## Linear Models

Geometric Algorithms Lecture 24

## Introduction

Recap Problem
$$A = \begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 1 \\ 1 & 0 & -1 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} 3 \\ 1 \\ -4 \end{bmatrix}$$

$$(arrange of the last of the second of the last of the$$

Find the projection of b onto 
$$Col(A)$$
.

Hint.  $rank(A) = 2$   $a_2 = a_1 + a_3$ 
 $Col((a_1, a_3)) = Col(A)$ 

# Answer AF P MXM

$$2: LS. Sol. For  $Ax = b$$$

$$\hat{x}$$
: L.S. sol. for  $A\hat{x} = \hat{b}$   
then  $A\hat{x} = (A\hat{x} + A\hat{x})A\hat{x} = A\hat{x}$ 

$$b = Ax = A(ATA)ATb$$

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$$C = \begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} 3 \\ 1 \\ -4 \end{bmatrix}$$

$$Col(C) = Col(A)$$

then 
$$A^{T}A^{\lambda} = (A^{T}A)^{A^{\lambda}}b$$

$$C^{T} = (101)^{3}$$

$$A^{\lambda} = b$$

$$A^{\lambda} = b$$

$$C^{T} = (101)^{3}$$

$$C^{T}b = (101)^{3}$$

#### Question

Find the matrix which implements orthogonal projection onto the span of  $\begin{bmatrix} 1 \\ -1 \\ 2 \end{bmatrix}$ .

#### Answer

$$\frac{1}{6} \begin{bmatrix} 1 & -1 & 2 \\ -1 & 1 & -2 \\ 2 & -2 & 4 \end{bmatrix}$$

$$\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \longrightarrow \begin{bmatrix} 2 \\ 1 \\ 0 \\ 0 \end{bmatrix} \qquad = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 1 & 1 \\ 0 & 1 & 6 \\ 2 & 1 \end{bmatrix}$$

$$= \frac{\left[ \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ -1 & 2 \end{bmatrix} \end{bmatrix}}{\left[ \begin{bmatrix} 1 & -1 & 2 \end{bmatrix} \begin{bmatrix} -1 & 1 \\ -1 & 2 \end{bmatrix} \end{bmatrix}} = \frac{\left[ \begin{bmatrix} 1 & -1 & 2 \\ -1 & 1 \end{bmatrix} \end{bmatrix}}{\left[ \begin{bmatrix} 0 & 1 \\ -1 & 1 \end{bmatrix} \end{bmatrix}}$$

$$= \frac{\left[ \begin{bmatrix} 0 & 0 \\ 0 \end{bmatrix} \begin{bmatrix} -1 & 2 \\ -1 & 1 \end{bmatrix} \end{bmatrix}}{\left[ \begin{bmatrix} 0 & -1 & 2 \\ -1 & 1 \end{bmatrix} \end{bmatrix}}$$

$$= \frac{\left[ \begin{bmatrix} 0 & 0 \\ 0 \end{bmatrix} \begin{bmatrix} -1 & 2 \\ -1 & 1 \end{bmatrix} \end{bmatrix}}{\left[ \begin{bmatrix} 0 & -1 & 2 \\ -1 & 1 \end{bmatrix} \end{bmatrix}}$$

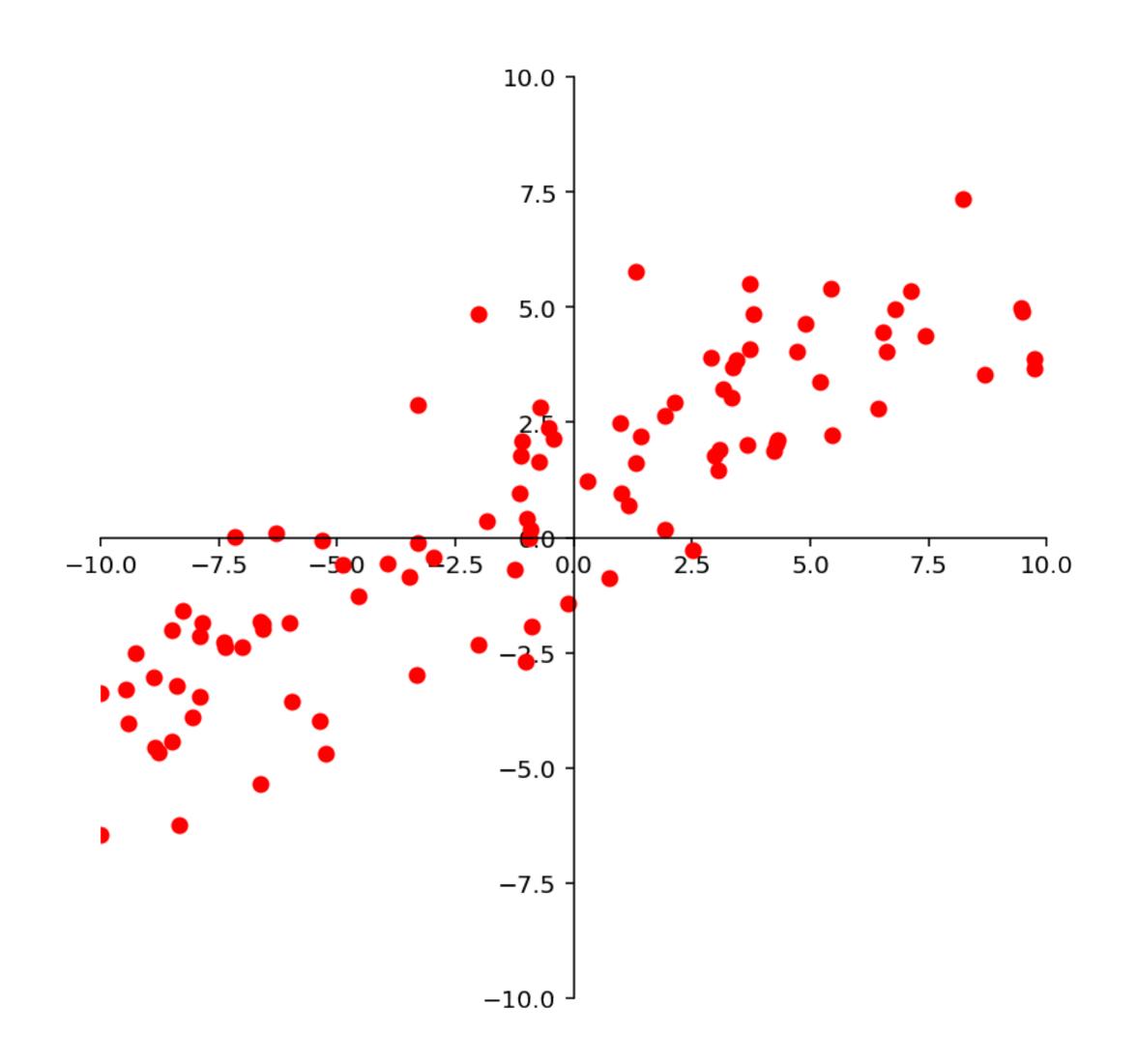
#### Objectives

- 1. Use the least square method to build linear models of noisy data.
- 2. Show how we can use linear algebraic methods to model with non-linear models.

#### Keywords

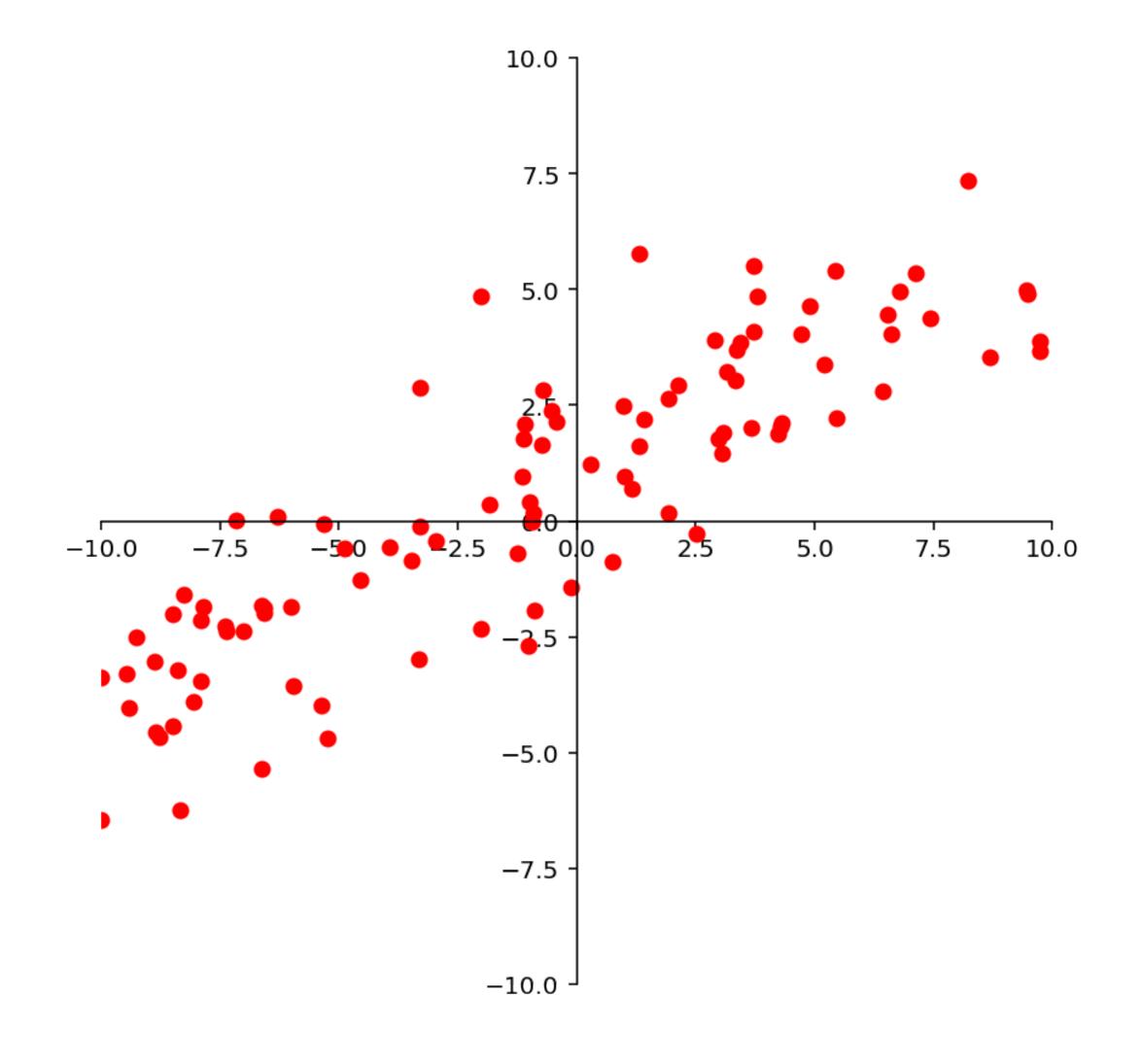
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line of best fit
independent/dependent variables
residuals
prediction
simple least squares regression
multiple regression
polynomial regression
models
model fitting
model parameters
design matrices
```

## A Warmup: Line of Best Fit



You're given a set of points in  $\mathbb{R}^2$ 

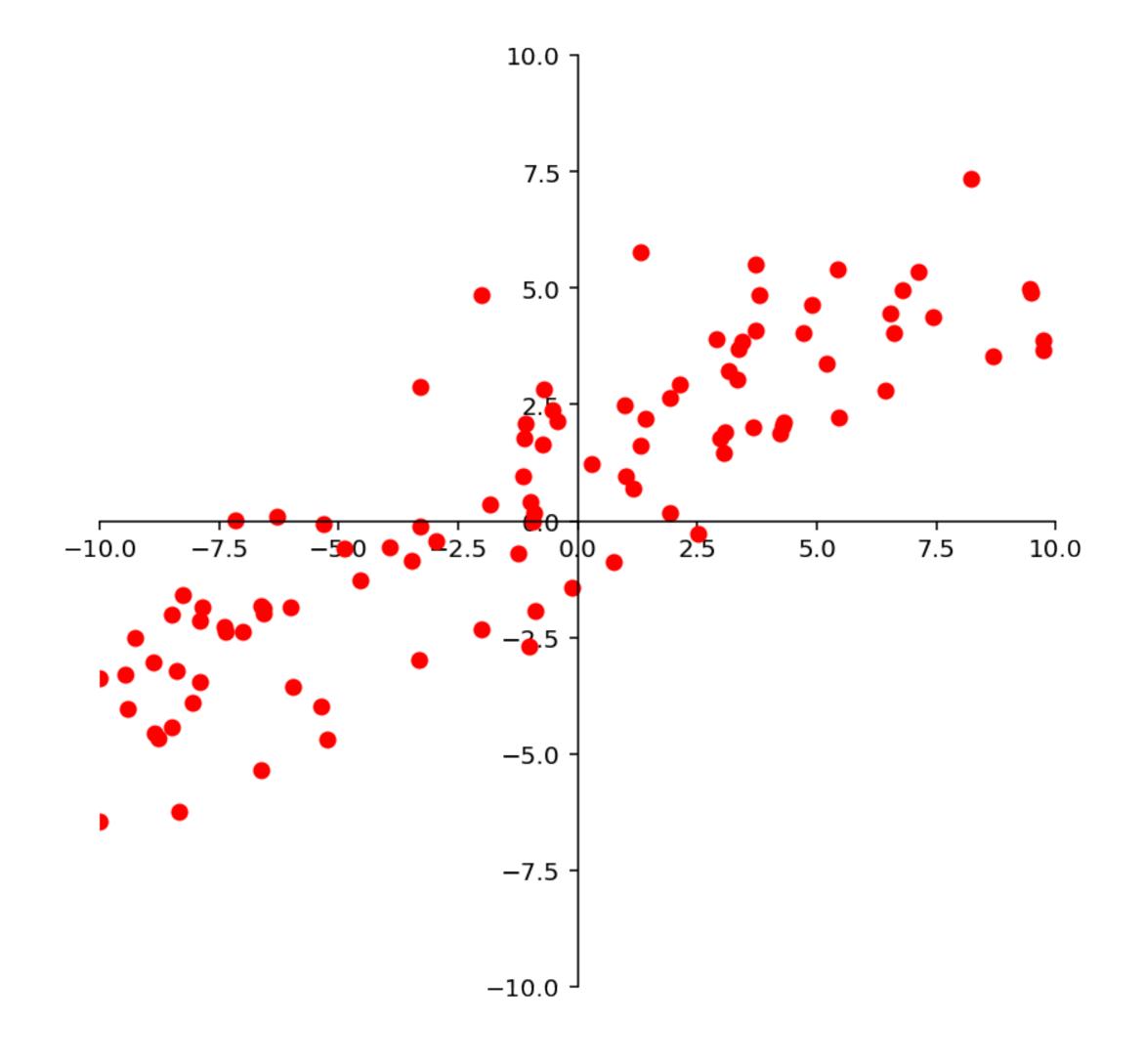
$$\{(x_1, y_1), \ldots, (x_k, y_k)\}$$



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**Example.** You collect (height, weight) data for a population.

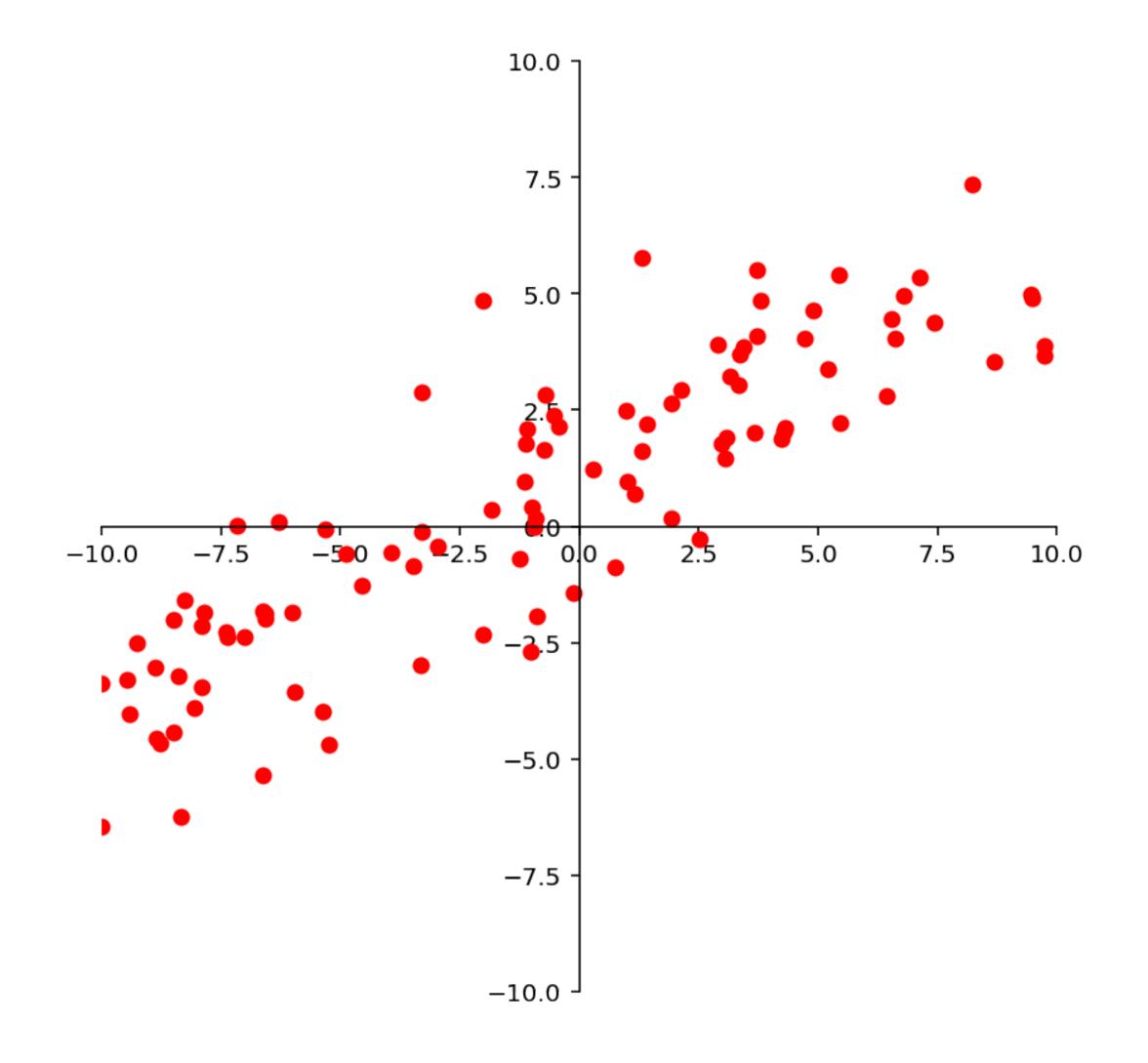


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You notice they *kind* of trend as a line.

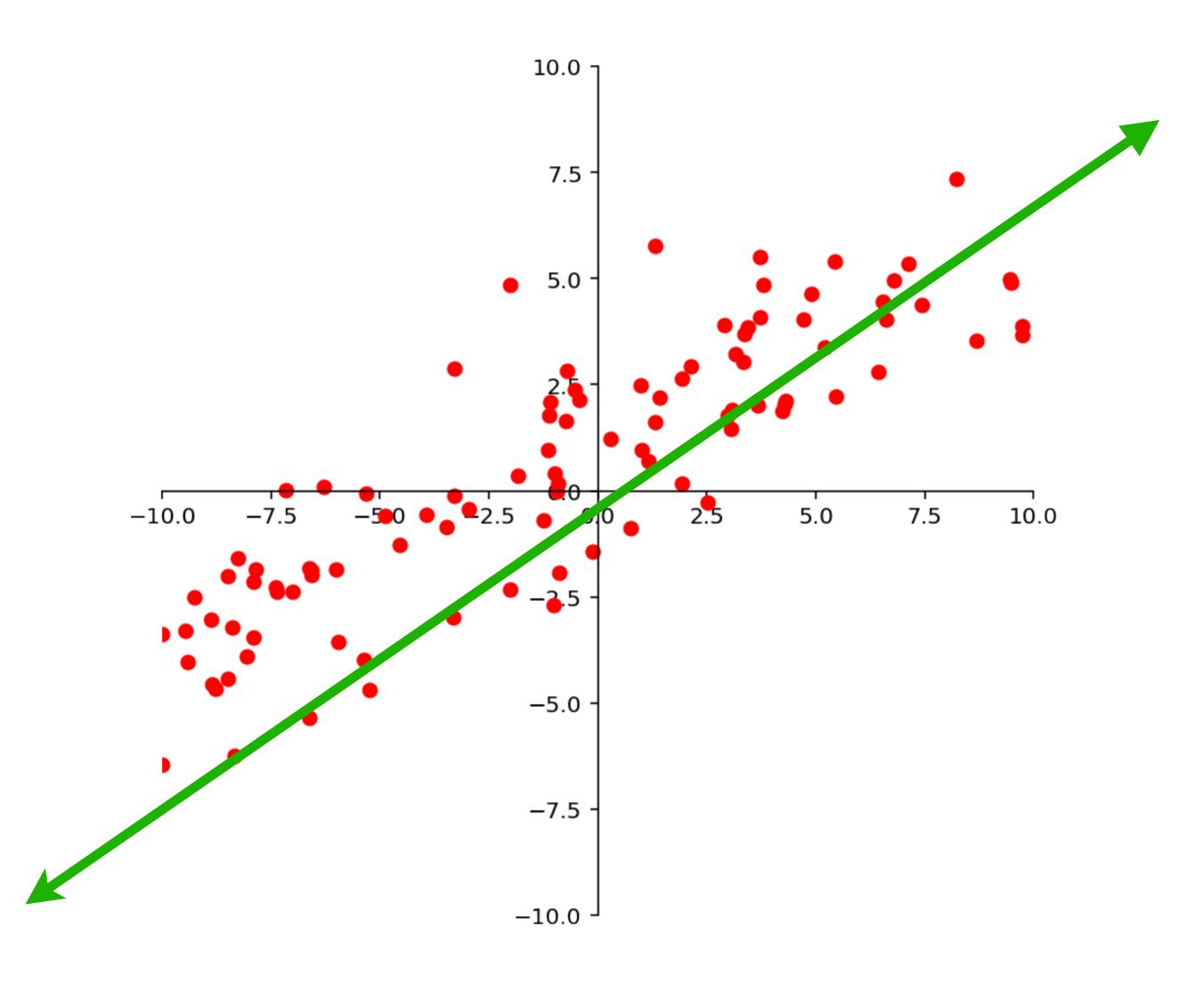


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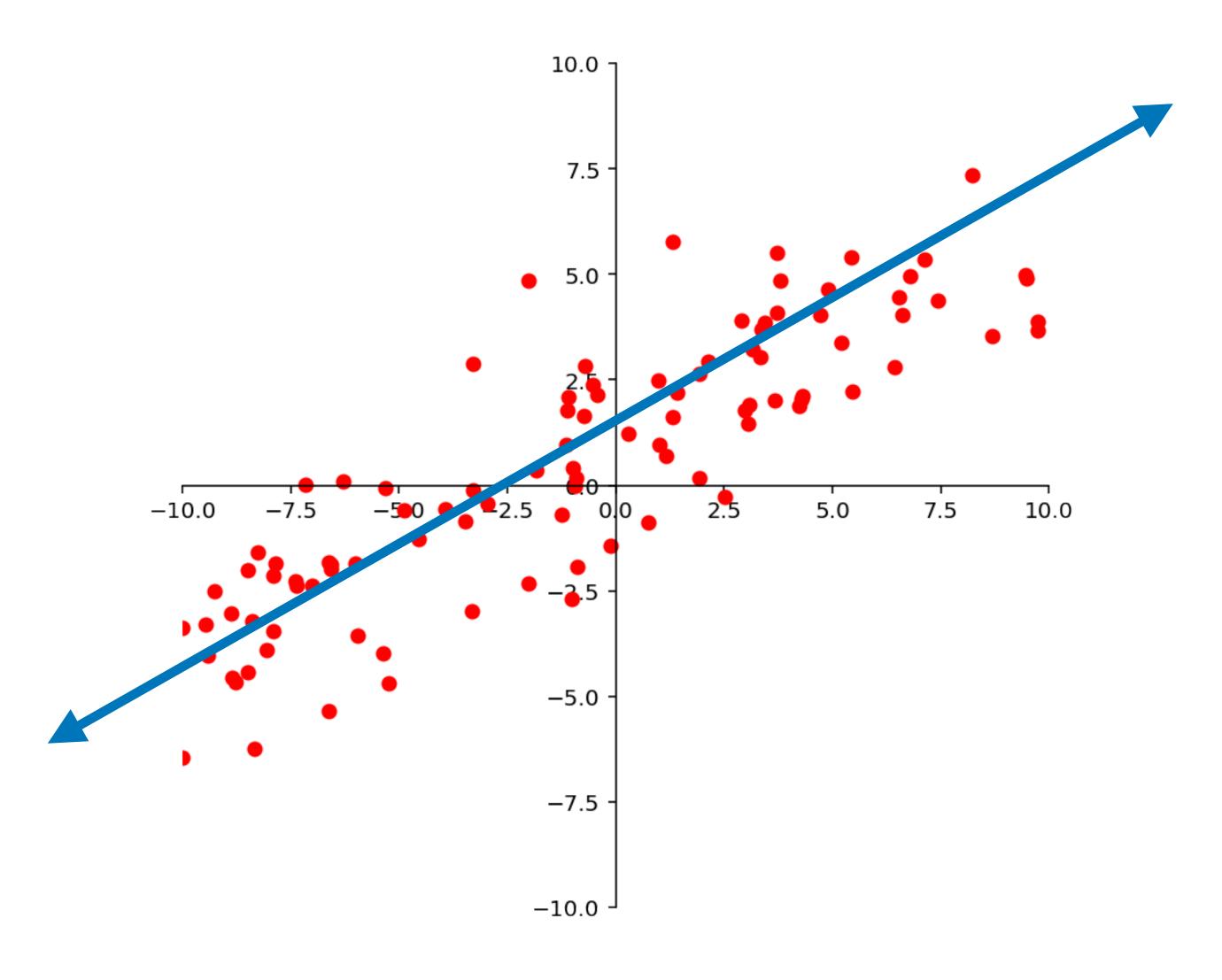


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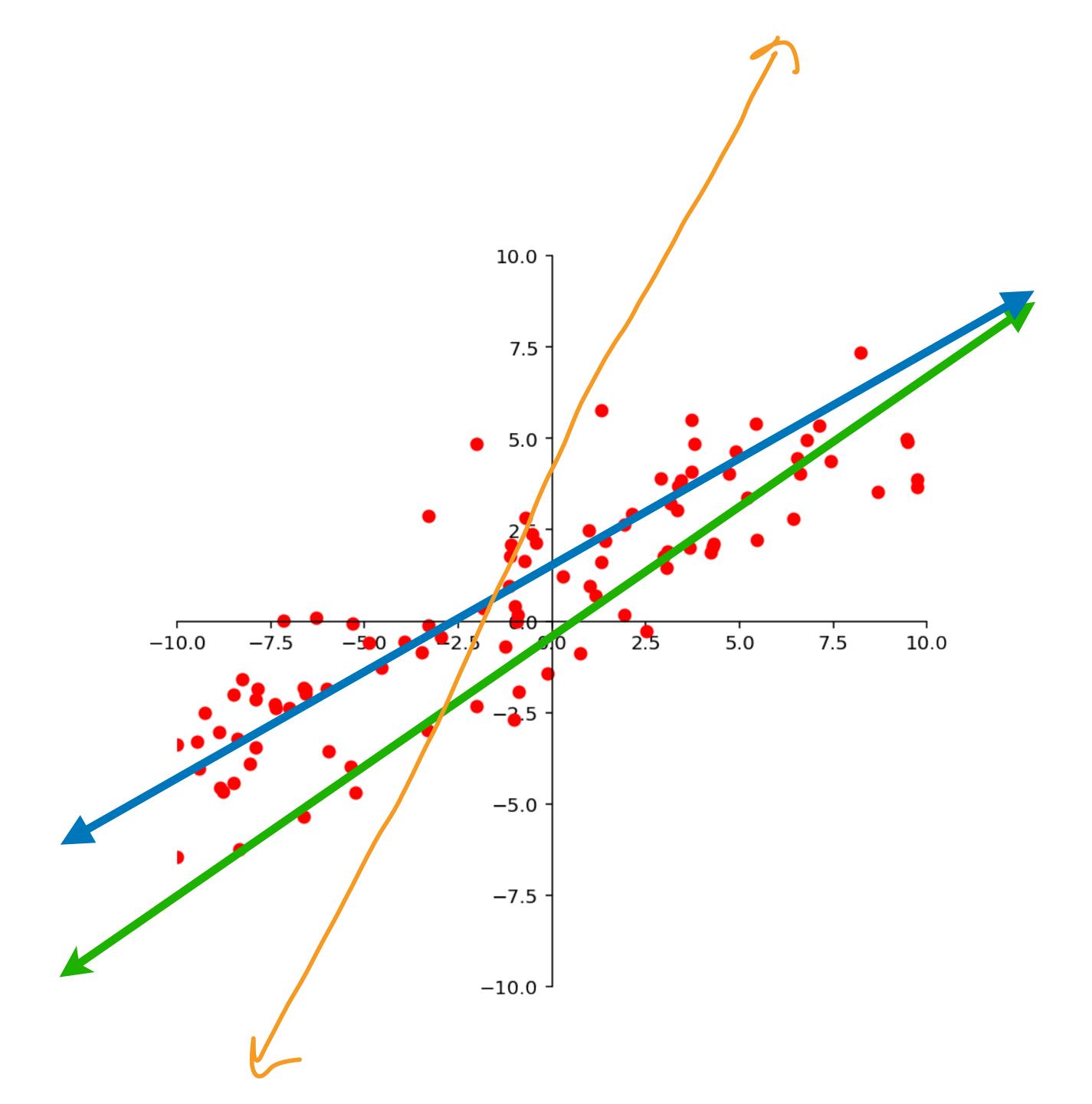
**Example.** You collect (height, weight) data for a population.

You notice they *kind* of trend as a line.



Question. Which line "best" describes the trend of the dataset?

Which one best models the dataset?



1. What is a model?

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We'll come back to this...

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2. What does "best" mean?

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We'll come back to this...

2. What does "best" mean?

This is a make-or-break question.

#### Least Squares Simple Linear Regression

**Problem.** Given a set of points  $\{(x_1,y_1),...,(x_n,y_n)\}$ , find the line

$$f(x) = \beta_0 + \beta_1 x$$

which <u>minimizes</u>

$$\sum_{i=1}^{n} (y_i - f(x_i))^2$$

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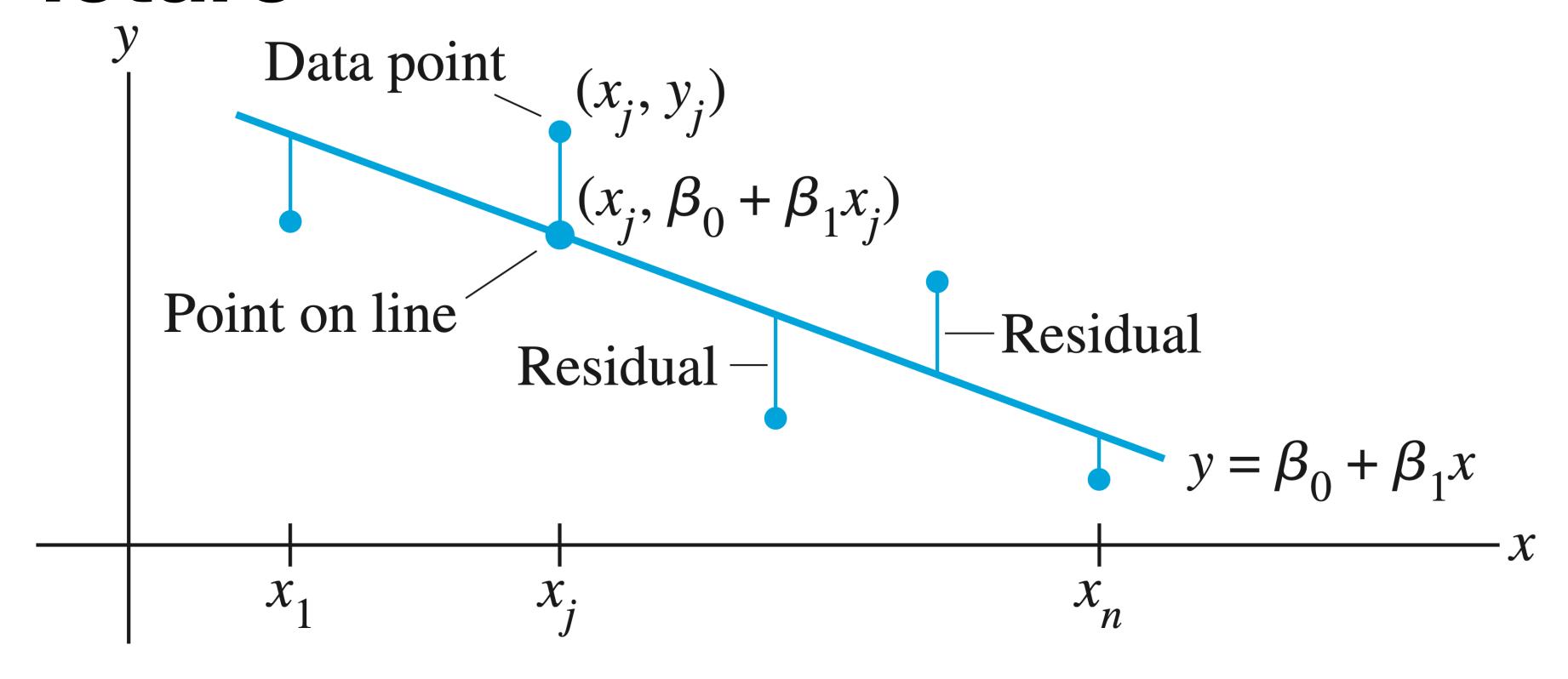
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$$y - interept$$

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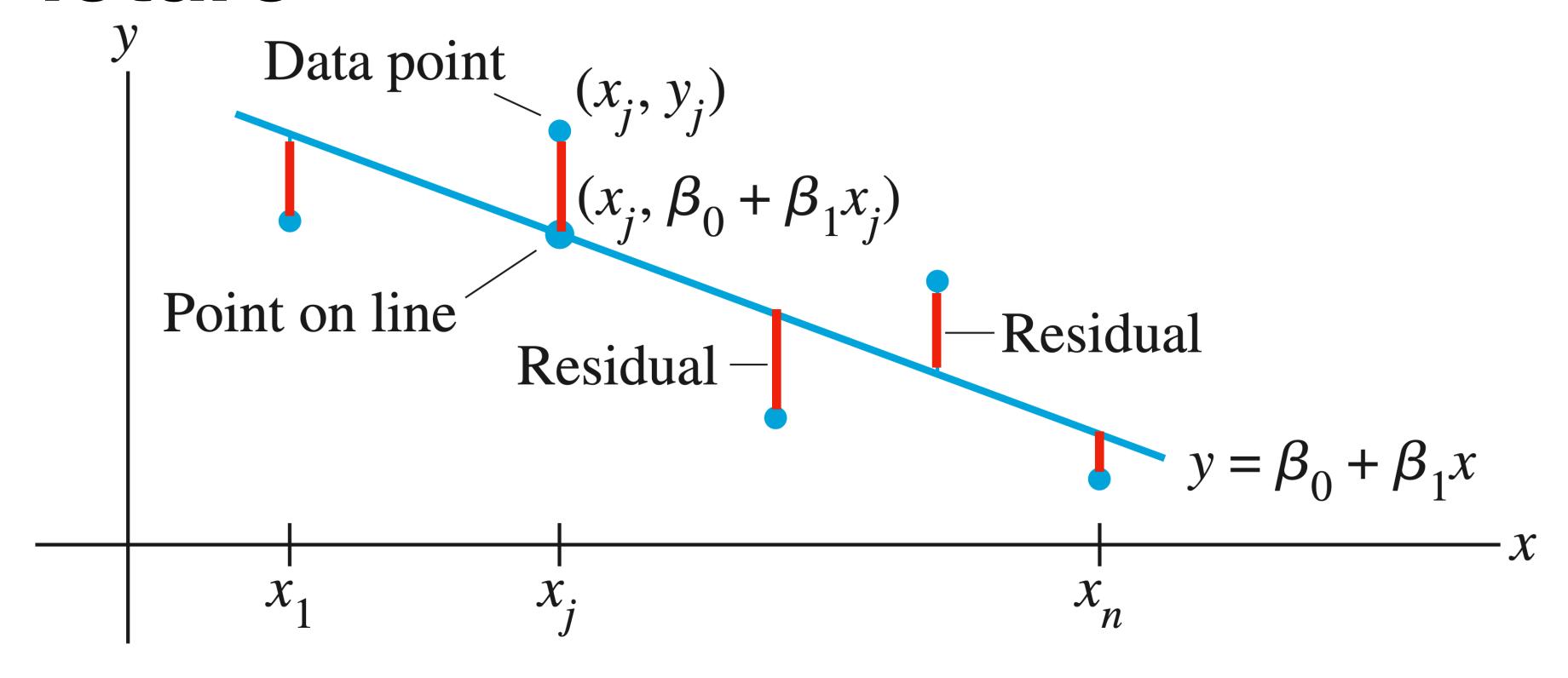
The "best" line minimizes the sum of squares of differences.

#### The Picture

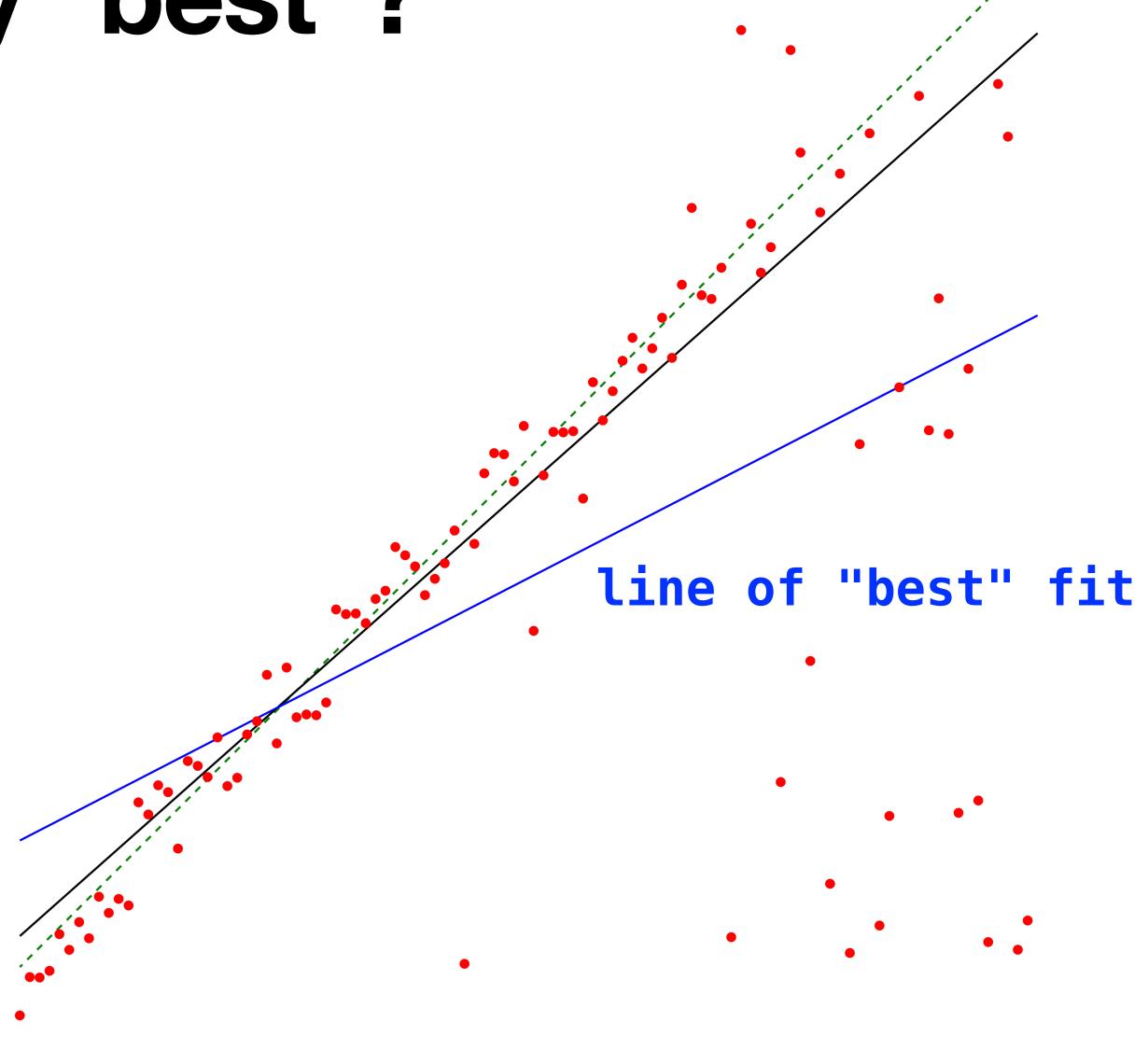


We want to find the line which makes the sum of these differences as small as possible.

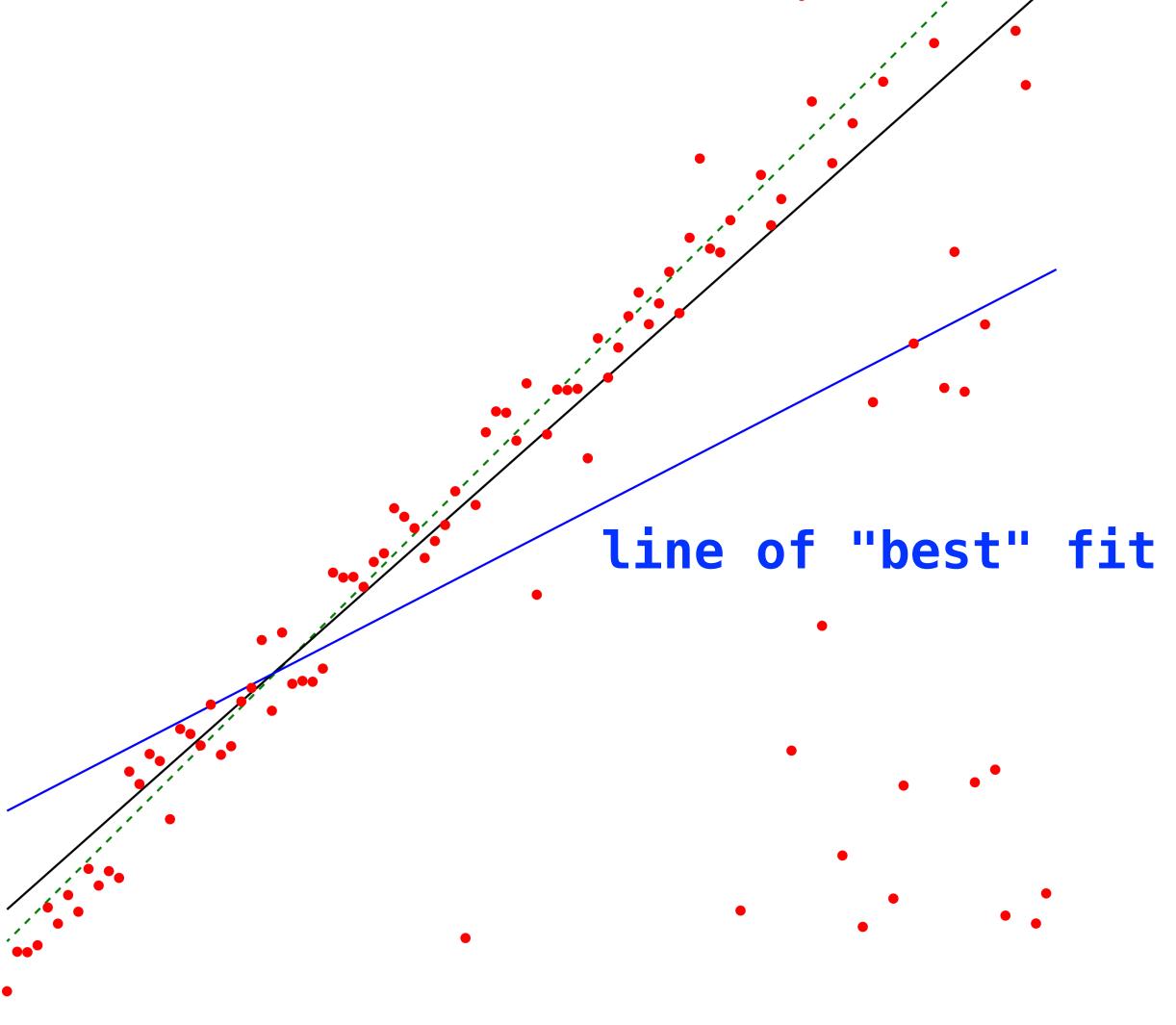
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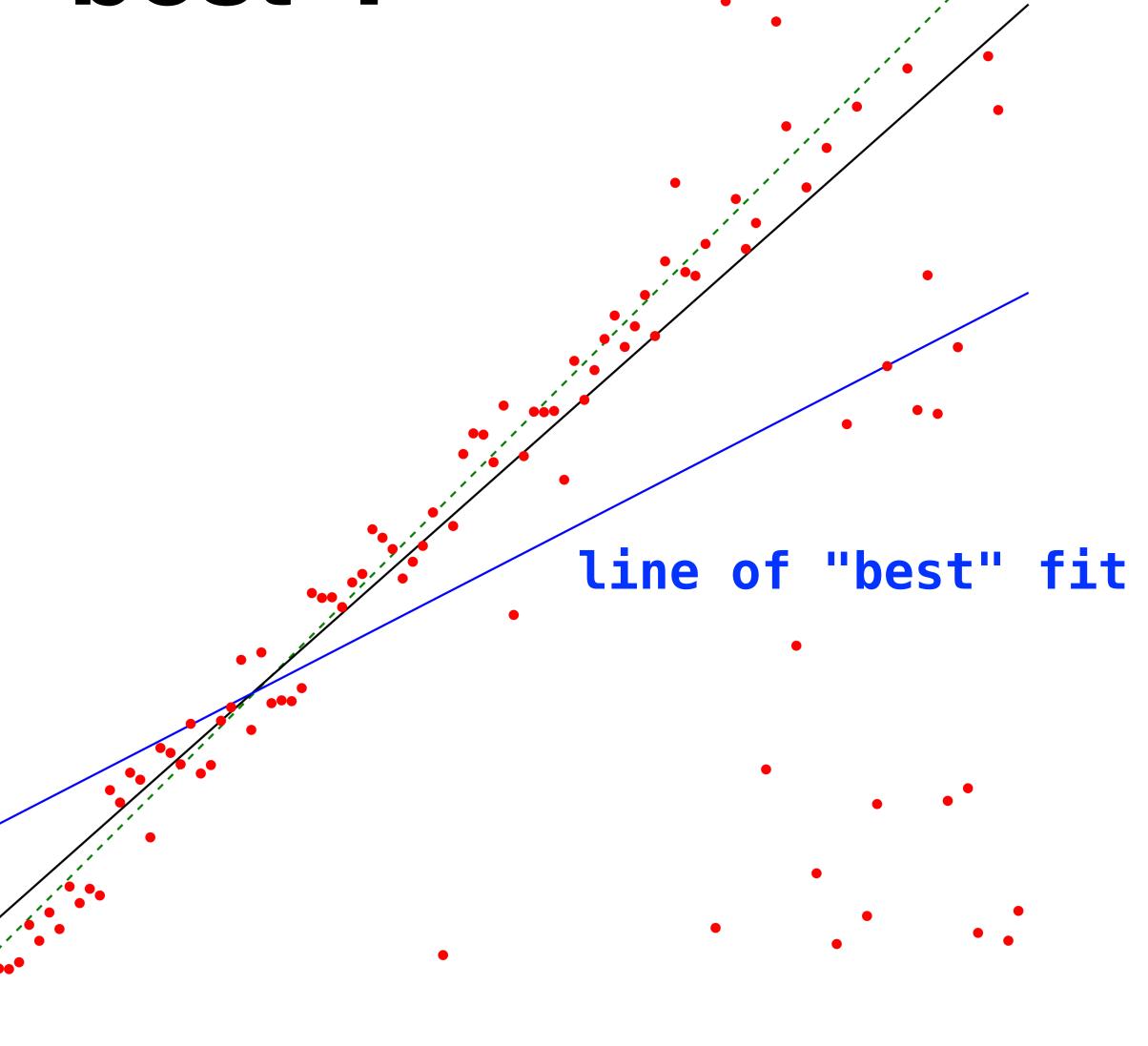


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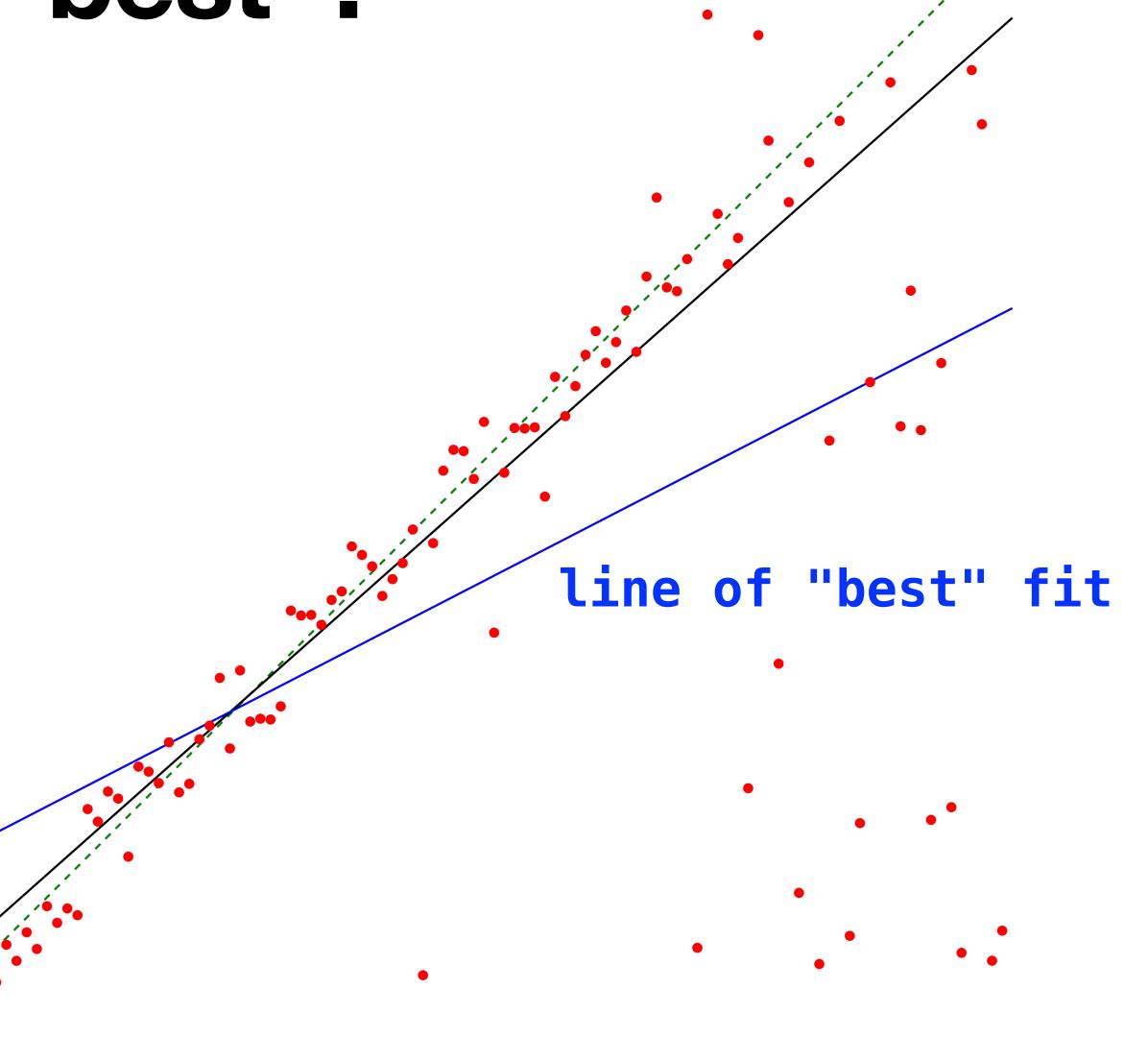
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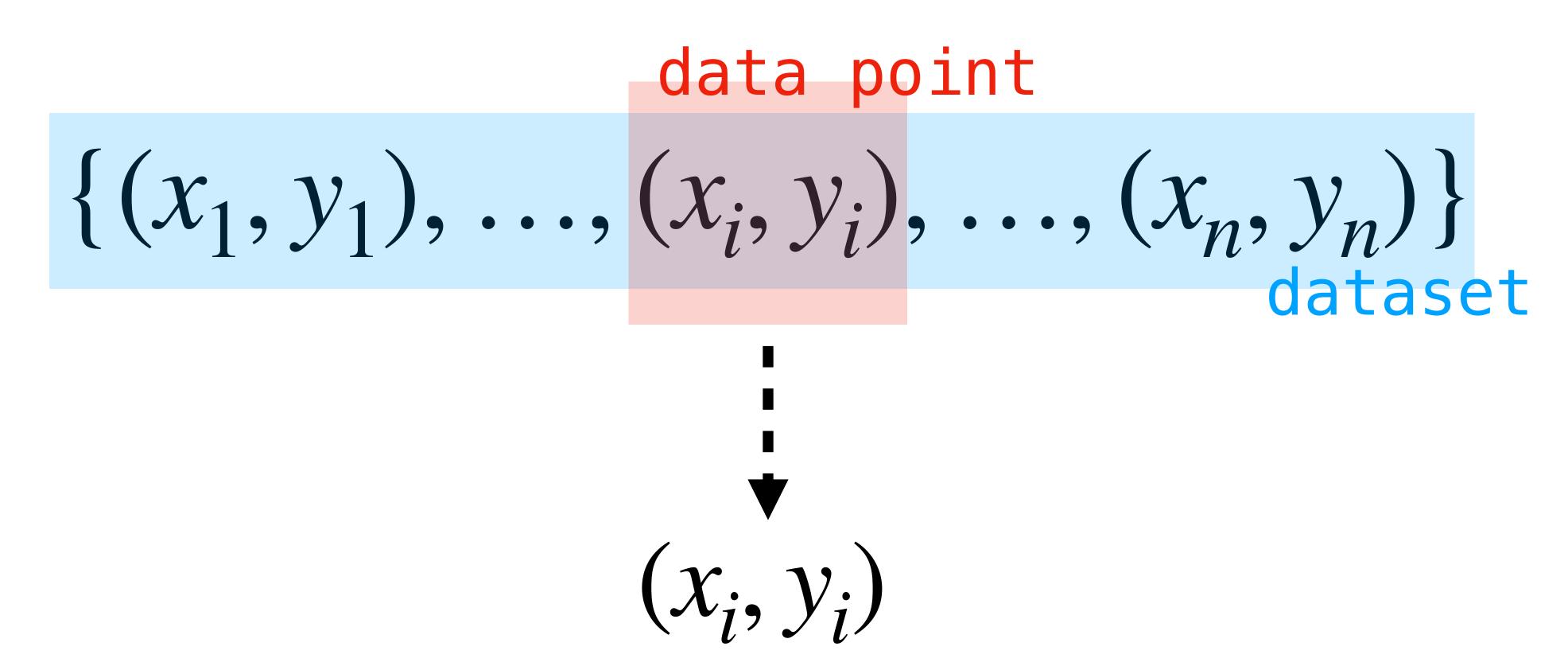
The point. We fix our notion of "best" first, and then we do calculations and derivations from there.

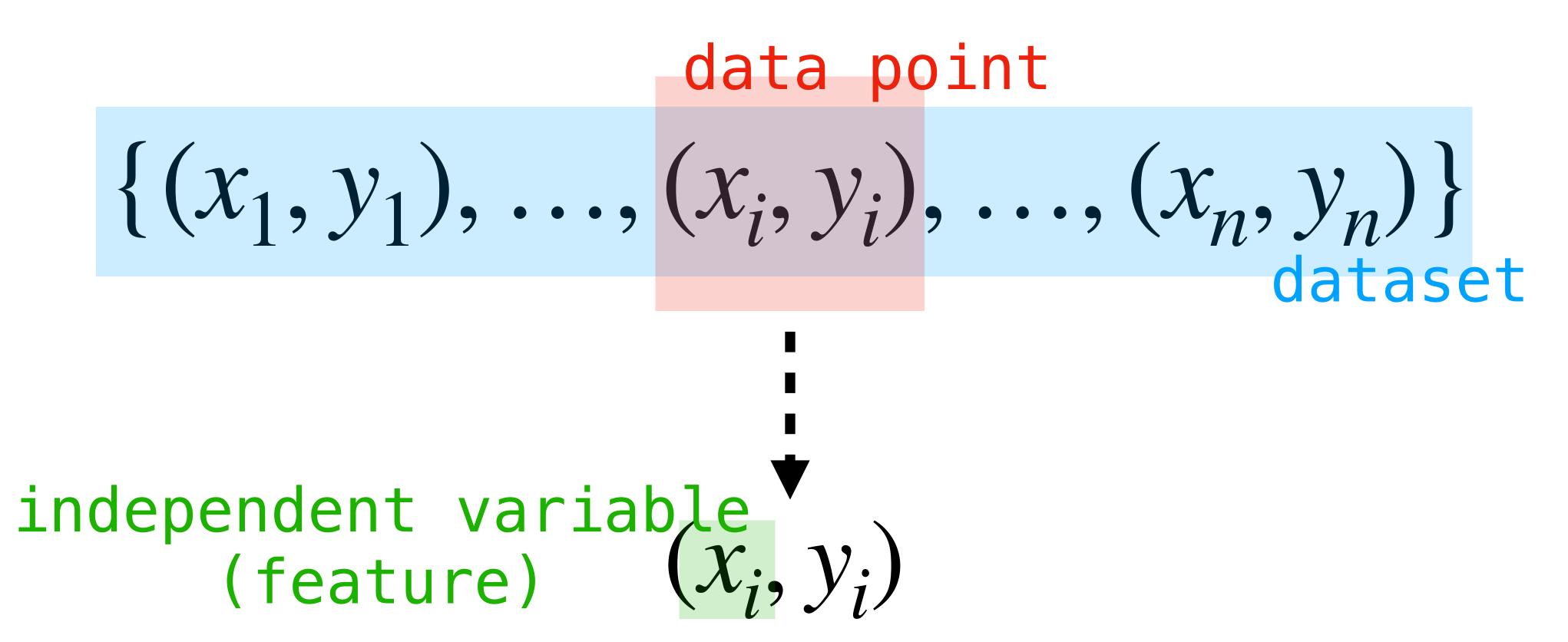


$$\{(x_1,y_1),\ldots,(x_i,y_i),\ldots,(x_n,y_n)\}$$

$$\{(x_1, y_1), \dots, (x_i, y_i), \dots, (x_n, y_n)\}\$$
dataset

$$\{(x_1,y_1),\ldots,(x_i,y_i),\ldots,(x_n,y_n)\}$$
data point
$$\{(x_1,y_1),\ldots,(x_i,y_i),\ldots,(x_n,y_n)\}$$
dataset





```
data point
     \{(x_1,y_1),\ldots,(x_i,y_i),\ldots,(x_n,y_n)\}
                                                dataset
independent variable (feature) (x_i, y_i) dependent variable (1961)
                                       (label)
```

#### Terminology: Models

$$f(x) = \beta_0 + \beta_1 x$$

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model parameters/ regression coefficients

$$f(x) = \beta_0 + \beta_1 x$$

$$\sum_{i=1}^{n} (y_i - f(x_i))^2$$

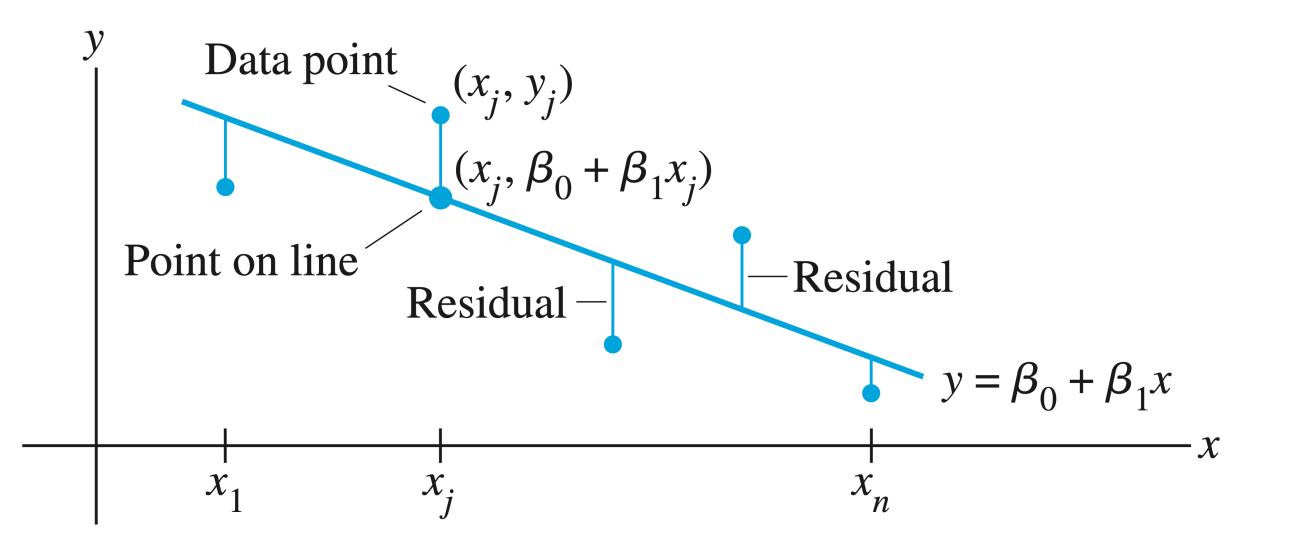
$$\sum_{i=1}^{n} (y_i - f(x_i))^2$$

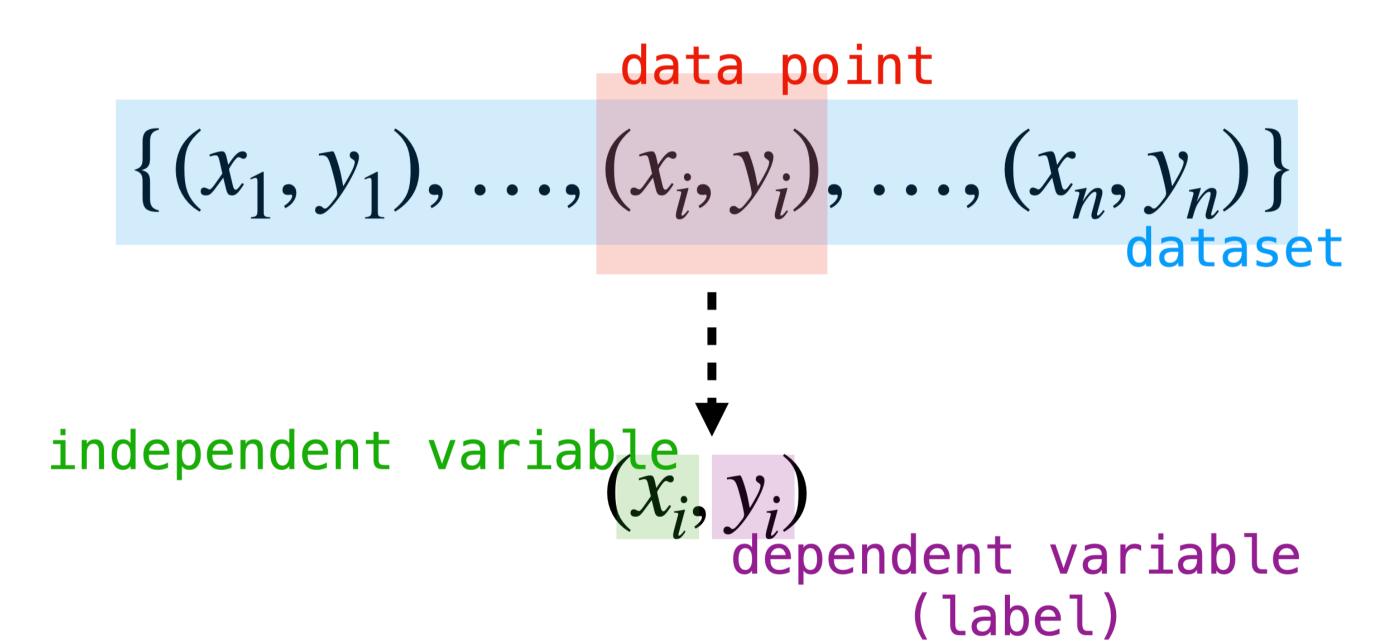
$$i=1$$

$$\sum_{i=1}^{n} \frac{\text{observation}}{y_i - f(x_i)^2}$$

$$\sum_{i=1}^{n} \frac{\text{observation}}{(y_i - f(x_i))^2}$$

# Terminology





model parameters/
regression coefficients
$$f(x) = \beta_0 + \beta_1 x$$

$$\sum_{i=1}^{n} \frac{\text{observation}}{(y_i - f(x_i))^2}$$

$$\sum_{i=1}^{n} \frac{y_i - f(x_i)^2}{\text{prediction}}$$

$$\beta_{1} = \frac{n \sum_{i=1}^{n} x_{i} y_{i} - \left(\sum_{i=1}^{n} x_{i}\right) \left(\sum_{i=1}^{n} y_{i}\right)}{n \sum_{i=1}^{n} x_{i}^{2} - \left(\sum_{i=1}^{n} x_{i}\right)^{2}} \qquad \beta_{0} = \frac{\sum_{i=1}^{n} y_{i} - \beta_{1} \sum_{i=1}^{n} x_{i}}{n}$$

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**Problem.** Find the least squares line for the dataset  $\{(x_1, y_1), ..., (x_n, y_n)\}$ .

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Solution (First attempt). Use these equations...

Don't memorize these.

$$\beta_{1} = \frac{\sum_{i=1}^{n} x_{i} \sum_{i=1}^{n} x_{i}}{\sum_{i=1}^{n} x_{i}} \left( \sum_{i=1}^{n} x_{i} \right) \left( \sum_{i=1}$$

**Problem.** Find the least squares line for the dataset  $\{(x_1, y_1), ..., (x_n, y_n)\}$ .

Solution (First attempt). Use these equations...

$$\sum_{i=1}^{n} (y_i - f(x_i))^2 \qquad ||A\mathbf{x} - \mathbf{b}||^2 = \sum_{i=1}^{n} ((A\mathbf{x})_i - \mathbf{b}_i)^2$$

$$\sum_{i=1}^{n} (y_i - f(x_i))^2$$

minimize for least-squares line

$$||A\mathbf{x} - \mathbf{b}||^2 = \sum_{i=1}^n ((A\mathbf{x})_i - \mathbf{b}_i)^2$$

minimize for least-squares method

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minimize for least-squares line

minimize for least-squares method

These expressions look very similar.

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minimize for least-squares line minimize for least-squares method

These expressions look very similar.

Can we <u>design</u> a matrix where finding a least squares solution gives us a least squares line?

$$\beta_0 + \beta_1 x_1 = y_1$$

$$\beta_0 + \beta_1 x_2 = y_2$$

$$\vdots$$

$$\beta_0 + \beta_1 x_n = y_n$$

In the "ideal" world, we could find parameters  $\beta_0$  and  $\beta_1$  such that all of these equations hold.

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$$\vdots$$

$$\beta_0 + \beta_1 x_n = y_n$$

This is a linear system in the variables  $eta_0$  and  $eta_1$ 

$$\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

In the "ideal" world, this matrix equation has a solution.

$$\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

In the "ideal" world, this matrix equation has a solution.

In reality this system is unlikely to have a solution, but maybe we can find an approximate solution.

$$\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

A Least Squares Problem 
$$\begin{bmatrix} 1 & X \\ 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \vec{\beta} \\ \beta_1 \end{bmatrix} = \begin{bmatrix} \mathbf{y} \\ y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

$$\|X\vec{\beta} - \mathbf{y}\|^2 = \sum_{i=1}^n ((\beta_0 + \beta_1 x_i) - y_i)^2$$

A Least Squares Problem 
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$$\|X\vec{\beta} - \mathbf{y}\|^2 = \sum_{i=1}^{n} ((\beta_0 + \beta_1 x_i) - y_i)^2$$

The sum of squares of residuals is the squared distances between  $X\beta$  and y.

**A Least Squares Problem**

$$\begin{bmatrix}
1 & X \\
1 & x_1 \\
1 & x_2 \\
\vdots & \vdots \\
1 & x_n
\end{bmatrix}
\begin{bmatrix}
\vec{\beta} \\
\beta_1
\end{bmatrix} = \begin{bmatrix}
y_1 \\
y_2 \\
\vdots \\
y_n
\end{bmatrix}$$

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Least squares solutions to this system give us parameters for least squares lines.

#### Just for Fun

$$\beta_1 = \frac{n\sum_i x_i y_i - \left(\sum_i x_i\right) \left(\sum_i y_i\right)}{n}$$

Let's derive it:

$$X = \begin{bmatrix} \hat{1} & \hat{x} \end{bmatrix}$$

$$X^{T}X = \begin{bmatrix} \hat{1} & \hat{1} \\ \hat{x}^{T} \end{bmatrix} \begin{bmatrix} \hat{1} & \hat{x} \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ \hat{x} & \hat{x} \end{bmatrix}$$

$$\left(X^{\top}X^{\top}\right) = \left(X^{\top}X^{\top}X^{\top}\right) - \left(X^{\top}X^{\top}X^{\top}\right)$$

$$X^{T} \dot{y} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \dot{y} = \begin{bmatrix} 1 \cdot y \\ x \cdot y \end{bmatrix}$$

$$n\sum_{i}x_{i}^{2}-\left(\sum_{i}x_{i}\right)^{2}$$

$$\begin{bmatrix} \times \cdot \times & -1 \cdot \times \\ -\times \cdot 1 & 1 \cdot 1 \end{bmatrix}$$

$$\frac{1}{N(x \cdot x) - (x \cdot 1)^2} \left[ \frac{1}{N(x \cdot x)} - \frac{1}{N(x \cdot x)} \right]$$

#### How To: Least Squares Line

$$\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

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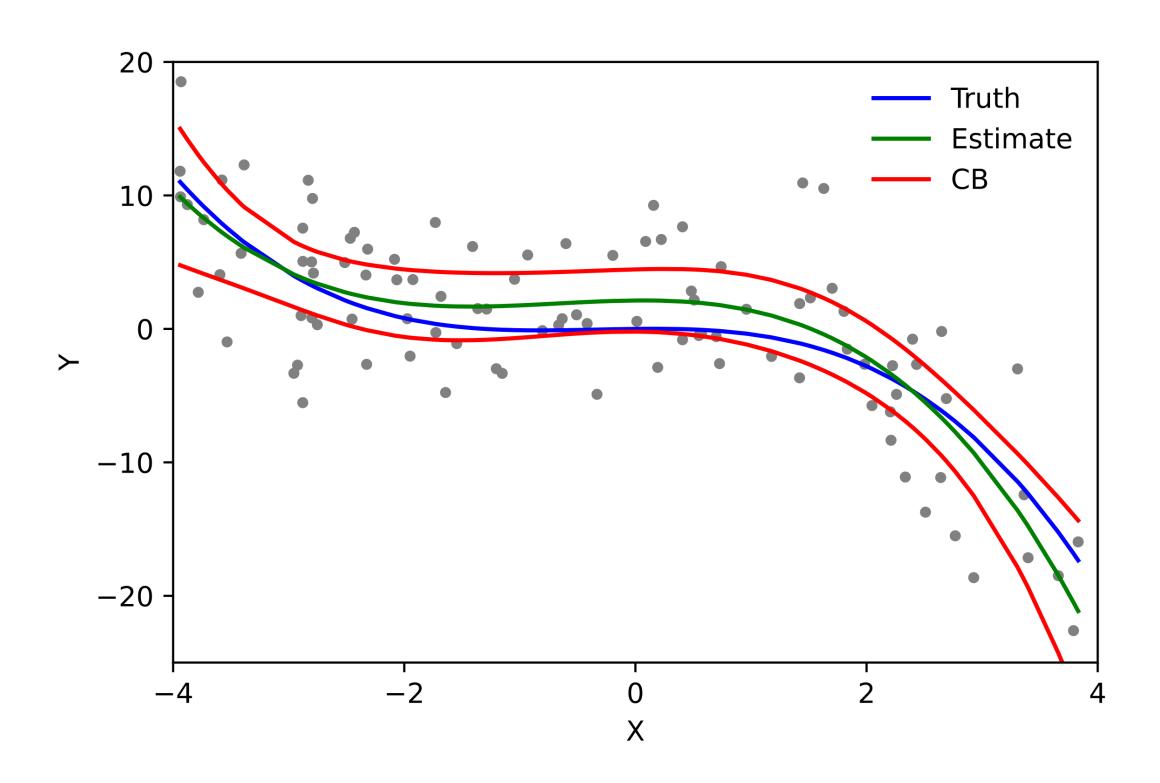
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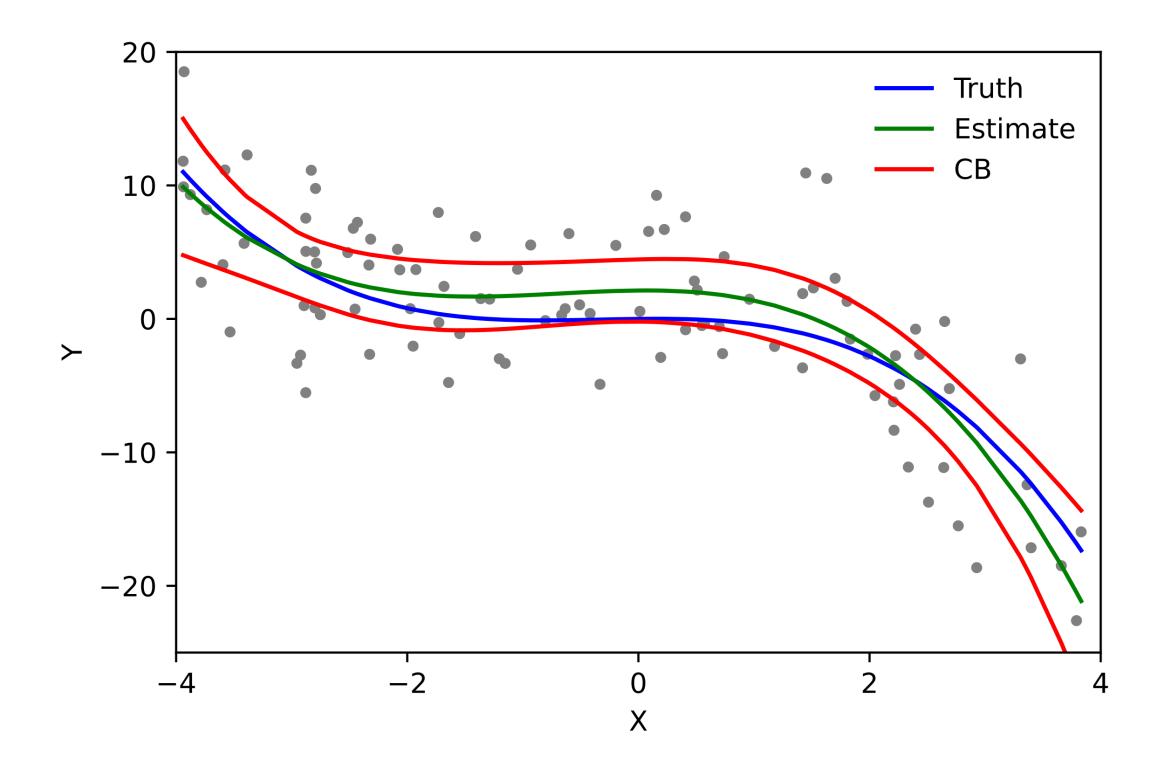
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**Problem.** Find the least squares line for the dataset  $\{(x_1, y_1), ..., (x_n, y_n)\}$ .

Solution. Find the least squares solution to the above equation.

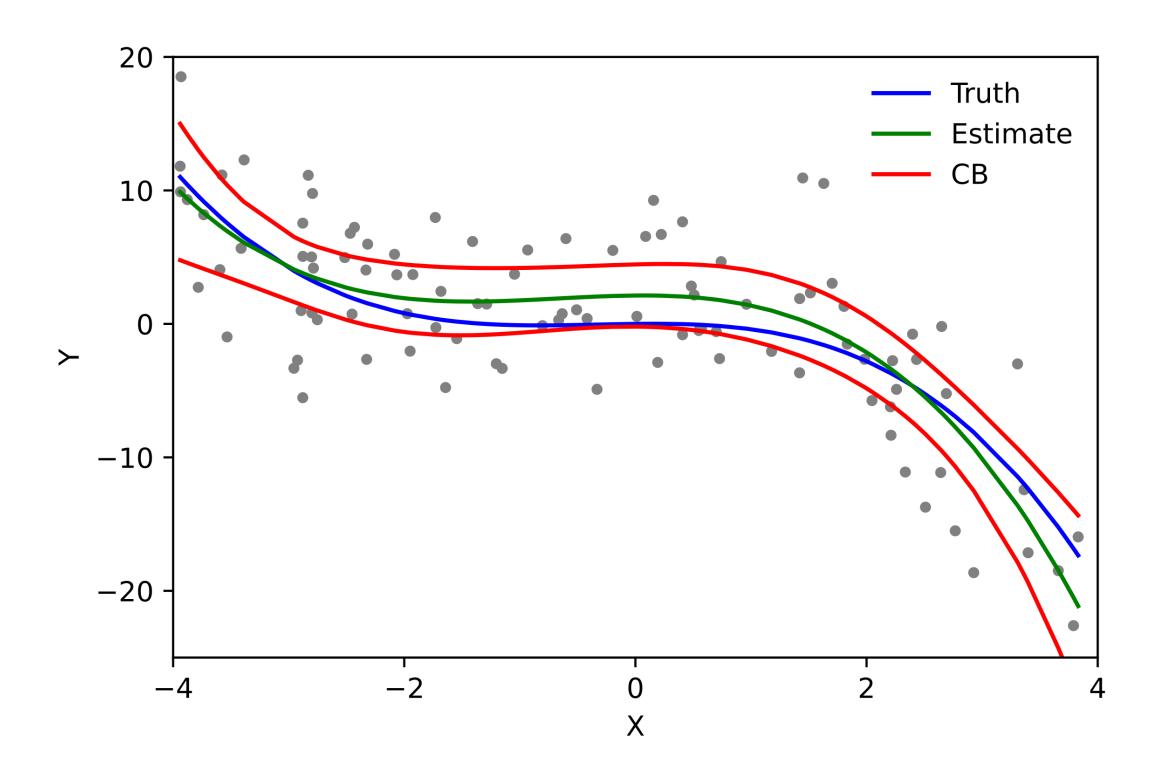


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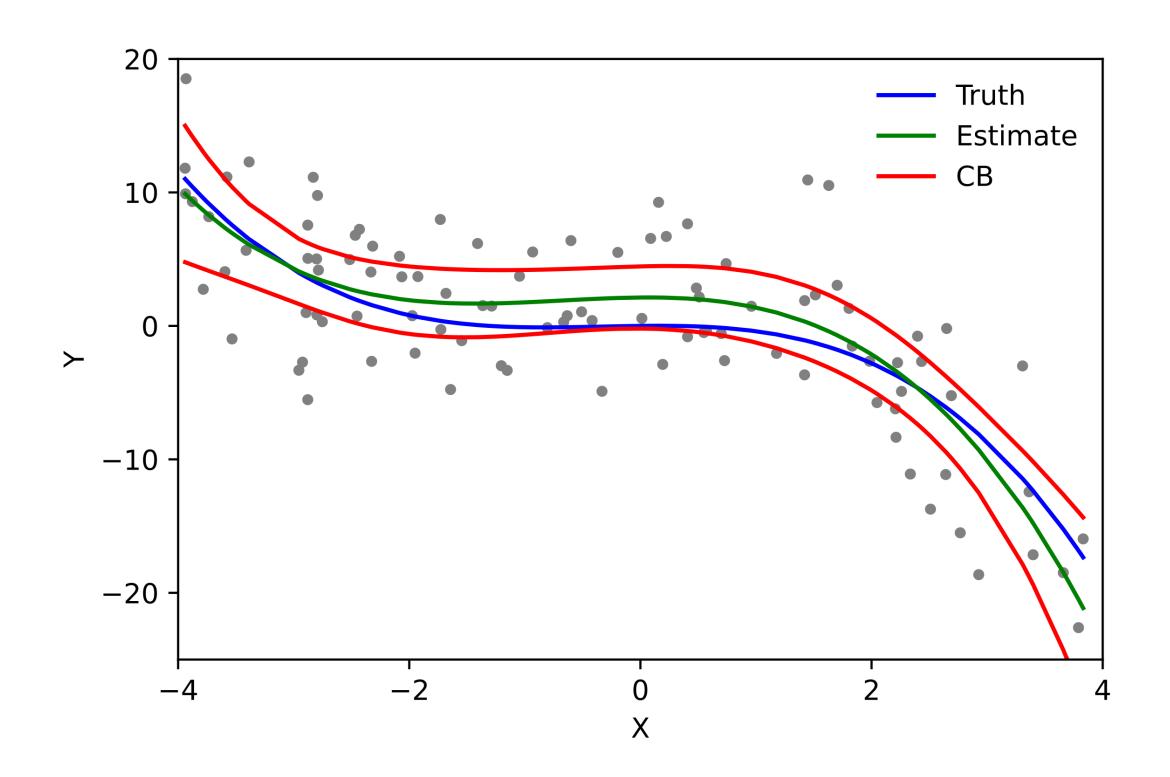
What we are estimating is a mathematical function



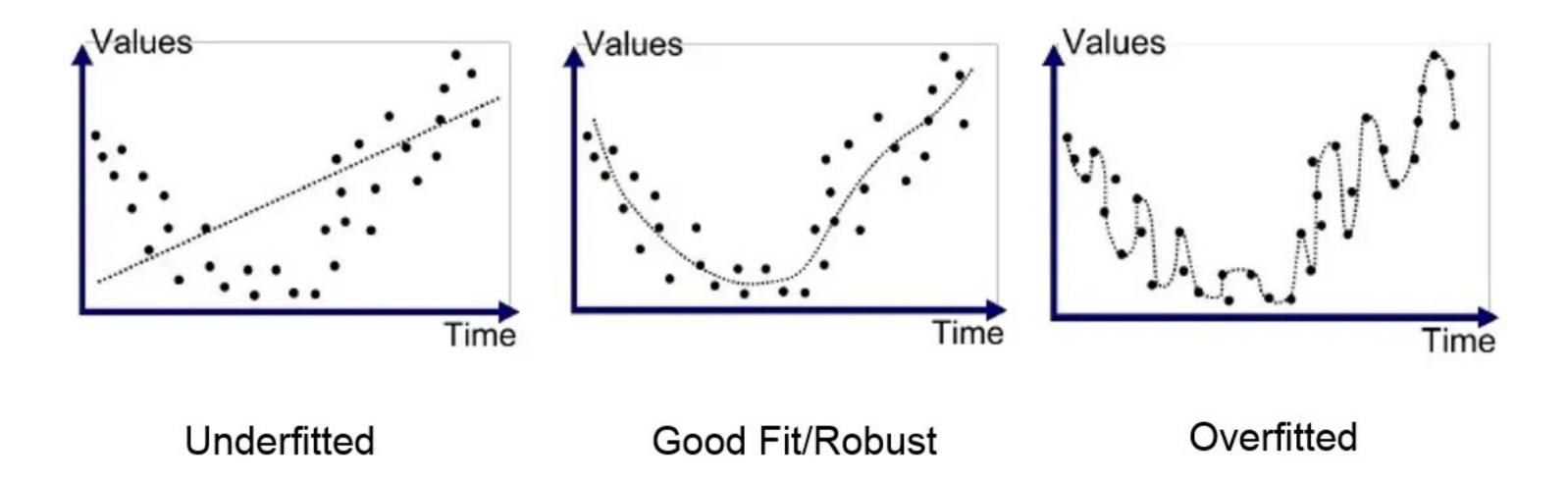
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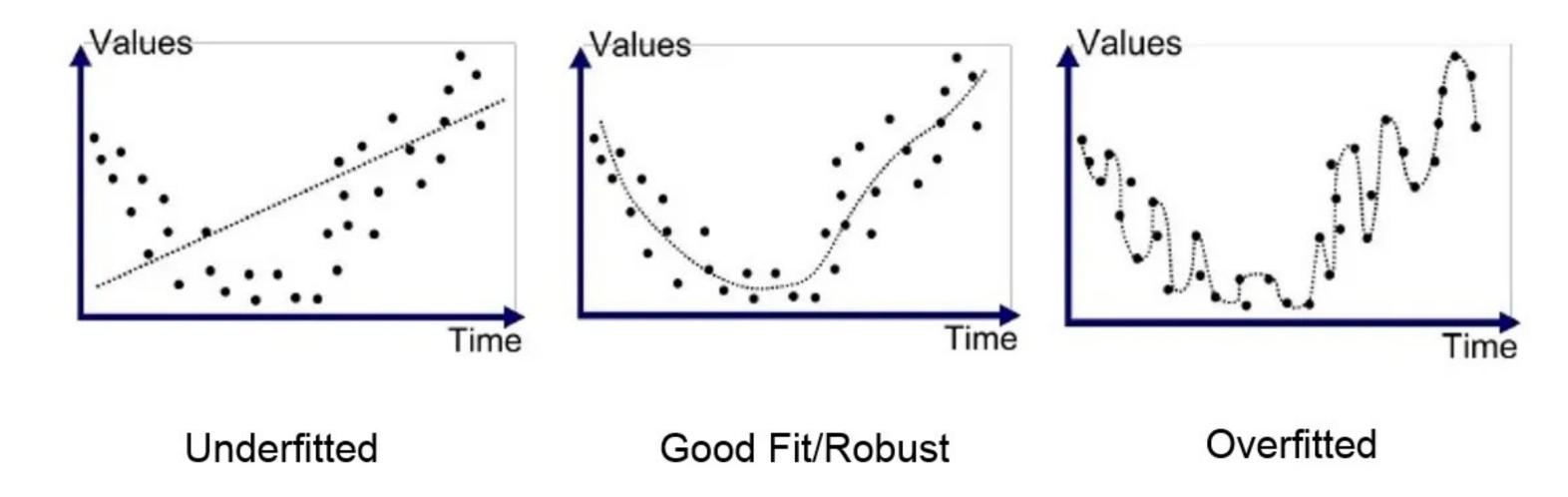
We think of the environment has providing us a function from our independent variables to our dependent variables.



#### Models

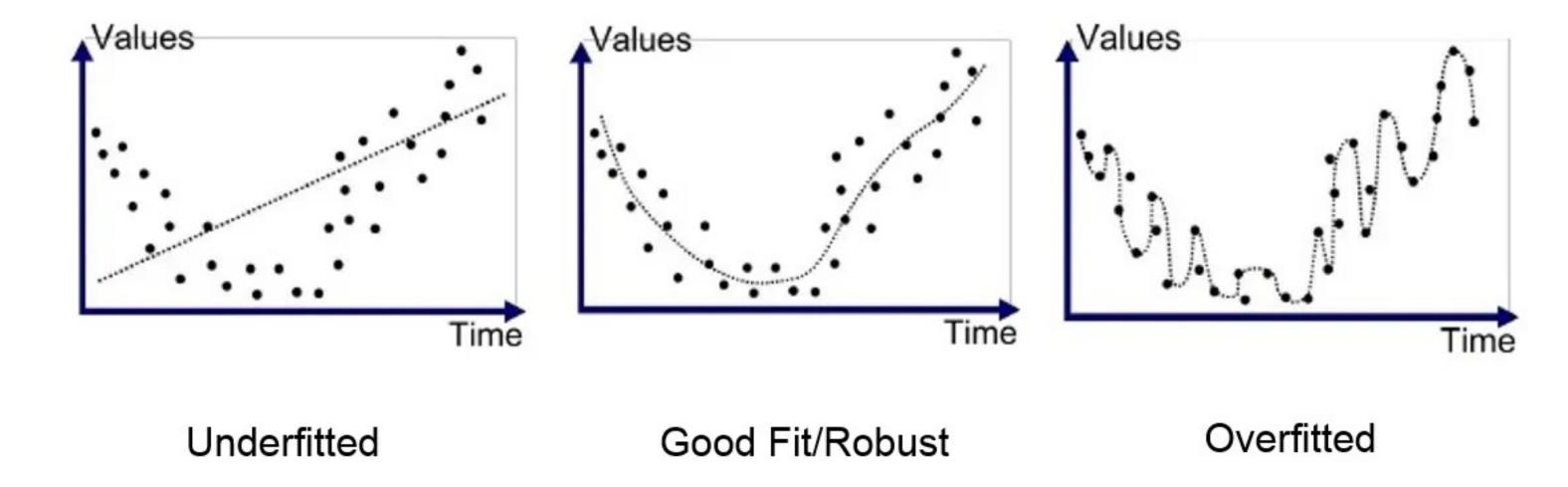


#### Models



Therefore, a model is a mathematical function.

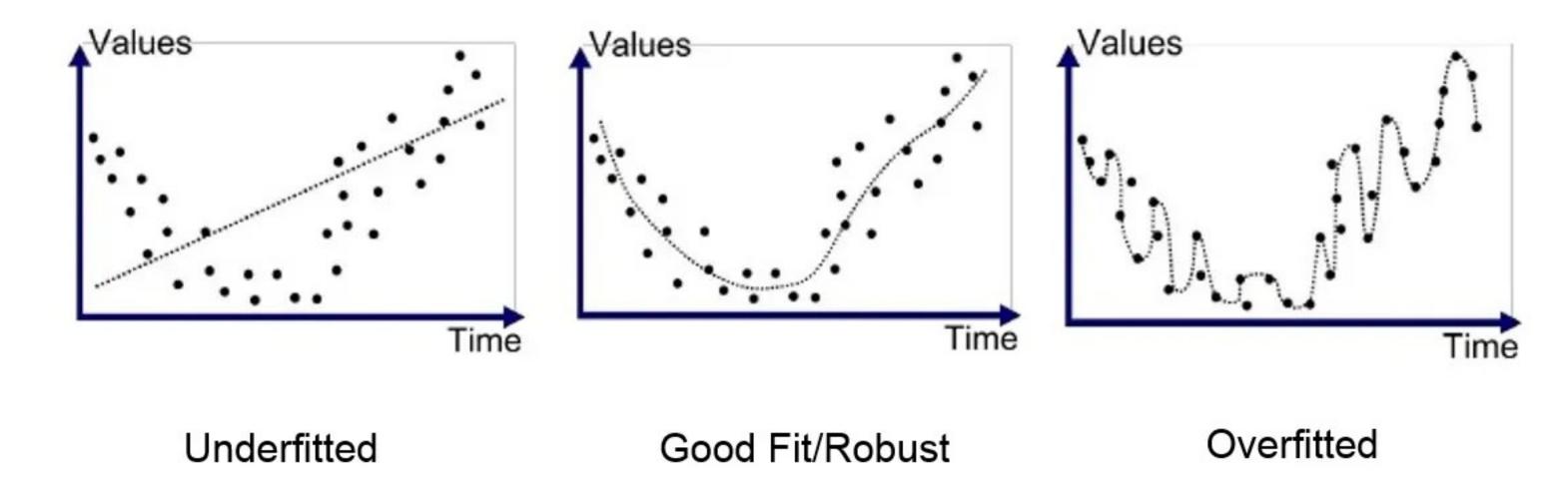
#### Models



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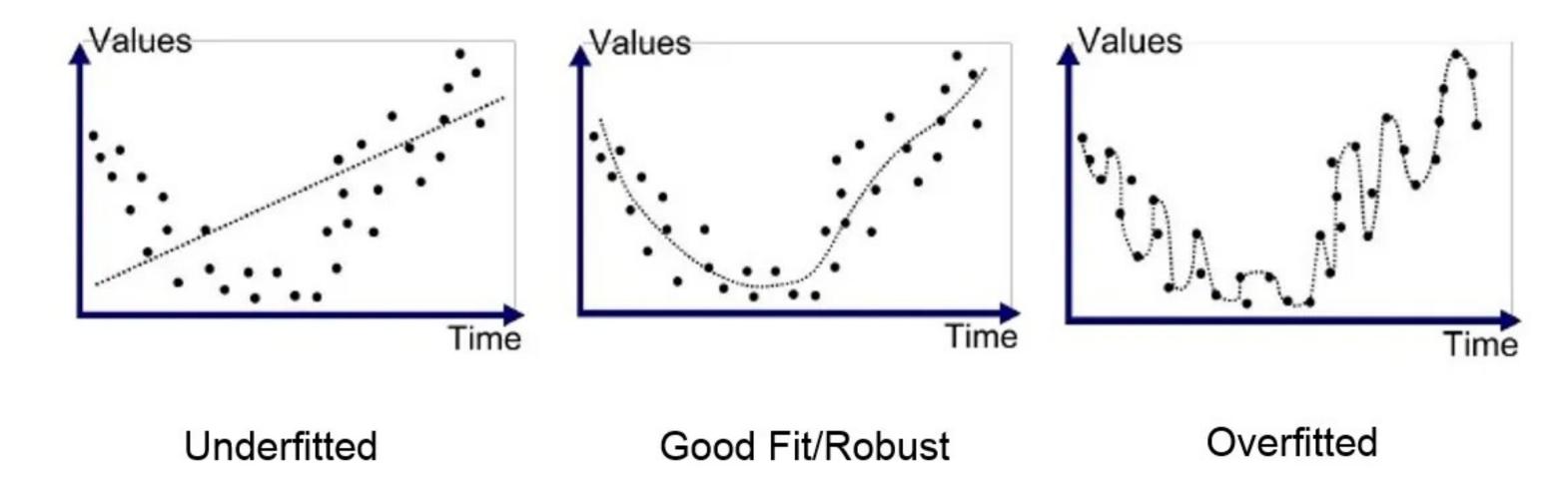


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But this would a bit boring if we just wanted to model data we've seen.

(Advanced) We pick models from weaker classes of functions so that they are more robust when we **predict** values using the model.

**Problem.** Given the data  $\{(x_1, y_1), ..., (x_k, y_k)\}$  use the line of best fit to predict the value of y' for the input x'.

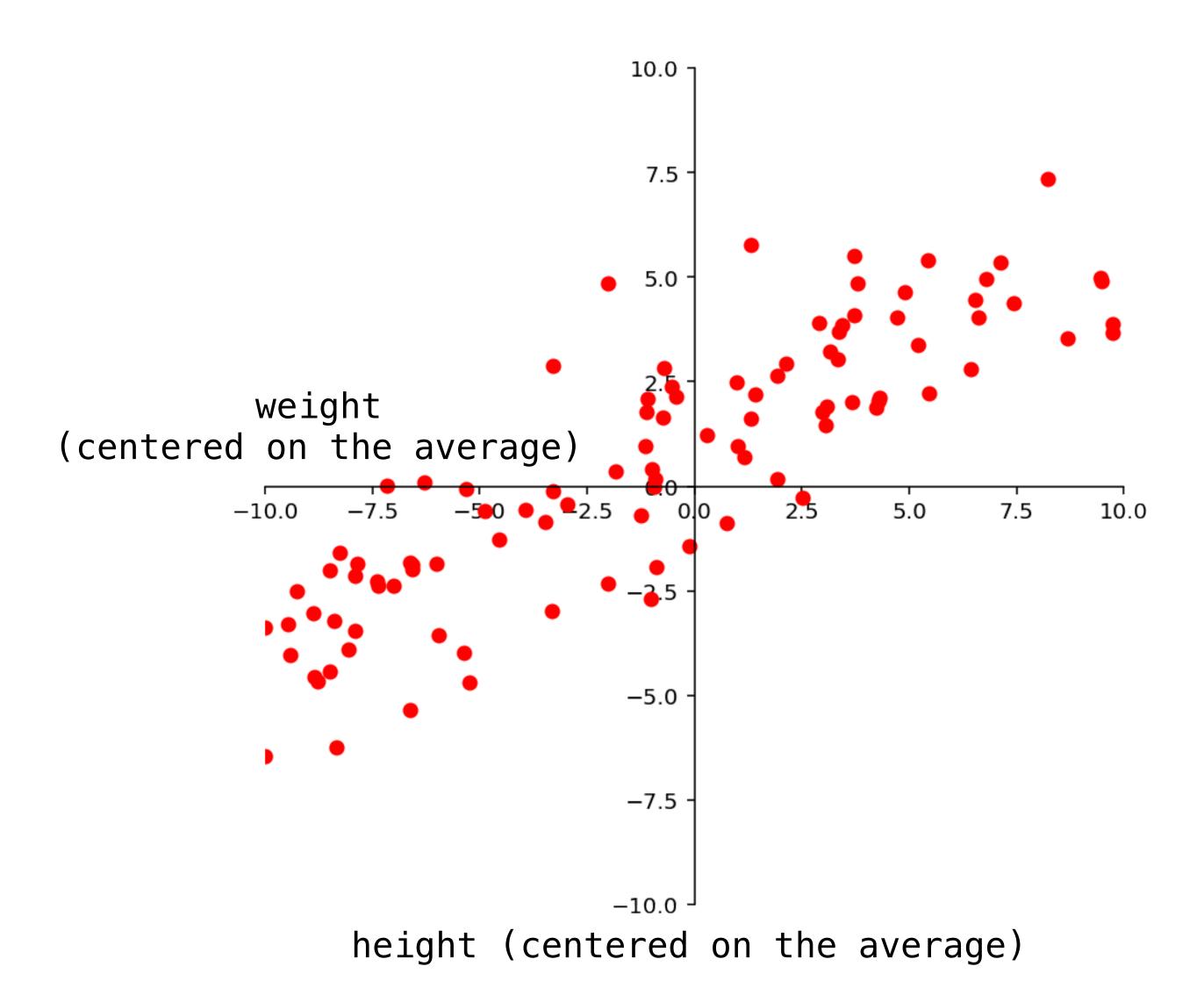
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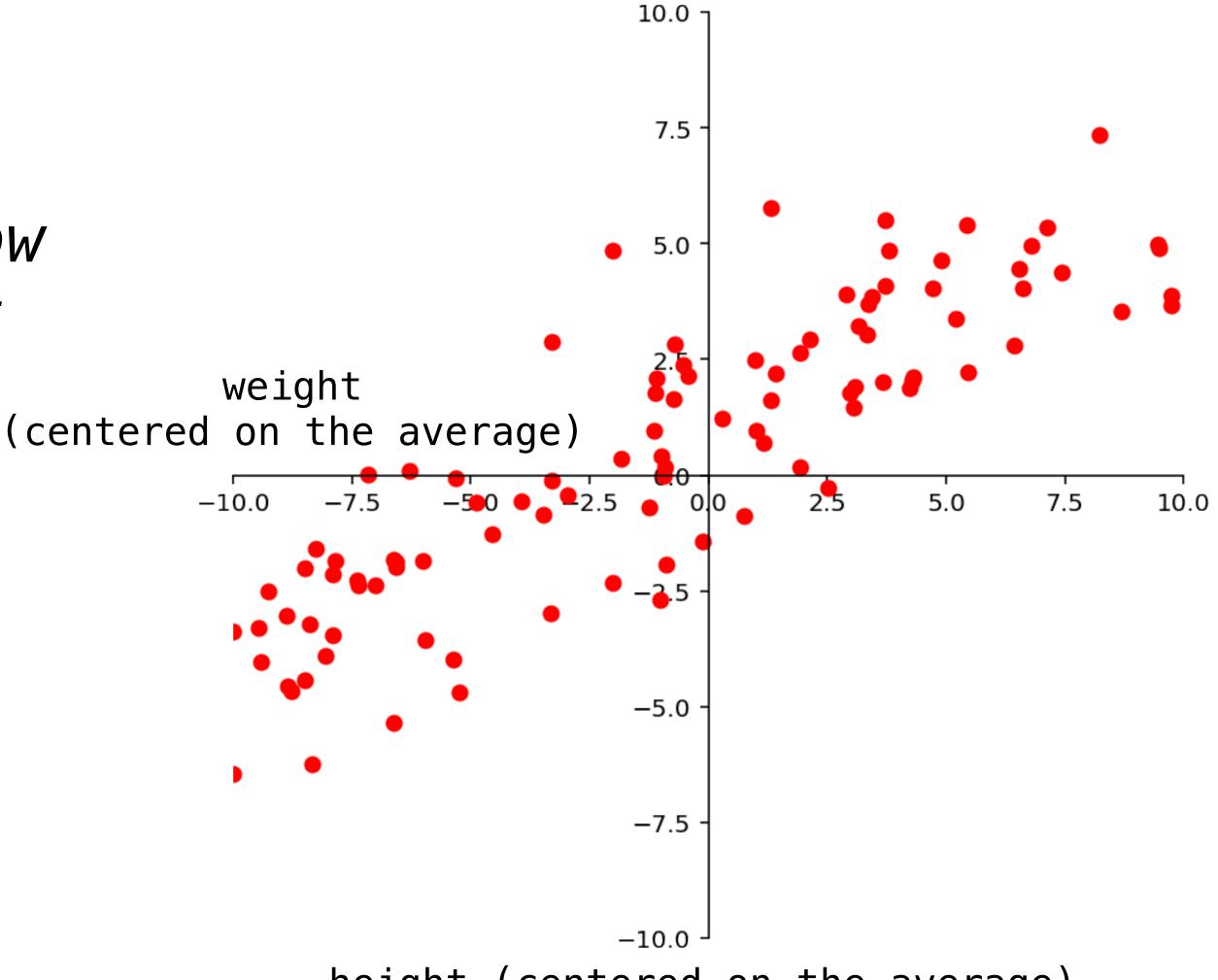
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This generalizes to any model fitting problem

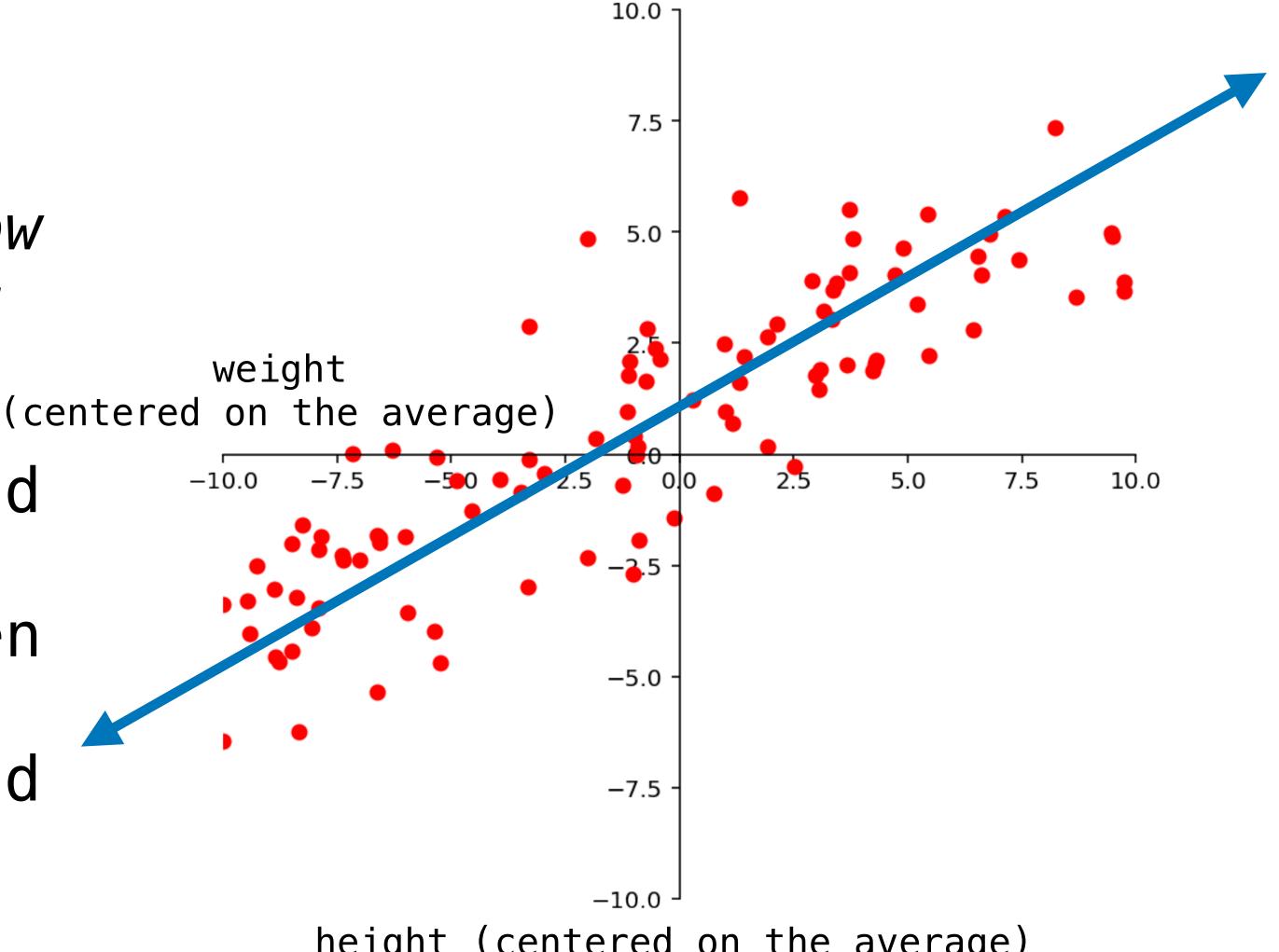


Suppose we know that person X weighs 150lb. How would we guess the height of person X?



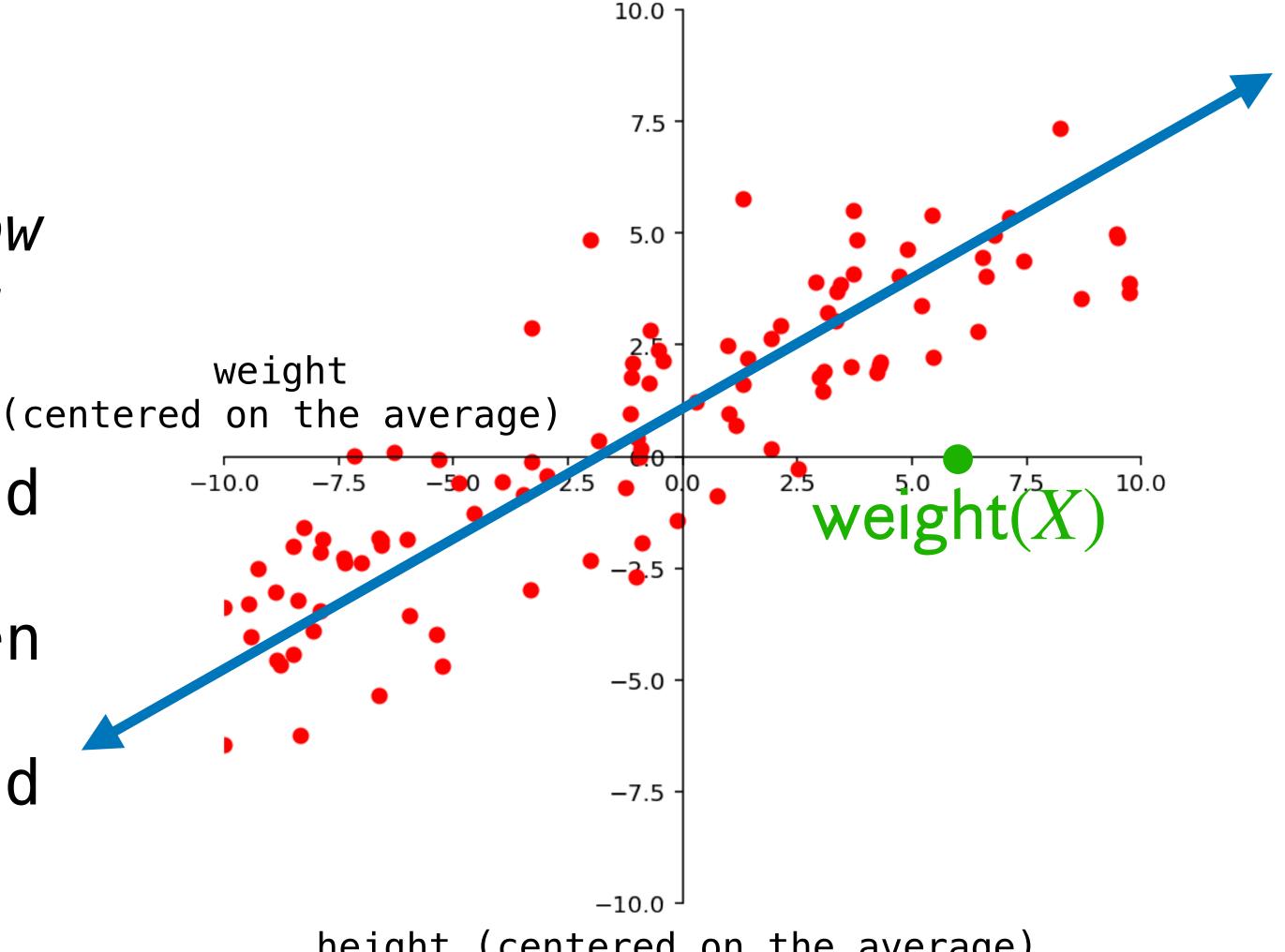
Suppose we know that person X weighs 150lb. How would we guess the height of person X?

If we know the heights and weights of a population (from which X comes), then we can find the line of best fit for that data and then use that function.



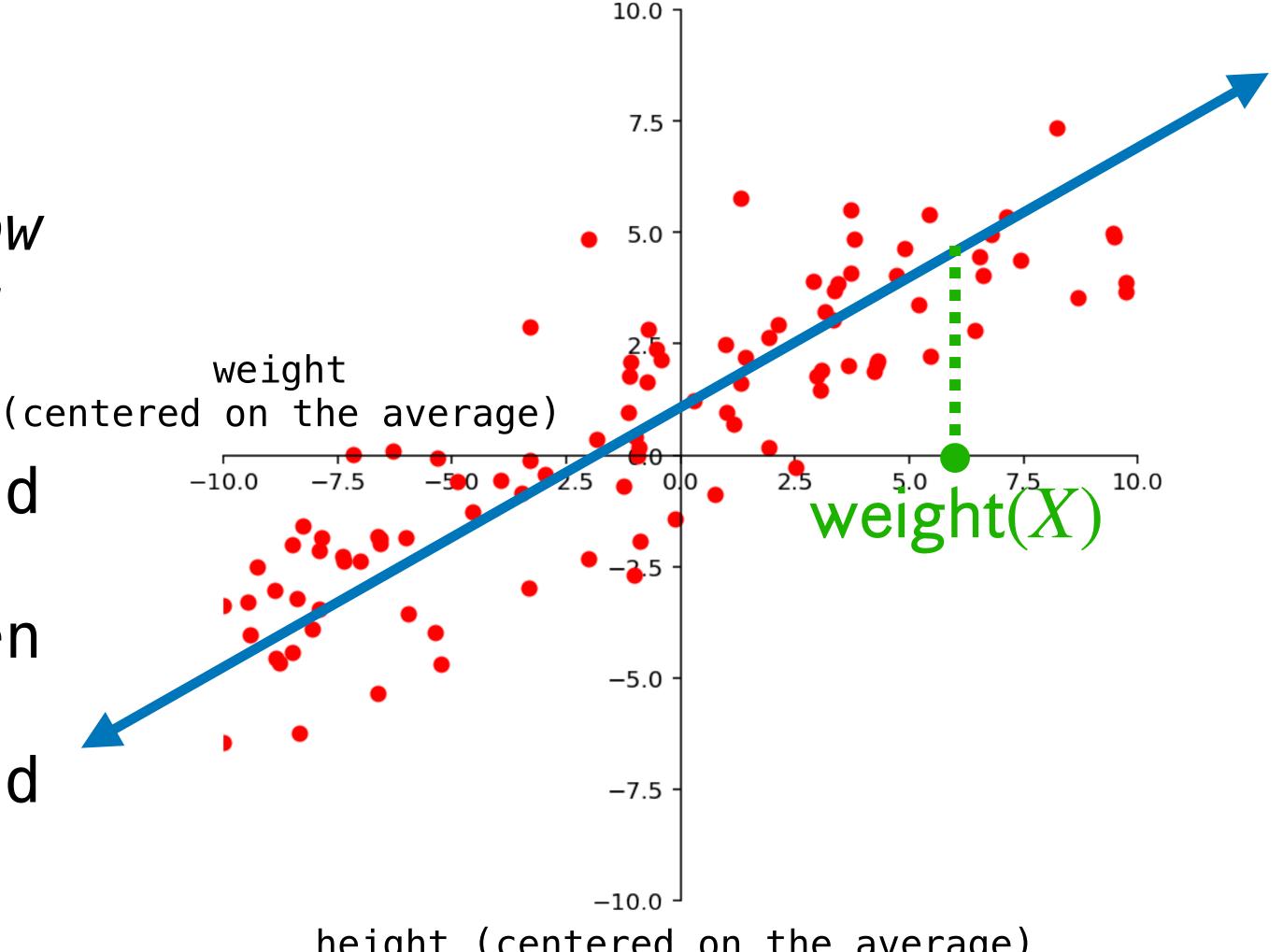
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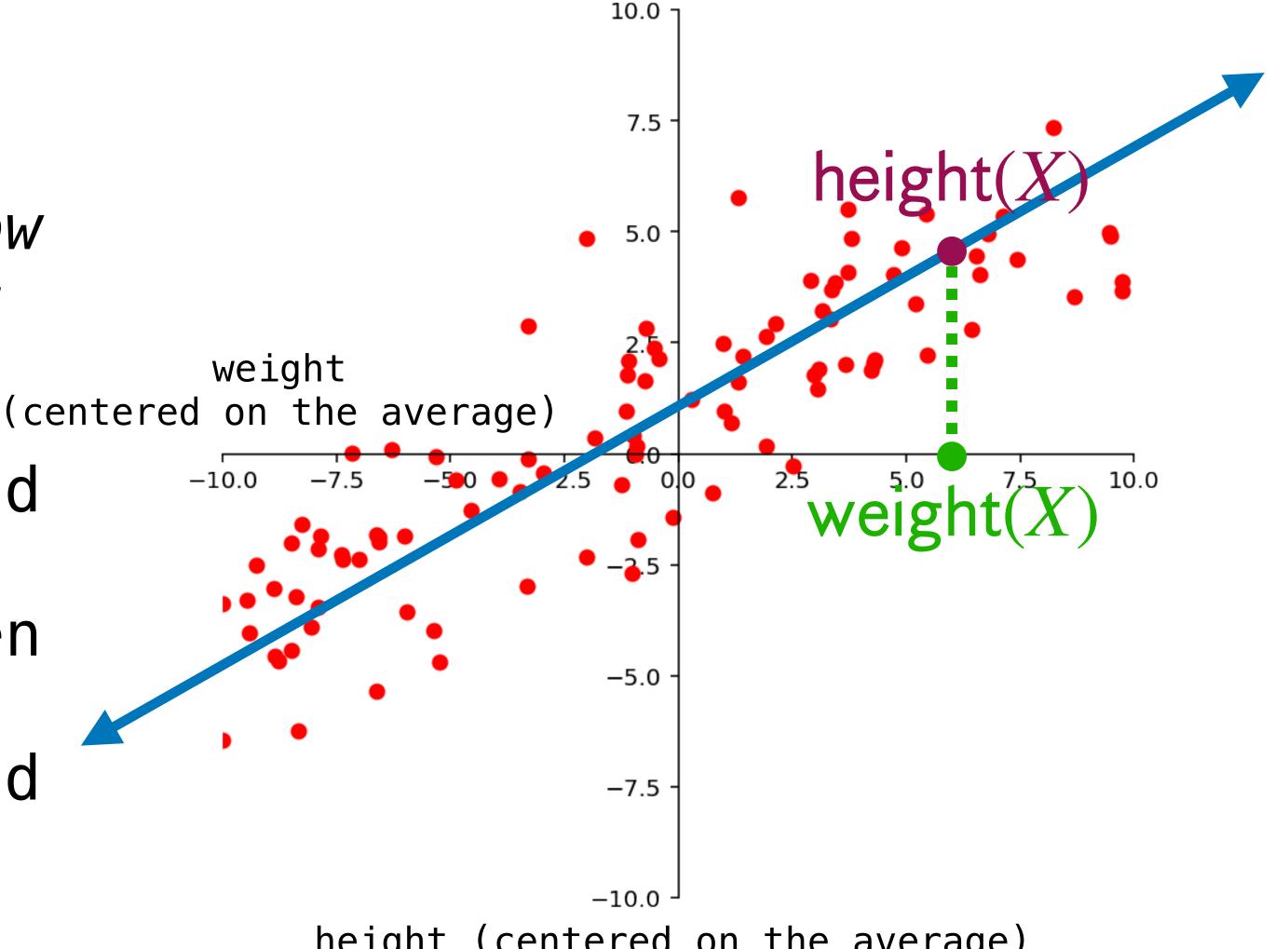
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Suppose we know that person X weighs 150lb. How would we guess the height of person X?

If we know the heights and weights of a population (from which X comes), then we can find the line of best fit for that data and then use that function.



#### Question

Find the line of best fit for the dataset

$$\{(0,3),(1,1),(-1,1),(2,3)\}$$

If you have time, graph your result and use it to "predict" the corresponding value for the input 4.

$$\{(0,3),(1,1),(-1,1),(2,3)\}$$

$$X = \begin{bmatrix} 1 & -1 & 7 \\ 1 & 0 & 7 \end{bmatrix}$$

$$X^{T}X = \begin{bmatrix} 1 & 1 & 1 \\ -1 & 0 & 1 \end{bmatrix}$$

$$Y = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 7 \end{bmatrix}$$

$$X^{T}y = \begin{bmatrix} 1 & 1 & 1 \\ -1 & 0 & 1 \end{bmatrix}$$

$$X^{T}y = \begin{bmatrix} 1 & 1 & 1 \\ -1 & 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 & 1 \\ 3 & 1 \end{bmatrix} = \begin{bmatrix} 8 \\ 6 \end{bmatrix}$$

$$\begin{bmatrix} 8 \\ 7 & 1 \end{bmatrix} = \begin{bmatrix} 8 \\ 6 \end{bmatrix}$$

$$\begin{bmatrix} 8 \\ 7 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 3 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\$$

# Linear Models and Least Squares Regression

1. What if we have *more than one* independent value?

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multiple regression, (hyper)plane of best fit

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e.g., polynomial regression

1. What if we have *more than one* independent value?

multiple regression, (hyper)plane of best fit

2. What if our data is not exactly linear.

e.g., polynomial regression

Figure 23.1

Terrain Data for Multiple Regression

**Dataset:**  $\{(x_1, y_1, z_1), ..., (x_k, y_k, z_k)\}$  where  $(x_i, y_i)$  is an longitude and latitude and  $z_i$  is an altitude.

**Problem:** Find the <u>plane</u> which "best" fits the data.

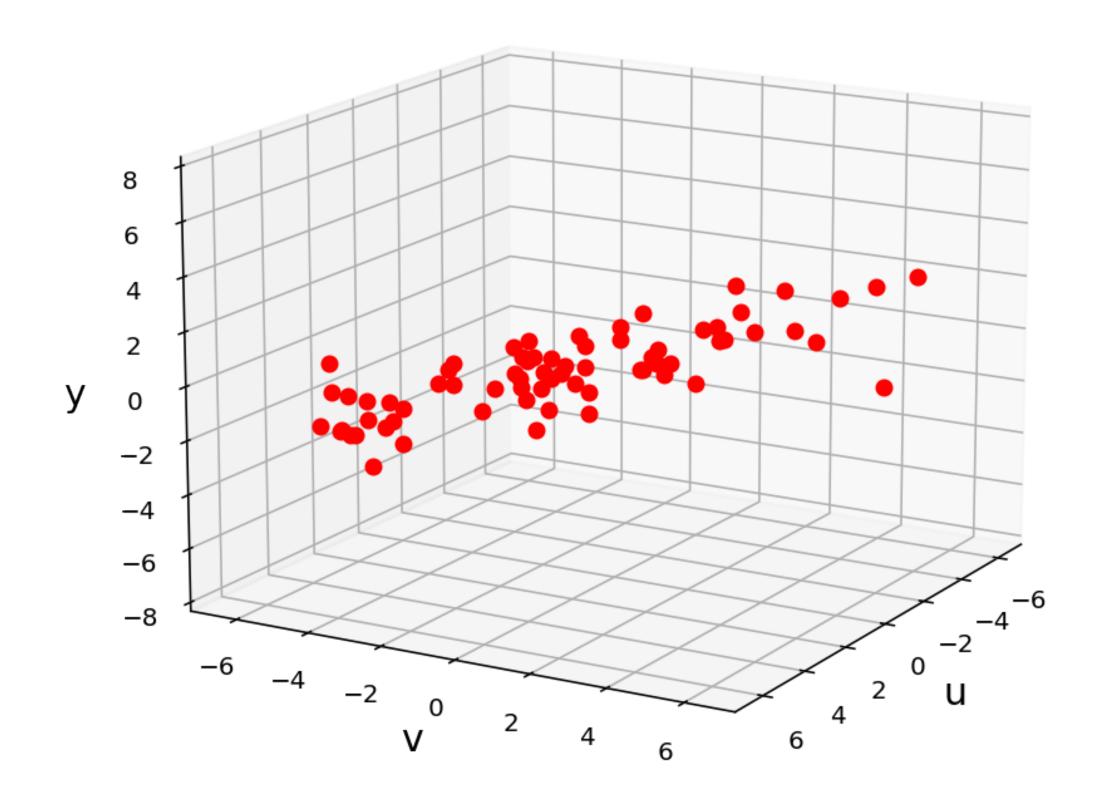


Figure 23.2

Multiple Regression Fit to Data

**Dataset:**  $\{(x_1, y_1, z_1), ..., (x_k, y_k, z_k)\}$  where  $(x_i, y_i)$  is an longitude and latitude and  $z_i$  is an altitude.

**Problem:** Find  $\beta_0, \beta_1, \beta_2$  such that

$$f(x, y) = \beta_0 + \beta_1 x + \beta_2 y$$

which minimizes

$$\sum_{i=1}^{k} (f(x_i, y_i) - z_i)^2$$

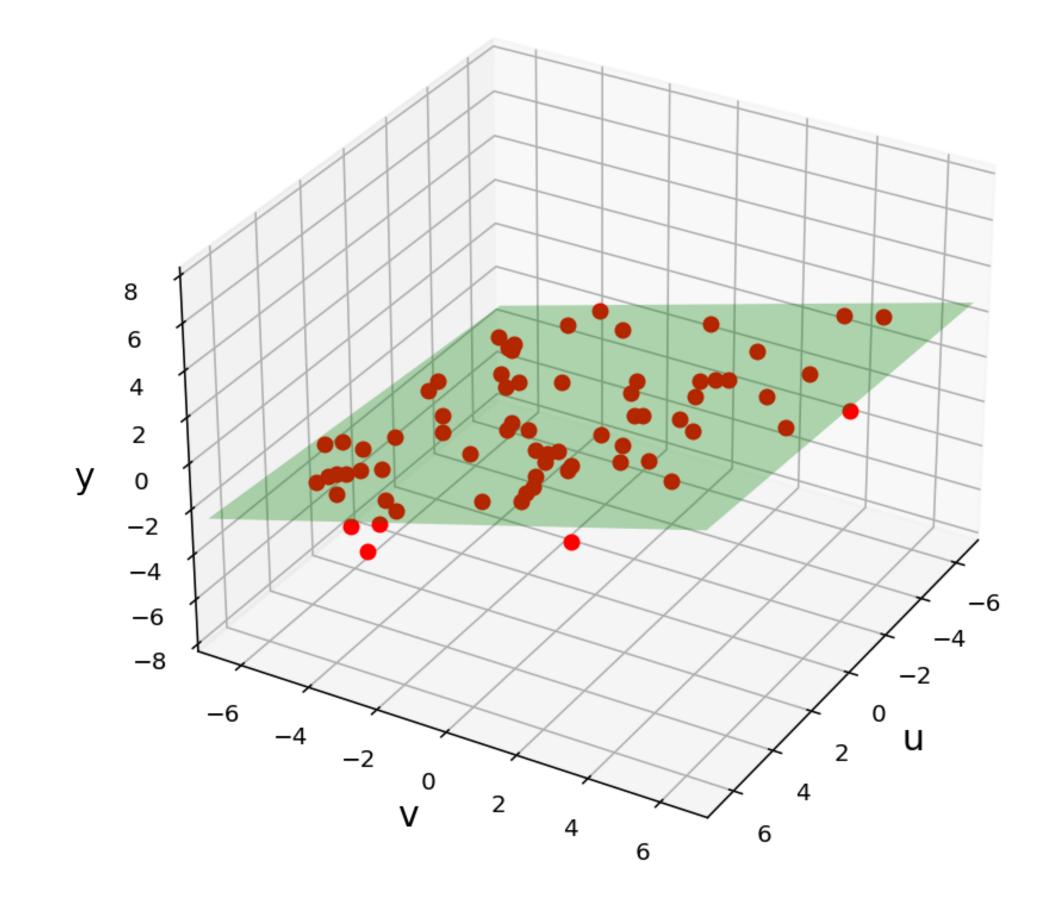


Figure 23.2

Multiple Regression Fit to Data

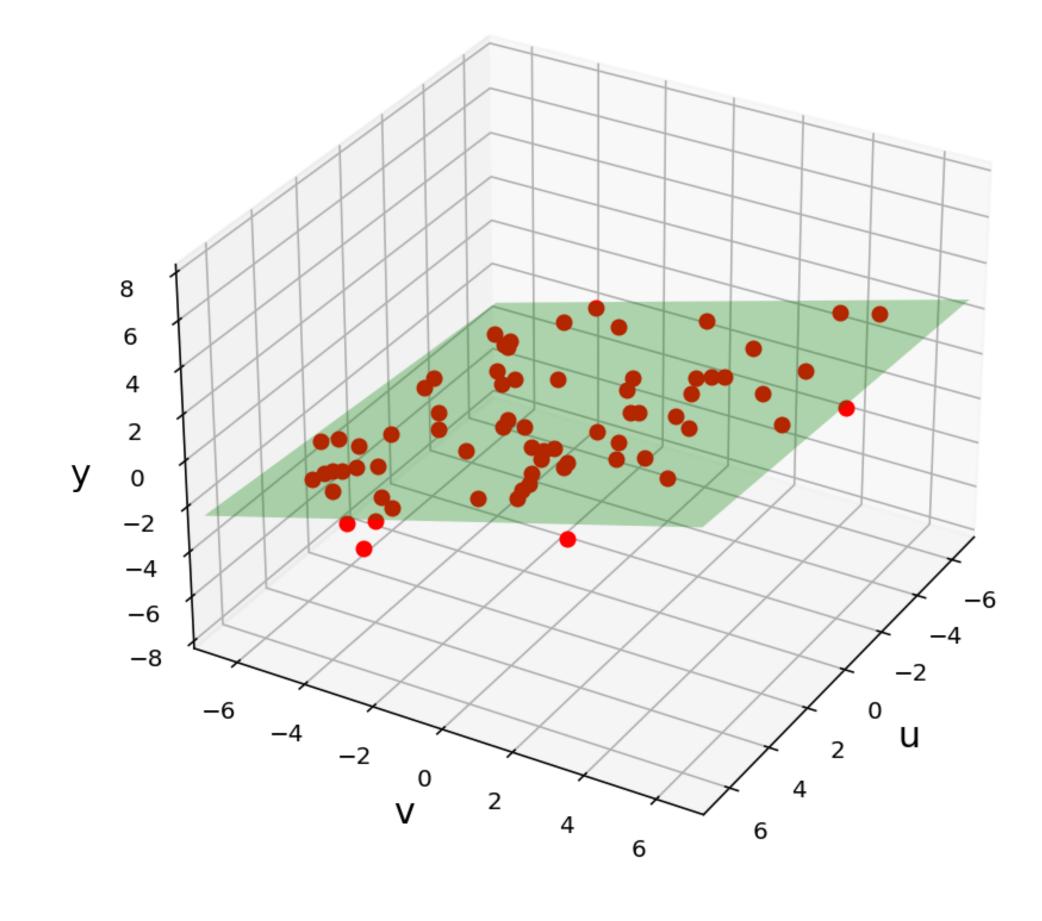
**Dataset:**  $\{(x_1, y_1, z_1), ..., (x_k, y_k, z_k)\}$  where  $(x_i, y_i)$  is an longitude and latitude and  $z_i$  is an altitude.

**Problem:** Find  $\beta_0, \beta_1, \beta_2$  such that

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f(x,y) is a good approximation of the altitude.

Figure 23.2

#### Multiple Regression Fit to Data

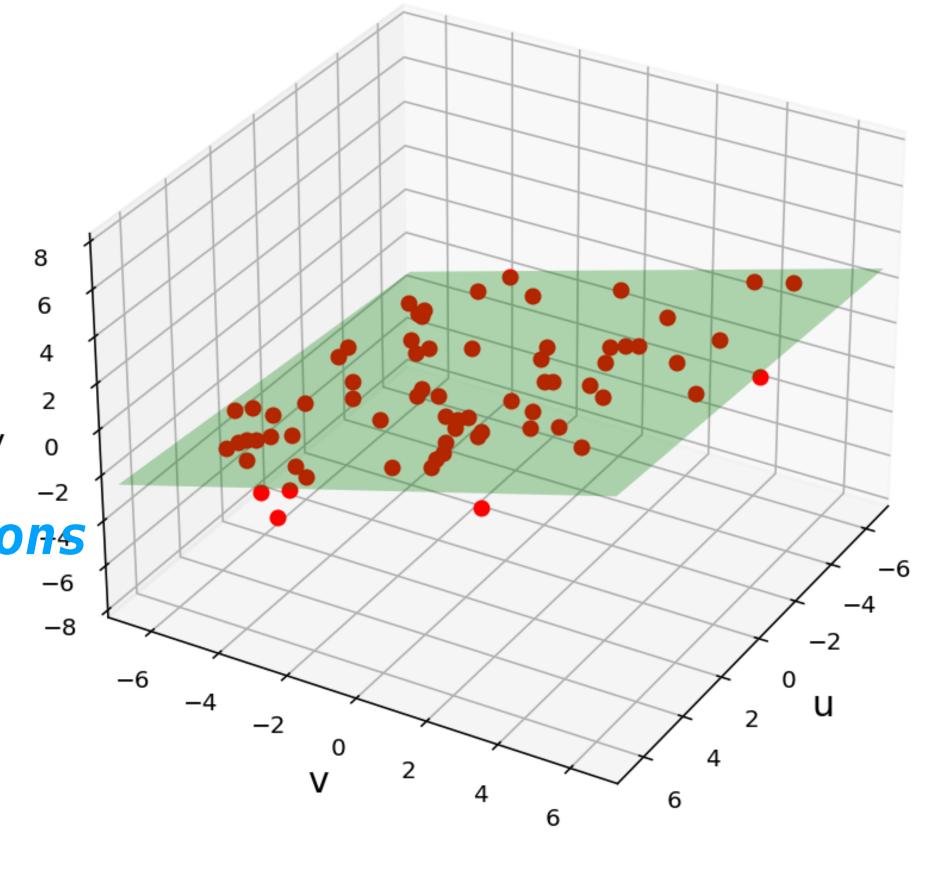
**Dataset:**  $\{(x_1, y_1, z_1), ..., (x_k, y_k, z_k)\}$  where  $(x_i, y_i)$  is an longitude and latitude and  $z_i$  is an altitude.

**Problem:** Find  $\beta_0, \beta_1, \beta_2$  such that

 $f(x,y) = \beta_0 + \beta_1 x + \beta_2 y$  recall: planes are given by linear equations

which minimizes

$$\sum_{i=1}^{k} (f(x_i, y_i) - z_i)^2$$



f(x,y) is a good approximation of the altitude.

**Dataset:**  $\{(x_1, y_1, z_1), ..., (x_k, y_k, z_k)\}$ where  $(x_i, y_i)$  is an longitude and

**Problem:** Find  $\beta_0, \beta_1, \beta_2$  such that

$$f(x, y) = \beta_0 + \beta_1 x + \beta_2 y$$

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Dataset: 
$$\{(x_1,y_1,z_1),...,(x_k,y_k,z_k)\}$$
  $\beta_0+\beta_1x_1+\beta_2y_1=z_1$  where  $(x_i,y_i)$  is an longitude and latitude and  $z_i$  is an altitude.  $\beta_0+\beta_1x_2+\beta_2y_2=z_2$  Problem: Find  $\beta_0,\beta_1,\beta_2$  such that

$$\beta_0 + \beta_1 x_k + \beta_2 y_k = z_k$$

Step 1: Set up an (almost assuredly inconsistent) system of linear equations in terms of the variables  $\beta_0, \beta_1, \beta_2$ 

#### This is still linear in the $\beta$ 's

**Dataset:**  $\{(x_1, y_1, z_1), ..., (x_k, y_k, z_k)\}$ where  $(x_i, y_i)$  is an longitude and

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**Dataset:**  $\{(x_1, y_1, z_1), ..., (x_k, y_k, z_k)\}$ 

$$f(x, y) = \beta_0 + \beta_1 x + \beta_2 y$$

which minimizes

$$\sum_{i=1}^{k} (f(x_i, y_i) - z_i)^2$$

where 
$$(x_i, y_i)$$
 is an longitude and latitude and  $z_i$  is an altitude. Problem: Find  $\beta_0, \beta_1, \beta_2$  such that 
$$f(x, y) = \beta_0 + \beta_1 x + \beta_2 y$$

$$\begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ \vdots & \vdots & \vdots \\ 1 & x_k & y_k \end{bmatrix} \begin{bmatrix} \vec{\beta}_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} \vec{z}_1 \\ \vec{z}_2 \\ \vdots \\ \vec{z}_k \end{bmatrix}$$

Step 2: Rewrite the system as a matrix equation.

**Dataset:**  $\{(x_1, y_1, z_1), ..., (x_k, y_k, z_k)\}$  where  $(x_i, y_i)$  is an longitude and latitude and  $z_i$  is an altitude.

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which minimizes

$$\sum_{i=1}^{k} (f(x_i, y_i) - z_i)^2$$

$$\hat{\vec{\beta}} = (X^T X)^{-1} X^T \mathbf{z}$$

**Step 3:** Find the least squares solution of this system and use as the parameters of your model.

### An Aside: Unique Least Squares

$$\begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ \vdots & \vdots & \vdots \\ 1 & x_k & y_k \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_k \end{bmatrix}$$

**Question (Conceptual).** Why can almost always assume that the columns of this matrix are linearly independent?

If the columns were linearly dependent, then one of our independent variables can be computed in terms of the others.

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First off, this is very unlikely.

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Second, this variable could be then be thought of as a dependent variable.

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Second, this variable could be then be thought of as a dependent variable.

It wouldn't contribute anything when using the least squares method.

1. What if we have *more than one* independent value?

multiple regression, (hyper)plane of best fit

2. What if our data is not exactly linear.

e.g., polynomial regression

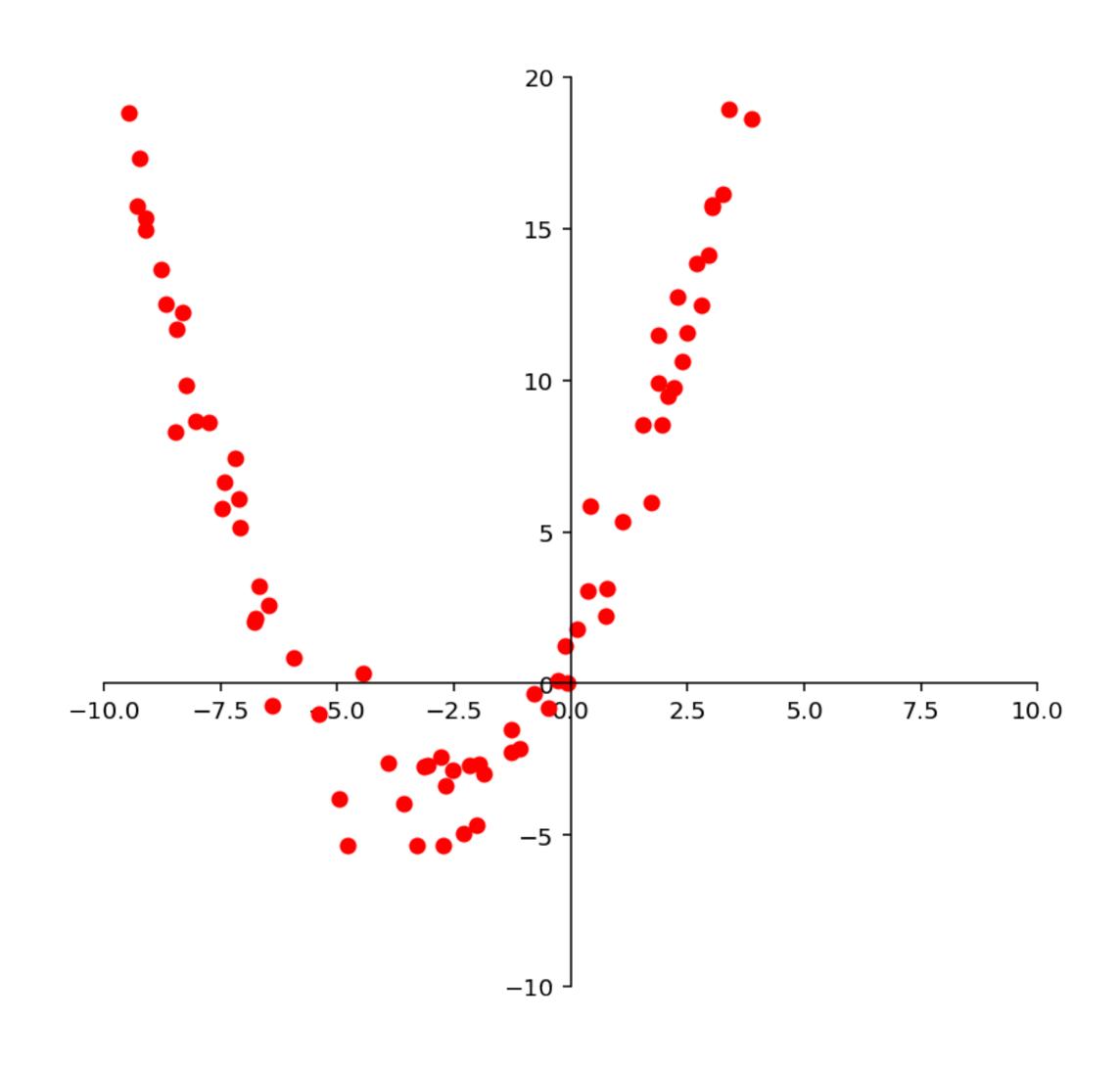
### "Vectors" of Generalization

1. What if we have *more than one* independent value?

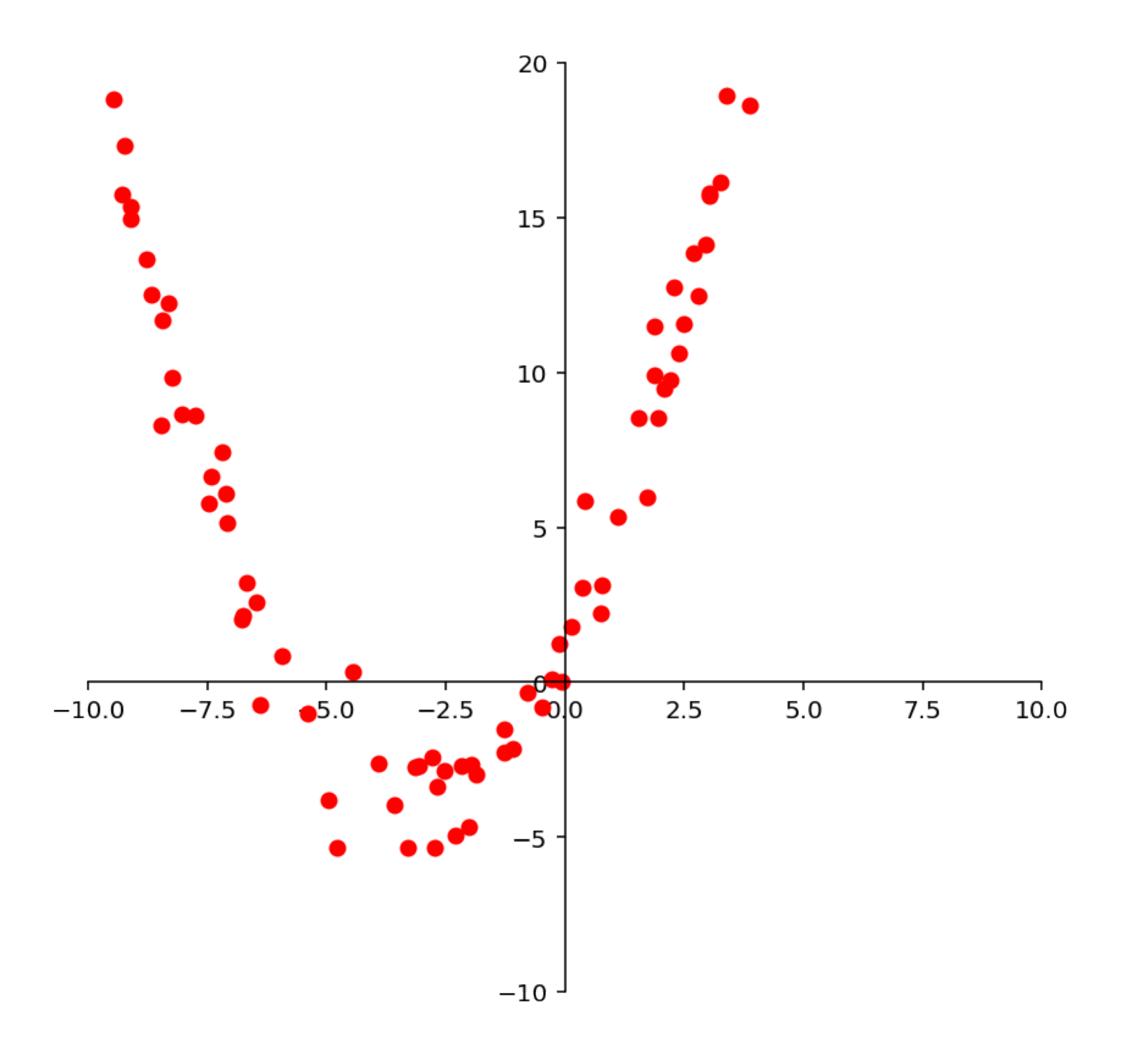
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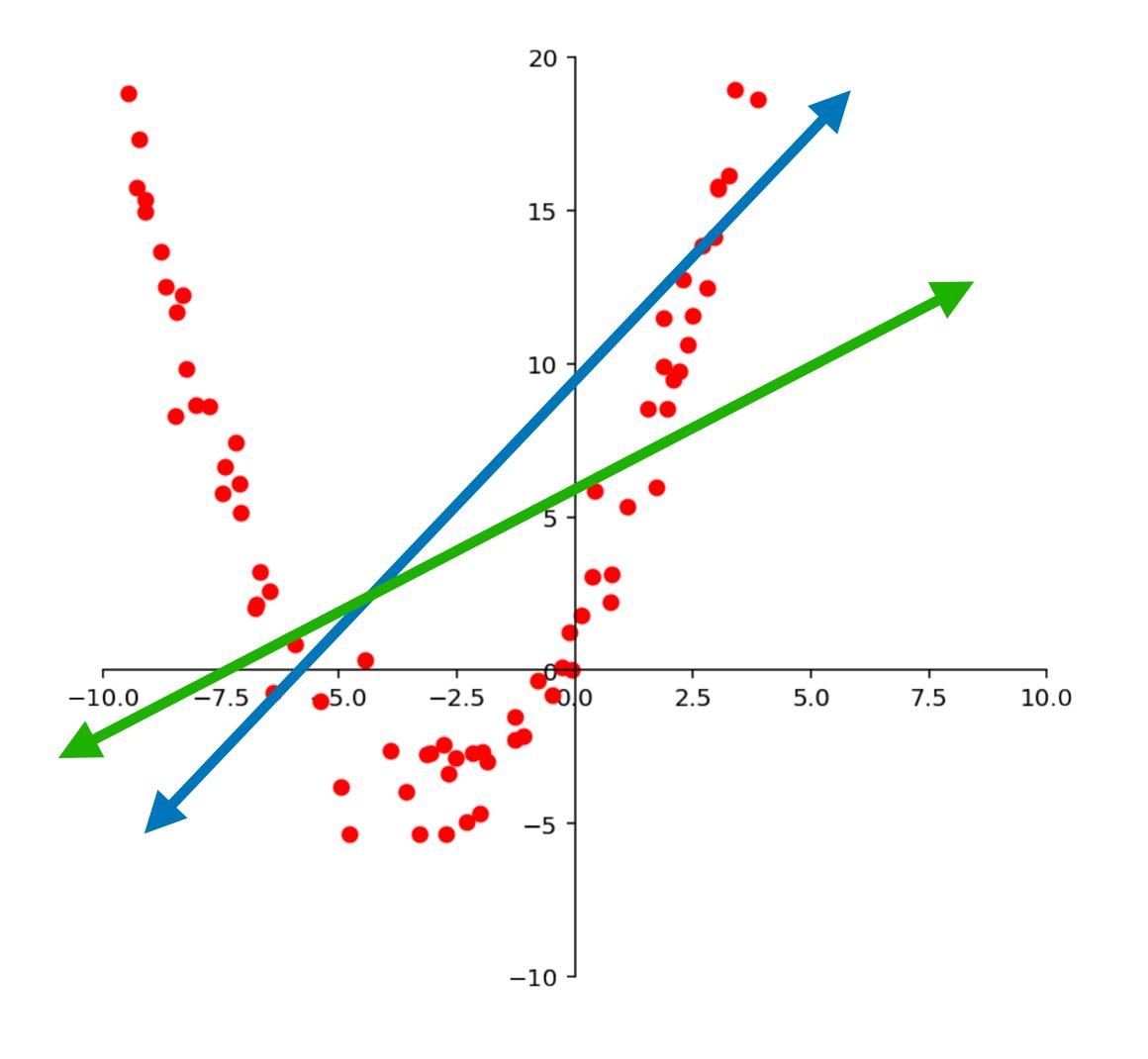


**Dataset:**  $\{(x_1, y_1), ..., (x_k, y_k)\}$ 



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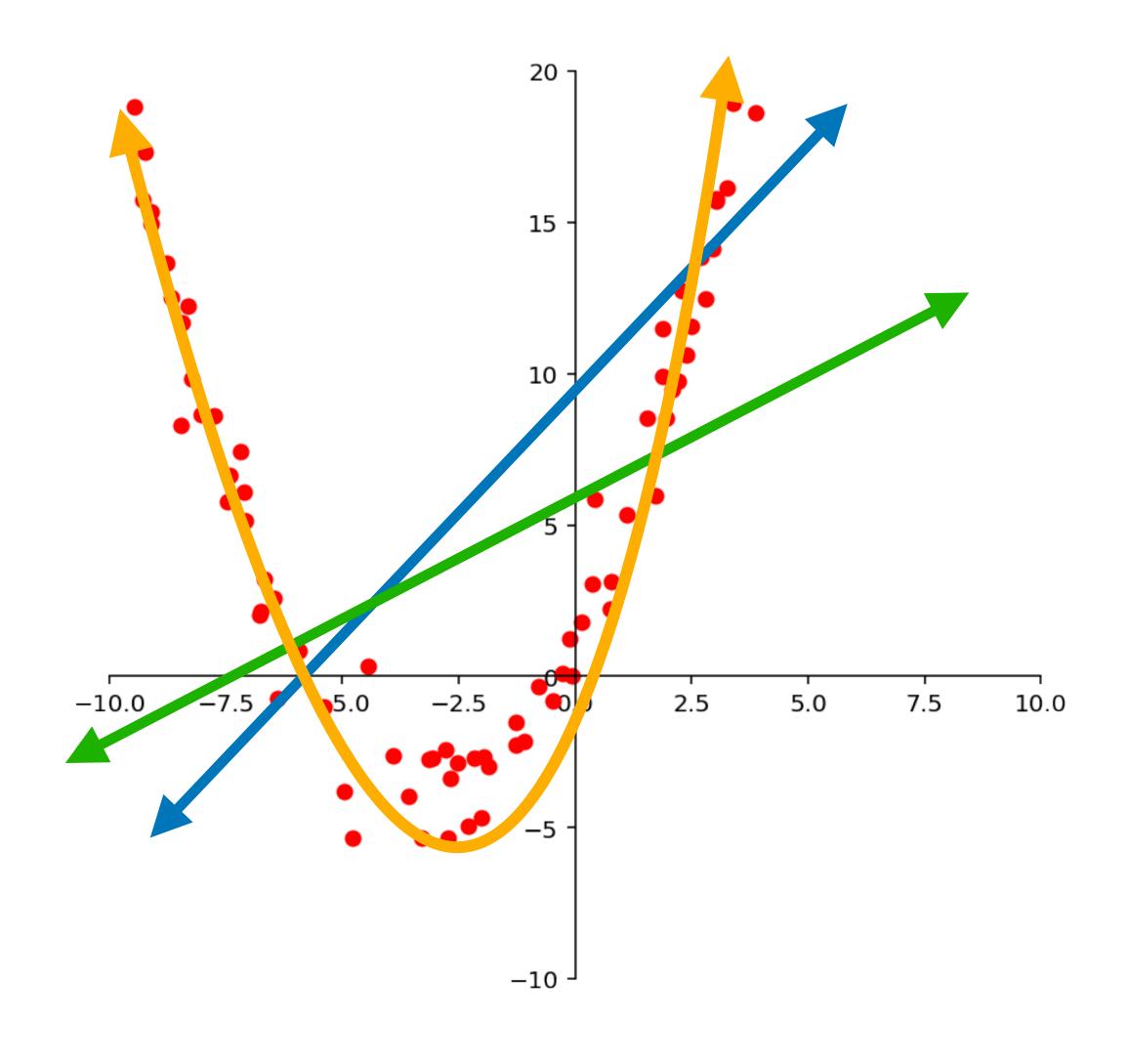
The issue: There is no good line to approximate this data.



**Dataset:**  $\{(x_1, y_1), ..., (x_k, y_k)\}$ 

The issue: There is no good line to approximate this data.

What about a parabola?



**Dataset:**  $\{(x_1, y_1), ..., (x_k, y_k)\}$ 

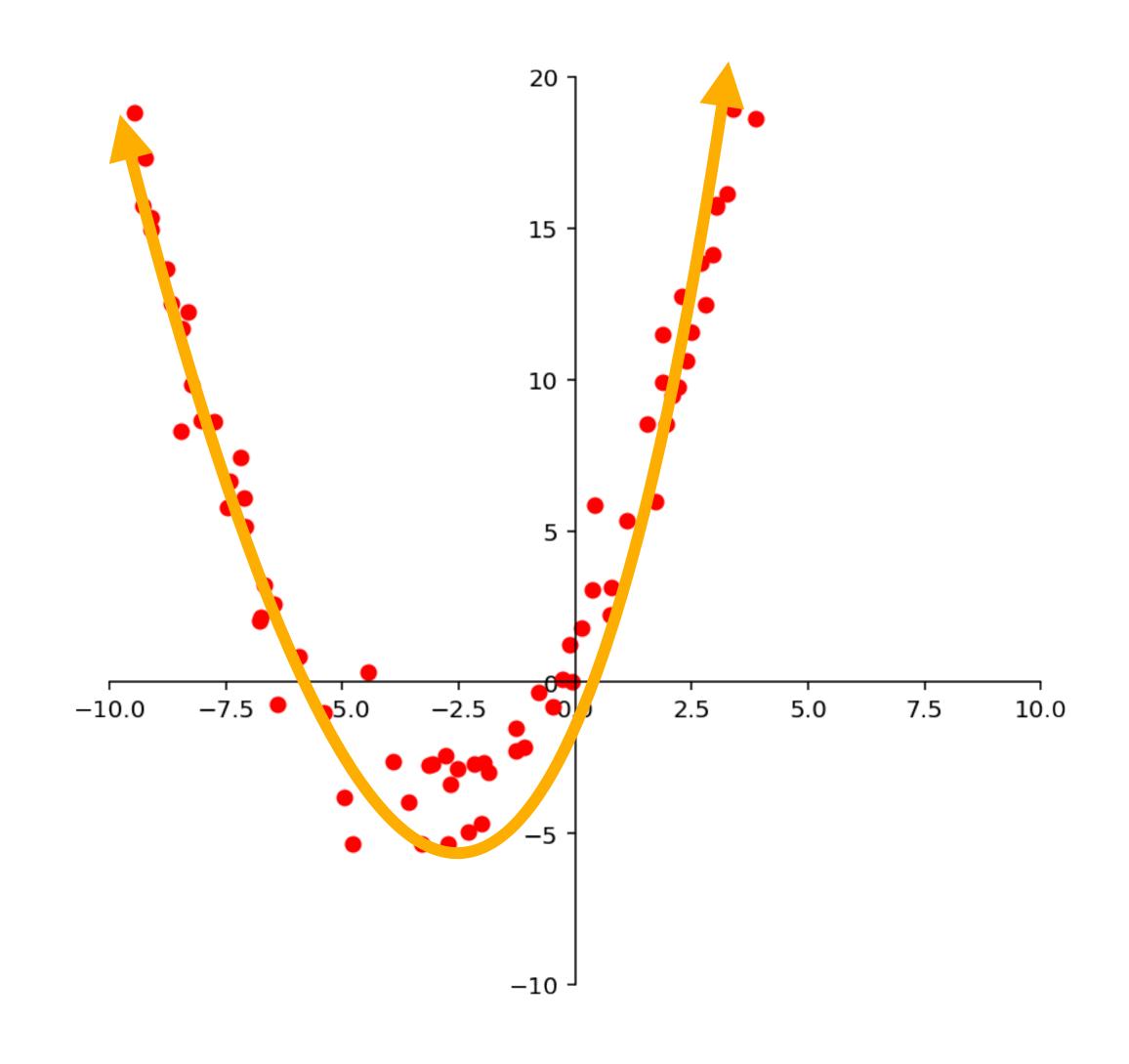
**Problem:** Find  $\beta_0, \beta_1, \beta_2$  such

that

$$f(x) = \beta_0 + \beta_1 x + \beta_2 x^2$$

minimizes

$$\sum_{i=1}^{k} (f(x_i) - y_i)^2$$



**Dataset:**  $\{(x_1, y_1), ..., (x_k, y_k)\}$ 

Problem: Find  $\beta_0, \beta_1, \beta_2$  such

that

$$f(x) = \beta_0 + \beta_1 x + \beta_2 x^2$$

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$$\beta_0 + \beta_1 x_1 + \beta_2 x_1^2 = y_1$$

$$\beta_0 + \beta_1 x_2 + \beta_2 x_2^2 = y_2$$

$$\vdots$$

$$\beta_0 + \beta_1 x_k + \beta_2 x_k^2 = y_k$$

**Step 1:** Set up an (almost assuredly inconsistent) system of linear equations in terms of the variables  $\beta_0, \beta_1, \beta_2$ 

**Dataset:** 
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Problem: Find 
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 such

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$$f(x) = \beta_0 + \beta_1 x + \beta_2 x^2$$

minimizes

$$\sum_{i=1}^{k} (f(x_i) - y_i)^2$$

This is still linear in the 
$$\beta$$
's 
$$\beta_0 + \beta_1 x_1 + \beta_2 x_1^2 = y_1$$

$$\beta_0 + \beta_1 x_2 + \beta_2 x_2^2 = y_2$$

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Step 2: Rewrite the system as a matrix equation.

**Dataset:**  $\{(x_1, y_1), ..., (x_k, y_k)\}$ 

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that

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

**Step 3:** Find the least squares solution of this system and use as the parameters of your model.

### Question

Find the parabola of best fit for the dataset  $\{(0,3),(1,1),(-1,1)\}$ 

Hint. Plot it

### Answer

 $\{(0,3),(1,1),(-1,1)\}$ 

### The Takeaway

We can use non-linear modeling functions as long as they are <u>linear in the parameters</u>.

Definition. A function  $f:\mathbb{R}^n\to\mathbb{R}$  is linear in the parameters  $\beta_1, ..., \beta_k$  if it can be written as  $f(\mathbf{x}) = \beta_1 \phi_1(\mathbf{x}) + \beta_2 \phi_2(\mathbf{x}) + ... + \beta_k \phi_k(\mathbf{x})$ 

$$f(\mathbf{x}) = \beta_1 \phi_1(\mathbf{x}) + \beta_2 \phi_2(\mathbf{x}) + \dots + \beta_k \phi_k(\mathbf{x})$$

for functions  $\phi_1, ..., \phi_k : \mathbb{R}^n \to \mathbb{R}$ 

Example: 
$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \mapsto \beta_2 e^{x_1} + \beta_3 \log(x_3)$$

$$\mathbf{y} = X \beta + \vec{\epsilon}$$

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So far, we have been considering inconsistent systems of the form  $\mathbf{y} = X\vec{\beta}$ .

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It is also common to make the system consistent by adding error terms (the  $\epsilon$ 's).

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It is also common to make the system consistent by adding error terms (the  $\epsilon$ 's).

(We won't use this view, this is mostly for your personal betterment, and because the notes use this notation occasionally.)

$$\frac{\text{design matrix}}{\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}}$$

So far, we have been considering inconsistent systems of the form  $\mathbf{y} = X\vec{\beta}$ .

It is also common to make the system consistent by adding error terms (the  $\epsilon$ 's).

(We won't use this view, this is mostly for your personal betterment, and because the notes use this notation occasionally.)

# We can build design matrices for function which are linear in their parameters.

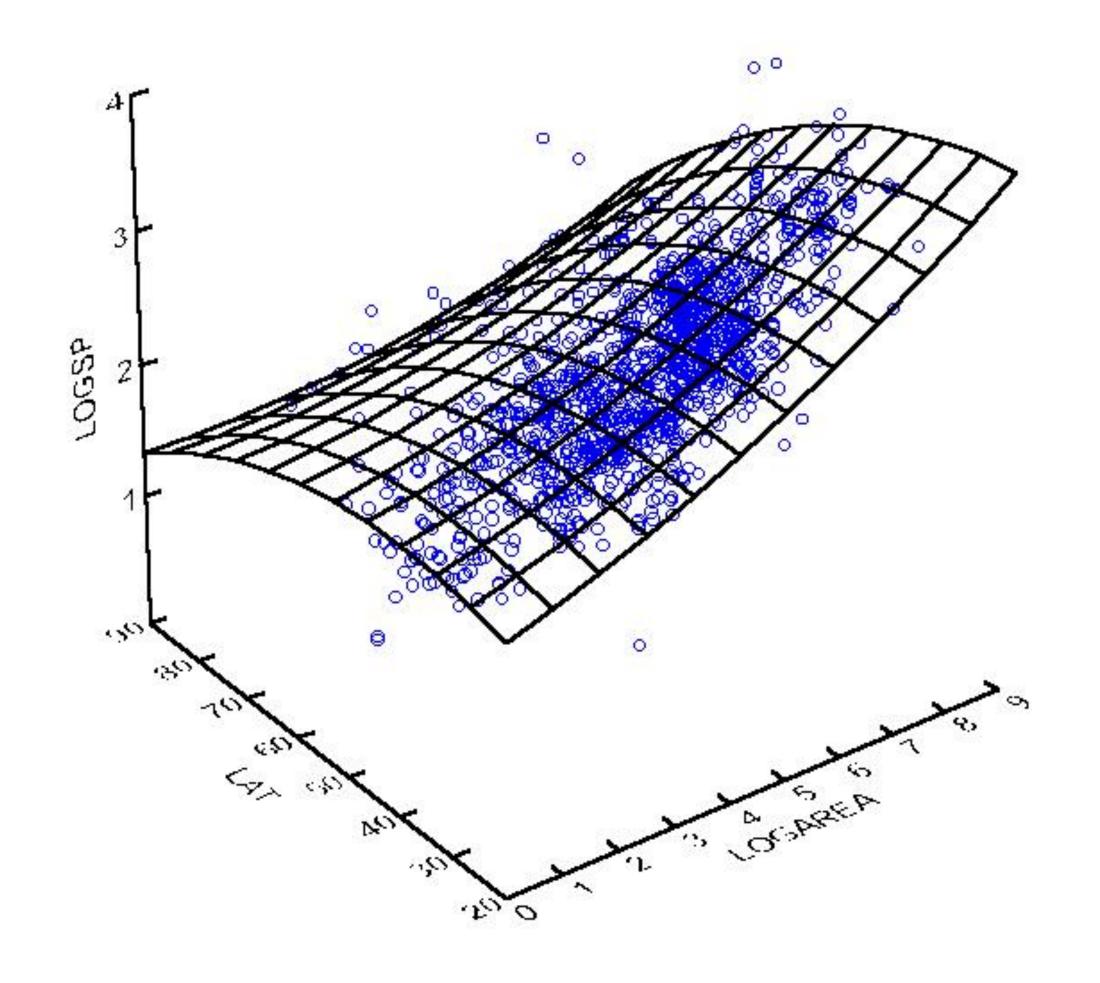
dataset:  $\{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_m, y_m)\}$  where  $\mathbf{x}_i \in \mathbb{R}^n$  and  $y_i \in \mathbb{R}$ 

Problem. Given a function

$$f_{\beta_1,\ldots,\beta_k}:\mathbb{R}^n\to\mathbb{R}$$

which is *linear in the* parameters  $\beta_1,...,\beta_k$ , find values for  $\beta_1,...,\beta_k$  which minimize

$$\sum_{i=1}^{k} (f_{\beta_1,\ldots,\beta_k}(\mathbf{x}_i) - y_i)^2$$



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 $\beta_1 \phi_1(\mathbf{x}_2) + \dots + \beta_k \phi_k(\mathbf{x}_2) = y_2$   
:

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**Step 1:** Set up an (almost assuredly inconsistent) system of linear equations in terms of the variables  $\beta_1, \ldots, \beta_k$ 

### This is still linear in the $\beta$ 's

**dataset:** 
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$$\sum_{i=1}^{k} (f_{\beta_1,\ldots,\beta_k}(\mathbf{x}_i) - y_i)^2$$

 $\begin{bmatrix} \phi_1(\mathbf{x}_1) & \phi_2(\mathbf{x}_1) & \dots & \phi_k(\mathbf{x}_1) \\ \phi_1(\mathbf{x}_2) & \phi_2(\mathbf{x}_2) & \dots & \phi_k(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{x}_m) & \phi_2(\mathbf{x}_m) & \dots & \phi_k(\mathbf{x}_m) \end{bmatrix} \begin{bmatrix} \vec{\beta}_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{bmatrix} = \begin{bmatrix} \mathbf{y}_1 \\ y_2 \\ \vdots \\ y_k \end{bmatrix}$ 

Step 2: Rewrite the system as a matrix equation.

dataset:  $\{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_m, y_m)\}$  where  $\mathbf{x}_i \in \mathbb{R}^n$  and  $y_i \in \mathbb{R}$ 

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

**Step 3:** Find the least squares solution of this system and use as the parameters of your model.

## How To: Design Matrices

### How To: Design Matrices

**Problem.** Find the design matrix for least squares regression with the function f in terms of the parameters  $\beta_1, \beta_2, ..., \beta_k$  given the dataset  $\{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_m, y_m)\}$ .

### How To: Design Matrices

**Problem.** Find the design matrix for least squares regression with the function f in terms of the parameters  $\beta_1, \beta_2, ..., \beta_k$  given the dataset  $\{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_m, y_m)\}$ .

**Solution.** First write  $f(\mathbf{x})$  as  $\beta_1\phi_1(\mathbf{x}) + ... + \beta_k\phi(\mathbf{x})$  where  $\phi_1, ..., \phi_k$  are potentially non-linear functions. Then build the matrix:

$$\begin{bmatrix} \phi_1(\mathbf{x}_1) & \phi_2(\mathbf{x}_1) & \dots & \phi_k(\mathbf{x}_1) \\ \phi_1(\mathbf{x}_2) & \phi_2(\mathbf{x}_2) & \dots & \phi_k(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{x}_m) & \phi_2(\mathbf{x}_m) & \dots & \phi_k(\mathbf{x}_m) \end{bmatrix}$$

### Question

Find the design matrix for the least squares regression with the function

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \mapsto \beta_1 \cos(x_1) + \beta_2 e^{-x_1 x_2} - \beta_1 x_3 + \beta_3$$

for the dataset

$$\mathbf{x}_1 = (0,0,0)$$
  $y_1 = 5$   
 $\mathbf{x}_2 = (\pi,3,1)$   $y_2 = 3$ 

## Answer: $\begin{bmatrix} 1 & 1 & 1 \\ -2 & e^{-3\pi} & 1 \end{bmatrix}$

$$\begin{bmatrix} 1 & 1 & 1 \\ -2 & e^{-3\pi} & 1 \end{bmatrix}$$

Many functions require large design matrices, e.g. multivariate polynomials have *a lot* of possible terms.

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Again, is least-squares error really what we want? What if we want to minimize something else?

Many functions require large design matrices, e.g. multivariate polynomials have *a lot* of possible terms.

We haven't actually talked about which modeling functions to use.

Again, is least-squares error really what we want? What if we want to minimize something else?

Concerns for another class.

### One Last Thing

Please through the last section of the notes "Multiple Regression in Practice"

It will be useful for Homework 12.