LEAST SQUARES SOLUTION TRICKS

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Contents

1. Least squares solution and minimum norm solution

Let us define the *least squares solution* and *minimum norm solution* of the matrix equation $A\mathbf{x} = \mathbf{b}$, where

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^n, \qquad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_k \end{bmatrix} \in \mathbb{R}^k,$$

and the matrix A has size $k \times n$.

Definition 1.1. *A vector* $\widetilde{\mathbf{x}} \in \mathbb{R}^n$ *is called a* least-squares solution *of the equation* $A\mathbf{x} = \mathbf{b}$ *if*

$$\|A\widetilde{\mathbf{x}} - \mathbf{b}\| = \min_{\mathbf{x}\in\mathbb{R}^n} \|A\mathbf{x} - \mathbf{b}\|. \tag{1.1}$$

Furthermore, we give a special name for the shortest least-squares solution (in general there may be many least-squares solutions). A vector $\widetilde{\mathbf{x}}_0$ *is called the* minimum norm solution *of* $A\mathbf{x} = \mathbf{b}$ *if* $\widetilde{\mathbf{x}}_0$ *is a least-squares solution of* $A\mathbf{x} = \mathbf{b}$ *and additionally satisfies*

$$\|\widetilde{\mathbf{x}}_0\| = \min\{\|\widetilde{\mathbf{x}}\| : \widetilde{\mathbf{x}} \textit{ is a least-squares solution of } A\mathbf{x} = \mathbf{b}\}. \tag{1.2}$$

The vector norm above is the Euclidean norm $\|\mathbf{x}\|^2 = x_1^2 + x_2^2 + \cdots + x_n^2$.

In the next two sections we explain how to compute these solutions in practice.

Date: Version 2, November 4, 2015.

2. Computing the least squares solution

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

$$Q(\mathbf{x}) = \|A\mathbf{x} - \mathbf{b}\|^2.$$

We want to find a minimizer $\widetilde{\mathbf{x}} \in \mathbb{R}^n$ for Q. In other words, we look for a vector $\widetilde{\mathbf{x}}$ for which it holds that

$$Q(\widetilde{\mathbf{x}}) = \min_{\mathbf{x}\in\mathbb{R}^n} Q(\mathbf{x}). \tag{2.1}$$

Note that Q is continuously differentiable in any variable x_j. Therefore, since $\widetilde{\mathbf{x}}$ is a minimizer, we have

$$0 = \frac{d}{dt}\|A(\widetilde{\mathbf{x}} + t\mathbf{w}) - \mathbf{b}\|^2\Big|_{t=0}$$

for any $\mathbf{w} \in \mathbb{R}^n$. (Why?)

We use the notation $\langle \mathbf{x}, \mathbf{y}\rangle$ for the inner product between two vertical vectors $\widetilde{\mathbf{x}} \in \mathbb{R}^n$ and $\widetilde{\mathbf{y}} \in \mathbb{R}^n$. The definition is

$$\langle \mathbf{x}, \mathbf{y}\rangle = \mathbf{x}^T\mathbf{y} = x_1y_1 + x_2y_2 + \cdots + x_ny_n.$$

Note that

$$\langle \mathbf{x}, \mathbf{x}\rangle = \mathbf{x}^T\mathbf{x} = x_1^2 + x_2^2 + \cdots + x_n^2 = \|\mathbf{x}\|^2.$$

Also, use matrix algebra to see that

$$\langle A\mathbf{x}, \mathbf{b}\rangle = (A\mathbf{x})^T\mathbf{b} = (\mathbf{x}^TA^T)\mathbf{b} = \mathbf{x}^T(A^T\mathbf{b}) = \langle \mathbf{x}, A^T\mathbf{b}\rangle.$$

Now use the linearity of the inner product to compute

$$\begin{aligned}
0 =&\frac{d}{dt}\|A(\widetilde{\mathbf{x}} + t\mathbf{w}) - \mathbf{b}\|^2\Big|_{t=0}\\
=&\frac{d}{dt}\langle A\widetilde{\mathbf{x}} + tA\mathbf{w} - \mathbf{b}, A\widetilde{\mathbf{x}} + tA\mathbf{w} - \mathbf{b}\rangle\Big|_{t=0}\\
=&\frac{d}{dt}\Big\{\|A\widetilde{\mathbf{x}}\|^2 + 2t\langle A\widetilde{\mathbf{x}}, A\mathbf{w}\rangle + t^2\|A\mathbf{w}\|^2\\
&\qquad - 2t\langle \mathbf{b}, A\mathbf{w}\rangle - 2\langle A\widetilde{\mathbf{x}}, \mathbf{b}\rangle + \|\mathbf{b}\|^2\Big\}\Big|_{t=0}\\
=&\Big\{2\langle A\widetilde{\mathbf{x}}, A\mathbf{w}\rangle + 2t\|A\mathbf{w}\|^2 - 2\langle \mathbf{b}, A\mathbf{w}\rangle\Big\}\Big|_{t=0}\\
=&2\langle A\widetilde{\mathbf{x}}, A\mathbf{w}\rangle - 2\langle \mathbf{b}, A\mathbf{w}\rangle\\
=&2\langle A^TA\widetilde{\mathbf{x}}, \mathbf{w}\rangle - 2\langle A^T\mathbf{b}, \mathbf{w}\rangle.
\end{aligned}$$

We conclude that the identity $\langle A^T A\widetilde{\mathbf{x}}, \mathbf{w}\rangle = \langle A^T\mathbf{b}, \mathbf{w}\rangle$ holds for any nonzero $\mathbf{w} \in \mathbb{R}^n$. Therefore, the minimizing vector must satisfy

$$A^T A\widetilde{\mathbf{x}} = A^T\mathbf{b}. \tag{2.2}$$

The identity (2.2) is called the *normal equation*. Now if the $n\times n$ matrix $A^T A$ happens to be invertible, we can compute the least squares solution as

$$\widetilde{\mathbf{x}} = (A^T A)^{-1}A^T\mathbf{b}. \tag{2.3}$$

If $A^T A$ is not invertible, there is no unique minimizer for Q and we cannot use formula (2.3). But even in that case we can compute the minimum norm solution!

3. Fitting a linear model to noisy data

Consider the following linear model describing the relationship between two scalar quantities $x \in \mathbb{R}$ and $x \in \mathbb{R}$:

$$y = a_0 x + b_0, \tag{3.1}$$

where $a_0, b_0 \in \mathbb{R}$ are parameters.

Assume given noisy data $y'_1, y'_2, \ldots, y'_n$ at points $x_1, x_2, \ldots, x_n$. More precisely,

$$y'_j = ax_j + b + \varepsilon_j, \tag{3.2}$$

where ε_j is some unknown error in the measurement.

We can solve for the parameters $a, b \in \mathbb{R}$ that give the model of the form (3.1) that best fits the data in the least-squares sense. Namely, write

$$A = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \in \mathbb{R}^n, \qquad \mathbf{y}' = \begin{bmatrix} y'_1 \\ y'_2 \\ \vdots \\ y'_n \end{bmatrix} \in \mathbb{R}^n,$$

and consider the linear system of equations defined by

$$A\begin{bmatrix} a \\ b \end{bmatrix} = \mathbf{y}'. \tag{3.3}$$

Now in general the equation (3.3) has no solutions because of the errors in (3.2). But if the matrix $(A^T A)$ is invertible, then we can use (2.3) to compute the least-squares solution as

$$\begin{bmatrix} \widetilde{a} \\ \widetilde{b} \end{bmatrix} = (A^T A)^{-1}A^T\mathbf{y}'.$$

4. Computing the minimum norm solution

We need a method for computing minimum norm solutions. For this, write A in the form of its SVD $A = UDV^T$ as explained in Section A. Recall that the singular values are ordered from largest to smallest as shown in (A.4), and let r be the largest index for which the corresponding singular value is nonzero:

$$r = \max\{j \mid 1 \leq j \leq \min(k,n),\ d_j > 0\}. \tag{4.1}$$

The definition of index r is essential in the following analysis, so we will be extra-specific:

$$d_1 > 0, \quad d_2 > 0, \quad \cdots \quad d_r > 0, \quad d_{r+1} = 0, \quad \cdots \quad d_{\min(k,n)} = 0.$$

Of course, it is also possible that all singular values are zero, in which case r is not defined and A is the zero matrix, or none of the singular values may be zero.

The next result gives a method to determine the minimum norm solution.

Theorem 4.1. *Let A be a $k \times n$ matrix and denote by $A = UDV^T$ the singular value decomposition of A. The minimum norm solution of the equation $A\mathbf{x} = \mathbf{b}$ is given by $A^+\mathbf{b}$ where*

$$A^+\mathbf{b} = VD^+U^T\mathbf{b},$$

and where

$$D^+ = \begin{bmatrix} 1/d_1 & 0 & \cdots & 0 & & \cdots & 0 \\ 0 & 1/d_2 & & & & & \vdots \\ \vdots & & \ddots & & & & \\ & & & 1/d_r & & & \\ & & & & 0 & & \\ \vdots & & & & & \ddots & \vdots \\ 0 & \cdots & & & & \cdots & 0 \end{bmatrix} \in \mathbb{R}^{n\times k}.$$

Proof. Write the singular matrix V in the form $V = [V_1 \quad V_2 \quad \cdots \quad V_n]$ and note that the column vectors $V_1, \ldots, V_n$ form an orthogonal basis for $\mathbb{R}^n$. We write $\mathbf{x} \in \mathbb{R}^n$ as a linear combination $\mathbf{x} = \sum_{j=1}^n a_j V_j = V\mathbf{a}$, and our goal is to find such coefficients $a_1, \ldots, a_n$ that $\mathbf{x}$ becomes a minimum norm solution.

Set $\mathbf{b}' = U^T\mathbf{b} \in \mathbb{R}^k$ and compute

$$\begin{aligned}\|A\mathbf{x}-\mathbf{b}\|^2 &= \|UDV^TV\mathbf{a}-U\mathbf{b}'\|^2\\ &= \|D\mathbf{a}-\mathbf{b}'\|^2\\ &= \sum_{j=1}^{r}(d_ja_j-\mathbf{b}'_j)^2+\sum_{j=r+1}^{k}(\mathbf{b}'_j)^2, \end{aligned} \tag{4.2}$$

where we used the orthogonality of U (namely, $\|U\mathbf{x}\| = \|\mathbf{x}\|$ for any vector $\mathbf{x} \in \mathbb{R}^k$). Now since d_j and $\mathbf{b}'_j$ are given and fixed, the expression (4.2) attains its minimum when $a_j = \mathbf{b}'_j/d_j$ for $j = 1, \ldots, r$. So any $\mathbf{x}$ of the form

$$\mathbf{x} = V\begin{bmatrix} d_1^{-1}\mathbf{b}'_1\\ \vdots\\ d_r^{-1}\mathbf{b}'_r\\ a_{r+1}\\ \vdots\\ a_n\end{bmatrix}$$

is a least-squares solution. The smallest norm $\|\mathbf{x}\|$ is clearly given by the choice $a_j = 0$ for $r < j \le n$, so the minimum norm solution is uniquely determined by the formula $\mathbf{a} = D^+\mathbf{b}'$. □

Definition 4.1. *The matrix A^+ is called the* pseudoinverse*, or the* Moore-Penrose inverse *of A.*

Appendix A. The singular value decomposition

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

$$A = UDV^T, \tag{A.1}$$

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

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

and $D \in \mathbb{R}^{k\times n}$ is a diagonal matrix. The right side of (A.1) is called the singular value decomposition (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: $D = \text{diag}(d_1, \ldots, d_k)$. If $k > n$ then

$$D = \begin{bmatrix} \text{diag}(d_1, \ldots, d_n) \\ \mathbf{0}_{(k-n)\times n} \end{bmatrix} = \begin{bmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & & \vdots \\ \vdots & & \ddots & \\ 0 & \cdots & \cdots & d_n \\ 0 & \cdots & \cdots & 0 \\ \vdots & & & \vdots \\ 0 & \cdots & \cdots & 0 \end{bmatrix}, \tag{A.2}$$

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

$$\begin{aligned} D &= [\text{diag}(d_1, \ldots, d_k), \mathbf{0}_{k\times(n-k)}] \\ &= \begin{bmatrix} d_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & d_2 & & \vdots & \vdots & & \vdots \\ \vdots & & \ddots & \vdots & \vdots & & \vdots \\ 0 & \cdots & \cdots & d_k & 0 & \cdots & 0 \end{bmatrix}. \end{aligned} \tag{A.3}$$

The diagonal elements d_j are nonnegative and in decreasing order:

$$d_1 \geq d_2 \geq \ldots \geq d_{\min(k,n)} \geq 0. \tag{A.4}$$

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:

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