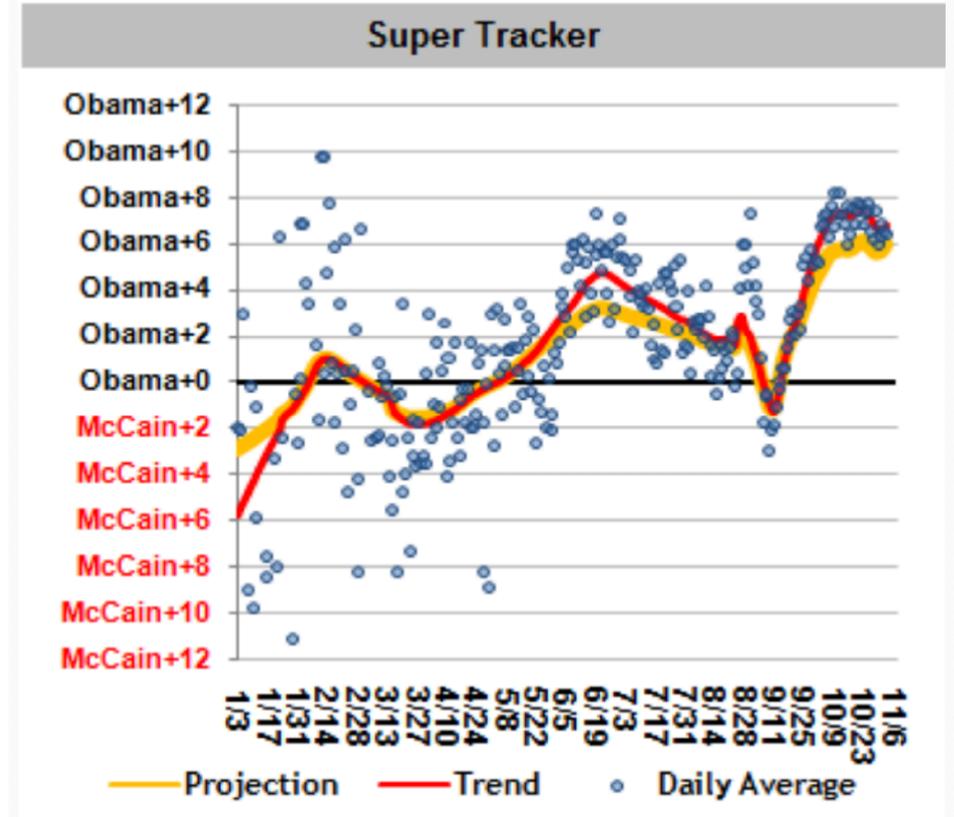
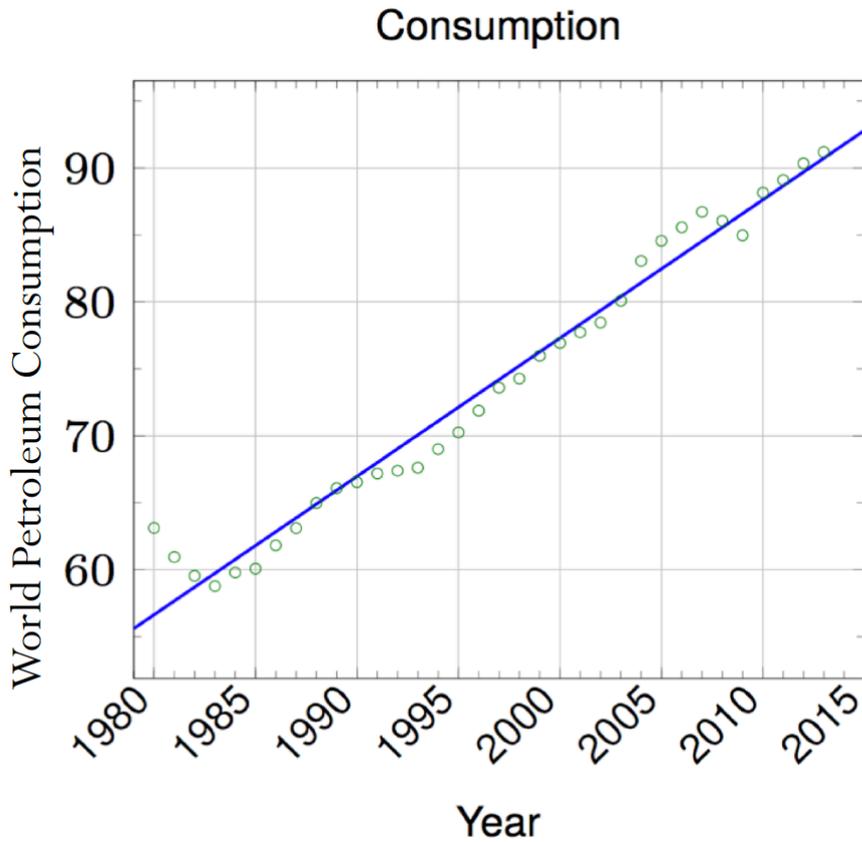


Least Squares and Data Fitting

Data fitting

How do we best fit a set of data points?



Linear Least Squares

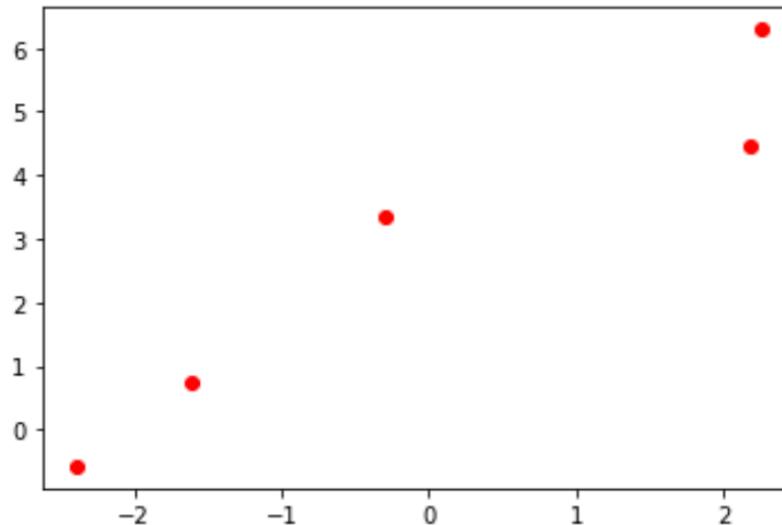
1) Fitting with a line

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

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

or in matrix form:

$$\begin{bmatrix} 1 & t_1 \\ \vdots & \vdots \\ 1 & t_m \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix} \quad \mathbf{A} \mathbf{x} = \mathbf{b}$$

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

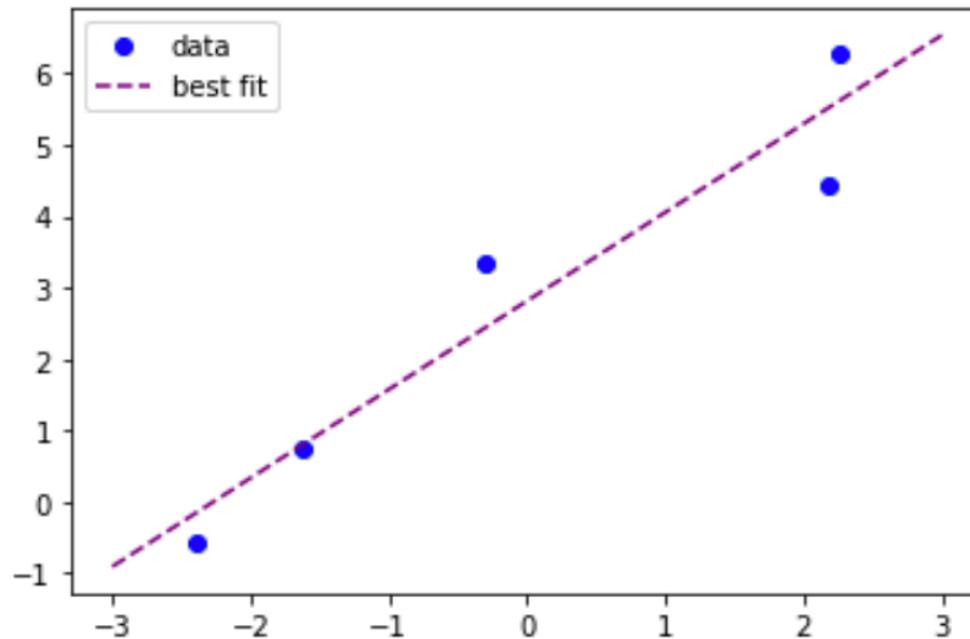
Note that this system of linear equations has more equations than unknowns –
OVERDETERMINED
SYSTEMS

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!**



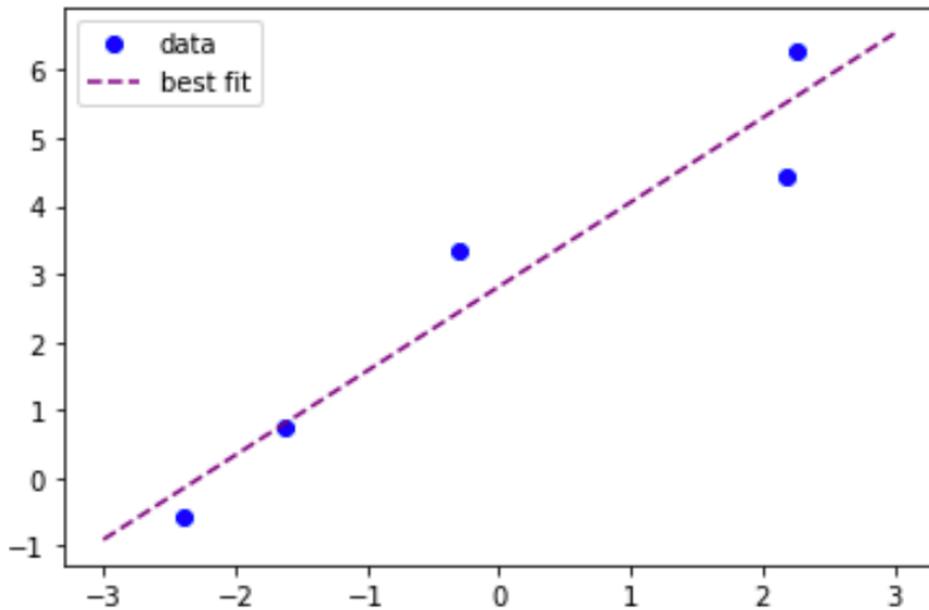
- Therefore, an overdetermined system is better expressed as

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

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 ϕ as the square of the 2-norm of the residual

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

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 ϕ 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

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

- 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

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

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

$$\nabla \phi(\mathbf{x}) = 2(\mathbf{A}^T \mathbf{b} - \mathbf{A}^T \mathbf{A} \mathbf{x})$$

Normal Equations – solve a linear system of equations

First order necessary condition:

$$\nabla \phi(\mathbf{x}) = 0 \rightarrow \mathbf{A}^T \mathbf{b} - \mathbf{A}^T \mathbf{A} \mathbf{x} = \mathbf{0} \rightarrow \mathbf{A}^T \mathbf{A} \mathbf{x} = \mathbf{A}^T \mathbf{b}$$

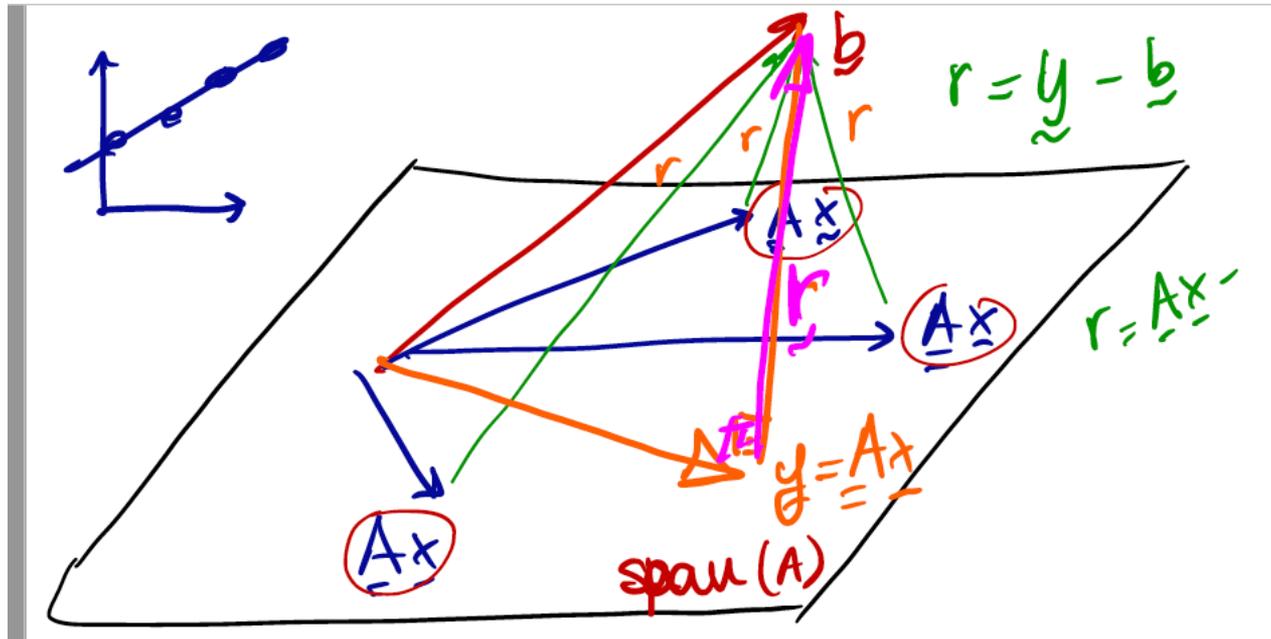
Second order sufficient condition:

$$D^2 \phi(\mathbf{x}) = 2\mathbf{A}^T \mathbf{A}$$

$2\mathbf{A}^T \mathbf{A}$ is a positive semi-definite matrix \rightarrow the solution is a minimum

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?



When $\mathbf{r} = \mathbf{b} - \mathbf{y} = \mathbf{b} - \mathbf{A} \mathbf{x}$ is orthogonal to all columns of \mathbf{A} , then \mathbf{y} is closest to \mathbf{b}

$$\mathbf{A}^T \mathbf{r} = \mathbf{A}^T (\mathbf{b} - \mathbf{A} \mathbf{x}) = 0 \longrightarrow \mathbf{A}^T \mathbf{A} \mathbf{x} = \mathbf{A}^T \mathbf{b}$$

Summary:

- \mathbf{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 $\mathbf{A} \mathbf{x} \cong \mathbf{b}$ *always* has solution.
- The Linear Least Squares solution \mathbf{x} minimizes the square of the 2-norm of the residual:

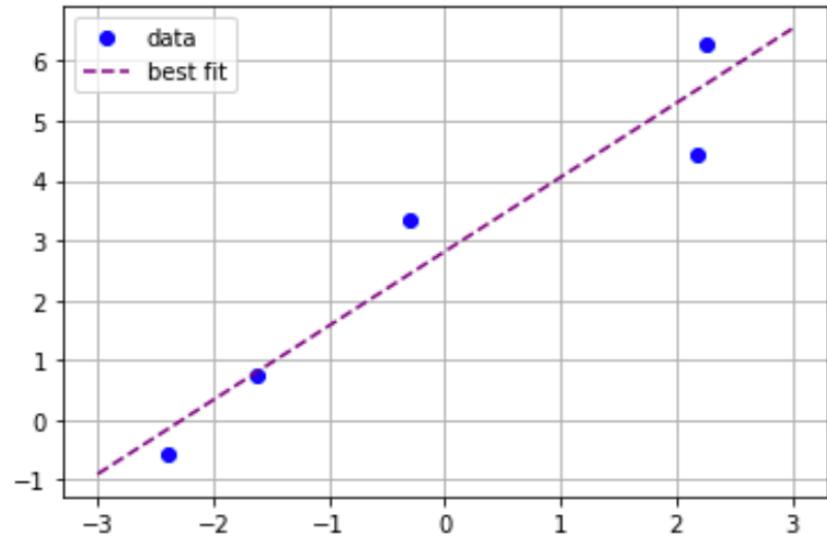
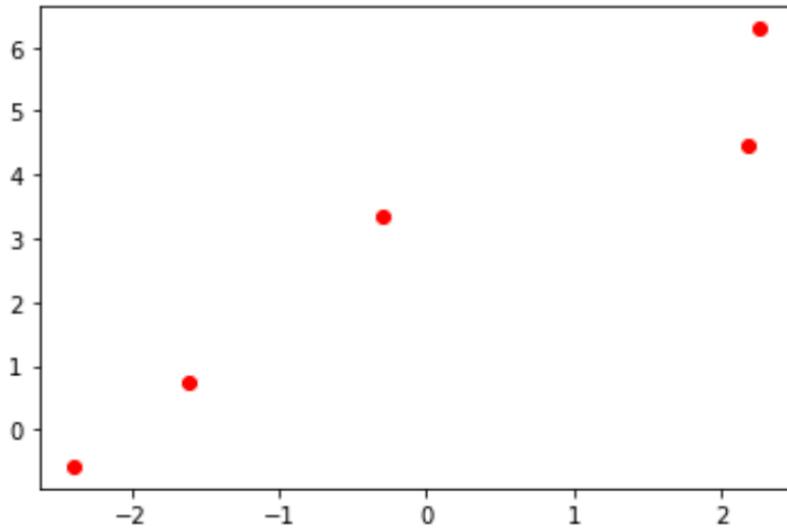
$$\min_{\mathbf{x}} \|\mathbf{b} - \mathbf{A} \mathbf{x}\|_2^2$$

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

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

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

Example:



t

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

b

```
array([ 0.74112251, -0.57768693,  3.33523097,  6.29377547,  4.44786481])
```

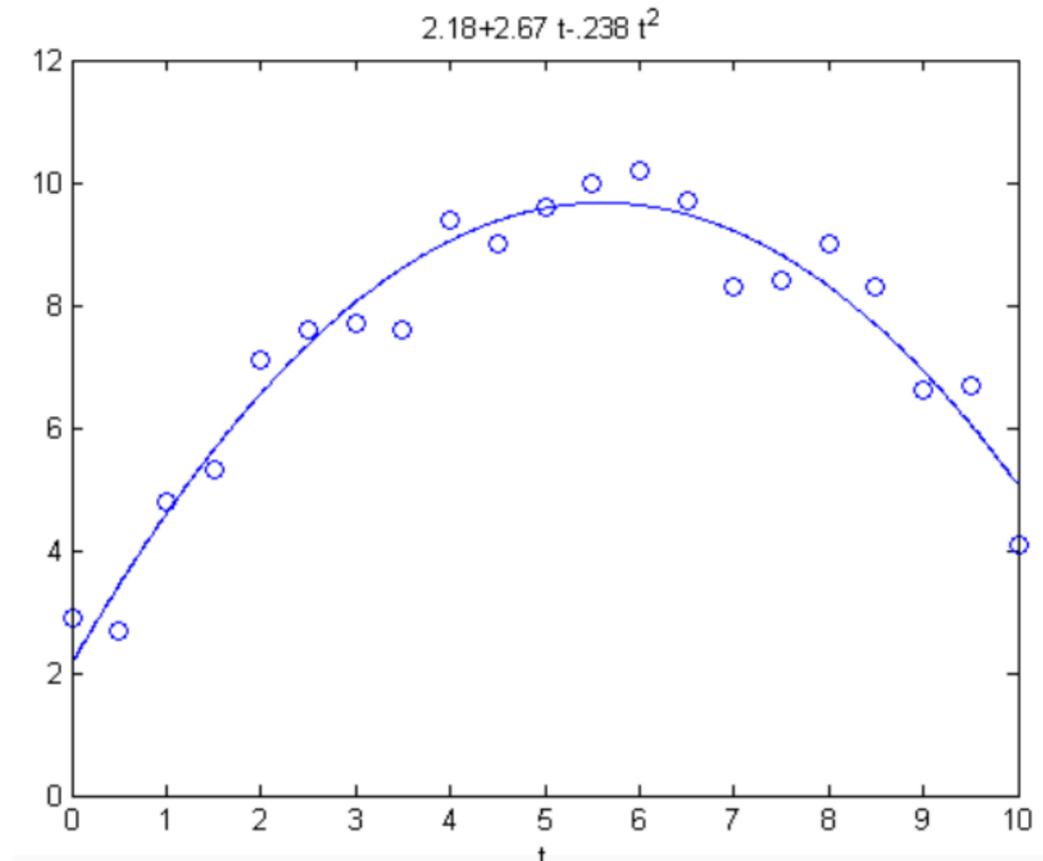
Solve: $A^T A x = A^T b$

x

```
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.

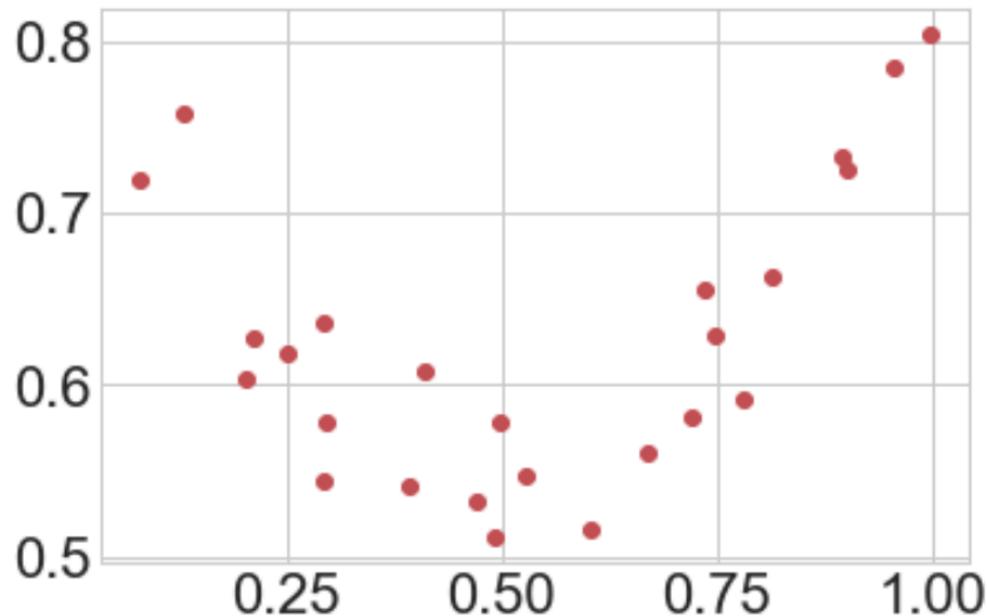


Linear Least Squares: The problem is **linear in its coefficients!**

Another examples

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

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

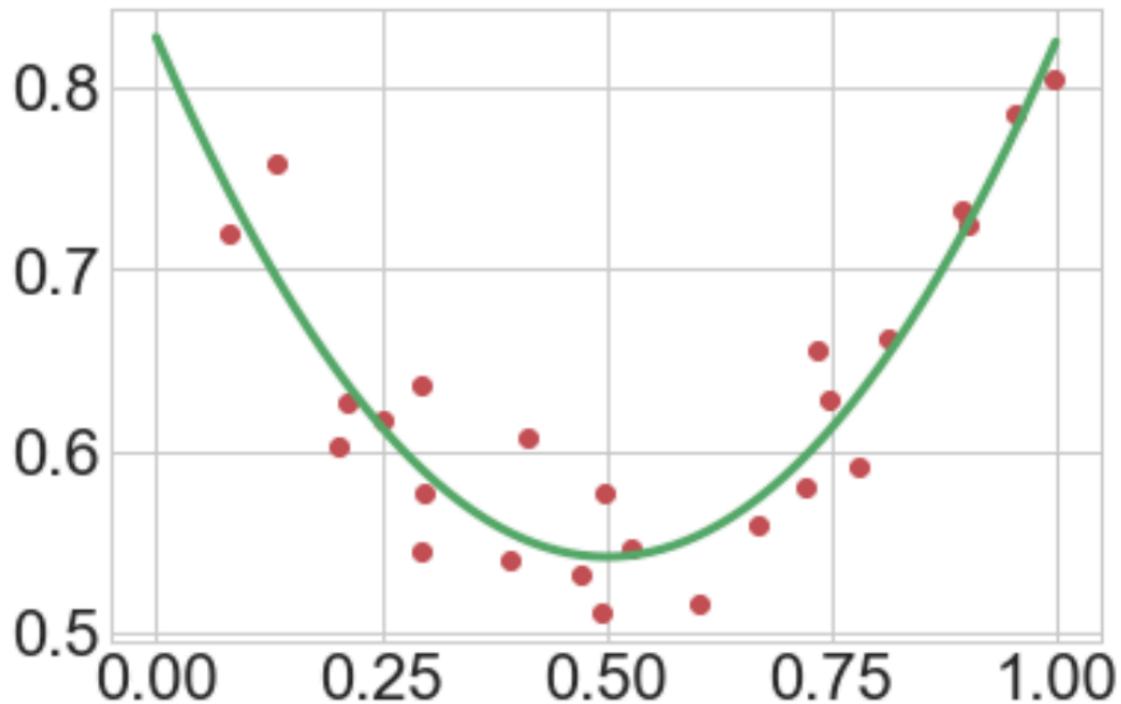


We would not want our “fit” curve to pass through the data points exactly as we are looking to model the general trend and not capture the noise.

Data fitting

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

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



Which function is not suitable for linear least squares?

A) $y = a + b x + c x^2 + d x^3$

B) $y = x(a + b x + c x^2 + d x^3)$

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

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

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

Computational Cost

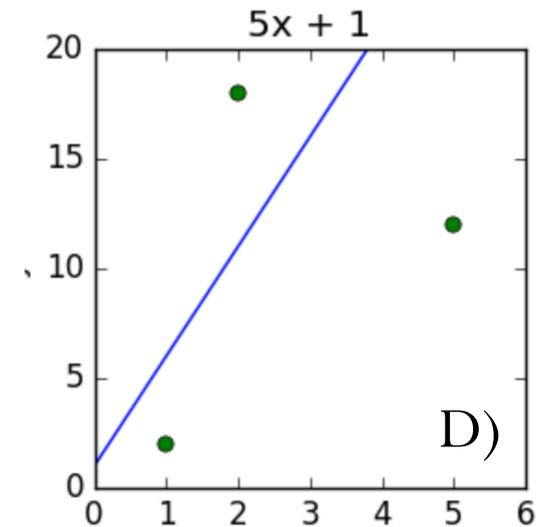
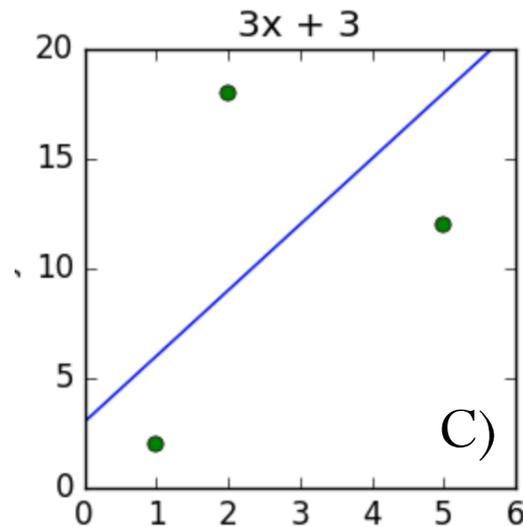
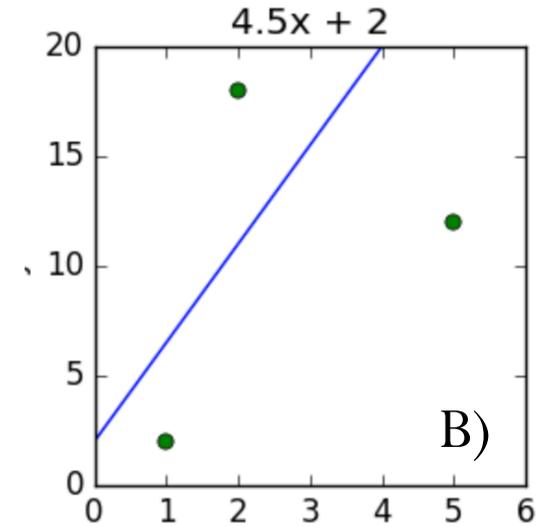
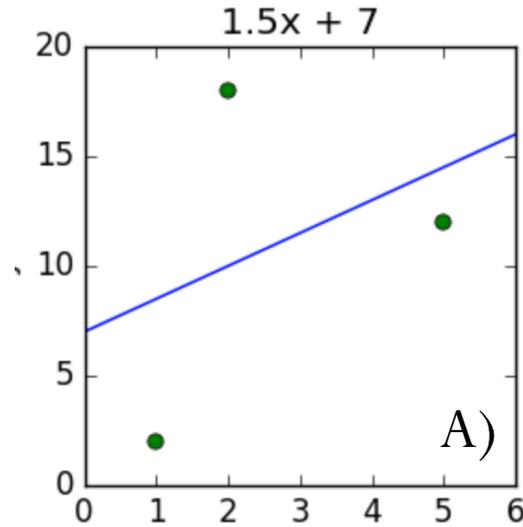
$$\mathbf{A}^T \mathbf{A} \mathbf{x} = \mathbf{A}^T \mathbf{b}$$

- Compute $\mathbf{A}^T \mathbf{A}$: $O(mn^2)$
- Factorize $\mathbf{A}^T \mathbf{A}$: LU $\rightarrow O\left(\frac{2}{3}n^3\right)$, Cholesky $\rightarrow O\left(\frac{1}{3}n^3\right)$
- Solve $O(n^2)$
- Since $m > n$ the overall cost is $O(mn^2)$

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)

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

- 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:

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

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

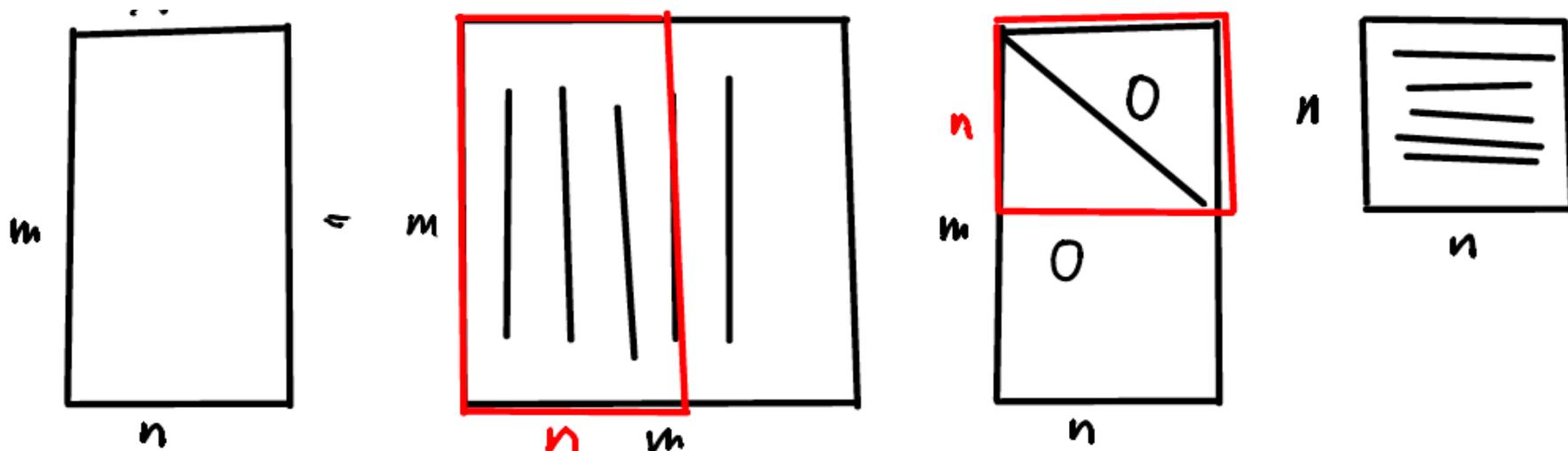
or better expressed in reduced form: $\mathbf{A} = \mathbf{U}_R \mathbf{\Sigma}_R \mathbf{V}^T$

Recall Reduced SVD $m > n$

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

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

$n \times n$



Shapes of the Reduced SVD

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

Hint: Remember the transpose on V !

The shape of U will be \times .

The shape of Σ will be \times .

The shape of V will be \times .

SVD to solve linear least squares problems

$$\mathbf{A} = \mathbf{U}_R \mathbf{\Sigma}_R \mathbf{V}^T$$

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

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

Normal equations: $\mathbf{A}^T \mathbf{A} \mathbf{x} = \mathbf{A}^T \mathbf{b} \rightarrow (\mathbf{U}_R \mathbf{\Sigma}_R \mathbf{V}^T)^T (\mathbf{U}_R \mathbf{\Sigma}_R \mathbf{V}^T) \mathbf{x} = (\mathbf{U}_R \mathbf{\Sigma}_R \mathbf{V}^T)^T \mathbf{b}$

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

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

$$(\mathbf{\Sigma}_R)^2 \mathbf{V}^T \mathbf{x} = \mathbf{\Sigma}_R \mathbf{U}_R^T \mathbf{b}$$

When can we take the inverse of the singular matrix?

$$(\Sigma_R)^2 V^T \mathbf{x} = \Sigma_R U_R^T \mathbf{b}$$

1) Full rank matrix ($\sigma_i \neq 0 \forall i$):

$$\text{rank}(\mathbf{A}) = n$$

$$V^T \mathbf{x} = (\Sigma_R)^{-1} U_R^T \mathbf{b}$$

Unique solution:

$$\mathbf{x} = V (\Sigma_R)^{-1} U_R^T \mathbf{b}$$

2) Rank deficient matrix ($\text{rank}(\mathbf{A}) = r < n$)

$$(\Sigma_R)^2 V^T \mathbf{x} = \Sigma_R U_R^T \mathbf{b} \quad \text{Solution is not unique!!}$$

Find solution \mathbf{x} such that $\min_{\mathbf{x}} \phi(\mathbf{x}) = \|\mathbf{b} - \mathbf{A} \mathbf{x}\|_2^2$

and also $\min_{\mathbf{x}} \|\mathbf{x}\|_2$

Solving Least Squares Problem with SVD (summary)

Cost of SVD:
 $O(m n^2)$

- Find \mathbf{x} that satisfies $\min_{\mathbf{x}} \|\mathbf{b} - \mathbf{A} \mathbf{x}\|_2^2$

- Find \mathbf{y} that satisfies $\min_{\mathbf{y}} \|\boldsymbol{\Sigma}_R \mathbf{y} - \mathbf{U}_R^T \mathbf{b}\|_2^2$

- Propose \mathbf{y} that is solution of $\boldsymbol{\Sigma}_R \mathbf{y} = \mathbf{U}_R^T \mathbf{b}$

Cost:

- Evaluate: $\mathbf{z} = \mathbf{U}_R^T \mathbf{b}$ \longrightarrow $m n$

- Set: $y_i = \begin{cases} \frac{z_i}{\sigma_i}, & \text{if } \sigma_i \neq 0 \\ 0, & \text{otherwise} \end{cases} \quad i = 1, \dots, n \longrightarrow n$

- Then compute $\mathbf{x} = \mathbf{V} \mathbf{y}$ $\longrightarrow n^2$

Solving Least Squares Problem with SVD (summary)

- If $\sigma_i \neq 0$ for $\forall i = 1, \dots, n$, then the solution $\mathbf{y} = \mathbf{V} (\boldsymbol{\Sigma}_R)^{-1} \mathbf{U}_R^T \mathbf{b}$ is unique (and not a “choice”).
- If at least one of the singular values is zero, then the proposed solution \mathbf{y} is the one with the smallest 2-norm ($\|\mathbf{y}\|_2$ is minimal) that minimizes the 2-norm of the residual $\|\boldsymbol{\Sigma}_R \mathbf{y} - \mathbf{U}_R^T \mathbf{b}\|_2$
- Since $\|\mathbf{x}\|_2 = \|\mathbf{V} \mathbf{y}\|_2 = \|\mathbf{y}\|_2$, then the solution \mathbf{x} is also the one with the smallest 2-norm ($\|\mathbf{x}\|_2$ is minimal) for all possible \mathbf{x} for which $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2$ is minimal.

Solving Least Squares Problem with SVD (summary)

Solve $\mathbf{A} \mathbf{x} \cong \mathbf{b}$ or $\mathbf{U}_R \mathbf{\Sigma}_R \mathbf{V}^T \mathbf{x} \cong \mathbf{b}$

$$\mathbf{x} \cong \mathbf{V} (\mathbf{\Sigma}_R)^+ \mathbf{U}_R^T \mathbf{b}$$

Example:

Consider solving the least squares problem $\mathbf{A} \mathbf{x} \cong \mathbf{b}$, where the singular value decomposition of the matrix $\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T$ 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) $O(m^2)$