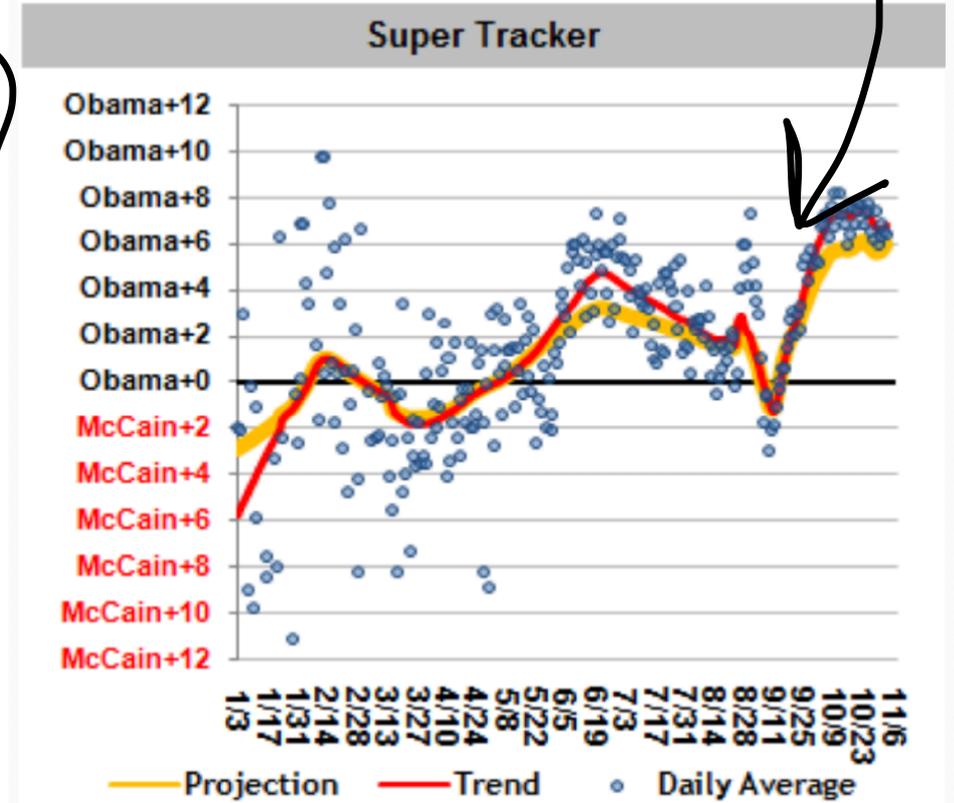
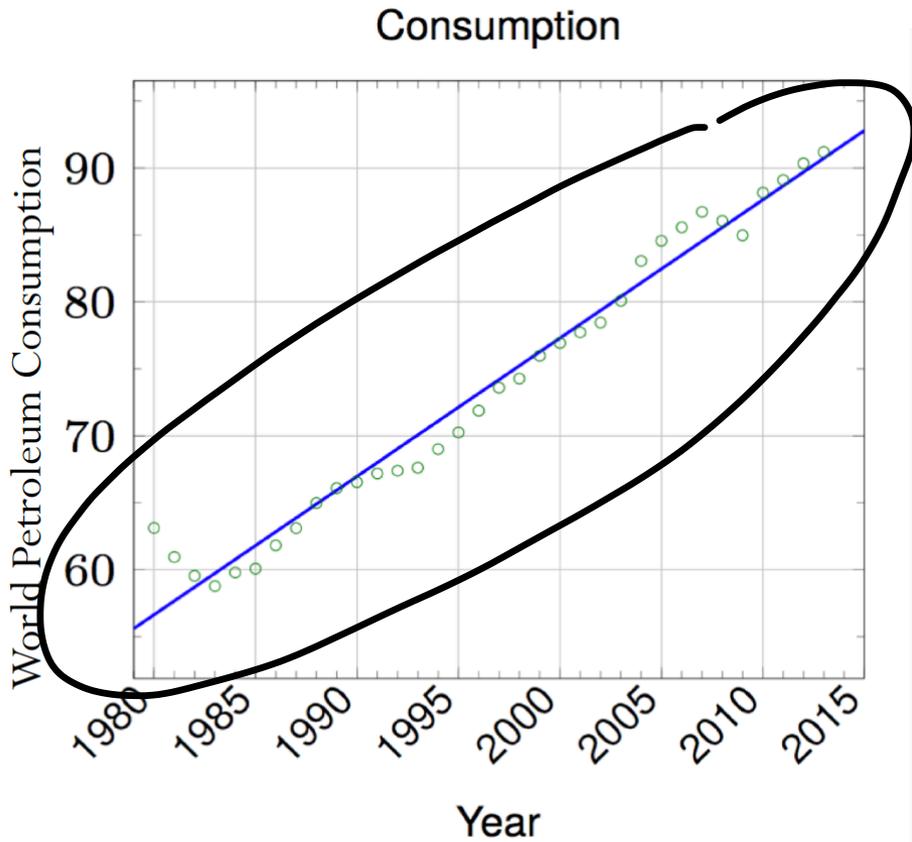


# Least Squares and Data Fitting

# Data fitting

How do we best fit a set of data points?



# Linear Least Squares

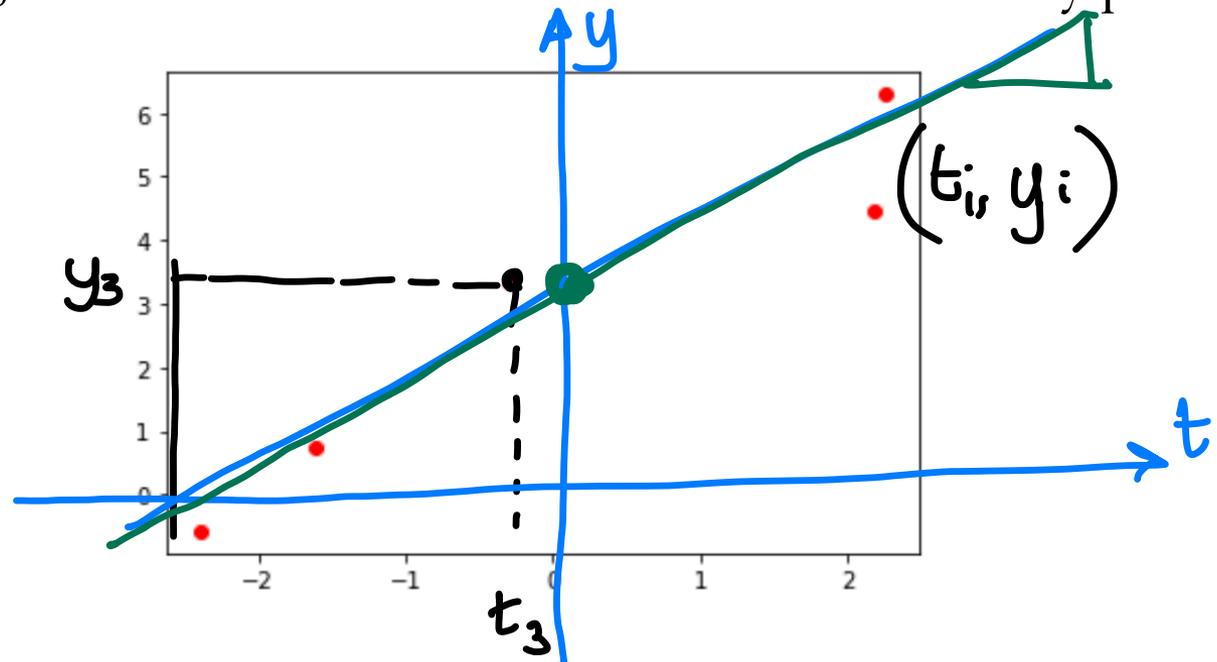
## 1) Fitting with a line

Given  $m$  data points  $\{\{t_1, y_1\}, \dots, \{t_m, y_m\}\}$ , we want to find the function

$$y = x_0 + x_1 t$$

that best fit the data (or better, we want to find the coefficients  $x_0, x_1$ ).

Thinking geometrically, we can think “what is the line that most nearly passes through all the points?”



Given  $m$  data points  $\{(t_1, y_1), \dots, (t_m, y_m)\}$ , we want to find  $x_0$  and  $x_1$  such that

$(t_i, y_i)$

$$y_i = x_0 + x_1 t_i$$

$$\forall i \in [1, m]$$

$$\begin{cases} y_1 = x_0 + x_1 t_1 \\ y_2 = x_0 + x_1 t_2 \\ y_3 = x_0 + x_1 t_3 \\ \vdots \\ y_m = x_0 + x_1 t_m \end{cases}$$

}

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$$

=

$$\begin{bmatrix} 1 & t_1 \\ 1 & t_2 \\ \vdots & \vdots \\ 1 & t_m \end{bmatrix}$$

$$\begin{bmatrix} x_0 \\ x_1 \end{bmatrix}$$

$\tilde{x}$   $n \times 1$

$\tilde{b}$   $m \times 1$

$\tilde{A}$   $m \times n$

$$\tilde{b} = \tilde{A} \tilde{x}$$

overdetermined!  $\boxed{m > n}$

$$\begin{matrix} \text{given} \nearrow & \tilde{b} & = & \tilde{A} & \tilde{x} \\ & & & \uparrow & \nwarrow \text{find} \\ & & & \text{given} & \end{matrix}$$

Given  $m$  data points  $\{\{t_1, y_1\}, \dots, \{t_m, y_m\}\}$ , we want to find  $x_0$  and  $x_1$  such that

$$y_i = x_0 + x_1 t_i \quad \forall i \in [1, m]$$

or in matrix form:

$$\begin{bmatrix} 1 & t_1 \\ \vdots & \vdots \\ 1 & t_m \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}$$

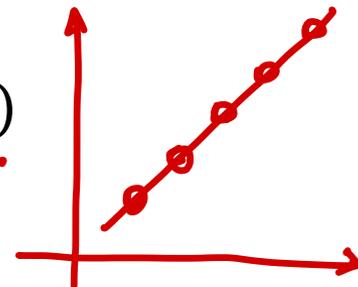
$m \times n$     $n \times 1$     $m \times 1$

$$\mathbf{A} \mathbf{x} = \mathbf{b}$$

Note that this system of linear equations has more equations than unknowns –  
OVERDETERMINED  
SYSTEMS

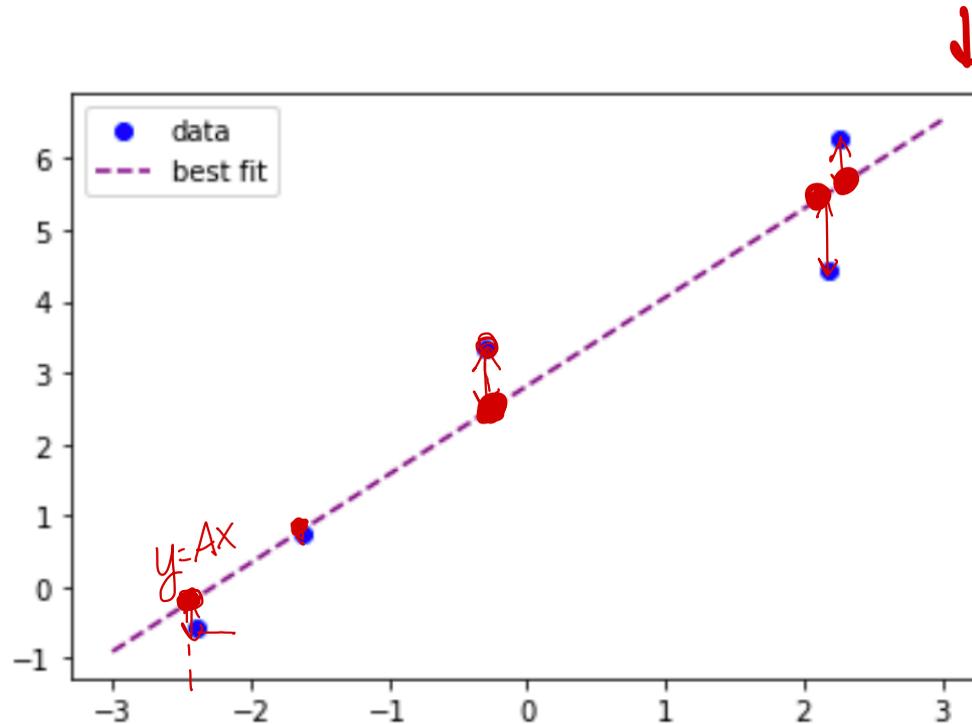
We want to find the appropriate linear combination of the columns of  $\mathbf{A}$  that makes up the vector  $\mathbf{b}$ .

If a solution exists that satisfies  $\mathbf{A} \mathbf{x} = \mathbf{b}$  then  $\mathbf{b} \in \text{range}(\mathbf{A})$



# Linear Least Squares

- In most cases,  $\mathbf{b} \notin \text{range}(\mathbf{A})$  and  $\mathbf{A} \mathbf{x} = \mathbf{b}$  **does not have an exact solution!**



We want to  
find  $\tilde{x}$  s.t  
 $y = Ax$  better  
approximates  
 $\tilde{b}$

- Therefore, an overdetermined system is better expressed as

$$\mathbf{A} \mathbf{x} \cong \mathbf{b}$$

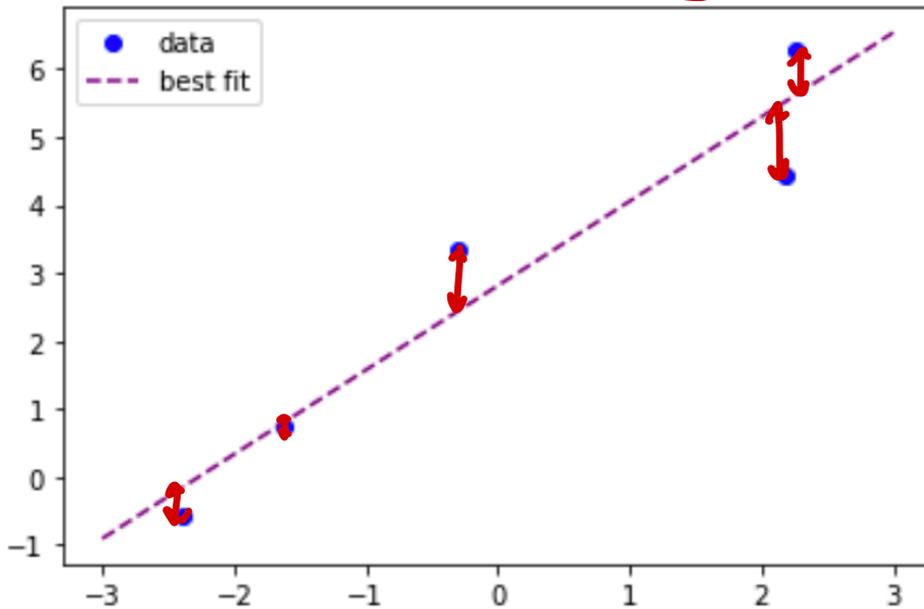
$$m > n$$

# Linear Least Squares

$$\begin{pmatrix} A & x \end{pmatrix} = b$$

- Least Squares: find the solution  $x$  that minimizes the residual

$\min \rightarrow r = b - Ax = \begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_5 \end{bmatrix} = \begin{bmatrix} b_1 - y_1 \\ b_2 - y_2 \\ \vdots \\ b_5 - y_5 \end{bmatrix}$



$r$  is a vector  
 $\min \|r\|$

- Let's define the function  $\phi$  as the square of the 2-norm of the residual

$\phi(x) = \|b - Ax\|_2^2$

# Linear Least Squares

- **Least Squares:** find the solution  $\mathbf{x}$  that minimizes the residual

$$\mathbf{r} = \mathbf{b} - \mathbf{A}\mathbf{x}$$

- Let's define the function  $\phi$  as the square of the 2-norm of the residual

$$\phi(\mathbf{x}) = \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2^2$$

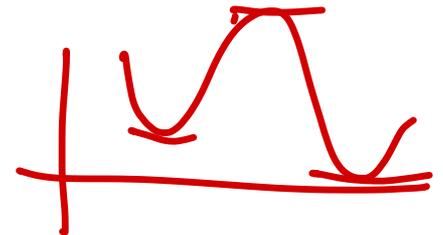
- Then the least squares problem becomes

$$\min_{\mathbf{x}} \phi(\mathbf{x})$$

1d opt  
1st order  
2nd order

- Suppose  $\phi: \mathcal{R}^m \rightarrow \mathcal{R}$  is a smooth function, then  $\phi(\mathbf{x})$  reaches a (local) maximum or minimum at a point  $\mathbf{x}^* \in \mathcal{R}^m$  only if

$$\nabla\phi(\mathbf{x}^*) = 0$$





# How to find the minimizer?

- To minimize the 2-norm of the residual vector

stationary



→ 1st order necessary cond

$$\min_x \phi(x) = \|b - Ax\|_2^2 = (b - Ax)^T (b - Ax)$$

$$\begin{aligned} \nabla \phi &= -A^T(b - Ax) + (b - Ax)^T(-A) \\ &= -A^T b + A^T Ax - A^T b + A^T Ax \end{aligned}$$

$$= 2(A^T Ax - A^T b)$$

$$\nabla \phi = 0$$

$$\underbrace{\begin{pmatrix} A^T & A \end{pmatrix}}_{n \times m} \underbrace{x}_{m \times 1} = \underbrace{\begin{pmatrix} A^T \end{pmatrix}}_{n \times m} \underbrace{b}_{m \times 1}$$

$n \times 1$

$$\nabla(\nabla \phi) = ?$$

$$\underbrace{A^T A}_{\text{given}} x = \underbrace{A^T b}_{\text{given}}$$

Normal Equations

lin sys

Find

$$\underline{A}^T \underline{A} \underline{x} = \underline{A}^T \underline{b} \rightarrow \text{Normal equation}$$

$\underline{x}$ : solution?

\*if matrix  $A$  is full rank:

$$A = \begin{bmatrix} & & \\ & & \\ & & \end{bmatrix}_{m \times n} \quad m > n \rightarrow \text{rank}(A) = n$$

$\text{rank}(A) = n \Rightarrow A$  has  $n$  L.I. columns

$\Rightarrow$  has  $n$  singular values  $> 0$

$\Rightarrow$  has  $n$  eigenvalues  $> 0$

$A^T A$  has  $n$  eigenvalues  $> 0$   
 $y^T A^T A y > 0$  for any  $y \neq 0 \Rightarrow A^T A$  is positive def. & symmetric

$$\underline{x} = (\underline{A}^T \underline{A})^{-1} \underline{A}^T \underline{b} \Rightarrow \text{unique}$$

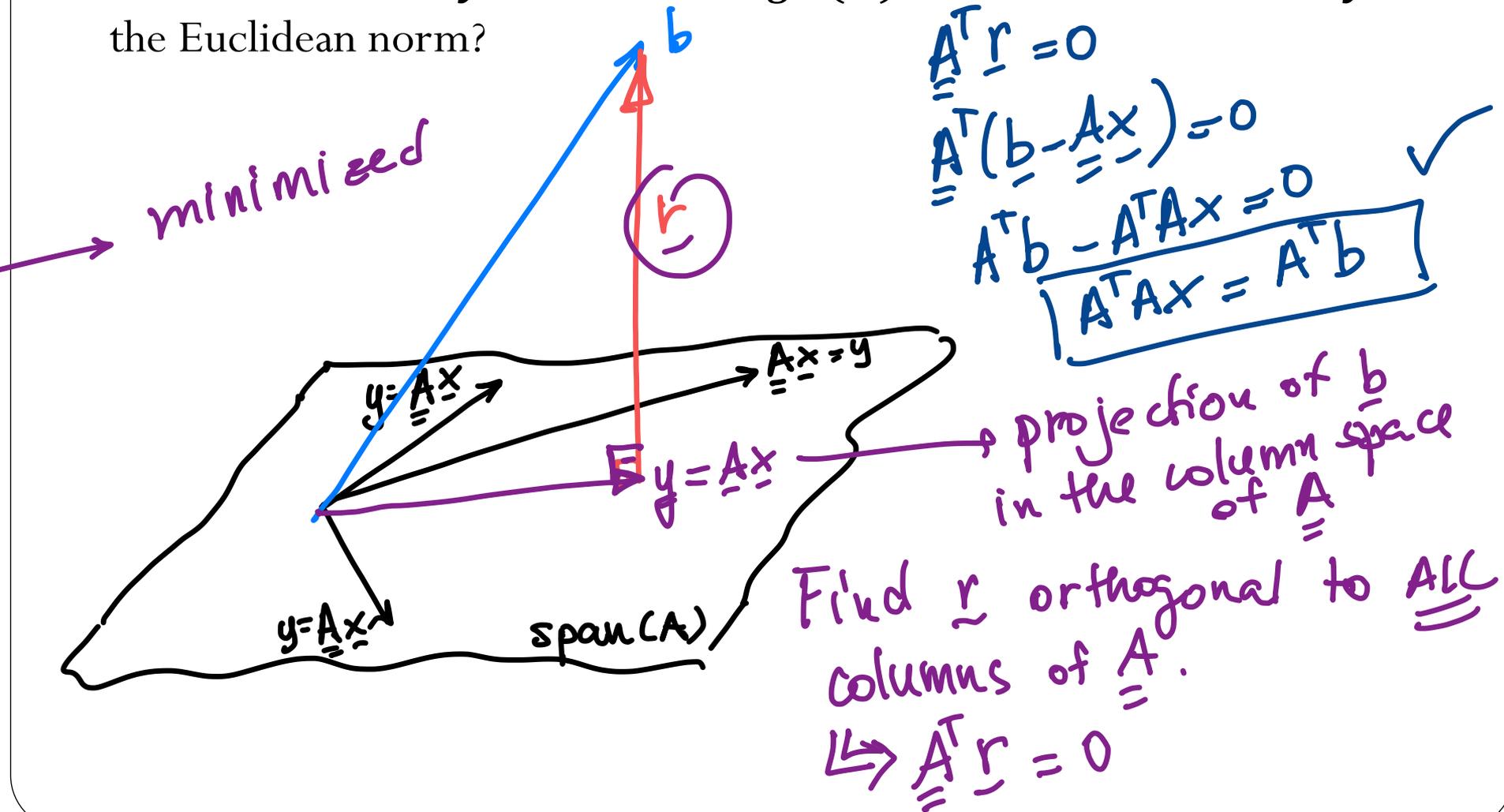
$\Leftrightarrow A^T A$  is invertible

$$\nabla \phi = 2(A^T A x - A^T b)$$
$$H = 2A^T A$$

$x$  is minimizer

# Linear Least Squares (another approach)

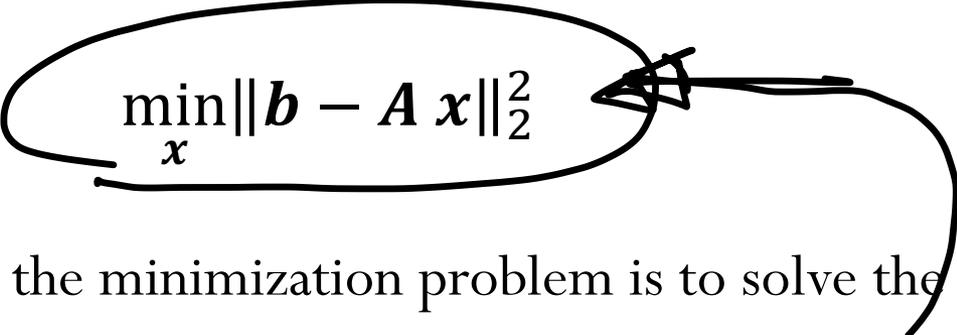
- Find  $\mathbf{y} = \mathbf{A} \mathbf{x}$  which is closest to the vector  $\mathbf{b}$
- What is the vector  $\mathbf{y} = \mathbf{A} \mathbf{x} \in \text{range}(\mathbf{A})$  that is closest to vector  $\mathbf{y}$  in the Euclidean norm?



# Summary:

- $A$  is a  $(m \times n)$  matrix, where  $m > n$ .
- $m$  is the number of data pair points.  $n$  is the number of parameters of the “best fit” function.
- Linear Least Squares problem  $A x \cong b$  *always* has solution.

- The Linear Least Squares solution  $x$  minimizes the square of the 2-norm of the residual:

$$\min_x \|b - A x\|_2^2$$


- One method to solve the minimization problem is to solve the system of Normal Equations

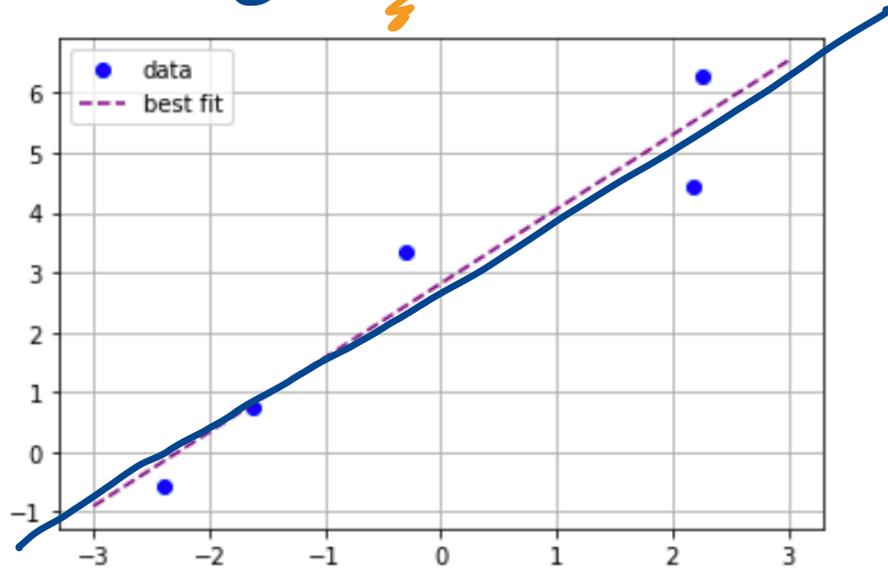
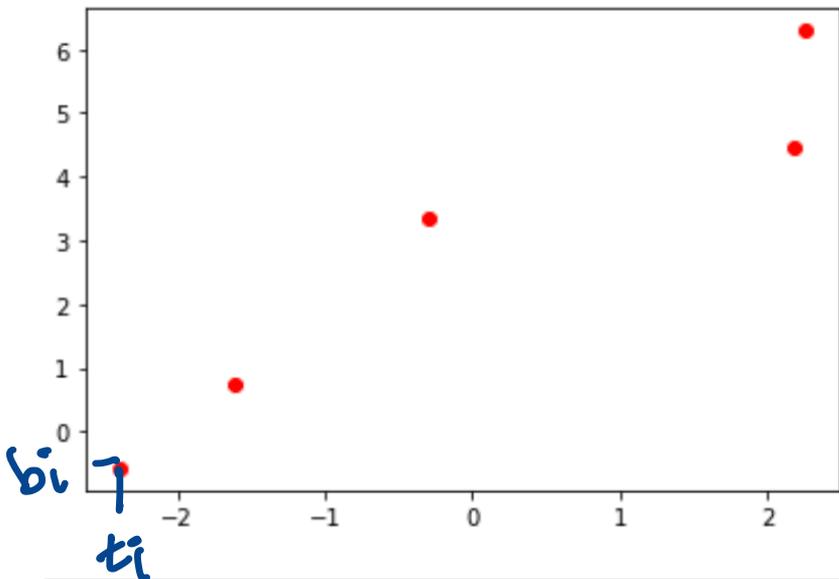
$$A^T A x = A^T b$$

$\rightarrow$   $x$  is unique  
matrix is full  
rank

- Let's see some examples and discuss the limitations of this method.

# Example:

$$y = \underbrace{x_0}_{\text{bias}} + \underbrace{x_1}_{\text{weight}} t$$



```
t
array([-1.61477467, -2.3970584 , -0.30372944,  2.26304537,  2.188127  ])
```

```
b
array([ 0.74112251, -0.57768693,  3.33523017,  6.29377547,  4.44786481])
```

Solve:  $A^T A x = A^T b$

$x = \text{la.solve}(A^T A, A^T b)$

$$A = \begin{bmatrix} 1 & t_1 \\ 1 & t_2 \\ \vdots & \vdots \\ 1 & t_5 \end{bmatrix}$$

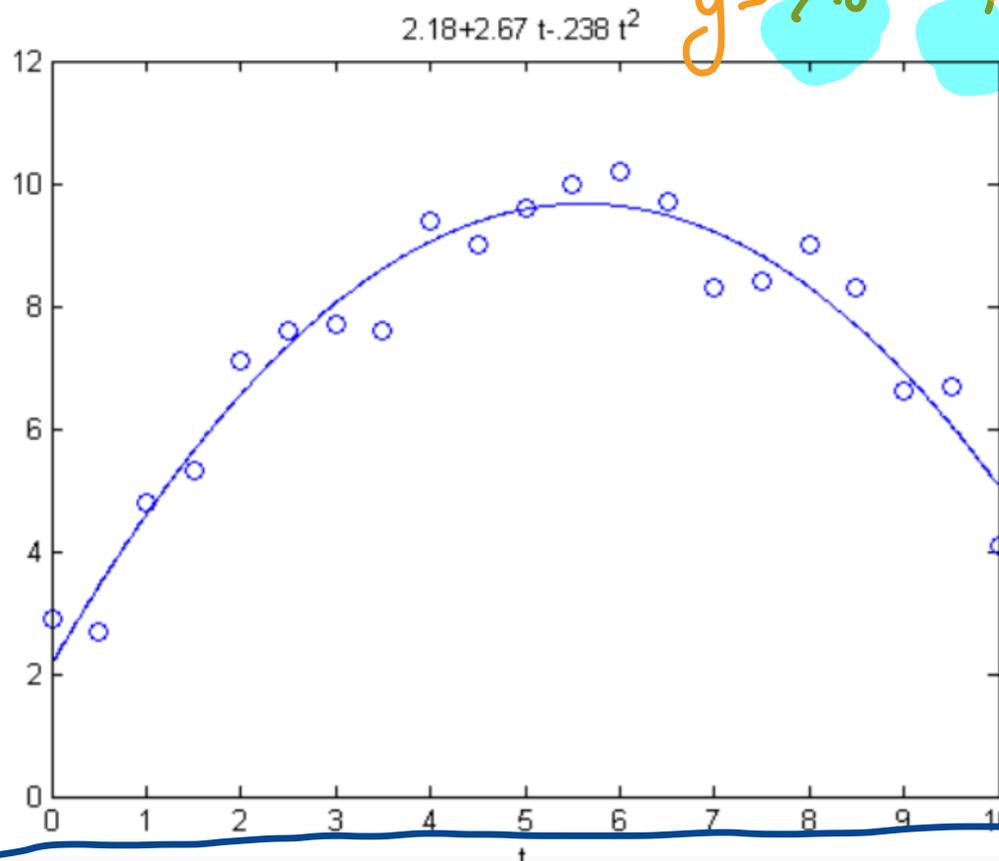
$5 \times 2$

$$b = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_5 \end{bmatrix}$$

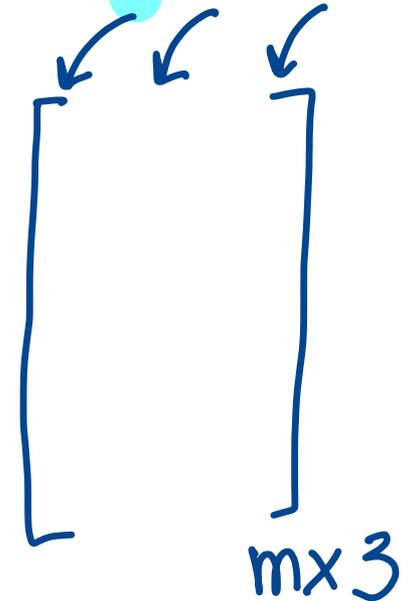
```
array([2.81441707, 1.24048133])
```

# Data fitting - not always a line fit!

- Does not need to be a line! For example, here we are fitting the data using a quadratic curve.



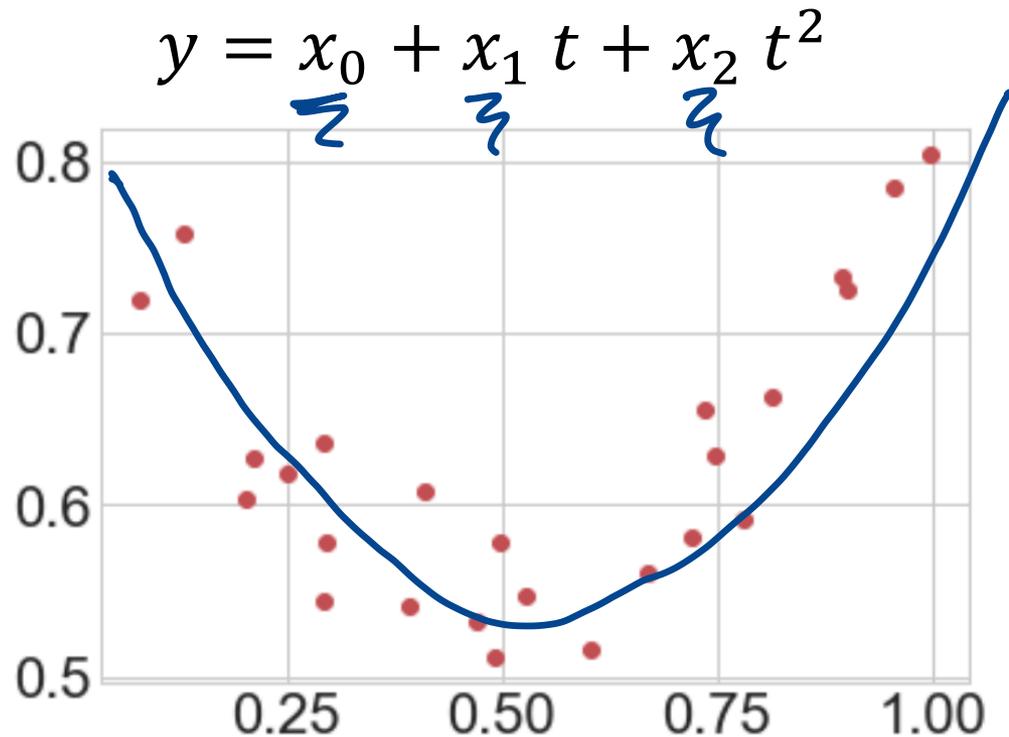
$$y = x_0 + x_1 t + x_2 t^2$$



Linear Least Squares: The problem is **linear in its coefficients!**

# Another example

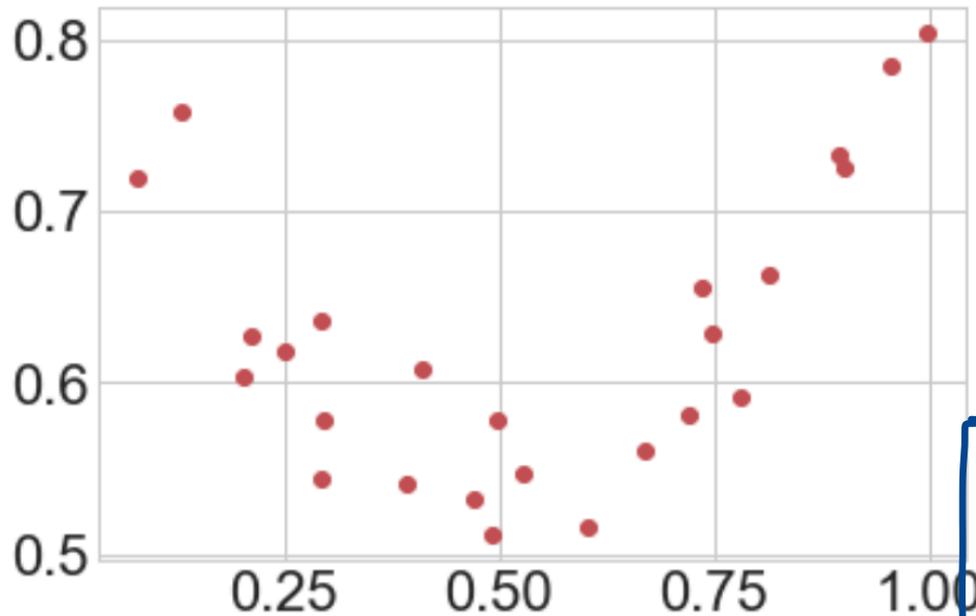
We want to find the coefficients of the quadratic function that best fits the data points:



We would not want our “fit” curve to pass through the data points exactly as we are looking to model the general trend and not capture the noise.

# Data fitting

$$y = x_0 + x_1 t + x_2 t^2$$



$m \times 1$

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$$

$$= \begin{bmatrix} 1 & t_1 & t_1^2 \\ 1 & t_2 & t_2^2 \\ \vdots & \vdots & \vdots \\ 1 & t_m & t_m^2 \end{bmatrix}$$

$$\stackrel{\text{A}}{=} \begin{bmatrix} t_1^2 \\ t_2^2 \\ t_3^2 \\ \vdots \\ t_m^2 \end{bmatrix}$$

$$\begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix}$$

3x1  
(1x1)

$$\begin{aligned} y_1 &= x_0 + x_1 t_1 + x_2 t_1^2 \\ y_2 &= x_0 + x_1 t_2 + x_2 t_2^2 \\ &\vdots \\ y_m &= x_0 + x_1 t_m + x_2 t_m^2 \end{aligned}$$

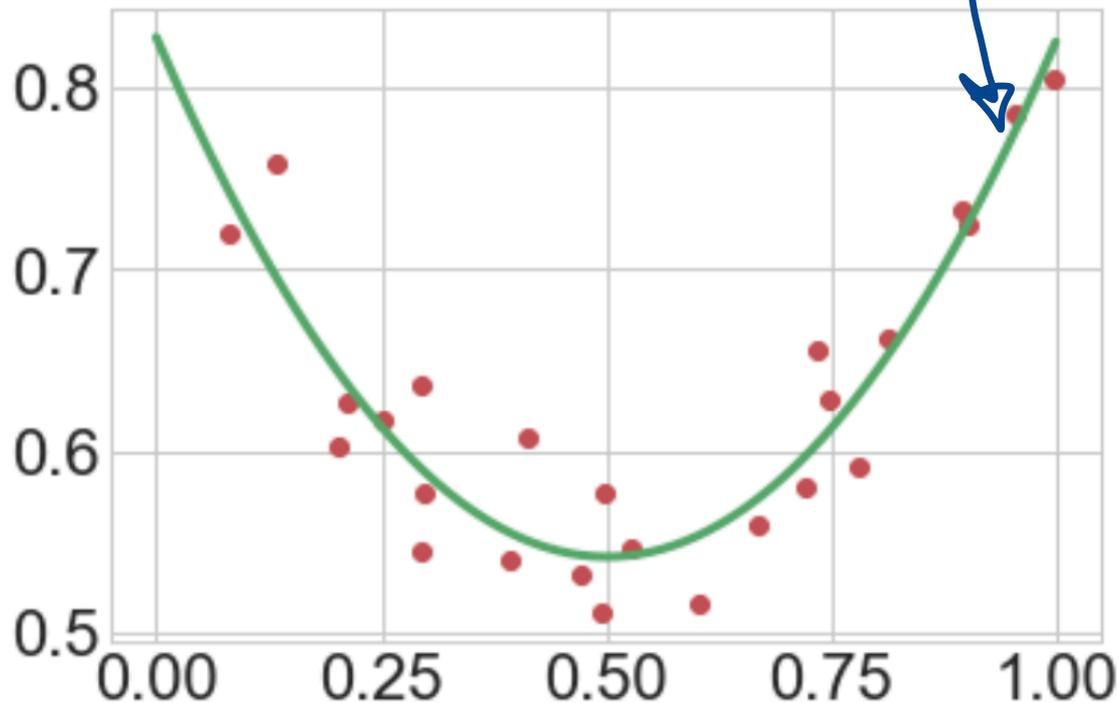


# Data fitting

$$\begin{bmatrix} 1 & t_1 & t_1^2 \\ \vdots & \vdots & \vdots \\ 1 & t_m & t_m^2 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}$$

$$\underline{\underline{A}} \underline{\underline{b}} \rightarrow \underline{\underline{A}} \underline{\underline{x}} \approx \underline{\underline{b}}$$

Solve:  $\mathbf{A}^T \mathbf{A} \mathbf{x} = \mathbf{A}^T \mathbf{b}$



Which function is not suitable for linear least squares?

A)  $y = a + bx + cx^2 + dx^3$

B)  $y = x(a + bx + cx^2 + dx^3)$

C)  $y = a \sin(x) + b / \cos(x)$

D)  $y = a \sin(x) + x / \cos(bx)$

E)  $y = a e^{-2x} + b e^{2x}$

$y = x_0 + x_1 t$

$y = x_0 + x_1 t + x_2 t^2$

$Ax = b$

$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$

$= \begin{bmatrix} e^{-2x_1} & e^{2x_1} \\ e^{-2x_2} & e^{2x_2} \\ \vdots & \vdots \\ \vdots & \vdots \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix}$

~~$\begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix} = \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix}$~~

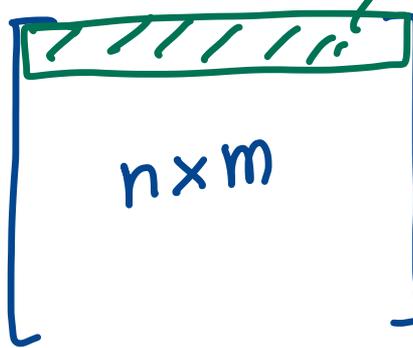
# Computational Cost

$$A^T A x = A^T b$$

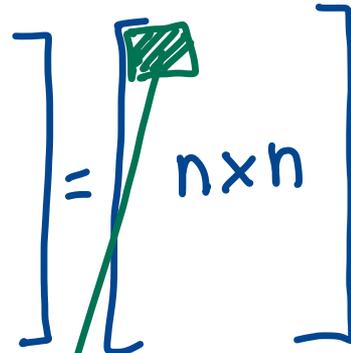
$A_{m \times n}$

inner product  
 $O(m)$

① Construct  $A^T A \Rightarrow$



$m \times n$



$n \times n$

② Factorize

$A^T A$   
 $n \times n$

$O(n^3)$

③ Solve

$O(n^2)$

overall cost:  $O(mn^2)$  ( $m \geq n$ )

$O(m)$

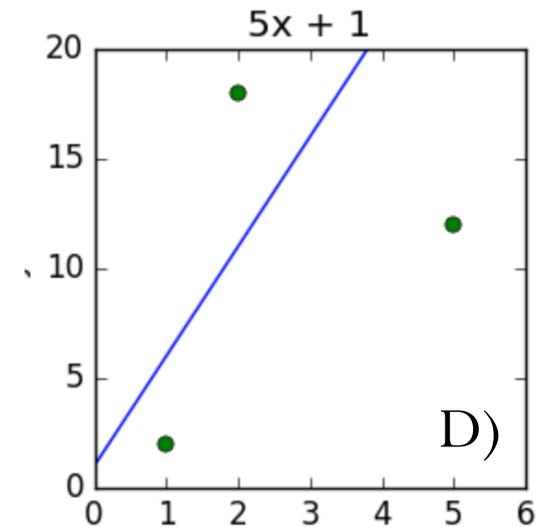
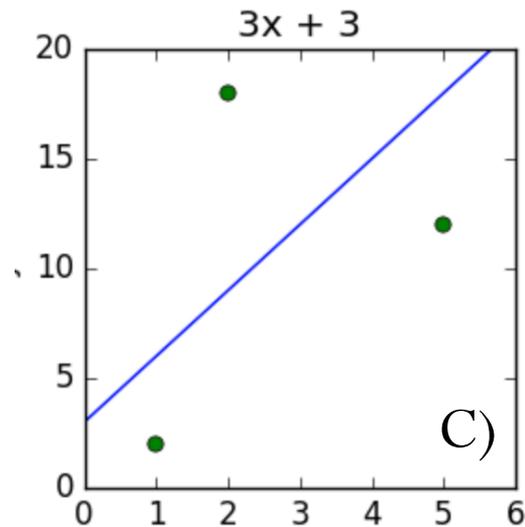
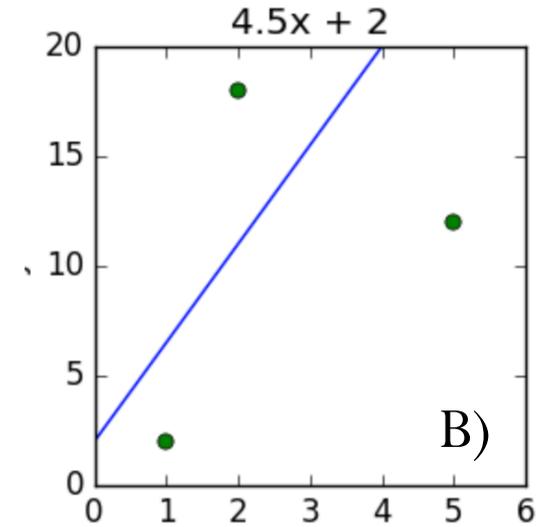
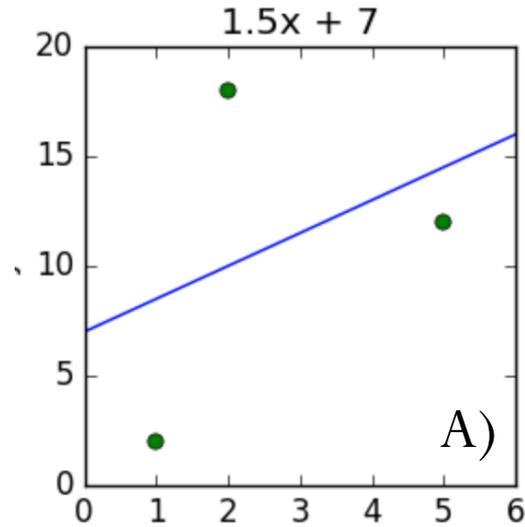
$n^2$  times

$O(mn^2)$

# Short questions

Given the data in the table below, which of the plots shows the line of best fit in terms of least squares?

$x$	1	2	5
$y$	2	18	12



# Short questions

Given the data in the table below, and the least squares model

$$y = c_1 + c_2 \sin(t\pi) + c_3 \sin(t\pi/2) + c_4 \sin(t\pi/4)$$

written in matrix form as

$$A \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} \cong \mathbf{y}$$

determine the entry  $A_{23}$  of the matrix  $\mathbf{A}$ .

Note that indices start with 1.

A)  $-1.0$

B)  $1.0$

C)  $-0.7$

D)  $0.7$

E)  $0.0$

$t_i$	$y_i$
0.5	0.72
1.0	0.79
1.5	0.72
2.0	0.97
2.5	1.03
3.0	0.96
3.5	1.00

# Solving Linear Least Squares with SVD

# What we have learned so far...

$\mathbf{A}$  is a  $m \times n$  matrix where  $m > n$

(more points to fit than coefficient to be determined)

Normal Equations:  $\mathbf{A}^T \mathbf{A} \mathbf{x} = \mathbf{A}^T \mathbf{b}$

- The solution  $\mathbf{A} \mathbf{x} \cong \mathbf{b}$  is unique if and only if  $\text{rank}(\mathbf{A}) = n$   
( $\mathbf{A}$  is full column rank)

- $\text{rank}(\mathbf{A}) = n \rightarrow$  columns of  $\mathbf{A}$  are *linearly independent*  $\rightarrow n$  non-zero singular values  $\rightarrow \mathbf{A}^T \mathbf{A}$  has only positive eigenvalues  $\rightarrow \mathbf{A}^T \mathbf{A}$  is a symmetric and positive definite matrix  $\rightarrow \mathbf{A}^T \mathbf{A}$  is invertible

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

- If  $\text{rank}(\mathbf{A}) < n$ , then  $\mathbf{A}$  is rank-deficient, and solution of linear least squares problem is *not unique*.

# Condition number for Normal Equations

Finding the least square solution of  $\mathbf{A} \mathbf{x} \cong \mathbf{b}$  (where  $\mathbf{A}$  is full rank matrix) using the Normal Equations

$$\mathbf{A}^T \mathbf{A} \mathbf{x} = \mathbf{A}^T \mathbf{b}$$

has some advantages, since we are solving a square system of linear equations with a symmetric matrix (and hence it is possible to use decompositions such as Cholesky Factorization)

However, the normal equations tend to worsen the conditioning of the matrix.

$$\text{cond}(\mathbf{A}^T \mathbf{A}) = (\text{cond}(\mathbf{A}))^2$$

**How can we solve the least square problem without squaring the condition of the matrix?**



# SVD to solve linear least squares problems

$\mathbf{A}$  is a  $m \times n$  rectangular matrix where  $m > n$ , and hence the SVD decomposition is given by:

$$\mathbf{A} = \begin{pmatrix} \vdots & \dots & \vdots \\ \mathbf{u}_1 & \dots & \mathbf{u}_m \\ \vdots & \dots & \vdots \end{pmatrix} \begin{pmatrix} \sigma_1 & & \\ & \dots & \\ & & \sigma_n \\ & & & 0 \\ & & & \vdots \\ & & & & 0 \end{pmatrix} \begin{pmatrix} \dots & \mathbf{v}_1^T & \dots \\ \vdots & \vdots & \vdots \\ \dots & \mathbf{v}_n^T & \dots \end{pmatrix}$$

We want to find the least square solution of  $\mathbf{A} \mathbf{x} \cong \mathbf{b}$ , where  $\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T$

or better expressed in reduced form:  $\mathbf{A} = \mathbf{U}_R \mathbf{\Sigma}_R \mathbf{V}^T$

# Recall Reduced SVD

$$m > n$$

$$A = U_R \Sigma_R V^T$$

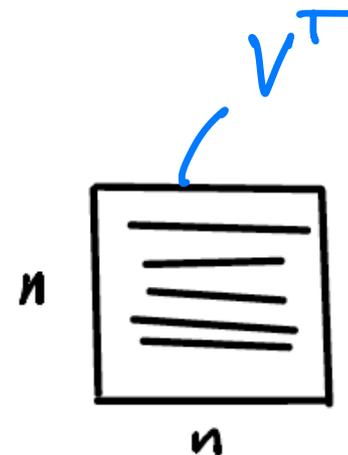
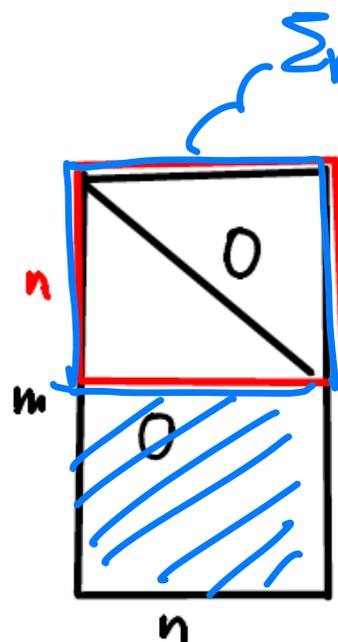
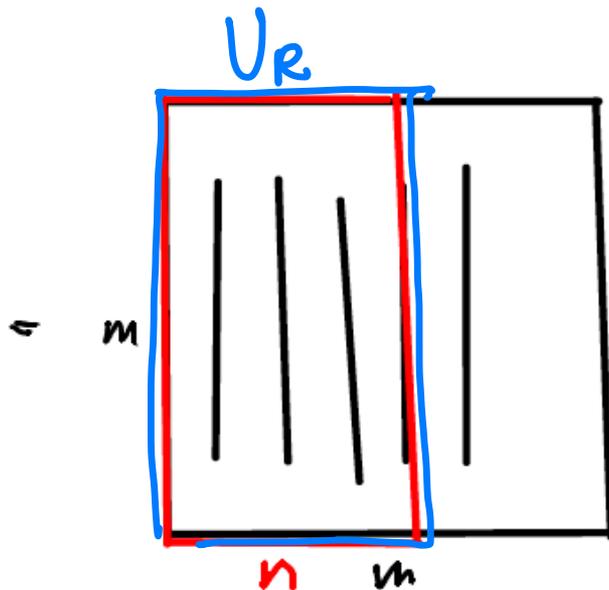
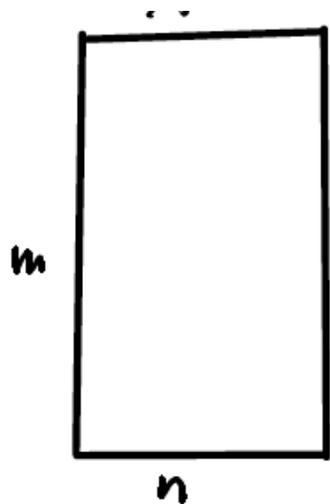
$m \times n$     $m \times n$     $n \times n$

$n \times n$

$U_R$

$\Sigma_R$

$V^T$



# Shapes of the Reduced SVD

Suppose you compute a reduced SVD  $A = U\Sigma V^T$  of a  $10 \times 14$  matrix  $A$ . What will the shapes of  $U$ ,  $\Sigma$ , and  $V$  be?

**Hint:** Remember the transpose on  $V$ !

The shape of  $U$  will be   $\times$  .

The shape of  $\Sigma$  will be   $\times$  .

The shape of  $V$  will be   $\times$  .

# SVD to solve linear least squares problems

$$A = U_R \Sigma_R V^T$$

$$A = \begin{pmatrix} \vdots & \dots & \vdots \\ \mathbf{u}_1 & \dots & \mathbf{u}_n \\ \vdots & \dots & \vdots \end{pmatrix} \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix} \begin{pmatrix} \dots & \mathbf{v}_1^T & \dots \\ \vdots & \vdots & \vdots \\ \dots & \mathbf{v}_n^T & \dots \end{pmatrix}$$

$$\underline{A} \underline{x} = \underline{b} \rightarrow \underline{A}^T \underline{A} \underline{x} = \underline{A}^T \underline{b}$$

$$(\underline{U}_R \underline{\Sigma}_R \underline{V}^T)^T (\underline{U}_R \underline{\Sigma}_R \underline{V}^T) \underline{x} = (\underline{U}_R \underline{\Sigma}_R \underline{V}^T)^T \underline{b}$$

$$(\underline{V}^T)^T \underline{\Sigma}_R^T \underbrace{\underline{U}_R^T \underline{U}_R}_{I} \underline{\Sigma}_R \underline{V}^T \underline{x} = (\underline{V}^T)^T \underline{\Sigma}_R^T \underline{U}_R^T \underline{b}$$

$$\underline{V} \underline{\Sigma}_R^T \underline{\Sigma}_R \underline{V}^T \underline{x} = \underline{V} \underline{\Sigma}_R^T \underline{U}_R^T \underline{b}$$

$$\underline{V} \underline{\Sigma}_R^2 \underline{V}^T \underline{x} = \underline{V} \underline{\Sigma}_R \underline{U}_R^T \underline{b} \Rightarrow$$

$$\boxed{\underline{\Sigma}_R^2 \underline{V}^T \underline{x} = \underline{\Sigma}_R \underline{U}_R^T \underline{b}}$$

$$\underline{\Sigma}_R^{-1} = ?$$

① Full rank  $A$      $A_{m \times n} : \text{rank}(A) = n$

$$\sum_r^2 V^T x = \sum_r U_r^T b \Rightarrow V^T x = \sum_r^{-1} U_r^T b$$

$$x = V \sum_r^{-1} U_r^T b$$

Diagram annotations for the equation above:  
-  $x$ : unique solution  
-  $V$ :  $n \times n$   
-  $\sum_r^{-1}$ :  $n \times n$   
-  $U_r^T$ :  $n \times n$   
-  $b$ :  $m \times 1$   
- The entire expression  $x = V \sum_r^{-1} U_r^T b$  is annotated as  $n \times m$ .

② Rank deficient     $A_{m \times n} : \text{rank}(A) = r < n$

$\sum_r^2 V^T x = \sum_r U_r^T b$   $\rightarrow$  solution is not unique

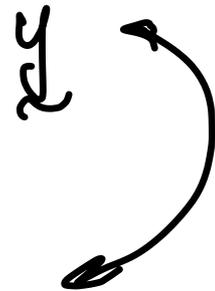
① Find  $\tilde{x}$  s.t.  $\min_x \|Ax - b\|_2^2$  ✓

⊕  $\min_x \|x\|_2$  ✓



In summary:

$$y_i = \begin{cases} \frac{u_i^T b}{\sigma_i}, & \text{if } i = 1, \dots, r \\ 0, & \text{if } i = r+1, \dots, n \end{cases}$$



Compute  $\tilde{x} \rightarrow \tilde{x} = V y = \sum_{i=1}^r (y_i) \tilde{v}_i$

$$\tilde{x} = \sum_{i=1}^n \left( \frac{u_i^T b}{\sigma_i} \right) \tilde{v}_i$$

$\sigma_i \neq 0$

$$A x = b$$

A is rank deficient

$$\tilde{x} = \sum_{i=1}^n \left( \frac{u_i^T b}{\sigma_i} \right) \tilde{v}_i$$

$\sigma_i \neq 0$

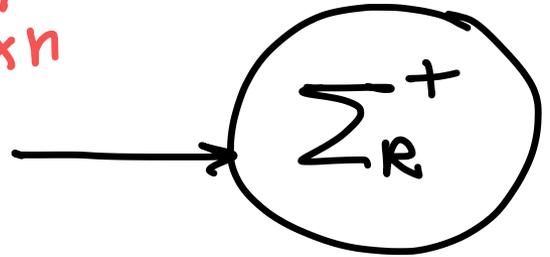
$$U_R^T b \quad \begin{matrix} \text{---} \\ \text{---} \\ \text{---} \end{matrix} \begin{matrix} m \times 1 \\ \\ \end{matrix} \implies O(mn)$$

$n \times m$

$$\Sigma_R^T z \quad \begin{matrix} \text{---} \\ \text{---} \\ \text{---} \end{matrix} \begin{matrix} n \times 1 \\ \\ \end{matrix} \xrightarrow{\Sigma \text{ is diag}} O(n)$$

$n \times n$

$$\Sigma_R^2 V^T x = \Sigma_R U_R^T b$$



$$V^T x = \Sigma_R^+ U_R^T b$$

$$\Sigma_R^+ = \Sigma_R^{-1} \text{ full rank}$$

$$\tilde{x} = V \Sigma_R^+ U_R^T b$$

$\tilde{x}$     $V$     $\Sigma_R^+$     $U_R^T b$

$$V y \quad \begin{matrix} \text{---} \\ \text{---} \\ \text{---} \end{matrix} \begin{matrix} n \times n \\ \\ \end{matrix} \implies O(n^2)$$

$n \times n$     $n \times 1$

SVD  $\Rightarrow O(mn^2)$

overall  $O(mn)$

$m \geq n$

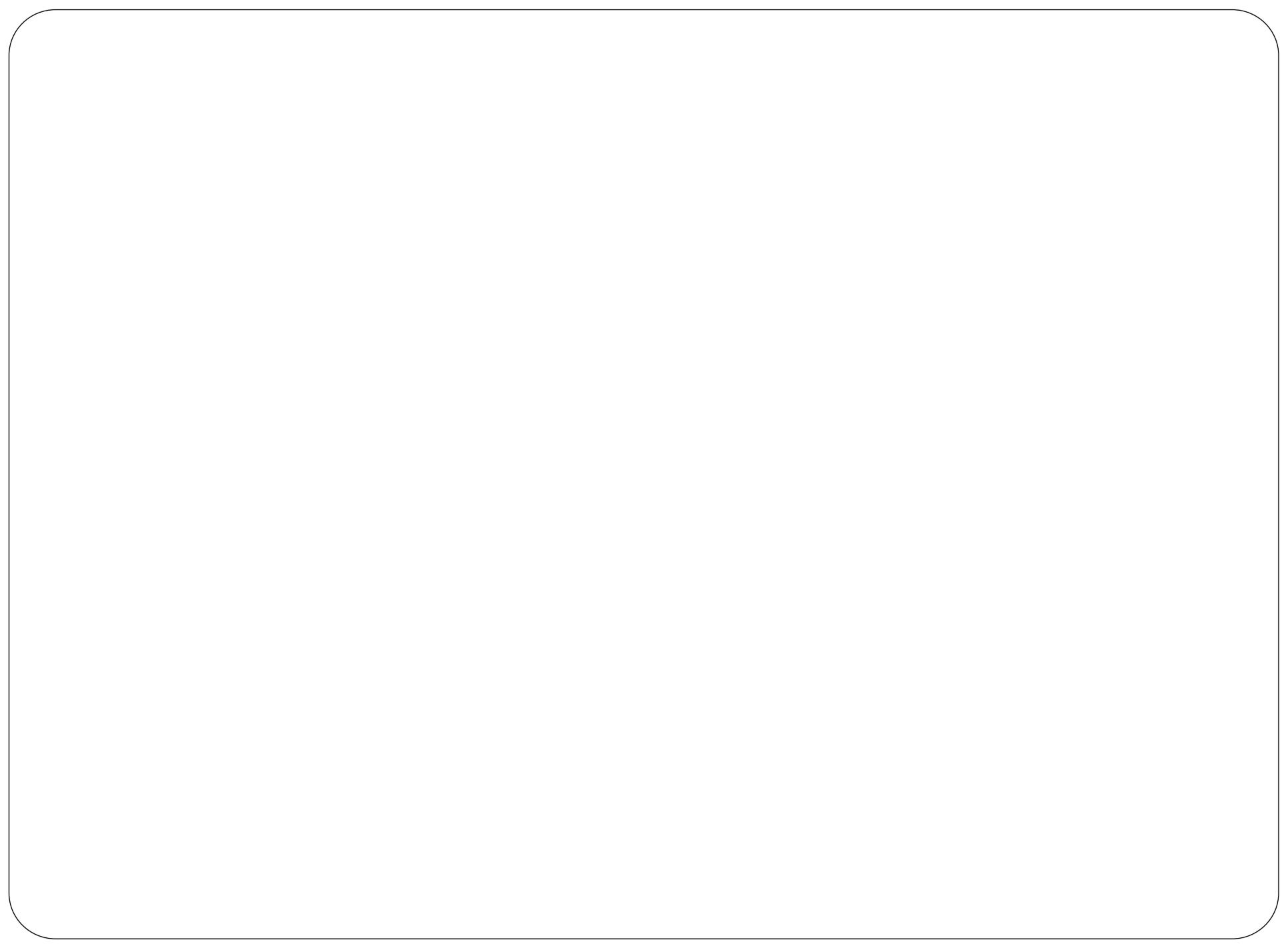


# Example:

Consider solving the least squares problem  $\mathbf{A} \mathbf{x} \cong \mathbf{b}$ , where the singular value decomposition of the matrix  $\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T \mathbf{x}$  is:

$$\begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 14 & 0 & 0 \\ 0 & 14 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \mathbf{x} \cong \begin{bmatrix} 12 \\ 9 \\ 9 \\ 10 \end{bmatrix}$$

Determine  $\|\mathbf{b} - \mathbf{A} \mathbf{x}\|_2$



# Example

Suppose you have  $\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T$  calculated. What is the cost of solving

$$\min_{\mathbf{x}} \|\mathbf{b} - \mathbf{A} \mathbf{x}\|_2^2 ?$$

- A)  $O(n)$
- B)  $O(n^2)$
- C)  $O(mn)$
- D)  $O(m)$
- E)  $O(m^2)$