Inverse Problems 1: convolution and deconvolution

Lesson 8: Tikhonov regularization, part II

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September 25, 2019

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Normal equations for Tikhonov regularization

Review

Tikhonov regularization

$$T_\alpha m = \underset{f \in \mathbb{R}^n}{\arg\min} \{\|Af - m\|^2 + \alpha \|f\|^2\}$$

Tikhonov regularization

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How to compute $T_\alpha m$?

Theorem

Let $A = UDV^T$, being U, V orthogonal matrices and $D = diag(d_1, \ldots, d_n)$, such that $d_1 \geq \ldots \geq d_n$. Suppose that $\exists r \leq n$: $d_r > 0$ and $d_{r+1} = \ldots = d_n = 0$. Let

$$\mathcal{D}_\alpha^+ = diag\left(\frac{d_1}{d_1^2 + \alpha}, \ldots, \frac{d_n}{d_n^2 + \alpha} \right).$$

Then, $T_\alpha = V \mathcal{D}_\alpha^+ U^T$

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Issue: the computation of U, D, V is numerically expensive.

Normal equations

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The solution $T_\alpha m$ can be computed as

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- Define the quadratic functional to be minimized:

$$Q_\alpha(f) = \|Af - m\|^2 + \alpha \|f\|^2.$$

- Then, if $f_\alpha = T_\alpha m$ is the minimum of Q_α, the following optimality condition must be satisfied:

$$\frac{d}{dt} Q_\alpha(f_\alpha + tw)\Big|_{t=0} = 0 \qquad \forall w \in \mathbb{R}^n$$

Normal equations - proof

- We rewrite the quadratic functional as follows:

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- using the transpose, $\quad \langle A^T Af_\alpha - A^T m + \alpha f_\alpha, w\rangle = 0 \quad \forall w \in \mathbb{R}^n$
- in conclusion, $\quad (A^T A + \alpha I)f_\alpha = A^T m$,
  and the matrix $A^T A + \alpha I$ is surely invertible.

Stacked version

The following formulation is equivalent to the normal equations:

Stacked form

$T_\alpha m$ is the unique least squares solution of $\begin{bmatrix} A \\ \sqrt{\alpha} I \end{bmatrix} f = \begin{bmatrix} m \\ 0 \end{bmatrix}$.

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- Let $\widetilde{A} = \begin{bmatrix} A \\ \sqrt{\alpha} I \end{bmatrix} \in \mathbb{R}^{2n \times n}$ and $\widetilde{m} = \begin{bmatrix} m \\ 0 \end{bmatrix} \in \mathbb{R}^{2n \times 1}$.

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- Analogously to the previous proof, one can show that the least squares solution (i.e., $f = \arg\min\{\|\widetilde{A} f - \widetilde{m}\|^2\}$) is the solution of the normal equations: $\widetilde{A}^T \widetilde{A} f = \widetilde{A}^T \widetilde{m}$

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- Analogously to the previous proof, one can show that the least squares solution (i.e., $f = \arg\min\{\|\widetilde{A}f - \widetilde{m}\|^2\}$) is the solution of the normal equations: $\widetilde{A}^T \widetilde{A} f = \widetilde{A}^T \widetilde{m}$
- we are not going to prove why such solution is unique
- One easily notices that:

$$\widetilde{A}^T \widetilde{A} = \begin{bmatrix} A^T & \sqrt{\alpha} I \end{bmatrix} \begin{bmatrix} A \\ \sqrt{\alpha} I \end{bmatrix} = A^T A + \alpha I, \quad \widetilde{A}^T \widetilde{m} = \begin{bmatrix} A^T & \sqrt{\alpha} I \end{bmatrix} \begin{bmatrix} m \\ 0 \end{bmatrix} = A^T m.$$

Implementation

Example 1

1. Set $n = 100$ and define the signal f and the point spread function PSF as in the previous lecture. Create the convolution matrix A.
2. Generate the noisy measurement $m_\delta = Af + \delta r$, being r a Gaussian random vector of n dimensions, $\|r\| = 1$. Consider $\delta = 10^{-2}$.
3. Compute the Tikhonov regularized solution associated to $\alpha = 0.1$ by employing the singular values, by the normal equations and by their stacked version.
4. Compare the results obtained by comparing the norm of the difference between the three version and by estimating the computational time required (use the commands `tic` and `toc`).
5. Replicate the same analysis for $n = 250, 500, 1000, 2000$.

Generalized Tikhonov regularization

Generalized Tikhonov

Remind: the formulation of Tikhonov involves a data fidelity term $\|Af - m\|$ and some a priori knowledge encoded by $\|f\|$. We assume to know that, among the possible solutions of $Af = m$, we are promoting the one of smallest norm.

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We can generalize the argument to incorporate different a priori information:

- we are interested in the solution f close to a known signal f_* (it minimizes $\|f - f_*\|$);

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Generalized Tikhonov regularization

$$T_\alpha m = \arg\min_{f \in \mathbb{R}^n} \{\|Af - m\|^2 + \alpha \|L(f - f_*)\|^2\}$$

Explicit formulas

It is easy to replicate the computation leading to the normal equations, obtaining

Generalized normal equations

The solution $T_\alpha m$ can be computed as

$$T_\alpha = (A^T A + \alpha L^T L)^{-1}(A^T m + \alpha L^T L f_*),$$

Explicit formulas

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Generalized normal equations

The solution $T_\alpha m$ can be computed as

$$T_\alpha = (A^T A + \alpha L^T L)^{-1}(A^T m + \alpha L^T L f_*),$$

or alternatively

Stacked form

$T_\alpha m$ is the least squares solution of $\begin{bmatrix} A \\ \sqrt{\alpha} L \end{bmatrix} f = \begin{bmatrix} m \\ \sqrt{\alpha} L f_* \end{bmatrix}.$

Exercise: try to prove both formulas

Implementation

Example 2

1. Set $n = 200$, let $n_1 = 2\left\lfloor \frac{n}{15} \right\rfloor$, $n_4 = 8\left\lfloor \frac{n}{15} \right\rfloor$, $n_5 = 10\left\lfloor \frac{n}{15} \right\rfloor$, $n_6 = 14\left\lfloor \frac{n}{15} \right\rfloor$ and define the signal f as

$$f = \begin{cases} 6 & \text{if } n_1 \leq n \leq n_4, \\ 4 - cos\left(\dfrac{2\pi n}{n_6 - n_5}\right) & \text{if } n_5 \leq n \leq n_6, \\ 5 & \text{elsewhere.} \end{cases}$$

2. create PSF by triple auto-convolution and normalization of $[1, 1, 1]$.
3. Generate the noisy measurement $m_\delta = Af + \delta r$, being r a Gaussian random vector, $\|r\| = 1$. Consider $\delta = 10^{-2}$.
4. Compute the Tikhonov regularized solution with $\alpha = 0.1$.
5. Compute the generalized Tikhonov solution by choosing $L = I$ and $f_* = 5$.

Implementation

Example 3

1. Create f as in Example 2, subtracting 5. Take PSF and m_δ as in Example 2.
2. Compute the Tikhonov regularized solution associated to $\alpha = 0.1$.
3. Compute the generalized Tikhonov solution by choosing $f_* = 0$ and by considering a matrix L obtained by discretization of the derivative operator by means of a finite difference scheme:

$$\frac{df}{dx}(x_i) \approx (Lf)_i = \frac{f(x_i) - f(x_{i-1})}{\Delta x} = \frac{f_i - f_{i-1}}{\Delta x}.$$

Hint: in our examples, $\Delta x = 1$. Then

$$(Lf)_i = f_i - f_{i-1} = [-1 \quad 1] \begin{bmatrix} f_{i-1} \\ f_i \end{bmatrix} = [0 \ldots -1 \quad 1 \ldots 0] \; f$$

Choice of the regularization parameter

If we knew the solution...

In applications, the noise level δ is fixed (and, approximatively, known).

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For Tikhonov, there exists an a priori parameter choice rule $\alpha = \alpha(\delta)$ which holds $\forall m_\delta : \|m - m_\delta\| \leq \delta$. Such rule is sub-obtimal in most of the cases. A posteriori rule: decide α according to m_δ.

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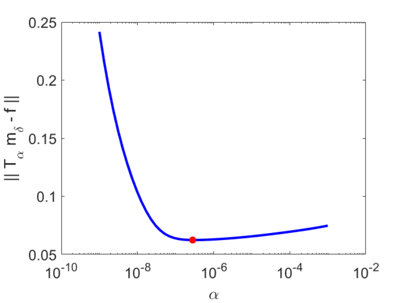

Idea

Take α such that $\| T_\alpha m_\delta - f \|$ is minimized.

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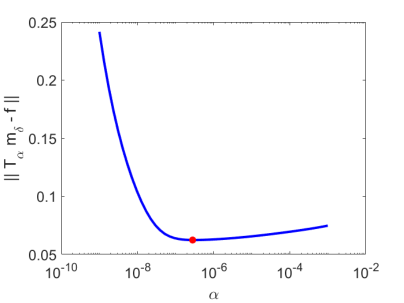

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Big problem: we need to know the exact solution!

Morozov's discrepancy principle

Consider the **residual**

$$r(\alpha) = \|Af_{\alpha,\delta} - m_\delta\|, \qquad f_{\alpha,\delta} = T_\alpha m_\delta.$$

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Theory: $r(\alpha)$ is an increasing function of $\alpha \in (0, \infty)$.

Its codomain is $(\|Pm_\delta\|, \|m_\delta\|)$, where P is the orthogonal projection on $range(A)^\perp$.

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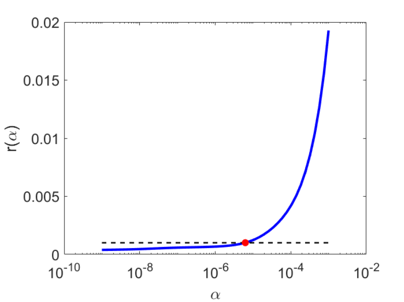

Morozov's discrepancy principle - in practice

Practical remarks:

- in application, δ is not always well known: we don't need high accuracy when solving $r(\alpha) = \delta$
- $f_{\alpha,\delta}$ is not extremely sensitive with respect to α
- alternative formulations of Morozov: $\|Af_{\alpha,\delta} - m\|^2 = \delta^2$ (which is equivalent), $r(\alpha) = \tau\delta$ (*rule of thumb*: $\tau = 1.2$).

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How to solve $r(\alpha) = \delta$?

1. generate several possible α (the command `logspace` is very useful), evaluate r in those points, minimize $|r(\alpha) - \delta|$;
2. iterative algorithms, e.g. (geometric) bisection, allow to compute very few values of $r(\alpha)$ to satisfy Morozov's principle up the a fixed tolerance.

L-curve method

A different idea

The parameter choice should detect the **perfect balance** between the two terms appearing in Tikhonov regularization:

$$f_{\alpha,\delta} = \arg\min_{f \in \mathbb{R}^n} \{\|Af - m_\delta\|^2 + \alpha\|f\|^2\}.$$

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What does *perfect balance* mean? We need to understand the tradeoff between data fidelity and a priori knowledge reliability.

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This is done by defining a parametric curve $(X(\alpha), Y(\alpha))$:
$X(\alpha) = \log(\|Af_{\alpha,\delta} - m\|)$.
$Y(\alpha) = \log(\|f_{\alpha,\delta}\|)$,

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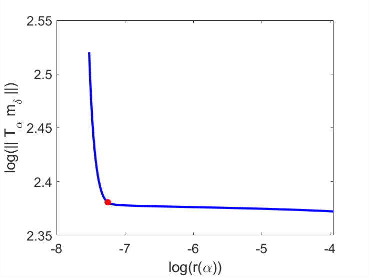

L-curve method - in practice

If the curve $(X(\alpha), Y(\alpha))$ has a shape similar to the letter L, then its "vertex" represent a good balance: a bigger α would cause a dramatic increas of the residual with no benefit for regularity, a smaller one would do the opposite.
Warning: that doesn't happen in any inverse problem!

L-curve method - in practice

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Warning: that doesn't happen in any inverse problem!

How to select the vertex?

- select some values of α (e.g. using `logspace`), compute X, Y and select the vertex by inspection;
- select some values of α, compute X, Y and select the point which is the closest to the origin of the graphic;
- more involved rules based on the slope of the curve.

Example 4

1. Create f as in Example 2, subtracting 5. Take PSF and m_δ as in Example 2, but use $\delta = 10^{-3}$.
2. Create a sampling of values of 60 αs from 10^{-9} to 10^{-2}, equally spaced in a logarithmic scale.
3. By employing the knowledge of the true solution, find which α gives the smallest relative error.
4. Show the residual as a function of α and automatically pick α satisfying Morozov's discrepancy principle. Is it close to the real value giving the smallest error?
5. Compute $X(\alpha)$, $Y(\alpha)$ and plot the L curve. Automatically select the vertex of the curve and the associated α. Is it close to the real value giving the smallest error?