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

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Summary

In this paper we propose a method for computation of the square root of the Helmholtz operator and its inverse that arise in downward extrapolation methods based on one-way wave equation. Our approach involves factorization of the discretized Helmholtz operator at each depth by extracting the matrix square root after performing the spectral projector in order to eliminate the evanescent modes. The computation of the square root of the discrete Helmholtz operator and its inverse is done using polynomial recursions and can be combined with low rank matrix approximations to reduce the computational cost for large problems. The resulting square root operator is able to model the propagating modes kinematically correctly at the angles of up to 90°. Preliminary results on convergence of iterations are presented in this abstract. Potential applications include seismic modeling, imaging and inversion.

Introduction

Downward extrapolation arises in seismic modeling and imaging. The big advantage of marching in depth is that it reduces the dimensionality of the modeling problem. The main disadvantage is that propagation angles above 90° can not be modeled. In downward extrapolation the goal is to solve the Helmholtz equation

$$\frac{\partial^2 p(\mathbf{x},z,\omega)}{\partial z^2} = -\left(\frac{\omega^2}{c^2(\mathbf{x},z)} + \nabla_{\mathbf{x}}^2\right) p(\mathbf{x},z,\omega) \tag{1}$$

by stepping in depth from the boundary data $p(\mathbf{x}, z = z_0, \omega)$ given at the surface of the model. This process is unstable due to the evanecent modes that can lead to the exponential growth of the solution. Sandberg & Beylkin (2009) proposed a stable method to solve this equation using spectral projection. Our approach is similar, except we will solve the one-way wave equation.

One way wave equation can be obtained by factoring the operator $\mathscr{H}_2 = \frac{\omega^2}{c^2(\mathbf{x},z)} + \nabla_{\mathbf{x}}^2$ in equation (1) and neglecting the terms that account for the scattering. The process is describeld in e.g. Grimbergen et al. (1998) and Wapenaar (1990). The one way wave equation is

$$\frac{\partial p^{\pm}}{\partial z} = \mp i \mathscr{H}_1 p^{\pm} \tag{2}$$

where p^+ and p^- are up and down going wave fields respectively, $p = p^+ + p^-$, and $\mathscr{H}_1 \mathscr{H}_1 p = \mathscr{H}_2 p$.

The one-way wave equation can be solved by stepping in depth by e.g. finite differences. In order to do that, $\mathscr{H}_1 = \mathscr{H}_2^{1/2}$ has to be computed at each depth step. For laterally varying media, the square root operator is a pseudo-differential operator. Most popular methods approximate this pseudo-differential operator by a diferential operator that is then discretized by finite differences. These approximations can model propagating modes at the angle up to some maximum angle from the vertical. It is of interest to compute $\mathscr{H}_1$ accurately, so as to ensure that the method can model the propagating waves at angles up to 90° in complex media. Also the computation needs to be fast.

The inverse of the square root operator $\mathscr{H}_1^{-1}$ is also sometimes necessary. For example, $\mathscr{H}_1^{-1}$ is necessary for (1) correct modeling of a volume injection source, e.g. an air gun source (Wapenaar (1990)), and (2) for the computation of the scattering operators coupling the up and down going wave fields, if one wants to model the scattering response of the medium. These operators can be expressed in terms of $\mathscr{H}_1$ and $\mathscr{H}_1^{-1}$.

Method and Theory

We adopt the approach of first discretizing the reduced Helmholtz operator $\mathscr{H}_2$ and then factorizing the discretized operator. If there is no attenuation in the medium, and apart from the boundary conditions, the discretized $\mathscr{H}_2$ is an indefinite real symmetric matrix that we will denote H_2. One way to compute the square root is to perform the eigenvalue decomposition (Grimbergen , 1995; Margrave et al. , 2002; Lin & Herrmann , 2007). This method, though accurate, is in general computationally intensive and becomes intractable for large 3D problems. For large problems, a polynomial recursion can be used instead. Combined with a low rank representation of matrices, (e.g., Xia , 2012), this makes it possible to compute the square root of a large matrix and its inverse fast with a small amount of storage.

The discretized $\mathscr{H}_1$, denoted H_1, can be computed from H_2 by the Shultz iteration (Higham , 2008):

$$\begin{aligned} Y_0 &= \frac{H_2}{\|H_2\|_2} \\ Z_0 &= I \\ Y_{k+1} &= \frac{1}{2} Y_k \left(3I - Z_k Y_k\right) \\ Z_{k+1} &= \frac{1}{2} Z_k \left(3I - Y_k Z_k\right) \end{aligned} \tag{3}$$

This iteration is shown to converge quadratically for matrices that do not have eigenvalues on the negative real axis as follows:

$$Y_k \longrightarrow \left(\frac{H}{\|H\|_2}\right)^{1/2} \qquad Z_k \longrightarrow \left(\frac{H}{\|H\|_2}\right)^{-1/2} \tag{4}$$

Since the Helmholtz matrix H_2 is indefinite, some of its eigenvalues are real and negative. The negative eigenvalues correspond to the evanescent modes, so they can be filtered out using the spectral projector described by Sandberg & Beylkin (2009). The projected Helmholtz matrix $\tilde{H}_2$ is symmetric positive semidefinite, so iteration (3) in principle converges to $\tilde{H}_1 = \tilde{H}_2^{1/2}$ and its pseudoinverse $\tilde{H}_1^{\dagger}$, however, since $\tilde{H}_2$ is singular, the problem is very ill-conditioned and in general $\tilde{H}_1^{\dagger}$ resulting from iteration (3) is inaccurate. A better way of computing $\tilde{H}_1^{\dagger}$ is to first find $\tilde{H}_2^{\dagger}$, the pseudoinverse of $\tilde{H}_2$ and then apply iteration (3) to extract the square root $\tilde{H}_1^{\dagger}$. The pseudoinverse can be computed e.g. by the polynomial recursion of Ben-Israel & Cohen (1966), which also converges quadratically.

The polynomial recursions described in the previous paragraphs involve operations such a matrix addition, multiplication and scaling that can be expensive for dense matrices. Partitioned low rank approximations, such as hiererchically semi-separable (HSS) representation, can be used to represent the matrices involved in the computation with less storage and speed up of the operations. Some methods for such matrices are described by e.g., Xia (2012) and Sheng et al. (2007). These studies provide analysis of the numerical cost of such algorithms. The complexity depends on the matrix size and the rank of the HSS approximation. The cost in polynomial recursions is dominated by the $O(nk^3)$ matrix-matrix multiplies, where k is the maximum rank of the off-diagonal block approximants.

Examples

In this section we show preliminary results of convergence tests of the polynomial recursions described in the previous section for spectral projected 1D Helmholtz matrix $\hat{H}_2$ of different size. Such matrix arises at each layer of 2D downward extrapolation problem. We test the iterations for the $n \times n$ matrix with $n = 251, 521, 1001, 2001$ and 2001. The matrices are obtained by discretizing the 1D Helmholtz operator in a homogeneous medium with velocity $v = 2000$ m/s at frequency $f = 9.992$ Hz. The lateral discretization step is $\Delta x = 2$ m, and a 21-point stencil with periodic boundary conditions is used in the discretization. The spectral projection is performed using polynomial recursion of Sandberg & Beylkin (2009). Then the pseudoinverse $\tilde{H}_2^{\dagger}$ is computed from the projected positive semidefinite matrix by Ben-Israel and Cohen iteration. The square root is then extracted from the projected matrix $\tilde{H}_2$ and its pseudoinverse $\tilde{H}_2^{\dagger}$ using Shultz iteration (3).

Figures 1, 2 and 3 show convergence of the pseudoinverse, square root and inverse square root interations for different matrix sizes. In all figures, Frobenius norm is used to compute the relative errors. Figure 1 shows the relative error between the pseudoinverse computed by the Ben-Israel and Cohen iteration and by Matlab function `pinv`. This iteration is known to converge slowly at the beginning, so finding a better starting point maybe a future research direction. Alternatively, it may be more beneficial to compute the pseudoinverse by the ULV decomposition as described by Sheng et al. (2007). In each

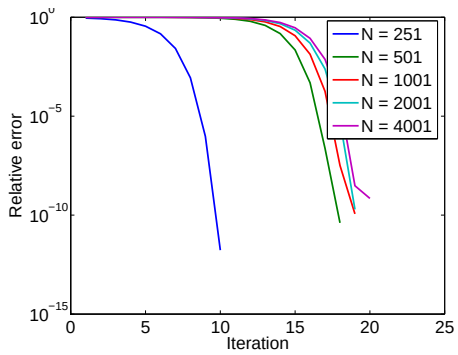
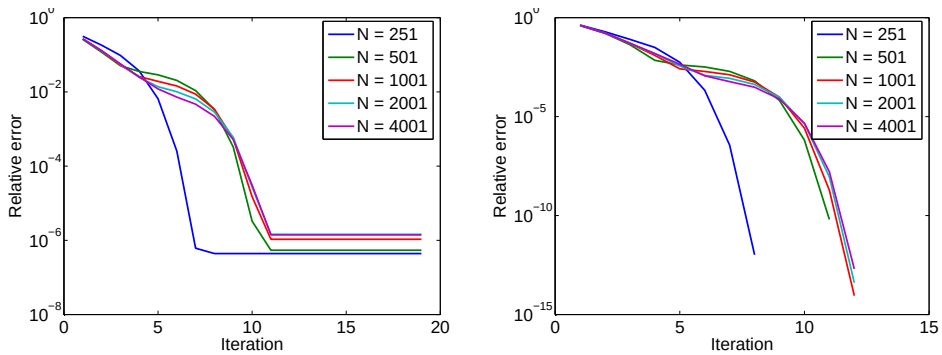


Figure 1 *Convergence of iteration for the pseudoinverse*



(a) (b)

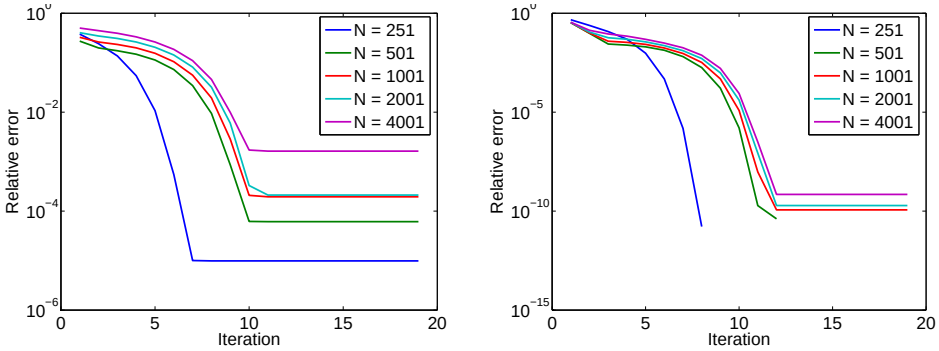
Figure 2 *Convergence of iteration for the square root*

of figures 2 and 3, image (a) shows the relative error between the square roots $\tilde{H}_1$ and $\tilde{H}_1^{\dagger}$ computed by the Shultz iteration and the square roots computed by the eigenvalue decomposition. Image (b) shows relative errors $\frac{\|\tilde{H}_1^2-\tilde{H}_2\|}{\|\tilde{H}_2\|}$ and $\frac{\|\tilde{H}_1^{\dagger 2}-\tilde{H}_2^{\dagger}\|}{\|\tilde{H}_2^{\dagger}\|}$. The convergence of the square root iteration is superlinear and fast. However, some precision loss is apparent for the inverse square root iteration, as the matrix grows and becomes more ill-conditioned. Possible strategies to avoid precision loss, e.g. preconditioning, remian to be explored.

Figure 4 shows the time slice of the down going wavefield from a monopole point source, i.e. with the application of the $\mathscr{H}_1^{-1}$ operator, generated by downward extrapolation with the square root operator computed as above. The source is the 10 Hz Ricker wavelet centered at time $t = 0.2$ sec, and is located in the middle of the computational grid at the range $x = 1000$ m at the top of the domain. The time slice is computed at $t = 0.5$ sec. The simulation parameters are the same as described in the previous paragraph.

Conclusions

Polynomial recursions can be a useful tool for computing functions of matrices, potentially leading to efficient seismic modeling, imaging, and inversion methods based on the one-way wave equation downward extrapolation that can handle steep dips and variable velocity media. Preliminary tests presented in the previous section look promising. Some convergence issues need to be explored and applications need to be developed.



(a) (b)

Figure 3 *Convergence of iteration for the pseudoinverse of the square root*

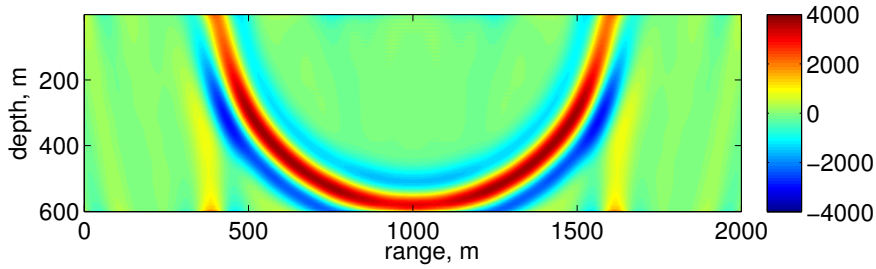


Figure 4 *A wavefield simulated from a point source.*

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References

A. Ben-Israel & D. Cohen, 1966. On iterative computation of generalized inverses and associated projections, J. SIAM Numer. Anal., **3**, pp. 410-419.

Grimbergen, 1995. One-way wave field operators in laterally varying media. M.Sc. Thesis, Delft University of Technology, Delft, The Netherlands.

J.L.T. Grimbergen, F.J. Dessing & K. Wapenaar, 1998. Modal expansion of one-way operators in laterally varying media, Geophysics, **63**, pp. 995-1005.

J. Higham, 2008. Finctions of matrices: theory and computations, SIAM.

T. Y. Lin & F.J. Herrmann, 2007. Compressed wavefield extrapolation, Geophysics, **72**, pp. SM77-SM93.

G.F. Margrave, M.P. Lamoureux, P. Gibson, R.A. Bale & J. Grossman, 2002. Exact wavefield extrapolation in 2D for v(x), CREWES Research Reports, http://www.crewes.com/ForOurSponsors/ResearchReports/2002/2002-13.pdf.

K. Sandberg & G. Beylkin, 2009. Full-wave-equation depth extrapolation migration, Geophysics, **74**, pp. WCA121-WCA128.

Z. Sheng, P. Dewilde, S. Chandrasekaran, 2007. Algorithms to solve hierarchically semi-separable systems, Operator Theory: Advances and Applications Volume 176, 255-294

C.P.A. Wapenaar, 1990. Representation of seismic sources in the one-way wave equations, Geophysics, **55**, pp.786-790.

J. Xia, 2012. On the complexity of some hierarchical structured algorithms. SIAM J. of Matrix Analysis and Applications, **33**(2), pp. 338-410.