5.7 Regularization methods for linear inverse problems

The primary difficulty with linear ill-posed problems is that the inverse image is undetermined due to small (or zero) singular values of \( A \). Actually the situation is a little worse in practice because \( A \) depends on our model of the measurement process and that is typically not precisely known—leading to a slight imprecision in the singular values. Usually that is not significant for the large singular values, but may lead to ambiguity in the small singular values so that we do not know if they are small or zero. As an introduction to regularization—which is one method for surmounting the problems associated with small singular vectors—we consider a framework for describing the quality of a reconstruction \( x \) in an inverse problem.

In the last section, we considered the linear problem

\[
b = Ax + n
\]

and focussed on the structure of the operator \( A \in \mathbb{R}^{m \times n} \). As far as the data are concerned, a reconstructed image \( \tilde{x} \) is good provided that it gives rise to “mock data” \( A\tilde{x} \) which are close to the observed data. Thus, one of the quantities for measuring the quality of \( \tilde{x} \) is the data misfit function or the square of the residual norm

\[
C(x) = ||b - Ax||^2
\]

However, from our previous considerations, we have seen that choosing \( \tilde{x} \) so as to minimize \( C(x) \) usually gives a poor reconstruction. If the rank of the operator \( A \) is less than \( n \), there are an infinite number of reconstructions, all of which minimize \( C(x) \), since the data are not affected by adding to a reconstruction any vector which lies in the null space of \( A \). In the presence of noise, finding the (possibly non-unique) minimum of \( C \) is undesirable as it leads to amplification of the noise in the directions of the singular vectors with small singular values. Instead, we usually regard the data as defining a “feasible set” of reconstructions for which \( C(x) \leq C_0 \) where \( C_0 \) depends on the level of the noise. Any reconstruction within the feasible set is to be thought of as being consistent with the data.

Since the data do not give us any information about some aspects of \( x \), it is necessary to include additional information which allows us to select from among several feasible reconstructions. Analytical solutions are available if we choose sufficiently simple criteria. One way of doing this is to introduce a second function \( \Omega(x) \) representing our aversion to a particular reconstruction. For example, we may decide that the solution of minimum norm should be chosen from among the feasible set. This can be done by choosing

\[
\Omega(x) = ||x||^2.
\]

Sometimes, we have a preference for reconstructions which are close to some default solution \( x^\infty \). This may be appropriate if we have historical information about the quantity. This can be done by choosing

\[
\Omega(x) = ||x - x^\infty||^2.
\]

More generally, it may not be the norm of \( x - x^\infty \) which needs to be small, but some linear operator acting on this difference. Introducing the operator \( L \) for this purpose, we can set

\[
\Omega(x) = ||L(x - x^\infty)||^2 = (x - x^\infty)^T L^T L (x - x^\infty)
\]

If the image space is \( n \) dimensional and the data space is \( m \) dimensional, the matrix \( A \) is of size \( m \times n \) and the matrix \( L \) is of size \( p \times n \) where \( p \leq n \). Typically, \( L \) is the identity matrix or a banded matrix approximation to the \((n-p)\)'th derivative. For example, an approximation to the first derivative is given by the matrix

\[
L_1 = \frac{1}{\Delta d} \begin{pmatrix}
-1 & 1 \\
-1 & 1 \\
... & ...
\end{pmatrix}
\]

while an approximation to the second derivative is

\[
L_2 = \frac{1}{(\Delta d)^2} \begin{pmatrix}
1 & -2 & 1 \\
1 & -2 & 1 \\
... & ... & ...
\end{pmatrix}
\]
where $\Delta d$ is the sampling interval between data.

In other cases, it may be appropriate to minimize some combination of the derivatives such as

$$\Omega(x) = a_0||x - x^\infty||^2 + \sum_{k=1}^q a_k||L_k(x - x^\infty)||^2$$  \hspace{1cm} (279)

where $L_k$ is a matrix which approximates the $k$'th derivative, and $a_k$ are non-negative constants. Such a quantity is also the square of a norm, called a Sobolev norm.

### 5.7.1 Tikhonov regularization

This is perhaps the most common and well-known of regularization schemes. We form a weighted sum of $\Omega(x)$ and $C(x)$ using a weighting factor, $\alpha^2$, and find the image $\tilde{x}$, which minimizes this sum, i.e.,

$$\tilde{x}_\alpha = \arg \min \left\{ \alpha^2||L(x - x^\infty)||^2 + ||b - Ax||^2 \right\}. \hspace{1cm} (280)$$

This is a whole family of solutions parameterized by the weighting factor $\alpha^2$. We call $\alpha$ the regularization parameter. If the regularization parameter is very large, the effect of the data misfit term $C(x)$ is negligible to that of $\Omega(x)$ and we find that $\lim_{\alpha \to \infty} \tilde{x}_\alpha = x^\infty$. With a large amount of regularization, we effectively ignore the data (and any noise on the data) completely and try to minimize the solution semi-norm which is possible by choosing the default solution. On the other hand, if $\alpha$ is small, the weighting placed on the solution semi-norm is small and the value of the misfit at the solution becomes more important. Of course, if $\alpha$ is reduced to zero, the problem reduces to the least-squares case considered earlier with its extreme sensitivity to noise on the data. A formal solution to the problem may readily be found. We set

$$\frac{\partial}{\partial x_{lk}} \left\{ \alpha^2(x - x^\infty)^T L^T L(x - x^\infty) + (b - Ax)^T (b - Ax) \right\} = 0 \hspace{1cm} (281)$$

for $k = 1, 2, \ldots, n$. This leads to the simultaneous equations

$$2\alpha^2 L^T L(x - x^\infty) - 2A^T (b - Ax) = 0, \hspace{1cm} (282)$$

or

$$(\alpha^2 L^T L + A^T A)x = \alpha^2 L^T Lx^\infty + A^T b. \hspace{1cm} (283)$$

Setting $\alpha = 0$ reduces this system of equations to the normal equations associated with the usual least squares problem. For non-zero values of $\alpha$, the additional term $\alpha^2 L^T L$ in the matrix on the left-hand side alters the eigenvalues (and eigenvectors) from those of $A^T A$ alone. So long as $\alpha^2 L^T L + A^T A$ is non-singular, there is a unique solution. The problem of image reconstruction is thus reduced to solving a (large) system of simultaneous equations with a symmetric positive definite coefficient matrix, and we shall later discuss ways of solving such systems of equations.

**An explicit solution of Tikhonov regularization** When the matrix $L$ happens to be the identity, Tikhonov regularization can be analyzed in an explicit form so that we can see clearly how the regularization parameter $\alpha$ affects the solution.

Let us suppose that we have computed the singular value decomposition of $A$ in the usual form

$$A = \sum_{l=1}^r \lambda_l u_l v_l^T, \hspace{1cm} (284)$$

then the left hand side of eq.(283) is written as

$$(\alpha^2 I + A^T A)\tilde{x} = \alpha^2 \sum_{l=1}^n \tilde{x}_l v_l + \sum_{l=1}^r \lambda_l^2 \tilde{x}_l v_l$$

$$= \sum_{l=1}^r (\alpha^2 + \lambda_l^2) \tilde{x}_l v_l + \alpha^2 \sum_{l=r+1}^n x_l^\infty v_l \hspace{1cm} (285)$$

where $\tilde{x}_l = v_l^T \tilde{x}$. The right hand side of eq.(283) is expressed by

$$\alpha^2 \tilde{x}^\infty + A^T b = \alpha^2 \sum_{l=1}^n x_l^\infty v_l + \sum_{l=1}^r \lambda_l b_l v_l$$

$$= \sum_{l=1}^r \left[ \alpha^2 x_l^\infty + \lambda_l^2 \left( \frac{b_l}{\lambda_l} \right) \right] v_l + \alpha^2 \sum_{l=r+1}^n x_l^\infty v_l \hspace{1cm} (286)$$
where \( x_{\infty} = v_{l}^T x_{\infty} \), \( b_l = u_{l}^T b \) and we have made use of the fact that \( I = \sum_{l=1}^{n} v_l v_l^T \), since the \( \{v_l\}_{l=1}^{n} \) form an orthonormal basis of \( R^n \). Equating (285) and (286) and using the linear independence of the vectors \( v_l \) we see that

\[
\tilde{x}_l = \left\{ \begin{array}{ll}
\frac{\alpha^2}{\alpha^2 + \lambda_l^2} x_{l\infty} + \frac{\lambda_l^2}{\alpha^2 + \lambda_l^2} \left( b_l \right) & \text{for } l = 1, 2, \ldots, r, \\
0 & \text{for } l = r + 1, \ldots, n.
\end{array} \right. \tag{287}
\]

Choosing the regularization parameter We have seen that \( \alpha \) sets the balance between minimizing the residual norm \( \|b - Ax_\alpha\| \) and minimizing the roughness \( \|x_\alpha - x_\infty\| \). The big question now is “how to choose \( \alpha \)?” Perhaps the most convenient graphical tool for setting \( \alpha \) is the “L-curve”. When we plot \( \log \|b - Ax_\alpha\| \) versus \( \log \|x_\alpha - x_\infty\| \) (for a discrete problem) we get the characteristic L-shaped curve with a (often) distinct corner separating vertical and horizontal parts of the curve. The rationale for using the L curve is that regularization is a trade-off between the data misfit and the solution seminorm. In the vertical part of the curve the solution seminorm \( \|L(x - x_\infty)\| \) is a very sensitive function of the regularization parameter because the solution is undergoing large changes with \( \alpha \) in an attempt to fit the data better. At these low levels of filtering, there are still components in the solution which come from dividing by a small singular value, which corresponds to having inadequate regularization. On the horizontal part, the solution is not changing by very much (as measured by the solution seminorm) as \( \alpha \) is changed. However, the data misfit is increasing sharply with more filtering. Along this portion, our preference for the more highly filtered solutions increases only slightly at the cost of a rapidly rising data misfit, and so it is desirable to choose a solution which lies not too far to the right of the corner.

5.7.2 Truncated Singular Value Decomposition (TSVD)

Let us suppose that the operator \( A \) has the singular value decomposition

\[
A = \sum_{l=1}^{r} \lambda_l u_l v_l^T. \tag{288}
\]

The truncated singular value decomposition (TSVD) method is based on the observation that for the larger singular values of \( A \), the components of the reconstruction along the corresponding singular vector is well-determined by the data, but the other components are not well-determined. An integer \( k \leq n \) is chosen for which the singular values are deemed to be significant and the solution vector \( \tilde{x} \) is chosen so that

\[
v_l^T \tilde{x} = \frac{u_l^T b}{\lambda_l} \text{ for } l = 1, \ldots, k. \tag{289}
\]

The components along the remaining singular-vector directions \( \{v_l\} \) for \( l = k + 1, \ldots, n \) are then chosen so that the total solution vector \( \tilde{x} \) satisfies some criterion of optimality, such as the minimization of a solution semi-norm of the form \( \Omega(x) = \|L(x - x_\infty)\|^2 \) as above. Let us denote by \( V_k \) the \( n \times (n - k) \) matrix whose columns are \( \{v_l\} \) for \( l = k + 1, \ldots, n \) so that \( V_k \) is the matrix whose columns span the effective null space of \( A \). The reconstruction which has zero projection in this effective null space is

\[
x' = \sum_{l=1}^{k} \left( \frac{u_l^T b}{\lambda_l} \right) v_l. \tag{290}
\]

The desired reconstruction \( \tilde{x} \) must be equal to the sum of \( x' \) and a vector which is the superposition of the columns of \( V_k \). This may be written as

\[
\tilde{x} = x' + \sum_{l=k+1}^{n} c_l v_l = x' + V_k c \tag{291}
\]

for a \( n - k \) element column vector \( c \). The solution semi-norm of this reconstruction is

\[
\Omega(\tilde{x}) = \|L(\tilde{x} - x_\infty)\|^2 = \|L(x' + V_k c - x_\infty)\|^2 = \|L(x' - x_\infty) + (LV_k)c\|^2 \tag{292}
\]

The vector \( c \) which minimizes this semi-norm is

\[
c = -(LV_k)^* L(x' - x_\infty) \tag{293}
\]
where the asterisk represents the Moore-Penrose inverse. i.e., for any matrix $A$, we define $A^\ast = (A^T A)^{-1} A^T$. This gives an explicit expression for the truncated singular value decomposition solution, namely

$$\tilde{x} = x' - V_k (LV_k)^\ast L(x' - x^\infty)$$

where $x'$ is given by (290) above. Note that some authors use the terminology truncated singular value decomposition to refer to the special case where $L$ is chosen to be the identity matrix, and call the general case derived above the modified truncated singular value decomposition.