Linear equations: Case of singular square matrix

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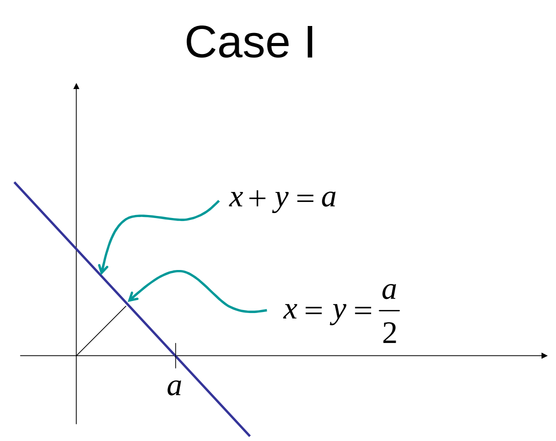
For a set of linear equations $\mathbf{Ax} = \mathbf{b}$ when $\mathbf{A}$ is square but singular, there are two cases:

- Case I: There are no solutions (so we look for the best approximation).
- Case II: There is a solution (in which case there are many solutions).

Example: Consider the equations:

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix} = x \cdot \begin{bmatrix} 1 \\ 1 \end{bmatrix} + y \cdot \begin{bmatrix} 1 \\ 1 \end{bmatrix} = (x+y) \cdot \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

Case I: When $a = b$, there are many solutions, since $\begin{bmatrix} a \\ a \end{bmatrix} = (x+y) \cdot \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ or $x + y = a$. One possible solution—the one that falls in the column space spanned by $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ -- is $x = y = \dfrac{a}{2}$. A vector that lies in the null space of $\mathbf{A}$ is $\begin{bmatrix} 1 \\ -1 \end{bmatrix}$. Thus, the set of possible solutions can be characterized as $\begin{bmatrix} a/2 \\ a/2 \end{bmatrix} + \alpha \cdot \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \begin{bmatrix} a/2 + \alpha \\ a/2 - \alpha \end{bmatrix}$. We might choose the solution that has minimum norm, which is easily shown to be $\alpha = 0$ or $x = y = \dfrac{a}{2}$. That is, the minimum norm solution is the one that falls in the column subspace spanned by $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$. This is illustrated geometically below.

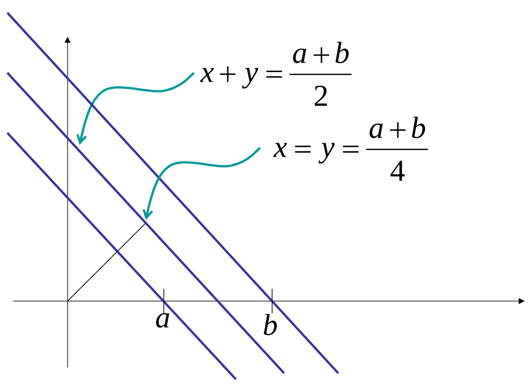


Case II: When $a \neq b$, there is no solution. The best approximate solution (in the mean-square sense) would minimize

$$\|\mathbf{b} - \mathbf{Ax}\|^2 = \left\| \begin{bmatrix} a-x-y \\ b-x-y \end{bmatrix} \right\|^2 = (a-x-y)^2 + (b-x-y)^2 .$$

This can be solved the conventional way (differentiation) to establish that the stationary point satisfies $x + y = \frac{a+b}{2}$. Thus, the LS approximation is not unique (it lies anywhere on a line falling midway between $x + y = a$ and $x + y = b$). So, we might again choose to pick the minimum-norm solution—examining the geometry, this is clearly at $x = y$, or $x = y = \frac{a+b}{4}$. This approaches the same solution as in Case I as $a \to b$. This case is illustrated below.

Case II



An alternative approach is to use the projection theorem. The minimization is restated as minimizing

$$\left\| \begin{bmatrix} a \\ b \end{bmatrix} - (x+y) \cdot \begin{bmatrix} 1 \\ 1 \end{bmatrix} \right\|^2 .$$

While the projection on the subspace spanned by $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ must be unique, this still does not uniquely specify $\mathbf{x}$. The orthogonality principle states that

$$[1 \quad 1]\left\{ \begin{bmatrix} a \\ b \end{bmatrix} - (x+y) \cdot \begin{bmatrix} 1 \\ 1 \end{bmatrix} \right\} = 0 \quad \text{or} \quad x + y = \frac{a+b}{2} .$$

Thus, this gives us the same answer as before—the projection theorem actually gives us many solutions—and we still have to minimize the norm to arrive at a unique answer.