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# APPLICATIONS OF GENERALIZED INVERSION IN GEOPHYSICS

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## Abstract

In this paper, an overview is given to applications of generalized inversion in the geophysical sciences. Since geophysical problems are often ill-posed with inadequate and inconsistent data, generalized inversion procedures are required. The analysis of non-Hermitian operators by Lanczos (1958, 1961) provides a framework for the solution of many inverse problems in geophysics. In addition, the conjugate gradient method of Hestenes and Stiefel (1952) and the related method of Lanczos (1950) allow for efficient iterative solutions of many large scale inverse problems in geophysics.

## Introduction

One of the objectives of geophysics is to infer properties of the Earth's atmosphere, oceans and solid interior using remotely recorded geophysical data. The forward problem in geophysics consists of computing geophysical field values given the physical parameters of the medium and the source configuration. For example, in seismology the field values are the vibrational displacement in the Earth, and the medium parameters are the Earth's elastic parameters and density.

The geophysical inverse problem consists of estimating the physical properties of the Earth from the observed geophysical data. Examples of geophysical inverse problems include seismic tomography of the Earth's interior (Aki and Richards, 1980, Chap. 13; Dziewonski, 1984; Nolet, 1987a), petroleum prospecting (Claerbout, 1976, 1985), inversion of gravity, magnetic and electromagnetic data (Lines, 1988, Chap. 5; Oldenburg; 1990, Madden, 1990), acoustic imaging in the oceans (Munk and Wunsch, 1979), and remote sensing of the atmosphere (Twomey, 1977).

In general, geophysical inverse problems are ill-posed due to the insufficient nature of the data, and appropriate techniques are required for their solution. The non-Hermitian analysis of Lanczos (1958, 1961, Chap. 3-5) has provided a framework for the solution of many geophysical inverse problems. Early applications of this work to geophysics include Jackson (1972), Wiggins (1972) and Madden (1972). For large scale geophysical inverse problems, the conjugate gradient method of Hestenes and Stiefel (1952) and the related method of Lanczos (1950) have provided efficient iterative solutions.

## Matrix Analogs and Geophysical Inversion

In many geophysical problems, the data is measured at discrete locations along the Earth's surface. In addition, time-variable geophysical data are often digitized to give discrete data in both time and location. The data vector can then be written as  $d_i$ ,  $i = 1, M$ . The medium properties, such as density, electrical conductivity, etc., can often be expanded in terms of a basis function expansion as  $m(\underline{x}) = \sum_{j=1}^{\infty} m_j B_j(\underline{x})$ .

If it can be assumed that the unknown medium parameters are bandlimited, then a finite expansion can be used. For discrete data and a finite basis expansion for the medium, a linearized matrix analog can be written

$$d_i = A_{ij} m_j \quad i = 1, M, \quad j = 1, N \quad (1)$$

where  $A_{ij}$  is the discretized data kernel,  $d_i$  are the data, and  $m_j$  are the coefficients of the basis function expansion for the medium parameters. For  $M < N$  or  $M > N$ , the matrix problem would be formally underdetermined or overdetermined, respectively. However, the solution ultimately depends on the rank, or the number of independent rows or columns, of  $A$ .

Lanczos (1958) solved equation (1) for the general non-Hermitian case by considering the coupled system with

$$S = \begin{bmatrix} 0 & A \\ \bar{A} & 0 \end{bmatrix}, \quad (2)$$

where  $\bar{A}$  is the Hermitian adjoint,  $\bar{A}_{ij} = A_{ji}^*$ , and  $*$  denotes complex conjugate.  $S$  is now a  $(N + M) \times (N + M)$  square Hermitian matrix. For this coupled system, standard eigenvalue/eigenvector analysis can be used to orthogonally decompose  $S$ . For the general case,  $A$  can be represented as

$$A = U\Lambda\bar{V}, \quad (3)$$

where  $U$  is an  $M \times p$  matrix with the  $p$  columns of  $U$  spanning the range space of  $A$ .  $V$  is an  $N \times p$  matrix where the  $p$  columns of  $V$  span the orthogonal complement of the nullspace of  $A$ .  $\Lambda$  is a diagonal  $p \times p$  matrix containing the singular values of  $A$ , which are also the nonzero, positive eigenvalues of  $S$ .

Eckart and Young (1939) provided an early example of the decomposition in equation (3) in terms of  $\bar{A}A$  and  $AA\bar{A}$  and cited earlier, more specialized work by Beltrami and Jordan (see Golub and Van Loan, 1989). Lanczos (1958, 1961, Chap. 3) made use of the coupled system of equation (2) to connect non-Hermitian and defective matrix analysis to Hermitian eigenvector/eigenvalue analysis and also applied it to construct the natural inverse of an arbitrary non-square matrix  $A$ . An algorithm for the singular value decomposition was given by Golub and Reinsch (1970) (see also, Dongarra, et al., 1979).

The natural inverse of Lanczos (1958, 1961, Chap. 3) for an arbitrary matrix satisfies the properties of the generalized inverse of Penrose (1955). In terms of the natural inverse, the general solution of equation (1) can be written

$$\underline{m} = V\Lambda^{-1}\bar{U}\underline{d} + V_0\underline{\eta}, \quad (4)$$

where the first term on the right-hand side is the best approximation solution, which also has minimum norm. The second term on the right-hand side is a solution component from the nullspace of  $A$ , spanned by the columns of  $V_0$  and perpendicular to the columns of  $V$ .  $\underline{\eta}$  is an arbitrary column vector of length  $N - p$ . If nullspace components exist, a nonunique general solution to equation (1) results. However, even with a non-unique general solution, the minimum norm component of the solution is always unique. For purely overdetermined problems, equation (4) reduces to the standard least squares solution. However, for the general case, the standard least squares solution can be singular.

Jackson (1972) and Madden (1972) applied the theory of Lanczos (1958, 1961, Chap. 3) to geophysical inverse problems with inaccurate, insufficient and inconsistent data. Wiggins (1972) gave applications of the natural inverse of Lanczos to the inversion for earth structure using seismic surface waves and free oscillations. Braile et al., (1974) applied the natural inverse to the inversion of gravity data. Wiggins et al., (1976) used generalized inversion to perform residual statics analysis of seismic prospecting data. Aki et al., (1977) used the Lanczos natural inverse, as well as stochastic, damped least squares, to perform one of the early seismic tomography experiments. A selection of papers applying generalized inversion methods to seismic, geopotential and electromagnetic data are included in Lines (ed.) (1988).

In practice, small but nonzero singular values can result in large deviations in the minimum norm solution of equation (1). One approach to moderate the effects of small singular values is to truncate them below a designated level (Wiggins, 1972). Another approach is to taper or filter the effects of the small singular values. This can be done by adding a small positive component to each of the singular values while constructing the natural inverse, or alternatively by using damped least squares (Aki and Richards, 1980, Chap. 13).

More systematic use of a priori data can be incorporated to stabilize geophysical inverse problems. A priori data can be used to reduce the non-uniqueness in the solution of equation (1), allowing the use of either equation (4) or more standard, least squares solutions of the resulting problem. A priori constraints can be in the form of hard or soft inequality constraints or bounds on the smoothness of the solution. Statistical approaches to stabilize ill-posed geophysical inverse problems have included stochastic inversion (Franklin, 1970; Aki and Richards, 1980, Chap. 13) and Bayesian inversion (Jackson,

1979; Jackson and Matsu'ura, 1985; Duijndam, 1988). Matsu'ura and Hirata (1982) incorporated a priori information within the natural inverse of Lanczos. Tarantola and Valette (1982) and Tarantola (1987) gave a general strategy for the incorporation of a priori statistical constraints in the solution of nonlinear inverse problems.

Recent tomographic investigations of the Earth have involved linearized systems which are large but sparse. For example, recent seismic tomography inversions for properties of the Earth's mantle have included up to  $O(10^6)$  travel-times and  $O(10^4 - 10^5)$  medium parameters (Dziewonski, 1984; Clayton and Comer, 1984; Spakman and Nolet, 1988). There are a number of iterative techniques for the approximate solution of large, sparse inverse problems. For example, the algebraic reconstruction technique, ART, and the simultaneous iterative reconstruction technique, SIRT, have been used in medical imaging as well as geophysics (Dines and Lytle, 1979; Herman, 1980).

Another class of solutions for large, sparse systems is based on projection methods such as the conjugate gradient method (Golub and Van Loan, 1989). Claerbout (1991) gives a number of applications of the conjugate gradient method in exploration seismology. As noted in the review by Hestenes (1990), the conjugate gradient method of Hestenes and Stiefel (1952) can be derived from the iteration method of Lanczos (1950), originally devised for finding eigenvalues (see also, Golub and Van Loan, 1989). The algorithm of Paige and Saunders (1982), called LSQR, has recently been applied in geophysics and uses a modified Lanczos method to iteratively solve unsymmetric and least squares problems. Van der Sluis and Van der Vorst (1987) and Spakman and Nolet (1988) have compared the LSQR and SIRT algorithms and found the LSQR algorithm to be computationally superior for large tomographic systems in geophysics. Applications of LSQR to seismic travel-time inversions have included Nolet (1985), Nolet (1987b), and Spakman and Nolet (1988). Nowack and Lutter (1988) applied the LSQR algorithm to the inversion of seismic amplitudes as well as travel-times.

### Continuous Operators and Geophysical Inversion

Many geophysical inverse problems can be more directly analyzed using continuous operators, and the work of Lanczos (1961, Chaps. 4,5) has been influential in this development (see Madden, 1972, 1990). Tarantola (1984, 1987, Chap. 7) derived continuous Hermitian adjoint operators for the seismic inverse problem using the bilinear identity. These adjoint operators can then be used within algorithms for the iterative update of the estimated medium parameters by the steepest descent or conjugate gradient methods. Even for linear differential operators, a nonlinear inverse problem often results for the inversion of model parameters, and a linearized, iterative approach is required. The physical interpretation of seismic imaging criteria and their adjoint implementations are described by Tarantola (1984, 1987). Applications to electromagnetic inverse problems are given by Madden and Mackie (1989) and Madden (1990). Finally, Nolet and Snieder (1990) used a modified Lanczos method (Lanczos, 1950) to solve geophysical inverse problems with continuous model parameterization by projection.

### Conclusion

This paper has provided a brief overview of some of the applications of generalized inversion in geophysics. The non-Hermitian analysis and natural inverse of Lanczos (1958, 1961) have provided a framework for many inverse problems in geophysics. For large scale, geophysical inverse problems, the conjugate gradient method of Hestenes and Stiefel (1952) and the related method of Lanczos (1950) have allowed for efficient iterative solutions.

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#### References

- Aki, K., Christofferson, A., and Husebye, E. S. (1977) "Determination of the three-dimensional seismic structure of the lithosphere," *J. Geophys. Res.*, **82**, pp. 277-296.
- \_\_\_\_\_ and Richards, P. G. (1980) *Quantitative Seismology, Theory and Methods*, W. H. Freeman, San Francisco.
- Braille, L. W., Keller, G. R., and Peeples, W. J. (1974) "Inversion of gravity data for two dimensional density distributions," *J. Geophys. Res.*, **79**, pp. 2017-2021.
- Claerbout, J. F. (1976) *Fundamentals of Geophysical Data Processing*, McGraw Hill, New York.
- \_\_\_\_\_ (1985) *Imaging the Earth's Interior*, Blackwell Scientific, Oxford UK.
- \_\_\_\_\_ (1991) *Earth Soundings Analysis: Processing Versus Inversion*, Blackwell Scientific, Oxford UK.
- Clayton, R. W., and Comer, P. (1984) "A tomographic analysis of mantle heterogeneities," *Terra Cognita*, **4**, pp. 282-283.
- Dines, K. A., and Lytle, R. J. (1979) "Computerized geophysical tomography," *Proc. IEEE*, **67**, pp. 1065-1073.
- Dongarra, J. J., Moler, C. B., Bunch, J. R., and Stewart, G. W. (1979) *LINPACK User's Guide*, Society of Industrial and Applied Mathematics, Philadelphia.
- Duijndam, A. J. W. (1988) "Bayesian estimation in seismic inversion." Part 1: principles, *Geophys. Prospecting*, **36**, pp. 878-898.
- Dziewonski, A. M., (1984) "Mapping the lower mantle: determination of lateral heterogeneity in P velocity up to degree and order 6," *J. Geophys. Res.*, **89**, pp. 5929-5952.
- Eckart, C., and Young, G. (1939) "A principle axis transformation for non-Hermitian matrices," *Bull. Am. Math. Soc.*, **45**, pp. 118-121.
- Franklin, J. N., (1970) "Well-posed stochastic extensions of ill-posed linear problems," *J. Math. Anal. and Appl.*, **31**, pp. 682-716.
- Golub, G. H., and Reinsch, C. (1970) "Singular value decomposition and least squares solutions," *Numer. Math.*, **14**, pp. 403-420.
- \_\_\_\_\_, and Van Loan, C. F. (1989) *Matrix Computations*, Johns Hopkins Press, Baltimore.
- Herman, G. T. (1980) *Image Reconstruction from Projections*, Academic Press, New York.
- Hestenes, M. R. (1990) "Conjugacy and gradients." in *A History of Scientific Computing*, (ed., S. G. Nash), ACM Press/Addison-Wesley, New York, pp. 167-179.
- \_\_\_\_\_, and Stiefel, E. (1952) "Method of conjugate gradients for solving linear systems," *J. Res. Nat. Bur. Stand.*, **49**, pp. 409-438.
- Jackson, D. D. (1972) "Interpretation of inaccurate, insufficient, and inconsistent data," *Geophys. J. R. Astr. Soc.*, **28**, pp. 97-109.

- \_\_\_\_\_ (1979) "The use of a priori data to resolve non-uniqueness in linear inversion," *Geophys. J. R. Astr. Soc.*, 57, pp. 137-157.
- \_\_\_\_\_, and Matsu'ura, M. (1985) "A Bayesian approach to nonlinear inversion," *J. Geophys. Res.*, 90, pp. 581-591.
- Lanczos, C. (1950) "An iteration method for the solution of the eigenvalue problem of linear differential and integral operators," *J. Res. Nat. Bur. Stand.*, 45, pp. 255-282.
- \_\_\_\_\_ (1958) "Linear systems in self-adjoint form," *Am. Math. Mon.*, 65, pp. 665-679.
- \_\_\_\_\_ (1961) *Linear Differential Operators*, Van Nostrand, New York.
- Lines, L. (ed.) (1989) *Inversion of Geophysical Data*, Society of Exploration Geophysicists, Tulsa, OK.
- Madden, T. R. (1972) "Transmission systems and network analogies to geophysical forward and inverse problems," Report No. 72-3, MIT Dept. of Earth and Planetary Sciences, Cambridge MA.
- \_\_\_\_\_, and Mackie, R. L. (1989) "Three-dimensional magnetotelluric modeling and inversion," *Proc. of the IEEE*, 77, pp. 318-333.
- \_\_\_\_\_ (1990) "Inversion of low frequency electromagnetic data, an example of non-linear inversions," in *Oceanic and Geophysical Tomography*, (eds. Y. Desaubies, A. Tarantola and J. Zinn-Justin), North-Holland Press, Amsterdam.
- Matsu'ura, M., and Hirata, N. (1982) "Generalized least-squares solutions to quasi-linear inverse problems with a priori information," *J. Phys. Earth*, 30, pp. 451-468.
- Munk, W., and Wunsch, C. (1979) "Ocean acoustic tomography: a scheme for large scale monitoring," *Deep Sea Res.*, 26A, pp. 439-464.
- Nolet, G. (1985) "Solving or resolving inadequate and noisy tomographic systems," *J. Comp. Phys.*, 61, pp. 463-482.
- \_\_\_\_\_ (ed.) (1987a) *Seismic Tomography*, Reidel Publ., Dordrecht Holland.
- \_\_\_\_\_ (1987b) "Seismic wave propagation and seismic tomography," in *Seismic Tomography*, (ed. G. Nolet), Reidel Publ., Dordrecht Holland.
- \_\_\_\_\_, and Snieder, R. (1990) "Solving large linear inverse problems by projection," *Geophys. J. Int.*, 103, pp. 565-568.
- Nowack, R. L., and Lutter, W. J. (1988) "Linearized rays, amplitude and inversion," *Pure and Applied Geophysics*, 128, pp. 401-421.
- Oldenburg, D. (1990) "Inversion of electromagnetic data: an overview of new techniques," *Surveys in Geophysics*, 11, pp. 231-270.
- Paige, C. C., and Saunders, M. A. (1982) "LSQR: an algorithm for sparse linear equations and sparse least squares," *ACM Trans. Math. Soft.*, 8, pp. 43-71, pp. 195-209.
- Penrose, R. A. (1955) "A generalized inverse for matrices," *Proc. Cambridge Phil. Soc.*, 51, pp. 406-413.
- Spakman, W., and Nolet, G. (1988) "Imaging algorithms, accuracy and resolution in delay time tomography," in *Mathematical Geophysics*, (eds. N. J. Vlaar, G. Nolet, M. J. R. Wortel and A. P. L. Cloetingh), Reidel Publ., Dordrecht Holland, pp. 155-187.
- Tarantola, A., and Valette, B. (1982) "Generalized non-linear inverse problems solved using the least squares criterion," *Rev. Geophys. and Space Phys.*, 20, pp. 219-232.

- \_\_\_\_\_ (1984) "Linearized inversion of seismic reflection data," *Geophys. Prosp.*, 32, pp. 998-1015.
- \_\_\_\_\_ (1987) *Inverse Problem Theory*, Elsevier, Amsterdam.
- Twomey, S. (1977) *Introduction to the Mathematics of Inversion in Remote Sensing and Indirect Measurements*, Elsevier, Amsterdam.
- Van der Sluis, A., and van der Vorst, H. A. (1987) "Numerical solution of large, sparse linear algebraic systems arising from tomographic problems," in *Seismic Tomography*, (ed G. Nolet), Reidel Publ., Dordrecht Holland, pp. 49-83.
- Wiggins, R. A. (1972) "General linear inverse problem—implication of surface waves and free oscillations for earth structure," *Rev. of Geophys. and Space Phys.*, 10, pp. 251-285.
- \_\_\_\_\_, Lerner, K. L., and Wisecup, R. D. (1976) "Residual statics analysis as a general linear inverse problem *Geophysics*," 41, pp. 922-938.