

Linear Models

Geometric Algorithms

Lecture 24

Practice Problem

$$B = \begin{bmatrix} 1 & 2 \\ 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$A = \begin{matrix} \vec{a}_1 & \vec{a}_2 & \vec{a}_3 \\ \begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 1 \\ 1 & 0 & -1 \end{bmatrix} \end{matrix}$$

$$\textcircled{1} B^T B \hat{x} = B^T \vec{b}$$

$$\textcircled{2} B \hat{x} \leftarrow \text{proj}_{\text{Col}(B)} \vec{b}$$

$$\mathbf{b} = \begin{bmatrix} 3 \\ 1 \\ -4 \end{bmatrix}$$

Find the projection of \mathbf{b} onto $\text{Col}(A) = \text{Col}(B)$

hint: $\vec{a}_2 - \vec{a}_1 = \vec{a}_3$

$$(B^T B)^{-1} = \frac{1}{6} \times$$

$$B^T B = \begin{bmatrix} 1 & 0 & 1 \\ 2 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 2 & 2 \\ 2 & 5 \end{bmatrix} \quad \begin{bmatrix} 5 & -2 \\ -2 & 2 \end{bmatrix}$$

Answer

$$A = \begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 1 \\ 1 & 0 & -1 \end{bmatrix}$$

$$\mathbf{b} = \begin{bmatrix} 3 \\ 1 \\ -4 \end{bmatrix}$$

$$B^T \vec{b} = \begin{bmatrix} 1 & 0 & 1 \\ 2 & 1 & 0 \end{bmatrix} \begin{bmatrix} 3 \\ 1 \\ -4 \end{bmatrix} = \begin{bmatrix} -1 \\ 7 \end{bmatrix}$$

$$\hat{x} = (B^T B)^{-1} B^T \vec{b} = \frac{1}{6} \begin{bmatrix} 5 & -2 \\ -2 & 2 \end{bmatrix} \begin{bmatrix} -1 \\ 7 \end{bmatrix} = \frac{1}{6} \begin{bmatrix} -19 \\ 16 \end{bmatrix}$$

$$\text{proj}_{\text{Col}(B)} \vec{b} = B \hat{x} = \begin{bmatrix} 1 & 2 \\ 0 & 1 \\ 1 & 0 \end{bmatrix} \left(\frac{1}{6} \right) \begin{bmatrix} -19 \\ 16 \end{bmatrix} = \frac{1}{6} \begin{bmatrix} -19 + 3 & 2 \\ 16 \\ -19 \end{bmatrix} = \frac{1}{6} \begin{bmatrix} 13 \\ 16 \\ -19 \end{bmatrix}$$

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

line of best fit

independent/dependent variables

residuals

prediction

simple least squares regression

multiple regression

polynomial regression

models

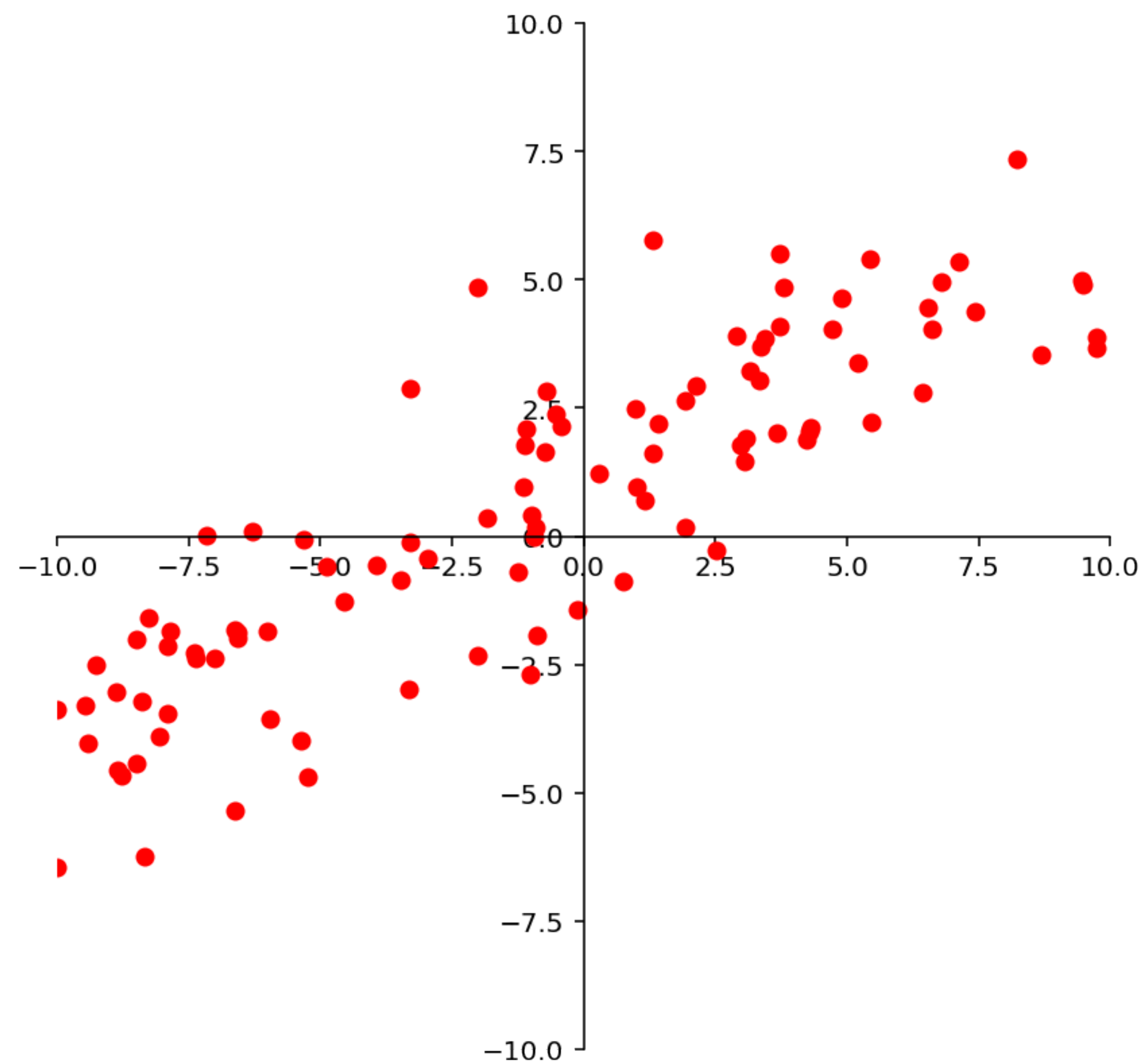
model fitting

model parameters

design matrices

Warm-up: Line of Best Fit

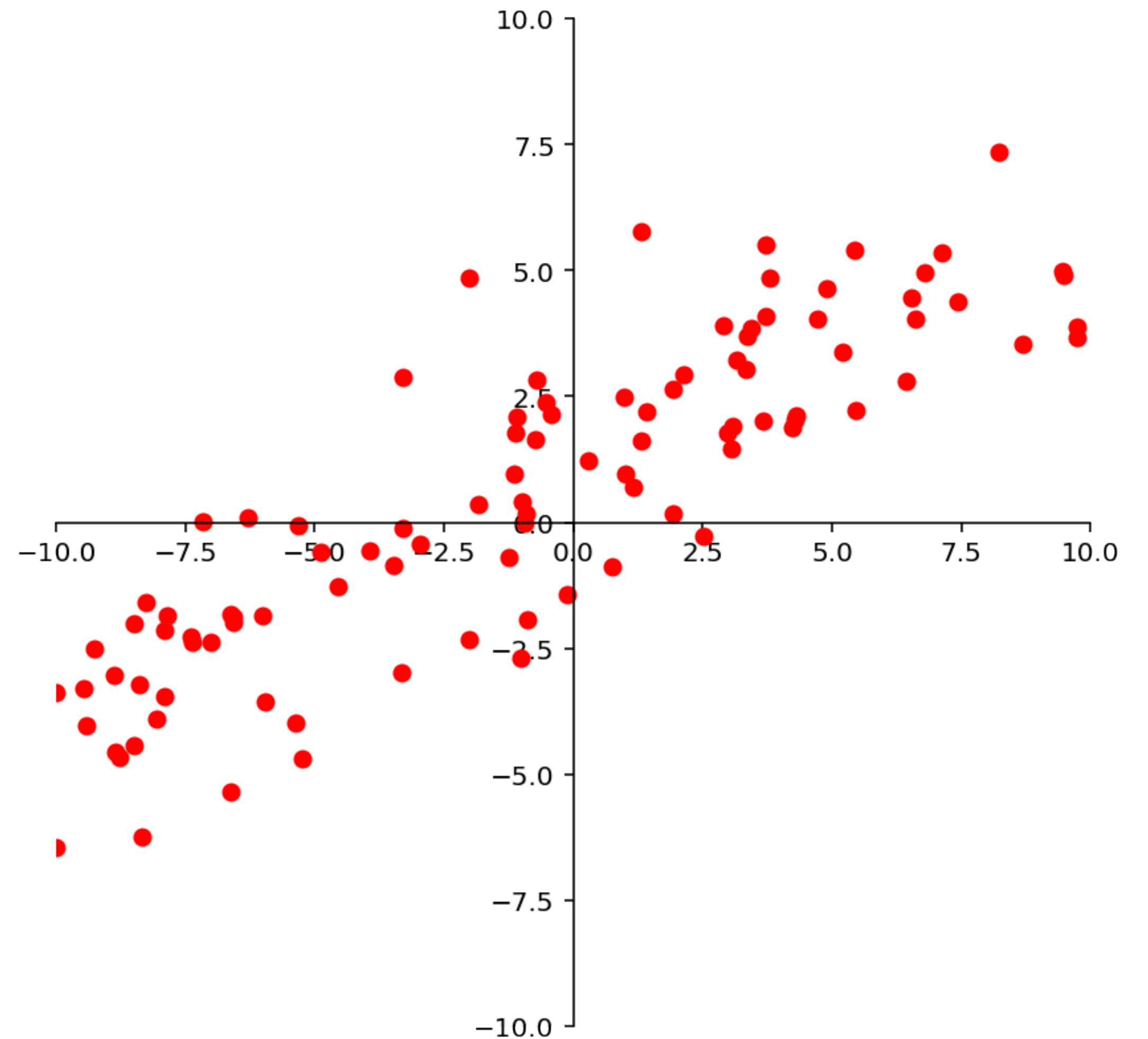
The Setup



The Setup

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

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

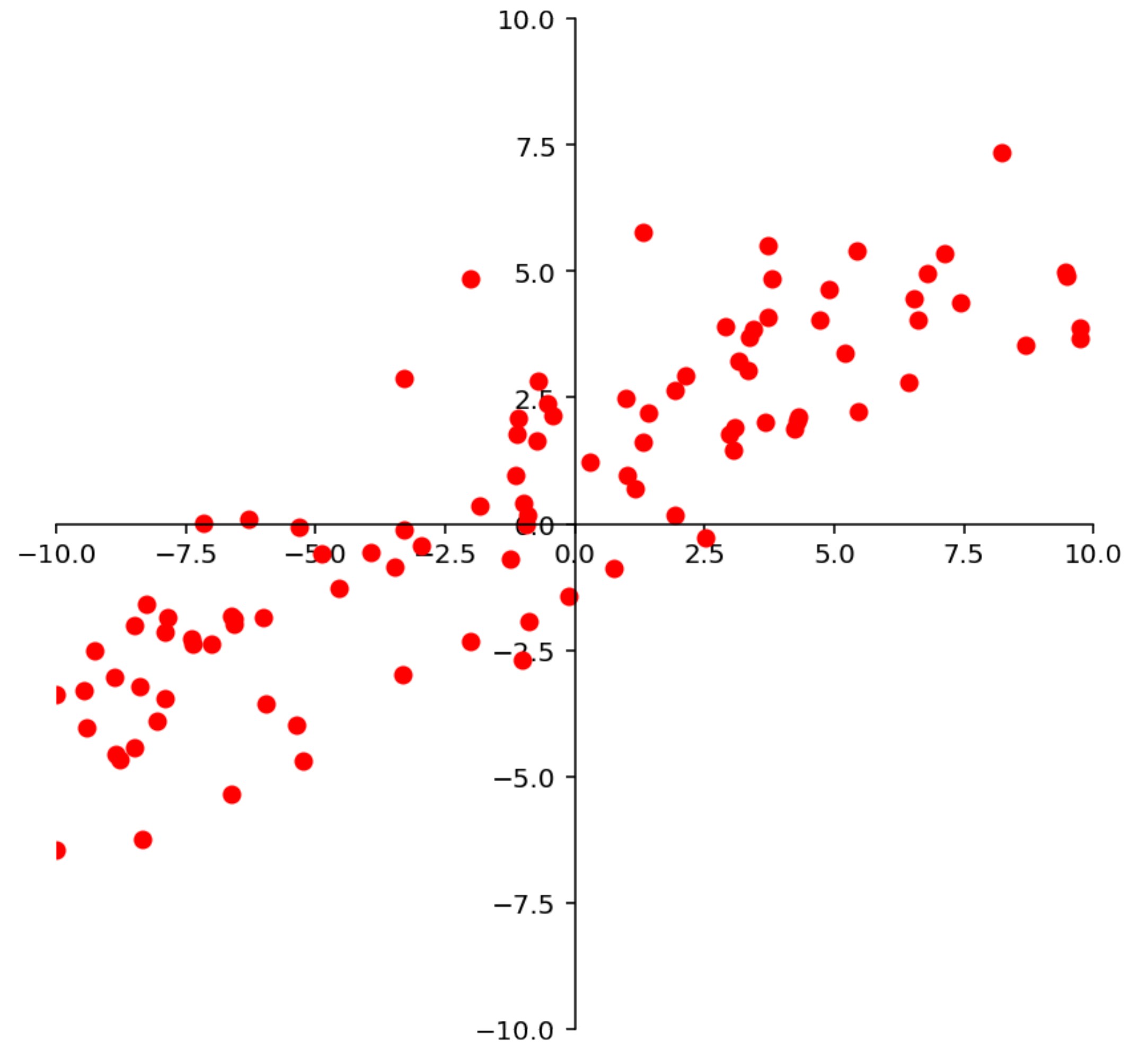


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Example. You collect (height, weight) data for a population.



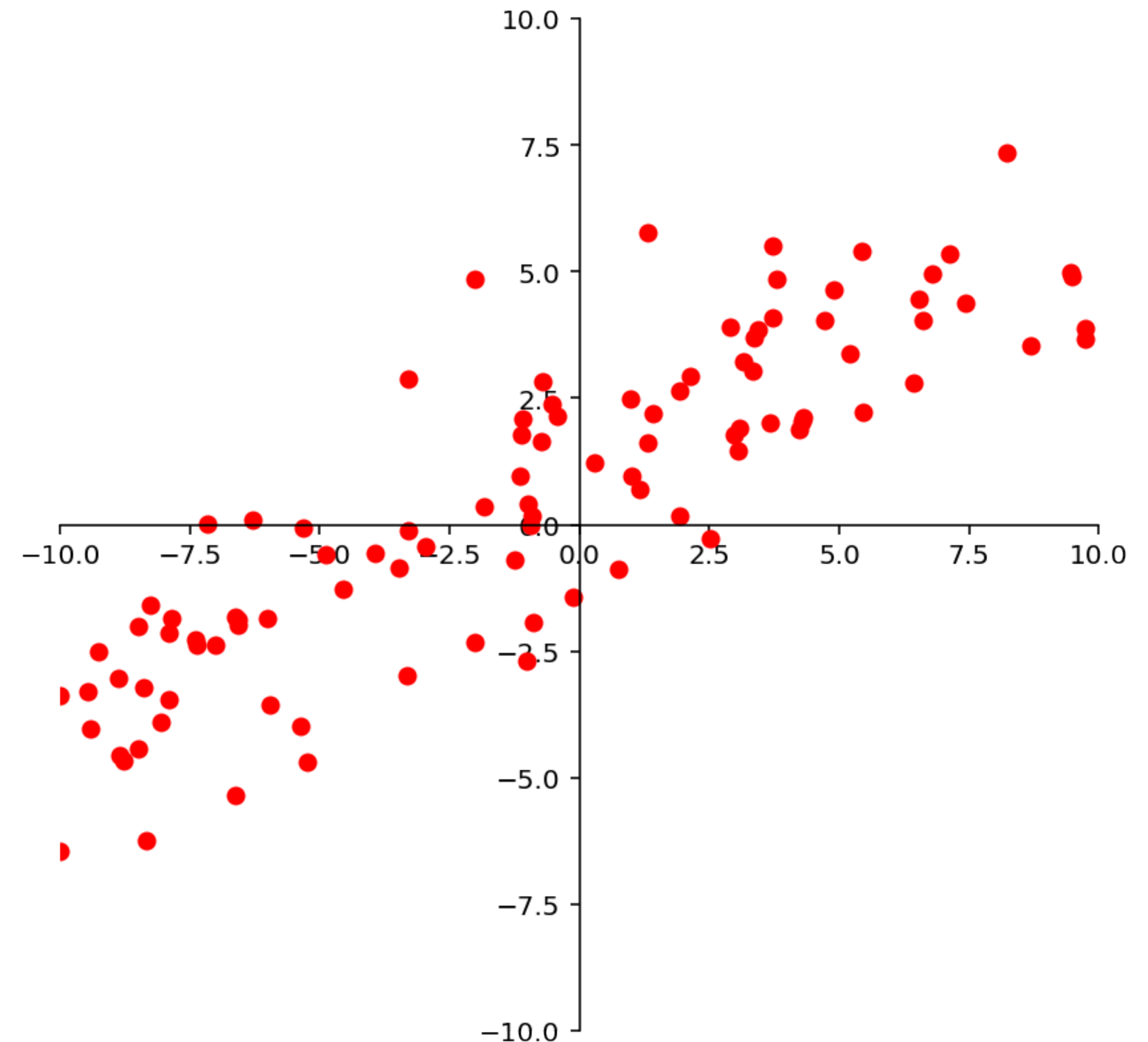
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You notice they *kind of* trend as a line.



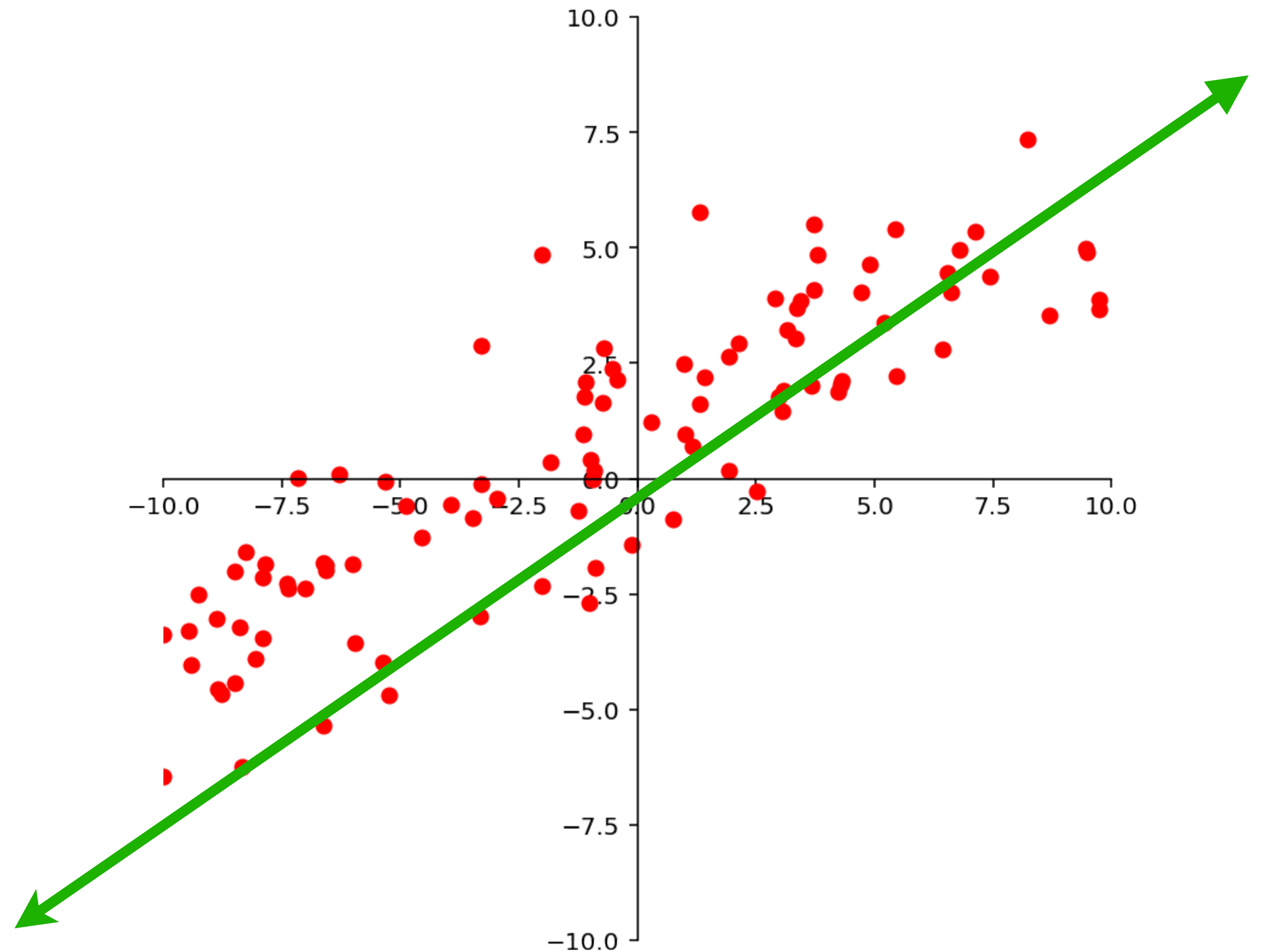
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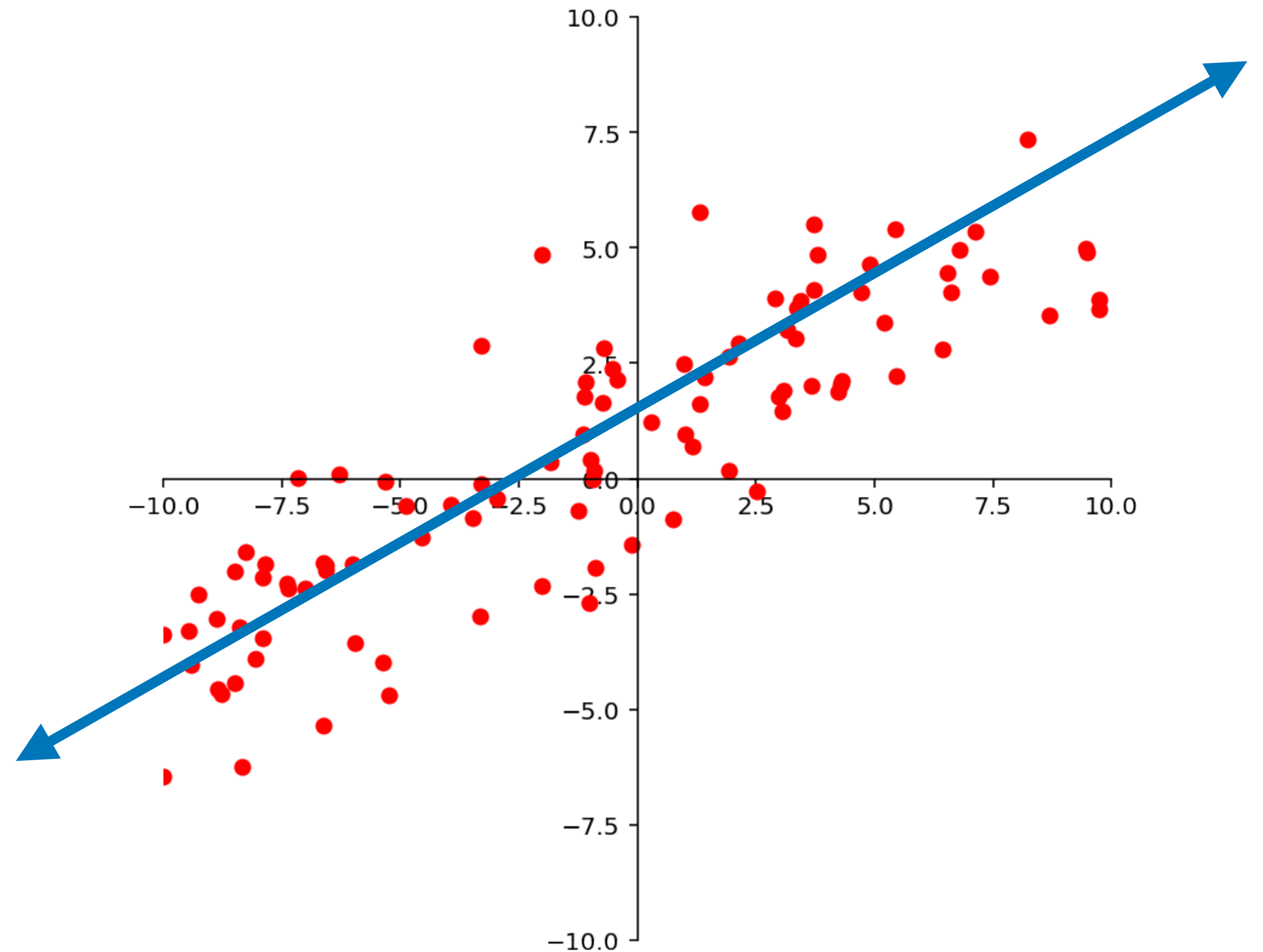
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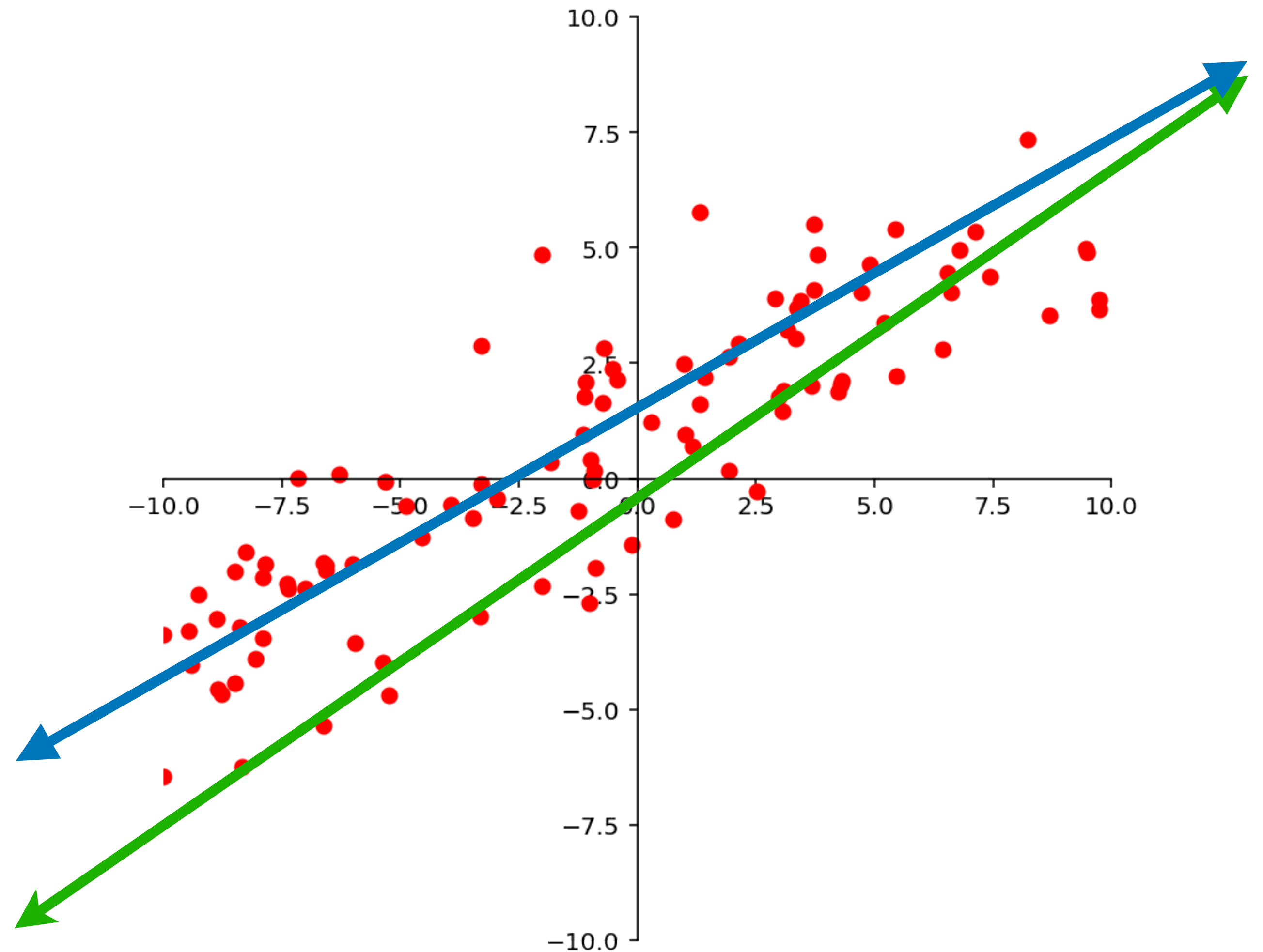
You notice they *kind of* trend as a line.



The Setup

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

Which one *best models* the dataset?



Two Important Questions

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1. What is a model?

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We'll come back to this...

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2. What does "best" mean?

Two Important Questions

1. What is a model?

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 $\{(x_1, y_1), \dots, (x_n, y_n)\}$, find the line

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

which minimizes

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

Least Squares Simple Linear Regression

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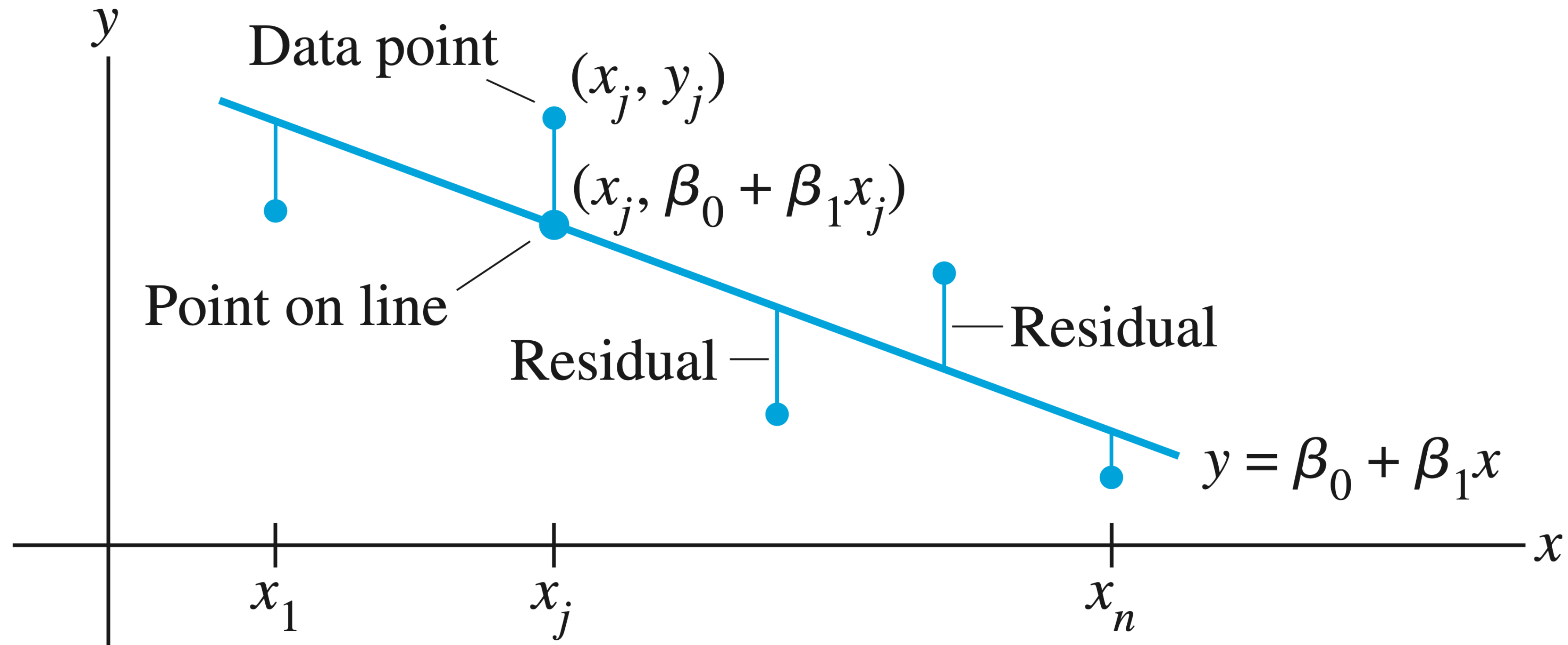
$$f(x) = \beta_0 + \beta_1 x$$

which minimizes

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

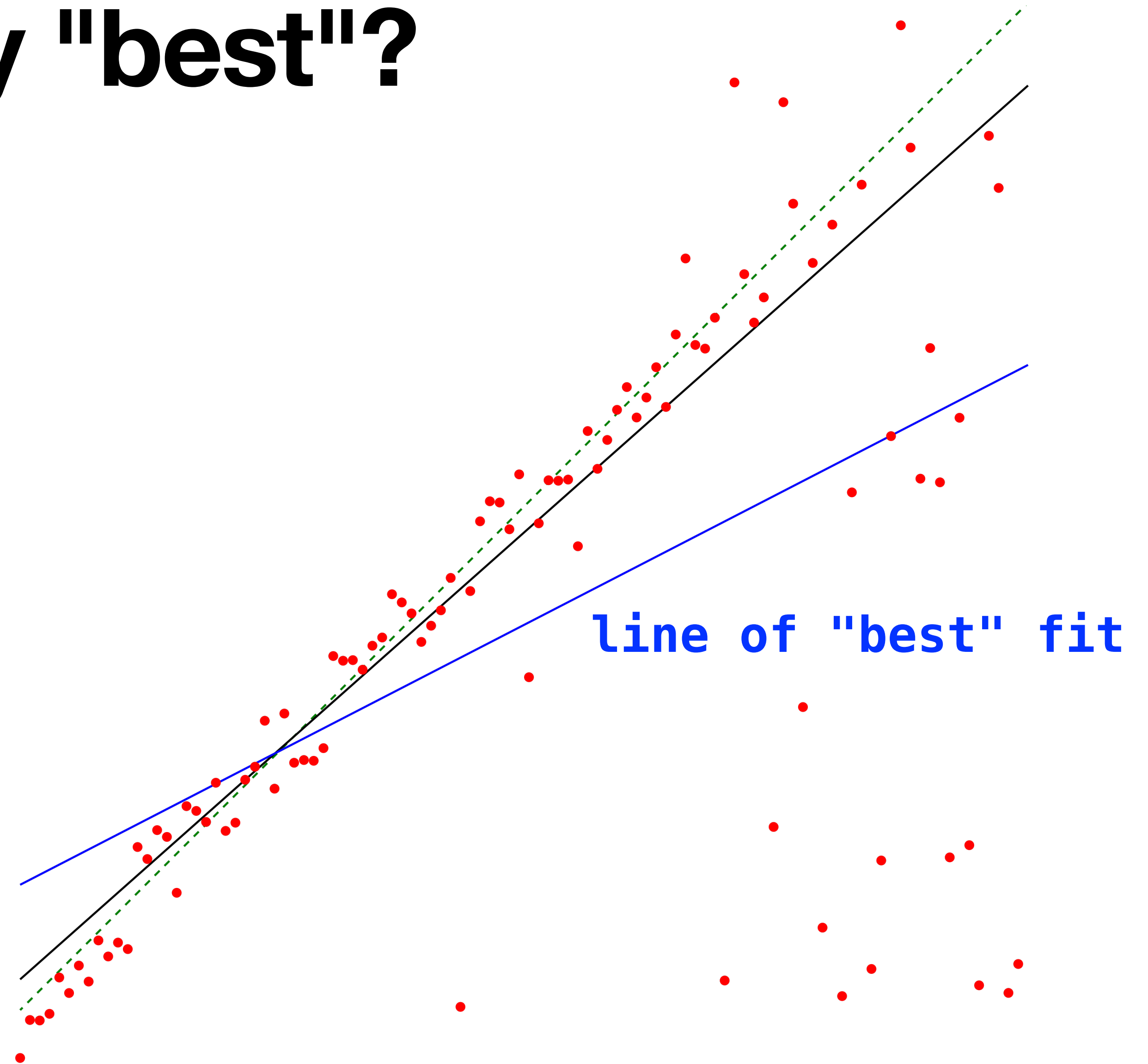
**The "best" line minimizes
the *sum of squares of
differences.***

The Picture



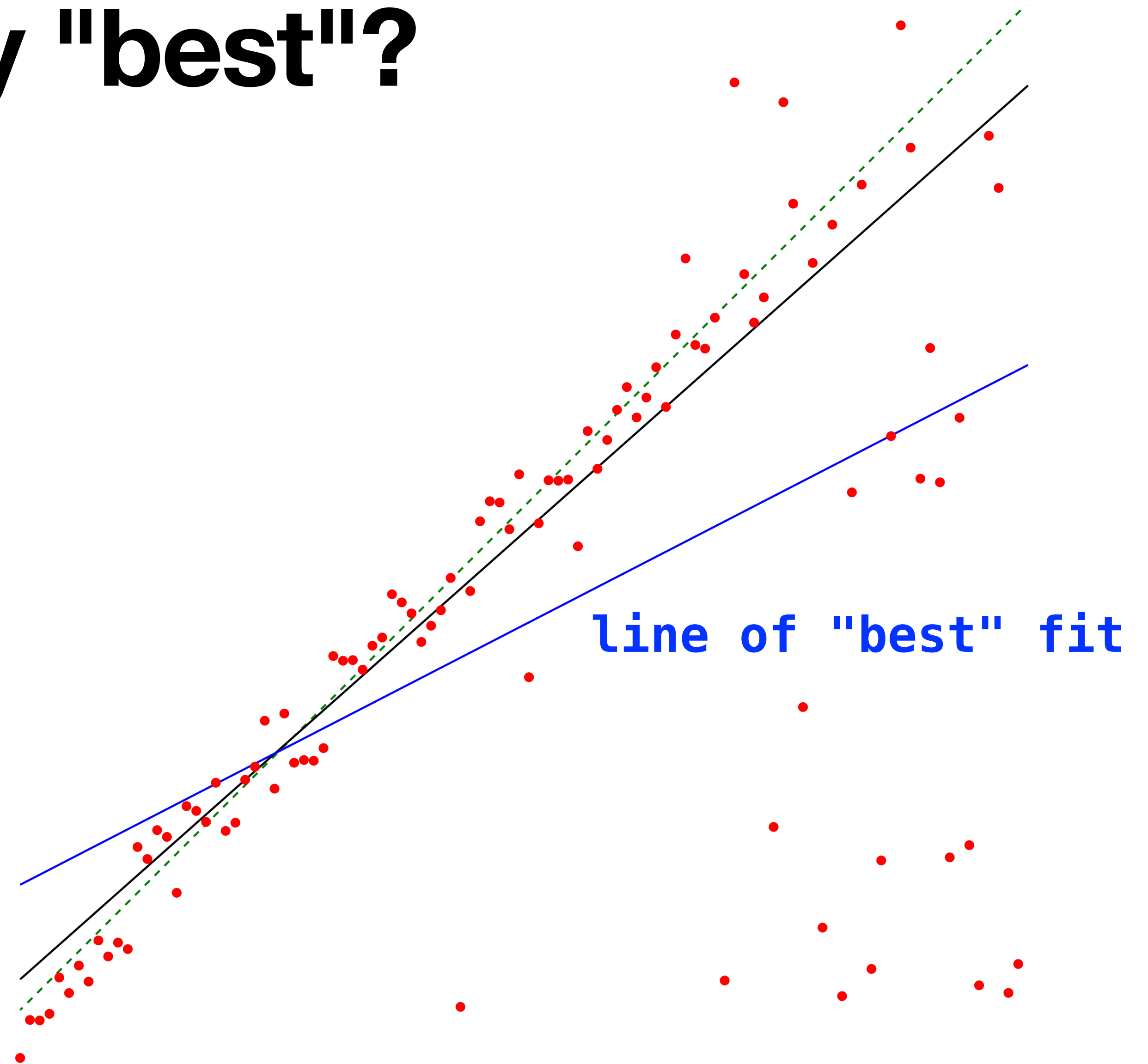
We want to find the line which makes the sum of these differences *as small as possible*.

An Aside: Is this really "best"?



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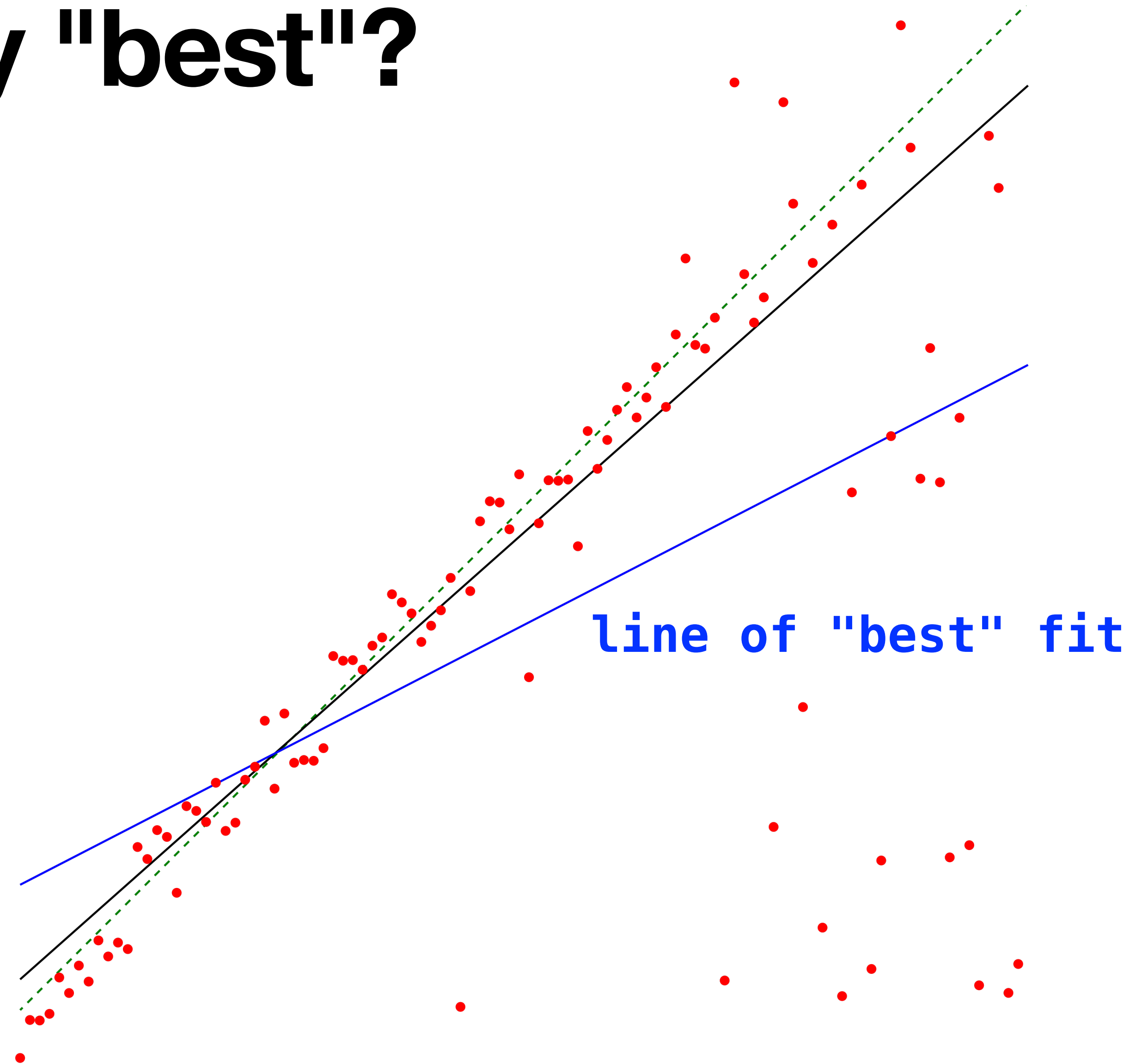
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An Aside: Is this really "best"?

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It depends on the data,
on the application
domain, etc.

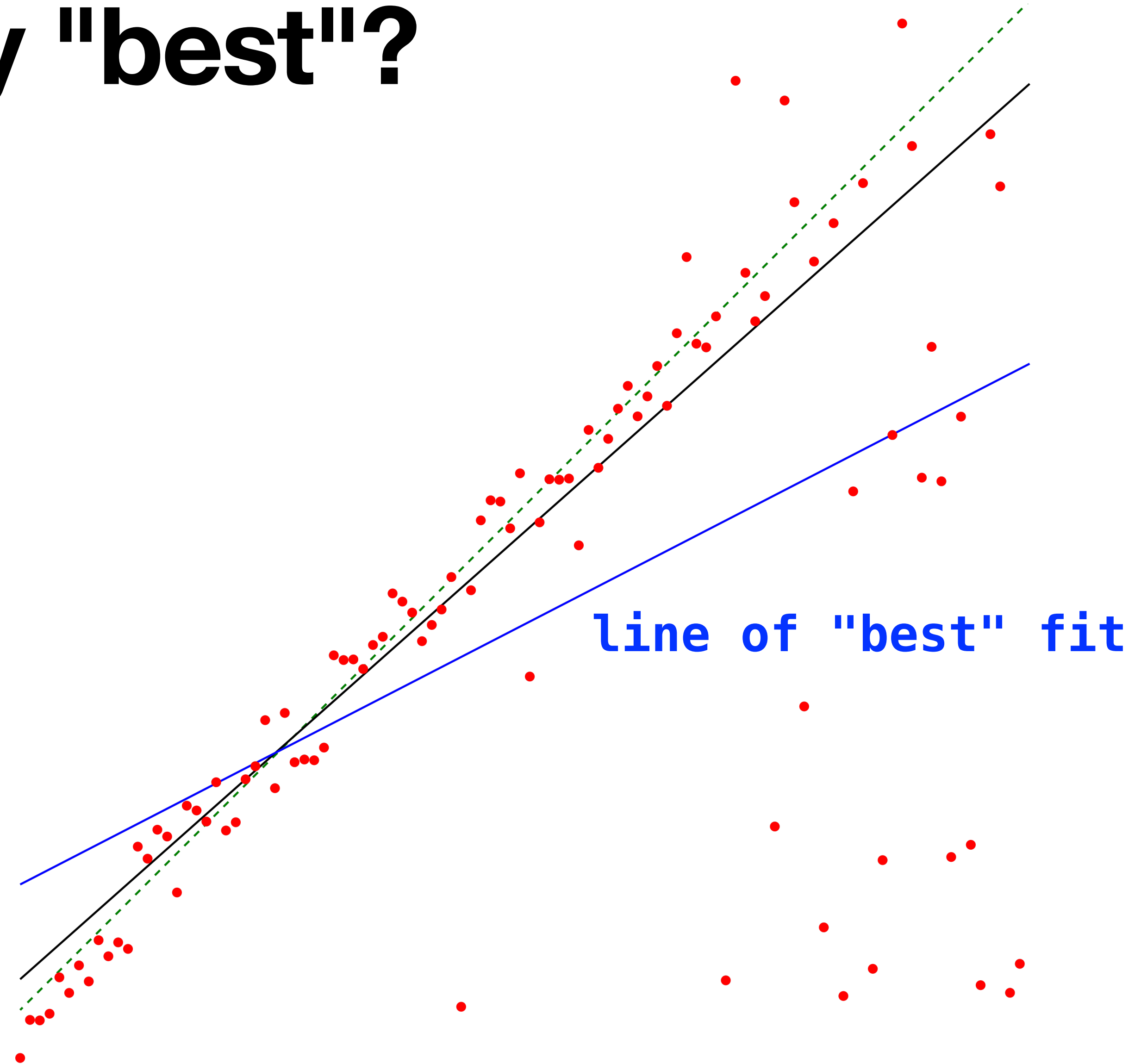


An Aside: Is this really "best"?

Who's to say...

It depends on the data,
on the application
domain, etc.

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



Terminology: Datasets

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

Terminology: Datasets

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dataset

Terminology: Datasets

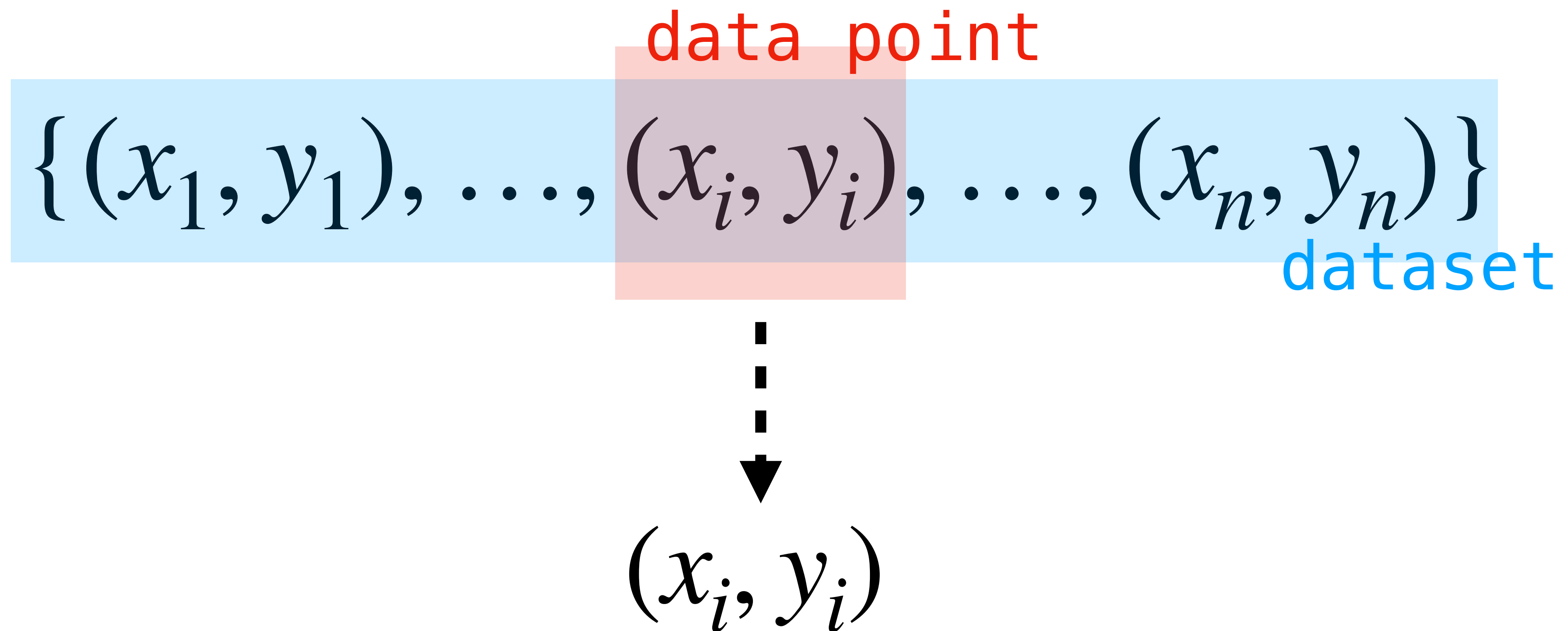
$\{(x_1, y_1), \dots, (x_i, y_i), \dots, (x_n, y_n)\}$

data point

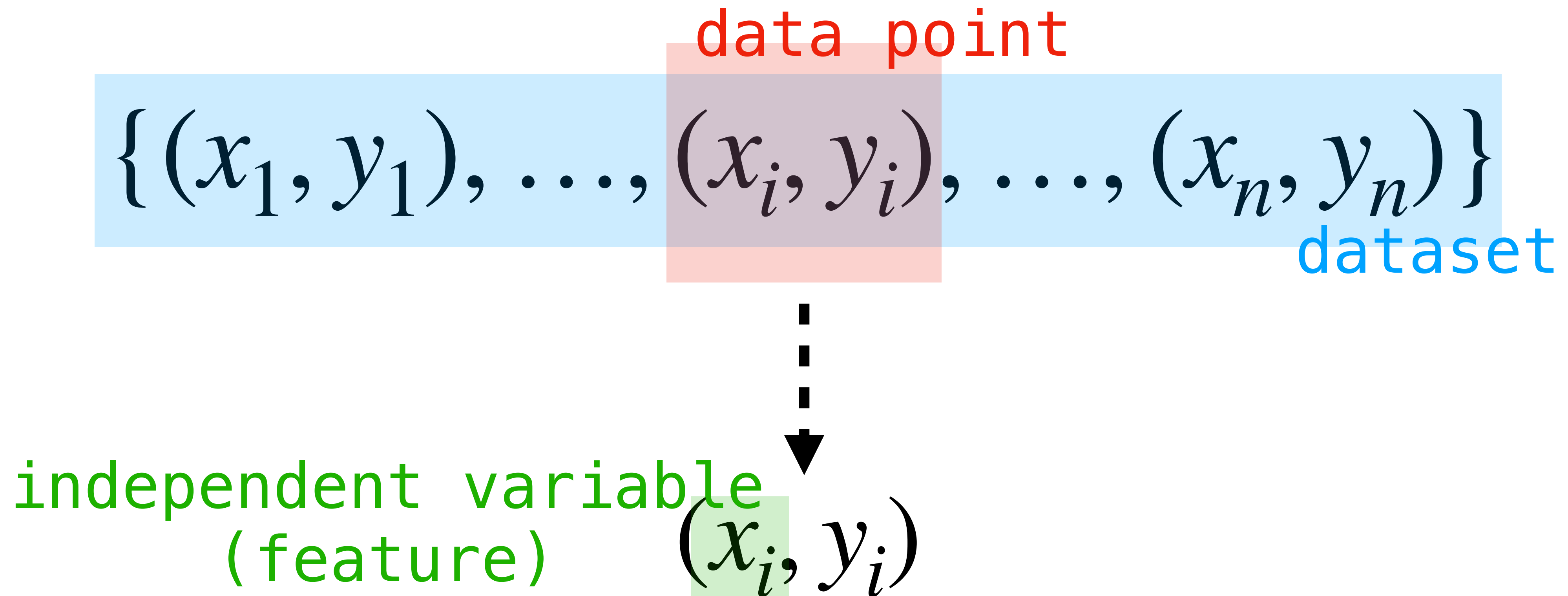
dataset

The diagram illustrates the terminology of datasets. A light blue rectangular background contains the mathematical expression for a dataset: $\{(x_1, y_1), \dots, (x_i, y_i), \dots, (x_n, y_n)\}$. The term 'dataset' is written in blue text at the bottom right of this background. A smaller, semi-transparent light red rectangle is positioned over the (x_i, y_i) term in the sequence. The text 'data point' is written in red above this red rectangle, indicating that a single element of the dataset is a data point.

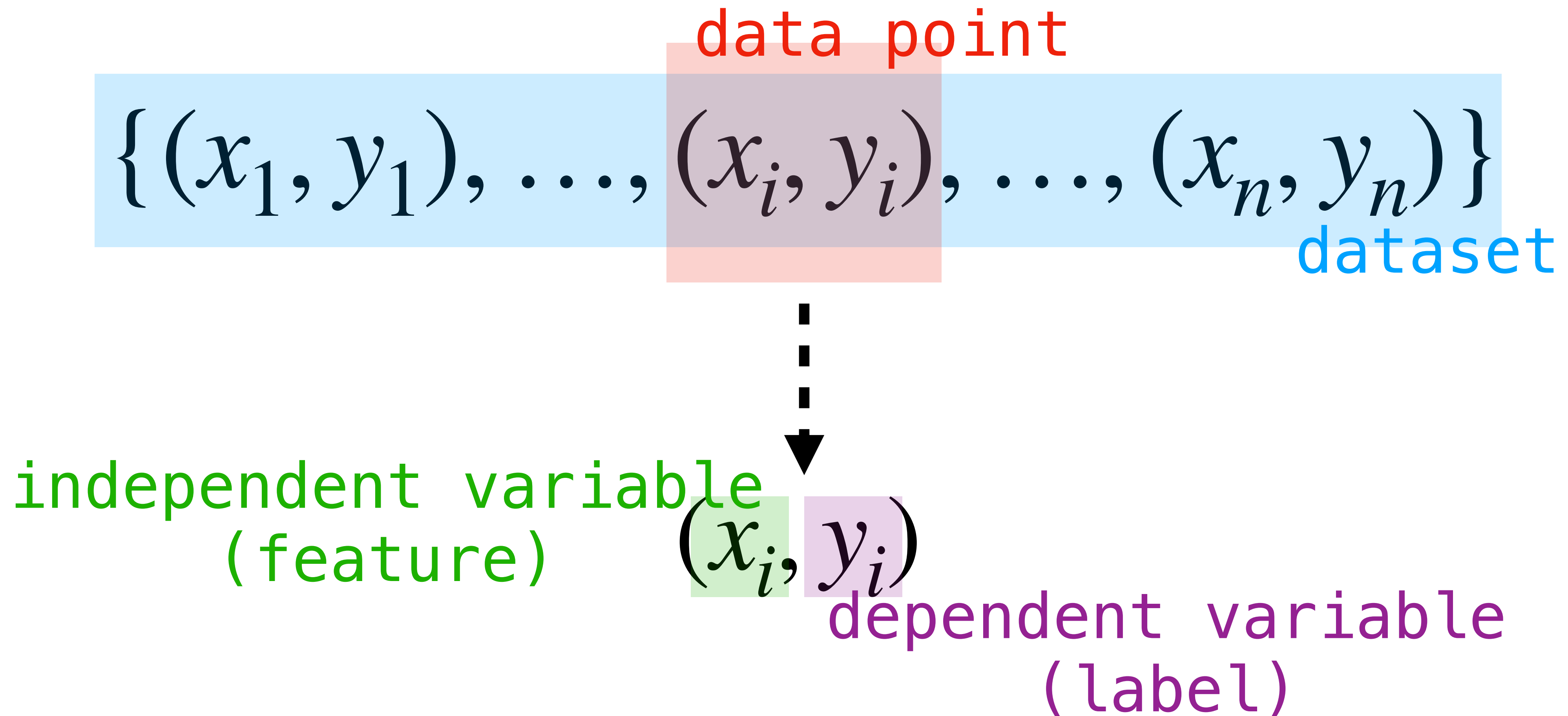
Terminology: Datasets



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Terminology: Datasets



Terminology: Models

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model

Terminology: Models

model parameters/
regression coefficients

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

model

Terminology: Least-Squares Error

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

Terminology: Least-Squares Error

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

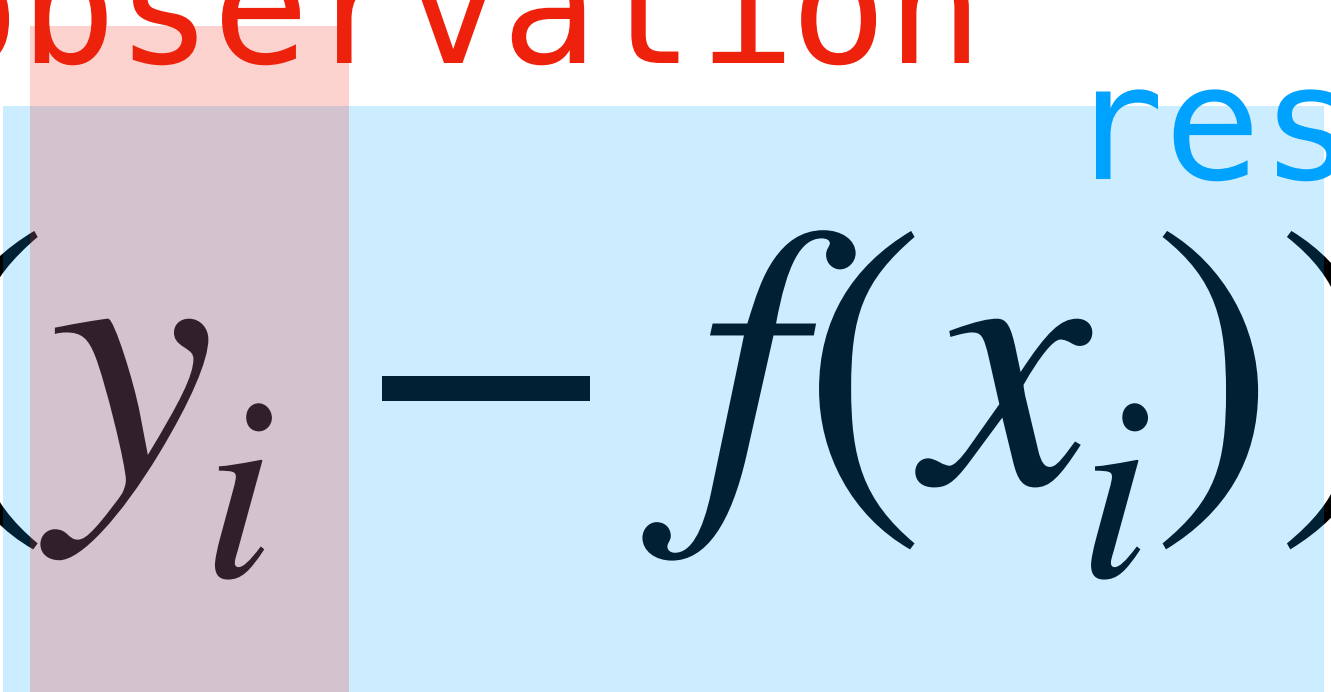
residual

Terminology: Least-Squares Error

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

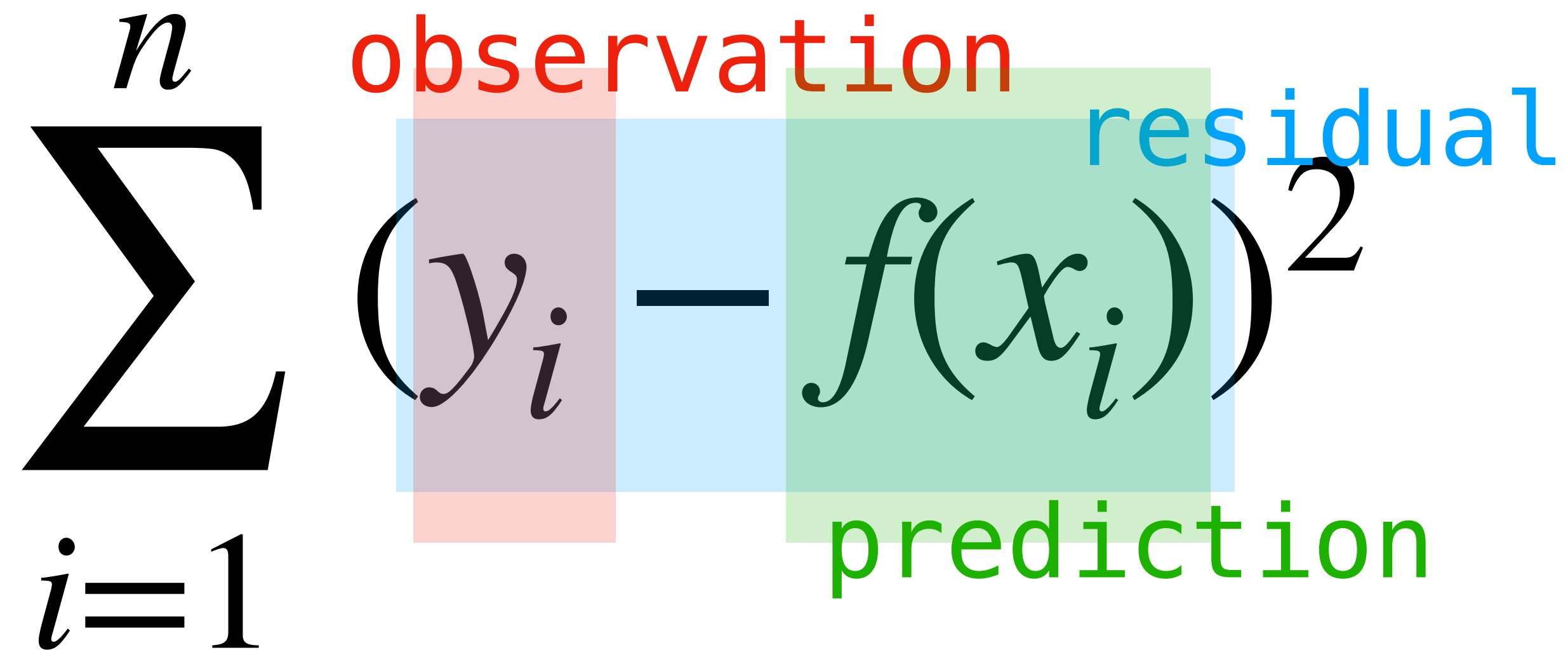
observation

residual



The diagram illustrates the components of the least-squares error formula. The summation symbol \sum is positioned to the left of the expression $(y_i - f(x_i))^2$. The index i is located below the summation symbol, and the total number of observations n is positioned above it. The term y_i is enclosed in a light red rectangular box, with the word "observation" written in red text above it. The term $f(x_i)$ is enclosed in a light blue rectangular box, with the word "residual" written in blue text above it. The entire expression is centered on the slide.

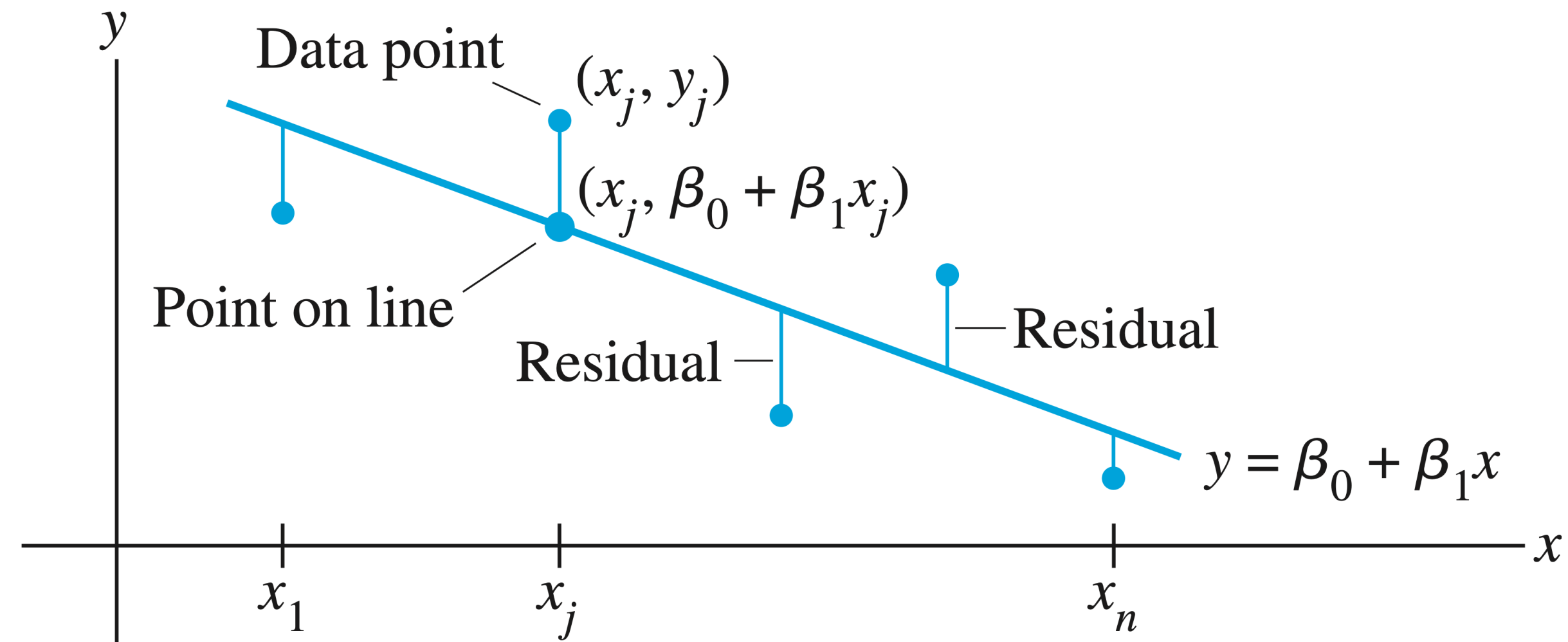
Terminology: Least-Squares Error



The diagram illustrates the least-squares error formula with color-coded components. The summation symbol \sum is large and black. The index $i=1$ is below it. The term y_i is inside a light purple box labeled "observation" in red. The minus sign $-$ is in a light blue box. The term $f(x_i)$ is inside a light green box labeled "prediction" in green. The entire expression is squared, with the exponent 2 in a light blue box labeled "residual" in blue.

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

Terminology



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

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

independent variable x_i

dependent variable (label) y_i

(x_i, y_i)

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

How to: Finding the Least Squares Line

$$\beta_1 = \frac{n \sum_{i=1}^n x_i y_i - \left(\sum_{i=1}^n x_i \right) \left(\sum_{i=1}^n y_i \right)}{n \sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i \right)^2} \quad \beta_0 = \frac{\sum_{i=1}^n y_i - \beta_1 \sum_{i=1}^n x_i}{n}$$

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

How to: Finding the Least Squares Line

Don't memorize these.

$$\beta_1 = \frac{\sum_{i=1}^n x_i y_i - \left(\sum_{i=1}^n x_i \right) \left(\sum_{i=1}^n y_i \right) / n}{\sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i \right)^2 / n} \quad \beta_0 = \frac{\sum_{i=1}^n y_i - \beta_1 \sum_{i=1}^n x_i}{n}$$

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An Observation

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

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

An Observation

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

minimize for least-squares line

$$\min_{\vec{x}} \|A\vec{x} - \vec{b}\|$$

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

minimize for least-squares method

An Observation

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minimize for least-squares method

These expressions look very similar.

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

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minimize for least-squares method

These expressions look very similar.

Can we design a matrix where finding a least squares solution gives us a least squares line?

A Least Squares Problem

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

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

$$\vdots$$

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

A Least Squares Problem

In the "ideal" world, we could find parameters β_0 and β_1 such that all of these equations hold.

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This would mean **all the points already lie on a single line.**

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This is a linear system in the variables β_0 and β_1

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

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

$$\vdots$$

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

A Least Squares Problem

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

A Least Squares Problem

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

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

A Least Squares Problem

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.

↙ design matrix

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

A Least Squares Problem

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

A Least Squares Problem

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

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

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

A Least Squares Problem

$$X\vec{\beta} = \vec{y}$$

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

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

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

Recall: The Normal Equations

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Theorem. The set of least-squares solutions of $A\mathbf{x} = \mathbf{b}$ is the same as the set of solutions to

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

Recall: The Normal Equations

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In particular, this set of solutions is nonempty

Recall: The Normal Equations

Theorem. The set of least-squares solutions of $A\mathbf{x} = \mathbf{b}$ is the same as the set of solutions to

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

In particular, this set of solutions is nonempty

(We just showed that if $\hat{\mathbf{x}}$ is a least squares solution then $A^T A \hat{\mathbf{x}} = A^T \mathbf{b}$)

Recall: Unique Least Squares Solutions

$(n \times k)$ $(k \times m)$ gives $n \times m$ matrix

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

If A has linearly independent columns, then its unique least squares solution is defined as above.

$$\begin{bmatrix} 1 & \dots & 1 \\ x_1 & \dots & x_n \end{bmatrix} \begin{bmatrix} 1 \\ \vdots \\ x_n \end{bmatrix} = \mathbf{x}$$

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

Just for Fun

$$\begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = (A^T A)^{-1} A^T \vec{b}$$

$$\beta_1 = \frac{n \sum_i x_i y_i - \left(\sum_i x_i \right) \left(\sum_i y_i \right)}{n \sum_i x_i^2 - \left(\sum_i x_i \right)^2}$$

Let's derive it:

$$A^T A = \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} n & x_1 + x_2 + \dots + x_n \\ x_1 + x_2 + \dots + x_n & x_1^2 + x_2^2 + \dots + x_n^2 \end{bmatrix}$$

$$(A^T A)^{-1} = \frac{1}{n(\sum_i x_i^2) - (\sum_i x_i)^2} \begin{bmatrix} \sum_i x_i^2 & -\sum_i x_i \\ -\sum_i x_i & n \end{bmatrix}$$

$$A^T \vec{b} = \begin{bmatrix} 1 & \dots & 1 \\ x_1 & \dots & x_n \end{bmatrix} \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} \sum_i y_i \\ \sum_i x_i y_i \end{bmatrix}$$

$$(A^T A)^{-1} A^T \vec{b} = \begin{bmatrix} \text{(something for } \beta_0 \text{)} \\ \frac{1}{\det(A^T A)} \left[(-\sum_i x_i)(\sum_i y_i) + n(\sum_i x_i y_i) \right] \end{bmatrix}$$

Exercise:
verify β_0 formula

How To: Least Squares Line

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

How To: Least Squares Line

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

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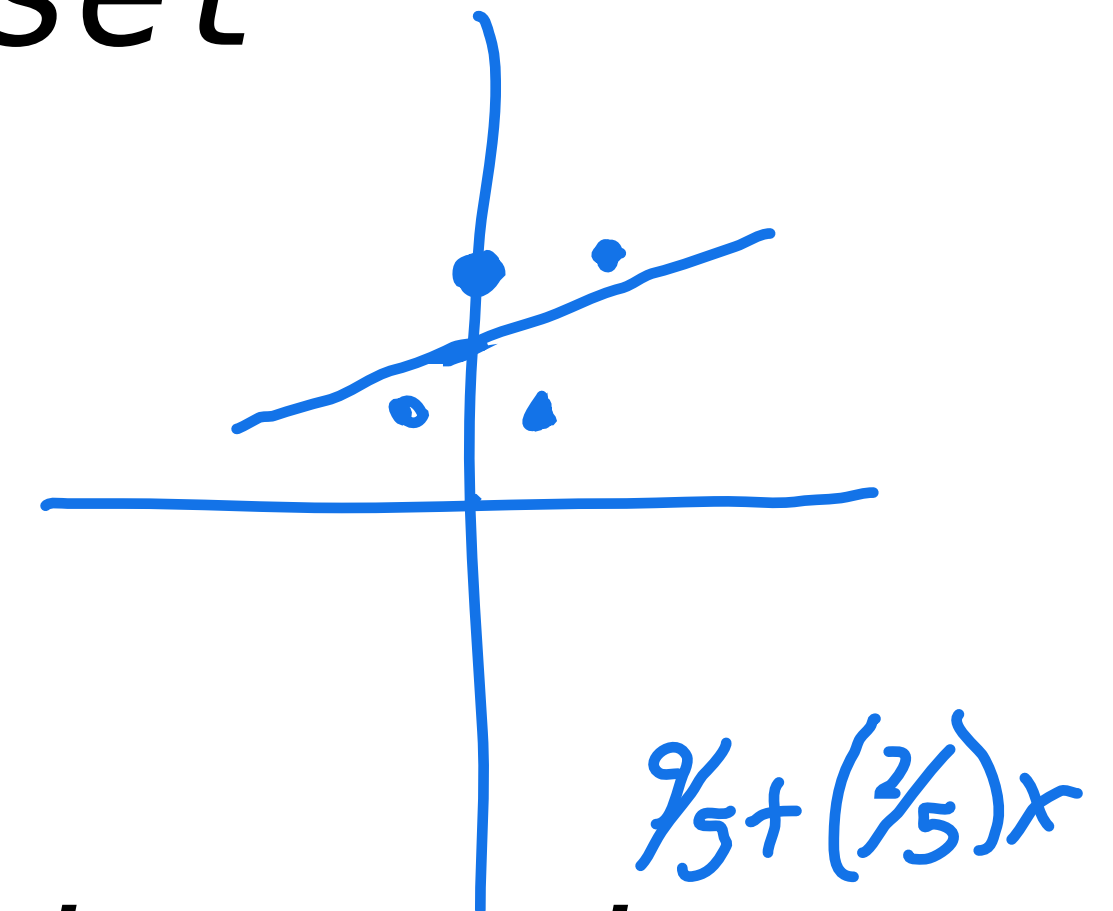
Solution. Find the least squares solution to the above equation.

Question

$$X \rightarrow \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & -1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} 3 \\ 1 \\ 1 \\ 3 \end{bmatrix} \leftarrow \vec{y}$$

Find the line of best fit for the dataset

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



by using the the least-squares method.

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

$$X^T X = \begin{bmatrix} 4 & 2 \\ 2 & 6 \end{bmatrix}$$

$$X^T \vec{y} = \begin{bmatrix} 8 \\ 6 \end{bmatrix}$$

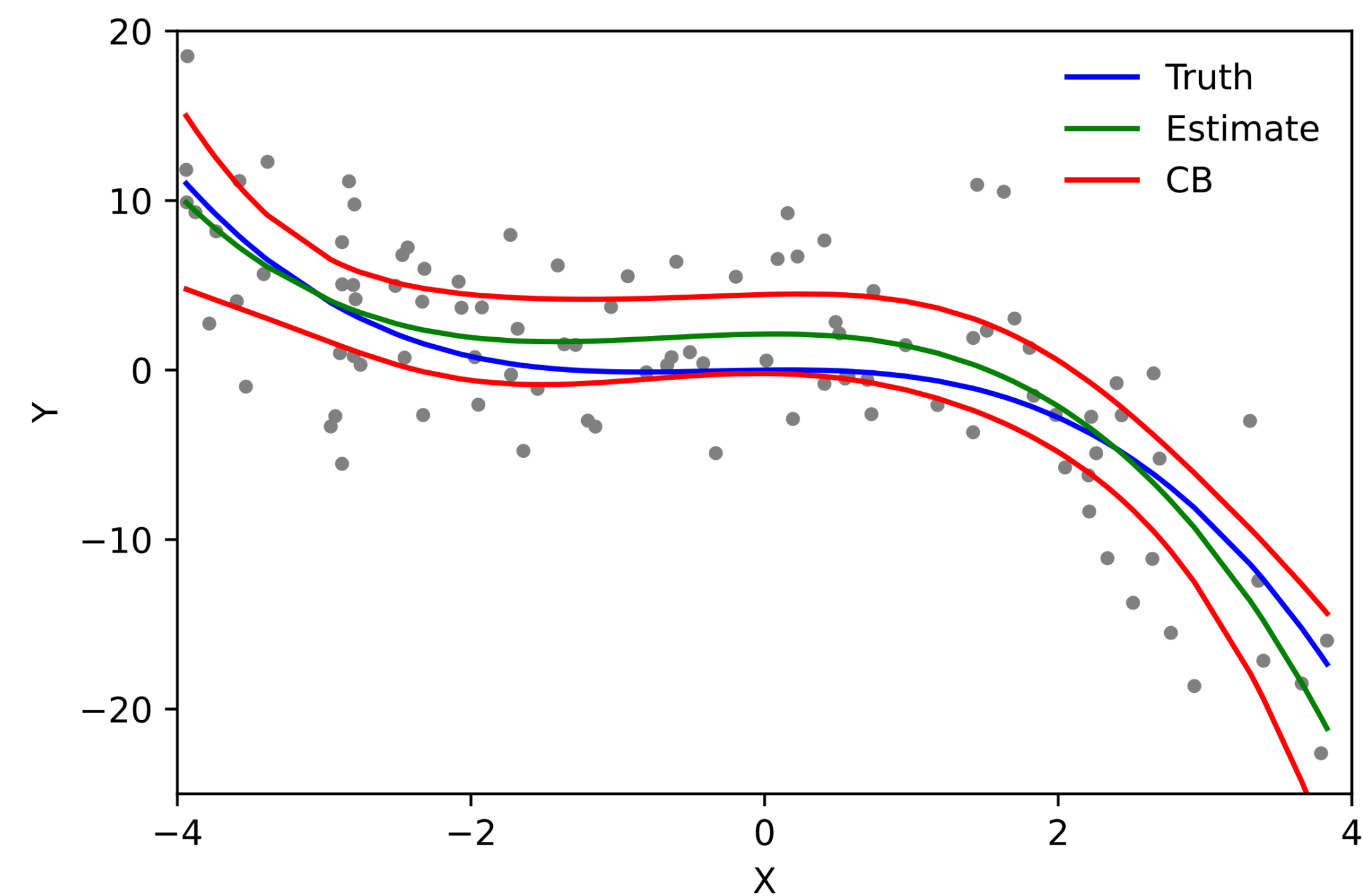
$$\begin{bmatrix} 4 & 2 & ; & 8 \\ 2 & 6 & ; & 6 \end{bmatrix} \sim \begin{bmatrix} 2 & 1 & 4 \\ 1 & 3 & 3 \end{bmatrix} \sim \begin{bmatrix} 1 & 3 & 3 \\ 0 & -5 & -2 \end{bmatrix}$$


$$-5\beta_1 = -2 \Rightarrow \beta_1 = \frac{2}{5} \qquad f(x) = \frac{9}{5} + \left(\frac{2}{5}\right)x$$

$$\beta_0 = 3 - 3\beta_1 = 3 - \frac{6}{5} = \frac{9}{5}$$

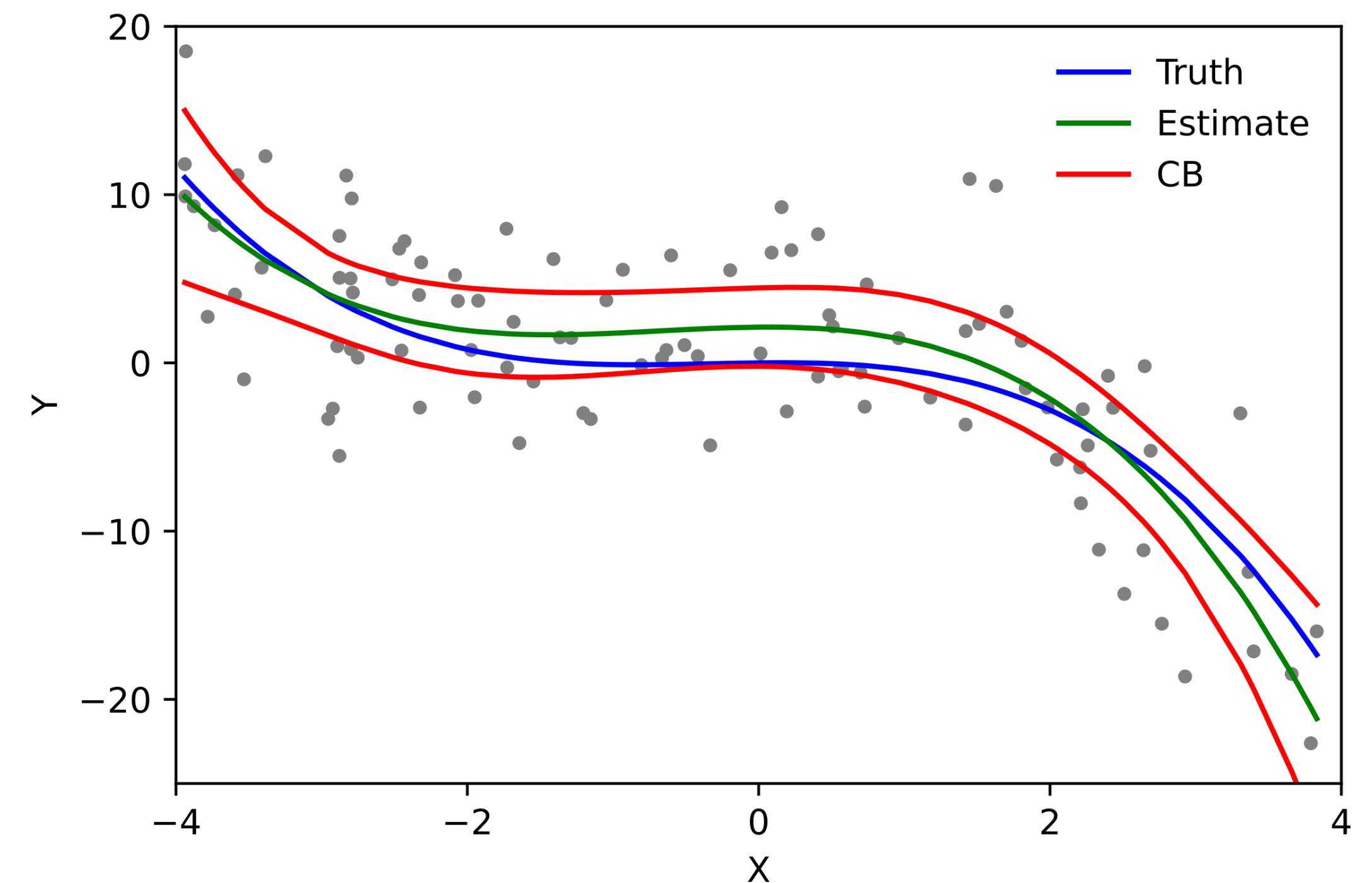
$$f(4) = \frac{9}{5} + \left(\frac{2}{5}\right)4 = \frac{9}{5} + \frac{8}{5} = \frac{17}{5}$$

General Regression



General Regression

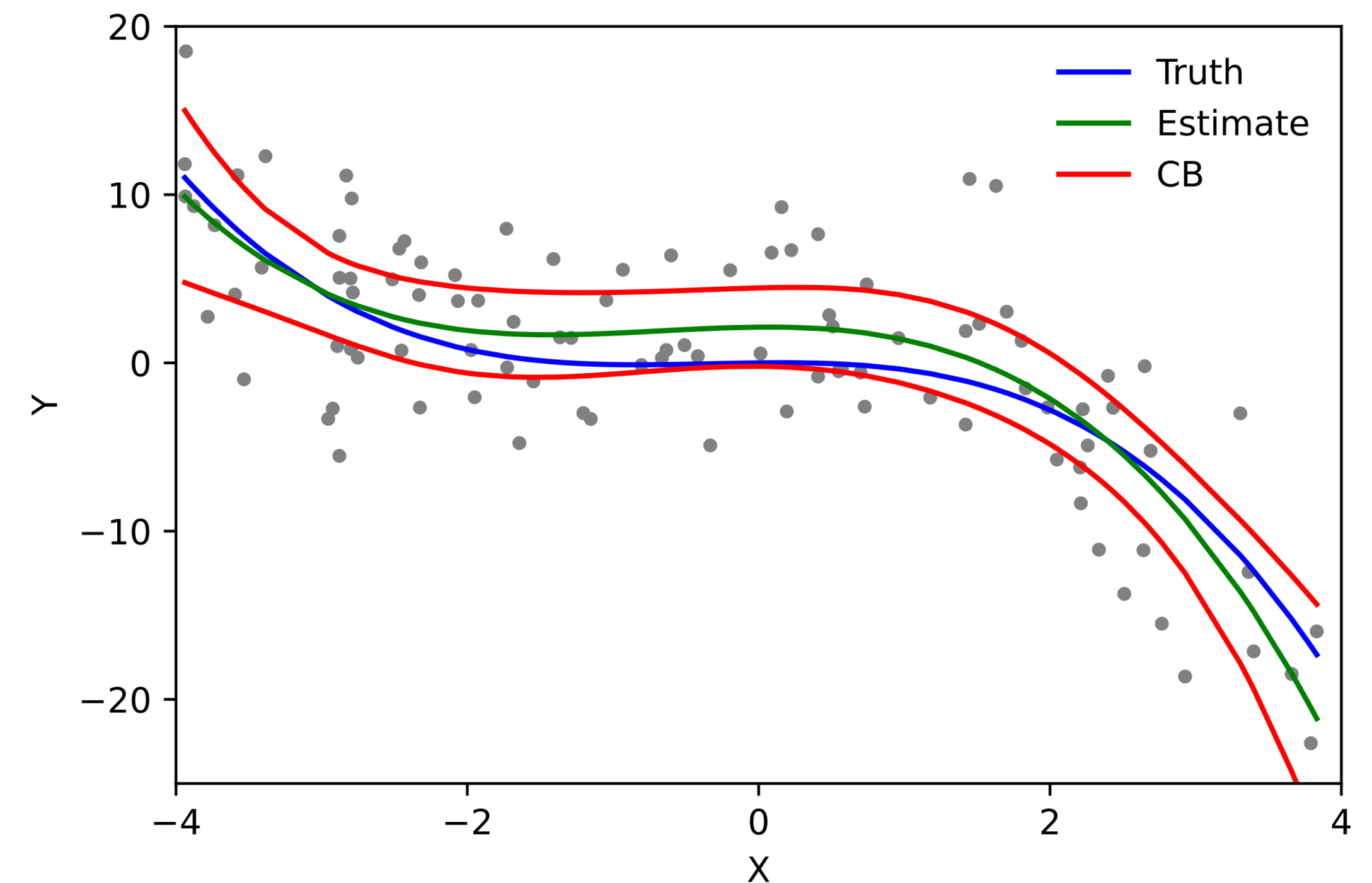
Regression is the process of estimating the relationships independent and dependent variables in a dataset.



General Regression

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What we are estimating is a mathematical function

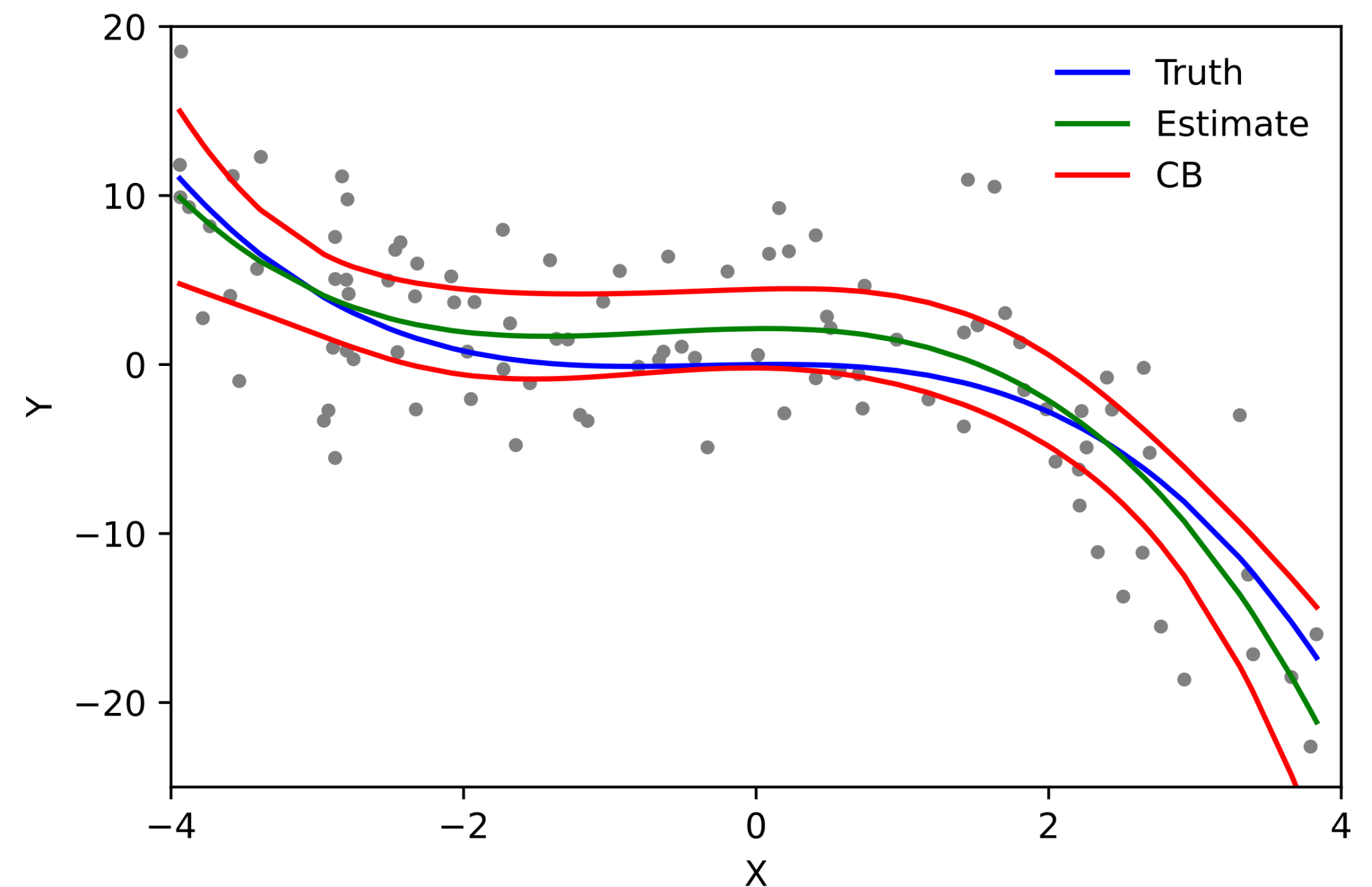


General Regression

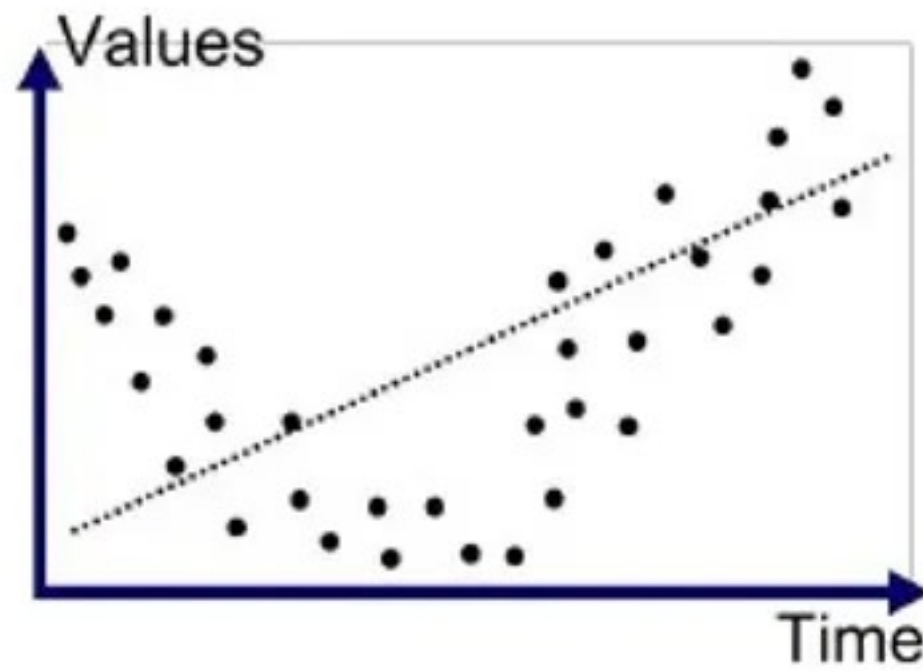
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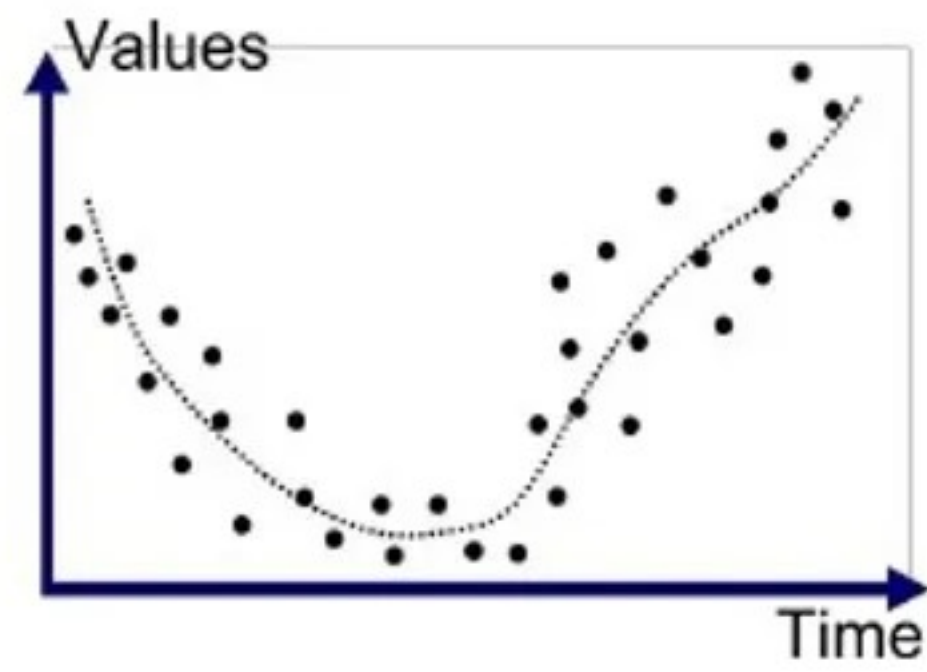
We think of the environment has providing us a function from our independent variables to our dependent variables.



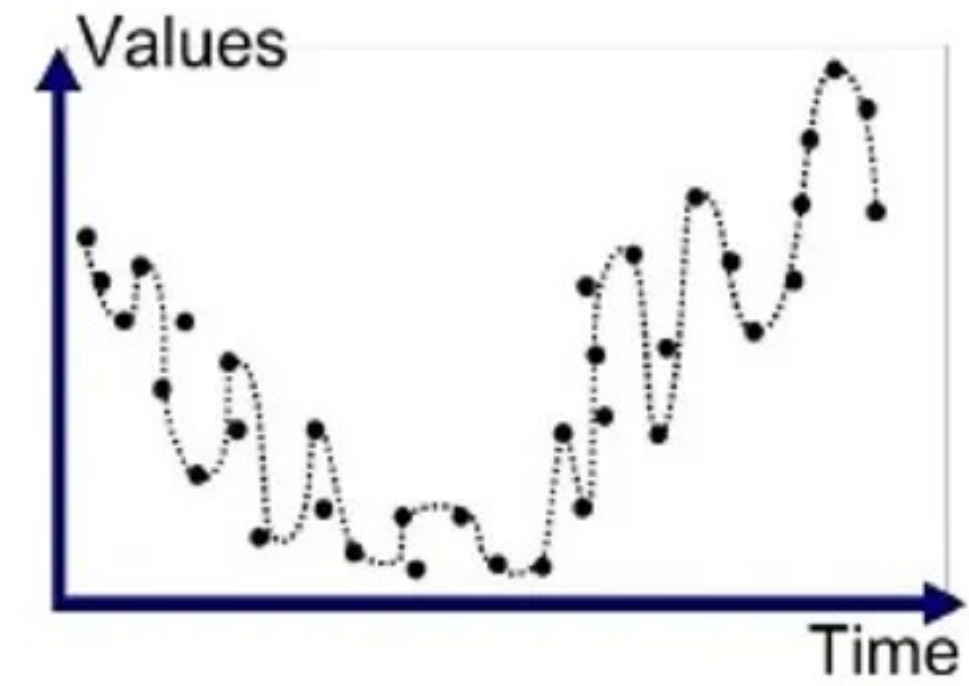
Models



Underfitted

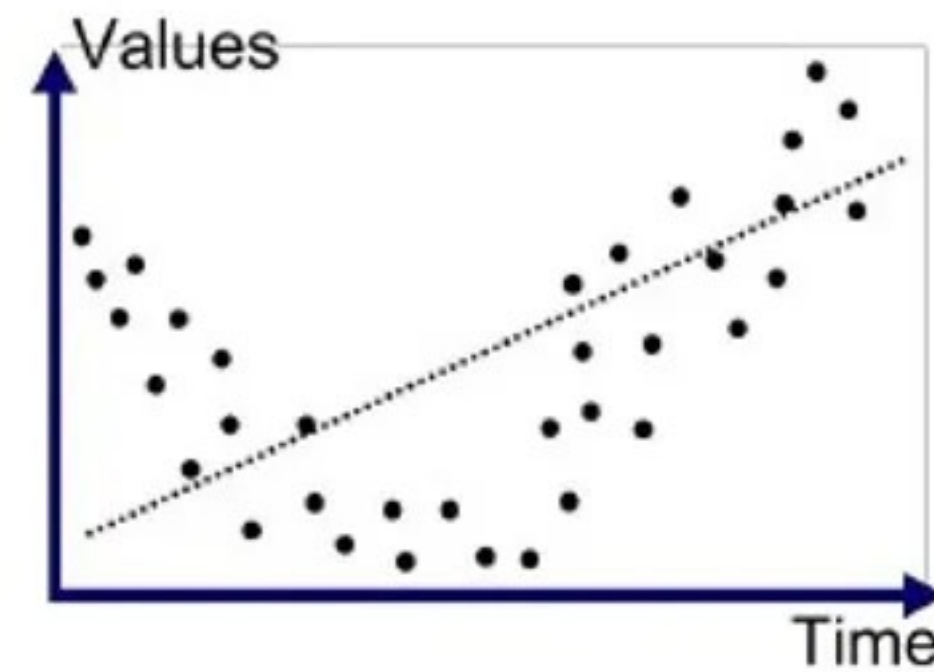


Good Fit/Robust

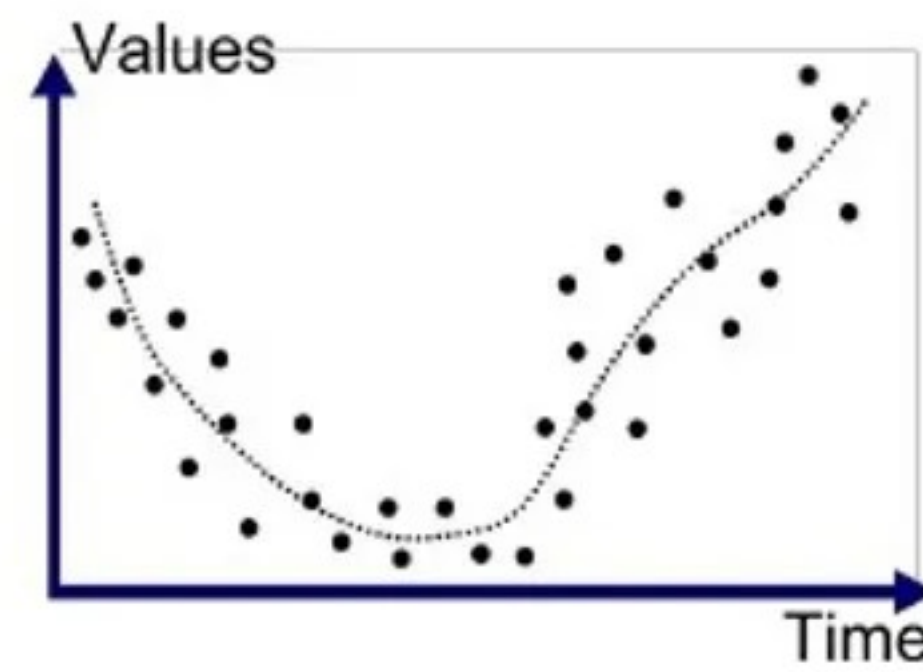


Overfitted

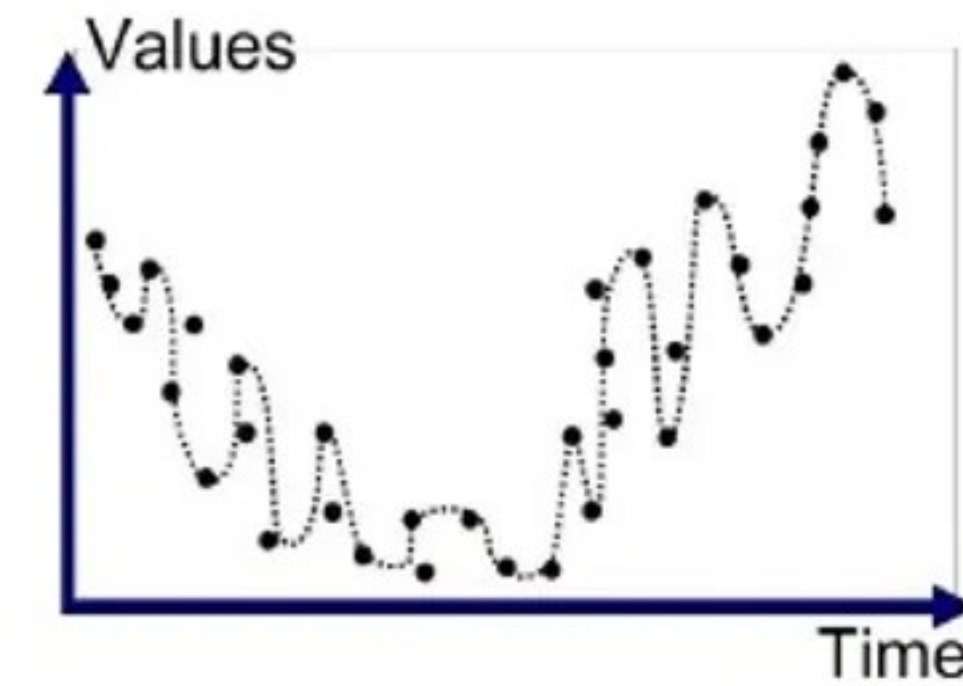
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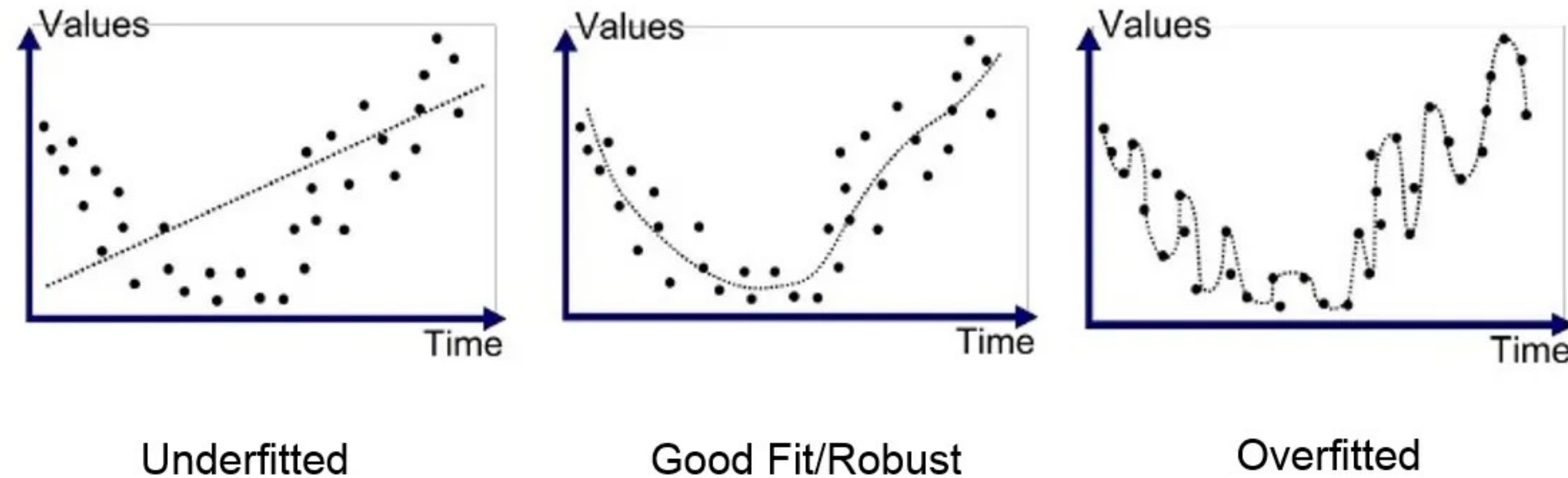


Overfitted

Therefore, a *model* is a mathematical function.

←
n datapoint
 (x_i, y_i)
deg ~~n~~ $n-1$ polynomial

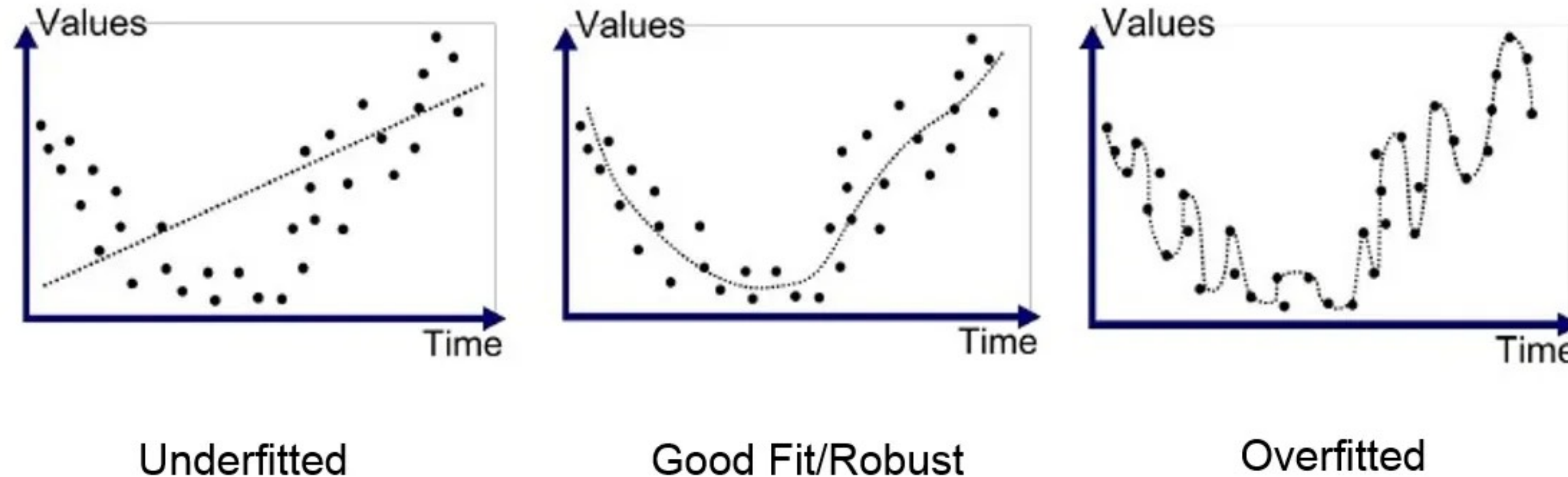
Models



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We're interested in finding mathematical functions that "correctly" model the data we've seen.

Models

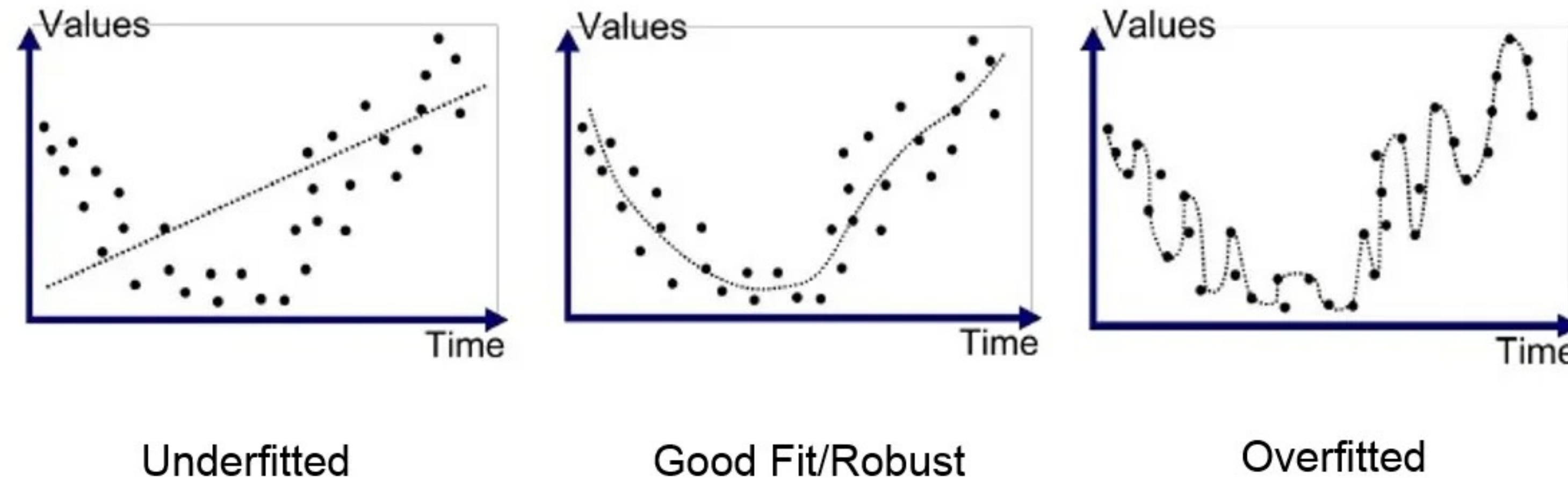


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Models



Therefore, a *model* is a mathematical function.

We're interested in finding mathematical functions that "correctly" model the data we've seen.

But this would be 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.*

How To: Prediction

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

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Solution. Find the best fit line $f(x) = \beta_0 + \beta_1 x$.
The predicted value of x' is $f(x')$.

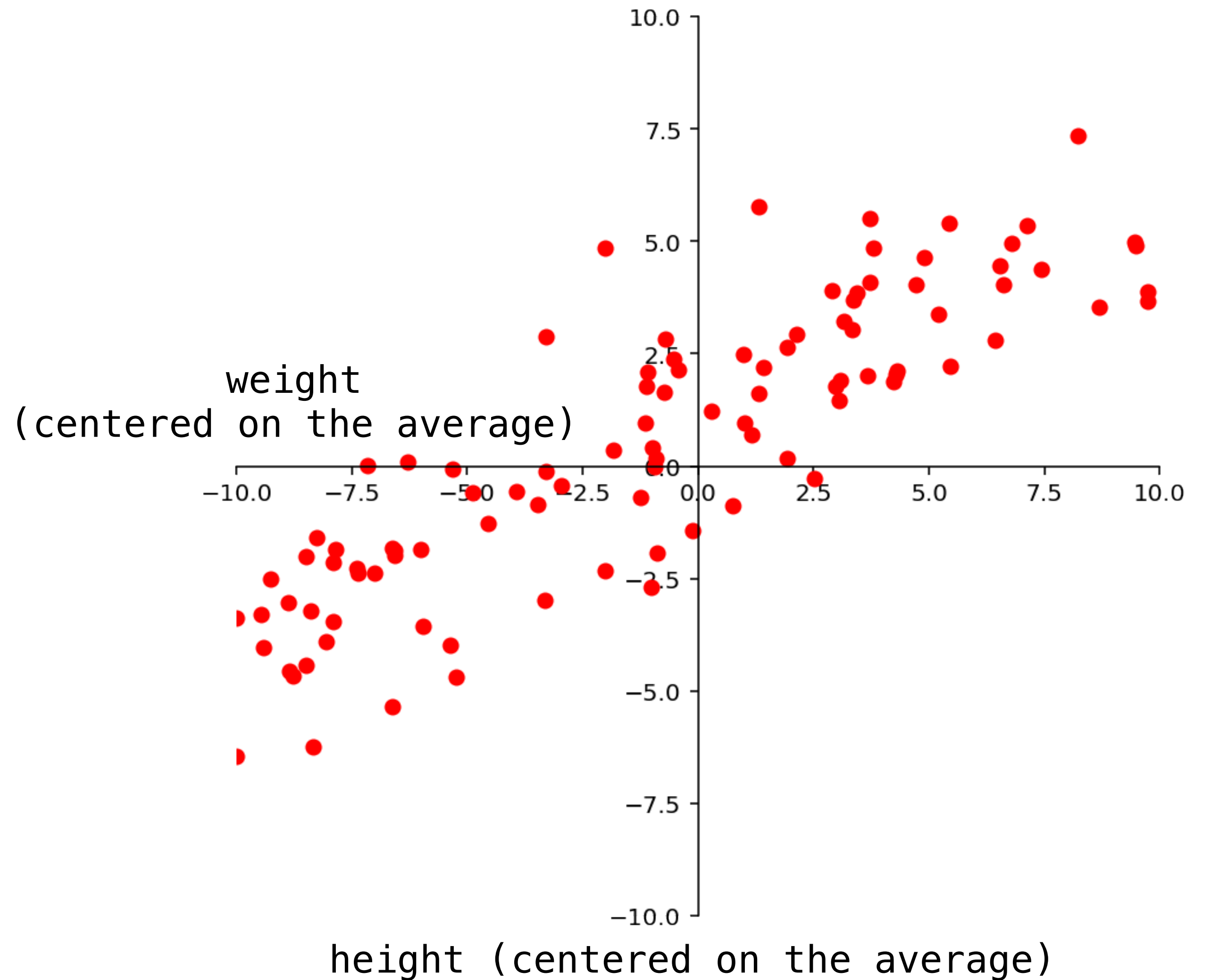
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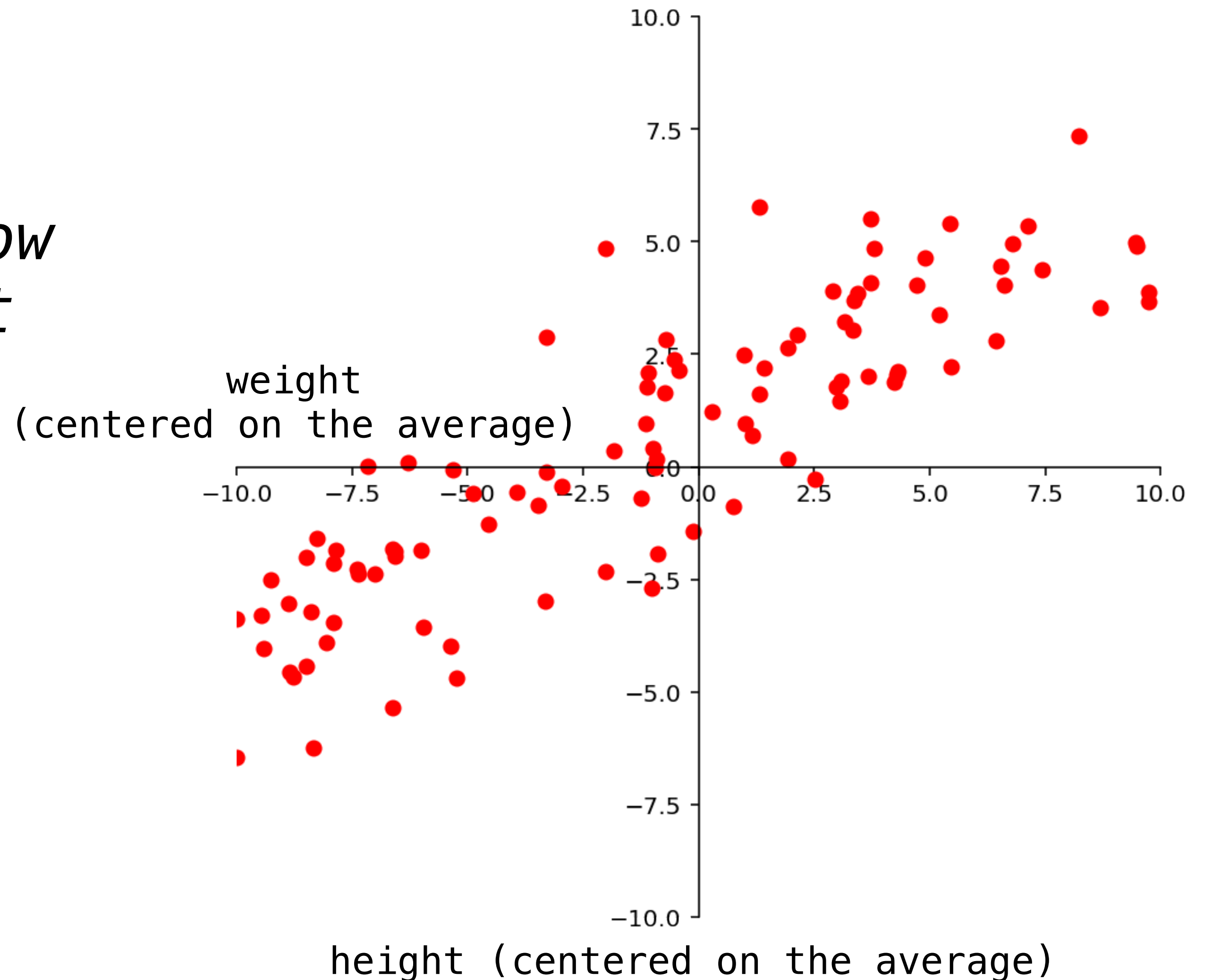
**This generalizes to any
model fitting problem**

Example: Height from Weight



Example: Height from Weight

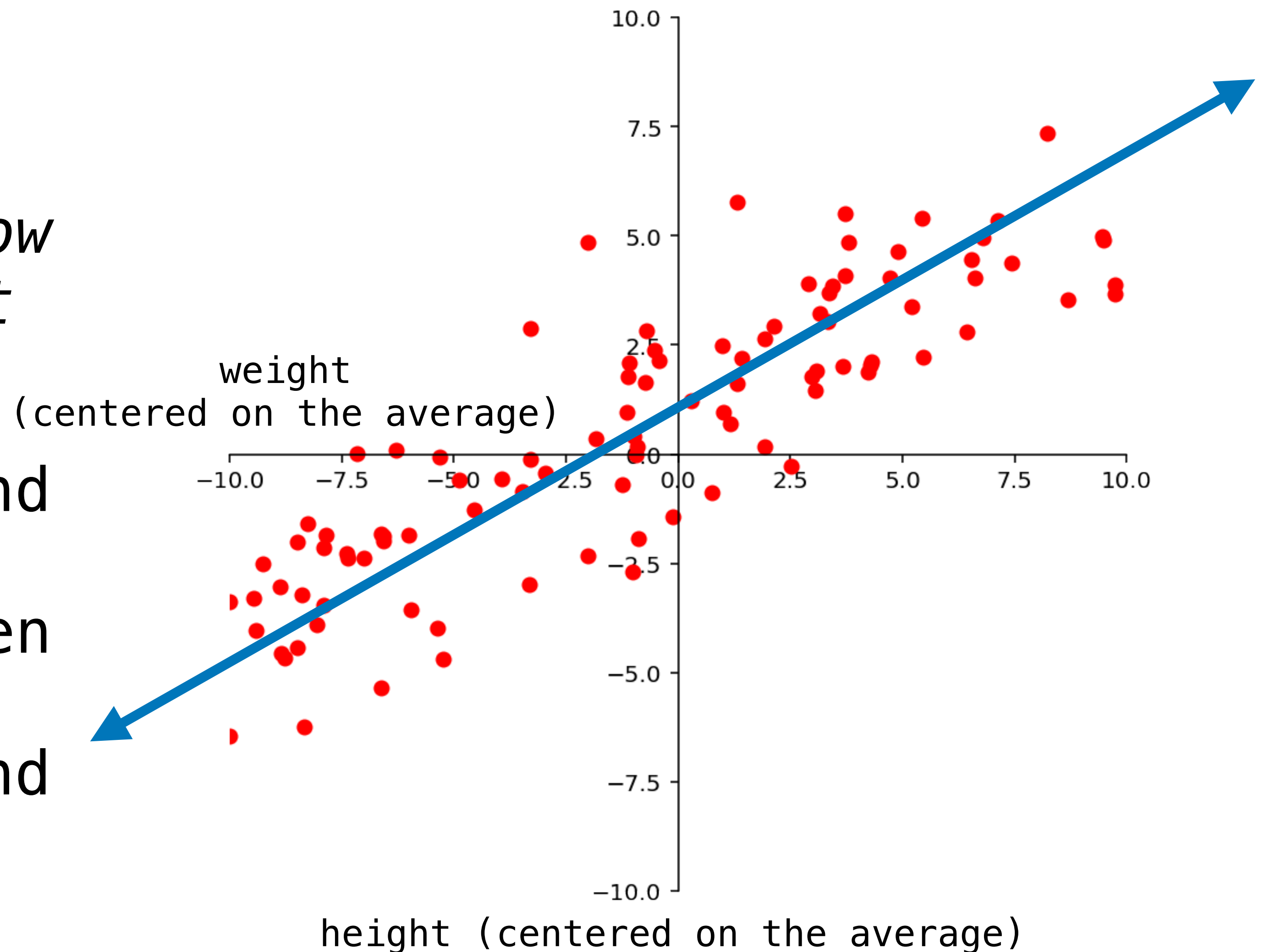
Suppose we know that person X weighs 150lb. *How would we guess the height of person X ?*



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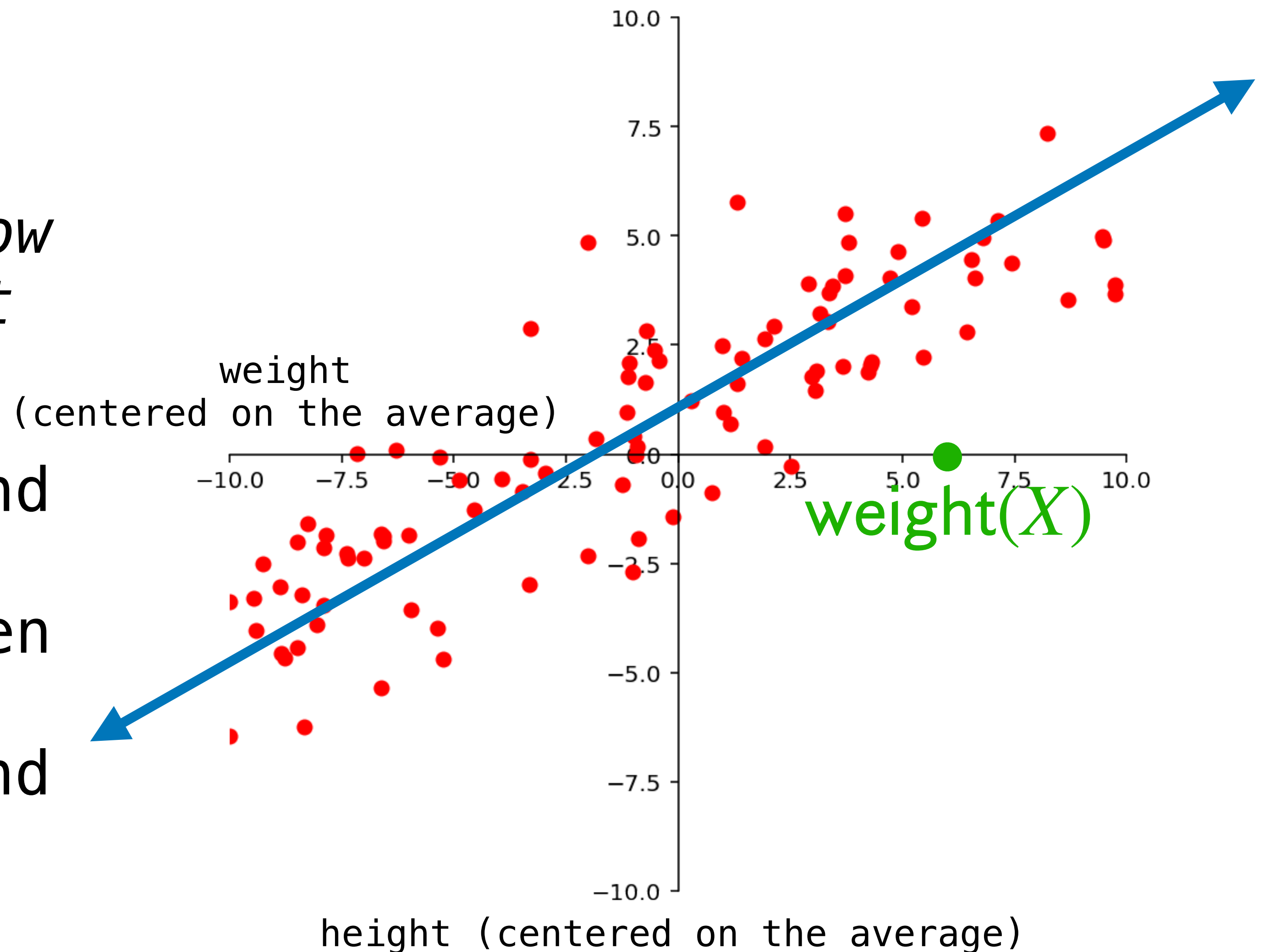
If we know the heights and weights of a population (from which X comes), then we can **find the line of best fit for that data** and then use that function.



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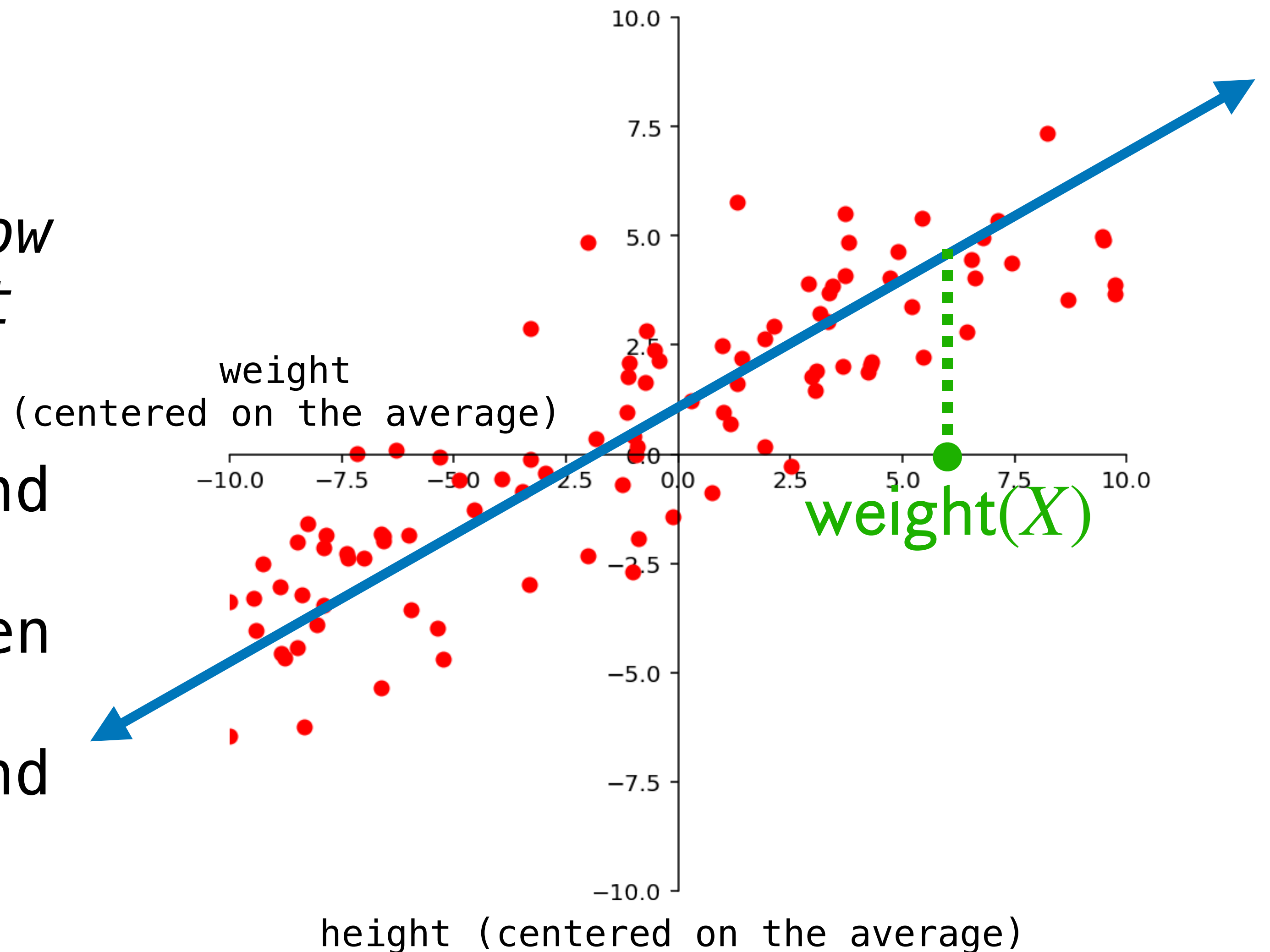
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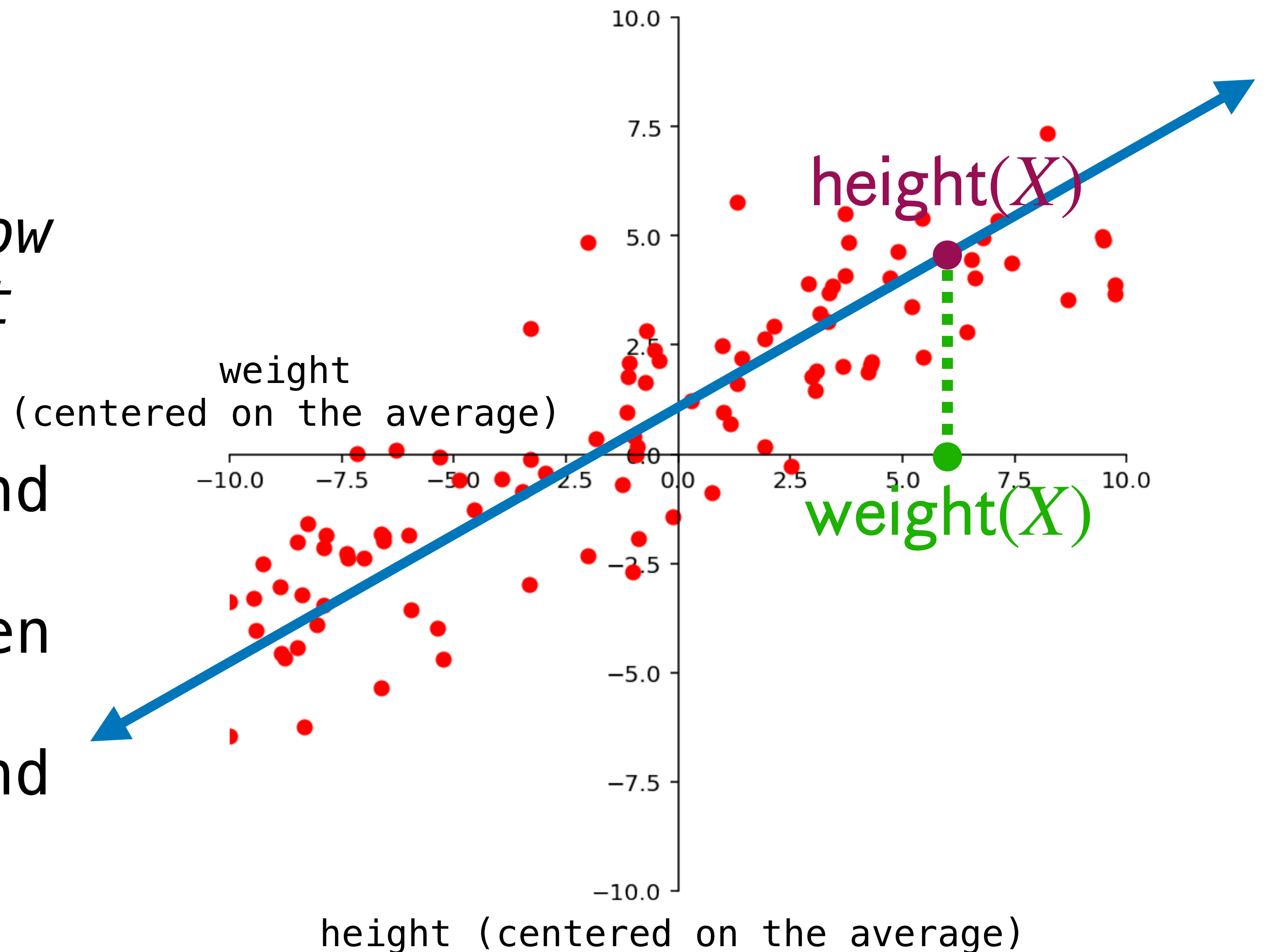
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Example: Height from Weight

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.

Answer

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

Linear Models and Least Squares Regression

"Vectors" of Generalization

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

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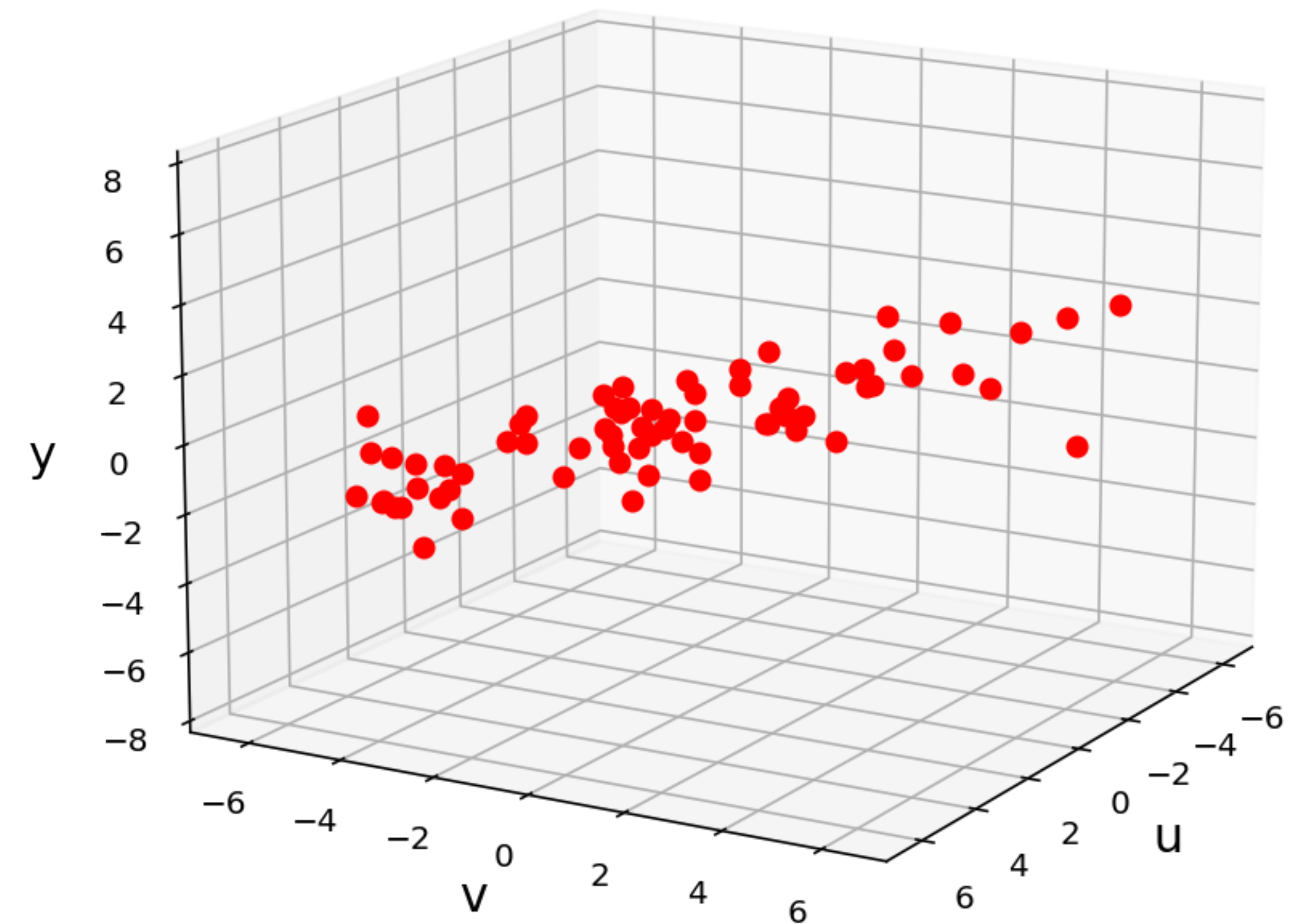
Example: Terrain Data

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

Problem: Find the plane
which "best" fits the
data.

Figure 23.1

Terrain Data for Multiple Regression



Example: Terrain Data

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

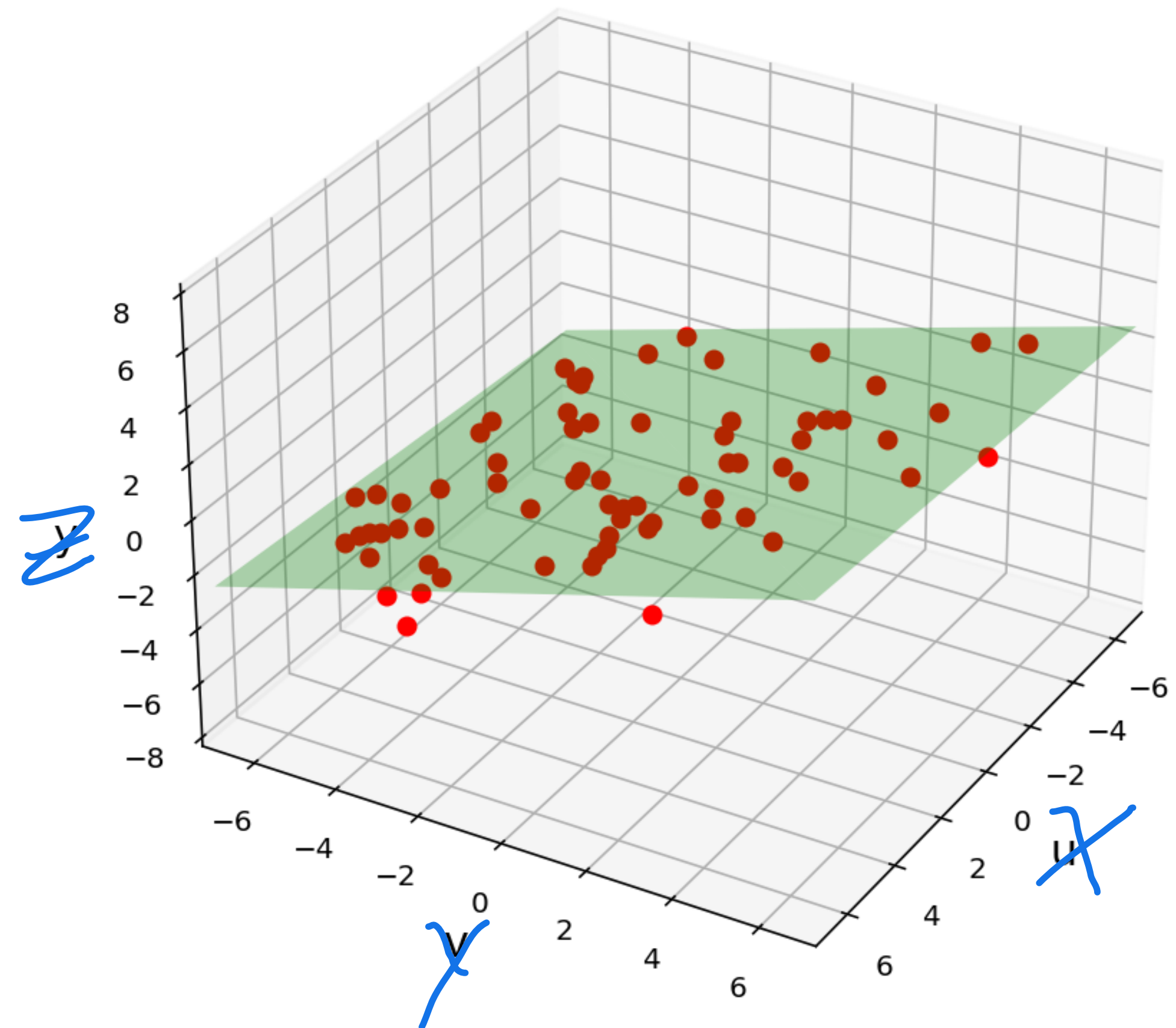
$$f(x, y) = \beta_0 + \beta_1 x + \beta_2 y$$

which minimizes

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

Figure 23.2

Multiple Regression Fit to Data



Example: Terrain Data

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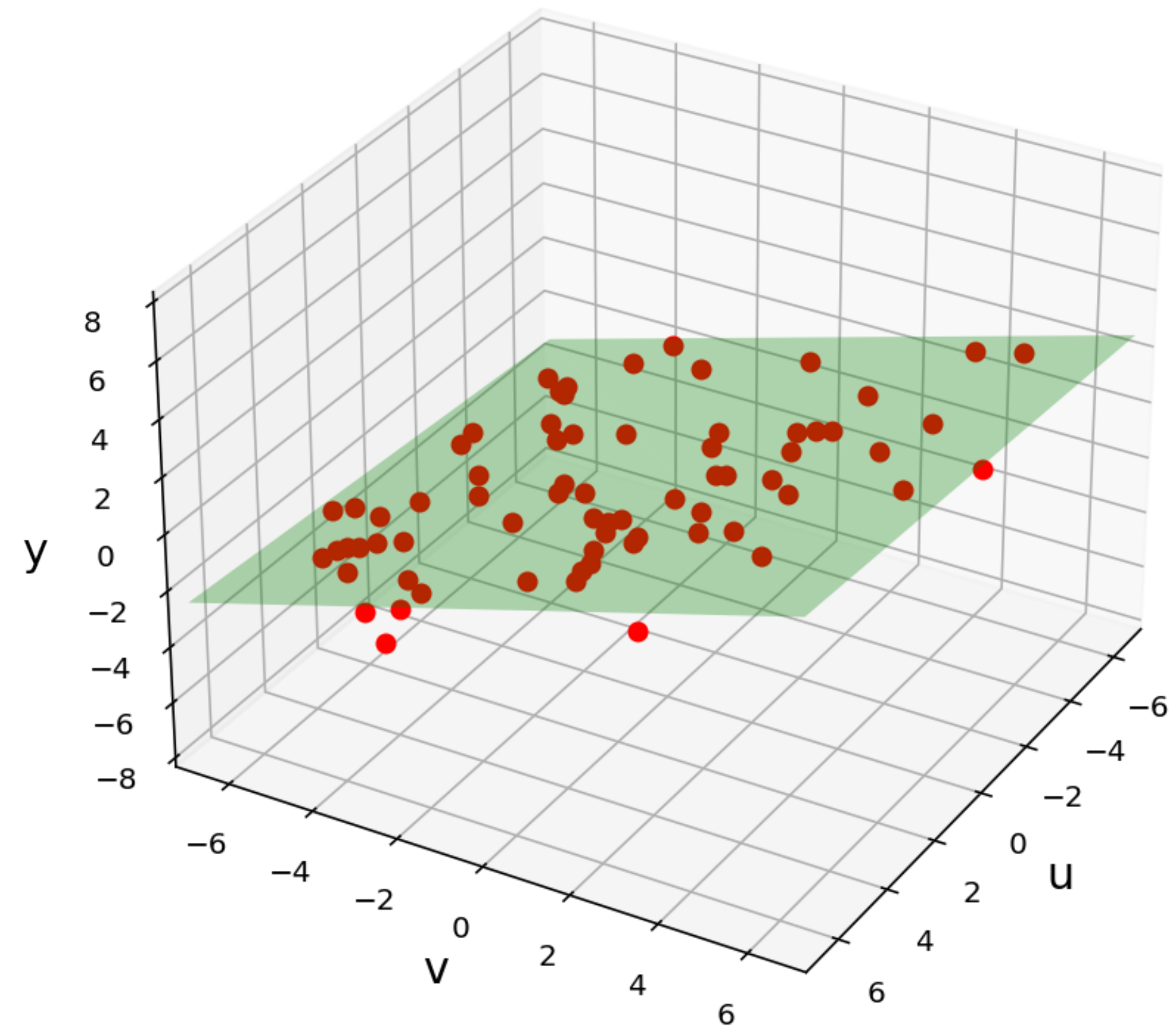
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$f(x, y)$ is a good approximation of the altitude.

Figure 23.2

Multiple Regression Fit to Data



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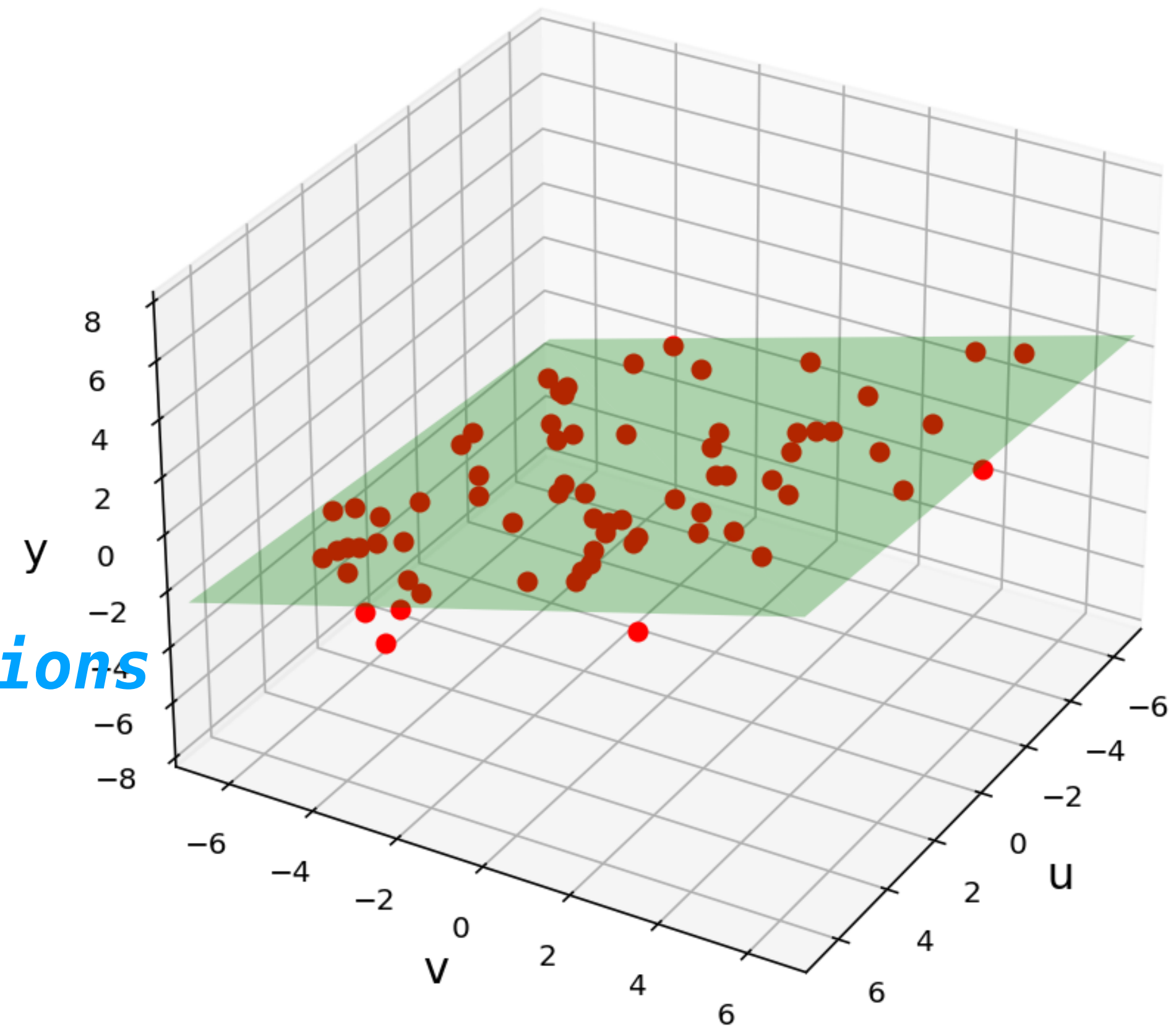
recall: planes are given by linear equations
which minimizes

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

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\vdots

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

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

Example: Terrain Data

This is still linear in the β 's

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$$\begin{bmatrix} 1 & \overset{\textcolor{blue}{X}}{x_1} & y_1 \\ 1 & x_2 & y_2 \\ \vdots & \vdots & \vdots \\ 1 & x_k & y_k \end{bmatrix} \begin{bmatrix} \overset{\textcolor{blue}{\vec{\beta}}}{\beta_0} \\ \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} \overset{\textcolor{blue}{Z}}{z_1} \\ z_2 \\ \vdots \\ z_k \end{bmatrix}$$

Step 2: Rewrite the system as a matrix equation.

Example: Terrain Data

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

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?*

Answer

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

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

First off, this is very unlikely.

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

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

"Vectors" of Generalization




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

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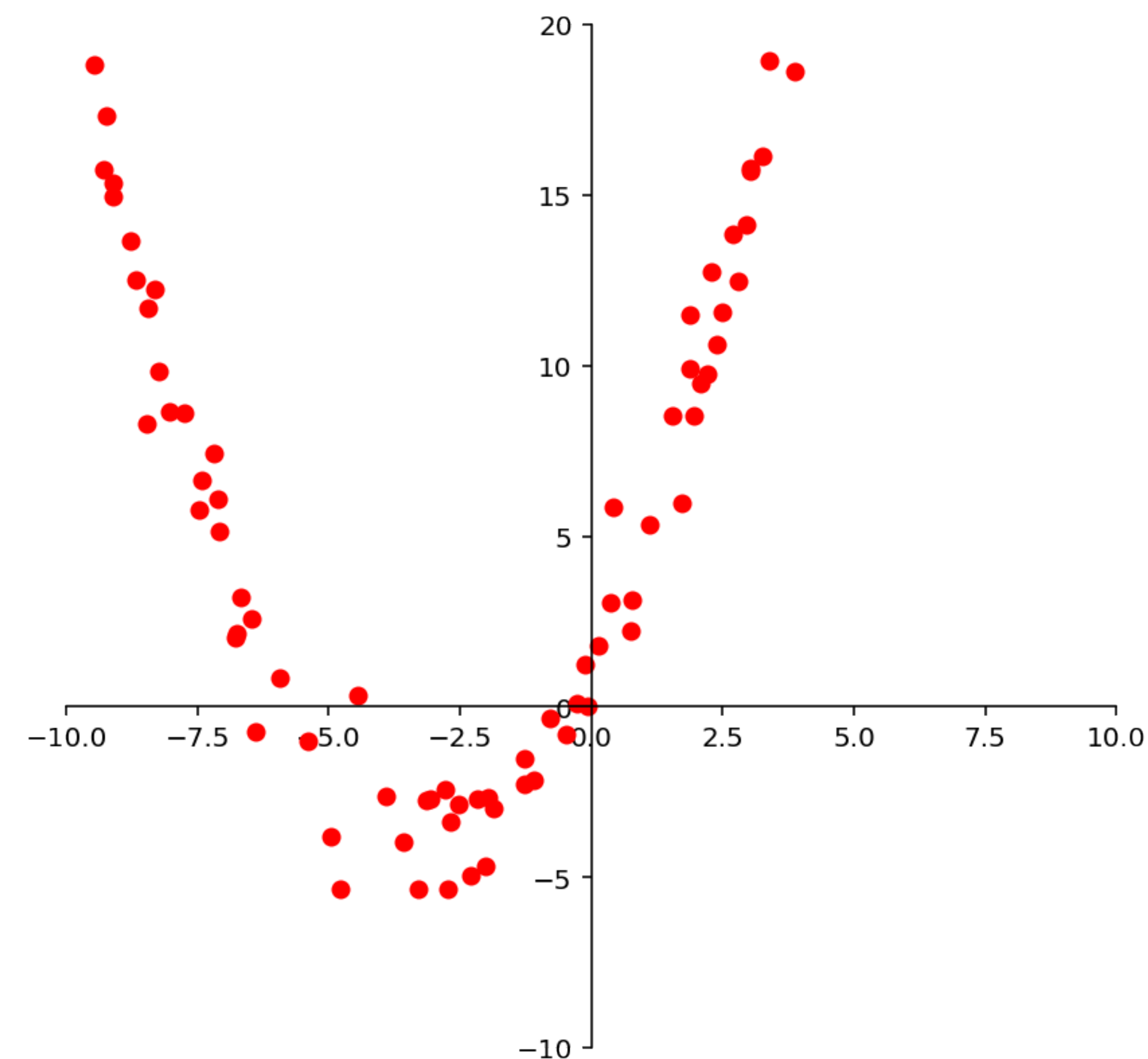
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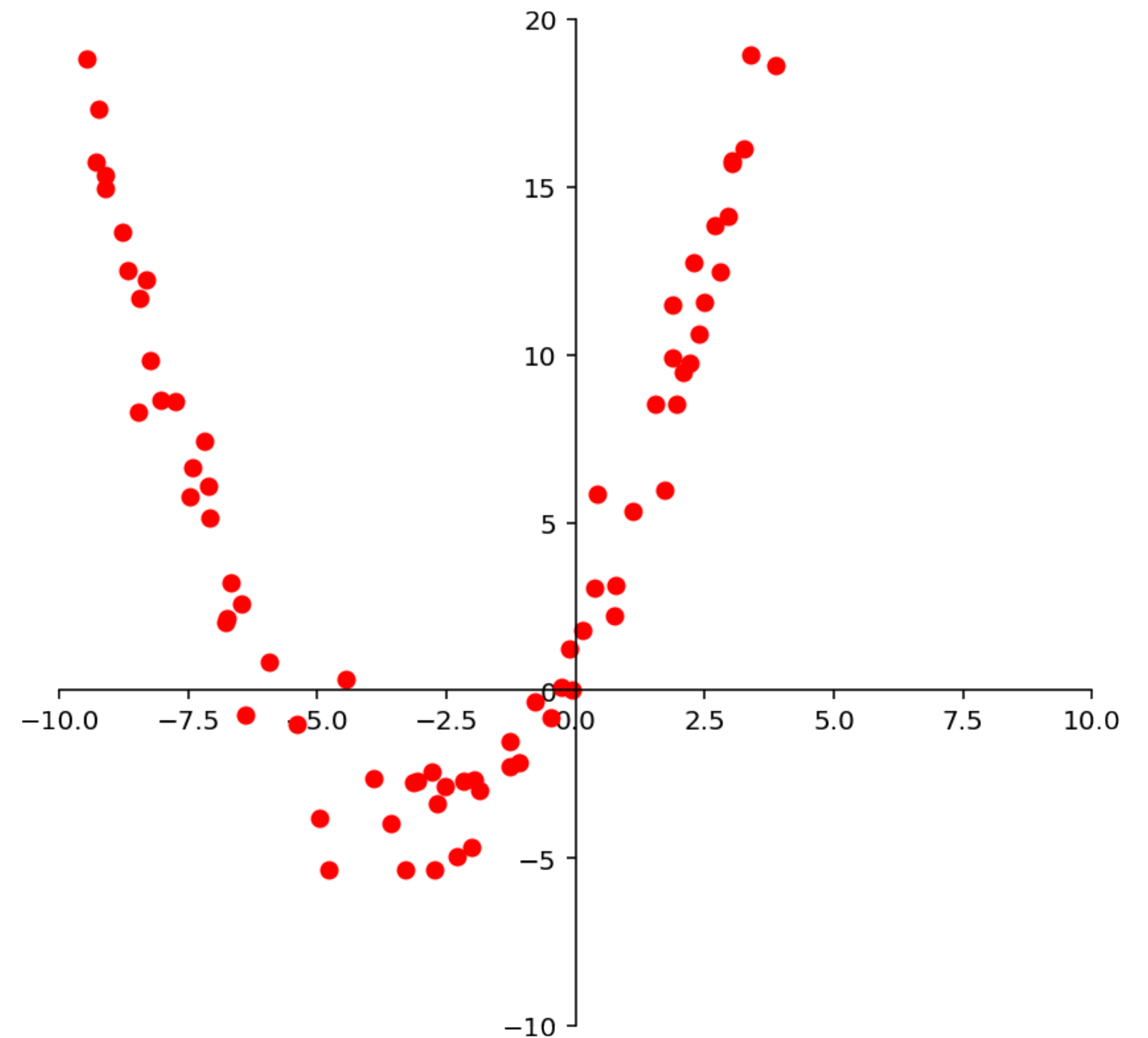
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Example: Best Fit Quadratic



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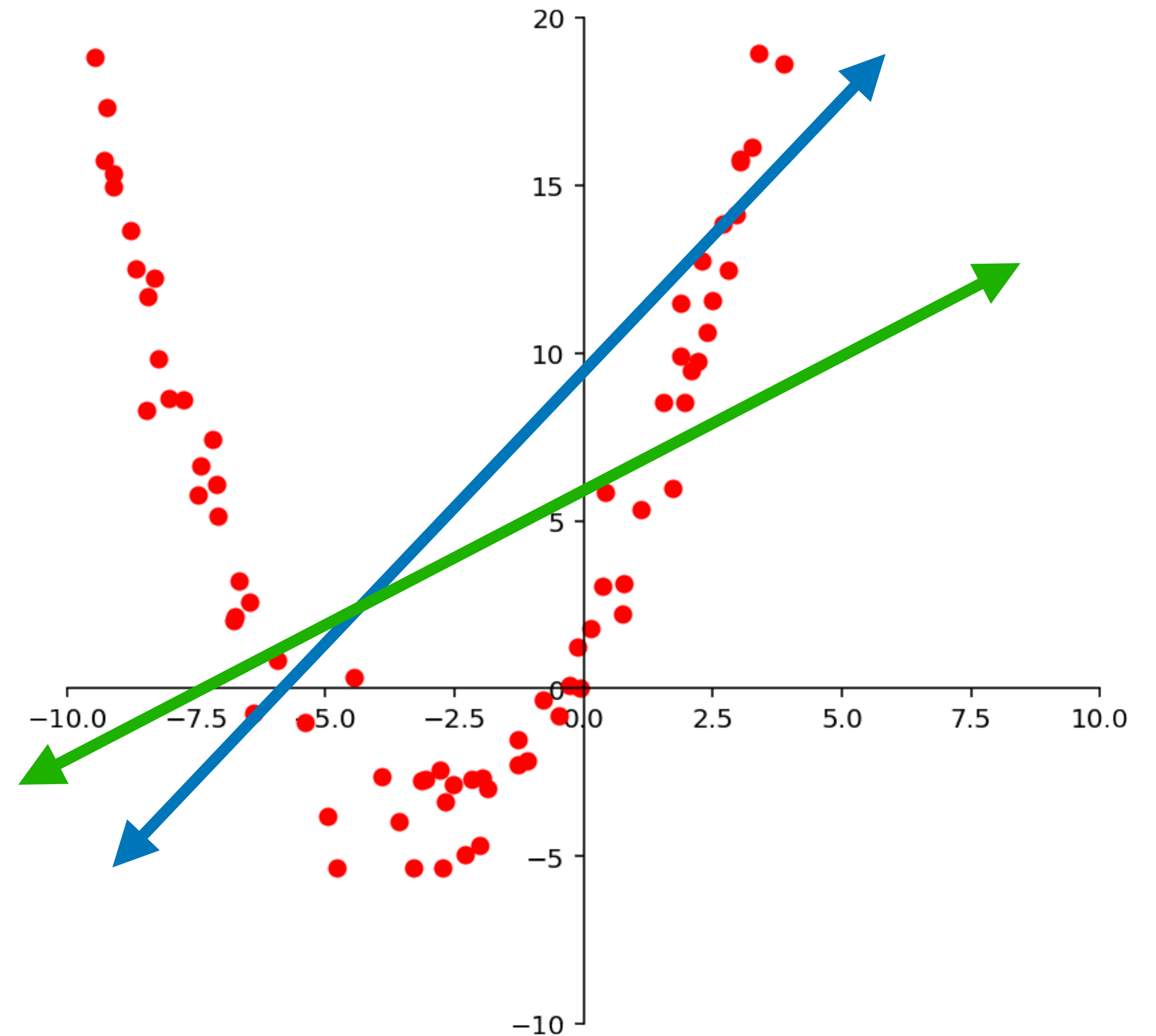
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Example: Best Fit Quadratic

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

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

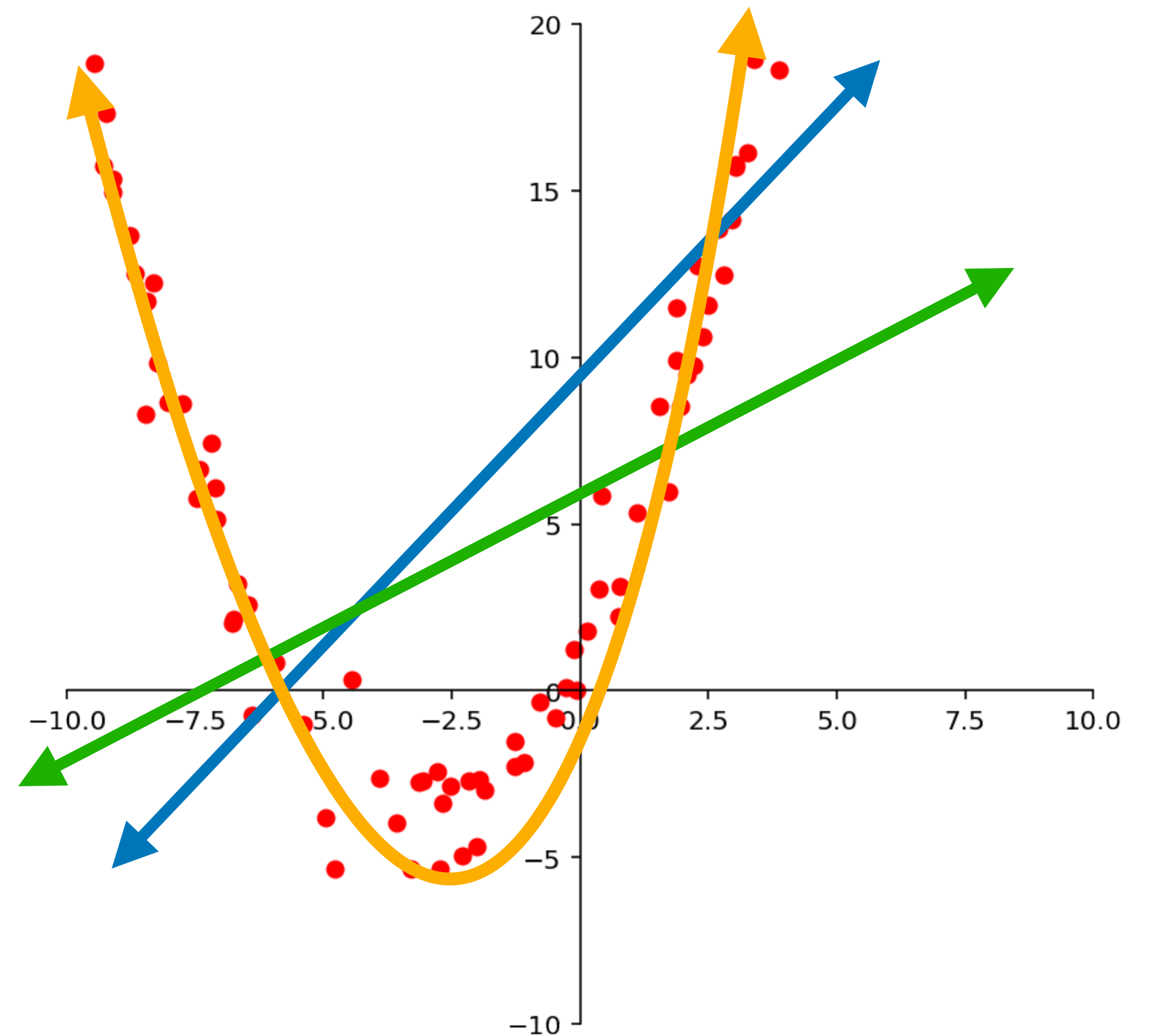


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What about a parabola?



Example: Best Fit Quadratic

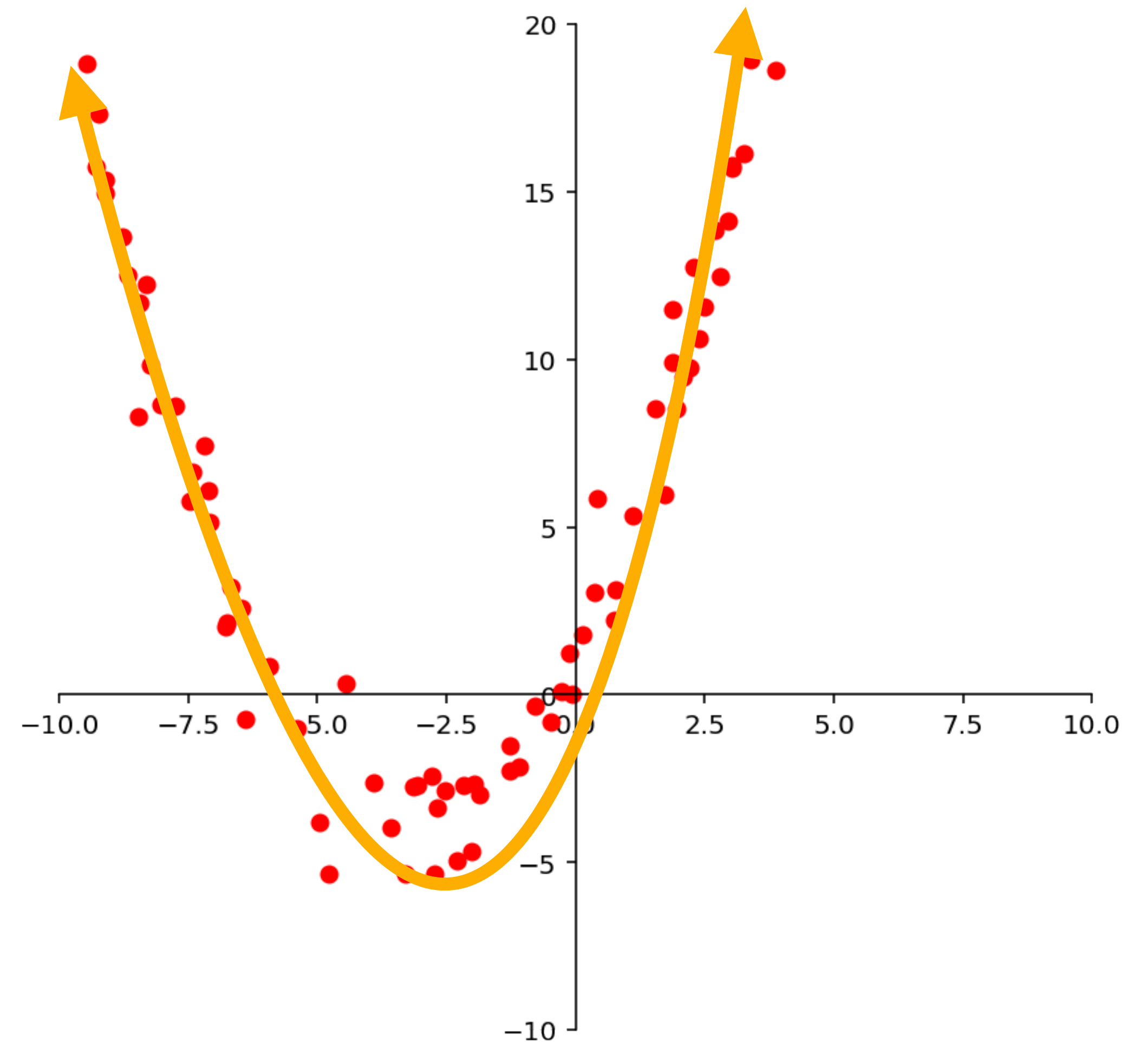
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The Takeaway

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

Linear in Parameters

Definition. A function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is **linear in the parameters** β_1, \dots, β_k if it can be written as

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

$$\vec{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

for functions $\phi_1, \dots, \phi_k: \mathbb{R}^n \rightarrow \mathbb{R}$

Example: $f(\vec{x}) = \beta_1 e^{x_1} \cos(x_2) + \beta_2 \sinh(x_1 + x_2)$

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

General Linear Regression

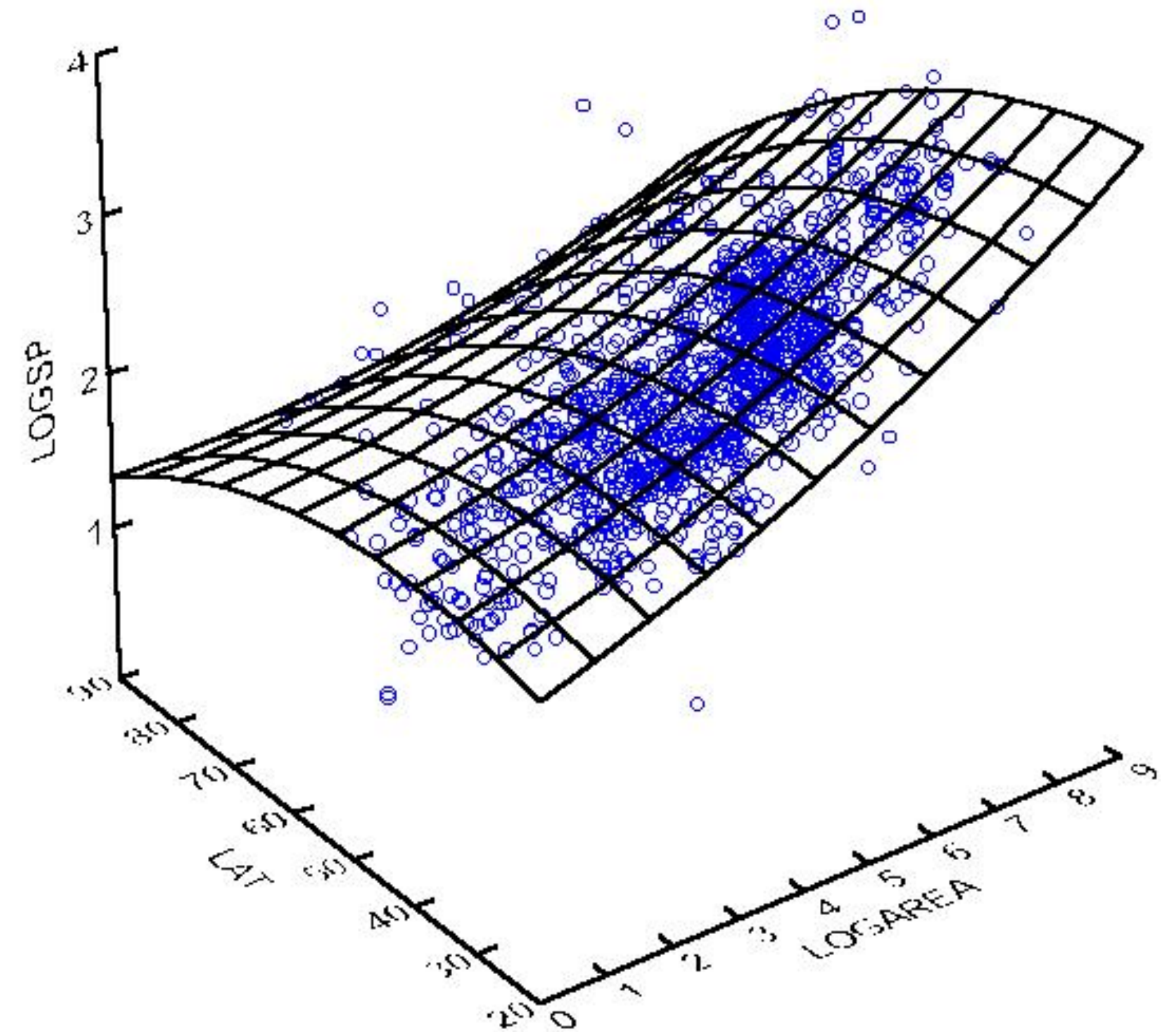
dataset: $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_m, y_m)\}$ where $\mathbf{x}_i \in \mathbb{R}^n$ and $y_i \in \mathbb{R}$

Problem. Given a function

$$f_{\beta_1, \dots, \beta_k} : \mathbb{R}^n \rightarrow \mathbb{R}$$

which is *linear in the parameters* β_1, \dots, β_k , find values for β_1, \dots, β_k which minimize

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



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

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$$\beta_1 \phi_1(\mathbf{x}_1) + \dots + \beta_k \phi_k(\mathbf{x}_1) = y_1$$

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

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$$\beta_1 \phi_1(\mathbf{x}_1) + \dots + \beta_k \phi_k(\mathbf{x}_1) = y_1$$

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

\vdots

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

Step 1: Set up an (almost assuredly inconsistent) system of linear equations in terms of the variables β_1, \dots, β_k

General Linear Regression

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

Problem. Given a function

$$f_{\beta_1, \dots, \beta_k} : \mathbb{R}^n \rightarrow \mathbb{R}$$

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design matrix

$$\overset{X}{\begin{bmatrix} \phi_1(\mathbf{x}_1) & \phi_2(\mathbf{x}_1) & \dots & \phi_k(\mathbf{x}_1) \\ \phi_1(\mathbf{x}_2) & \phi_2(\mathbf{x}_2) & \dots & \phi_k(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{x}_m) & \phi_2(\mathbf{x}_m) & \dots & \phi_k(\mathbf{x}_m) \end{bmatrix}} \begin{bmatrix} \vec{\beta} \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{bmatrix} = \begin{bmatrix} \mathbf{y} \\ y_1 \\ y_2 \\ \vdots \\ y_k \end{bmatrix}$$

Step 2: Rewrite the system as a matrix equation.

General Linear Regression

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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

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

How To: Design Matrices

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

Solution. First write $f(\mathbf{x})$ as $\beta_1\phi_1(\mathbf{x}) + \dots + \beta_k\phi_k(\mathbf{x})$ where ϕ_1, \dots, ϕ_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

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

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

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

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

$$\beta_1 (\cos(x_1) - x_3) + \beta_2 (e^{-x_1 x_2}) + \beta_3 (1)$$

ϕ_1

ϕ_2

ϕ_3

$$\vec{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

for the dataset

$$\mathbf{x}_1 = (0, 0, 0) \quad y_1 = 5$$

$$\mathbf{x}_2 = (\pi, 3, 1) \quad y_2 = 3$$

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

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Concerns for another class.