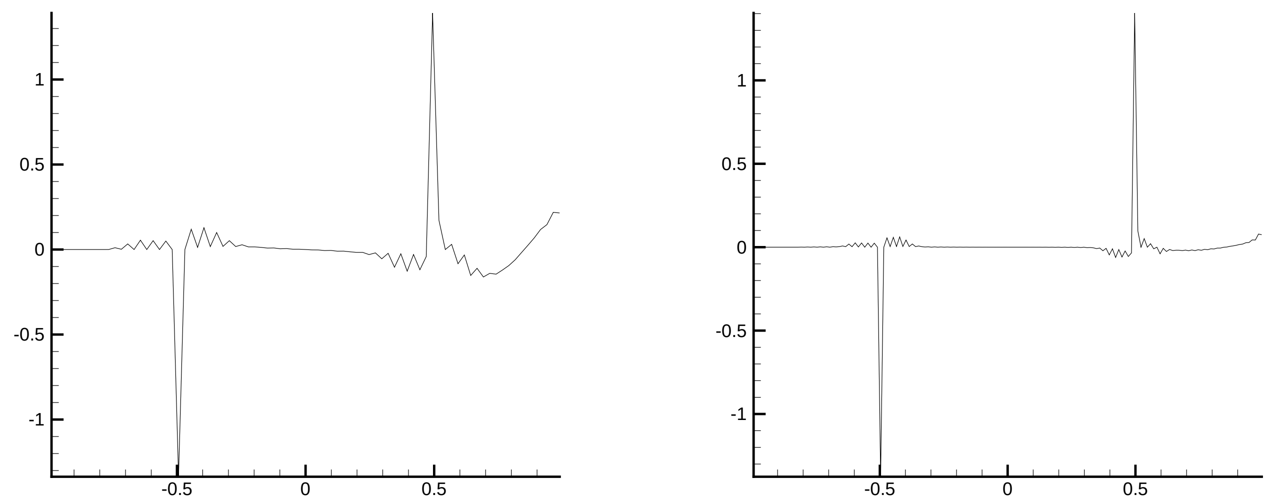
- Nonlinear scale-free detection: MinMod detection

$$\text{mm}\{S_N^{\sigma=lin}, S_N^{exp}\} = \begin{cases} \min\left(|S_N^{\sigma=lin}(x)|, |S_N^{exp}(x)|\right) & \text{if } S_N^{\sigma=lin} \times S_N^{exp} > 0 \\ 0 & \text{otherwise} \end{cases}$$

Edges are barriers for propagation of smoothness at a given scale

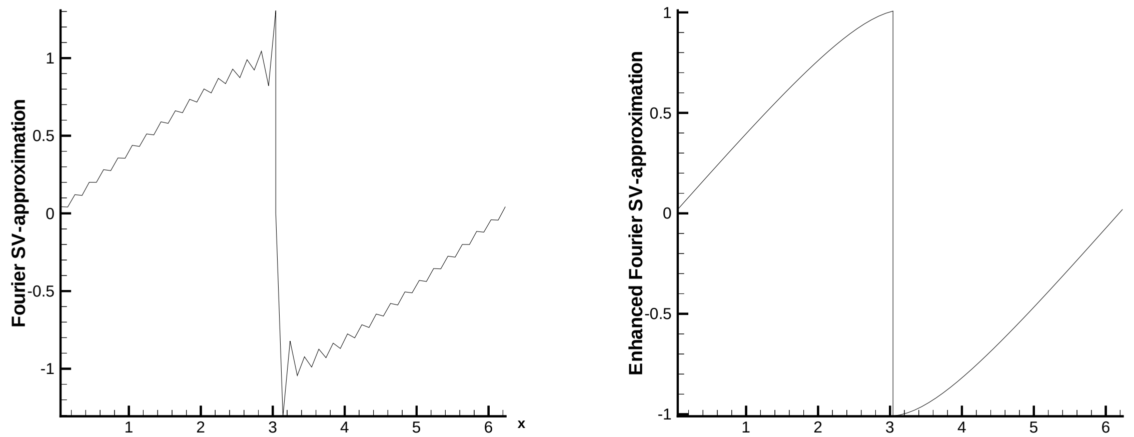


Enhanced edge detection using conjugate sums, $S_N^\sigma[f](x) = \frac{1}{c_\sigma}\sum \sigma(\frac{|k|}{N}) sgn(k) \widehat{f}_k e^{ikx}$

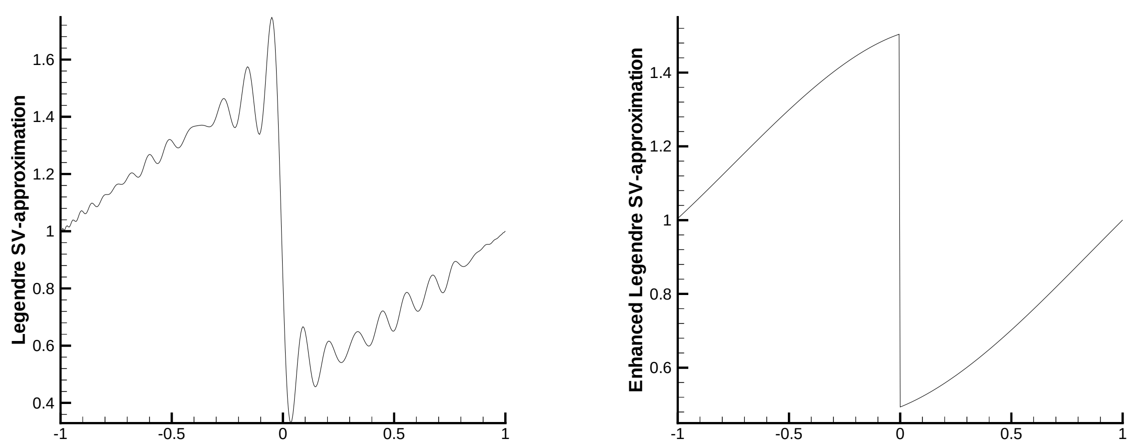


Minmod detection $mm\{S_N^{\sigma=lin}, S_N^{exp}\}$, for $f_b(x)$ with $N = 40$ and $N = 80$ gridpoints.

Enhanced Spectral Viscosity method: Burgers' eq.

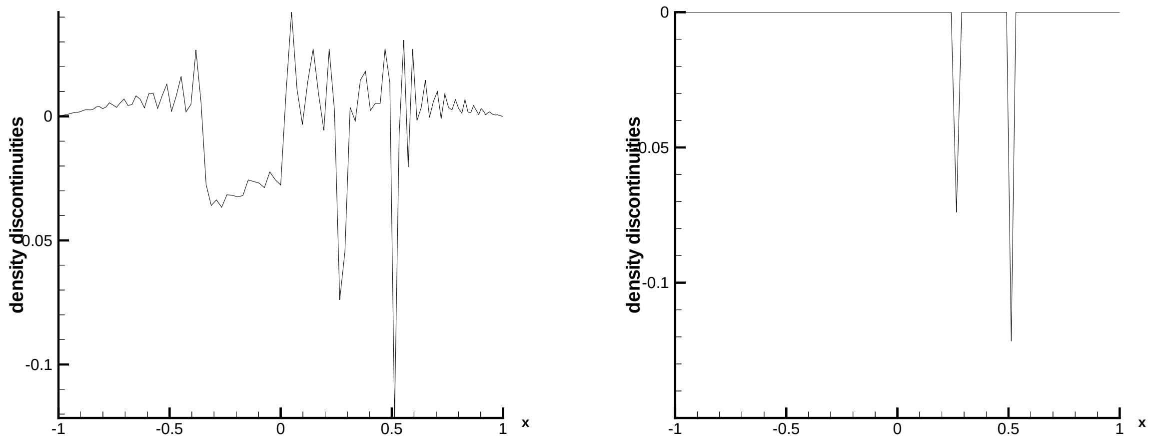


The solution to the inviscid Burgers equation with periodic boundary conditions at time $T = 1$ using (left) the Fourier SV-approximation and (right) the enhanced Fourier SV-approximation for $N = 64$.

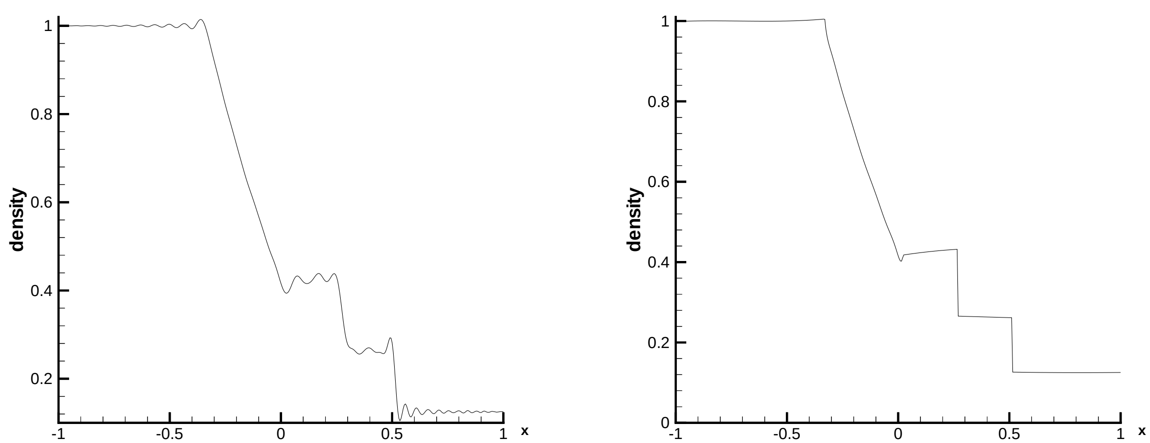


The solution to the inviscid Burgers equation with periodic boundary conditions at time $t = 1.5$ using (left) the Legendre SV-approximation and (right) the enhanced Legendre SV-approximation for $N = 64$.

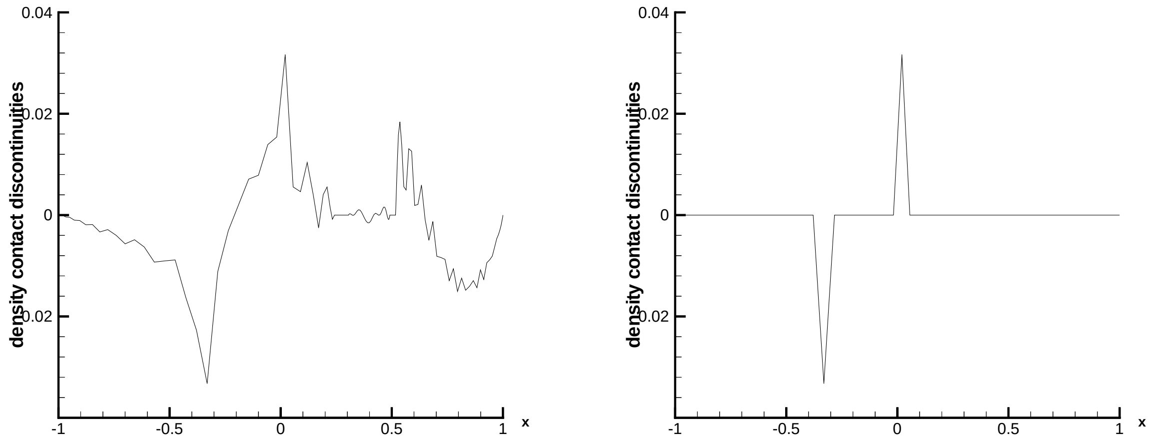
Enhanced Legendre SV-method (Riemann problem)



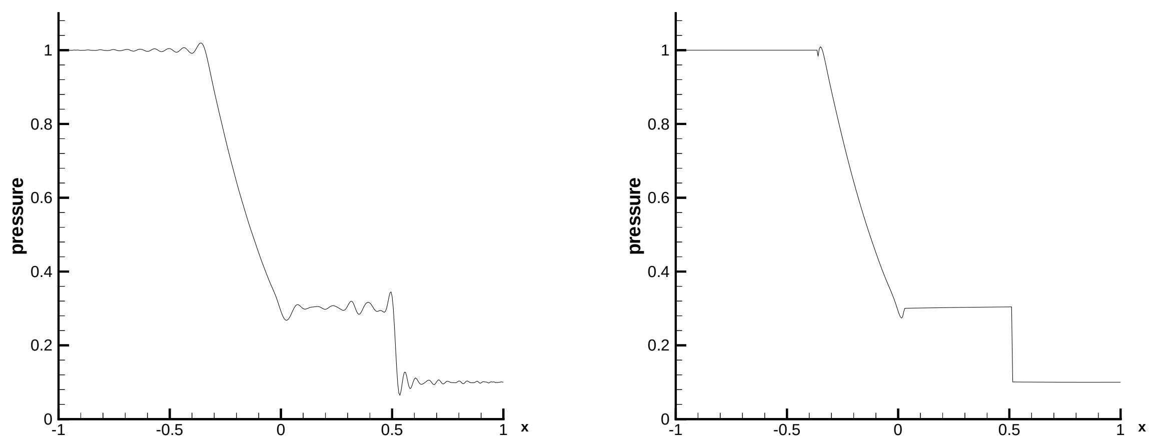
Detection of the shock discontinuities using the ‘concentrated’ method (left) and the enhanced edge detection method (right). $N = 128$ modes.



Density profile using the Legendre SV-method (left) and the enhanced version (right).



Detection of the contact discontinuities using the ‘concentrated’ method (left) and the enhanced edge detection method (right).



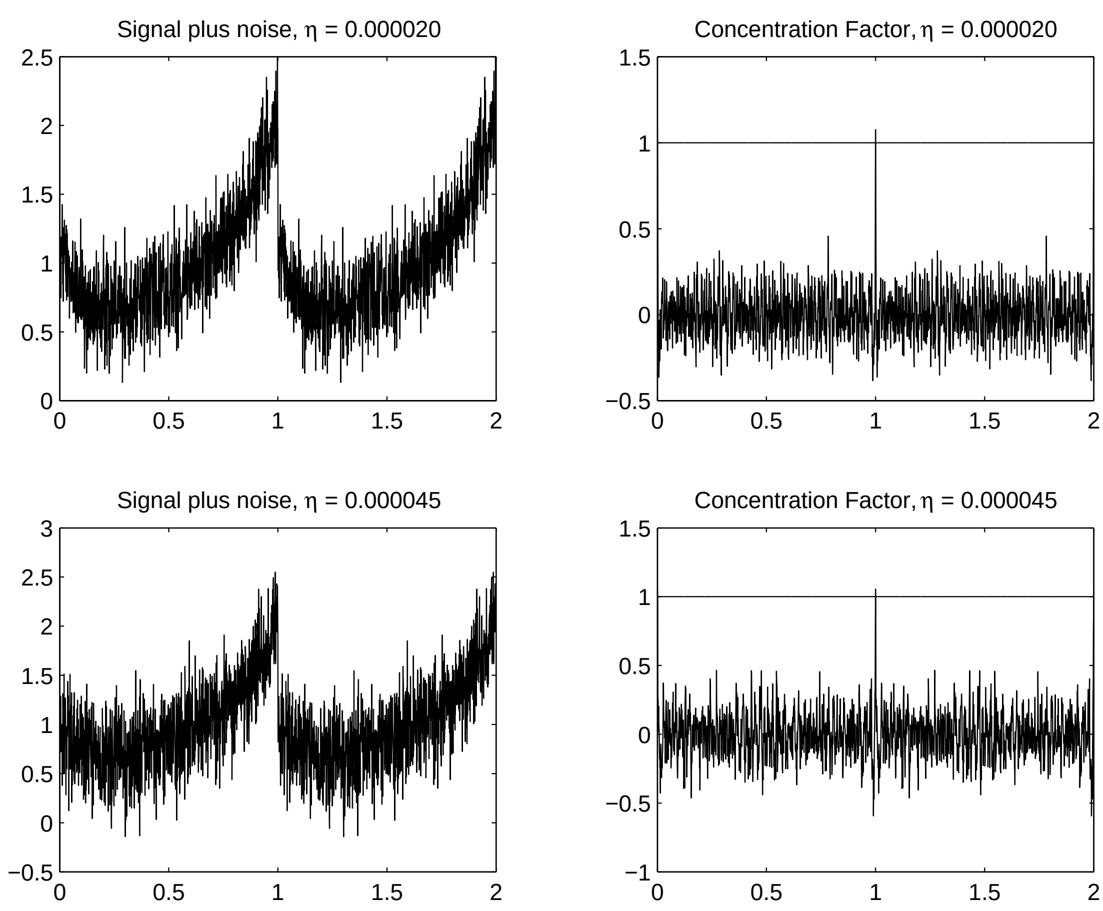
Pressure profile using the Legendre SV-method (left) and the enhanced version (right).

Adding noise: $\widehat{f}_k \sim \frac{i}{k}e^{-ik\xi} + \widehat{r}_k, \quad \eta := E(|\widehat{r}_k|)^2$

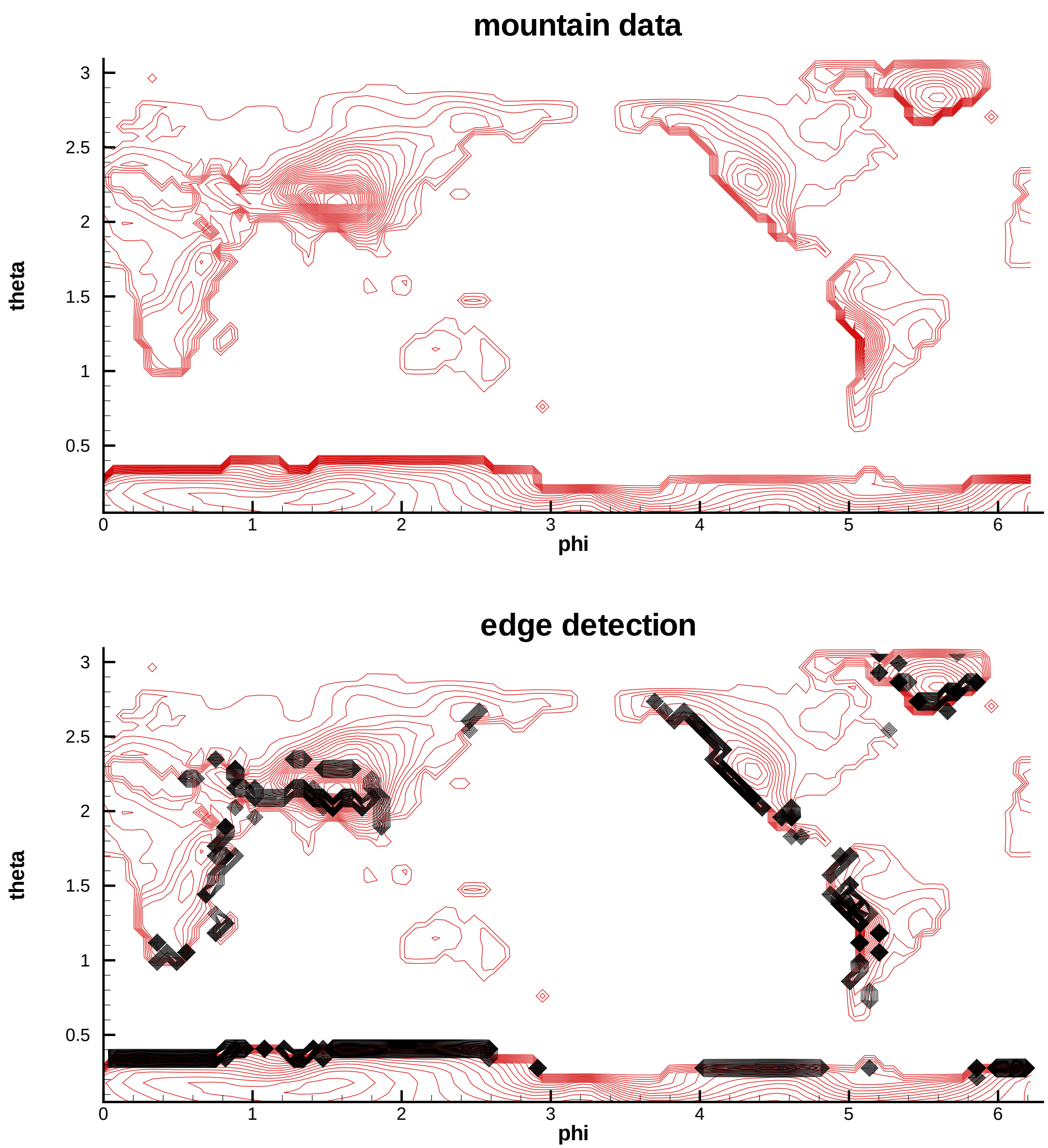
- A new small scale: white noise with variance $\eta := E(|\widehat{r}_k|)^2$:

$$\sigma(\theta) \sim \frac{N\theta}{1+\beta\eta(N\theta)^2}, \qquad c_\sigma \sim \begin{cases} N & \eta = 0 \text{(noiseless)} \\ \frac{1}{\sqrt{\eta}}\tan^{-1}(\sqrt{\eta}N) & \eta > 0 \end{cases}$$

Separation of scales: smoothness scale $\mathcal{O}(1/N) \ll$ Noise $\mathcal{O}(\eta) \ll$ edges $\mathcal{O}(1)$



2D setup: Detection of edges in earth topography



- Nonlinear enhancement: 48 latitudinal $\times$ 96 longitudinal gridpoints

II. Adaptive mollifiers. Reconstruction between edges.

- One-parameter finite order mollifiers: $\psi_\delta(x) := \frac{1}{\delta}\psi(\frac{x}{\delta})$

  p vanishing moments: $\psi_\delta * f - f = \mathcal{O}(\delta^{p+1}) \downarrow 0$ fixed order p

- Two-parameter spectrally accurate mollifiers (*Gottlieb-ET. 1985*):

⊙ Starting with... $\psi(x) = \psi_p(x) := \rho(x)D_p(x)$

∘ D_p — Dirichlet kernel of degree p, $D_p = \frac{\sin(p+\frac{1}{2})x}{2\pi\sin(x/2)}$

∘ $\rho(x) \in C_0^\infty(-\pi,\pi)$ cut-off with $\rho(0) = 1$ (important!)

$$\boxed{\psi_{p,\delta} := \frac{1}{\delta}\psi_p(\frac{x}{\delta}) = \frac{1}{\delta}\rho(\frac{x}{\delta})D_p(\frac{x}{\delta})}\Bigg|\,supp\Big(\psi_{p,\delta}\Big) = \delta$$

∘ Spectral order: increasing # of vanishing moments, $p = p_N$

...

Adaptive mollifiers — direction of smoothness

⊙ Set δ so $f(x-y)\psi_{p,\delta}(y)$ admits largest domain of smoothness:

$$\boxed{\delta \sim \mathsf{d}(x) := \mathrm{dist}(x, singsupp(f))}$$

- How to find $\mathsf{d}(x)$? – detection of edges from part I ...
- δ is fixed; so where does the spectral accuracy come from?

⊙ Choose $p = p_N$ — with increasing # of vanishing moments ...

- 'Optimal' solution of the moment problem modulo spectrally small error:

$$\int x^j \psi_{p,\delta}(x)dx = \int x^j \rho(x) D_p(x)dx = \left\{ \begin{array}{ll} 1, & j = 0 \\ 0, & j \geq 1 \end{array} \right\} + Const_s \cdot {p_N}^{-s}, \ \forall s$$

$$\boxed{\text{theoretical bound}: \quad p = p_N \sim \sqrt{N} \qquad \textit{Gottlieb-ET. '85}}$$

Spectrally accurate mollifiers

$$\psi_{p,\delta} * S_N f(x) - f(x) \;=\; \int S_N(\rho D_p)(y) f(x-\delta y)dy - f(x) = \ldots$$

$$\ldots \text{Trunction } \mathcal{I} \longleftrightarrow \;=\; \Big[\int \Big[(S_N - I)(\rho D_p)(y)\Big] f(x-\delta y)dy +$$

$$\text{Regularization } \mathcal{II} \longleftrightarrow \quad +\Big[\int D_p(y)\rho(y)\Big[f(x-\delta y) - f(x)\Big]dy$$

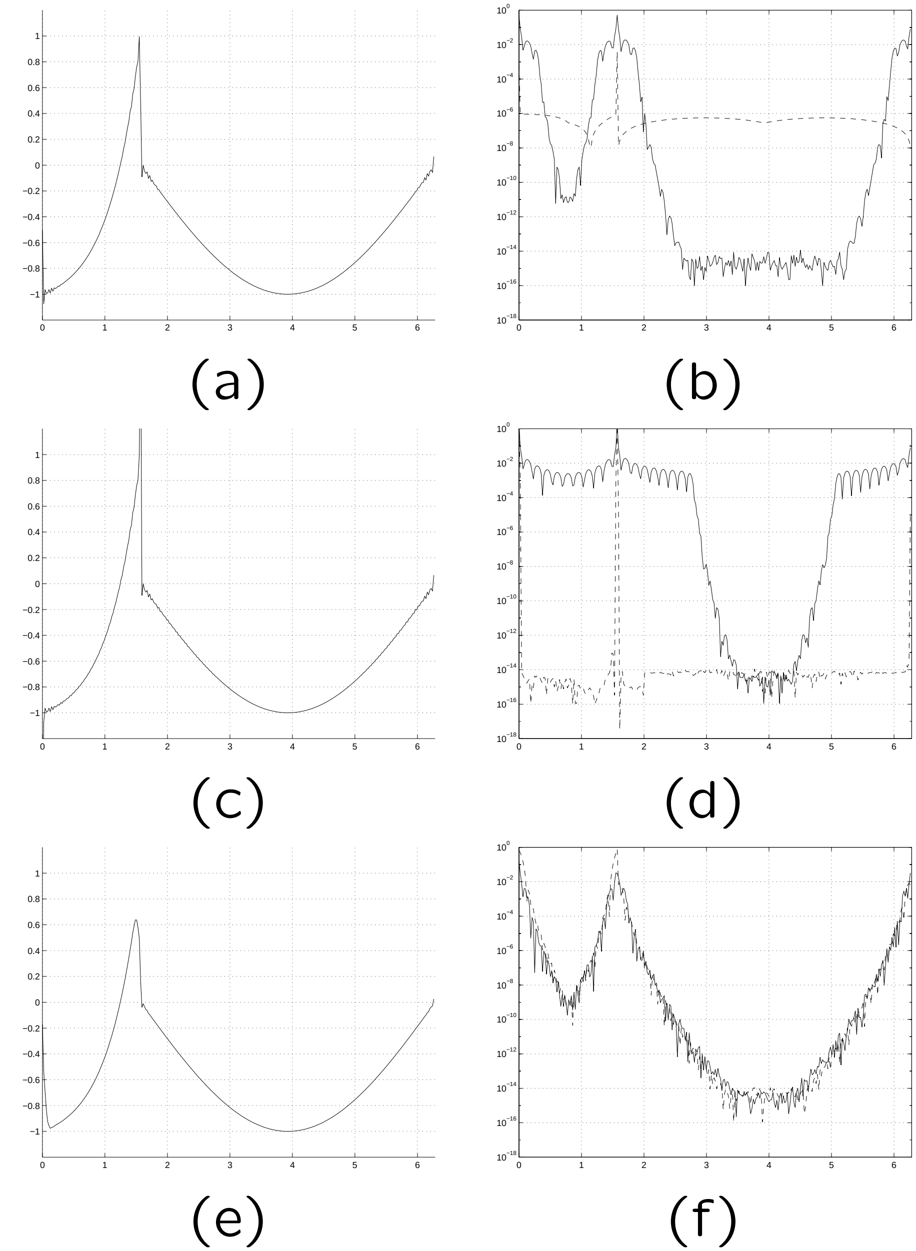
⊙ Spectrally small <u>truncation</u> $\mathcal{I}$: $\quad \|\rho\|_{C^s} \times \left(\frac{p}{N}\right)^s, \quad \forall s$

⊙ Spectrally small <u>regularization</u> $\mathcal{II}$: $\quad \|\rho f\|_{C^s(x-\delta, x+\delta)} \times \left(\frac{1}{p}\right)^s, \quad \forall s$

• Spectrally accurate mollifier: $\left(\frac{p}{N}\right)^s \sim \left(\frac{1}{p}\right)^s : \Longrightarrow \boxed{p_N \sim \sqrt{N}}$

$\Longrightarrow$ Error of order $\quad \sim Const_s\left(\frac{1}{\sqrt{N}}\right)^s, \qquad Const_s \sim \|\rho f\|_{C^s(x-\delta, x+\delta)}, \quad \underline{\forall s}$

Spectrally small error bound, but computations show otherwise for $d(x) \ll 1 \ldots$



Recovery of $f_2(x)$ from its first $N = 128$ Fourier modes, on the left, and the corresponding regularization errors (dashed) and truncation errors (solid) on the right, using the spectral mollifier $\psi_{p,\delta}$ based on various choices of p_N's:

$$\text{(a)-(b) } p_N = N^{0.5}, \text{ (c)-(d) } p_N = N^{0.8}, \text{ (e)-(f) } p_N = N\mathrm{d}(x)/\pi\sqrt{e}.$$

Exponential accuracy revisited: $\psi_{p,\delta} = \frac{1}{\delta}\rho(\frac{x}{\delta})D_p(\frac{x}{\delta})$

- *ET.-Tanner 2001*: Adaptive choice: $p = p_N \sim \mathsf{d}(x)N$

$$\int x^j \psi_{p,\delta}(x)dx \sim \left\{ \begin{array}{ll} 1 & j=0 \\ 0 & j>0 \end{array} \right\} + \mathcal{O}(e^{-Const.\sqrt{\mathsf{d}(x)N}}), \ \ \delta = \mathsf{d}(x), \ \ p \sim \mathsf{d}(x)N$$

⊙ G_2 Gevrey regularity of cut-off $\rho(x) = e^{\frac{\alpha x^2}{x^2-\pi^2}}$: $\|\rho\|_{C^s} \sim (s!)^2\eta^{-s}$

- Exponential accuracy $$\boxed{\left|\psi_{p,\delta} \star S_N f(x) - f(x)\right| \leq C_\rho \cdot \mathsf{d}(x)N \cdot e^{-Const.\sqrt{\mathsf{d}(x)N}}}$$

- The discrete case — high-order 'expolants'

$$\boxed{\left|\frac{\pi}{N}\sum_{\nu=0}^{2N-1}\psi_{p,\delta}(x-y_\nu)f(y_\nu) - f(x)\right| \leq Const \cdot (\mathsf{d}(x)N)^2 e^{-C\sqrt{\mathsf{d}(x)N}}}$$

Exponential accuracy except near edges where $\mathsf{d}(x) \sim 1/N$: normalization ...

Adaptivity – sharper resolution near edges

- Gottlieb: Gegenbauer mollifiers – uniform high accuracy *up to* the edges
- Our approach: *adaptive order* (ENO,...) by normalization ...
- How to normalize? enforce exact vanishing moments ...

$$\psi_{p,\delta} \longmapsto \frac{\psi_{p,\delta}}{\int \psi_{p,\delta}} : \rho \longrightarrow \tilde{\rho} := \frac{\rho}{\int \psi_{p,\delta}}$$

... exponential accuracy away from edges $\mathrm{d}(x) >> 1/N$

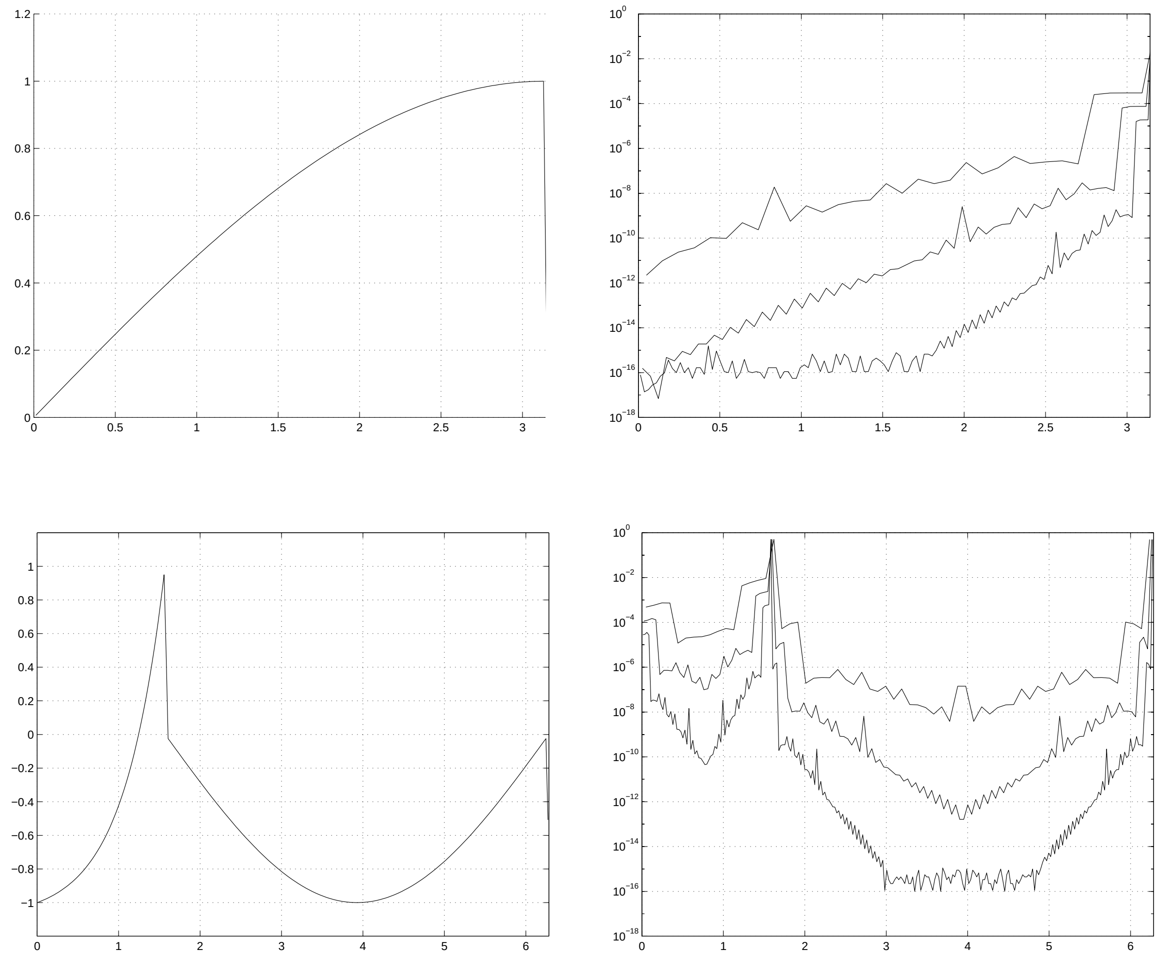
$$\tilde{\rho}(0) = 1 + Const.e^{-\eta\sqrt{\delta(x)N}}$$

- Adaptive mollifier of *variable* order $r \sim \mathrm{d}(x)N$

$$f(x) - \psi_{p,\delta} * S_N f(x) = f(x) - f * S_N \psi_{p,\delta}(x) \leq Const.(\mathrm{d}(x))^{r+1}$$

provided we normalize

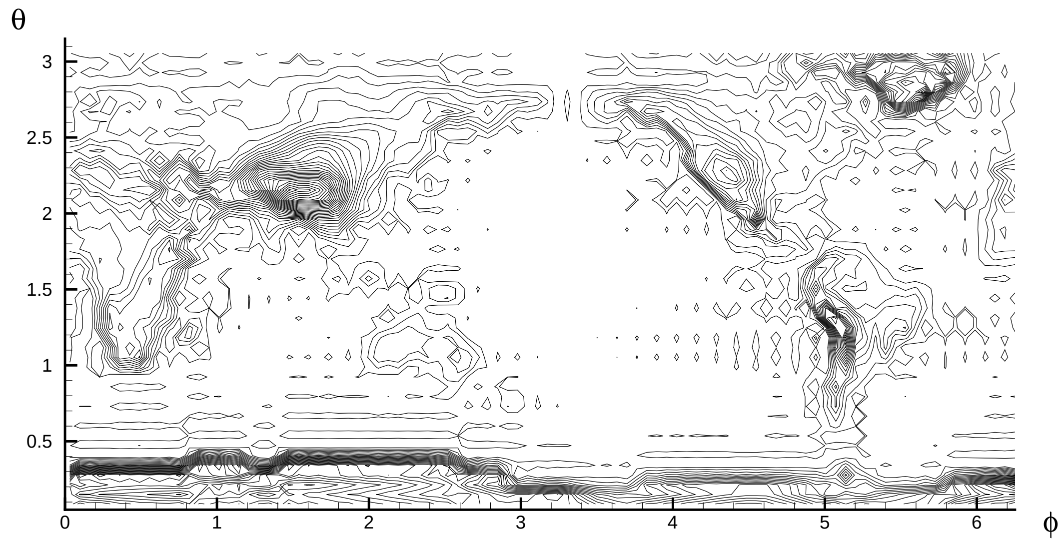
$$\int_{-\pi}^{\pi} \psi_{p,\delta}(x) S_N(x^j)dx = \begin{cases} 1, & j = 0 \\ 0, & j = 1, 2, \ldots, r \end{cases}$$

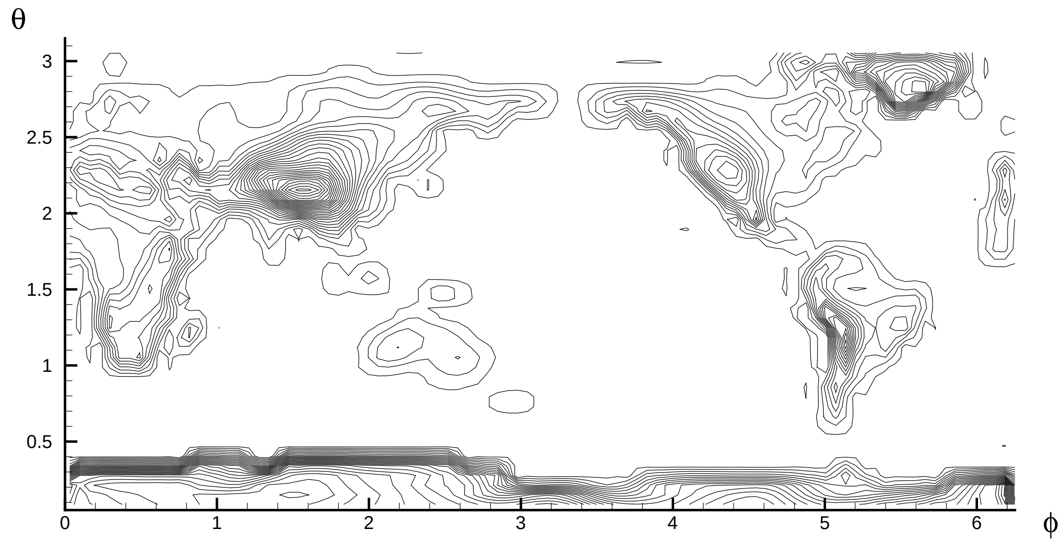


(Left): Recovery of $f(x)$ from its $N = 128$-modes spectral projections; Normalized mollifier, $\psi_{p,\theta}$ of degree $p = \mathsf{d}(x)N/\pi\sqrt{e}$

(Right): Log error for recovery of $f(x)$ based on $N = 32, 64, 128$ modes.

2D Reconstruction of earth topography





Spectral reconstruction vs. localized reconstruction

EPILOGUE

- Adaptive filters (vs. mollifiers):

$$S_N^\sigma f = \frac{1}{2\pi}\sum_{|k|\leq N} \sigma(\frac{|k|}{N})\widehat{f}(k)e^{ikx}$$

based on an adaptive G_2-filter:

$$\sigma = \sigma_p(\theta) = \begin{cases} exp\Big(\frac{\xi^p}{\xi^2-1}\Big), & |\xi| \leq 1 \\ \\ 0, & |\xi| > 1. \end{cases}, \qquad p_N = (\eta \mathsf{d}(x)N)^{1/2},$$

- 2D detection and reconstruction of piecewise Radon data

- More about noisy data

- More about spectral (and hierarchical) viscosity:

http://www.cscamm.umd.edu/~tadmor/spectral_viscosity/

THANK YOU