Chapter 5

Tikhonov regularization

Tikhonov regularization is typically the method of first choice for linear problems. It provides some smoothing, and generalized Tikhonov regularization provides an opportunity to incorporate known properties of the solution into the solution method. As we shall see in this chapter, it is simple to implement, but introduces the classic question, "How can I choose the regularization parameter?" Two popular but not always reliable methods for selecting the regularization parameter, the Morozov discrepancy principle and the L-curve method, are explained in Section 5.4. In fact, there is no known method for choosing the regularization parameter that results in an optimal solution, but it is important to be aware of these widely used methods. The results of using Tikhonov regularization on our three guiding examples is demonstrated in this chapter and through the exercises.

5.1 Classical Tikhonov regularization

The Tikhonov regularized solution of equation $\mathbf{m} = A\mathbf{f} + \varepsilon$ is the vector $T_\alpha(\mathbf{m}) \in \mathbb{R}^n$ that minimizes the expression

$$\|AT_\alpha(\mathbf{m}) - \mathbf{m}\|^2 + \alpha\|T_\alpha(\mathbf{m})\|^2,$$

where $\alpha > 0$ is called a regularization parameter. We denote

$$T_\alpha(\mathbf{m}) = \underset{\mathbf{z}\in\mathbb{R}^n}{\arg\min}\left\{\|A\mathbf{z} - \mathbf{m}\|^2 + \alpha\|\mathbf{z}\|^2\right\}. \tag{5.1}$$

Tikhonov regularization can be understood as a balance between two requirements:

(i) $T_\alpha(\mathbf{m})$ should give a small residual $AT_\alpha(\mathbf{m}) - \mathbf{m}$.

(ii) $T_\alpha(\mathbf{m})$ should be small in L^2-norm.

The regularization parameter $\alpha > 0$ can be used to "tune" the balance.

Note that in inverse problems there are typically infinitely many choices of $T_\alpha(\mathbf{m})$ satisfying (i), and one of the roles of (ii) is to make the solution unique.

Theorem 5.1. *Let A be a $k \times n$ matrix. The Tikhonov regularized solution for equation $\mathbf{m} = A\mathbf{f} + \varepsilon$ is given by*

$$T_\alpha(\mathbf{m}) = V \mathcal{D}_\alpha^+ U^T \mathbf{m}, \tag{5.2}$$

where $A = UDV^T$ is the SVD, and

$$\mathcal{D}_\alpha^+ = \operatorname{diag}\left(\frac{d_1}{d_1^2 + \alpha}, \ldots, \frac{d_{\min(k,n)}}{d_{\min(k,n)}^2 + \alpha} \right) \in \mathbb{R}^{n \times k}. \tag{5.3}$$

Proof. Write $T_\alpha(\mathbf{m}) \in \mathbb{R}^n$ as linear combination of column vectors of the matrix V: $T_\alpha(\mathbf{m}) = \sum_{j=1}^n a_j V_j = V\mathbf{a}$. Set $\mathbf{m}' = U^T \mathbf{m}$ and compute

$$\begin{aligned}
&\|AT_\alpha(\mathbf{m}) - \mathbf{m}\|^2 + \alpha \|T_\alpha(\mathbf{m})\|^2 \\
&= \|UDV^T V\mathbf{a} - UU^T \mathbf{m}\|^2 + \alpha \|V\mathbf{a}\|^2 \\
&= \|D\mathbf{a} - \mathbf{m}'\|^2 + \alpha \|\mathbf{a}\|^2 \\
&= \sum_{j=1}^r (d_j a_j - \mathbf{m}'_j)^2 + \sum_{j=r+1}^k (\mathbf{m}'_j)^2 + \alpha \sum_{j=1}^n a_j^2 \\
&= \sum_{j=1}^r \left(d_j^2 + \alpha\right) \left(a_j^2 - 2\frac{d_j \mathbf{m}'_j}{d_j^2 + \alpha} a_j \right) + \alpha \sum_{j=r+1}^n a_j^2 + \sum_{j=1}^k (\mathbf{m}'_j)^2 &(5.4) \\
&= \sum_{j=1}^r \left(d_j^2 + \alpha\right) \left(a_j - \frac{d_j \mathbf{m}'_j}{d_j^2 + \alpha} \right)^2 + \alpha \sum_{j=r+1}^n a_j^2 &(5.5) \\
&\quad - \sum_{j=1}^r \frac{(d_j \mathbf{m}'_j)^2}{d_j^2 + \alpha} + \sum_{j=1}^k (\mathbf{m}'_j)^2,
\end{aligned}$$

where completing the square in the leftmost term in (5.4) yields (5.5). Our task is to choose such values for the parameters $a_1, \ldots, a_n$ that (5.5) attains its minimum. Clearly the correct choice is

$$a_j = \begin{cases} \dfrac{d_j}{d_j^2 + \alpha} \mathbf{m}'_j\,, & 1 \le j \le r, \\ 0, & r+1 \le j \le n, \end{cases}$$

or, in short, $\mathbf{a} = \mathcal{D}_\alpha^+ \mathbf{m}'$. $\square$

Recall from Section 4.2 that the TSVD solution is given by

$$\mathcal{L}_\alpha(\mathbf{m}) = V D_\alpha^+ U^T \mathbf{m} = \sum_{i=1}^{r_\alpha} \frac{\mathbf{u_i}^T \mathbf{m}}{d_i} \mathbf{v_i}, \tag{5.6}$$

where the $\mathbf{u_i}$ and $\mathbf{v_i}$ are the columns of the matrices U and V, respectively, while

$$T_\alpha(\mathbf{m}) = V \mathcal{D}_\alpha^+ U^T \mathbf{m} = \sum_{i=1}^r \left(\frac{d_i^2}{d_i^2 + \alpha} \right) \frac{\mathbf{u_i}^T \mathbf{m}}{d_i} \mathbf{v_i} = \sum_{i=1}^r \left(\frac{d_i}{d_i^2 + \alpha} \right) (\mathbf{u_i}^T \mathbf{m}) \mathbf{v_i}. \tag{5.7}$$

Recall that $r_\alpha \le r$. Thus, we see that the entries of $\mathcal{D}_\alpha^+$ effectively weight the contributions of the vectors in the SVD, and if the regularization parameter α is sufficiently small (smaller than the smallest singular value), the Tikhonov regularized solution is essentially the same as the solution obtained by the SVD. By increasing α, less weight is placed on the small singular values, which also correspond to the highly oscillatory right singular vectors.

5.2 Normal equations and stacked form

Consider the quadratic functional $Q_\alpha : \mathbb{R}^n \to \mathbb{R}$ defined by

$$Q_\alpha(\mathbf{f}) = \|A\mathbf{f} - \mathbf{m}\|^2 + \alpha\|\mathbf{f}\|^2.$$

It can be proven that Q_α has a unique minimum for any $\alpha > 0$. The minimizer $T_\alpha(\mathbf{m})$ (i.e., the Tikhonov regularized solution of $\mathbf{m} = A\mathbf{f} + \varepsilon$) satisfies

$$0 = \frac{d}{dt}\left\{\|A(T_\alpha(\mathbf{m}) + t\mathbf{w}) - \mathbf{m}\|^2 + \alpha\|T_\alpha(\mathbf{m}) + t\mathbf{w}\|^2\right\}\bigg|_{t=0}$$

for any $\mathbf{w} \in \mathbb{R}^n$.

Compute

$$\begin{aligned}
&\frac{d}{dt}\|A(T_\alpha(\mathbf{m}) + t\mathbf{w}) - \mathbf{m}\|^2\bigg|_{t=0} \\
&= \frac{d}{dt}\langle AT_\alpha(\mathbf{m}) + tA\mathbf{w} - \mathbf{m}, AT_\alpha(\mathbf{m}) + tA\mathbf{w} - \mathbf{m}\rangle\bigg|_{t=0} \\
&= \frac{d}{dt}\Big\{\|AT_\alpha(\mathbf{m})\|^2 + 2t\langle AT_\alpha(\mathbf{m}), A\mathbf{w}\rangle + t^2\|A\mathbf{w}\|^2 \\
&\qquad\qquad -2t\langle \mathbf{m}, A\mathbf{w}\rangle - 2\langle AT_\alpha(\mathbf{m}), \mathbf{m}\rangle + \|\mathbf{m}\|^2\Big\}\bigg|_{t=0} \\
&= 2\langle AT_\alpha(\mathbf{m}), A\mathbf{w}\rangle - 2\langle \mathbf{m}, A\mathbf{w}\rangle,
\end{aligned}$$

and

$$\begin{aligned}
&\frac{d}{dt}\alpha\langle T_\alpha(\mathbf{m}) + t\mathbf{w}, T_\alpha(\mathbf{m}) + t\mathbf{w}\rangle\bigg|_{t=0} \\
&= \alpha\frac{d}{dt}\left\{\|T_\alpha(\mathbf{m})\|^2 + 2t\langle T_\alpha(\mathbf{m}), \mathbf{w}\rangle + t^2\|\mathbf{w}\|^2\right\}\bigg|_{t=0} \\
&= 2\alpha\langle T_\alpha(\mathbf{m}), \mathbf{w}\rangle.
\end{aligned}$$

Thus, we have $\langle AT_\alpha(\mathbf{m}) - \mathbf{m}, A\mathbf{w}\rangle + \alpha\langle T_\alpha(\mathbf{m}), \mathbf{w}\rangle = 0$, and by taking the transpose,

$$\langle A^T AT_\alpha(\mathbf{m}) - A^T\mathbf{m}, \mathbf{w}\rangle + \alpha\langle T_\alpha(\mathbf{m}), \mathbf{w}\rangle = 0.$$

This results in the variational form

$$\langle (A^T A + \alpha I)T_\alpha(\mathbf{m}) - A^T\mathbf{m}, \mathbf{w}\rangle = 0. \tag{5.8}$$

Since (5.8) holds for any nonzero $\mathbf{w} \in \mathbb{R}^n$, we necessarily have $(A^T A + \alpha I)T_\alpha(\mathbf{m}) = A^T\mathbf{m}$. So the Tikhonov regularized solution $T_\alpha(\mathbf{m})$ satisfies

$$T_\alpha(\mathbf{m}) = (A^T A + \alpha I)^{-1}A^T\mathbf{m}, \tag{5.9}$$

and actually (5.9) can be used for computing $T_\alpha(\mathbf{m})$ defined in the basic situation (5.1).

In the generalized case of (5.14) we get by a similar computation,

$$T_\alpha(\mathbf{m}) = (A^T A + \alpha L^T L)^{-1} A^T \mathbf{m}. \tag{5.10}$$

Next we will derive a computationally attractive *stacked form* version of (5.2).

We rethink problem (5.2) so that we have two measurements on $\mathbf{f}$ that we minimize simultaneously in the least-squares sense. Namely, we consider both equations $A\mathbf{f} = \mathbf{m}$ and $\mathbf{f} = 0$ as independent measurements of the same object $\mathbf{f}$, where $A \in \mathbb{R}^{k\times n}$. Now we stack the matrices and right-hand sides so that the regularization parameter $\alpha > 0$ is involved correctly:

$$\begin{bmatrix} A \\ \sqrt{\alpha} \end{bmatrix} \mathbf{f} = \begin{bmatrix} \mathbf{m} \\ 0 \end{bmatrix}. \tag{5.11}$$

We write (5.11) as $\widetilde{A}\mathbf{f} = \widetilde{\mathbf{m}}$ and solve for $T_\alpha(\mathbf{m})$ defined in (5.10) in MATLAB by

$$\mathbf{f} = \widetilde{A} \backslash \widetilde{\mathbf{m}}, \tag{5.12}$$

where \ stands for finding the least-squares solution. This is a good method for medium-dimensional inverse problems, where n and k are of the order $\sim 10^3$. Formula (5.12) is applicable to higher-dimensional problems than formula (5.2) since there is no need to compute the SVD for (5.12).

Why would (5.12) be equivalent to (5.9)? In general, a computation similar to the above shows that a vector $\mathbf{z}_0$, defined as the minimizer

$$\mathbf{z}_0 = \arg\min_{\mathbf{z}} \|B\mathbf{z} - \mathbf{b}\|^2,$$

satisfies the normal equations $B^T B\mathbf{z}_0 = B^T\mathbf{b}$. In this case the minimizing $\mathbf{z}_0$ is called the least-squares solution to equation $B\mathbf{z} = \mathbf{b}$. In the context of our stacked form formalism, the least-squares solution of (5.11) satisfies the normal equations

$$\widetilde{A}^T \widetilde{A}\mathbf{f} = \widetilde{A}^T \widetilde{\mathbf{m}}.$$

However,

$$\widetilde{A}^T \widetilde{A} = \begin{bmatrix} A^T & \sqrt{\alpha} I \end{bmatrix} \begin{bmatrix} A \\ \sqrt{\alpha} I \end{bmatrix} = A^T A + \alpha I$$

and

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

so it follows that $(A^T A + \alpha I)\mathbf{f} = A^T\mathbf{m}$.

As an example, consider the tomographic measurement matrix A constructed in Section 2.3.5 for the resolution 50×50 and with 50 projection directions. We can use the stacked form approach (5.11) and (5.12) to avoid the expensive computation of the SVD of A.

5.3 Generalized Tikhonov regularization

Sometimes we have a priori information about the solution of the inverse problem. For example, we may know that $\mathbf{f}$ is close to a vector $\mathbf{f}_* \in \mathbb{R}^n$; then we minimize

$$T_\alpha(\mathbf{m}) = \underset{\mathbf{z} \in \mathbb{R}^n}{\arg\min} \left\{ \|A\mathbf{z} - \mathbf{m}\|^2 + \alpha \|\mathbf{z} - \mathbf{f}_*\|^2 \right\}. \tag{5.13}$$

Another typical situation is that $\mathbf{f}$ is known to be smooth. Then we minimize

$$T_\alpha(\mathbf{m}) = \underset{\mathbf{z}\in\mathbb{R}^n}{\arg\min}\left\{\|A\mathbf{z}-\mathbf{m}\|^2 + \alpha\|L\mathbf{z}\|^2\right\} \tag{5.14}$$

or

$$T_\alpha(\mathbf{m}) = \underset{\mathbf{z}\in\mathbb{R}^n}{\arg\min}\left\{\|A\mathbf{z}-\mathbf{m}\|^2 + \alpha\|L(\mathbf{z}-\mathbf{f}_*)\|^2\right\}, \tag{5.15}$$

where L is a discretized differential operator.

For example, in dimension one, representing the vector $\mathbf{f}$ as a continuous function f with $f(s_j) = \mathbf{f_j}$, we can discretize the derivative of the continuum by the difference quotient

$$\frac{df}{ds}(s_j) \approx \frac{f(s_{j+1}) - f(s_j)}{\Delta s} = \frac{\mathbf{f}_{j+1} - \mathbf{f}_j}{\Delta s}.$$

This leads to the discrete differentiation matrix

$$L = \frac{1}{\Delta s}\begin{bmatrix} -1 & 1 & 0 & 0 & 0 & \cdots & & 0 \\ 0 & -1 & 1 & 0 & 0 & \cdots & & 0 \\ 0 & 0 & -1 & 1 & 0 & \cdots & & 0 \\ \vdots & & & & \ddots & & & \\ \vdots & & & & & \ddots & & \\ 0 & & \cdots & & 0 & -1 & 1 & 0 \\ 0 & & \cdots & & 0 & 0 & -1 & 1 \\ 1 & & \cdots & & 0 & 0 & 0 & -1 \end{bmatrix}. \tag{5.16}$$