A single formulation for least squares, orthogonal projections, exact and approximate solutions

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For a square invertible matrix $A = [\vec{a}_1 \cdots \vec{a}_n]$, $A\vec{x} = \vec{b}$ has the solution $\vec{x} = A^{-1}\vec{b}$.

One way to describe this is that $\vec{b}$ is a linear combination of the columns of A, where

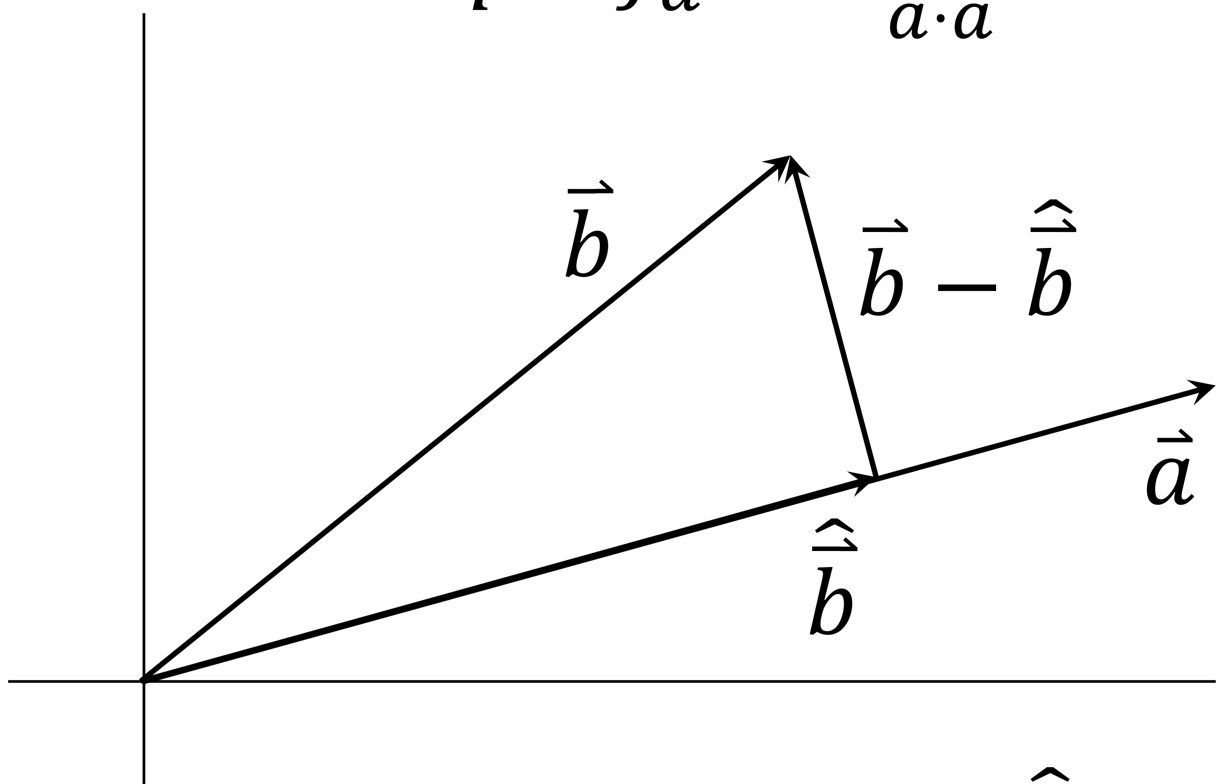
$$\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \vec{x} = A^{-1}\vec{b}$$

is the amounts of each column needed to build $\vec{b}$:

$$x_1\vec{a}_1 + \cdots + x_n\vec{a}_n = \vec{b}$$

Typically, a little later comes the idea of projecting one vector $\vec{b}$ onto another $\vec{a}$:

$$\hat{\vec{b}} = proj_{\vec{a}}\vec{b} = \frac{\vec{b}\cdot\vec{a}}{\vec{a}\cdot\vec{a}}\vec{a}.$$



Important is the fact that $\vec{b} - \hat{\vec{b}} \perp \vec{a}$.

More generally, where the columns of $A = [\vec{a}_1 \cdots \vec{a}_n]$ are orthogonal (and non-zero),

$$\hat{\vec{b}} = proj_{Col\ A}\vec{b} = \frac{\vec{b}\cdot\vec{a}_1}{\vec{a}_1\cdot\vec{a}_1}\vec{a}_1 + \cdots + \frac{\vec{b}\cdot\vec{a}_n}{\vec{a}_n\cdot\vec{a}_n}\vec{a}_n$$

$$= [\vec{a}_1 \cdots \vec{a}_n]\begin{bmatrix} \frac{\vec{b}\cdot\vec{a}_1}{\vec{a}_1\cdot\vec{a}_1} \\ \vdots \\ \frac{\vec{b}\cdot\vec{a}_n}{\vec{a}_n\cdot\vec{a}_n} \end{bmatrix} = A\hat{\vec{x}},$$

where $\hat{\vec{x}}$ is weightings of the columns of A in building $\vec{b}$ as well as we can.

Similar to before,

$$\vec{b} - \hat{\vec{b}} \perp Col\ A$$

that is,

$$\vec{b} - A\hat{\vec{x}} \perp Col\ A$$

that is,

$$A^T\left(\vec{b} - A\hat{\vec{x}}\right) = \vec{0}$$

which leads to

$$A^T A\hat{\vec{x}} = A^T\vec{b}.$$

This equation can also be found by minimizing the error $\left\|\vec{b} - A\vec{x}\,\right\|$.

So in general, the best solution $\hat{\vec{x}}$ to $A\vec{x} = \vec{b}$ (where the columns of A are linearly independent) is the least squares solution

$$\hat{\vec{x}} = (A^T A)^{-1} A^T \vec{b}.$$

There are four cases:

	Columns of $m \times n$ matrix A Orthogonal	Span R^m
Case 1	No	No
Case 2	No	Yes
Case 3	Yes	No
Case 4	Yes	Yes

The question is how the solutions to $A\vec{x} = \vec{b}$ for these four cases are related to

$$\hat{\vec{x}} = (A^T A)^{-1} A^T \vec{b}$$

and/or to

$$\hat{\vec{b}} = proj_{Col\,A} \vec{b} = A\hat{\vec{x}} = A(A^T A)^{-1} A^T \vec{b}\,.$$

Case 1

Columns of A are not orthogonal.

Columns of A do not span R^m.

$$\hat{\vec{x}} = (A^T A)^{-1} A^T \vec{b}$$

so that

$$\hat{\vec{b}} = proj_{Col\ A} \vec{b} = A\hat{\vec{x}} = A(A^T A)^{-1} A^T \vec{b}\ .$$

Case 2

Columns of A are not orthogonal.

Columns of A do span R^m.

(So A is square and invertible)

$$\hat{\vec{x}} = (A^T A)^{-1} A^T \vec{b} = A^{-1} (A^T)^{-1} A^T \vec{b} = A^{-1} \vec{b}$$

so that

$$\hat{\vec{b}} = proj_{Col\,A} \vec{b} = A \hat{\vec{x}} = A\left(A^{-1} \vec{b}\right) = \vec{b}.$$

Case 2

Columns of A are not orthogonal.

Columns of A do span R^m.

(So A is square and invertible)

$$\hat{\vec{x}} = (A^T A)^{-1} A^T \vec{b} = A^{-1}(A^T)^{-1} A^T \vec{b} = A^{-1}\vec{b}$$

so that

$$\hat{\vec{b}} = proj_{Col\,A}\vec{b} = A\hat{\vec{x}} = A\left(A^{-1}\vec{b}\right) = \vec{b}.$$

I think we usually make this observation with our students.

Case 3

Columns of A are orthogonal.

Columns of A do not span R^m.

First,

$$A^T A = \begin{bmatrix} \vec{a}_1^T \\ \vdots \\ \vec{a}_n^T \end{bmatrix} [\vec{a}_1 \cdots \vec{a}_n]$$

$$= \begin{bmatrix} \vec{a}_1^T \vec{a}_1 & & \\ & \ddots & \\ & & \vec{a}_n^T \vec{a}_n \end{bmatrix}$$

So

$$(A^TA)^{-1}A^T = \begin{bmatrix} \frac{1}{\vec{a}_1\cdot\vec{a}_1} & & \\ & \ddots & \\ & & \frac{1}{\vec{a}_n\cdot\vec{a}_n} \end{bmatrix} \begin{bmatrix} \vec{a}_1^T \\ \vdots \\ \vec{a}_n^T \end{bmatrix} = \begin{bmatrix} \frac{\vec{a}_1^T}{\vec{a}_1\cdot\vec{a}_1} \\ \vdots \\ \frac{\vec{a}_n^T}{\vec{a}_n\cdot\vec{a}_n} \end{bmatrix}$$

so that

$$\hat{\vec{x}} = (A^TA)^{-1}A^T\vec{b} = \begin{bmatrix} \frac{\vec{b}\cdot\vec{a}_1}{\vec{a}_1\cdot\vec{a}_1} \\ \vdots \\ \frac{\vec{b}\cdot\vec{a}_n}{\vec{a}_n\cdot\vec{a}_n} \end{bmatrix}.$$

Then

$$\hat{\vec{b}} = A\hat{\vec{x}} = [\vec{a}_1 \cdots \vec{a}_n]\begin{bmatrix} \frac{\vec{b}\cdot\vec{a}_1}{\vec{a}_1\cdot\vec{a}_1} \\ \vdots \\ \frac{\vec{b}\cdot\vec{a}_n}{\vec{a}_n\cdot\vec{a}_n} \end{bmatrix}$$

$$= \frac{\vec{b}\cdot\vec{a}_1}{\vec{a}_1\cdot\vec{a}_1}\vec{a}_1 + \cdots + \frac{\vec{b}\cdot\vec{a}_n}{\vec{a}_n\cdot\vec{a}_n}\vec{a}_n$$

which is what we found earlier when we projected $\vec{b}$ onto the column space of A.

Then

$$\hat{\vec{b}} = A\hat{\vec{x}} = [\vec{a}_1 \cdots \vec{a}_n]\begin{bmatrix} \frac{\vec{b}\cdot\vec{a}_1}{\vec{a}_1\cdot\vec{a}_1} \\ \vdots \\ \frac{\vec{b}\cdot\vec{a}_n}{\vec{a}_n\cdot\vec{a}_n} \end{bmatrix}$$

$$= \frac{\vec{b}\cdot\vec{a}_1}{\vec{a}_1\cdot\vec{a}_1}\vec{a}_1 + \cdots + \frac{\vec{b}\cdot\vec{a}_n}{\vec{a}_n\cdot\vec{a}_n}\vec{a}_n$$

which is what we found earlier when we projected $\vec{b}$ onto the column space of A.

I am not sure that we always make this connection with our students.

<u>Case 4</u>

Columns of A <u>are</u> orthogonal.
Columns of A <u>do</u> span R^m.

Same as case 3, except that $\hat{\vec{b}} = \vec{b}$ exactly, since the columns of A span R^m.

The point is that every one of the four cases we typically consider can be viewed as a special case of the least squares solution $\hat{\vec{x}}$ to $A\vec{x} = \vec{b}$:

$$\hat{\vec{x}} = (A^T A)^{-1} A^T \vec{b}$$

$$\hat{\vec{b}} = proj_{Col\,A} \vec{b} = A\hat{\vec{x}} = A(A^T A)^{-1} A^T \vec{b}$$

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Questions?