1 Overview

Main ideas:

1. definition of a least-squares solution of a (not necessarily consistent) system and least-squares error
2. general procedure for finding a least squared solution
3. criteria for uniqueness of least-squares solution
4. finding a least-squares solution of $Ax = b$ when the columns of A are orthogonal
5. (finding a least-squares solution using a QR factorization–omit)

Examples in text:

1. find a least-squares solution of an inconsistent system
2. find the general form of a least-squares solution for an inconsistent system
3. determine the least squared error of a least-squares solution
4. find a least-squares solution of a system $Ax = b$ where the columns of A are othogonal
5. (find a least-squares solution using a QR factorization)

2 Discussion and Worked Examples

2.1 Finding an Approximate Solution to an Inconsistent System of Equations

When a system of equations is created to model observed phenomena, there is a possibility that the system is inconsistent, due to measurement error. In such a case, it is useful to find an *approximate* solution.

Suppose A is an $m \times n$ matrix and b a vector in $\mathbb{R}^m$ such that $Ax = b$ is inconsistent. We wish to find $\tilde{x}$ in $\mathbb{R}^n$ such that

$$\|b - A\tilde{x}\| \quad \leq \quad \|b - Ax\| \qquad \text{for all } x \text{ in } \mathbb{R}^n$$

i.e. the distance between $A\tilde{x}$ and b is less than or equal to the distance between Ax and b for any vector x in $\mathbb{R}^n$. In this case, $\tilde{x}$ is called a *least-squares solution* and the distance between $A\tilde{x}$ and b is called the *least-squares error*.

(Do we know that such a vector exists? If it does exist, will it be unique??)

A reformulation allows us to use the results we have proven in the last couple of sections. The inconsistency of $Ax = b$ means that b is not in the column space of A. We wish to find the vector Ax in the column space of A that is closest to b. By the Best Approximation Theorem, this is the projection of b onto $\operatorname{col} A$. Thus the least-squares solution is the solution to the equation $Ax = \operatorname{proj}_{\operatorname{col} A} b$. This system is certainly consistent, since $\operatorname{proj}_{\operatorname{col} A} b$ is in the column space of A. However, A is not necessarily invertible (not even necessarily square) so the solution may not be unique.

Example Find a least-squares solution (and the least-squares error) to $Ax = b$, where

$$A \;=\; \begin{bmatrix} 2 & 1 \\ -2 & 2 \\ 2 & 1 \end{bmatrix} \qquad b = \begin{bmatrix} -5 \\ 8 \\ 1 \end{bmatrix}$$

The columns of A are clearly linearly independent and actually orthogonal. Further b does not lie in the column space of A. We want to find a vector $\tilde{x}$ in $\mathbb{R}^2$ such that $A\tilde{x}$ is the projection of b onto col$A$. Since we have an orthogonal basis for the column space of A, we can easily compute the projection

$$\text{proj}_{\text{col}A}b \quad = \quad -\frac{24}{12}\begin{bmatrix}2\\-2\\2\end{bmatrix} + \frac{12}{6}\begin{bmatrix}1\\2\\1\end{bmatrix} \quad = \quad \begin{bmatrix}-4\\4\\-4\end{bmatrix} + \begin{bmatrix}2\\4\\2\end{bmatrix} \quad = \quad \begin{bmatrix}-2\\8\\-2\end{bmatrix}$$

Now we solve the system $Ax = \text{proj}_{\text{col}A}b$.

$$\begin{bmatrix}2 & 1 & -2\\-2 & 2 & 8\\2 & 1 & -2\end{bmatrix} \quad \to \ \ldots \ \to \quad \begin{bmatrix}1 & 0 & -2\\0 & 1 & 2\\0 & 0 & 0\end{bmatrix}$$

So the solution is $\tilde{x} = (-2, 2)$. Can you see how we should have known this without looking at the augmented matrix and row reducing?

Now we find the least-squares error by computing the distance between $A\tilde{x}$ and b.

$$A\tilde{x} - b \quad = \quad \begin{bmatrix}-2\\8\\-2\end{bmatrix} - \begin{bmatrix}-5\\8\\1\end{bmatrix} \quad = \quad \begin{bmatrix}3\\0\\-3\end{bmatrix}$$

So the least-squares error is $\|A\tilde{x} - b\| \quad = \quad 3\sqrt{2}$.

This example worked out very nicely because the columns of A were orthogonal. If the columns of A are not orthogonal, it is not as easy to compute the projection of b onto the column space of A. We next discuss a more general way of finding a least-squares solution that does not rely on having an orthogonal basis for the column space of A.

2.2 General Procedure for Obtaining a Least-squares Solution

As in the previous section, assume that A in an $m \times n$ matrix and b is a vector in $\mathbb{R}^m$, not necessarily in the column space of A. We aim to find a vector $\tilde{x}$ in $\mathbb{R}^n$ such that $A\tilde{x}$ is a best approximation (in the column space of A) to b. In other words we want to solve $Ax = \text{proj}_{\text{col}A}b$.

When we do not have an orthogonal basis for the column space of A, we cannot directly compute the projection of b onto the column space of A. However, we can *characterize* the projection vector. It is the unique vector Ax in the column space of A such that $b - Ax$ is in $(\text{col}A)^\perp$. Since $(\text{col}A)^\perp \ = \ \text{null}A^T$,

$$b - Ax \ \text{ in } (\text{col}A)^\perp \quad \Leftrightarrow \quad b - Ax \text{ in null}A^T \quad \Leftrightarrow \quad A^T(b - Ax) = 0 \quad \Leftrightarrow \quad A^Tb = A^T(Ax)$$

Thus we simply need to solve the equation $(A^TA)x \ = \ (A^Tb)$.

Example Find a least-squares solution (and the least-squares error) to $Ax = b$, where

$$A \quad = \quad \begin{bmatrix}2 & 1\\-2 & 0\\2 & 3\end{bmatrix} \qquad\qquad b = \begin{bmatrix}-5\\8\\1\end{bmatrix}$$

We will solve the equation $(A^TA)x = (A^Tb)$. Well,

$$A^TA \quad = \quad \begin{bmatrix}2 & -2 & 2\\1 & 0 & 3\end{bmatrix}\begin{bmatrix}2 & 1\\-2 & 0\\2 & 3\end{bmatrix} \quad = \quad \begin{bmatrix}12 & 8\\8 & 10\end{bmatrix} \qquad \text{and} \qquad A^Tb \quad = \quad \begin{bmatrix}2 & -2 & 2\\1 & 0 & 3\end{bmatrix}\begin{bmatrix}-5\\8\\1\end{bmatrix} \quad = \quad \begin{bmatrix}-24\\-2\end{bmatrix}$$

So we set up the augmented matrix and row reduce

$$\begin{bmatrix} 12 & 8 & -24 \\ 8 & 10 & -2 \end{bmatrix} \longrightarrow \ \dots \ \longrightarrow \begin{bmatrix} 1 & 0 & -4 \\ 0 & 1 & 3 \end{bmatrix}$$

Thus $(-4, 3)$ is the unique solution, thus $\tilde{x} = (-4, 3)$. (Notice that since $A^T A$ is a 2×2 invertible matrix we could also have computed $(A^T A)^{-1}(A^T b)$.) Now we find the least-squares error, $\|b - A\tilde{x}\|$.

$$b - A\tilde{x} \ = \ \begin{bmatrix} -5 \\ 8 \\ 1 \end{bmatrix} - \begin{bmatrix} 2 & 1 \\ -2 & 0 \\ 2 & 3 \end{bmatrix} \begin{bmatrix} -4 \\ 3 \end{bmatrix} = \begin{bmatrix} -5 \\ 8 \\ 1 \end{bmatrix} - \begin{bmatrix} -5 \\ 8 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Thus the least-squares error is zero. What does this mean? This means that b is actually in the column space of A, so $\tilde{x}$ is an exact solution!

Example Find all least-squares solutions (and the least-squares error) to $Ax = b$ where

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix} \qquad b = \begin{bmatrix} 7 \\ 2 \\ 3 \\ 6 \\ 5 \\ 4 \end{bmatrix}$$

We need to solve $(A^T A)x \ = \ A^T b$, so we compute:

$$A^T A \ = \ \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 6 & 3 & 3 \\ 3 & 3 & 0 \\ 3 & 0 & 3 \end{bmatrix}$$

$$A^T b \ = \ \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 7 \\ 2 \\ 3 \\ 6 \\ 5 \\ 4 \end{bmatrix} = \begin{bmatrix} 27 \\ 12 \\ 15 \end{bmatrix}$$

Thus we row reduce

$$\begin{bmatrix} 6 & 3 & 3 & 27 \\ 3 & 3 & 0 & 12 \\ 3 & 0 & 3 & 15 \end{bmatrix} \longrightarrow \ \dots \ \longrightarrow \begin{bmatrix} 1 & 0 & 1 & 5 \\ 0 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

The solutions of $(A^T A)x \ = \ A^T b$ are of the form:

$$x \ = \ \begin{bmatrix} -x_3 + 5 \\ x_3 - 1 \\ x_3 \end{bmatrix} \ = \ \begin{bmatrix} 5 \\ -1 \\ 0 \end{bmatrix} + x_3 \begin{bmatrix} -1 \\ 1 \\ 1 \end{bmatrix}$$

Thus the general least-squares solution of $Ax = b$ has the form

$$\tilde{x} \ = \ \begin{bmatrix} 5 \\ -1 \\ 0 \end{bmatrix} + t \begin{bmatrix} -1 \\ 1 \\ 1 \end{bmatrix} \qquad \text{for } t \text{ in } \mathbb{R}$$

To find the least-squares error, first compute $A\tilde{x}$ and $b - A\tilde{x}$

$$A\tilde{x} \;=\; \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 5-t \\ t-1 \\ t \end{bmatrix} \;=\; \begin{bmatrix} 4 \\ 4 \\ 4 \\ 5 \\ 5 \\ 5 \end{bmatrix} \qquad b - A\tilde{x} \;=\; \begin{bmatrix} 7 \\ 2 \\ 3 \\ 6 \\ 5 \\ 4 \end{bmatrix} - \begin{bmatrix} 4 \\ 4 \\ 4 \\ 5 \\ 5 \\ 5 \end{bmatrix} \;=\; \begin{bmatrix} 3 \\ -2 \\ -1 \\ 1 \\ 0 \\ -1 \end{bmatrix}$$

Thus the least-squared error is

$$\|b - A\tilde{x}\| \;=\; \sqrt{9+4+1+1+0+1} \;=\; 4$$

2.3 Uniqueness of Least-squared Solutions

Recall our two characterizations of least-squared solutions: a least-squared solution to a system $Ax = b$ is a solution to

$$Ax \;=\; \mathrm{proj}_{\mathrm{col}A} b \qquad \text{or equivalently} \qquad (A^T A)\, x \;=\; (A^T b)$$

From the first characterization, it is clear that a least-squared solution always exists, regardless of what b is, (because the projection of b onto col$A$ is in col$A$), and the solution will be unique if and only if the columns of A are linearly independent. Now look at the second characterization. Since the matrix $A^T A$ is square, the second equation has a unique solution (regardless of what b is) if and only if $A^T A$ is invertible. In this case, the solution is clearly $(A^T A)^{-1} A^T b$. Thus we have outlined the proof of the following theorem:

Theorem. *Let A be an $m \times n$ matrix. Then the following are equivalent:*

1. *The system $Ax = b$ has a unique least-squares solution for all b in $\mathbb{R}^m$.*
2. *The columns of A are linearly independent.*
3. *The matrix $A^T A$ is invertible.*

When a system has a unique least-squares solution the solution is given by

$$\tilde{x} \;=\; (A^T A)^{-1} A^T b$$