Advanced Methods in Applied Statistics

The L-curve and its use in the numerical treatment of inverse problems

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Date:
March 7th, 2018

Motivation

The L-curve and its use in the numerical treatment of inverse problems by P. C. Hansen (2001) outlines a graphical procedure (the L-curve) that can handle inverse problems which are ill-posed. The L-curve is a visual way of dealing with the trade-off between the size of a regularized solution and its fit to the given data as the regularization parameter varies. This summary will illustrate the method of the paper by using an example:

Suppose we are trying to locate a treasure which has been buried under the ground. In our treasure hunt, we have a tool to measure vertical gravity anomalies (d) and we know that the treasure can be identified as a place with a negative density anomaly. We conduct 60 measurements at the locations s along the distance x between 0 and 100 m. Thus, the measured gravity anomaly function ($d(s)$) can be described as:

$$d(s) = \int_{0}^{100} g(x-s)m(x)\mathrm{d}x \tag{1}$$

where $g(x-s)$ is a well-known convolution kernel (not important here) applied on the density anomaly function $m(x)$. As we want to estimate $m(x)$, this is an inverse problem which can be written on the form $\mathbf{Gm} = \mathbf{d}$ where $\mathbf{G}$ is a 60x60 matrix. As the problem is on a matrix form, the least squares solution is given by (Aster et al., 2011):

$$\mathbf{m} = \left(\mathbf{G}^{\mathrm{T}}\mathbf{G}\right)^{-1}\mathbf{G}^{\mathrm{T}}\mathbf{d} \tag{2}$$

The solution is plotted in Fig. 1, and it is evident that it is an unstable solution (ill-posed problem). This can be further verified by checking if the matrix condition number increases as the number of discretization steps increases (which it does) (Aster et al., 2011). This is defined as a *discrete ill-posed problem.* So in order to accurately locate the buried treasure, we need to use *Tikhonov regularization.*

Method and Results

Tikhonov regularization is one way of dealing with discrete ill-posed problems. The least squares solution is similar to Eq. 2, but now it also includes the smoothing term $\alpha^2\mathbf{I}$ (0 order Tikhonov matrix):

$$\mathbf{m} = \left(\mathbf{G}^{\mathrm{T}}\mathbf{G} + \alpha^2\mathbf{I}\right)^{-1}\mathbf{G}^{\mathrm{T}}\mathbf{d}, \tag{3}$$

where $\mathbf{I}$ is the identity matrix and α is a regularization parameter between 0 and 1. So we need to estimate the Tikhonov matrix that provides the best solution. This is done by plotting calculations of the solution norm $||\mathbf{m}||_2$ as a function of the residual norm $||\mathbf{Gm} - \mathbf{d}||_2$ for an array of α values. By plotting this on a ln-ln scale we have a L-curve as seen in Fig. 2. If α is too high, then the model will not fit the data properly (large residual norm), and if α is too low, then the fit will be good, but it will be dominated by data errors (large solution norm). Thus, the best value of α is then found when both the solution and residual norm are minimal. hence, at the kink or at the place with the highest curvature (this can be automated or found manually). In Fig. 2, $\alpha = 1.3 \cdot 10^{-4}$ is the most optimal parameter. By using Eq. 3, the solution to the inverse problem using a 0 order Tikhonov regularization is provided in Fig. 1. We can see that we now a more smooth and stable solution which shows a negative density anomaly in the center of the domain. We have hereby located the treasure.

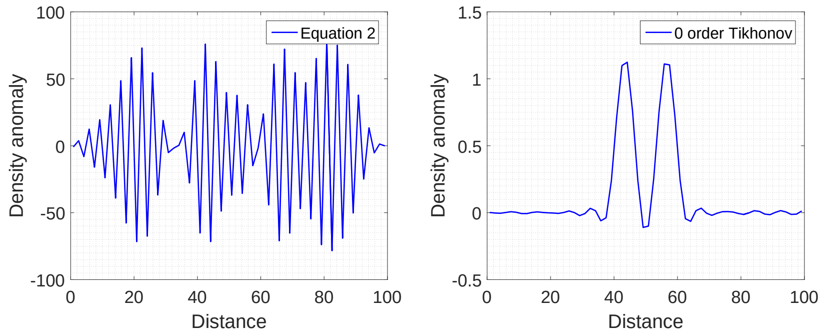

Figure 1: The estimated density anomaly $m(x)$. Left figure shows the raw least squares solution (Eq. 2) and the right figure shows a 0 order Tikhonov solution (Eq. 3).

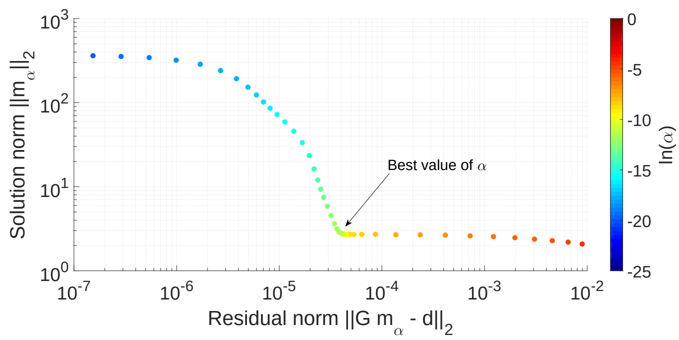

Figure 2: The solution norm $||\mathbf{m}_\alpha||_2$ as a function of the residual norm $||\mathbf{G}\mathbf{m}_\alpha - \mathbf{d}||_2$ for an array of α values. The best value of α is found at the kink.

Bibliography

Aster, R. C., Borchers, B. and Thurber, C. H. (2011), *Parameter Estimation and Inverse Problems*, Elsevier: Academic Press.

P. C. Hansen (2001), *The L-curve and its use in the numerical treatment of inverse problems*, WIT Press.