

Chapter 1

Characteristics of Inverse Problems

The fields of inverse problems and statistics have significant overlap, though their literatures remain largely disjoint. Our goal in this manuscript is to present an introduction to the field of inverse problems with statistical content introduced, and connections between the two fields highlighted, wherever appropriate, in the hopes that this will facilitate the exchange of ideas between these two closely tied fields.

1.1 Preliminaries

We begin with the following linear statistical model with Gaussian noise:

$$\mathbf{b} = \mathbf{A}\mathbf{x} + \boldsymbol{\epsilon}, \quad (1.1)$$

where \mathbf{b} is the $m \times 1$ model output, or observation, vector; \mathbf{x} is the $n \times 1$ vector of unknown model parameters; \mathbf{A} is the $m \times n$ forward model matrix, which sometimes requires a separate set of observations; and $\boldsymbol{\epsilon}$ is an $m \times 1$ independent and identically distributed (iid) Gaussian random vector with variance σ^2 across all entries, which we denote $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$. We will assume that $m \geq n$ and that \mathbf{A} has full column rank.

In the statistics literature, \mathbf{b} is called the *response vector*, \mathbf{A} the *design matrix*, and \mathbf{x} the *unknown parameter vector*. Moreover, for statistical problems it is typically the case that $m \gg n$ and that the measured data consists both of the response vector \mathbf{b} and of the elements of \mathbf{A} , which are called the *explanatory variables*.

The term *inverse problem* is used in many contexts, however, classically, inverse problems are *ill-posed*, which means not *well-posed*, a term first defined by Jacques Hadamard [10]. The definition, adjusted for our notation and situation, is given as follows.

Definition 1.1. *The discrete mathematical model $\mathbf{b} = \mathbf{A}\mathbf{x}$ is said to be well-posed if*

1. *for all model output \mathbf{b} there exists a solution \mathbf{x} to $\mathbf{A}\mathbf{x} = \mathbf{b}$;*

2. the solution \mathbf{x} is unique; and
3. the solution \mathbf{x} is stable with respect to perturbations in \mathbf{b} ; that is, if $\tilde{\mathbf{b}}$ is a perturbation of \mathbf{b} with corresponding solution $\tilde{\mathbf{x}}$, then $\|\mathbf{x} - \tilde{\mathbf{x}}\|/\|\mathbf{x}\|$ is of the same order of magnitude as, or is smaller than, $\|\mathbf{b} - \tilde{\mathbf{b}}\|/\|\mathbf{b}\|$.

Condition 3 gives a suitable definition of stability for the examples that we consider in this text, however it may not be a suitable definition for all discrete inverse problems. In the continuous setting, where the focus is instead on the underlying continuously defined mathematical model $b = Ax$, a precise definition of stability can be given. In this case, Hadamard's condition 3 becomes

3. the solution x is stable with respect to perturbations in b ; that is, the inverse mapping $b \mapsto x$ is continuous.

In an introductory course on linear algebra or statistics, students study linear regression, which often leads to a linear system $\mathbf{b} = \mathbf{A}\mathbf{x}$ that fails condition 1 of Definition 1.1. To see this consider the next example.

Example 1.2 Suppose as a scientist you want to find a formula to estimate the weight b in kilograms of a lion by using its length ℓ in meters. You have five samples: $(b, \ell) = (420, 2.4), (350, 2.0), (310, 2.1), (280, 1.8)$, and $(75, 1.3)$. We assume a model of the form

$$b_i = x_1 + x_2 \ell_i + \epsilon_i, \quad (1.2)$$

where $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$. Gathering the data in matrix form $\mathbf{b} = \mathbf{A}\mathbf{x}$ yields

$$\begin{bmatrix} 420 \\ 350 \\ 310 \\ 280 \\ 75 \end{bmatrix} = \begin{bmatrix} 1 & 2.4 \\ 1 & 2.0 \\ 1 & 2.1 \\ 1 & 1.8 \\ 1 & 1.3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}. \quad (1.3)$$

We plot this data in Figure 1.1. Visually, you can see that the data has a linear trend, but also that there is no single line that interpolates all data points. Or in other words, (1.3) does not have a solution. This fact can be verified by performing Gaussian elimination on the augmented system $[\mathbf{A}|\mathbf{b}]$. Thus (1.3) is an ill-posed problem because it fails conditions 1 and 2. We can overcome this deficiency by computing the least squares solution, or equivalently by solving the normal equations $\mathbf{A}^T \mathbf{A} \hat{\mathbf{x}} = \mathbf{A}^T \mathbf{b}$, yielding the best-fit line $b = -303.08 + 307.34\ell$, also plotted with the data in Figure 1.1. We will discuss least squares in more detail in a moment. ■

The last example would not be considered a classical inverse problem. As was mentioned above, it is typical in inverse problems that the noise free equation $\mathbf{b} = \mathbf{A}\mathbf{x}$ in (1.1) is obtained from the numerical discretization of a continuously defined physical model $b = Ax$, where b and x are functions and A is an operator between function spaces. In many important applications, and in the examples

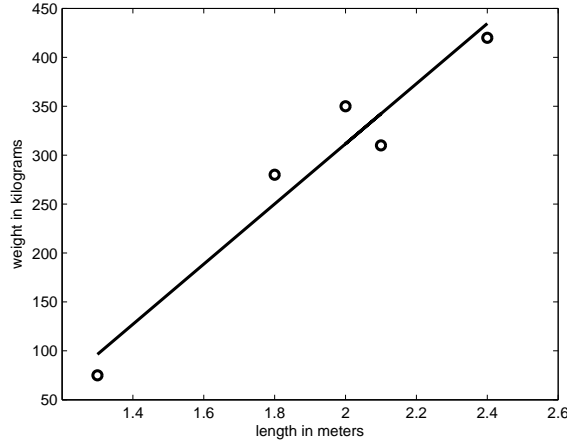


Figure 1.1. Scatter plot of lion length and weight data (ℓ_i, b_i) together with a plot of the best fit line.

considered in this book, this continuous model takes the form of a Fredholm first kind integral equation

$$b(s) = Ax(s) \stackrel{\text{def}}{=} \int_{\Omega} a(s, s')x(s') ds', \quad (1.4)$$

where Ω is the domain over which x is defined, and a is known as the *kernel*. In the examples considered in this text, either $\Omega = [0, 1]$ or $\Omega = [0, 1] \times [0, 1]$.

To obtain a matrix-vector equation $\mathbf{b} = \mathbf{A}\mathbf{x}$ from (1.4), we must perform a numerical discretization. We assume $\Omega = [0, 1]$ and use the midpoint quadrature rule, which for a general function f defined on $[0, 1]$ has the form

$$\int_0^1 f(s') ds' = h \sum_{j=1}^n f(s'_j) + E_n, \quad (1.5)$$

where $h = 1/n$, $s'_j = (j - \frac{1}{2})/n$, and E_n is the quadrature error. Assuming the same grid for the s variable, i.e. $s_j = s'_j$, if we define $b_i \stackrel{\text{def}}{=} b(s_i)$, $x_j \stackrel{\text{def}}{=} x(s'_j)$, and $a_{ij} = a(s_i, s'_j)$, and apply (1.5) to (1.4), ignoring E_n , we obtain

$$b_i = h \sum_{j=1}^n a_{ij}x_j, \quad i = 1, \dots, m. \quad (1.6)$$

Equation (1.6) can be written in matrix-vector form $\mathbf{b} = \mathbf{A}\mathbf{x}$, where $\mathbf{b} \in \mathbb{R}^m$, $\mathbf{x} \in \mathbb{R}^n$, and $\mathbf{A} \in \mathbb{R}^{m \times n}$ with entries $[\mathbf{A}]_{ij} = a_{ij}$.

For many examples in imaging, $m = n$ and the matrix \mathbf{A} is invertible. However, the resulting model $\mathbf{b} = \mathbf{A}\mathbf{x}$ will fail condition 3 of Definition 1.1, which will be the case for the next example.

Example 1.3 An application that we will repeatedly turn to in this manuscript, and that can be modeled as a Fredholm first kind integral equation, is image deblurring. In this section, we present a one-dimensional (1D) test problem. The ease of computation and visualization in the 1D case makes the illustration of certain concepts more straightforward. We will discuss the two-dimensional image deblurring problem later.

Often in image deblurring problems, the blur is the same everywhere in the image, in which case we say that it is spatially invariant. The assumption of a spatially invariant blur simplifies (1.4) so that it has convolution form

$$b(s) = \int_0^1 a(s-s')x(s')ds'. \quad (1.7)$$

Applying the mid-point quadrature rule to (1.7), as above, with kernel function

$$a(s) = \frac{1}{\sqrt{2\pi\gamma^2}} \exp\left(-\frac{s^2}{2\gamma^2}\right), \quad \gamma > 0, \quad (1.8)$$

yields the system of linear equations

$$b_i = h \sum_{j=1}^n a_{i-j} x_j, \quad i = 1, \dots, m, \quad (1.9)$$

where $a_{i-j} = a((i-j)h)$. Compare with (1.6).

As with (1.6), equation (1.9) can be written as $\mathbf{b} = \mathbf{A}\mathbf{x}$ with $\mathbf{b} \in \mathbb{R}^m$, $\mathbf{x} \in \mathbb{R}^n$, and $\mathbf{A} \in \mathbb{R}^{m \times n}$ with entries

$$[\mathbf{A}]_{ij} = \frac{h}{\sqrt{2\pi\gamma^2}} \exp\left(-\frac{((i-j)h)^2}{2\gamma^2}\right). \quad (1.10)$$

From this model, we can generate noisy data using (1.1) with $m = n = 80$ and σ^2 chosen so that the signal-to-noise ratio (SNR), $\|\mathbf{A}\mathbf{x}\|/\sqrt{n\sigma^2}$, is 50. Both \mathbf{x} and \mathbf{b} are plotted on the left in Figure 1.2.

Example 1.4 The relationship between integration and its inverse, differentiation, also illustrates a failure of condition 3 of Definition 1.1 nicely. The Second Fundamental Theorem of Calculus states that if

$$b(s) = \int_0^s x(s')ds', \quad (1.11)$$

then $\frac{d}{ds}b(s) = x(s')$. Unknown to most is that the inverse problem of obtaining x from b defined in (1.11) is ill-posed. To see this, let's proceed as in the last example and discretize (1.11) using midpoint quadrature. We have

$$b_i = \int_0^{s_i} x(s')ds' \approx h \sum_{j=1}^i x(s'_j), \quad i = 1, \dots, n.$$

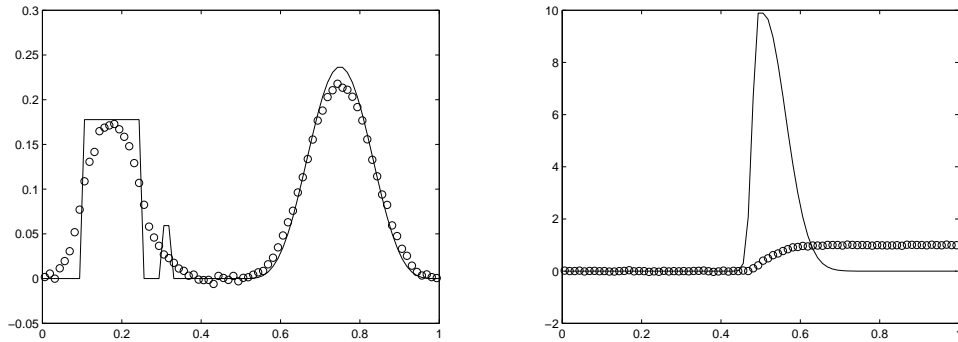


Figure 1.2. One dimensional deblurring (left) and kernel reconstruction (right) examples. The true image \mathbf{x} is given by the solid line and the blurred and noisy data \mathbf{b} is given by the circles.

Letting \mathbf{x} be the $n \times 1$ vector with j th entry $x(s'_j)$ yields $\mathbf{b} = \mathbf{A}\mathbf{x}$ with

$$\mathbf{A} = h \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 1 & 1 & \ddots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 1 & 1 & \cdots & 1 \end{bmatrix}_{n \times n}. \quad (1.12)$$

We will leave it as an exercise to show that

$$\mathbf{A}^{-1} = h^{-1} \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ -1 & 1 & \ddots & \ddots & 0 \\ 0 & -1 & 1 & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & -1 & 1 \end{bmatrix}_{n \times n}. \quad (1.13)$$

Next, let's tie (1.11) to a specific application. Note that in the previous example, the kernel a was assumed to be known. However, in any image deblurring problem involving a kernel, an estimate of the kernel is needed before the inverse problem can be solved. In radiography, the kernel is estimated by passing a step function through the imaging instrument. If a convolution model is assumed, and the step function has the form

$$\chi_t(s') = \begin{cases} 1 & s' > t, \\ 0 & s' \leq t, \end{cases}$$

with $t \in [0, 1]$, then the output has the form (ignoring for a moment the finite

computational domain):

$$\begin{aligned} b(s) &= \int_{-\infty}^{\infty} a(s-s') \chi_t(s') ds' \\ &= \int_t^{\infty} a(s-s') ds' \\ &= \int_{-\infty}^s a(s'-t) ds' \end{aligned}$$

Restricting to the computational domain $[0,1]$, we use the model

$$b(s) = \int_0^s a(s'-t) ds',$$

which is equivalent to (1.11) with $x(s') = a(s'-t)$.

As a numerical test problem, we synthetically generates a kernel, which defines \mathbf{x} , and then, as in the previous example, generated synthetic data \mathbf{b} with an SNR of 50 via (1.1) with \mathbf{A} defined by (1.12). The result is plotted in Figure 1.2. ■

1.2 The Least Squares Estimator

In the 1D examples above, the goal is to estimate the true image \mathbf{x} given data \mathbf{b} and the model matrix \mathbf{A} . First we recall that the probability density function for a general Gaussian random variable $\mathbf{w} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C})$ is given by

$$p(\mathbf{w}) = \frac{1}{\sqrt{(2\pi)^n \det(\mathbf{C})}} \exp\left(-\frac{1}{2}(\mathbf{v} - \boldsymbol{\mu})^T \mathbf{C}^{-1}(\mathbf{v} - \boldsymbol{\mu})\right). \quad (1.14)$$

Then the statistical model defined by (1.1) implies that

$$p(\mathbf{b}|\mathbf{x}, \sigma^2) = \frac{1}{\sqrt{(2\pi)^n \sigma^{2n}}} \exp\left(-\frac{\|\mathbf{Ax} - \mathbf{b}\|^2}{2\sigma^2}\right). \quad (1.15)$$

A common approach for estimating \mathbf{x} given \mathbf{b} is to maximize the likelihood function, which is defined $L(\mathbf{x}|\mathbf{b}, \sigma^2) = p(\mathbf{b}|\mathbf{x}, \sigma^2)$, with respect to \mathbf{x} . Equivalently, we can minimize the negative log-likelihood $-\ln L(\mathbf{x}|\mathbf{b})$, whose minimizer is also the minimizer of

$$\ell(\mathbf{x}) = \frac{1}{2}\|\mathbf{Ax} - \mathbf{b}\|^2, \quad (1.16)$$

and hence is also the least squares solution. The least squares solution can be expressed as the solution of the normal equations

$$\mathbf{A}^T \mathbf{Ax} = \mathbf{A}^T \mathbf{b}, \quad (1.17)$$

a fact whose proof we relegate to the exercises. We assume that \mathbf{A} has full column rank, so that $\mathbf{A}^T \mathbf{A}$ is invertible and the least squares solution is given by

$$\mathbf{x}_{\text{LS}} = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{b}. \quad (1.18)$$

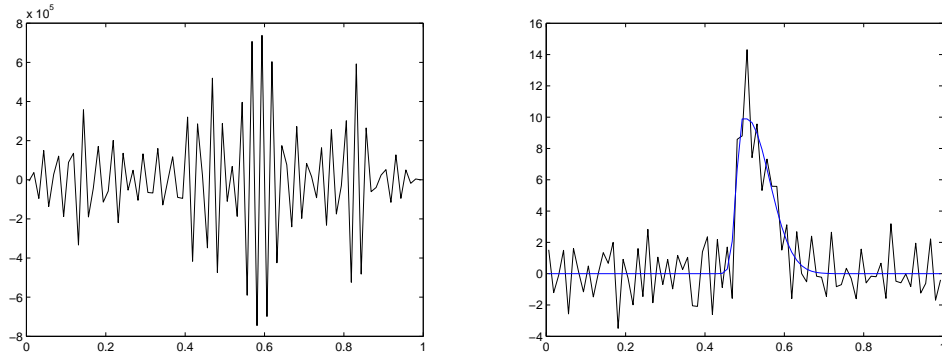


Figure 1.3. The least squares solution \mathbf{x}_{LS} for the one-dimensional deblurring example.

Thus if \mathbf{A} is invertible, then $\mathbf{x}_{\text{LS}} = \mathbf{A}^{-1}\mathbf{b}$.

The reader with any experience studying inverse problems will not be surprised that the least squares solutions for the above examples are poor. To illustrate, we plot the least squares solutions in Figure 1.3, and note that in both cases, highly oscillatory components degrade the reconstruction. In addition, for the deblurring example, the oscillatory components completely dominate, making the magnitude of the least squares solution more than 10^7 times larger than for the true image. To see that both examples fail condition 3 of Definition 1.1, in the deblurring case $\|\mathbf{Ax} - \mathbf{b}\|/\|\mathbf{Ax}\| = 0.024$ and $\|\mathbf{x} - \mathbf{x}_{\text{LS}}\|/\|\mathbf{x}\| = 5.25 \times 10^{13}$, while for the PSF reconstruction case $\|\mathbf{Ax} - \mathbf{b}\|/\|\mathbf{Ax}\| = 0.021$ and $\|\mathbf{x} - \mathbf{x}_{\text{LS}}\|/\|\mathbf{x}\| = 0.60$. Given these results, we say that the deblurring example is severely ill-posed, while the PSF reconstruction problem is only mildly ill-posed.

From a statistical viewpoint, we note that (1.1) implies $\mathbf{b} \sim \mathcal{N}(\mathbf{Ax}, \sigma^2\mathbf{I})$. Moreover, for a general $n \times 1$ normal random vector $\mathbf{v} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C})$ if $\mathbf{w} = \mathbf{Bv}$, where \mathbf{B} is an $m \times n$ matrix, $\mathbf{w} \sim \mathcal{N}(\mathbf{B}\boldsymbol{\mu}, \mathbf{BCB}^T)$. Thus from (1.18) we have

$$\mathbf{x}_{\text{LS}} \sim \mathcal{N}(\mathbf{x}, \sigma^2(\mathbf{A}^T\mathbf{A})^{-1}), \quad (1.19)$$

and hence, while the variance of each pixel of the data \mathbf{b} is σ^2 , for the i^{th} component of \mathbf{x}_{LS} the variance is $[\sigma^2(\mathbf{A}^T\mathbf{A})^{-1}]_{ii}$, which will be large for large i in typical examples in inverse problems. As a result, the least squares solution will typically be far from the true image \mathbf{x} , which is again supported by the plots in Figure 1.3.

1.3 The Singular Value Decomposition and Ill-Conditioning

In order to understand why the least squares solutions are so poor, we turn to the singular value decomposition (SVD) of the design matrix:

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T, \quad (1.20)$$

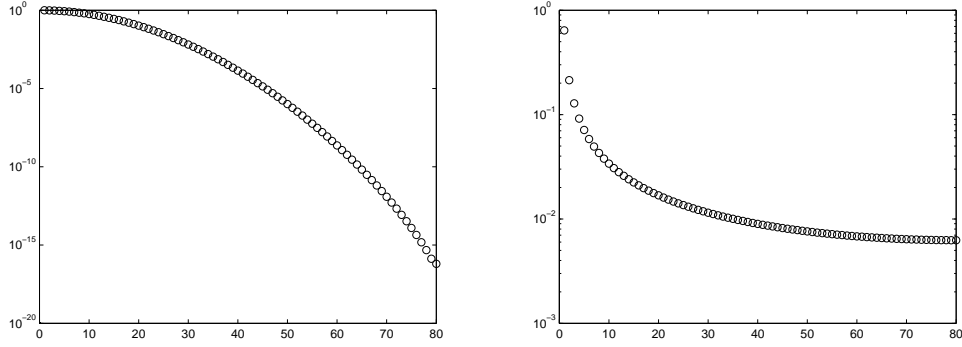


Figure 1.4. A plot of singular values of \mathbf{A} for the one-dimensional deblurring example (left) and the PSF reconstruction example (right). The y-axis is on the log scale.

where \mathbf{U} is an $m \times m$ matrix with columns given by the orthonormal eigenvectors of $\mathbf{A}\mathbf{A}^T$; \mathbf{V} is an $n \times n$ matrix with columns given by the orthonormal eigenvectors of $\mathbf{A}^T\mathbf{A}$; and $\mathbf{\Sigma}$ is an $m \times n$ diagonal matrix with diagonal entries $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n \geq 0$, which are called the singular values of \mathbf{A} and are the square roots of the eigenvalues of $\mathbf{A}^T\mathbf{A}$. The columns of $\mathbf{U} = [\mathbf{u}_1, \dots, \mathbf{u}_m]$ and $\mathbf{V} = [\mathbf{v}_1, \dots, \mathbf{v}_n]$ are called the left and right singular vectors of \mathbf{A} , respectively, and are orthonormal so that $\mathbf{U}^T\mathbf{U} = \mathbf{I}_m$ and $\mathbf{V}^T\mathbf{V} = \mathbf{I}_n$.

Although \mathbf{A} may not have an inverse, its pseudo-inverse always exists and is defined

$$\mathbf{A}^\dagger = \mathbf{V}\mathbf{\Sigma}^\dagger\mathbf{U}^T, \quad (1.21)$$

where $\mathbf{\Sigma}^\dagger$ is the $n \times m$ matrix with diagonal values $\sigma_1^{-1} \geq \sigma_2^{-1} \geq \dots \geq \sigma_r^{-1} > 0$, where r is the smallest positive singular value. Detail on the SVD and the pseudo-inverse can be found in [9]. For discretized first kind Fredholm integral equations (called discrete inverse problems in [13]), the singular values decay continuously to 0 as i increases, with a large number clustered near 0. To illustrate, we plot the singular values of \mathbf{A} in both cases in Figure 1.4. Note that the singular values drop to zero much more rapidly in the deblurring example, which partially explains the much worse results for the least squares solutions presented in Figure 1.3. The lower bound of the singular values in the simple integration (kernel reconstruction) example isn't much below the grid size h .

We can also say something about typical behavior of the left and right singular vectors, \mathbf{u}_i and \mathbf{v}_i , respectively, for discretized first kind Fredholm integral equations; namely, they behave like the Fourier basis in the sense that as i increases, \mathbf{u}_i and \mathbf{v}_i become more oscillatory. This fact is demonstrated for several examples in [13]. We leave its verification for the 1D deblurring example considered above to the exercises.

1.3.1 Statistical Properties of the Least Squares Estimator

We now return to the least squares solution and view it in light of the above discussion. Given our assumptions regarding \mathbf{A} , it can be shown (see Exercise 4) that

$$\mathbf{x}_{\text{LS}} = \sum_{i=1}^n \frac{\mathbf{u}_i^T \mathbf{b}}{\sigma_i} \mathbf{v}_i \quad (1.22)$$

$$= \mathbf{x} + \sum_{i=1}^n \frac{\mathbf{u}_i^T \boldsymbol{\epsilon}}{\sigma_i} \mathbf{v}_i. \quad (1.23)$$

From (1.23) and the above discussion, we see that due to the spectral properties of a typical noise realization $\boldsymbol{\epsilon}$, $(\mathbf{v}_i^T \boldsymbol{\epsilon})/\sigma_i$ will be large for large i , which serves to amplify the more oscillatory components in the second term in (1.23). This coincides with what we observe in the least squares solutions in Figure 1.3, where high frequency components dominate.

A more detailed analysis of the interplay between the noise $\boldsymbol{\epsilon}$, the data \mathbf{b} , and the spectral properties of \mathbf{A} , through its SVD, is possible using the discrete Picard condition; the interested reader should see [13] for details, as well as the exercises for a Picard analysis of the deblurring example considered in this chapter.

We can also use the SVD to shed further light on the distributional statement (1.19) for \mathbf{x}_{LS} . Replacing \mathbf{A} with its the SVD in (1.19) yields

$$\mathbf{x}_{\text{LS}} \sim \mathcal{N}(\mathbf{x}, \sigma^2 \mathbf{V} \boldsymbol{\Sigma}^{-2} \mathbf{V}^T), \quad (1.24)$$

where $\boldsymbol{\Sigma}^{-2} = (\boldsymbol{\Sigma}^T \boldsymbol{\Sigma})^{-1}$.

From (1.24), we can see that $E[\mathbf{x}_{\text{LS}}] = \mathbf{x}$, and hence the least squares estimator is *unbiased*. However, in the orthonormal basis defined by the columns of \mathbf{V} (the right singular vectors), (1.24) can be restated in a component-wise fashion as follows:

$$\mathbf{v}_i^T \mathbf{x}_{\text{LS}} \sim \mathcal{N}(\mathbf{v}_i^T \mathbf{x}, \sigma^2 / \sigma_i^2), \quad i = 1, \dots, n, \quad (1.25)$$

which directly shows that for $0 < \sigma_i^2 \ll \sigma^2$ (i large), one can expect high variability in the corresponding oscillatory mode \mathbf{v}_i . Thus although the least squares estimator is unbiased, its *total variance*, which is given by

$$\text{tr}(\sigma^2 \mathbf{V} \boldsymbol{\Sigma}^{-2} \mathbf{V}^T) = \sigma^2 \sum_{i=1}^n 1/\sigma_i^2, \quad (1.26)$$

where ‘tr’ denotes the matrix trace, will be extremely large, which is undesirable.

Example 1.5 In order to make the above concepts more concrete, we consider a two dimensional example. First we define the matrix \mathbf{A} via its SVD: let $\mathbf{v}_1 = [1/\sqrt{2}, 1/\sqrt{2}]^T$, $\mathbf{v}_2 = [-1/\sqrt{2}, 1/\sqrt{2}]^T$, and

$$\mathbf{A} = \mathbf{v}_1 \mathbf{v}_1^T + 10^{-2} \mathbf{v}_2 \mathbf{v}_2^T$$

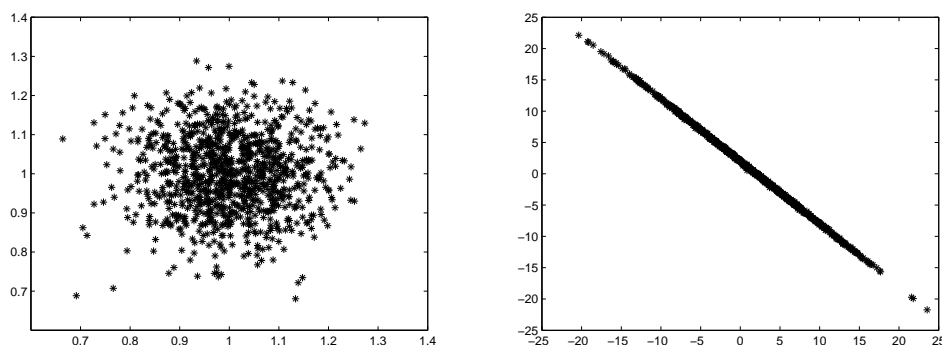


Figure 1.5. On the left are 1000 realizations from the data model $\mathbf{b} = \mathbf{A}\mathbf{x} + \boldsymbol{\epsilon}$, and on the right are plots of the corresponding 1000 least squares solutions $\mathbf{A}^{-1}\mathbf{b}$. Both the true solution \mathbf{x} and the noise-free data $\mathbf{A}\mathbf{x}$ are $[1, 1]^T$.

Note that we have used the summation form of the SVD (see Exercise 1.3). Hence \mathbf{v}_1 and \mathbf{v}_2 are both the left and right singular vectors and the singular values are $\sigma_1 = 1$ and $\sigma_2 = 10^{-2}$. Furthermore, as in the above cases, the smaller singular value corresponds to the ‘higher frequency’ vector.

Now suppose $\mathbf{x} = [1, 1]^T$, then $\mathbf{b} = \mathbf{A}\mathbf{x} = [1, 1]^T$ and $\mathbf{A}^{-1}\mathbf{b} = [1, 1]^T$. However, if we add a small amount of noise to \mathbf{b} using (1.1) with $\boldsymbol{\epsilon} = [0.026, 0.075]^T$ (a truncated realization of an iid Gaussian distribution with variance $\sigma^2 = 0.01$) then $\mathbf{A}^{-1}\mathbf{b} = [-1.400, 3.501]^T$, which is far from $[1, 1]^T$.

Let us use the SVD discussion above to explore this problem more deeply. First, we plot 1000 realizations from the statistical model $\mathbf{b} = \mathbf{A}\mathbf{x} + \boldsymbol{\epsilon}$ with $\sigma^2 = 0.01$ on the left in Figure 1.5. Note that the \mathbf{b} samples have a relatively small variance centered around $[1, 1]^T$. Next, on the right in Figure 1.5, we plot \mathbf{x}_{LS} for each realization of the data. Note that the noise free solution $[1, 1]^T$ is contained within the data cloud, but that the variance is high in the direction of \mathbf{v}_2 , while in the direction of \mathbf{v}_1 it is relatively small. This coincides with (1.25), which says that the variance of \mathbf{x}_{LS} in the direction \mathbf{v}_1 is $\sigma^2/\sigma_1^2 = 0.01$, while in the direction \mathbf{v}_2 it is $\sigma^2/\sigma_2^2 = 100$. We computationally verified this for our experiment by computing the sample variance of $\mathbf{v}_1^T \mathbf{x}_{\text{LS}}$ and $\mathbf{v}_2^T \mathbf{x}_{\text{LS}}$ for all least squares solutions, which were 0.01 and 99.73, respectively. Additionally, note that

$$\mathbf{A} = \begin{bmatrix} 0.505 & 0.495 \\ 0.495 & 0.505 \end{bmatrix},$$

which, though non-singular, has columns that are ‘nearly’ linearly dependent, both well-approximating the singular vector \mathbf{v}_1 . This agrees with our observations above since variance values for $\mathbf{v}_1^T \mathbf{x}_{\text{LS}}$ and $\mathbf{v}_2^T \mathbf{x}_{\text{LS}}$ of 0.01 and 100, respectively, suggest that the least squares solution is well-resolved in the direction of \mathbf{v}_1 and poorly resolved in the direction of \mathbf{v}_2 . ■

Exercises

1.1. *This simple linear regression problem was written in the fall of 2011 by former University of Montana Math PhD students (and now PhD's) John Hossler, Marylesa Howard, and Jordan Purdy:* In baseball two commonly collected statistics for pitchers are batting average against (AVG) and walks plus hits per inning pitched (WHIP). Suppose we believe that a linear relationship exists between AVG and WHIP, and in particular, we believe we can predict a pitcher's WHIP from their AVG. AVG and WHIP data for 30 Major League Baseball (MLB) pitchers from the 2011 regular season (through September 2) are provided in `BaseballData.m`. Use this data to answer the following questions. You may find it easiest to modify `SimpleLinearModel.m` used for Example 1.2.

- Plot the batting average (AVG) against corresponding walks plus hits per inning pitched (WHIP) such that AVG predicts WHIP (AVG on x-axis, WHIP on y-axis).
- Write out by hand the first four rows of the design matrix. Construct the entire design matrix in MATLAB. Include an intercept in your model.
- Compute the least squares estimate. Note that \mathbf{x}_{LS} is a 2×1 vector.
- Using the model created in part (c), plot the model on the data plot from part (a). This model predicts a pitcher's WHIP given his batting average against.
- For each observed data point, the residual is that observed value (WHIP) minus the corresponding predicted value (predicted WHIP) from the model. Calculate the thirty residuals and plot them against their corresponding AVG value. On the same graph, plot the line $y = 0$. Comment on whether a pattern is distinguishable or whether there is random scatter in the residual plot. A pattern in the residuals may suggest a different model or a linear model with different error structure is more appropriate, for this data set. While random scatter does not verify our choice of this linear model is correct, it does suggest this model may be useful for analysis.

1.2. The *midpoint quadrature rule* for a function f defined on $[a, b]$ is defined by

$$\int_a^b f(x)dx = (b-a)f\left(\frac{a+b}{2}\right) + \frac{f''(\eta)}{24}(b-a)^3, \quad (1.27)$$

where $a \leq \eta \leq b$.

- Write your own MATLAB code applying midpoint quadrature with $n = 100$ grid points to approximate $\int_0^{2\pi} \cos x \, dx = 1$.
- Determine an upper bound for the quadrature error in part (a) using (1.27) (n times) and then verify that the inequality holds.

- c. Modify `Deblur1d.m` so that it implements midpoint quadrature on the convolution model (1.7) with kernel

$$a(s) = \begin{cases} 100s + 10, & -\frac{1}{10} \leq s \leq 0, \\ -100s + 10, & 0 \leq s \leq \frac{1}{10}, \\ 0, & \text{otherwise.} \end{cases}$$

to obtain $\mathbf{b} = \mathbf{A}\mathbf{x}$. Plot a on $[-1, 1]$. Is the deblurring problem ill-posed with this kernel? Support your answer.

1.3. *More on the simple integration/kernel reconstruction inverse problem.*

- a. Show that \mathbf{A} defined by (1.12) has inverse \mathbf{A}^{-1} defined by (1.13). Use induction on n .
- b. Show that \mathbf{A}^{-1} corresponds to the discretization of $\frac{d}{ds}$ on the grid $\{s'_j\}_{j=1}^n$, where recall that $s'_j = (j - \frac{1}{2})/n$, with a zero Dirichlet boundary condition on the left (i.e., $x(s'_0) = 0$) and a zero Neumann boundary condition on the right (i.e., $x(s'_{n+1}) = x(s'_n)$). Use the forward difference approximation of the derivative:

$$\frac{d}{ds}x(s'_j) \approx \frac{x(s'_j) - x(s'_{j-1})}{h}.$$

- c. Replace \mathbf{A} by \mathbf{A}^{-1} in `PSFrecon.m`. How do the results change? Is $\mathbf{b} = \mathbf{A}^{-1}\mathbf{x}$ an ill-posed problem, i.e. does it fail any of the three conditions of Definition 1.1?

1.4. *The Singular Value Decomposition.* Let \mathbf{A} be $m \times n$, with $m \geq n$, and suppose it has singular value decomposition $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$. Let \mathbf{u}_i be the i th column of \mathbf{U} , \mathbf{v}_i be the i column of \mathbf{V} , and σ_i the i diagonal element of $\mathbf{\Sigma}$.

- a. If the rank of \mathbf{A} is $r \leq n$, show that

$$\mathbf{A}\mathbf{v}_i = \begin{cases} \sigma_i \mathbf{u}_i, & i = 1, \dots, r \\ \mathbf{0}, & i = r + 1, \dots, n, \end{cases} \quad \mathbf{A}^T \mathbf{u}_i = \begin{cases} \sigma_i \mathbf{v}_i, & i = 1, \dots, r \\ \mathbf{0}, & i = r + 1, \dots, m. \end{cases}$$

- b. Show that (1.20) can be written $\mathbf{A} = \sum_{i=1}^n \mathbf{u}_i \sigma_i \mathbf{v}_i^T$ and write down the equivalent expression for \mathbf{A}^\dagger defined in (1.21).
- c. Substitute (1.20) into (1.18) to prove (1.22) and hence that $\mathbf{x}_{\text{LS}} = \mathbf{A}^\dagger \mathbf{b}$.

1.5. *The Singular Value Decomposition.* Define $\mathbf{A} = \begin{bmatrix} 1 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}$.

- a. Compute the singular value decomposition of \mathbf{A} by hand: $\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^T$, where $\mathbf{U} \in \mathbb{R}^{3 \times 3}$ is orthogonal, $\mathbf{S} \in \mathbb{R}^{3 \times 2}$ is diagonal, and $\mathbf{V} \in \mathbb{R}^{2 \times 2}$ is orthogonal.
- b. Using the columns of \mathbf{U} and \mathbf{V} as basis elements, write down bases for the four subspaces: the column space $C(\mathbf{A})$, the row space $C(\mathbf{A}^T)$, the null space $N(\mathbf{A})$, and the left null space $N(\mathbf{A}^T)$.

- c. Using the SVD you computed in (a), compute the pseudo-inverse \mathbf{A}^\dagger of \mathbf{A} , and then use it to compute the least squares solution $\mathbf{x}_{LS} = \mathbf{A}^\dagger \mathbf{b}$ of

$$\begin{bmatrix} 1 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}.$$

1. Compare the solution in (c) with the solution of the normal equations, $\mathbf{A}^T \mathbf{A} \mathbf{x} = \mathbf{A}^T \mathbf{b}$. The two solutions should agree.

1.6. *The discrete Picard condition.* For parts (a)-(d), use `Deblur1d.m`.

- Create plots verifying that the singular vectors of the design matrix \mathbf{A} become more oscillatory as i increases. Plot, for example, right singular vectors 1-8.
- A Picard plot for a discretized inverse problem is a plot of the values of σ_i , $|\mathbf{u}_i^T \mathbf{b}|$, and $|\mathbf{u}_i^T \mathbf{b}|/\sigma_i$. Picard plots are used extensively in [13] for analyzing discrete inverse problems. For the 1D deblurring example, create the Picard plot with a legend, first using the noise-free data and then using noisy data. Verify in both cases the *discrete Picard condition*: Ignoring the part of the Picard plot where $|\mathbf{u}_i^T \mathbf{b}|$ levels off due either to numerical round-off (in the noise-free case) or to the presence of noise in \mathbf{b} , the discrete Picard condition is satisfied if the remaining values of $|\mathbf{u}_i^T \mathbf{b}|$, on average, decay faster than σ_i , i.e. $|\mathbf{u}_i^T \mathbf{b}|/\sigma_i$ is decreasing. Motivate the discrete Picard condition by appealing to (1.22).
- Plot the variance values in (1.25). What do they tell you about the statistical properties of the least squares solution.
- Show that even in the absence of noise, the least squares solution for the deblurring example remains poor. This is due to the fact that the deblurring example is so ill-conditioned that even round-off errors, which are on the order of machine precision (approximately 10^{-16}), are amplified.
- Repeat a-c using `PSFrecon.m`.

1.7. *Multivariate Gaussian distribution.*

- Suppose $\mathbf{v} = (v_1, v_2, \dots, v_n)$ is an independent and identically distributed standard Normal random vector, i.e. $v_i \sim \mathcal{N}(0, 1)$ for $i = 1, \dots, n$. Given $p(v_i) = 1/\sqrt{2\pi} \exp(-v_i^2/2)$, show that

$$p_{\mathbf{v}}(\mathbf{v}) = \frac{1}{\sqrt{(2\pi)^n}} \exp\left(-\frac{1}{2}\|\mathbf{v}\|^2\right)$$

- Let $\mathbf{w} = \mathcal{N}(\boldsymbol{\mu}, \mathbf{C})$. Note that $\mathbf{w} = \boldsymbol{\mu} + \mathbf{C}^{1/2} \mathbf{v}$, where \mathbf{v} is as in (a). Then the inverse transformation yields $\mathbf{v} = \mathbf{C}^{-1/2}(\mathbf{w} - \boldsymbol{\mu})$ and

$$p(\mathbf{w}) = p_{\mathbf{v}}(\mathbf{C}^{-1/2}(\mathbf{w} - \boldsymbol{\mu})) \cdot \det(\mathbf{C}^{-1/2}).$$

Use this to derive the multivariate Gaussian probability density function (1.14).

- c. Use (b) to deriving the probability density for $p(\mathbf{b}|\mathbf{x}, \sigma^2)$ in (1.15).

1.8. *Deriving the least squares normal equations.*

- a. A function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is convex if its Hessian $\nabla^2 f(\mathbf{x})$ is positive semi-definite for all \mathbf{x} and is strictly convex if $\nabla^2 f(\mathbf{x})$ is positive definite for all \mathbf{x} . Moreover, the set of minimizers of a convex function f is the set on which the gradient of f is zero, i.e., those vectors \mathbf{x} satisfying $\nabla f(\mathbf{x}) = \mathbf{0}$, and this set has a single member (and hence f a unique minimizer) if f is strictly convex. Use these facts to show that the minimizers of $\ell(\mathbf{x}) = \frac{1}{2} \|\mathbf{Ax} - \mathbf{b}\|^2$, with respect to \mathbf{x} , are the solutions of (1.17) and derive conditions on \mathbf{A} that guarantee that $\ell(\mathbf{x})$ has a unique minimizer.
- b. Show that the projection of \mathbf{b} onto the column space of \mathbf{A} , which we assume has full column rank, has the form \mathbf{Ax}_{LS} , where \mathbf{x}_{LS} is the least squares solution. Note that the projection formula can be found in an elementary linear algebra text.

1.9. *Sampling from Gaussian probability densities.*

- a. Let \mathbf{v} be a random n -vector with mean $\boldsymbol{\mu} = E[\mathbf{v}]$ (here E is the expected value function) and covariance

$$\mathbf{C} = \text{cov}(\mathbf{v}) = E[(\mathbf{v} - \boldsymbol{\mu})(\mathbf{v} - \boldsymbol{\mu})^T].$$

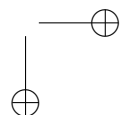
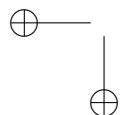
Use the linearity of the expected value function to show that if \mathbf{B} is an $m \times n$ matrix, the mean and covariance of $\mathbf{w} = \mathbf{Bv}$ are $\mathbf{B}\boldsymbol{\mu}$ and \mathbf{BCB}^T , respectively. Thus if $\mathbf{v} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C})$, then $\mathbf{w} = \mathbf{Bv}$ is also normally distributed with distribution $\mathbf{w} \sim \mathcal{N}(\mathbf{B}\boldsymbol{\mu}, \mathbf{BCB}^T)$.

- b. Show, using part (a), that if \mathbf{R} is a square root matrix for \mathbf{C} , i.e. $\mathbf{C} = \mathbf{R}^T \mathbf{R}$, and if $\mathbf{v} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ then $\mathbf{w} = \boldsymbol{\mu} + \mathbf{R}^T \mathbf{v}$ has distribution $\mathbf{w} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C})$.
- c. Use MATLAB and part (b) to compute and plot 1000 samples from the random vector $\mathbf{w} \sim \mathcal{N}\left(\begin{bmatrix} 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}\right)$.
- d. If $\mathbf{w} = (w_1, \dots, w_k)$ is a random vector such that $w_i \sim \mathcal{N}(0, 1)$ for $i = 1, \dots, k$, then $Q = \sum_{i=1}^k w_i^2$ is a $\chi^2(k)$ random variable. Verify that, approximatively, a correct amount of the sampled points are located inside the confidence regions given by the 95% and 99% limits of the $\chi^2(2)$ distribution, computed using the `chi2inv` function.

1.10. *Sampling the least squares solution.*

- a. Use the results in Exercise 9 part (a) to prove (1.19). **Hint:** first show that $\mathbf{x}_{\text{LS}} = \mathbf{x} + (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \boldsymbol{\epsilon}$, where $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$.
- b. In the m-file `TwoVarTest.m`, which was used to generate Figure 1.5, samples of \mathbf{x}_{LS} are computed by first sampling $\mathbf{b} \sim \mathcal{N}(\mathbf{Ax}, \sigma^2 \mathbf{I})$ and then computing the corresponding least squares solution \mathbf{x}_{LS} via (1.18). Add a line of code that also samples \mathbf{x}_{LS} using the approach in part

- (a), then plot the two collections of samples together in different color to verify that the sample distributions look roughly the same. Also, compare their sample mean and covariance matrices using MATLAB's `mean` and `cov` functions.
- c. Create normalized histograms (using the `hist` function) from the samples of $\mathbf{v}_1^T \mathbf{x}_{LS}$ and $\mathbf{v}_2^T \mathbf{x}_{LS}$ computed in `TwoVarTest.m` and then graph the resulting sample probability densities together with the analytic true normal densities given by (1.25).



Chapter 2

Regularization by Filtering

In the last chapter, we introduced two examples, both obtained by numerically discretizing an integral equation, that characterize ill-posed inverse problems. We showed that for these problems the standard least squares solution is poor and, through an SVD analysis, why this is the case.

In this chapter, we present several methods which modify the least squares solution in such a way that the new solutions provide a significant improvement. Specifically, these methods filter out the singular vectors with low magnitude in the noise-free signal \mathbf{Ax} (and therefore small signal-to-noise ratio in the data \mathbf{b}) but which lead to large variance in the least squares solution. These techniques are known as *regularization methods* and we interpret them as a ‘filtered’ SVD, or spectral filtering method.

The filters that we introduce are dependent upon a single unknown parameter, known as the *regularization parameter*. Hence the practical usefulness of the regularization methods depends upon there being effective techniques for estimating the regularization parameter. Thus we also present several *regularization parameter choice methods*.

2.1 Spectral Filtering Methods

To motivate our discussion, we return to Example 1.5, where we considered the problem of estimating $\mathbf{x} = [x_1, x_2]^T$ from data $\mathbf{b} = [b_1, b_2]^T$ generated by the model

$$\begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} 0.505 & 0.495 \\ 0.495 & 0.505 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \end{bmatrix},$$

where $\epsilon_1, \epsilon_2 \stackrel{iid}{\sim} \mathcal{N}(0, 0.01)$.

Recall our example: suppose $\mathbf{x} = [1, 1]^T$, then in the noise-free case, $\mathbf{b} = \mathbf{Ax} = [1, 1]^T$ and $\mathbf{A}^{-1}\mathbf{b} = [1, 1]^T$, while if $\mathbf{b} = \mathbf{Ax} + \boldsymbol{\epsilon} = [1.026, 1.075]^T$, then $\mathbf{A}^{-1}\mathbf{b} = [-1.400, 3.501]^T$. Thus after adding a small amount of noise, the least squares solution is far from the solution $[1, 1]^T$ in the noise-free case. From our

discussion in the previous chapter, this is due to high variance in the solution in the direction of the singular vector $\mathbf{v}_2 = [-1/\sqrt{2}, 1/\sqrt{2}]$.

Given this, a natural idea is to remove (or filter) the singular vector \mathbf{v}_2 from the model, so that instead \mathbf{A} is replaced by

$$\mathbf{A}_{\text{filt}} = \sigma_1 \mathbf{v}_1 \mathbf{v}_1^T = \begin{bmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{bmatrix}.$$

The filtered least squares solution for the data $\mathbf{b} = [1.026, 1.075]^T$ is then given by

$$\mathbf{x}_{\text{filt}} = \mathbf{A}_{\text{filt}}^\dagger \mathbf{b} = \sigma_1^{-1} (\mathbf{v}_1^T \mathbf{b}) \mathbf{v}_1 = \begin{bmatrix} 1.0505 \\ 1.0505 \end{bmatrix},$$

where ‘ \dagger ’ denotes pseudo-inverse [9], which is much nearer to the noise free solution $[1, 1]^T$ than $\mathbf{A}^{-1} \mathbf{b}$.

2.1.1 The Truncated Singular Value Decomposition

The approach of removing the singular vectors from the model that lead to large variance in the least squares solution, as we did in the previous example, can be generalized to higher dimensional problems. For the problems of interest to us, if

$$\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T = \sum_{i=1}^n \mathbf{u}_i \sigma_i \mathbf{v}_i^T, \quad (2.1)$$

the singular vectors that lead to high variance in the least squares solution correspond to the larger values of i . Removing the singular vectors for $i \geq k$ from the model amounts to replacing $\mathbf{\Sigma}$ in (2.1) by the $m \times n$ diagonal matrix $\mathbf{\Sigma}_k$ with diagonal entries $(\sigma_1, \sigma_2, \dots, \sigma_k, 0, \dots, 0)$, yielding

$$\mathbf{U} \mathbf{\Sigma}_k \mathbf{V}^T = \sum_{i=1}^k \mathbf{u}_i \sigma_i \mathbf{v}_i^T.$$

This is known as the truncated singular value decomposition of \mathbf{A} and it leads to the *TSVD regularized solution*

$$\mathbf{x}_k = \mathbf{V} \mathbf{\Sigma}_k^\dagger \mathbf{U}^T \mathbf{b} = \sum_{i=1}^k \frac{\mathbf{u}_i^T \mathbf{b}}{\sigma_i} \mathbf{v}_i, \quad (2.2)$$

where ‘ \dagger ’ denotes pseudo-inverse. Compare (2.2) with the analogous expression for the least squares solution (1.22).

The TSVD appears in many of the standard texts on inverse problems; see e.g., [12, 13, 14, 16, 27], and in the statistical literature, it is known as *principal component regression* [20]. The parameter k is known as the *regularization parameter*, and the choice of its value is a nontrivial task that we address in Section 2.2. Nonetheless, to illustrate the effectiveness of the TSVD, we plot \mathbf{x}_k for $k = 24$ in the

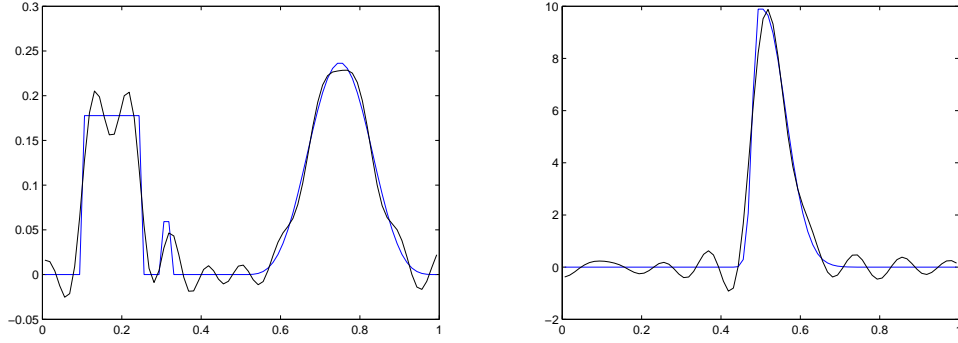


Figure 2.1. A plot of the TSVD reconstruction \mathbf{x}_k for $k = 24$ in the deblurring case (left) and for $k = 20$ in the kernel reconstruction case (right) together with the true image.

deblurring case and $k = 20$ in the kernel reconstruction case in Figure 2.1, which yields a good visual reconstruction of \mathbf{x} .

The TSVD is an example of the general class of *spectral filtering methods*, which have the filtered SVD form

$$\mathbf{x}_\nu = \mathbf{V}\Phi_\nu\Sigma^\dagger\mathbf{U}^T\mathbf{b} \quad (2.3)$$

where Φ_ν is an $n \times n$ diagonal matrix with diagonal entries $[\Phi_\nu]_{ii} = \phi_i^{(\nu)}$ for $i = 1, \dots, n$. The $\phi_i^{(\nu)}$'s are known as *filter factors*, are parameterized by the variable ν , and are chosen so that $\phi_i^{(\nu)} \approx 1$ for large singular values and $\phi_i^{(\nu)} \approx 0$ for small singular values.

For the TSVD, $\nu = k$ in (2.3) and

$$\phi_i^{(k)} = \begin{cases} 1 & i = 1, \dots, k \\ 0 & i = k + 1, \dots, n. \end{cases}$$

We define $\Phi_k = \text{diag}(\phi_1^{(k)}, \dots, \phi_n^{(k)})$, then (2.3) takes the form

$$\mathbf{x}_k = \mathbf{V}\Phi_k\Sigma^\dagger\mathbf{U}^T\mathbf{b}, \quad (2.4)$$

which is equivalent to (2.2).

2.1.2 Tikhonov Regularization

Tikhonov regularization is probably the most commonly used form of regularization, and it appears in every text on the subject of inverse problems. These include [1, 5, 7, 12, 13, 14, 16, 27], as well as many others. The Tikhonov regularized solution is defined by

$$\mathbf{x}_\alpha = \arg \min_{\mathbf{x}} \left\{ \frac{1}{2} \|\mathbf{Ax} - \mathbf{b}\|^2 + \frac{\alpha}{2} \|\mathbf{x}\|^2 \right\}, \quad (2.5)$$

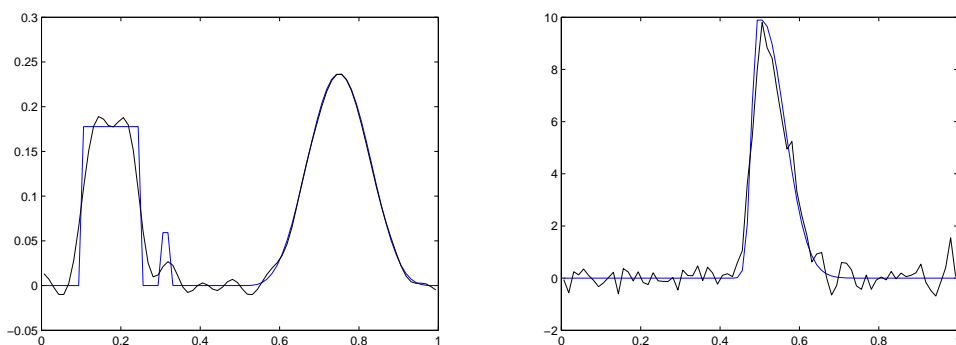


Figure 2.2. A plot of the Tikhonov reconstruction \mathbf{x}_α for $\alpha = 0.005$ in the deblurring case (left) and $\alpha = 0.0002$ in the kernel reconstruction case (right), together with the true image.

which can be equivalently expressed as the solution of the pseudo-normal equations for (2.5):

$$(\mathbf{A}^T \mathbf{A} + \alpha \mathbf{I}) \mathbf{x} = \mathbf{A}^T \mathbf{b}. \quad (2.6)$$

Comparing (2.6) with the least squares normal equations (1.17), we see that the addition of the penalty term $\frac{\alpha}{2} \|\mathbf{x}\|^2$ in (2.5) has the effect of uniformly increasing the eigenvalues of the coefficient matrix; namely from σ_i^2 for $\mathbf{A}^T \mathbf{A}$ in (1.17) to $\sigma_i^2 + \alpha$ for $\mathbf{A}^T \mathbf{A} + \alpha \mathbf{I}$ in (2.6). This makes the computation of \mathbf{x}_α more stable than the computation of the least squares solution. Statisticians might recognize (2.5), (2.6) as *ridge regression* [19].

Tikhonov regularization can also be written as a spectral filtering method with filter factors

$$\phi_i^{(\alpha)} = \sigma_i^2 / (\sigma_i^2 + \alpha).$$

Hence, \mathbf{x}_α can be written in the form (2.3) with $\nu = \alpha$ and

$$\Phi_\alpha = \text{diag} \left(\frac{\sigma_1^2}{\sigma_1^2 + \alpha}, \dots, \frac{\sigma_n^2}{\sigma_n^2 + \alpha} \right). \quad (2.7)$$

The proof of the equivalence of (2.5), (2.6), and (2.3) with $\nu = \alpha$ and (2.7) is left to the exercises.

As was the case for the TSVD, we choose a value of the regularization parameter α that yields a good visual reconstruction of \mathbf{x} . For $\alpha = 0.005$ in the deblurring case and $\alpha = 0.0002$ in the kernel reconstruction case, the corresponding Tikhonov regularized solution \mathbf{x}_α is plotted in Figure 2.2. Less subjective methods for choosing α are presented in Section 2.2.

2.1.3 Iterative Regularization

For inverse problems, iterative methods applied to the problem of minimizing $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2$ often exhibit *semi-convergence*; that is, if \mathbf{x}_k is the k th iteration of the algorithm

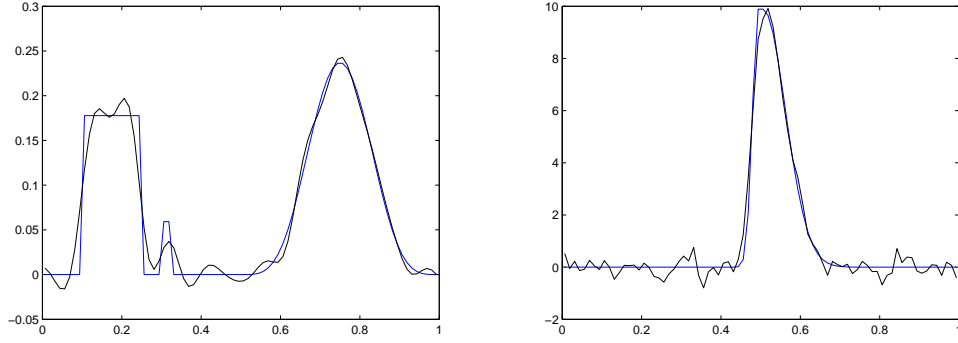


Figure 2.3. The Landweber reconstruction \mathbf{x}_k is plotted, together with the true image, on the left in the deblurring case with $k = 300$, and on the right in the kernel reconstruction case with $k = 3000$.

– not to be confused with \mathbf{x}_k defined by the TSVD – in early iterations $\|\mathbf{x}_k - \mathbf{x}\|^2$ decreases, but then eventually begins to increase as $\mathbf{x}_k \rightarrow \mathbf{x}_{\text{LS}} = \mathbf{A}^{-1}\mathbf{b}$, which you'll recall is noise corrupted. The early stopping of such iterations is known as *iterative regularization*, where the iteration count k is the regularization parameter.

To illustrate, we consider the simplest iterative regularization method, which is known as the Landweber iteration [5, 7]:

$$\mathbf{x}_k = \mathbf{x}_{k-1} - \tau \mathbf{A}^T (\mathbf{A} \mathbf{x}_{k-1} - \mathbf{b}), \quad (2.8)$$

where $0 < \tau < 1/\sigma_1$ to guarantee convergence.

If $\mathbf{x}_0 = \mathbf{0}$, it can be shown that (2.8) can be written in the form (2.3) with filter factors

$$\phi_i^{(k)} = 1 - (1 - \tau \sigma_i^2)^k \quad (2.9)$$

for $i = 1, \dots, n$. Thus \mathbf{x}_k can be written in the form of (2.3):

$$\mathbf{x}_k = \mathbf{V} \Phi_k \Sigma^\dagger \mathbf{U}^T \mathbf{b}, \quad (2.10)$$

where $\Phi_k = \text{diag}(\phi_1^{(k)}, \dots, \phi_n^{(k)})$. Given our assumption regarding the value of τ , we see that $\phi_i \rightarrow 1$ as $i \rightarrow \infty$. Hence the filtering becomes less pronounced as the iteration proceeds and eventually converges to \mathbf{x}_{LS} . Moreover, the closer τ is to $1/\sigma_1$ the faster will be the convergence.

In Figure 2.3, we plot the Landweber solution for the deblurring example with $\tau = 0.9$ after 300 iterations. The choice of the stopping iteration k corresponds to the regularization parameter in this case. Objective methods for choosing k are discussed in Section 2.2.

Other iterative methods applied to the problem of minimizing $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2$ can be used in the same fashion, i.e., early stopping of their iterations can be used as a regularization method. Some even have the filtered SVD form (2.3), such as the steepest descent method (same as (2.8) but with $\tau = \tau_k$ iteration dependent), and

conjugate gradient iteration. However, even for such relatively simple algorithms, the corresponding SVD analysis quickly becomes complicated [21].

2.1.4 Statistical Properties of Filtered Solutions

Just as in the least squares case, we can make a distributional statement about estimators obtained from filtered solutions. A general filtered solution has the form $\mathbf{x}_\nu = \mathbf{V}\Phi_\nu \Sigma^\dagger \mathbf{U}^T \mathbf{b}$, where $\nu = \alpha$ in the case of Tikhonov regularization and $\nu = k$ in the case of TSVD and truncated Landweber iterations. Recalling that $\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T$ and $\mathbf{b} \sim \mathcal{N}(\mathbf{Ax}, \sigma^2 \mathbf{I})$, we therefore have

$$\mathbf{x}_\nu \sim \mathcal{N}(\mathbf{V}\Phi_\nu \mathbf{V}^T \mathbf{x}, \sigma^2 \mathbf{V}\Phi_\nu \Sigma^{-2} \Phi_\nu \mathbf{V}^T), \quad (2.11)$$

where $\Sigma^{-2} \stackrel{\text{def}}{=} (\Sigma^T \Sigma)^{-1}$. The *bias* of the estimator \mathbf{x}_ν is given by

$$\text{bias}[\mathbf{x}_\nu] = \mathbf{x} - E[\mathbf{x}_\nu] = \mathbf{V}(\mathbf{I} - \Phi_\nu) \mathbf{V}^T \mathbf{x} = \sum_{i=1}^n (1 - \phi_i^{(\nu)}) (\mathbf{v}_i^T \mathbf{x}) \mathbf{v}_i. \quad (2.12)$$

Notice that \mathbf{x}_ν is unbiased only if $\phi_i = 1$ for all i , which corresponds to the least squares solution (or no filtering).

However, while filtering introduces bias, it reduces the total variance in the estimator, which is given by

$$\text{tr}(\sigma^2 \mathbf{V}\Phi_\nu \Sigma^{-2} \Phi_\nu \mathbf{V}^T) = \sigma^2 \sum_{i=1}^n (\phi_i^{(\nu)} / \sigma_i)^2. \quad (2.13)$$

For multivariate random vectors, the *mean square error* for \mathbf{x}_ν is defined [23]

$$\begin{aligned} \text{MSE}(\nu) &= E[\|\mathbf{x}_\nu - \mathbf{x}\|^2] \\ &= \text{tr}(\sigma^2 \mathbf{V}\Phi_\nu \Sigma^{-2} \Phi_\nu \mathbf{V}^T) + \|\text{bias}[\mathbf{x}_\nu]\|^2 \\ &= \sigma^2 \sum_{i=1}^n (\phi_i^{(\nu)} / \sigma_i)^2 + \sum_{i=1}^n (1 - \phi_i^{(\nu)})^2 (\mathbf{v}_i^T \mathbf{x})^2. \end{aligned} \quad (2.14)$$

Thus to minimize the MSE, the filter factor $\phi_i^{(\nu)}$ should be chosen to balance the competing desires for small variance and small bias in the estimator.

A similar treatment of the statistical properties of regularized solutions can be found in [23, 25]. Moreover, regularization methods exist that strive to balance the desire for small bias and variance, notably the method of Backus and Gilbert [2], which we do not present here, but which can also be found in [23, 25].

2.2 Regularization Parameter Selection Methods

The practical usefulness of the regularization approaches presented above hinges on there being methods for choosing the regularization parameter. For a given regularization technique with filter factors parameterized by ν , yielding regularized solution \mathbf{x}_ν , a natural choice for ν is the value that minimizes $\text{MSE}(\mathbf{x}_\nu)$ defined in (2.14). Unfortunately, the computation of an estimator for $\text{MSE}(\mathbf{x}_\nu)$ is infeasible in general, since in practice we do not know \mathbf{x} .

2.2.1 The Unbiased Predictive Risk Estimator

A related approach is to instead minimize the *predictive risk*, which is defined

$$E[\|\mathbf{A}\mathbf{x}_\nu - \mathbf{A}\mathbf{x}\|^2], \quad (2.15)$$

where ν is the regularization parameter (α or k in our examples). Since the unknown \mathbf{x} is in (2.15), we can't use it directly, but we can replace (2.15) by an unbiased estimator that does not contain \mathbf{x} . The resulting method is appropriately known as the *unbiased predicative risk estimator* (UPRE) method; it was first introduced in [18], but can also be found in [27].

To obtain the estimator for (2.15), we first define \mathbf{A}_ν to be the regularization matrix such that $\mathbf{x}_\nu = \mathbf{A}_\nu \mathbf{b}$, where $\mathbf{A}_\nu = \mathbf{U}\Phi_\nu \Sigma^\dagger \mathbf{V}^T$. Then, given that $\mathbf{A}\mathbf{A}_\nu$ is symmetric in the cases of interest to us,

$$\begin{aligned} E[\|\mathbf{A}\mathbf{x}_\nu - \mathbf{A}\mathbf{x}\|^2] &= E[\|\mathbf{A}\mathbf{A}_\nu \mathbf{b} - \mathbf{A}\mathbf{x}\|^2] \\ &= E[\|(\mathbf{A}\mathbf{A}_\nu - \mathbf{I})\mathbf{A}\mathbf{x} + \mathbf{A}\mathbf{A}_\nu \boldsymbol{\epsilon}\|^2] \\ &= \|(\mathbf{A}\mathbf{A}_\nu - \mathbf{I})\mathbf{A}\mathbf{x}\|^2 + E[2\boldsymbol{\epsilon}^T \mathbf{A}\mathbf{A}_\nu (\mathbf{A}\mathbf{A}_\nu - \mathbf{I})\mathbf{A}\mathbf{x} + \boldsymbol{\epsilon}^T (\mathbf{A}\mathbf{A}_\nu)^2 \boldsymbol{\epsilon}] \\ &= \|(\mathbf{A}\mathbf{A}_\nu - \mathbf{I})\mathbf{A}\mathbf{x}\|^2 + E[\boldsymbol{\epsilon}^T (\mathbf{A}\mathbf{A}_\nu)^2 \boldsymbol{\epsilon}] \\ &= \|(\mathbf{A}\mathbf{A}_\nu - \mathbf{I})\mathbf{A}\mathbf{x}\|^2 + \text{tr}((\mathbf{A}\mathbf{A}_\nu)^2). \end{aligned} \quad (2.16)$$

The last equality follows from the fact that for a symmetric matrix \mathbf{B} and white noise vector \mathbf{v} , $E[\mathbf{v}^T \mathbf{B} \mathbf{v}] = \text{tr}(\mathbf{B})$ [27, Lemma 7.2].

A similar calculation to that for deriving (2.16) gives us that

$$E[\|\mathbf{A}\mathbf{x}_\nu - \mathbf{b}\|^2] = \|(\mathbf{A}\mathbf{A}_\nu - \mathbf{I})\mathbf{A}\mathbf{x}\|^2 + \text{tr}((\mathbf{A}\mathbf{A}_\nu)^2) - 2\sigma^2 \text{tr}(\mathbf{A}\mathbf{A}_\nu) + m\sigma^2,$$

and hence,

$$E[\|\mathbf{A}\mathbf{x}_\nu - \mathbf{A}\mathbf{x}\|^2] = E[\|\mathbf{A}\mathbf{x}_\nu - \mathbf{b}\|^2] + 2\sigma^2 \text{tr}(\mathbf{A}\mathbf{A}_\nu) - m\sigma^2. \quad (2.17)$$

Finally, we define

$$U(\nu) = \|\mathbf{A}\mathbf{x}_\nu - \mathbf{b}\|^2 + 2\sigma^2 \text{tr}(\mathbf{A}\mathbf{A}_\nu) - m\sigma^2, \quad (2.18)$$

which is an unbiased estimator of the predictive risk for given ν . Choosing the ν that minimizes $U(\nu)$ defines the UPRE regularization parameter choice method.

With the SVD of \mathbf{A} in hand, we can simplify (2.18). In particular, note that since $\mathbf{A}_\nu = \mathbf{V}\Phi_\nu \Sigma^\dagger \mathbf{U}^T$ (see (2.3)), so that

$$\mathbf{A}\mathbf{A}_\nu = \mathbf{U}\Sigma\mathbf{V}^T\mathbf{V}\Phi_\nu\Sigma^\dagger\mathbf{U}^T = \mathbf{U}\Sigma\Phi_\nu\Sigma^\dagger\mathbf{U}^T,$$

and hence

$$\begin{aligned} U(\nu) &= \|(\mathbf{U}\Sigma(\Phi_\nu - \mathbf{I})\Sigma^\dagger\mathbf{U}^T\mathbf{b})\|^2 + 2\sigma^2 \text{tr}(\mathbf{U}\Sigma\Phi_\nu\Sigma^\dagger\mathbf{U}^T) - m\sigma^2 \\ &= \sum_{i=1}^n [((\phi_i^{(\nu)} - 1)\mathbf{u}_i^T \mathbf{b})^2 + 2\sigma^2 \phi_i^{(\nu)}] - m\sigma^2, \end{aligned} \quad (2.19)$$

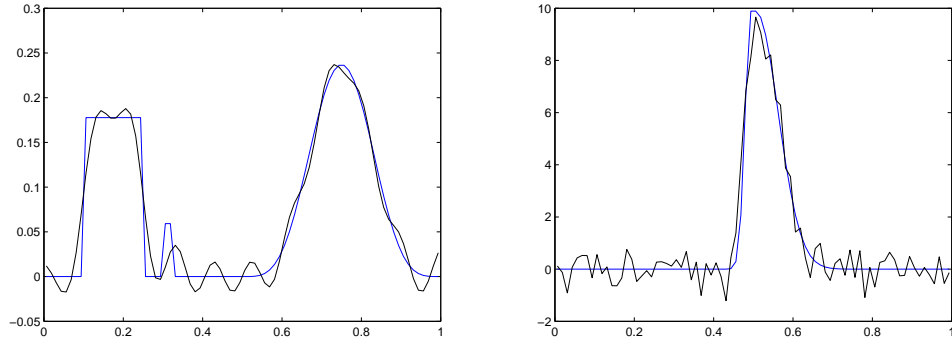


Figure 2.4. On the left is a plot of the TSVD reconstruction \mathbf{x}_k with the UPRE choice of $k = 22$ in the deblurring example. On the right is a plot of the Tikhonov reconstruction \mathbf{x}_α with the UPRE choice of $\alpha = 0.00011$ for the kernel reconstruction example.

the verification of which we leave as an exercise. The ‘ $-m\sigma^2$ ’ term can be ignored since it does not depend upon ν .

For each of the filters above, we can write down the specific UPRE functions; for TSVD and Tikhonov regularization they are given, respectively, by

$$U(k) = \sum_{i=k+1}^n (\mathbf{u}_i^T \mathbf{b})^2 + 2\sigma^2 k \quad (2.20)$$

$$U(\alpha) = \sum_{i=1}^n \frac{\alpha^2 (\mathbf{u}_i^T \mathbf{b})^2}{(\sigma_i^2 + \alpha)^2} + 2\sigma^2 \sum_{i=1}^n \frac{\sigma_i^2}{\sigma_i^2 + \alpha}. \quad (2.21)$$

The expression for U for the Landweber iteration it is left to the exercises.

We apply UPRE to the problem of choosing k for TSVD and α for Tikhonov regularization for the 1D deblurring example. For a specific noise realization, the UPRE choice for k was 22, while for α it was 0.00011. The corresponding reconstructions are given in Figure 2.4.

2.2.2 Generalized Cross Validation

One of the limitations of the UPRE selection method is that it requires knowledge of the noise variance σ^2 .

A method similar to UPRE that does not require σ^2 is generalized cross validation (GCV). GCV was originally introduced in [29], is very commonly used in inverse problems (see, e.g., [1, 13, 14, 27]), and is an approximation of leave-one-out cross validation (LOOCV).

The idea behind LOOCV is as follows. First, we define $\mathbf{A}^{[i]} \mathbf{x} = \mathbf{b}^{[i]}$ to be the linear system that results after the i^{th} element of \mathbf{b} and the i^{th} row of \mathbf{A} are removed, and $\mathbf{x}_\nu^{[i]} = \mathbf{A}_\nu^{[i]} \mathbf{b}^{[i]}$, where $\mathbf{A}_\nu^{[i]}$ is the regularization matrix for the modified

system. Finally, we define the LOOCV choice of regularization parameter ν to be the minimizer of

$$V(\nu) = \frac{1}{m} \sum_{i=1}^m ([\mathbf{A}\mathbf{x}_\nu^{[i]}]_i - b_i)^2,$$

i.e., the value of ν that yields the best overall prediction of the removed data points.

Evaluating the function V at a single ν involves solving m large-scale inverse problems, and hence, LOOCV is infeasible to implement for the problems of interest to us. However, a feasible approximation of V exists. We derive it by first noting that V can be equivalently written as (see [1] for details)

$$V(\nu) = \frac{1}{m} \sum_{i=1}^m \left(\frac{[\mathbf{A}\mathbf{x}_\nu - \mathbf{b}]_i}{1 - [\mathbf{A}\mathbf{A}_\nu]_{ii}} \right)^2.$$

For many large-scale problems, the diagonal values of $\mathbf{A}\mathbf{A}_\nu$ are infeasible to compute. Thus the GCV approximation of $V(\nu)$ replaces $1 - [\mathbf{A}\mathbf{A}_\nu]_{ii}$ by $(m - \text{tr}(\mathbf{A}\mathbf{A}_\nu))/m$ for all i to obtain

$$G(\nu) = \frac{m \|\mathbf{A}\mathbf{x}_\nu - \mathbf{b}\|^2}{[\text{tr}(\mathbf{I} - \mathbf{A}\mathbf{A}_\nu)]^2}. \quad (2.22)$$

The GCV choice of $\nu > 0$ is then the one that minimizes $G(\nu)$.

Simplifying (2.22) using the SVD as we did for UPRE above, we obtain

$$G(\nu) = \frac{\sum_{i=1}^n ((\phi_i^{(\nu)} - 1) \mathbf{u}_i^T \mathbf{b})^2}{(m - \sum_{i=1}^n \phi_i^{(\nu)})^2}, \quad (2.23)$$

which for TSVD and Tikhonov regularization has the form, respectively, of

$$G(k) = \left(\sum_{i=k+1}^n (\mathbf{u}_i^T \mathbf{b})^2 \right) / (m - k)^2 \quad (2.24)$$

$$G(\alpha) = \left(\sum_{i=1}^n \frac{\alpha^2 (\mathbf{u}_i^T \mathbf{b})^2}{(\sigma_i^2 + \alpha)^2} \right) / \left(m - \sum_{i=1}^n \frac{\sigma_i^2}{\sigma_i^2 + \alpha} \right)^2, \quad (2.25)$$

The expression for the Landweber iteration it is left to the reader.

We apply the GCV method to the 1D deblurring example, for the same noise realization as was used for UPRE, and obtain $k = 25$ for the TSVD solution and $\alpha = 0.0012$ for the Tikhonov solution. The two reconstructions, \mathbf{x}_k and \mathbf{x}_α , are plotted in Figure 2.5

2.2.3 The Discrepancy Principle

Next, we present the *discrepancy principle* (DP), which is a standard regularization parameter selection method for inverse problems; see e.g., [1, 7, 13, 14, 16, 27]. DP advocates choosing ν so that the sum of squared residuals $\|\mathbf{A}\mathbf{x}_\nu - \mathbf{b}\|^2$ is equal to the noise level $E[\|\epsilon\|^2]$, and it is equivalent to the method of moments in statistics on the

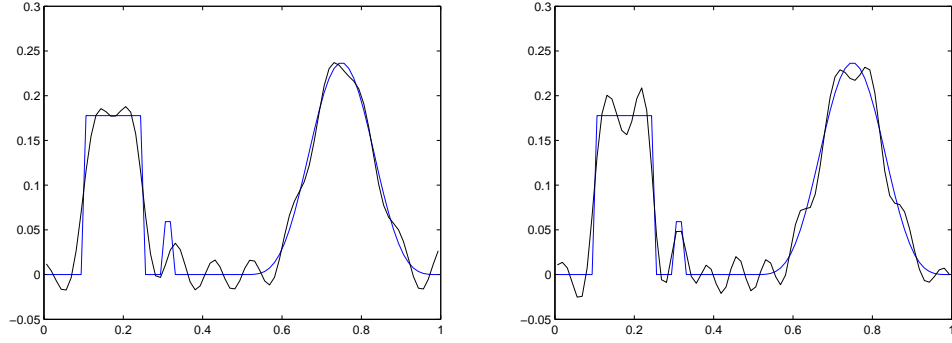


Figure 2.5. On the left is a plot of the TSVD reconstruction \mathbf{x}_k with the GCV choice of $k = 25$. On the right is a plot of the Tikhonov reconstruction \mathbf{x}_α with the GCV choice of $\alpha = 0.0012$.

second moment of the distribution. Since given our assumptions, $E[\|\epsilon\|^2] = m\sigma^2$, this amounts to solving to nonlinear equation

$$0 = D(\nu) \stackrel{\text{def}}{=} \|\mathbf{A}\mathbf{x}_\nu - \mathbf{b}\|^2 - m\sigma^2. \quad (2.26)$$

The function D simplifies using the SVD to

$$D(\nu) = \sum_{i=1}^n [(\phi_i^{(\nu)} - 1)\mathbf{u}_i^T \mathbf{b}]^2 - m\sigma^2. \quad (2.27)$$

which for TSVD and Tikhonov regularization has the form, respectively, of

$$D(k) = \sum_{i=k+1}^n (\mathbf{u}_i^T \mathbf{b})^2 - m\sigma^2 \quad (2.28)$$

$$D(\alpha) = \sum_{i=1}^n \frac{\alpha^2 (\mathbf{u}_i^T \mathbf{b})^2}{(\sigma_i^2 + \alpha)^2} - m\sigma^2. \quad (2.29)$$

We apply DP to the problem of choosing k for TSVD and α for Tikhonov regularization for the deblurring example. For the same noise realization as in the UPRE and GCV cases, the value of k chosen was 23, while the value for α was 0.0023. The corresponding reconstructions are plotted in Figure 2.6.

Note that when using DP for TSVD or Landweber iterations, you can choose the first k such that $D(k) \leq 0$. For Tikhonov regularization, on the other hand, a root finding algorithm such as the secant method or Newton's method can be used; note that $D(\alpha)$ is a differentiable function of α . Alternatively, a minimization algorithm can be used to compute the minimizer of $D(\nu)^2$, which will work even in cases where $D(\nu) > 0$ for all $\nu > 0$.

The expression for D for the Landweber iteration it is left to the exercises.

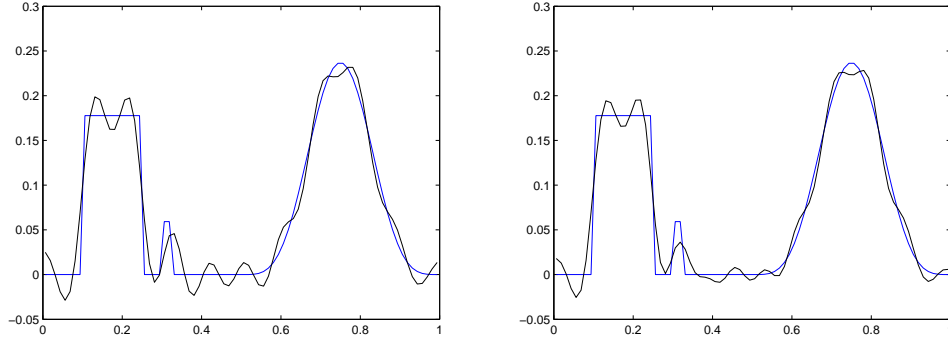


Figure 2.6. On the left is a plot of the TSVD reconstruction \mathbf{x}_k with the GCV choice of $k = 23$. On the right is a plot of the Tikhonov reconstruction \mathbf{x}_α with the GCV choice of $\alpha = 0.0023$.

2.2.4 The L-curve Criterion

The *L-curve method* is a heuristic developed in [11] that is widely used and that has been found to work well on many examples in inverse problems. We consider it here only as a method for choosing the Tikhonov regularization parameter α . It can also be used for choosing the TSVD parameter k , but it is a more involved procedure that we leave to [13] and the references therein.

The effectiveness of the L-curve method hinges on the fact that for a variety of inverse problems the parameterized curve

$$\left(\xi(\alpha) \stackrel{\text{def}}{=} \log \|\mathbf{x}_\alpha\|^2, \rho(\alpha) \stackrel{\text{def}}{=} \log \|\mathbf{A}\mathbf{x}_\alpha - \mathbf{b}\|^2 \right), \quad (2.30)$$

has a distinct L-shape. The corner of the curve corresponds, roughly, to the transition point between the values of α near 0 for which $\|\mathbf{x}_\alpha\|$ is large and $\|\mathbf{A}\mathbf{x}_\alpha - \mathbf{b}\|$ is small (too little regularization), and the large values of α for which $\|\mathbf{x}_\alpha\|$ is small and $\|\mathbf{A}\mathbf{x}_\alpha - \mathbf{b}\|$ is large (too much regularization). The L-curve method chooses α corresponding to the corner, or point of maximum curvature, along the curve (2.30), since this will often correspond to the value of α at which this transition occurs. We plot the L-curve for the 1D deblurring example on the left in Figure 2.7.

The equation for the curvature for a parametric curve of the form $(\xi(\alpha), \rho(\alpha))$ can be found in standard texts on analytic geometry and is given by

$$C(\alpha) = \frac{\rho(\alpha)' \xi(\alpha)'' - \rho(\alpha)'' \xi(\alpha)'}{(\rho'(\alpha)^2 + \xi'(\alpha)^2)^{3/2}}.$$

For the parametric curve defined by (2.30), $C(\alpha)$ can be expressed entirely in terms of $s(\alpha) \stackrel{\text{def}}{=} \|\mathbf{x}_\alpha\|^2$, $r(\alpha) \stackrel{\text{def}}{=} \|\mathbf{A}\mathbf{x}_\alpha - \mathbf{b}\|^2$ and $s'(\alpha)$ [27]:

$$C(\alpha) = -\frac{r(\alpha)s(\alpha)[\alpha r(\alpha) + \alpha^2 s(\alpha)] + [r(\alpha)s(\alpha)]^2/s'(\alpha)}{[r(\alpha)^2 + \alpha^2 s(\alpha)^2]^{3/2}}. \quad (2.31)$$

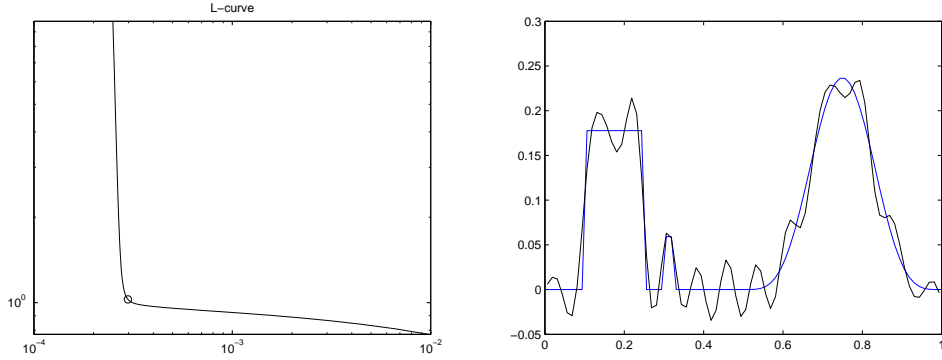


Figure 2.7. On the left is a plot of the curve $(\log \|\mathbf{x}_\alpha\|^2, \log \|\mathbf{A}\mathbf{x}_\alpha - \mathbf{b}\|^2)$ for the 1D image deblurring test problem. The L-curve choice of the regularization parameter $\alpha = 0.00035$ corresponds to the circle at the corner of the curve. On the right is a plot of the corresponding Tikhonov reconstruction \mathbf{x}_α .

Using the SVD, we can derive the following formula for $s'(\alpha)$:

$$s'(\alpha) = \sum_{i=1}^n \frac{-2\sigma_i^2(\mathbf{u}_i^T \mathbf{b})^2}{(\sigma_i^2 + \alpha)^3}. \quad (2.32)$$

The L-curve choice for the regularization parameter α is the value that maximizes the curvature C defined by (2.31). For the 1D deblurring test case, the L-curve choice was $\alpha = 0.00035$, which corresponds to the circle in left-hand plot in Figure 2.7. The resulting Tikhonov solution \mathbf{x}_α is plotted on the right in Figure 2.7.

Remarks: A regularization method is said to be convergent if, roughly speaking, as the noise level (in our case represented by σ^2) goes to 0, the methods choose values of ν such that \mathbf{x}_ν converges to \mathbf{x} . An in-depth analysis of the convergence properties of the above methods can be found in [27]. To summarize that analysis, UPRE, GCV, and DP are convergent methods, with UPRE having the best convergence properties, followed by GCV, and then DP. We remind the reader that both UPRE and DP require an estimate of σ^2 , while GCV does not. The L-curve method is shown to be non-convergent in [27], an important result that one should weigh when choosing a regularization parameter selection method. Nonetheless, the L-curve method is frequently used and has been shown to work reasonably well on a large number of examples in inverse problems, including the one in this chapter.

It is also worth mentioning that since the data \mathbf{b} is a random vector, the value of ν given by the above methods will also be random. For this reason, a Monte Carlo analysis of the above four regularization parameter selection methods is useful. Such an analysis can be found for GCV, DP, and the L-curve in [13].

2.3 Summary

In this chapter, we showed how to overcome the stability issues associated with inverse problems, as described in Chapter 1, using a technique known as regularization.

We began with an example with two unknowns, where we removed (filtered) the singular value/vector from the design matrix that were the cause of high variance in the least squares solution. This example motivated the truncated singular value decomposition (TSVD) method of regularization, in which the singular vectors of the design matrix are removed for singular values below some threshold. We then introduced some other common regularization methods that can be viewed as filtered singular value decomposition (SVD) methods: Tikhonov regularization and the truncated Landweber iteration.

We derived a formula for the variance of general filtered SVD regularized solutions, which shows that when regularization is used, the variance in the estimator decreases, and hence stability improves, however at the cost of increased bias in the estimator.

In all cases, the particular filter used was parameterized by a single unknown parameter ν (either α or k in our examples), known as the regularization parameter. In order for the filtering methods to be practically useful, methods for the choice of ν are required. Thus we presented several regularization parameter selection methods. The first was the unbiased predictive risk estimator method, which sought ν that minimizes an unbiased estimator of the predictive risk $E[\|\mathbf{Ax}_\nu - \mathbf{Ax}\|^2]$. The second method, called generalized cross validation, approximates the leave-on-out cross validation method for the choosing ν . The third method we presented was the discrepancy principle (DP), which seeks ν that matches the sum of squared residuals to the noise level, i.e., $\|\mathbf{Ax}_\nu - \mathbf{b}\|^2 = m\sigma^2$. And finally, we presented the L-curve method for Tikhonov regularization, which seeks the value of α that maximizes the curvature along the curve $(\log \|\mathbf{x}_\alpha\|^2, \log \|\mathbf{Ax}_\alpha - \mathbf{b}\|^2)$.

We implemented all four regularization parameter selection methods on a one-dimensional deblurring example and found them to perform well.

Exercises

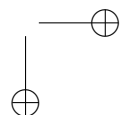
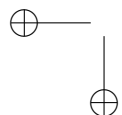
- 2.1.
 - a. Define $\ell(\mathbf{x})$ to be the penalized least squares function in (2.5). Show that $\nabla \ell(\mathbf{x}) = \mathbf{0}$ yields (2.6) and hence that the solutions of (2.5) and (2.6) coincide. Argue, moreover, that the solution is unique.
 - b. Use the SVD of the matrix \mathbf{A} to show that the solutions of (2.6) (and hence of (2.5)) can be written in filtered SVD form (2.3) with Tikhonov filter (2.7).
- 2.2.
 - a. Create plots of the *relative error* function $f(\alpha) = \|\mathbf{x}_\alpha - \mathbf{x}_{\text{true}}\|/\|\mathbf{x}_{\text{true}}\|$ within both `DeblurTikhonov.m` and `PSFreconTikhonov.m` (use MATLAB's `logspace` function). Then estimate from the plots which α minimizes the relative error.

- b. Repeat part (a) with `DeblurTSVD.m` and `PSFreconTSVD.m`.
 - c. Repeat part (a) with `DeblurLandweber.m` and `PSFreconLandweber.m`.
- 2.3. Show that (2.8) can be written as (2.3) with ϕ_i defined by (2.9). *Hint:* First show that for $\mathbf{x}_0 = \mathbf{0}$, (2.8) can be written $\mathbf{x}_k = \sum_{j=0}^{k-1} (\mathbf{I} - \tau \mathbf{A}^T \mathbf{A})^j (\tau \mathbf{A}^T \mathbf{b})$. Then substitute the SVD of \mathbf{A} into the expression.
- 2.4.
 - a. Verify that (2.11) holds assuming $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$, $\mathbf{b} \sim \mathcal{N}(\mathbf{Ax}, \sigma^2 \mathbf{I})$, and $\mathbf{x}_\nu = \mathbf{V}\mathbf{\Phi}_\nu \mathbf{\Sigma}^\dagger \mathbf{U}^T \mathbf{b}$. Use the fact that for a general $n \times 1$ normal random vector $\mathbf{v} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C})$ if $\mathbf{w} = \mathbf{B}\mathbf{v}$, where \mathbf{B} is an $m \times n$ matrix, $\mathbf{w} \sim \mathcal{N}(\mathbf{B}\boldsymbol{\mu}, \mathbf{B}\mathbf{C}\mathbf{B}^T)$.
 - b. Use (2.11) to derive the distribution for $\mathbf{v}_i^T \mathbf{x}_\nu$ akin to (1.25).
- 2.5.
 - a. Find the expressions for the MSE defined by (2.14) for the TSVD, Tikhonov, and Landweber regularized solutions.
 - b. Create plots of $\text{MSE}(\alpha)$, using MATLAB's `logspace` function, within both `DeblurTikhonov.m` and `PSFreconTikhonov.m`. Then estimate from the plots which α minimizes the MSE.
 - c. Repeat part (a) with `DeblurTSVD.m` and `PSFreconTSVD.m`.
 - d. Repeat part (a) with `DeblurLandweber.m` and `PSFreconLandweber.m`.
 - e. If you have done Exercise 2, how do the MSE and relative error curves compare? Plot the curves for `DeblurTikhonov.m` and `PSFreconTikhonov.m` separately.
- 2.6.
 - a. Modify `DeblurTikhonov.m` and `PSFreconTikhonov.m` so that (some subset of) the following curves are plotted together, (all on the same numerical grid created using `logspace`):
 - i. the UPRE curve $U(\alpha)$ defined by (2.21),
 - ii. the GCV curve $G(\alpha)$ defined by (2.25),
 - iii. the DP curve $D(\alpha)^2$ defined by (2.29), and
 - iv. the L-curve curvature function $-C(\alpha)$ defined by (2.31).
 - b. Repeat part a, (i)-(iii), with `DeblurTSVD.m` and `PSFreconTSVD.m`.
 - c. Repeat part a, (i)-(iii), with `DeblurLandweber.m` and `PSFreconLandweber.m`.
 - d. If you have done Exercises 2 and/or 5, how do the curves you've plotted compare to the *relative error* and/or the MSE? Plot the curves for the deblurring and kernel reconstruction test cases separately.
- 2.7.
 - a. Derive formulas for $U(k)$, $G(k)$, $D(k)$ defined by (2.19), (2.23), and (2.27), respectively, for the Landweber iteration.
 - b. Using `DeblurLandweber.m`, compute Landweber iterations and report the iterations at which $U(k)$ and $G(k)$ first increase, and $D(k)$ first drops below zero. Plot the corresponding reconstructions.
- 2.8.
 - a. Use the SVD of \mathbf{A} to verify the step (2.19).
 - b. Use the SVD of \mathbf{A} to verify that (2.22) and (2.23) are equivalent.
 - c. Use the SVD of \mathbf{A} to verify that (2.26) and (2.27) are equivalent.

- 2.9. In exercise 1.2, you were asked to modify `Deblur1d.m` so that the convolution kernel

$$a(s) = \begin{cases} 100s + 10, & -\frac{1}{10} \leq s \leq 0, \\ -100s + 10, & 0 \leq s \leq \frac{1}{10}, \\ 0, & \text{otherwise.} \end{cases}$$

is used instead to define **A**. Use Tikhonov regularization together with the L-curve criterion to reconstruct **x** from observations **b**. Compare your results with those obtained using GCV. Which yields a lower relative error?



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