Gaussian spectral rules for second order finite-differ

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References


Motivations

In remote sensing applications (geophysics, radar imaging, medical tomography, etc.) the solution is only needed at a few points (receivers).

- Usually finite-difference schemes match Maclauren series in even order schemes: three point stencil in 1-D, five-points stencil in 2-D stencils for higher order schemes.
- Conventional approach to grid optimization: adaptive grids based on minimization of the truncation error – improves constants but not much.
- Superconvergence: at some points the convergence order can be higher.
- Ill-posedness of the inverse impedance problems: small variations in impedances (Dirichlet to Neumann map) results in exponentially fast decay of the solution of the inverse problem.
Can it be used in a constructive way?
Main results

- A grid optimization approach for second order finite-difference methods yields exponential convergence at a priori selected points without amplifying higher modes and increasing the stencil. The constructed schemes are spectrally accurate up to those points.

- Area of application: linear second order PDEs and systems (elliptic, parabolic, and hyperbolic) in remote sensing.

- Practical examples: frequency domain Maxwell equations for elastic or acoustic logging in 3-D inhomogeneous anisotropic media and 2-D hyperbolic problems of acoustic logging. Speedup more than one order.
Model problem and finite-differences

- Two-point problem:

\[ Aw - \frac{d^2w}{dx^2} = 0, \quad \frac{dw}{dx}|_{x=0} = -\varphi, \quad w(l) = 0. \]

\(\varphi\)-vector, \(w\)-vector-function of \(x, x \in [0, l]\).

Example: the Laplace eq. in \(R^2\), \(A = -\frac{d^2}{dy^2}\).

- Three-point finite-difference approximation

\[ A w_i - \frac{1}{\hat{h}_i} \left( \frac{w_{i+1} - w_i}{h_i} - \frac{w_i - w_{i-1}}{h_{i-1}} \right) = 0, \quad i = \]

\[ \frac{w_2 - w_1}{h_1} - \hat{h}_1 Aw_1 = -\varphi, \quad w_{k+1} = 0. \]

- How to find an optimal grid for the approximation of the Neumann map at \(x = 0\), i.e., minimize \(\|w_1 - w(0)\|\)?
Discrete and continuous Neumann-to-Dirichlet maps

- Neumann-to-Dirichlet map in terms of the impedance function:

\[ w(0) = f(A)\varphi. \]

- Discrete Neumann-to-Dirichlet map:

\[ w_1 = f_k(A)\varphi. \]

- Let \( \text{sp}(A) \subset [\lambda_{min}, \lambda_{max}] \), \( \|\varphi\| = 1 \), then:

\[
\|w(0) - w_1\| \leq \max_{\lambda \in \text{sp}(A)} |f_k(\lambda) - f(\lambda)| \leq \max_{\lambda \in [\lambda_{min}, \lambda_{max}]} |f_k(\lambda) - f(\lambda)|.
\]
Discrete and continuous impedance problem:

**Cont. problem:**

\[ \lambda u - \frac{d^2 u}{dx^2} = 0, \quad \frac{du}{dx} |_{x=0} = -1, \quad w(l) = 0. \]

\[ f(\lambda) = u(0) |_{\lambda} = \lambda^{-1/2} \tanh(l \sqrt{\lambda}). \]

**Disc. problem**

\[ \lambda u_i - \frac{1}{\hat{h}_i} \left( \frac{u_{i+1} - u_i}{h_i} - \frac{u_i - u_{i-1}}{h_{i-1}} \right) = 0, \quad i = 2 \]

\[ \frac{u_2 - u_1}{h_1} - \hat{h}_1 \lambda u_1 = -1, \quad u_{k+1} = 0. \]

\[ f_k(\lambda) = u_1 |_{\lambda} = \sum_{i=1}^{k} \frac{y_i}{\lambda - \theta_i}, \]

\( \theta_i = \text{FD eigenvalues}, \quad \sqrt{y_i} = \text{the FD eigenfunctions at } x_1. \)
Optimal grids

• Stieltjes continued fraction representation

\[ f_k(\lambda) = \frac{1}{\hat{h}_1 \lambda + \frac{1}{h_1 + \frac{1}{\hat{h}_2 \lambda + \ldots + \frac{1}{h_{k-1} + \frac{1}{\hat{h}_k \lambda + \ldots}}}}}. \]

• Ideal algorithm: find \( h_i, \hat{h}_i, \) \( i = 1 \ldots k \) minimizing

\[ \max_{\lambda_{\min} \leq \lambda \leq \lambda_{\max}} |f(\lambda) - f_k(\lambda)|. \]

The closed form solution is known only for \( f = \lambda^{-1/2} \) (semiinfinite case, Zolotarjov 1877).
Gaussian finite-difference rules

Find $h_i, \hat{h}_i, i = 1 \ldots k$ such that some $2k$ functionals $f_k(\lambda)$ coincide.

- Simple Padé ($l < \infty$):

\[ \frac{d^i}{d\lambda^i} [f_k(\lambda) - f(\lambda)] \bigg|_{\lambda=0} = 0, \quad i = 0, \ldots, 2k - 1 \]

- The Padé–Chebyshev:

\[ \int_{\lambda_1}^{\lambda_2} \lambda^i [f_k(\lambda) - f(\lambda)] \rho(\lambda) d\lambda = 0, \quad i = 0, \ldots, 2k \]

- Multipoint Padé:

\[ [f_k(\lambda) - f(\lambda)]|_{\lambda_j} = 0, \quad j = 1, \ldots, 2k. \]
Two-stage algorithm

- Compute Galerkin or Padé impedance in terms of the poles and

\[ f_k = \sum_{i=1}^{k} \frac{y_i}{\lambda - \theta_i}. \]

- Find \( h_1, \ldots, h_k \) and \( \hat{h}_1, \ldots, \hat{h}_k \):

\[
\sum_{i=1}^{k} \frac{y_i}{\lambda - \theta_i} \equiv \frac{1}{\hat{h}_1 \lambda + \frac{1}{h_1 + \frac{1}{\hat{h}_2 \lambda + \ldots + \frac{1}{h_{k-1} + \frac{1}{\hat{h}_k \lambda}}}}}
\]
Quadratures

• Krein-Kac measure:

\[ d\hat{x} = dx \sum_{i=1}^{k} \hat{h}_i \delta(x - x_i). \]

\[ f_k \to f \iff \hat{x} \to x. \]

• 2k nonlinear moment equations (for simple Padé):

\[
\begin{align*}
\int_{0}^{l} d\hat{x}^{-1} &= \int_{0}^{l} dx, \\
\int_{0}^{l} d\hat{x}^{-1} \int_{0}^{l} d\hat{x} \int_{\hat{x}^{-1}} d\hat{x}^{-1} &= \int_{0}^{l} dx \int_{0}^{l} dx \int_{0}^{l} dx \\
\int_{0}^{l} d\hat{x}^{-1} \int_{0}^{l} d\hat{x} \int_{\hat{x}^{-1}} d\hat{x}^{-1} \cdots &= \int_{0}^{l} dx \int_{0}^{l} dx \int_{0}^{l} dx \cdots
\end{align*}
\]
The first two are the same as for the Gauss-Lobatto-Legendre's scheme:

\[ x_k = \int_0^l dx = l, \quad \sum_{i=1}^k \hat{h}_i (x_i - l)^2 = \int_0^l (x - l)^2 dx = \frac{l^2}{3}. \]
Elliptic problems on unbounded domains: optimal geometric grids

- The Laplace equation on \([0, \infty] \times [0, 1]\):

\[
-\frac{\partial^2 w(x, y)}{\partial y^2} - \frac{\partial^2 w(x, y)}{\partial x^2} = 0,
\]

\[
\frac{\partial w}{\partial x} \bigg|_{x=0} = -\varphi(y), \quad w \big|_{x=+\infty} = 0, \quad w(x, 0) = 0, \quad w(x, 1) = 0.
\]

- Semidiscretization: the FD scheme along \(x\). If \(\varphi \in L^2[0, 1]\), then the semidiscrete error at \(x = 0\) is \(O\left(\max_{\lambda \in [0, \infty]} |f_k(\lambda) - \lambda^{-1/2}|\right)\).

- Optimal geometric grid: \(h_i = e^{\sqrt{k}(i-\frac{1}{2})}\), \(\hat{h}_{i+1} = \sqrt{h_i h_{i+1}}\), \(i = 1, \ldots\). Then

\[
|f_k(\lambda) - \lambda^{-1/2}|_{\lambda \in [0, \infty]} = O\left(e^{-\pi \sqrt{k}}\right).
\]

- Elliptic problems with variable coefficients asymptotically equivalent to the Laplace equation near singularities and at infinity, so our geometric grid is optimal asymptotically.
**Elliptic and hyperbolic problems in bounded domains**

- For $l < \infty$ and $0 < \lambda_{\text{min}} < \lambda_{\text{max}} < \infty$ (elliptic problems) superexponential convergence

\[
\max_{\lambda \in [\lambda_{\text{min}}, \lambda_{\text{max}}]} |f_k(\lambda) - f(\lambda)| < O \left(e^{-ck \log k}\right)
\]

with $c > 0$ depending on $\lambda_{\text{min}}$ and $\lambda_{\text{max}}$.

- For hyperbolic problems $A$ is indefinite, i.e., $\lambda_{\text{min}} < 0$ and there can be (resonances) of $f(\lambda)$ in $[\lambda_{\text{min}}, \lambda_{\text{max}}]$

\[
\max_{\lambda \in [\lambda_{\text{min}}, \lambda_{\text{max}}]} |f_k(\lambda) - f(\lambda)| < O \left(e^{c(n-k) \log k}\right),
\]

$n \equiv$ two points per wavelength.
Implementation: piecewise-homogeneous with rectangular interfaces

- Subdivision: domains are decomposed on rectangular homogeneous (checkerboard).
- Approximation of Dirichlet-to-Neumann map for each subdomain via conjugation conditions via interfaces.
- Tensor product grids for every rectangular subdomain → reduction approximation problems.
- 1-D optimal grids are computed a priori and stored in memory.
- Result: exponential convergence at subdomain corners.
Connection with the Spectral Galerkin

- Spectral Galerkin (Element) Method: \( u \approx u_k \in S, \) \( S \) is a good subspace of polynomials, trigonometric functions etc. Exponential convergence.

Let \( \theta_i \) and \( z_i(x) \) are Galerkin (Rayleigh-Ritz) eigenvalues and eigenfunctions, then

\[
\begin{align*}
    u_k &= \sum_{i=1}^{k} \frac{z_i(x)z_i(0)}{\lambda - \theta_i}, \\
    f_S(\lambda) &= u(0)|_\lambda = \sum_{i=1}^{k} \frac{z_i(0)^2}{\lambda - \theta_i}.
\end{align*}
\]

- The finite-difference and spectral galerkin method: for any subspace \( S \), such three-point finite-difference scheme with the same impedance,

\[
f_k(\lambda) \equiv f_S(\lambda).
\]

- Instead of working with full matrices requiring FFT and other techniques, the same results can be obtained with the three-point finite-difference scheme.
Matching impedance

- Continuous problem: Let $\nabla \cdot \sigma \nabla u = 0$ in $\Omega \subset \mathbb{R}^2$, then Dirichlet transmission operator (DN) $\Lambda_\sigma$ is defined as $\Lambda_\sigma u \big|_{\partial \Omega} = \sigma \frac{\partial u}{\partial \nu} \big|_{\partial \Omega}$.

- Let $u_k$ be obtained after the discretization on $k^2$ nodes in $\Omega$ using the FDM or FEM scheme.

Normally the scheme coefficients chosen to achieve the second order accuracy globally, i.e., $\|u - u_k\|_\Omega = O(k^{-2})$.

The are $O(k)$ independent grid parameters per surface node.

Can we find such parameters of the grid that the discrete DN EXPONENTIALLY, i.e.,

$$\|\Lambda_k^\sigma - \Lambda_\sigma\| = O(e^{-ck}), \ c > 0$$
Cost vs. benefits

• Cost:
  solution of discrete inverse problems, i.e., optimization of grid parameters of the PDE a priori. Can be reduced using domain decomposition approach:
  
  \[ \Omega = \bigcup \omega_i, \]

  then from exponential convergence of DN for every \( \omega_i \) separately for convergence of the global solution restricted on \( S = \bigcup \partial \omega_i \).

• Benefit:
  Exponentially convergent FD schemes using only simplest low order of second derivatives (i.e. 5-point scheme for 2-D, 7-point for 3-D). Traditionally this can be only achieved by spectral methods with full course, the spectral methods converge exponentially at all points, while only at a subset.)
Summary

• **New approach:** use schemes with the same finite-difference step location of the nodes from the point of view of the approximation at a priori selected points (receivers) for the required frequency band.

• **Results:** exponential superconvergence at receivers with the same cost as for the second order schemes.

• **Current applications:** elliptic and hyperbolic PDEs with piecewise coefficients and rectangular homogeneous subdomains (acoustic and electromagnetic logging problems). Observed speedup more than one order.

• **Ongoing research:** non rectangular interfaces and general vari...