Application of matrix square root and its inverse to downward wavefield extrapolation

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Motivation

- Downward wavefield extrapolation
- Matrix functions
- Low rank matrix compression (HSS)
- Combine to explore and develop efficient algorithms for modeling/imaging
In downward extrapolation, the goal is to solve Helmholtz equation

$$\frac{\partial^2 p(x, z, \omega)}{\partial z^2} = -\left(\frac{\omega^2}{c^2(x, z)} + \nabla_x^2\right)p(x, z, \omega)$$

by stepping in depth from the boundary data $p(x, z = z_0, \omega)$.

Main advantage: reduction in dimensionality of extrapolation problem

Main difficulty: evanescent modes
**Introduction**

Full wave equation depth extrapolation (Sandberg & Beylkin, 2009; Sandberg, Beylkin & Vassiliou, 2010)

- Operator $\mathcal{H}_2 = \frac{\omega^2}{c^2(x,z)} + \nabla^2_x$ is projected to its non-negative invariant subspace:

$$\mathcal{H}_2 \rightarrow \mathcal{P}\mathcal{H}_2\mathcal{P}$$

- Downward extrapolation equation:

$$\frac{\partial^2 p(x, z, \omega)}{\partial z^2} = -\mathcal{P}\mathcal{H}_2\mathcal{P} p(x, z, \omega) \quad (2)$$

- Spectral projector is computed by:

$$\mathcal{P} = \frac{1}{2}(I + \text{sign}(\mathcal{H}_2))$$

where $\text{sign}(\mathcal{H}_2)$ is found by recursion (e.g. Kenney & Laub, 1995)

$$S_0 = \frac{\mathcal{H}_2}{\|\mathcal{H}_2\|_2}, \quad S_{k+1} = \frac{3}{2}S_k - \frac{1}{2}S_k^3$$

- Efficiency is achieved by low rank matrix compression (PLR, HSS), estimated cost $\sim O(N)$
Introduction

One way wave equation:
- Similar approach can be used in one way wave equation extrapolation
- Square root operator $\mathcal{H}_1 = \mathcal{H}_2^{1/2}$ can be computed by polynomial recursion
- Filtering of evanescent waves is still necessary
- Modeling of all propagating modes is possible
- Efficiency for large problems with matrix compression

Other uses:
- Correct modeling of a volume injection (e.g. air gun) source and scattering operators (e.g. Wapenaar, 1990)
- These require computation of inverse square root $\mathcal{H}_2^{-1/2}$
The one way wave equation is obtained by factoring the operator $\mathcal{H}_2 = \frac{\omega^2}{c^2(x,z)} + \nabla_x^2$, and then neglecting the terms that account for the scattering (e.g. Grimbergen et al., 1998; Wapenaar, 1990):

$$\frac{\partial p^\pm}{\partial z} = \mp i\mathcal{H}_1 p^\pm$$

where $p^+, p^-$ - down and up going fields: $p = p^+ + p^-$, $\mathcal{H}_1$ - propagator, $\mathcal{H}_1 \mathcal{H}_1 p = \mathcal{H}_2 p$.

Extrapolation is done by finite differences or matrix exponentiation by scaling and squaring algorithm.
One way wave equation

- $\mathcal{H}_1 = \mathcal{H}_2^{1/2}$ is a non-local pseudo-differential operator
- Approximate square root by a polynomial or rational function $\Rightarrow$ paraxial wave equation
  - Efficient with finite differences and operator splitting
  - Propagating modes up to certain angle from the main propagation direction
- Modal decomposition of the discretized operator $\mathcal{H}_2$ (e.g. Grimbergen et al.; Margrave et al., 2002; Lin & Herrmann, 2007)
  - Discretize $\mathcal{H}_2 \rightarrow \mathcal{H}_2$ by finite differences
  - All propagating modes in the main propagation direction
  - Requires eigenvalue decomposition, not practical for large problems
- Our goal: use polynomial recursion with matrix compression instead of modal decomposition
Square root calculation

- Assume:
  - Absorbing boundary conditions in $x$ are decoupled, $H_2$ is self-adjoint
  - Negative eigenvalues have been removed by spectral projector: $\tilde{H}_2 = \mathcal{P}H_2\mathcal{P}$ - no evanescent modes
- Principal root of matrix $H$ with no nonpositive eigenvalues can be computed by Shultz iteration (Higham, 2008):

  $$
  Y_0 = \frac{H}{\|H\|_2}, \quad Z_0 = I
  $$

  $$
  Y_{k+1} = \frac{3}{2}Y_k - \frac{1}{2}Y_kZ_kY_k
  $$

  $$
  Z_{k+1} = \frac{3}{2}Z_k - \frac{1}{2}Z_kY_kZ_k
  $$

- Derived by applying polynomial recursion for matrix sign function to $\begin{bmatrix} 0 & H \\ I & 0 \end{bmatrix}$ and Newton’s method
- $Y_k \rightarrow \left(\frac{H}{\|H\|_2}\right)^{1/2}, \quad Z_k \rightarrow \left(\frac{H}{\|H\|_2}\right)^{-1/2}$ quadratically
The square root polynomial recursion is poorly conditioned since $\tilde{H}_2$ has zeros eigenvalues (numerically they are very small complex numbers).

Shultz iteration applied to $\tilde{H}_2$: $Y_k \rightarrow \left(\frac{\tilde{H}_2}{\|\tilde{H}_2\|_2}\right)^{1/2}$ in $\sim O(10)$ with high accuracy.

$Z_k$ part causes the iteration eventually to diverge, since $\tilde{H}_2$ does not have an inverse $\Rightarrow$ careful stopping criterion is needed.

Stopping criterion we use: (a) difference between iterates $\|Y_{k+1} - Y_k\|$, (b) misfit $\|\tilde{H}_1^2 - \tilde{H}_2\|$, (c) update direction.
Pseudo inverse $\tilde{H}_1^\dagger$ is needed to implement volume injection source as a boundary condition:

$$S^{\pm}(x, z = 0, \omega) = \frac{i\omega^2}{2} \tilde{H}_1^\dagger I(x, z = z_0, \omega)$$

(e.g. Wapenaar, 1990)

To compute pseudo inverse $\tilde{H}_1^\dagger$:

- Compute $H_2^{-1}$, e.g. by recursion (Ben Israel and Cohen, 1966): well conditioned, stable, quadratic convergence, known to be slow initially
- Apply spectral projector to $H_2^{-1}$: $H_2^{-1} \rightarrow \tilde{H}_2^\dagger = \mathcal{P} H_2^{-1} \mathcal{P}$
- Compute pseudo inverse of $\tilde{H}_1^\dagger$ by Shultz iteration from $\tilde{H}_2^\dagger$

Evanescent modes are discarded in all calculations.
Figure 1: Convergence of iteration for the square root, relative error $= \frac{\|\tilde{H}^2_1 - \tilde{H}_2\|}{\|\tilde{H}_2\|}$
Figure 2: Convergence of iteration for the matrix inverse, relative error $= \frac{\|H_2^{-1} - \text{pinv}(H_2)\|}{\|\text{pinv}(H_2)\|}$
Figure 3: Convergence of iteration for the pseudo inverse of square root, relative error $= \frac{\|\tilde{H}_1^\dagger - \tilde{H}_2^\dagger\|}{\|\tilde{H}_2^\dagger\|}$
Figure 4: Structure of example $H_2$ matrix and its inverse: 1-d case, simple finite differences
Figure 5: Rank representation of the inverse

- Diagonal blocks have full rank
- Off-diagonal blocks have rank 1
Matrices that have HSS structure

- Have large blocks with low numerical rank
- Often arise in solutions of PDEs, e.g. integral operators:

\[
u(x) = \int K(x, y) f(y) dy,
\]

where \( K(x, y) \) decays fast away from \( x = y \) or is smooth
- Discretized Helmholtz operator (and functions of thereof) have HSS structure. This has been proven for some functions \( \text{(e.g. Beylkin et al., 1999 - sign function)} \)
- Seismic data being the Green’s function can also be represented with HSS \( \text{(Kumar et al., 2013)} \)
Off-diagonal blocks have low numerical rank

Each low rank approximation is a product of
- a tall matrix
- a small matrix and
- a thin matrix

The hierarchy is organized in a binary tree

Xia, 2012, Lyons, 2005
Hierarchically semiseparable (HSS) representation of matrices allows us to

- Store dense matrices with less memory
- Do matrix operations - multiplication, addition, scaling, etc. - fast (e.g. $O(n)$ vs $O(n^3)$ flops)
- Results are also HSS matrices
- Approximate but can be made arbitrarily accurate by increasing the rank of the block approximants
Compression

Xia, 2012, Lyons, 2005

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Compression

- Store only lowest $U$’s and $V$’s in the hierarchy
- Store $B$’s, $R$’s, $W$’s for each level
  - small matrices, much smaller than $U$’s and $V$’s
- Higher $U$’s and $V$’s are determined from lower $U$’s and $V$’s via $R$’s and $W$’s
- Store the lowest $D$’s in the hierarchy as dense matrices
- Optimized for matrix-vector multiplication

Xia, 2012, Lyons, 2005
Compression

Xia, 2012, Lyons, 2005

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### Complexity of algorithms for HSS matrix operations (Sheng et al., 2007):

<table>
<thead>
<tr>
<th>Operation</th>
<th>Cost with HSS</th>
<th>Cost without HSS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix-vector multiplication</td>
<td>$O(nr^2)$</td>
<td>$O(n^2)$</td>
</tr>
<tr>
<td>Matrix-matrix multiplication</td>
<td>$O(nr^3)$</td>
<td>$O(n^3)$</td>
</tr>
<tr>
<td>Matrix addition</td>
<td>$O(nr^2)$</td>
<td>$O(n^2)$</td>
</tr>
<tr>
<td>LU decomposition</td>
<td>$O(nr^3)$</td>
<td>$O(n^3)$</td>
</tr>
<tr>
<td>Matrix inverse</td>
<td>$O(nr^3)$</td>
<td>$O(n^3)$</td>
</tr>
<tr>
<td>Transpose</td>
<td>$O(nr)$</td>
<td>$O(n^2)$</td>
</tr>
<tr>
<td>HSS construction</td>
<td>$O(nr)$</td>
<td>Not applicable</td>
</tr>
</tbody>
</table>

- $r$ is maximum rank of off-diagonal blocks
- Efficient implementation is non-trivial
- Current implementation in Matlab (MSN toolbox and Lina Miao)
Examples

True model: 2D SEG model, background model: smoothed 2D SEG model

Absorbing boundary conditions: taper the wavefield at each depth step (Serjan et al., 1985)

Model parameters:

- 85 grid points \times 338 grid points, model size 840 \times 3370 m
- Spacing: \Delta x = \Delta z = 10 m
- Source: Ricker wavelet with central frequency 15 Hz
- Sources: 100 m spacing from x = 100 m to x = 3300 m at depth z = 0 m
- Receivers: at every grid point at depth z = 0 m

Data is generated by the linearized constant density acoustic frequency domain forward modeling operator.
Figure 6: True velocity model
Figure 7: True velocity model
Figure 8: Model perturbation
Figure 9: Wavefield time slice at $t = 0.35$ sec, source $x = 1500$ m
Figure 10: One way wave equation migration result
Figure 11: Model perturbation
Figure 12: Reverse time migration result
Future work

- Implementation of matrix compression – currently use Matlab implementation that is not optimal
- Do more tests with HSS compression: precision seems to depend on HSS approximation accuracy, and does not get worse with increase of matrix size
- 3D implementation
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