Q_5: **Reconstruction from practical data.** Given the noisy data $m = \mathcal{A}f + \varepsilon$, how to approximate f in a noise-robust fashion?

3.5 The SVD for matrices

In practice the continuum measurement model (1.1) of the form $\mathbf{m} = \mathcal{A}f + \varepsilon$ needs to be approximated by a discrete model of the form $\mathbf{m} = A\mathbf{f} + \varepsilon$, where A is a matrix, $\mathbf{f} \in \mathbb{R}^n$, and $\mathbf{m} \in \mathbb{R}^k$. Let us now discuss a tool that allows explicit analysis of Hadamard's conditions in this finite-dimensional setting, namely, *singular value decomposition* (*SVD*) of A.

We know from matrix algebra that any matrix $A \in \mathbb{R}^{k\times n}$ can be written in the form

$$A = UDV^T, \tag{3.12}$$

where $U \in \mathbb{R}^{k\times k}$ and $V \in \mathbb{R}^{n\times n}$ are orthogonal matrices, that is,

$$U^T U = UU^T = I, \quad V^T V = VV^T = I,$$

and $D \in \mathbb{R}^{k\times n}$ is a diagonal matrix. The rigt-hand side of (3.12) is called the SVD of matrix A, and the diagonal elements d_j are the *singular values* of A. The properties of d_j, and the columns u_i of U, and the columns V_i of V correspond to those of the SVE.

In the case $k = n$ the matrix D is square-shaped: $D = \operatorname{diag}(d_1, \ldots, d_k)$. If $k > n$, then

$$D = \begin{bmatrix} \operatorname{diag}(d_1,\ldots,d_n) \\ \mathbf{0}_{(k-n)\times n} \end{bmatrix} = \begin{bmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & & \vdots \\ \vdots & & \ddots & \\ 0 & \cdots & \cdots & d_n \\ 0 & \cdots & \cdots & 0 \\ \vdots & & & \vdots \\ 0 & \cdots & \cdots & 0 \end{bmatrix}, \tag{3.13}$$

and in the case $k < n$ the matrix D takes the form

$$\begin{aligned} D &= [\operatorname{diag}(d_1,\ldots,d_k), \mathbf{0}_{k\times(n-k)}] \\ &= \begin{bmatrix} d_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & d_2 & & \vdots & \vdots & & \vdots \\ \vdots & & \ddots & \vdots & \vdots & & \vdots \\ 0 & \cdots & \cdots & d_k & 0 & \cdots & 0 \end{bmatrix}. \end{aligned} \tag{3.14}$$

The diagonal elements d_j are nonnegative and in decreasing order:

$$d_1 \ge d_2 \ge \cdots \ge d_{\min(k,n)} \ge 0. \tag{3.15}$$

Note that some or all of the d_j can be equal to zero.

Recall the definitions of the following linear subspaces related to the matrix A:

$$\begin{aligned} \operatorname{Ker}(A) &= \{\mathbf{f} \in \mathbb{R}^n \,:\, A\mathbf{f} = 0\}, \\ \operatorname{Range}(A) &= \{\mathbf{m} \in \mathbb{R}^k \,:\, \text{there exists } \mathbf{f} \in \mathbb{R}^n \text{ such that } A\mathbf{f} = \mathbf{m}\}, \\ \operatorname{Coker}(A) &= (\operatorname{Range}(A))^\perp \subset \mathbb{R}^k. \end{aligned}$$

See Figure 3.3 for a diagram illustrating these concepts.

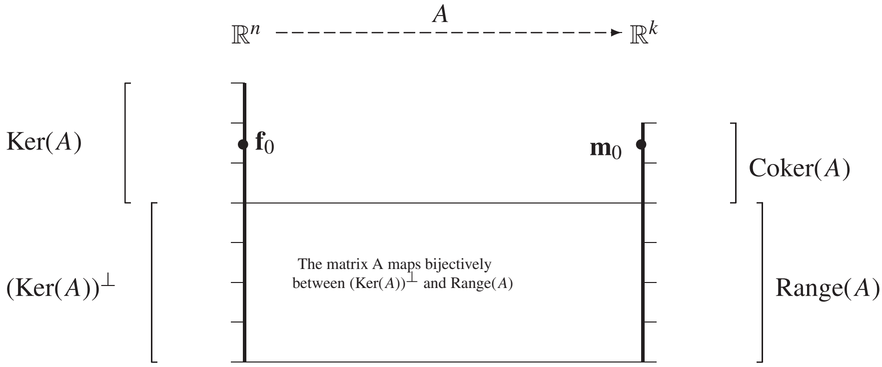

Figure 3.3. This diagram illustrates various linear subspaces related to a matrix mapping $\mathbb{R}^n$ to $\mathbb{R}^k$. The two thick vertical lines represent the linear spaces $\mathbb{R}^n$ and $\mathbb{R}^k$; in this schematic picture we have $n = 7$ and $k = 6$. Furthermore, $\dim(\text{Ker}(A)) = 3$ and $\dim(\text{Range}(A)) = 4$ and $\dim(\text{Coker}(A)) = 2$. Note that the four-dimensional orthogonal complement of Ker(A) in R^n is mapped in a bijective manner to Range(A). The points $\mathbf{f}_0 \in \text{Ker}(A)$ and $\mathbf{m}_0 \in \text{Coker}(A)$ are used in the text.

Failure of Hadamard's existence and uniqueness conditions can now be detected from the matrix D. If $k > n$, then $\dim(\text{Range}(A)) < k$ and we can choose a nonzero $\mathbf{m}_0 \in \text{Coker}(A)$ as shown in Figure 3.3. Even in the case $\varepsilon = 0$ we have problems since there does not exist any $\mathbf{f} \in \mathbb{R}^n$ satisfying $A\mathbf{f} = \mathbf{m}_0$, and consequently the existence condition H_1 fails since the output $A^{-1}\mathbf{m}_0$ is not defined for the input $\mathbf{m}_0$. In case of nonzero random noise the situation is even worse since even though $A\mathbf{f} \in \text{Range}(A)$, it might happen that $A\mathbf{f} + \varepsilon \notin \text{Range}(A)$. If $k < n$, then $\dim(\text{Ker}(A)) > 0$ and we can choose a nonzero $\mathbf{f}_0 \in \text{Ker}(A)$ as shown in Figure 3.3. Then even in the case $\varepsilon = 0$ we have a problem of defining $A^{-1}\mathbf{m}$ uniquely since both $A^{-1}\mathbf{m}$ and $A^{-1}\mathbf{m} + \mathbf{f}_0$ satisfy $A(A^{-1}\mathbf{m}) = \mathbf{m} = A(A^{-1}\mathbf{m} + \mathbf{f}_0)$. Thus the uniqueness condition H_2 fails unless we specify an explicit way of dealing with the nullspace of A. Note that if $d_{\min(k,n)} = 0$, then both conditions H_1 and H_2 fail.

The above problems with existence and uniqueness are quite clear since they are related to integer-valued dimensions. In contrast, ill-posedness related to the continuity condition H_3 is more tricky in our finite-dimensional context. Consider the case $n = k$ so A is a square matrix, and assume that A is invertible. In that case we can write

$$A^{-1}\mathbf{m} = A^{-1}(A\mathbf{f} + \varepsilon) = \mathbf{f} + A^{-1}\varepsilon, \tag{3.16}$$

where the error $A^{-1}\varepsilon$ can be bounded by

$$\|A^{-1}\varepsilon\| \leq \|A^{-1}\|\|\varepsilon\|.$$

Now if $\|\varepsilon\|$ is small and $\|A^{-1}\|$ has reasonable size, then the error $A^{-1}\varepsilon$ is small. However, if $\|A^{-1}\|$ is large, then the error $A^{-1}\varepsilon$ can be huge even when ε is small. This is the kind of amplification of noise we see in Figures 2.5, 2.9, and 2.19.

Note that if $\varepsilon = 0$ in (3.16), then we do have $A^{-1}\mathbf{m} = \mathbf{f}$ even if $\|A^{-1}\|$ is large. However, in practice the measurement data always has some noise, and even computer simulated data is corrupted with roundoff errors. Those inevitable perturbations prevent using $A^{-1}\mathbf{m}$ as a reconstruction method for an ill-posed problem.

To define ill-posedness related to the continuity condition H_3 rigorously, we must consider the relative sizes of the singular values. Consider the case $n = k$ and $d_n > 0$, when we do not have the above problems with existence or uniqueness. It seems that nothing is wrong since we can invert the matrix A as

$$A^{-1} = VD^{-1}U^T, \qquad D^{-1} = \operatorname{diag}\left(\frac{1}{d_1}, \ldots, \frac{1}{d_k}\right),$$

and define $\mathcal{R}(\mathbf{m}) = A^{-1}\mathbf{m}$ for any $\mathbf{m} \in \mathbb{R}^k$. The problem comes from the *condition number*

$$\operatorname{Cond}(A) := \frac{d_1}{d_k} \tag{3.17}$$

being large. Namely, if d_1 is several orders of magnitude greater than d_k, then numerical inversion of A becomes difficult since the diagonal inverse matrix D^{-1} contains floating point numbers of very different sizes. This in turn leads to uncontrollable amplification of truncation errors.

Strictly mathematically speaking, though, A is an invertible matrix even in the case of large condition number. For a rigorous definition, we must return to the continuum problem approximated by the matrix model. Suppose that we model the continuum measurement by a sequence of matrices A_k having size $k \times k$ for $k = k_0, k_0+1, k_0+2, \ldots$ so that the approximation to the forward problem becomes better as k grows. Then we say that condition H_3 fails if

$$\lim_{k\to\infty} \operatorname{Cond}(A_k) = \infty. \tag{3.18}$$

Thus, the ill-posedness cannot be rigorously detected from one approximation matrix A_k but only from the sequence $\{A_k\}_{k=k_0}^{\infty}$. Theorem 3.3 tells us further that the ill-posedness of the problem is not evident from a single approximation matrix A_k to the operator $\mathcal{A}$, but only from a sequence of approximations.

3.6 SVD for the guiding examples

We start with the one-dimensional convolution example introduced in Section 2.1. We compute the singular values of measurement matrices for the two resolutions $k = n = 64$ and $k = n = 128$. See Figure 3.4 for a logarithmic plot of the singular values. The singular values decrease very quickly towards zero but nevertheless stay positive; this is a sign of ill-posedness.

Next we consider the heat propagation model discussed in Section 2.2. Singular values of the matrix A defined by (3.6) for $T = 0.1$ and $T = 0.4$ are shown in Figure 3.5. The distribution of the singular values does not change significantly with Δx, but does have some dependence on the final time T. It is an exercise to compute the condition number of A.

Finally, Figure 3.6 shows singular values of a measurement matrix related to the X-ray tomography problem. The matrix is the one constructed in Section 2.3.5 for the resolution 50×50 and with 50 projection directions.