Iterative Helmholtz Solvers

Accuracy of iterative Helmholtz solutions

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Outline

Aim and Impact

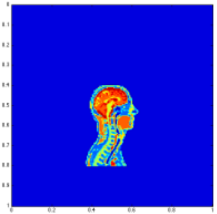
- Alert solver developers to keep accuracy of solution in mind
- Research sharper error bounds
- Allows a priori theoretical error estimation
- Research pollution through spectral methods
- Pinpoint pollution in 2D and 3D

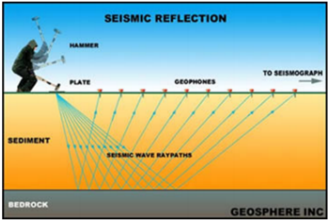
Introduction - The Helmholtz Equation

- Homogeneous Helmholtz equation + BC's

$$(-\nabla^2 - k^2)\, u(\mathbf{x}) = \mathbf{0}, \mathbf{x} \in \Omega \subseteq \mathbb{R}^n$$

- k is the wave number: $k = \frac{2\pi}{\lambda}$
- Practical applications in seismic and medical imaging[1]





[1]Source: https://earthquake.usgs.gov/image &
http://math.mit.edu/icg/resources/teaching/18.336-spring2014/

Introduction - Analytical Model

- Analytical 1D model problem

$$-\frac{d^2u}{dx^2} - k^2\,u = \delta(x - \frac{L}{2}),$$
$$u(0) = 0, u(L) = 0,$$
$$x \in \Omega = [0, L] \subseteq \mathbb{R},$$

- Sturm-Liouville + Green's function $\Rightarrow$ exact solution

$$G(x, L/2) = \frac{2}{L}\sum_{j=1}^{\infty}\frac{\sin(j\pi L/2)}{j^2\pi^2 - k^2/L^2}\sin(j\pi x/L)$$
$$\lambda_j = j^2\pi^2 - k^2$$
$$k \neq \frac{j\pi}{L}$$
$$j = 1, 2, 3, \ldots$$

Introduction - Numerical Model

- Discretization on $\Omega = [0, 1]$
- Most used second-order finite difference with $h = \frac{1}{n}$
- $k \approx \lfloor 2\pi/\#\text{gpw} \rfloor \Rightarrow kh$ is the grid resolution
- Rule of thumb $kh = 0.625$
- We obtain a linear system $A\hat{u} = f$

$$
\begin{aligned}
A &= \frac{1}{h^2}\text{tridiag}[-1 \;\; 2-(kh)^2 \;\; -1], \\
\hat{\lambda}_j &= \frac{1}{h^2}\left[2 - 2\cos(j\pi h) - k^2h^2\right], \\
j &= 1, 2, 3, \ldots, n-1, \\
A &\in \mathbb{R}^{(n-1)\times(n-1)}.
\end{aligned}
$$

- A is real, symmetric, normal, indefinite, tridiagonal and sparse

Introduction - Spectral Properties

- Near-null eigenvalues near intersection with origin
- The index where this happens for the analytical case is

$$\lambda_{j_{\min}} = 0 \Rightarrow j^2\pi^2 \approx k^2\pi^2,$$
$$\Rightarrow j_{\min} = \lfloor \frac{k}{\pi} \rfloor \text{ or } \lceil \frac{k}{\pi} \rceil.$$

- The index where this happens for the numerical case is

$$\hat{\lambda}_{\hat{j}_{\min}} = 0 \Rightarrow \frac{1}{h^2}\left[2 - 2\cos(j\pi h)\right] \approx k^2$$
$$\Rightarrow \hat{j}_{\min} = \text{round}\left[\frac{\arccos(1-\kappa^2)}{\pi h}\right]$$

- Near-null eigenvalues ⇒ convergence issues ⇒ Deflation
- Near-null eigenvalues ⇒ accuracy issues ⇒ Pollution
- Our aim: study both cause and effect simultaneously

Pollution - Introduction

- Numerical dispersion due to different numerical wave number
- Pollution error accumulates
- Non-accurate error estimates
- Total error is (Babuska, I., et al., 1997)
  $\frac{\|u-\hat{u}\|}{\|u\|} \leq C_1 kh + C_2 k^3 h^2,\ kh < 1$
- Phase error is $\left|\tilde{k} - k\right| = \mathcal{O}(k^2 h^2)$
- Error grows with k
- Set $k^3 h^2 < 1$ or use higher-order discretization

Pollution - Error Bound - I

- Take $k = \frac{2\pi}{\lambda}$, $\lambda = \frac{2\pi}{\omega n} \Rightarrow k = \omega n$
- Second order FD scheme for (Runborg, O., 2012)

$$\underbrace{\frac{-u_{j+1} + 2u_j - u_{j-1}}{h^2}}_{A} - \underbrace{\frac{\omega^2 n^2 h^2 u_j}{h^2}}_{B} = 0$$

- Solution for exact ωn: $u(x) = e^{i\omega n x_j}$ (1)
- Solution for numerical $\omega \tilde{n}$: $u_j = e^{i\omega \tilde{n} x_j}$ (2)
- Substitute (1) into A & (2) into B

$$-u_{j+1} + 2u_j - u_{j-1} = e^{i\omega \tilde{n} x_j} 2\left[1 - \cos\left(\omega \tilde{n} h\right)\right] \qquad (3)$$

- If $\tilde{n}$ solves (3) then

$$\frac{2(1 - \cos\left(\omega \tilde{n} h\right))}{h^2} - \omega^2 n^2 h^2 = 0 \qquad (4)$$

Pollution - Error Bound - II

- Expand cosine, substitute in (4) and divide by ω^2

$$\tilde{n}^2 - n^2 + \mathcal{O}(\omega^2 h^2) = 0$$

- Error due to different wave speed $\tilde{n}$ is

$$|\tilde{n} - n| = \mathcal{O}(\omega^2 h^2), \text{ for } \tilde{n} \approx n$$

- Error due to dispersion

$$\left| e^{i\omega n x_j} - e^{i\omega \tilde{n} x_j} \right| = \left| 1 - e^{i(\tilde{n}-n)x_j} \right| \leq C\omega \left| \tilde{n} - n \right| \leq C\omega^3 h^2$$

- Total error for the model problem

$$\text{Rel. err.} = \frac{\|u - \hat{u}\|}{\|u\|} \leq C_1 kh + C_2 k^3 h^2, \; kh < 1$$

Pollution - Error

Relative error between exact and numerical solution for $kh = 0.625$

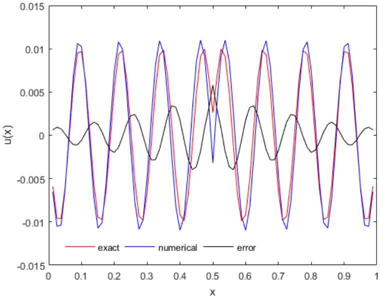
k	n	Rel. error	k^3h^2
100	160	0.5770	39
200	320	1.9347	78
300	480	4.2584	117
400	640	1.1925	156
500	800	0.9783	195

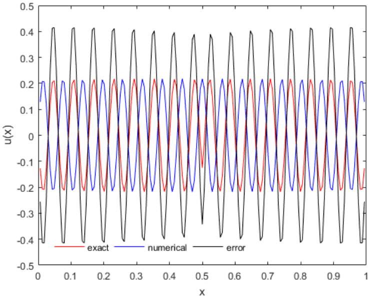
k	n	Rel. error	k^3h^2
102	164	62.0447	39
139	224	3.8516	53
212	332	1.1111	80
312	500	38.5703	121
485	776	172.9903	189

- Large and unregular error
- k^3h^2 bound is not sharp

Pollution - 1D

Exact and numerical solution for $k = 100$ (L) and $k = 102$ (R)





Pollution - Dispersion Correction

- Accuracy comes with uneconomical linear systems
- Recall phase error is $\left|\tilde{k} - k\right| = \mathcal{O}(k^2 h^2)$
- Dispersion correction by setting (Babuska, I., et al., 1997)

$$\tilde{k} = \sqrt{\frac{2(1 - \cos(kh))}{h^2}}$$

- Construct matrix A using $\tilde{k}$ instead of k
- Correction with $\tilde{k}$ possible in 1D
- In higher dimensions infinite directions

Pollution - Error

Relative error and index $j_{\text{min}}, \hat{j}_{\text{min}}$ of the smallest analytical and numerical eigenvalue for $kh = 0.625$ using k (L) and $\tilde{k}$ (R)

k	j_{min}	$\hat{j}_{\text{min}}$	Rel. error
100	32	32	0.5770
200	64	65	1.9347
300	95	97	4.2584
400	127	129	1.1925
500	159	162	0.9783

$\tilde{k}$	j_{min}	$\hat{j}_{\text{min}}$	Rel. error
98	32	32	0.0685
197	64	64	0.0681
295	95	95	0.0680
394	127	127	0.0678
492	159	159	0.0680

- Pollution if kernel misaligned
- Spectral effect of $\tilde{k}$ on kernel
- Sign of smallest eigenvalue also matters

Our Approach - Introduction

- Primary literature focus on differences k and $\tilde{k}$
- Not much literature on role of eigenvalues
- Our aim: shed light on role of near nullspace eigenvalue(s)
- Main hypothesis: the accuracy of the near nullspace numerical eigenvalues are related to the pollution
- We propose an error bound incorporating the eigenvalues

Our Approach - Spectral Properties

- We use eigenvalues to obtain theoretical sharper bound
- Total error now becomes

$$\frac{\|u - \hat{u}\|}{\|u\|} \leq \frac{\sqrt{\left(\frac{2\pi^2}{3}\frac{1}{\hat{\lambda}^2_{\hat{j}_{\min}}} + \frac{\pi^2}{2{\lambda_{j_{\min}}}^2}\right)}}{\|u\|}$$

- Error grows with discrepancy between $\lambda_{j_{\min}}$ and $\hat{\lambda}_{\hat{j}_{\min}}$.
- As k increases $\Rightarrow j_{\min} \neq \hat{j}_{\min}$

Our Approach - New Upper Bound

Construction of upper bound:

1. Orthonormalize basis and evaluate at discrete points
2. Rewrite error as

$$\|u - \hat{u}\| = \left\| 2 \sum_{j=1}^{n} \sin(j\pi x') \left(\frac{1}{\lambda_j} - \frac{1}{\hat{\lambda}_j} \right) \right\|,$$

$$= \sqrt{4 \sum_{j=1}^{n} \sin(j\pi x')^2 \left(\frac{1}{\lambda_j} - \frac{1}{\hat{\lambda}_j} \right)^2}$$

3. Compute $\lambda_{j_{\min}}$ and $\hat{\lambda}_{\hat{j}_{\min}}$
4. Find recursive relation for ratio's between eigenvalues
5. Express and bound sum in terms of ratio

$$\|u - \hat{u}\| \leq \sqrt{\left(\frac{2\pi^2}{3} \frac{1}{\hat{\lambda}^2_{\hat{j}_{\min}}} + \frac{\pi^2}{2\lambda_{j_{\min}}{}^2} \right)}$$

Our Approach - Preliminary Results

Relative error and new bound (E) for $kh = 0.625$

k	n	Rel. error	E
100	160	0.5770	5.0369
200	320	1.9347	3.2117
300	480	4.2584	4.7559
400	640	1.1925	1.4373
500	800	0.9783	1.7980

k	n	Rel. error	E
102	164	62.0447	67.9444
139	224	3.8516	4.6088
212	332	1.1111	1.7703
312	500	38.5703	43.0448
485	776	172.9903	191.9262

- New bound (E) sharper
- Allows detailed study of error in terms of spectrum
- Connect results to convergence

Our Approach - Alternate Correction

- Use information from eigenvalues instead of $\tilde{k}$
- Solve system

$$A_c u = f, \text{ where } A_c = A + cI,$$
$$c = -\lambda_{\mathbf{j}_{\text{min}}} + \hat{\lambda}_{\hat{\mathbf{j}}_{\text{min}}},$$

- Note this correction also possible in higher dimensions

Our Approach - Error

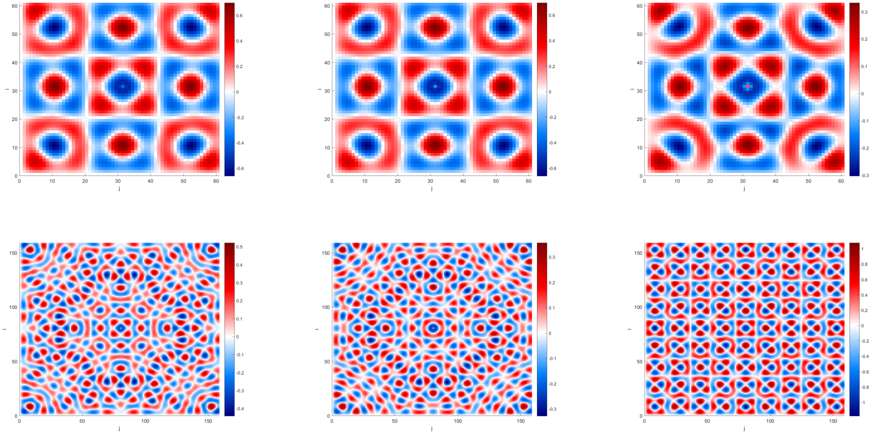
Relative error and index $j_{\text{min}}, \hat{j}_{\text{min}}$ of the smallest analytical and numerical eigenvalue for $kh = 0.625$ using eigenvalue correction

k	j_{min}	$\hat{j}_{\text{min}}$	Rel. error
100	32	32	0.0747
200	64	64	0.0946
300	95	95	0.0344
400	127	127	0.0213
500	159	159	0.0100

- No pollution if kernel aligned
- Drawback: requires smallest analytical and numerical eigenvalue
- Use to study sharper pollution progression in 2D & 3D

Our Approach - Dispersion Correction (2D)

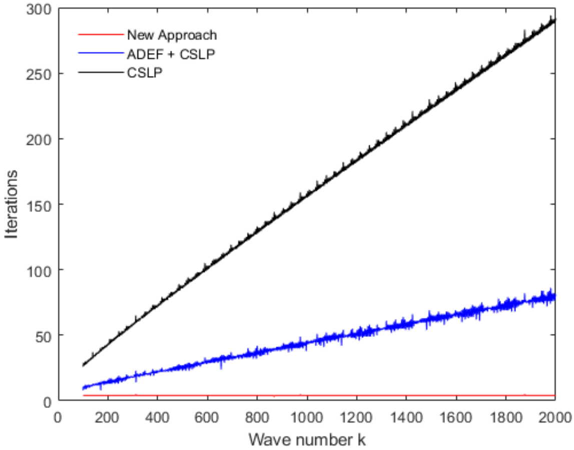
Exact (L), Adjusted Numerical (C) and Unadjusted Numerical (R) Solution for $k = 30$ (Top) and $k = 100$ (Bottom)



Conclusion

- Fast solvers may lead to inaccurate solutions
- Phase differences 'pollute' the numerical solution
- Bound error using smallest eigenvalues
- For the first time: dispersion correction in 2D without increasing problem size and/or switching to higher-order schemes.
- Relate error to convergence properties

Next Up - Accelerated Convergence



References

- Upcoming articles
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- Further reading

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