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Multipenalty and composed merit functions in Tikhonov-type regularization applied to atmospheric source identification problems

Multi-penalização e funções de mérito compostas em regularização do tipo Tikhonov aplicadas a problemas identificação de fontes atmosféricas

Roseane Alves de Souza Albani[I], Vinícius Viana Luiz Albani[II], Antônio José da Silva Neto[I]

[I] Universidade do Estado do Rio de Janeiro, Instituto Politécnico, Nova Friburgo, RJ, Brazil
[II] Universidade Federal de Santa Catarina, Departamento de Matemática, Florianóplis, SC, Brazil

ABSTRACT

We propose a technique to simplify the minimization of the objective function arising in Tikhonov-type regularization when there are multiple observations, like multiphysics identification problems, and multiple penalty terms. It breaks the original problem into two or more minimizations that are performed sequentially and recursively. In this preliminary work, we consider the case of two minimization steps. We apply the estimation technique to the identification of pollutant emission sources in the atmosphere, considering the data from the Copenhagen experiment.

Keywords: Inverse problems; Tikhonov-type regularization; Multipenalty; Composed merit functions

RESUMO

Propomos uma técnica para simplificar a minimização da função objetivo que surge na regularização do tipo Tikhonov quando há múltiplas observações, como problemas de identificação multi-física, e múltiplos termos de penalidade. A técnica divide o problema original em duas ou mais minimizações que são executadas sequencialmente e recursivamente. Neste trabalho preliminar consideramos o caso de duas etapas de minimização. Aplicamos a técnica de estimativa na identificação de fontes de emissão de poluentes na atmosfera considerando os dados do experimento de Copenhague.

Palavras-chave: Problemas inversos; Regularização do tipo Tikhonov; Multipenalização; Funções de mérito compostas

1 INTRODUCTION

In many applications, we have access to different observations of the same object by using a combination of measurement techniques. For example, in medical imaging, we can combine the information obtained by computer tomography and magnetic resonance imaging to obtain more accurate diagnosis. Finding ways of combining different measurement techniques to better estimate a given object or quantity is the subject of intense research in many fields, such as Geophysics, Medical Imaging, etc.

Moreover, the observations can be corrupted by noise sources with different distributions, such as impulsive noise and Gaussian noise. In these cases, the way the noise is accounted for in merit functions is different. In all these cases, each set of observations can be represented by a corresponding parameter-to-solution operator or data misfit functional, which leads us to composed merit functions.

Depending on the nature of the unknown quantity, it is possible to include *a priori* data in the penalty term of Tikhonov-type regularization. This leads us to the multipenalty regularization, where different prior characteristics of the unknown are included in the search for a solution by different penalty terms.

In this work, we consider the problem of multipenalty regularization combined with composed merit functions in Tikhonov-type regularization. This is in general a hard-to-solve optimization problem. Since this is a preliminary work, we will focus on the case when the merit function has two terms, and the penalty term also has two terms. To address this task, we will consider an algorithm that breaks the minimization into two steps that are implemented recursively until reaching an equilibrium. As we shall see, the algorithm will converge, under appropriate conditions. See, for example, Albani and Zubelli (2020). The proposed technique is tested with an atmospheric source identification problem, where different noise sources are considered.

2 THE PROPOSED ESTIMATION MODEL

Let us consider the operators $F_j : A \subset X \to Y_j$, $(j = 1,\cdots, m)$, representing different phenomena that associate the unknonw parameter $x \in A$ to the data y_j $(j = 1,\cdots, m)$ The set A must be such that $A \subset D(F_j)$ for each $j = 1,\cdots, m$. The sets X and $Y_j(j = 1,\cdots, m)$ are normed vector spaces.

We want to solve the problem of finding $x^\dagger$ in A, such that:

$$F_j(x^\dagger) = y_j, \tag{1}$$

for all $j = 1,\cdots, m$. In general, for each $j = 1, \cdots, m$, we have access only to noisy observations $y_j^{\delta j}$ of the y_j's satisfying:

$$||y_j^{\delta_j} - y_j||_{Y_j} \leq \delta_j, \tag{2}$$

with $\delta_j > 0$ the jth noise level. As this problem may not be well-posed, we apply Tikhonov regularization. Notice that, we also assume that a series of different characteristics must be accounted for in the search for a solution. This information is incorporated as the convex and differentiable penalty terms of the Tikhonov-type regularization functional denoted as $f_j : A \subset X \to \mathbb{R}_+ \,(j = 1,\cdots, m)$. We assume, by simplicity that the number of penalty terms is the same number of functionals F_j.

Therefore, the approximate solutions obtained by Tikhonov-type regularization are obtained by finding the solution of the minimization problem below:

$$\text{Min}\left\{\sum_{j=1}^{m}\left[\beta_j||F_j(\mathbf{x}) - y_j^{\delta_j}||_{Y_j}^{p_j} + \alpha_j f_j(\mathbf{x})\right] \;:\; \mathbf{x} \in A\right\}, \tag{3}$$

where $\beta_j > 0$ defines a weight for each merit function and $\alpha_j > 0$ represents the regularization parameter corresponding to the functional $f_j(j = 1,\cdots, m)$.

There are many tasks arising in this approach. The first and more basic one is to unify the representation of the unknown involving different physical phenomena. Another one is to choose appropriately the parameters α_j and β_j $(j = 1,\cdots, m)$.

Since minimizing the Tikhonov-type functional in Eq. (3) can be computationally intensive we focus on this task. For the choice of the parameters α_j $(j = 1,\cdots, m)$, we can use discrepancy principles. For example, for each $j = 1$, minimize: $||F_j(\mathbf{x}) - y_j^{\delta_j}||_{Y_j}^{p_j} + \alpha_j f_j(\mathbf{x})$, δ_j and denote the minimizer by $x_{\alpha j}$. We want to find positive values for α_j and β_j $(j = 1,\cdots, m)$, such that, for $\tau > 1$ the following inequalities hold,

$$||F_j(x_\alpha^\delta) - y_j^{\delta_j}||_{Y_j} \le \tau\delta_j, \qquad j = 1,\cdots, m. \tag{4}$$

Appropriate treatment of this problem is beyond the scope of this work, but we can refer to Albani et al. (2016, 2017); Anzengruber & Ramlau (2010); Morozov (1966) as theoretical texts that consider discrepancy-based choices of regularization parameters.

As mentioned above, we focus on the problem with $m = 2$. Thus, we break the minimization problem in Eq. (3) into two steps by defining two artificial variables, namely, ${x_1}^k$ and ${x_2}^k$, where k denotes the kth iterate. Thus, for each $k = 1,2,\cdots$, perform the iterations:

$$x_1^k \in \operatorname{argmin}\left\{\beta_1||F_1(x) - y_1^{\delta_1}||_{Y_1}^2 + \alpha_1 f_1(x) + \frac{\varepsilon}{2}||x - x_2^{k-1}||_X^2\right\}$$

$$x_2^k \in \operatorname{argmin}\left\{\beta_2||F_2(x) - y_2^{\delta_2}||_{Y_2}^2 + \alpha_2 f_2(x) + \frac{\varepsilon}{2}||x - x_1^k||_X^2\right\}$$

Under appropriate hypotheses (Albani and Zubelli (2020); Scherzer et al., (2008)), we expect that $\lim_{k\to\infty} x_1^k = \lim_{k\to\infty} x_2^k = \tilde{x}$. Notice that, if $\tilde{x}$ exists, it can be an approximation of the solution to the minimization in Eq. (3), as it minimizes:

$$\beta_1\left|\left|F_1(x) - y_1^{\delta_1}||_{Y_1}^2 + \beta_2\right|\right| F_2(x) - y_2^{\delta_2}||_{Y_2}^2 + \alpha_1 f_1(x) + \alpha_2 f_2(x) + \varepsilon||x - \tilde{x}||_X^2.$$

3 THE SOURCE IDENTIFICATION PROBLEM

3.1 The dispersion problem

The estimation technique is applied to the source identification problem, considering atmospheric releases. The direct problem is given by the dispersion of a pollutant from a point source during a certain period over a flat terrain. This process is mathematically described by an advection-diffusion partial differential equation (PDE) solution that accounts for parametric models of the wind field and turbulent diffusion profiles. The scalar-valued concentration is denoted by $C(x, y, z)$ and solves the following PDE:

$$\mathbf{u} \cdot \nabla C - \nabla \cdot (\mathbf{K}\nabla C) = \sum_{j=1}^{n} \mathbb{S}_j, \tag{5}$$

with $(x, y, z) \in \Omega$, where $\Omega = [x_{\min}, x_{\max}] \times [y_{\min}, y_{\max}] \times [z_0, h]$ is the computational domain that accounts for a portion of the Atmospheric Boundary Layer (ABL). The boundary conditions are:

$$\mathbf{n} \cdot \nabla C = 0, \tag{6}$$

at $z = z_0$ and $z = h$ with $\mathbf{n}$ representing the outward normal, and

$$C = 0 \text{ elsewhere.} \tag{7}$$

In the left-hand side of the PDE, the first term represents the pollutant transport driven by the wind field u, and the second represents the turbulent diffusion. We assume that the wind field is given by $u = (u, v, w)$ with its components given by $u = |u|\cos(\theta)$, $v = |u|\sin(\theta)$, and $w = 0$, θ is the angle of the wind direction. The diffusion tensor $\mathbf{K}$ is defined by a 3D-diagonal matrix, with the diagonal components given by K_x, K_y, and K_z accounting for turbulent diffusion with respect to the x-, y-, and z-directions, respectively. In the PDE right-hand side, there are the n point sources $\mathbb{S}\_j$ $(j = 1, \ldots, n)$: $\mathbb{S}j(x, y, z) = Q_j\, \delta(x - x_j^S)\delta(y - y_j^s)\delta(z - z_j^s)$, δ is the Dirac delta distribution, (x_j^s, y_j^s, z_j^s) are the sources' locations coordinates, and Q_j is the emission rate.

Notice that denotes the surface roughness length and is the ABL height. The boundary conditions in Eqs. (6)–(7) assume, respectively, no gradient, or flux, at the bottom and top of the ABL, and the concentration goes to zero when we are sufficiently far from the source.

To save computational time, we take advantage of the linear structure of the emission source problem and solve an adjoint-state PDE for each concentration observation. See, Albani et al. (2020). The PDE problem is solved by the Galerkin Least-square (GLS) finite element method (FEM) (Hughes et al., (1989)), such as in Albani & Albani (2020). For more details on the setup of the dispersion problem including the PDE parameters, we refer to Albani et al. (2020).

3.2 Source identification

Denote by the vector C^{obs} that contains the measured concentrations of some pollutant emitted from a set of unknown sources. We want to find the parameters, namely, the sources' locations and strengths, that generated these observations, assuming that the dispersion is determined by the PDE problem in Eqs. (5)–(7). In what follows, the number of sources is set as $n = 1$. The set of unknown parameters is denoted by $\Theta^s = (x^s, y^s, z^s, Q^s)$ and the set of numerical concentrations evaluated at the measurement locations is $C(\Theta^s)$.

We assume that the measurements are corrupted by two noise sources: Gaussian and impulsive noise. This is addressed by accounting for two data misfit functions, for the Gaussian noise we use the ℓ_2-norm: $||x||_{\ell_2}^2 = \sum_{j=1}^{N} x_j^2$, and for the impulsive noise, the ℓ_2-norm is approximated by the $\ell_{1.01}$-norm $||x||_{\ell_{1.01}}^2 = \sum_{j=1}^{N} |x_j|^{1.01}$.

We also use the negative form of the Boltzmann-Shannon entropy, from Information Theory and Thermodynamics, as the penalty term (Vogel, 2002):

$$S(x) = \sum_{j=1}^{N} x_j \log(x_j),$$

if $x_j > 0$. Thus, the source estimation solution is given by the minimizer of the Tikhonov functional

$$\mathcal{F}(\Theta) = \beta_1 \frac{||C(\Theta) - C^{obs}||_{\ell_2}^2}{||C^{obs}||_{\ell_2}^2} + \beta_2 \frac{||C(\Theta) - C^{obs}||_{\ell_{1.01}}^{1.01}}{||C^{obs}||_{\ell_{1.01}}^{1.01}} + \alpha S(\Theta + \Theta_0) \quad (8)$$

For the minimization, repeat the iterations below until convergence:

$$\Theta_1^k \in \operatorname{argmin}\left\{\frac{1}{2}\frac{||C(\Theta) - C^{obs}||_{\ell_2}^2}{||C^{obs}||_{\ell_2}^2} + \alpha S(\Theta + \Theta_0) + \frac{\alpha}{20}||\Theta - \Theta_2^{k-1}||_{\ell_2}^2\right\}$$

$$\Theta_2^k \in \operatorname{argmin}\left\{\frac{1}{2}\frac{||C(\Theta) - C^{obs}||_{\ell_{1.01}}^{1.01}}{||C^{obs}||_{\ell_{1.01}}^{1.01}} + \alpha S(\Theta + \Theta_0) + \frac{\alpha}{20}||\Theta - \Theta_1^{k}||_{\ell_2}^2\right\}$$

Notice that we set $\mathcal{E}$ as 10% of α, for simplicity.

4 NUMERICAL RESULTS

4.1 The experimental dataset and PDE parameters

To test the proposed estimation technique, we use the Copenhagen experiment dataset. The experiment was carried out in the Copenhagen area during 1978/79 accounting for unstable and neutral atmospheric conditions. At 115 *m* of height, SF_6 was released from a tower without buoyancy and its concentration was measured by an array of sensors located at 2-3 *m* above the surface level, distributed over concentric arcs with radii of 2, 4, and 6 *Km*, with the source located at the center. The concentration was averaged for 20 minutes and measured three consecutive times, leading to a sampling time of 1 hour. The sampling site had a roughness length (z_0) of 0.6 [*m*]. The wind speed and direction, and temperature were measured at several heights at the emission site. For more details, we refer to Gryning (1981); Gryning & Lyck (1984, 2002).

In the numerical solution of the dispersion problem, we used the wind intensity |u| and the vertical eddy diffusion coefficient K_z proposed in Ulke (2000), considering unstable conditions ($h/L > 0$). They are given, respectively, as follows,

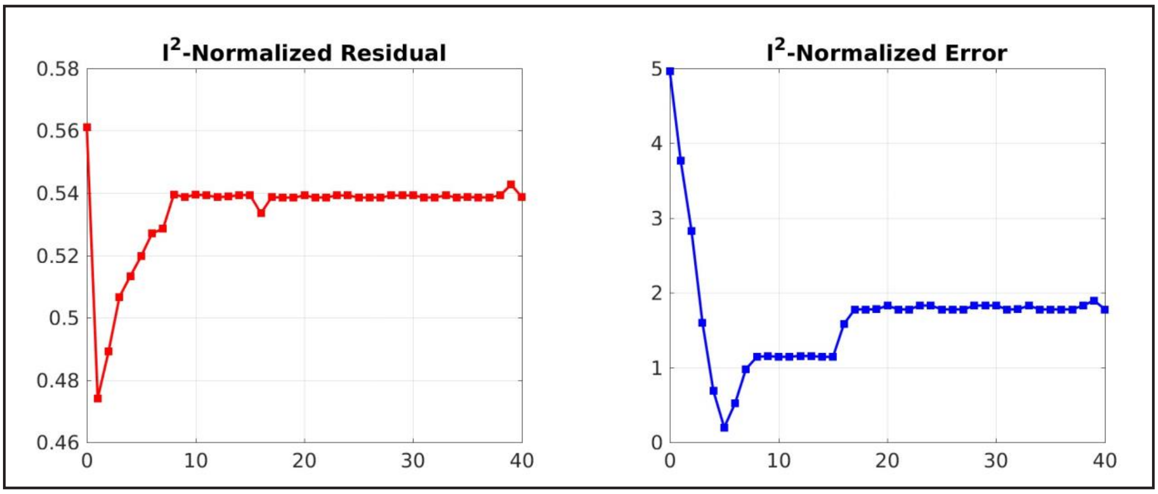
$$|\mathbf{u}(z)| = \frac{u_{*0}}{\kappa}\left\{\ln\left(\frac{z}{z_0}\right) + \ln\left(\frac{1+\mu_0^2}{1+\mu^2}\right) + 2\ln\left(\frac{1+\mu_0}{1+\mu}\right) + 2[\arctan(\mu) - \arctan(\mu_0)] + \frac{2L}{33h}(\mu^3 - \mu_0^3)\right\} \quad (9)$$

With $\mu(z) = \left(1 - 22\frac{h}{L}\frac{z}{h}\right)^{\frac{1}{4}}$ and $\mu_0 = \mu(z_0)$, and

$$K_z(z) = \kappa u_* h\mu\frac{z}{h}\left(1 - \frac{z}{h}\right) \quad (10)$$

Considering the meteorological information from 19-Oct-1978, we set $h = 1120\ m$, $u_* = 0.39\ m/s$, $L = -108$ and the average of the wind direction angle $\theta = 290°$. Moreover, the other diffusion coefficients were set as $K_x = K_y = 50\ m^2/s$, accordingly to (Arya, 2001, p. 272) (unstable conditions).

Figure 1 – Evolution of the normalized residual (left) and error (right) with respect to the number of iterations. The evaluation was made after performing the two minimization steps and 40 iterations

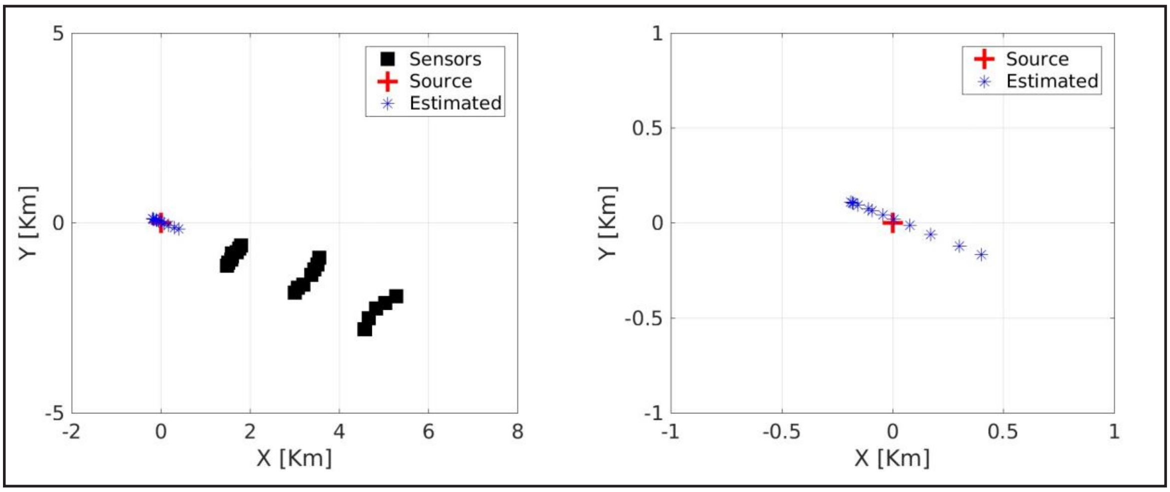


Source: the authors (2023)

The optimization steps were performed by the particle swarm optimization algorithm from the global optimization toolbox of MATLAB. The following settings were used, *Swarm size population* was 100, the *Self Adjustment Weight* was one, the *Social Adjustment Weight* was 0.5, the *Inertial range* was of $[0.1,1.2]$, and the *Function Tolerance* was of 10^{-30}. The computational domain was $\Omega = [-2.0,0.0] \times [-5.0,5.0] \times [0.0006,1.120]Km$. The regularization parameter was set as $\alpha = 10^{-4}$.

The estimated source parameter values can be found in Table 1. Figure 1 presents the evolution of the ℓ^2-normalized error and residual with respect to the iterations. We performed 40 iterations comprising the two minimization steps. Figure 2 presents the evolution of the estimated source locations in the *xy*-plane in comparison to the true source location and the sensors used to measure the pollutant concentration.

Figure 2 – Evolution of the estimated position of the source compared with the true location (red cross) and the locations of the sensors (filled squares in the left panel)



Source: the authors (2023)

Table 1 – Estimated source parameters (x, y, z, and Q) with corresponding ℓ^2-normalized errors and residuals considering the initial step (Initial), the estimation with the lowest error (Best), the mean of estimations in the first (Mean 1) and second (Mean 2) plateaus in the error panel in Fig. 1, and the parameter actual values (True)

	x (Km)	y (Km)	z (Km)	Q (g/s)	Residual	Error
Initial	0.550	-0.150	0.150	3.500	0.561	4.965
Best	0.008	0.019	0.125	1.750	0.520	0.199
Mean 1	-0.107	0.072	0.127	1.767	0.538	1.127
Mean 2	-0.178	0.104	0.120	1.754	0.539	1.792
True	0	0	0.115	3.200	-	-

By Fig. 1, we can say that the algorithm possibly attained an equilibrium after 17 steps. Unfortunately, this equilibrium did not contain the best estimation, that occurred at the 6th iterate. The solution with the smallest residual, i.e., the 2nd iterates, had an error value considerably larger than the following iterates. This is due to overfitting, as the data is corrupted by noise. Possible ways to improve the algorithm performance are the following, we can use some discrepancy principle to refine the selection of the regularization parameter α and we can set some threshold value for the residual, where the algorithm only keeps the estimated values that are below the threshold. The main difficulty with this procedure is to set the threshold avoiding overfitting. In the present experiment, a potential threshold value is 0.53.

5 CONCLUSIONS

We proposed an estimation technique that can be applied to problems with multiple observations and penalty terms. The main difficulty is to guarantee the algorithm's accuracy. Although the algorithm converged, the stable solution was not the best one. This can be addressed by forcing the algorithm to keep only the iterates with residuals below some previously stated threshold. Another feature that can also be used to improve performance is reducing the search region by adding some prior information. The present results are preliminary, and in future research, we will add the features mentioned above, and we will apply this technique to other problems.

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Authorship Contributions

1 – Roseane Alves de Souza Albani

Universidade do Estado do Rio de Janeiro - DSc. in Mechanical Engineering
https://orcid.org/0000-0002-2091-194X - roseanealves75@gmail.com
Contribution: Conceptualization, Data curation, Formal Analysis, Investigation, Methodology, Resources, Software, Visualization, Writing – original draft, Writing – review editing.

2 - Vinícius Viana Luiz Albani

Universidade Federal de Santa Catarina - DSc. in Mathematics
https://orcid.org/0000-0002-5751-5895 - v.albani@ufsc.br
Contribution: Conceptualization, Data curation, Formal Analysis, Investigation, Methodology, Resources, Software, Visualization, Writing – original draft, Writing – review editing.

3 – Antônio José da Silva Neto

Universidade do Estado do Rio de Janeiro - PhD in Mechanical Engineering.
https://orcid.org/0000-0002-9616-6093 - ajsn@uerj.iprj.br
Contribution: Conceptualization, Data curation, Formal Analysis, Investigation, Methodology, Resources, Software, Visualization, Writing – original draft, Writing – review editing.

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