

AN INVERSE PROBLEM APPROACH FOR THE IDENTIFICATION OF THE REFRACTIVE INDEX IN THE HELMHOLTZ EQUATION

Matheus de Lara Todt¹, Hilbeth P. A. de Deus¹,

¹*Dept. of Mechanics, Federal University of Technology - PR
R. Dep. Heitor Alencar Furtado, 5000, CEP 81280-340, Curitiba, Paraná, Brazil
todt@alunos.utfpr.edu.br, azikri@utfpr.edu.br*

Abstract. The Identification of parameters for differential equations is one of the most common types of discrete inverse problems. Formulations like these can be used to calculate the thermal conductivity of a material, the drag coefficient in a body during freefall and the diffusion of matter through a certain media. Following this trend, this paper shows how the refraction index of a pre-established domain can be calculated applying inverse problem techniques to the Helmholtz equation. As the main endeavor in inverse problems arise from the necessity of solving matrices with large condition number, this work contains an overall review and a numerical comparison between classical and more recent regularization schemes to solve these ill-posed matrices. In order to validate the results, the problem was also solved in a direct manner using the Finite Elements Method. Results include numerical examples for uniform and non-uniform mesh grids.

Keywords: Discrete Inverse Problems, Helmholtz Equation, Finite Elements Method, Regularization Schemes.

1 Introduction

The Helmholtz Equation is a partial differential equation that is associated with a large variety of physical phenomena such as: vibrations, electromagnetism and other oscillatory disciplines. In the study of acoustic systems, the equation models the sound pressure field in the frequency domain. As the Helmholtz Equation is a time independent PDE, its use reduces a problem exclusively to spatial dependency. The drawback of this modelling approach is that it can only be used if the signal of the system is harmonic [1, 2].

The Helmholtz equation can also be used in inverse problems of parameter identification. In these types of applications, partial differential equations coefficients (e.g. thermal conductivity in the heat equation and diffusion of matter in Fick's Law) can be estimated given that there is experimental data about the solution of the PDE [3-5]. In this paper, it's shown that the Helmholtz can be used to retrieve information about the refractive index in a media given that there is data on the pressure field and the source terms acting in this media.

In Hansen [6] it's mentioned that the main issue that arises from these inverse problem formulations is the ill-posedness of the numerical formulation. According to Hadamard [7], this means that: there may not exist a solution for the problem; there is not a unique solution; or the solution of the problem is not stable. For the inverse problem analyzed in this work, the main concern is the stability: small perturbations of the input data (the pressure field and the source terms) can result in big fluctuations in the results (refractive index).

In this context, this paper also covers a brief overview of a few regularization techniques that can be used to suppress the effects of these perturbations in order to achieve more consistent results.

2 Problem formulation and procedures

The problem formulation consists in a boundary value problem (BVP) for the Helmholtz equation. From the BVP, the problem is then discretized in two different ways, one for the forward problem and another one for the inverse problem.

In this paper, we approach the discretization of the forward and the inverse problems through the finite element method (FEM), as it is done in many papers presented in the literature. But there are other numerical methods being used in other works, such as the finite difference method and boundary methods [8, 9].

Following the FEM implementation, the forward problem is well-posed and does not need any type of regularization before it can be solved. So, a few discrete points from its solution can be used as the pressure field input for the inverse problem.

On the other hand, the inverse problem linear system cannot be immediately solved, as its stiffness matrix is ill-conditioned. Therefore, a regularization must be done. This is done by the means of the Tikhonov regularization [6, 10, 11]. To calculate the optimal Tikhonov regularization parameter two different methods were used: the L-curve criterion [6, 12-15] and a fixed-point approach proposed by Bazan [16], based on the discrepancy principle.

Ultimately, with the inverse problem solved, a comparison can be done between the refractive index used as input in the forward problem and the refractive index obtained as the solution of the inverse problem.

This whole process is done for uniform and non-uniform mesh grids.

2.1 Forward problem

The general idea of the proposed forward problem is to solve the Helmholtz equation given a certain input data (the wave number, the refractive index and the source terms).

Considering the unidimensional case, with $x \in \Omega = (0, L)$, where $\Omega \subset \mathbb{R}^1$ is the domain with boundary $\partial\Omega$, the boundary value problem for the Helmholtz equation can be formally written as

$$\begin{aligned} \nabla^2 u(x) + \kappa^2 n u(x) &= p(x) \quad \text{in } \Omega \\ u(0) &= u_0 \quad \text{in } \partial\Omega \\ u(L) &= u_L \quad \text{in } \partial\Omega \end{aligned} \quad (1)$$

where $u \in H^1(\Omega)$ is the sound pressure, $n \in L^\infty(\Omega)$ is the refractive index, $p \in L^\infty(\Omega)$ is the source term and κ is the wave number.

The forward problem can then be defined as: find the $u \in H^1(\Omega) \forall \phi \in H^1(\Omega)$ that satisfies the weak formulation of eq. (1):

$$-\int_{\Omega} \nabla u(x) \nabla \phi(x) dx + \kappa^2 \int_{\Omega} n u(x) \phi(x) dx = \int_{\Omega} p(x) \phi(x) dx \quad (2)$$

Using the finite elements method, u can be approximated to a finite dimensional space, V^h , using basis functions. Thus, $u(x) \approx u^h = u_i \phi_i(x)$. The problem can then be fully rewritten in its discrete weak formulation, for each element $\Omega_e \subset \Omega$, as:

Find $u^h \in V^h \subset H^1$ such that

$$\left(\kappa^2 \int_{\Omega_e} n(x) \phi_i(x) \phi_j(x) dx - \int_{\Omega_e} \nabla \phi_i(x) \nabla \phi_j(x) dx \right) u_i = \int_{\Omega_e} p(x) \phi_k(x) dx \quad (3)$$

hence, the forward problem narrows down to solving the linear equation

$$\mathbb{K}u = f \quad (4)$$

2.2 Inverse problem

In the formulation of the inverse problem, we aim the calculation of the refractive index. So, in this case, discrete points of the pressure field are used as input and the refractive index is the output. The finite element approximation is also used to interpolate the refractive index. Therefore $n(x) \approx n^h = n_j \phi_j(x)$.

Applying these changes, the discrete weak form yields

$$\left(\kappa^2 \int_{\Omega_e} u^h(x) \phi_j(x) \phi_k(x) dx \right) n_j = \int_{\Omega_e} p(x) \phi_k(x) dx + \int_{\Omega_e} u^h(x) \nabla \phi_k(x) dx \quad (5)$$

And the linear equation takes the form of

$$\mathbb{K}^* \mathbf{n} = \mathbf{f}^* \quad (6)$$

2.3 Regularization schemes

In inverse problems the input data, being it experimental or numerical, usually contains a considerably amount of noise. This is expected because experimental setups are not perfect, there may be noise generated in measurements due to human error, imprecision of equipment or even randomness. When the input data comes from another numerical simulation, like this present paper, there can also be noise related to rounding and truncation.

Considering a linear system of the form $\mathbf{Ax} = \mathbf{b}$, the upper bound of the solution error can be, according to Allaire and Kaber [16], written as

$$\frac{\|\tilde{x} - x\|_2}{\|x\|_2} \leq \text{cond}(\mathbf{A}) \left\{ \frac{\|\tilde{\mathbf{A}} - \mathbf{A}\|_2}{\|\mathbf{A}\|_2} + \frac{\|\tilde{\mathbf{b}} - \mathbf{b}\|_2}{\|\mathbf{b}\|_2} \right\} + \mathcal{O}(\epsilon^2) \quad (7)$$

where $\text{cond}(\mathbf{A}) = \|\mathbf{A}\|_2 \|\mathbf{A}^{-1}\|_2$ is the condition number of matrix \mathbf{A} and $(\tilde{\cdot})$ refers to a noisy term.

Matrices with $\text{cond}(\mathbf{A}) \gg 1$, are called ill-conditioned and linear systems involving them lack stability [6]. In this context, it's needed a method that can suppress the noise effects without prejudice to the overall physics of the problem. One such method is the Tikhonov regularization.

According to Hansen and O'Leary [13], the generalized Tikhonov regularization consists in

$$\min\{\|\mathbf{Ax} - \mathbf{b}\|_2^2 + \lambda^2 \|\mathbf{x}\|_2^2\} \quad (8)$$

where λ is the parameter responsible for controlling the weight in the minimization of $\|\mathbf{x}\|_2$ relative to the minimization of $\|\mathbf{Ax} - \mathbf{b}\|_2$. In some cases, the seminorm $\|\mathbf{Lx}\|_2$ is used instead of the L^2 norm of the solution [11, 13, 16]. But if \mathbf{L} is chosen to be the identity matrix, the formulation is reduced to the one shown in eq. (8).

A wide range of different methods are proposed in the literature for the identification of the optimal value for the λ parameter, such as in the works of Wu [18], Bazán [16], Reginska [14], and many others.

In this present paper, only the L-curve criterion [6, 12-15] and the fixed-point approach proposed by Bazán [16] are going to be used.

2.4 The L-Curve Criterion

The L-curve is graphic device, very commonly used to identify the optimal λ parameter. According to Hansen [12], the method consists in a log-log plot between the regularized solution norm ($\|x_\lambda\|_2^2$) and the regularized residual norm ($\|\mathbf{Ax}_\lambda - \mathbf{b}\|_2^2$), which means that the curve represents a trade-off between two quantities that should be controlled. The name of the curve comes from it's very characteristic L-shape.

In Hansen and O'Leary [13], it's suggested that the optimal trade-off point is the in the "corner", i.e., the region of maximum curvature, of the L-shaped curve. The reason behind this choice lies in the fact that the corner of the curve separates two regions: one dominated by perturbation errors and another by regularization errors. Therefore, choosing the corner means that the regularization will be effective enough to suppress the noise but will not lead to large regularization errors. There are a few other methods to estimate λ from the L-curve but the maximum curvature methodology seems to be the best choice in most cases, as shown in Johnston and Gulrajani [15].

In order to find the corner, Hansen and O’Leary [13] proposes the use of the expression

$$K = 2 \frac{\eta \rho \lambda^2 \eta' \rho + 2 \lambda \eta \rho + \lambda^4 \eta \eta'}{\eta' (\lambda^2 \eta^2 + \rho^2)^{3/2}} \quad (9)$$

where K is the curvature of the plot, $\eta = \|x_\lambda\|_2^2$ and $\rho = \|Ax_\lambda - b\|_2^2$. The corner of the curve can then be computed by taking the maximum of K .

The advantages of the L-curve criterion are in its robustness and efficiency in the treatment of noise. However, the method also has some disadvantages. According to Hanke [19] the L-Curve criterion fails when the analyzed problems have very smooth solutions and in Vogel [13], it’s mentioned that the λ_t parameter, calculated by the L-Curve criterion, deviates from the optimal parameter λ_{opt} as n , the rank of A , increases.

2.5 GDP-FP

According to Bazán [16] the Generalized Discrepancy Principle (GDP) equation can be written as

$$G(\lambda) = \|\tilde{A}x_\lambda - \tilde{b}\|_2^2 - (\delta_x + \delta_A \|Lx_\lambda\|_2)^2 = 0 \quad (10)$$

where δ_x and δ_A are the explicit values of noise for x and A , respectively.

From eq. (10), Bazán [16] shows that taking

$$\vartheta(\lambda) = \frac{\|\tilde{A}x_\lambda - \tilde{b}\|_2}{\delta_x + \delta_A \|Lx_\lambda\|_2}, \xi(\lambda) = \frac{\lambda^2}{\vartheta(\lambda)} \text{ and } \zeta(\lambda) = \sqrt{\xi(\lambda)} \quad (11)$$

a stable fixed-point expression can be derived, and it reads as

$$\zeta(\lambda) = \frac{\lambda}{\sqrt{\vartheta(\lambda)}} = \lambda \quad (12)$$

The GDP-FP algorithm consists in iterating eq. (12) from an initial guess, λ_0 , until convergence, i.e., $|\lambda_{j+1} - \lambda_j| \leq \epsilon |\lambda_j|$, where ϵ is a user defined threshold.

The method is very advantageous, if compared to Newton-like methods, because it doesn’t require the calculation of derivatives. However, one evident downside, is that differently from the L-Curve, it requires knowledge about the explicit noise values δ_x and δ_A .

3 Results

The forward problem was solved, for different mesh grids, by taking $\kappa = 0$, $p(x) = 0$, $u(0) = u(L) = 0$, $n(x) = 1$ and by approximating u^h by linear basis functions. The pressure field solution of the forward problem was used as input to the inverse problem. In order to have a square stiffness matrix, n^h was also approximated by linear basis functions.

The whole FEM script was written in MATLAB. The L-Curve method was used, also in MATLAB, by the means of the REGULARIZATION TOOLS package [21].

Figure (1) shows a comparison between the refractive index achieved by the GDP-FP and the L-Curve methods for mesh grids with 25, 50, 75 and 100 elements.

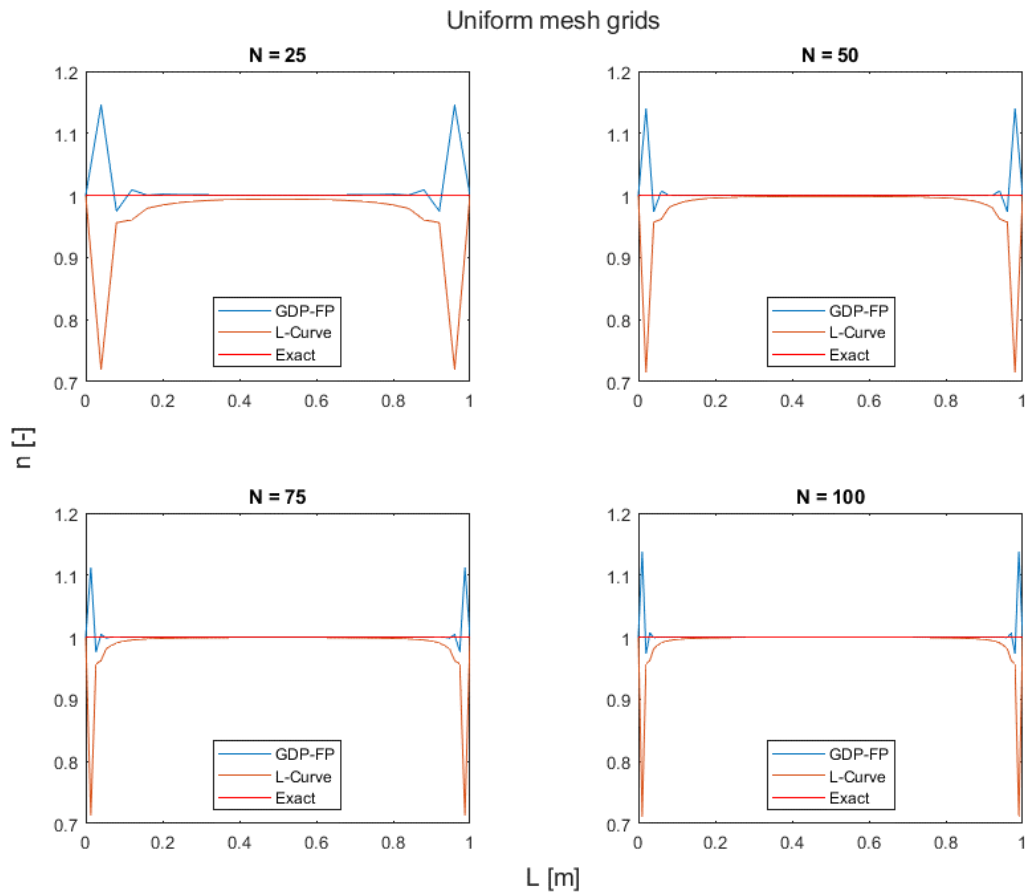


Figure 1. Inverse problem results for uniform mesh grids of different sizes.

For the uniform mesh grids, the results show that both regularization methods were able to approximate the exact value of n very well in the centermost region of the domain. The main deviation from the exact solution was near the boundaries but increasing the number of elements is shown to be effective in reducing the area of effect of these instabilities.

The maximum amplitude of the peaks, i.e. errors, was shown to be lower for the GDP-FP than the L-curve method, 13.7% to 28.8%, respectively, for the mesh grid with 100 elements. But the transition from the boundary instabilities to the well approximated region was smoother for the L-curve method.

In the comparison with non-uniform grid, fig. (2), the size of each element was randomized, in order to amplify the perturbations in the solution. As expected, even for a large number of elements ($N = 200$), numerical instabilities were introduced to the solution. Even then, both regularization methods presented a similar behavior, as the position of their peaks is matching, with the only difference being their amplitude. The largest deviations from the exact solution were, similarly to the uniform-mesh, near the boundaries.

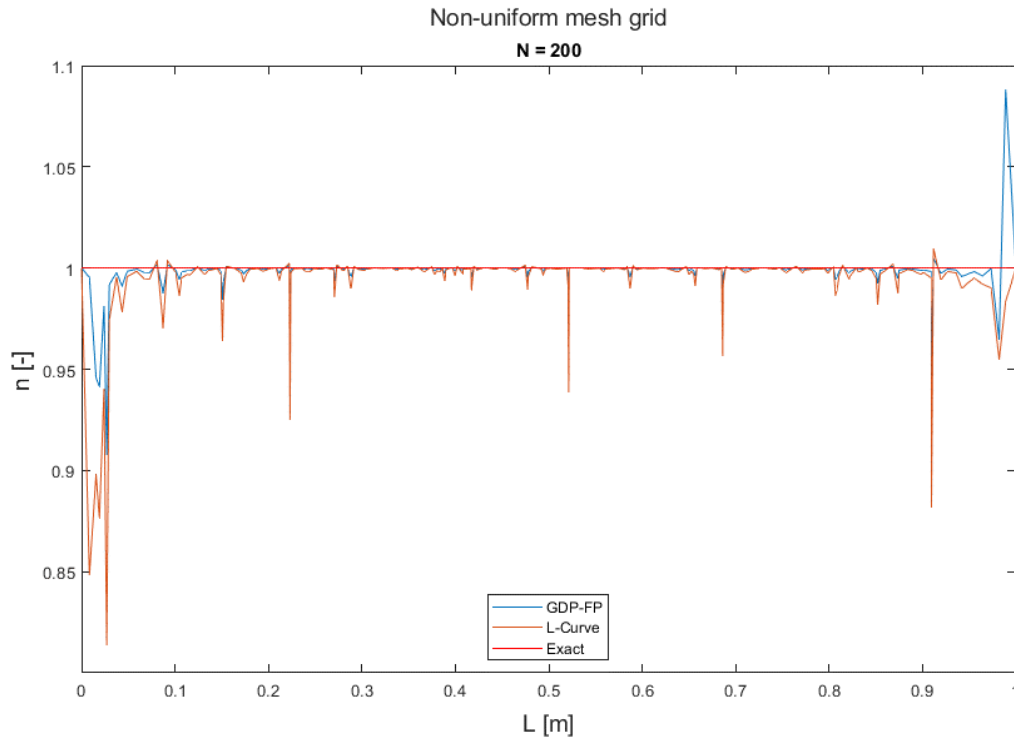


Figure 2. Inverse problem results for a non-uniform mesh $N=200$.

4 Conclusions

In this paper an inverse problem of parameter identification was analyzed by the means of the Helmholtz equation. Given that problems of this sort are instable and require regularization, a brief review was done about the Tikhonov regularization and two different methods of inferring the Tikhonov parameter.

Following the use of the regularization schemes, the parameter identification technique was successful in retrieving information about a physical parameter with only a few discrete data points as input.

Suggestions to future works include: approximation of the refractive index by higher order basis functions, which will result in rectangular stiffness matrices; the input data on the refractive index can be a function, instead of a constant; error estimates may be used to infer levels of numerical noise acting on the system, this can supplement the evaluation of the GDP-FP algorithm; other regularization methods other than the L-Curve and the GDP-FP can also be evaluated.

Acknowledgements. The authors would like to thank the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - Brasil (CAPES) for the partial financial support, under grant number 695237/2022-00, to this research paper.

Authorship statement. The authors hereby confirm that they are the sole liable persons responsible for the authorship of this work, and that all material that has been herein included as part of the present paper is either the property (and authorship) of the authors, or has the permission of the owners to be included here.

References

- [1] N. A. Gumerov and R. Duraiswami. *Fast Multipole Methods for the Helmholtz Equation in Three Dimensions*. Elsevier, 2004.
- [2] A. Figueroa, M. Telenko Jr., L. Chen and S. F. Wu. "Determining structural damping and vibroacoustic characteristics of a non-symmetrical vibrating plate in free boundary conditions using the modified Helmholtz equation least squares method", *Journal of Sound and Vibration*, vol 495, 2021.
- [3] Chleboun, J., P. Příkryl, K. Segeth, J. Šístek and T. Vejchodský. "Computational approaches to some inverse problems from engineering practice". *Programs and Algorithms of Numerical Mathematics*. vol. 17, pp. 215-230. 2015.

- [4] F. D. M. Neto and A. J. S. Neto, *An introduction to Inverse problems with applications*. Springer, 2013.
- [5] V. Isakov. *Inverse problems for Partial Differential Equations*. Springer, 1998.
- [6] P. C. Hansen. *Discrete Inverse Problems: Insight and Algorithms*. SIAM, 2010.
- [7] J. Hadamard. “Sur les problèmes aux dérivées partielles et leur signification physique”. *Princeton University Bulletin*, vol. XIII, n. 4, pp. 49-52, 1902.
- [8] M. Bonnet and A. Constantinescu. “Inverse problems in elasticity”. *Inverse Problems*, vol. 21, n. 2, 2005.
- [9] G. D. Egbert, A. Kelbert. “Computational recipes for electromagnetic inverse problems”. *Geophysical Journal International*, vol 189, n. 1, pp. 251-267, 2012.
- [10] A. Kirsch. *An Introduction to the Mathematical Theory of Inverse Problems*. Springer, 2010.
- [11] G. H. Golub, P. C. Hansen, D. P. O’Leary, “Tikhonov Regularization and Total Least Squares”. *SIAM J. Matrix Anal. Appl.*, vol. 21, n. 1, pp. 185-194, 1999.
- [12] P.C. Hansen. “The L-curve and its use in the numerical treatment of inverse problems”. In: *Computational Inverse Problems in Electrocardiology*. pp. 119-142, 2001.
- [13] P. C. Hansen and D. P. O’Leary. “The Use of the L-Curve in the Regularization of Discrete Ill-Posed Problems”. *SIAM Journal on Scientific Computing*, vol. 14, n. 6, pp. 1487–1503, 1993.
- [14] T. Reginska. “A regularization parameter in discrete ill-posed problems”. *SIAM J. Sci. Comput.* vol. 17, n. 3, 740-749, 1996.
- [15] P. R. Johnston and R. M. Gulrajani, "Selecting the Corner in the -Curve Approach to Tikhonov Regularization". *IEEE Transactions on Biomedical Engineering*, vol. 47, n. 9, 2000.
- [16] F. S. V. Bazán. “Simple and Efficient Determination of the Tikhonov Regularization Parameter Chosen by the Generalized Discrepancy Principle for Discrete Ill-Posed Problems”. *J. Sci. Comput.* 2013.
- [17] G. Allaire and S. M. Kaber, *Numerical Linear Algebra*. Springer, 2008.
- [18] L. Wu. “A parameter choice method for Tikhonov regularization”. *Electronic Transactions on Numerical Analysis*, vol. 16, pp. 107-128, 2003.
- [19] M. Hanke. “Limitations of the L-Curve Method in Ill-posed Problems”. *BIT Numerical Mathematics*, vol. 36, 287-301, 1996.
- [20] C. R. Vogel. “Non-convergence of the L-curve regularization parameter selection method”. *Inverse Problems*, vol. 12, 535-547. 1996.
- [21] P. C. Hansen, *Regularization Tools Version 4.0 for Matlab 7.3*, Numerical Algorithms, 46 (2007), pp. 189-194.