CS450: Numerical Analysis

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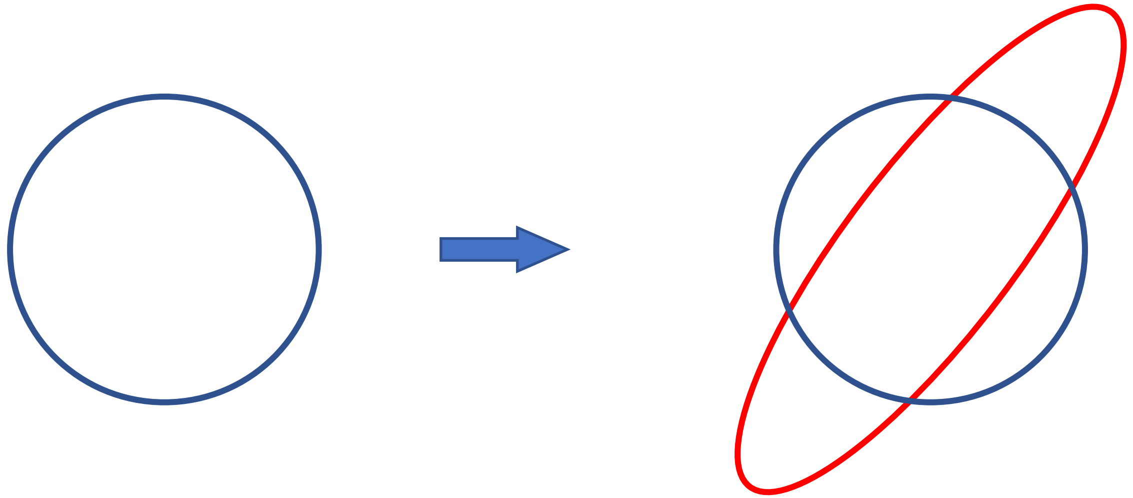
Matrix Norm

- What does matrix multiplication do to a linear (sub)space?
  - Rotation & stretching
- What does matrix norm mean?
  - How much a particular linear operator A stretch a unit ball
  - This unit ball depends on which norm we used for defining it



Matrix Norms (cont'd)

- Given a vector norm $\|\cdot\|$
  - The matrix norm induced by this vector norm is given as

$$\|\boldsymbol{A}\| = \max_{\|\boldsymbol{x}\|=1} \|\boldsymbol{A}\boldsymbol{x}\|$$

    - Different vector norms can induce different matrix norms for the same matrix
  - Examples
    - When the norm is L-1 norm, $\|\boldsymbol{A}\|_{\mathbf{1}} = \max_j \sum_{i=1}^{m} |a_{ij}|$: the maximum absolute column sum of the matrix
    - When the norm is L-∞ norm, $\|\boldsymbol{A}\|_{\infty} = \max_i \sum_{j=1}^{n} |a_{ij}|$: the maximum absolute row sum of the matrix

Matrix Norms (cont'd)

- When the norm is the Euclidean norm $\|\cdot\|_2$
  - The matrix norm induced by this vector norm is given as

$$\|\boldsymbol{A}\|_{\mathbf{2}} = \max_{\boldsymbol{x}\neq\mathbf{0}} \frac{\|\boldsymbol{A}\boldsymbol{x}\|_2}{\|\boldsymbol{x}\|_2} = \max_{\|\boldsymbol{x}\|_2=1} \|\boldsymbol{A}\boldsymbol{x}\|_{\mathbf{2}}$$

    - This is called the spectral norm of matrix $\boldsymbol{A}$

Matrix Condition Number

- Given a matrix $\boldsymbol{A}$, the condition number is

$$\kappa(\boldsymbol{A}) = \|\boldsymbol{A}\| \cdot \|\boldsymbol{A}^{-\mathbf{1}}\|$$

- Definition: a $n \times n$ matrix $\boldsymbol{A}$ is said to be nonsingular/invertible if $\boldsymbol{A}^{-1}$ exists such that $\boldsymbol{A}\boldsymbol{A}^{-1} = \boldsymbol{A}^{-1}\boldsymbol{A} = \boldsymbol{I}$; otherwise, it is singular
- Large $\kappa(\boldsymbol{A})$ implies the matrix is nearly singular

Matrix Condition Number (cont'd)

- Is small determinant a good indicator for singularity?
- What is determinant really doing?

Matrix Condition Number (cont'd)

- Given a matrix $\boldsymbol{A}$, the condition number is

$$\kappa(\boldsymbol{A}) = \|\boldsymbol{A}\| \cdot \|\boldsymbol{A}^{-1}\|$$

- Estimating $\|\boldsymbol{A}\|$ is generally easy, but estimating $\|\boldsymbol{A}^{-1}\|$ is usually challenging
- Example: how to quickly estimate $\|\boldsymbol{A}^{-1}\|$ for the following matrix?

$$\boldsymbol{A} = \begin{bmatrix} 0.913 & 0.659 \\ 0.457 & 0.330 \end{bmatrix}$$

Matrix Condition Number (cont'd)

- Estimating $\|\boldsymbol{A}^{-1}\|$ is usually challenging, we can try to find a pair $\boldsymbol{z}$ and $\boldsymbol{y}$, such that $\boldsymbol{Az} = \boldsymbol{y}$, then

$$\|\boldsymbol{z}\| = \left\|\boldsymbol{A}^{-1}\boldsymbol{y}\right\| \leq \left\|\boldsymbol{A}^{-1}\right\| \cdot \|\boldsymbol{y}\|$$

- Since $\frac{\|\boldsymbol{z}\|}{\|\boldsymbol{y}\|} \leq \left\|\boldsymbol{A}^{-1}\right\|$, if the ratio $\frac{\|\boldsymbol{z}\|}{\|\boldsymbol{y}\|}$ is relatively large, it provides a good estimation for $\left\|\boldsymbol{A}^{-1}\right\|$

Matrix Condition Number (cont'd)

- Example: how to quickly estimate $||\boldsymbol{A}^{-1}||$ for the following matrix?

$$\boldsymbol{A} = \begin{bmatrix} 0.913 & 0.659 \\ 0.457 & 0.330 \end{bmatrix}$$

- Since $\boldsymbol{y} = [0, 1.5]$, $\boldsymbol{z} = [-7780, 10780]$ is a candidate pair for $\boldsymbol{Az} = \boldsymbol{y}$

$$||\boldsymbol{A}^{-1}||_1 \approx \frac{||\boldsymbol{z}||_1}{||\boldsymbol{y}||_1} \approx 1.238 \times 10^4$$

- Hence the condition number is

$$\kappa(\boldsymbol{A}) = ||\boldsymbol{A}||_1 \cdot ||\boldsymbol{A}^{-1}||_1 \approx 1.370 \times 1.238 \times 10^4 = 1.696 \times 10^4$$

Linear System

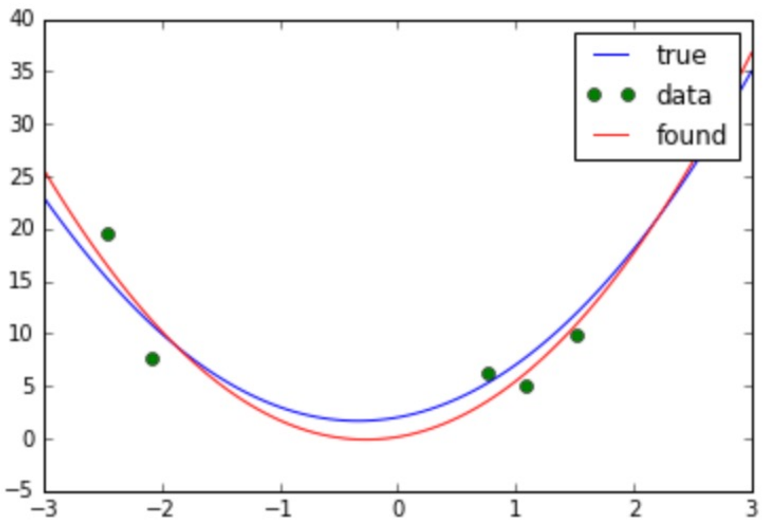
- Suppose we want to solve a linear system $\boldsymbol{Ax} = \boldsymbol{b}$, with $\boldsymbol{A}$ and $\boldsymbol{b}$ being known, what does this mean?
  - What does $\boldsymbol{Ax}$ mean?
  - What does $\boldsymbol{Ax} = \boldsymbol{b}$ mean?
- What happens if $\boldsymbol{A}$ is not a square matrix?

Linear Least Square

- Instead of solving $\boldsymbol{Ax} = \boldsymbol{b}$, we aim to find $\boldsymbol{x}$ to minimize $||\boldsymbol{Ax} - \boldsymbol{b}||_{\boldsymbol{2}}$
  - Generally, a perfect fitting may not be possible, and we look for an approximation
  - In data science, this is called Linear Regression
- Motivating examples: Room renting price

Linear Least Square (Cont’d)

- Motivating examples: Does linear least square only deals with “linear”?
- Data fitting: Non-linearity



Solving the Linear Least Square

- How to find $\boldsymbol{x}^* = \mathrm{argmin}_{\boldsymbol{x}} \|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}\|_2$ where $\boldsymbol{A} \in R^{m \times n}$?
  - The residual error can be written as

$$Err(\boldsymbol{x}) = (\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b})^T(\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b})$$

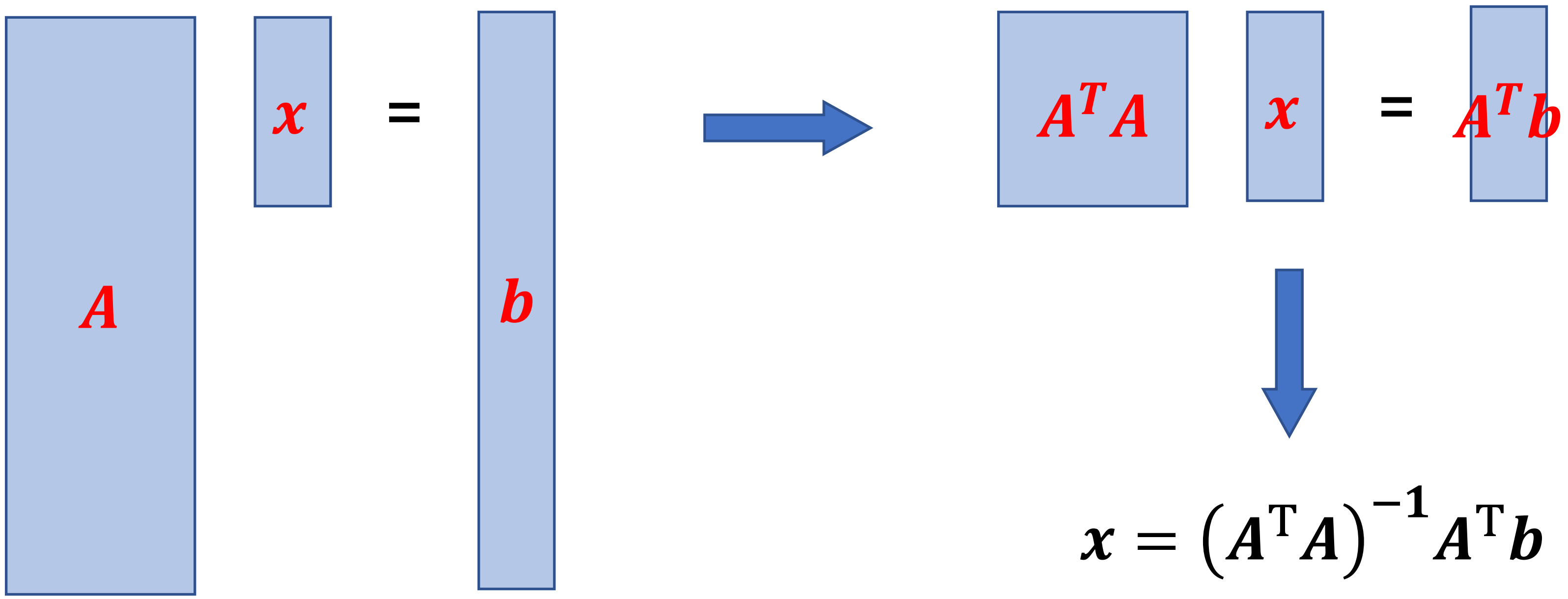
  - Let $\frac{\partial Err(\boldsymbol{x})}{\partial \boldsymbol{x}} = 2\boldsymbol{A}^T(\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}) = \boldsymbol{0}$, which is equivalent to $(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})\boldsymbol{x} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{b}$
  - If $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$ is nonsingular, we obtain the solution as

$$\boldsymbol{x} = (\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{b}$$

  - This is known as the normal equation

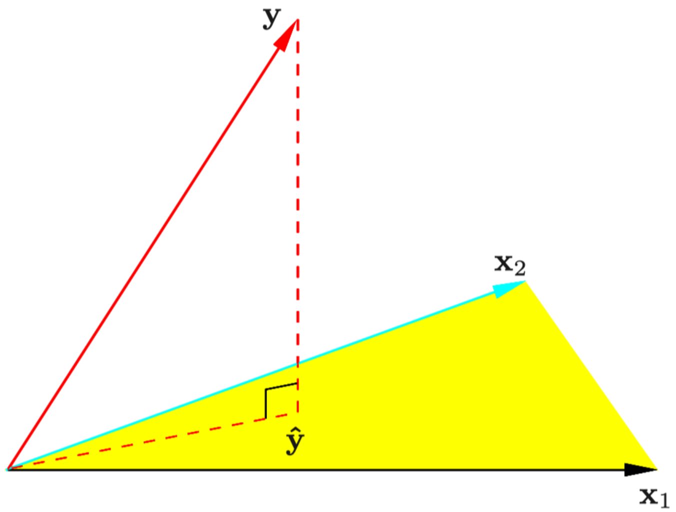
Solving the Linear Least Square (cont'd)

- An algebraic view of the minimizer
  - Typically, the matrix $\boldsymbol{A}$ is a tall matrix, and the solution procedure of linear regression is somewhat like the following



$$\boldsymbol{x} = \left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{b}$$

Solving the Linear Least Square (cont'd)



- A geometric point of view
  - A square matrix $\boldsymbol{P}$ is called a projector if $\boldsymbol{P}^2 = \boldsymbol{P}$
    - It project a vector onto the space of span(P) but leave whatever already in it
  - The linear least square operates at minimizing the error between the label vector $\boldsymbol{b}$ and the space spanned by the data points $\boldsymbol{a}_1, \dots, \boldsymbol{a}_n$

Example

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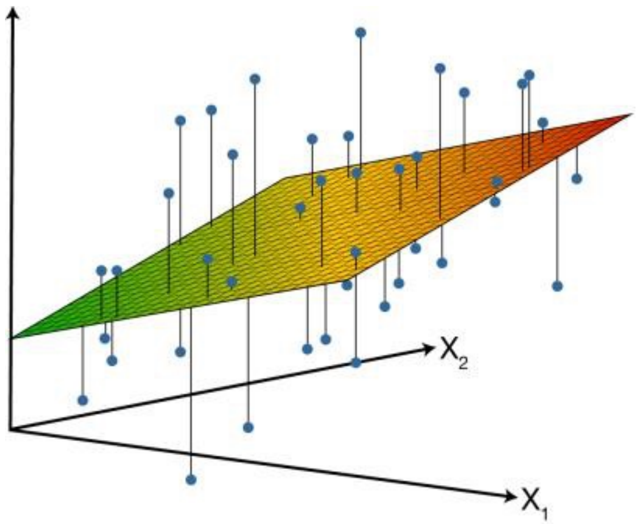
- Pull strength of a wired bond against wire length and die height:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$$



Hastie. et al. 2009

$$\mathbf{X} = \begin{bmatrix} 1 & 2 & 50 \\ 1 & 8 & 110 \\ 1 & 11 & 120 \\ 1 & 10 & 550 \\ 1 & 8 & 295 \\ 1 & 4 & 200 \\ 1 & 2 & 375 \\ 1 & 2 & 52 \\ 1 & 9 & 100 \\ 1 & 8 & 300 \\ 1 & 4 & 412 \\ 1 & 11 & 400 \\ 1 & 12 & 500 \\ 1 & 2 & 360 \\ 1 & 4 & 205 \\ 1 & 4 & 400 \\ 1 & 20 & 600 \\ 1 & 1 & 585 \\ 1 & 10 & 540 \\ 1 & 15 & 250 \\ 1 & 15 & 290 \\ 1 & 16 & 510 \\ 1 & 17 & 590 \\ 1 & 6 & 100 \\ 1 & 5 & 400 \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} 9.95 \\ 24.45 \\ 31.75 \\ 35.00 \\ 25.02 \\ 16.86 \\ 14.38 \\ 9.60 \\ 24.35 \\ 27.50 \\ 17.08 \\ 37.00 \\ 41.95 \\ 11.66 \\ 21.65 \\ 17.89 \\ 69.00 \\ 10.30 \\ 34.93 \\ 46.59 \\ 44.88 \\ 54.12 \\ 56.63 \\ 22.13 \\ 21.15 \end{bmatrix}$$

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 2 & 8 & \cdots & 5 \\ 50 & 110 & \cdots & 400 \end{bmatrix} \begin{bmatrix} 1 & 2 & 50 \\ 1 & 8 & 110 \\ \vdots & \vdots & \vdots \\ 1 & 5 & 400 \end{bmatrix}$$

$$= \begin{bmatrix} 25 & 206 & 8{,}294 \\ 206 & 2{,}396 & 77{,}177 \\ 8{,}294 & 77{,}177 & 3{,}531{,}848 \end{bmatrix}$$

$$\mathbf{X}'\mathbf{y} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 2 & 8 & \cdots & 5 \\ 50 & 110 & \cdots & 400 \end{bmatrix} \begin{bmatrix} 9.95 \\ 24.45 \\ \vdots \\ 21.15 \end{bmatrix} = \begin{bmatrix} 725.82 \\ 8{,}008.47 \\ 274{,}816.71 \end{bmatrix}$$

$$\begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_2 \end{bmatrix} = \begin{bmatrix} 25 & 206 & 8{,}294 \\ 206 & 2{,}396 & 77{,}177 \\ 8{,}294 & 77{,}177 & 3{,}531{,}848 \end{bmatrix}^{-1} \begin{bmatrix} 725.82 \\ 8{,}008.37 \\ 274{,}811.31 \end{bmatrix}$$

$$= \begin{bmatrix} 0.214653 & -0.007491 & -0.000340 \\ -0.007491 & 0.001671 & -0.000019 \\ -0.000340 & -0.000019 & +0.0000015 \end{bmatrix} \begin{bmatrix} 725.82 \\ 8{,}008.47 \\ 274{,}811.31 \end{bmatrix}$$

$$= \begin{bmatrix} 2.26379143 \\ 2.74426964 \\ 0.01252781 \end{bmatrix}$$

$$\hat{y} = 2.26379 + 2.74427x_1 + 0.01253x_2$$

Potential Issue

- We talked about all these by assuming that we can solve the normal equation
- What is the condition number of this linear system?

```
n = 5

A = np.random.randn(5, 5) * 10**-np.linspace(0, -5, n)
la.cond(A)
```

```
1157203.022995764
```

```
la.cond(np.dot(A.T, A))
```

```
1339118843597.7017
```

Conditioning of Rectangular Matrix

- Given an overdetermined system $\boldsymbol{Ax} = \boldsymbol{b}$ where $\boldsymbol{A} \in R^{m\times n}, m > n$ and $\mathrm{rank}(\boldsymbol{A}) = n$,
  - recall that $\kappa(\boldsymbol{A}) = \|\boldsymbol{A}\|_2 \cdot \|\boldsymbol{A}^{-\boldsymbol{1}}\|_2$
  - we can calculate $\|\boldsymbol{A}\|_2$, but $\boldsymbol{A}$ is not invertable, therefore, …
  - we define a pseudoinverse of $\boldsymbol{A}$ by $\boldsymbol{A}^{+} = (\boldsymbol{A}^{T}\boldsymbol{A})^{-\boldsymbol{1}}\boldsymbol{A}^{T}$, note that $\boldsymbol{A}^{+}\boldsymbol{A} = \boldsymbol{I}$
- Then, the condition number of a rectangular matrix $\boldsymbol{A}$ is defined as

$$\kappa(\boldsymbol{A}) = \|\boldsymbol{A}\|_2 \cdot \|\boldsymbol{A}^{+}\|_2$$

  - What if $\mathrm{rank}(\boldsymbol{A}) < n$? $\kappa(\boldsymbol{A}) = \infty$
  - We also define $\kappa(\boldsymbol{A}) = \sigma_{max}/\sigma_{min}$, is it still true here?

Example (1)

- Calculate the condition number of the following rectangular matrix $\boldsymbol{A}$

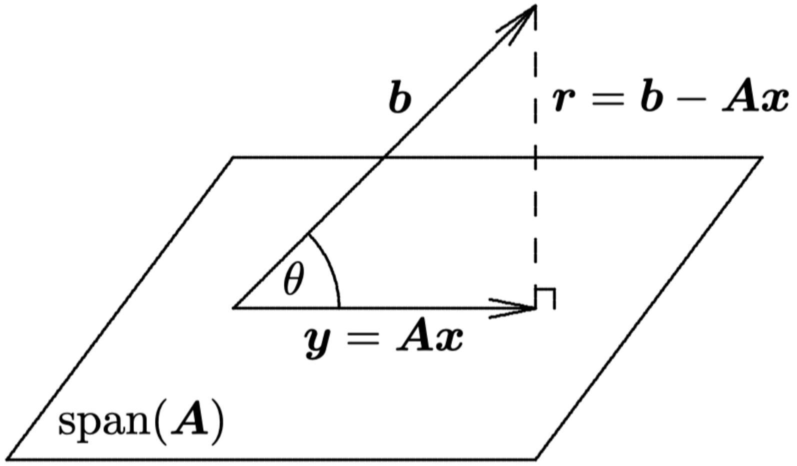
$$\boldsymbol{A}\boldsymbol{x} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \cong \begin{bmatrix} 1237 \\ 1941 \\ 2417 \\ 711 \\ 1177 \\ 475 \end{bmatrix} = \boldsymbol{b}.$$

$$\Rightarrow \quad \boldsymbol{A}^{+} = (\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T = \frac{1}{4}\begin{bmatrix} 2 & 1 & 1 & -1 & -1 & 0 \\ 1 & 2 & 1 & 1 & 0 & -1 \\ 1 & 1 & 2 & 0 & 1 & 1 \end{bmatrix}$$

- Consequently, $\|\boldsymbol{A}\|_2 = 2$ and $\|\boldsymbol{A}^{+}\|_2 = 1$, which gives $\kappa(\boldsymbol{A}) = \|\boldsymbol{A}\|_2 \cdot \|\boldsymbol{A}^{+}\|_2 = 2$

Conditioning of Linear Least Square

- Back to the problem of finding $\boldsymbol{x}^* = \mathrm{argmin}_{\boldsymbol{x}} ||\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}||_2$ where $\boldsymbol{A} \in R^{m \times n}$
- Unlike the conditioning of a linear system $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$, which only depends on the condition of the $\boldsymbol{A}$; the conditioning/sensitivity of the solution to an LSQ depends on both $\boldsymbol{A}$ and $\boldsymbol{b}$
  - It is more stable when $\boldsymbol{b}$ lies near span($\boldsymbol{A}$)
  - It is sensitive if $\boldsymbol{b}$ lies near orthogonal to span($\boldsymbol{A}$)



Conditioning of LSQ: A Closer Look (1)

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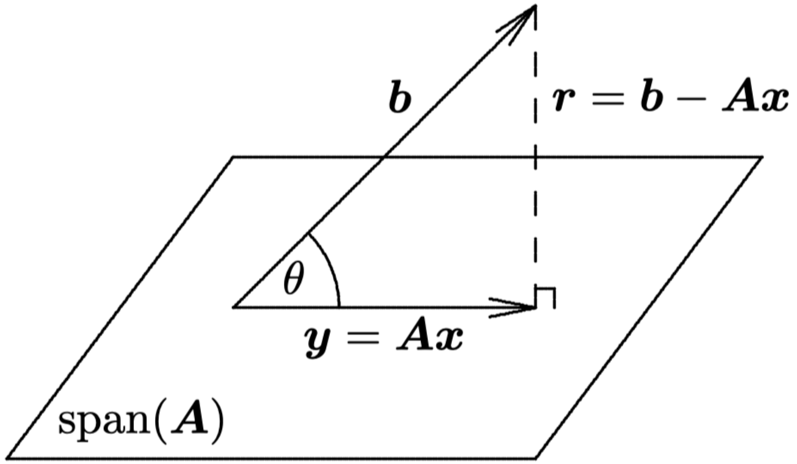
- Recall that solution of the normal equation $\boldsymbol{A}^T\boldsymbol{A}\boldsymbol{x} = \boldsymbol{A}^T\boldsymbol{b}$ solves the LSQ
- For a perturbation on the RHS, it gives $\boldsymbol{A}^T\boldsymbol{A}(\boldsymbol{x} + \Delta\boldsymbol{x}) = \boldsymbol{A}^T(\boldsymbol{b} + \Delta\boldsymbol{b})$, i.e., $\boldsymbol{A}^T\boldsymbol{A}\Delta\boldsymbol{x} = \boldsymbol{A}^T\Delta\boldsymbol{b}$. As such, $\Delta\boldsymbol{x} = (\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T\Delta\boldsymbol{b} = \boldsymbol{A}^+\Delta\boldsymbol{b}$, and this leads to:

$$\begin{aligned}
\frac{\|\Delta\boldsymbol{x}\|_2}{\|\boldsymbol{x}\|_2} &\leq \|\boldsymbol{A}^+\|_2 \frac{\|\Delta\boldsymbol{b}\|_2}{\|\boldsymbol{x}\|_2} \\
&= \operatorname{cond}(\boldsymbol{A}) \frac{\|\boldsymbol{b}\|_2}{\|\boldsymbol{A}\|_2 \cdot \|\boldsymbol{x}\|_2} \frac{\|\Delta\boldsymbol{b}\|_2}{\|\boldsymbol{b}\|_2} \\
&\leq \operatorname{cond}(\boldsymbol{A}) \frac{\|\boldsymbol{b}\|_2}{\|\boldsymbol{A}\boldsymbol{x}\|_2} \frac{\|\Delta\boldsymbol{b}\|_2}{\|\boldsymbol{b}\|_2} \\
&= \operatorname{cond}(\boldsymbol{A}) \frac{1}{\cos(\theta)} \frac{\|\Delta\boldsymbol{b}\|_2}{\|\boldsymbol{b}\|_2}.
\end{aligned}$$

- What determines θ?
- What values of θ are bad?



Conditioning of LSQ: A Closer Look (2)

- Recall that solution of the normal equation $\boldsymbol{A}^T\boldsymbol{A}\boldsymbol{x} = \boldsymbol{A}^T\boldsymbol{b}$ solves the LSQ
- What about there is a perturbation to matrix $\boldsymbol{A}$ (i.e., $\boldsymbol{A}$ becomes $\boldsymbol{A} + \boldsymbol{E}$)?

$$\frac{\|\Delta \boldsymbol{x}\|_2}{\|\boldsymbol{x}\|_2} \leq \left([\mathrm{cond}(\boldsymbol{A})]^2 \tan(\theta) + \mathrm{cond}(\boldsymbol{A})\right) \frac{\|\boldsymbol{E}\|_2}{\|\boldsymbol{A}\|_2}$$

- Two notable behaviors
  - If $\theta \approx 0$, the condition number is cond($\boldsymbol{A}$)
  - Otherwise, cond($\boldsymbol{A}$)^2