Linear Models

Geometric Algorithms
Lecture 24

CAS CS 132

Introduction

Recap Problem

$a_1 \quad a_2 \quad a_3$

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

Find the (orthogonal) projection of $\mathbf{b}$ onto Col(A).

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

$\text{Col}([a_1 \;\; a_3]) = \text{Col}(A)$

Answer

$A \in \mathbb{R}^{m \times n}$

$$\hat{b} = A(A^T A)^{-1} A^T \vec{b}$$

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

given L.S. solution $\hat{x}$

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

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

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

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

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

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

$$(C^T C)^{-1} = \begin{bmatrix} 1/2 & 0 \\ 0 & 1/3 \end{bmatrix}$$

$$C^T b = \begin{bmatrix} -1 \\ 8 \end{bmatrix}$$

$$\hat{b} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1/2 & 0 \\ 0 & 1/3 \end{bmatrix} \begin{bmatrix} -1 \\ 8 \end{bmatrix}$$

Question

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

Answer

$$\operatorname{proj}_{\operatorname{span}\{\vec{u}\}} \vec{r} = \frac{\langle r, u \rangle}{\langle u, u \rangle} \vec{u} \qquad \vec{u} = \begin{bmatrix} 1 \\ -1 \\ 2 \end{bmatrix} \qquad \frac{1}{6}\begin{bmatrix} 1 & -1 & 2 \\ -1 & 1 & -2 \\ 2 & -2 & 4 \end{bmatrix}$$

$$[1\ 0\ 0]\begin{bmatrix} 1 \\ -1 \\ 2 \end{bmatrix} = 1$$

$$\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \mapsto \frac{\langle e_1, u \rangle}{\langle u, u \rangle} \vec{u} = \frac{1}{6}\begin{bmatrix} 1 \\ -1 \\ 2 \end{bmatrix}$$

$$[1\ -1\ 2]\begin{bmatrix} 1 \\ -1 \\ 2 \end{bmatrix} = 1 + 1 + 4 = 6$$

$$\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \mapsto \frac{\langle e_2, u \rangle}{\langle u, u \rangle} \vec{u} = \frac{-1}{6}\begin{bmatrix} 1 \\ -1 \\ 2 \end{bmatrix}$$

$$\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \mapsto \frac{2}{6}\begin{bmatrix} 1 \\ -1 \\ 2 \end{bmatrix}$$

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

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

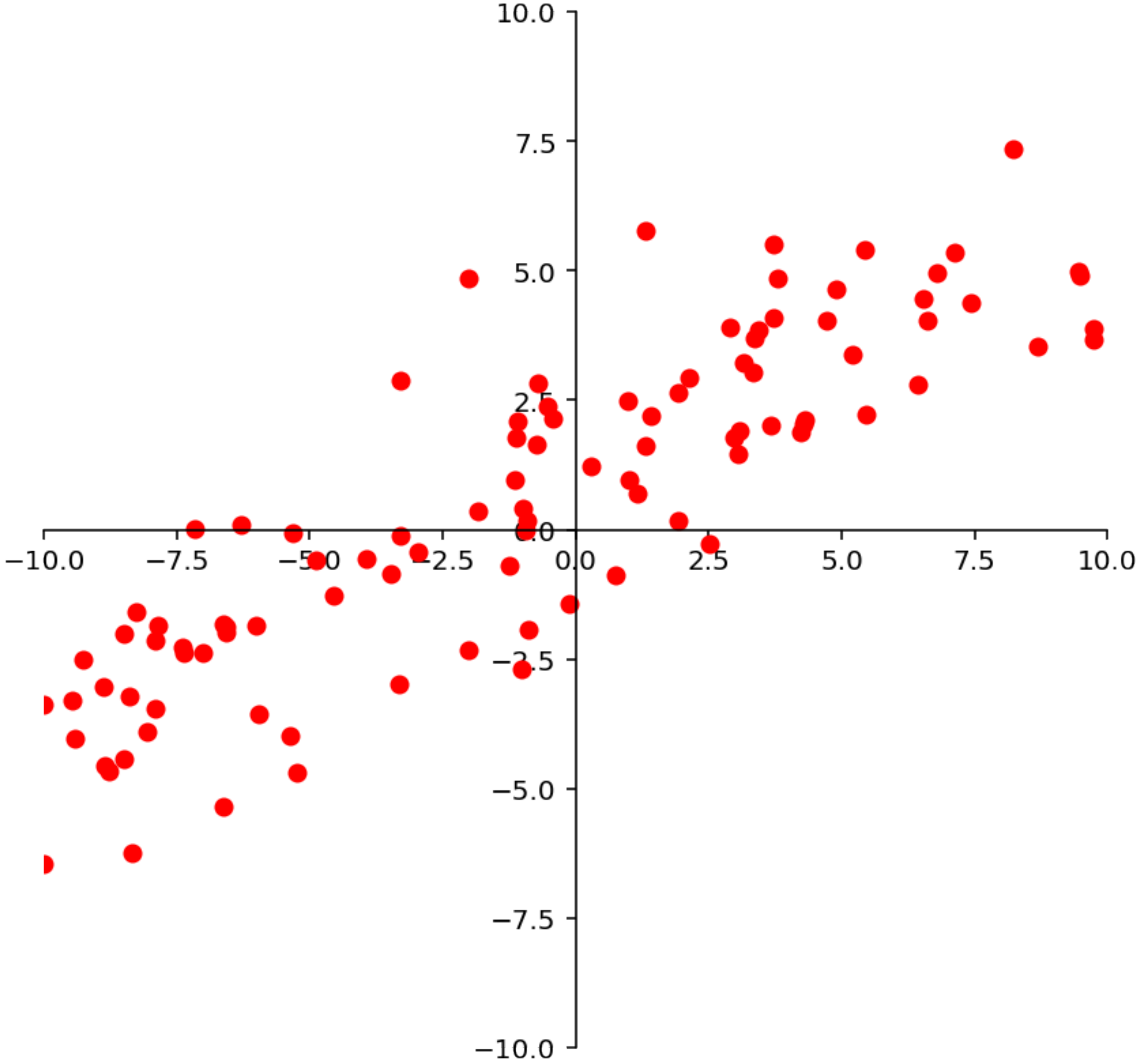
model fitting

model parameters

design matrices

A Warmup: Line of Best Fit

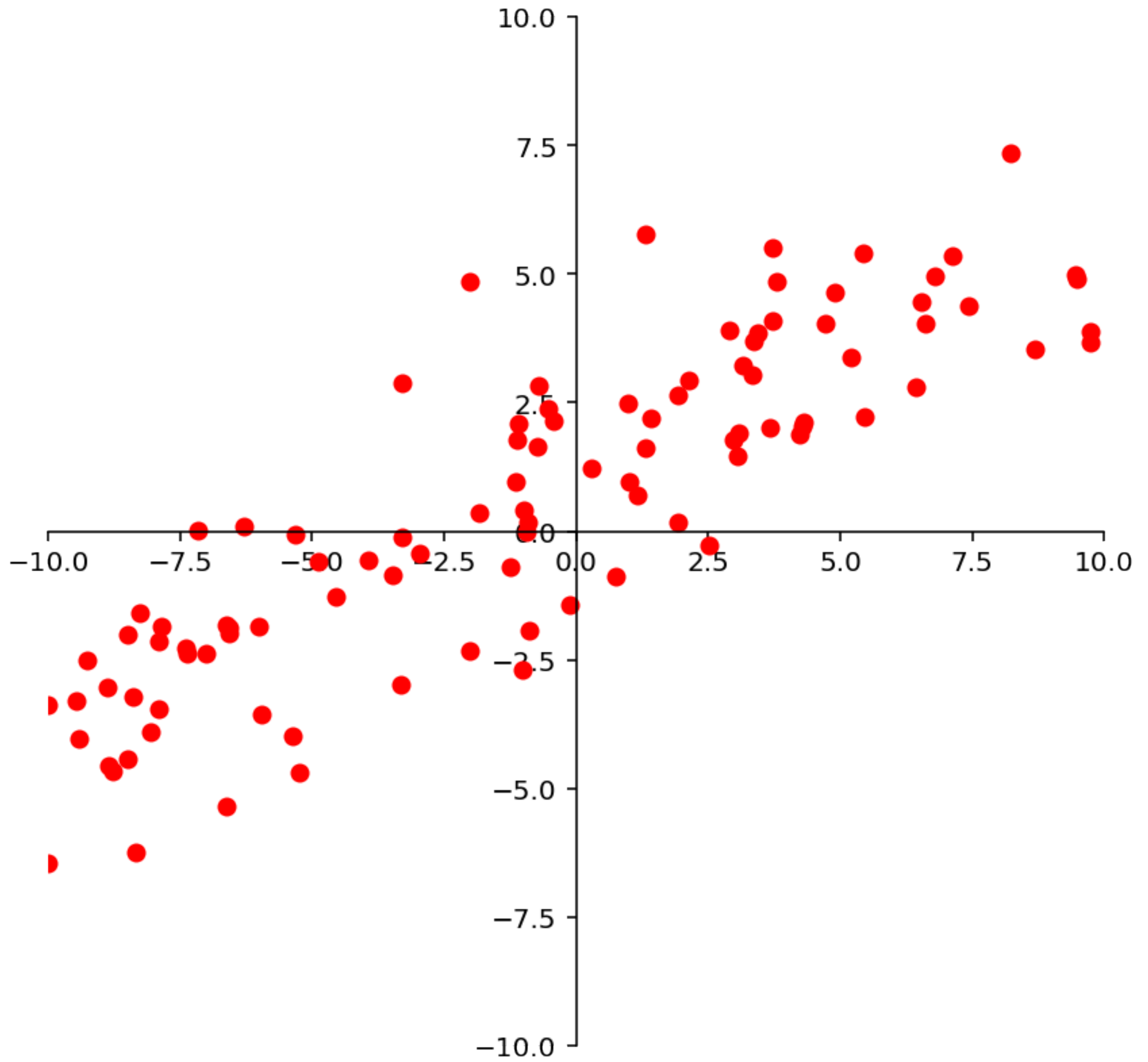
The Setup



The Setup

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

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



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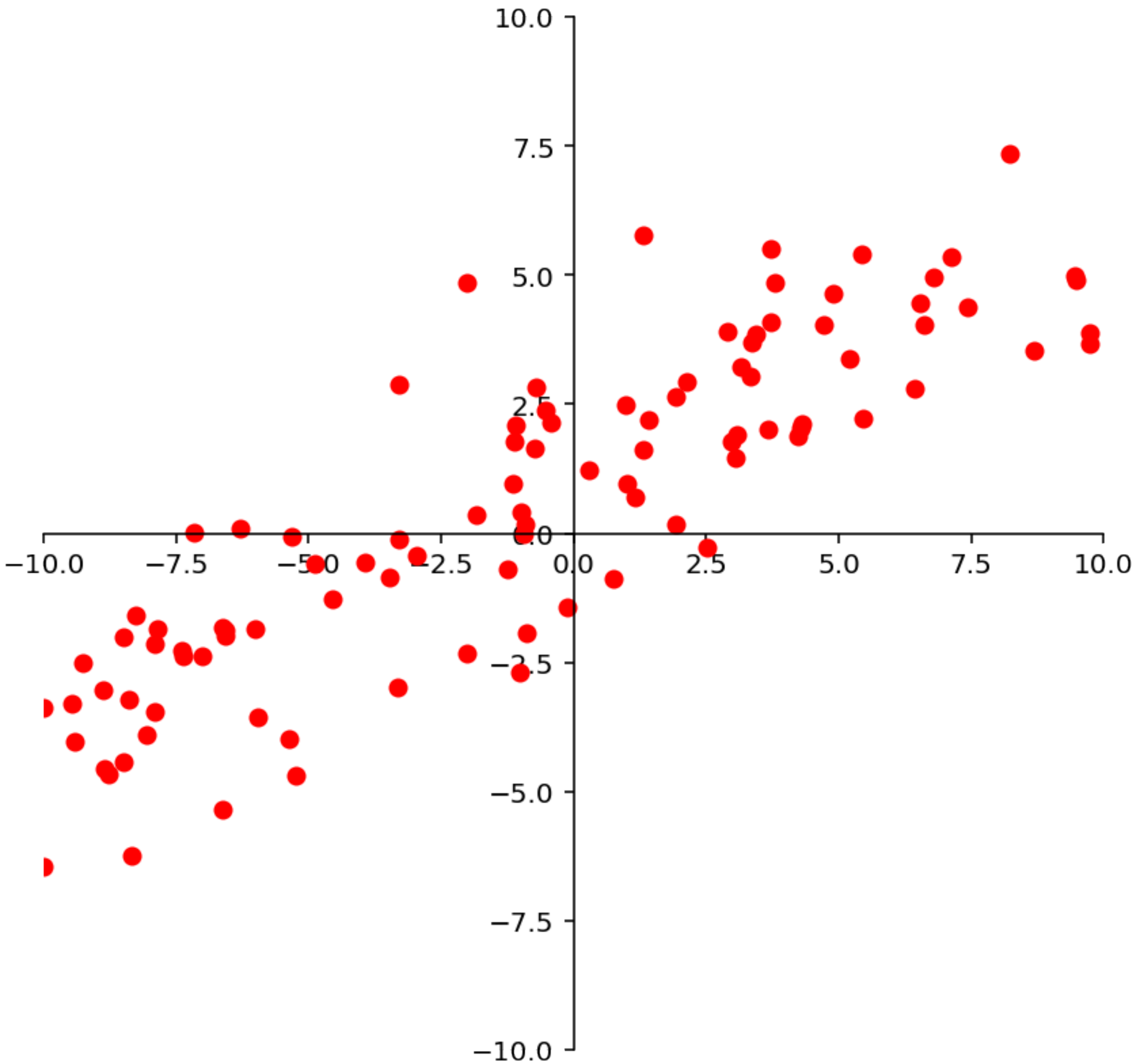
Example. You collect (height, weight) data for a population.



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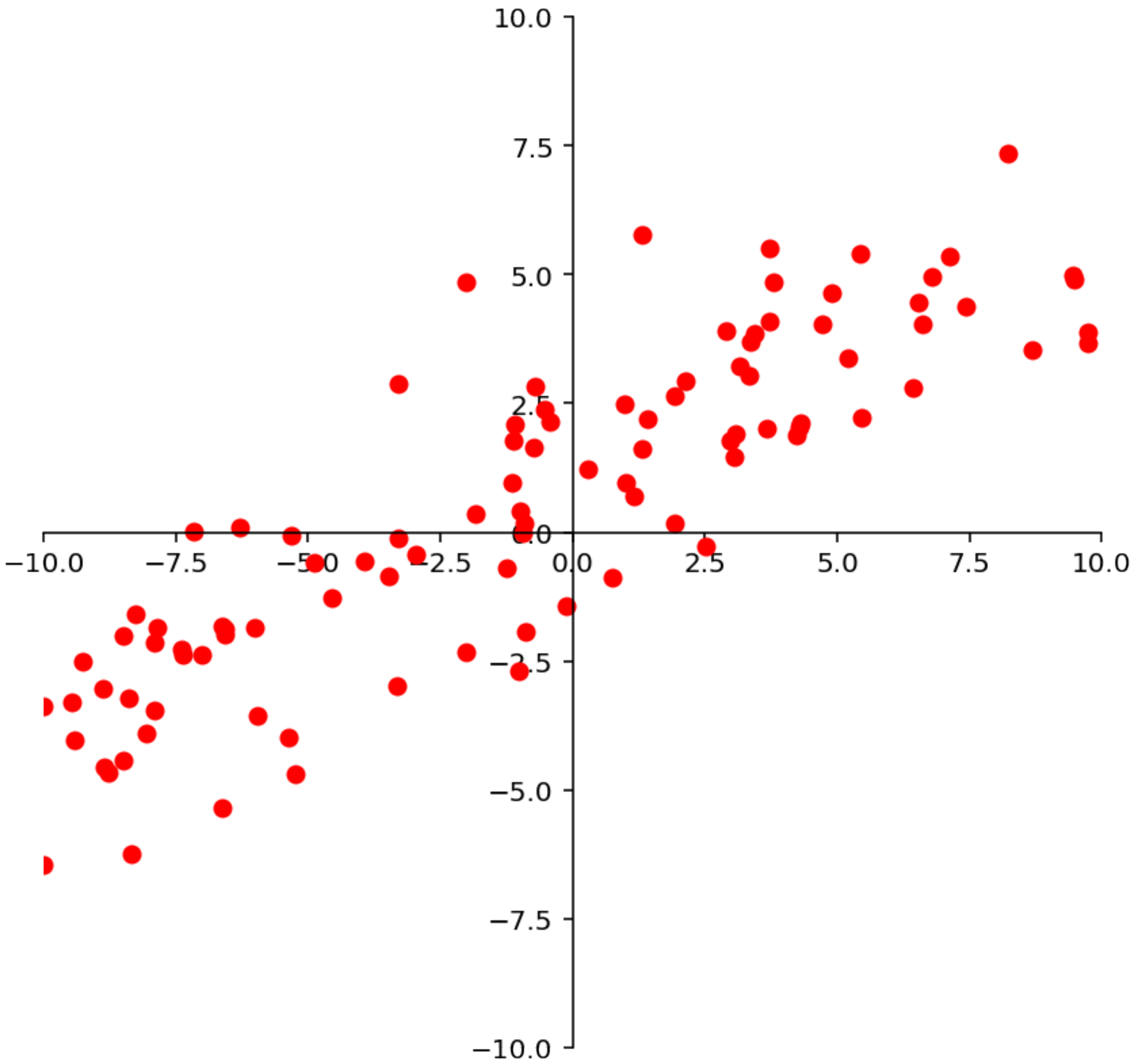
You notice they *kind of* trend as a line.



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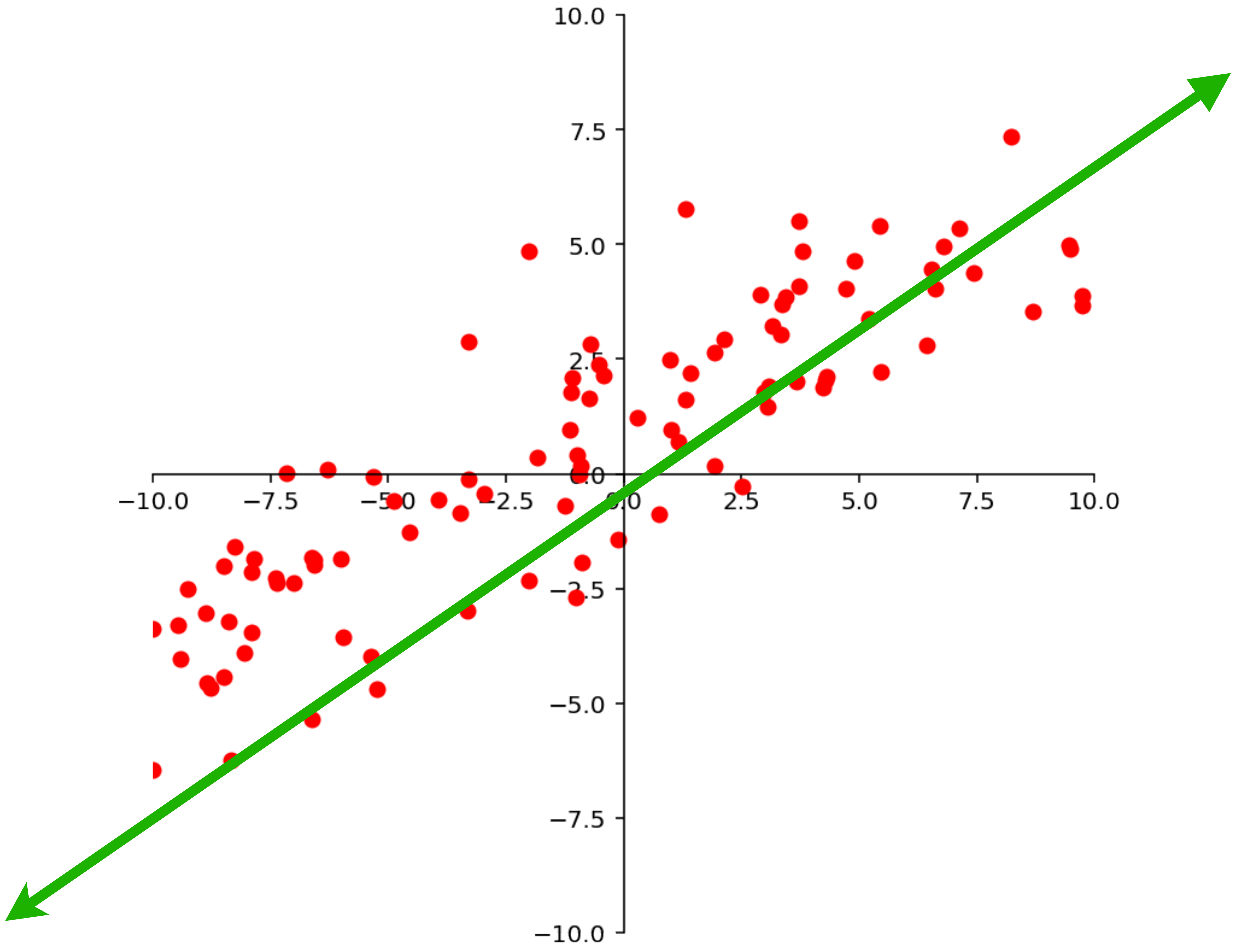

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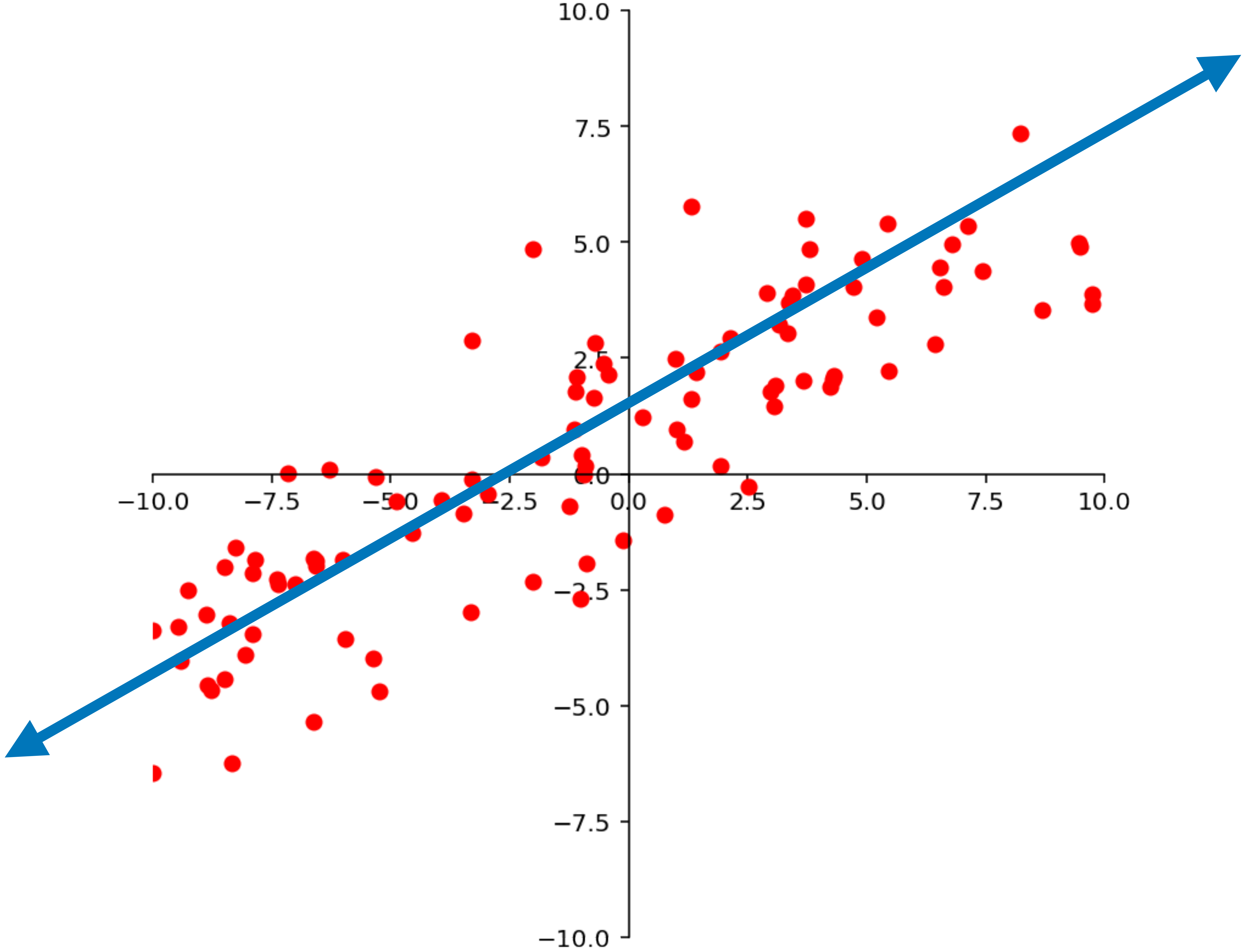
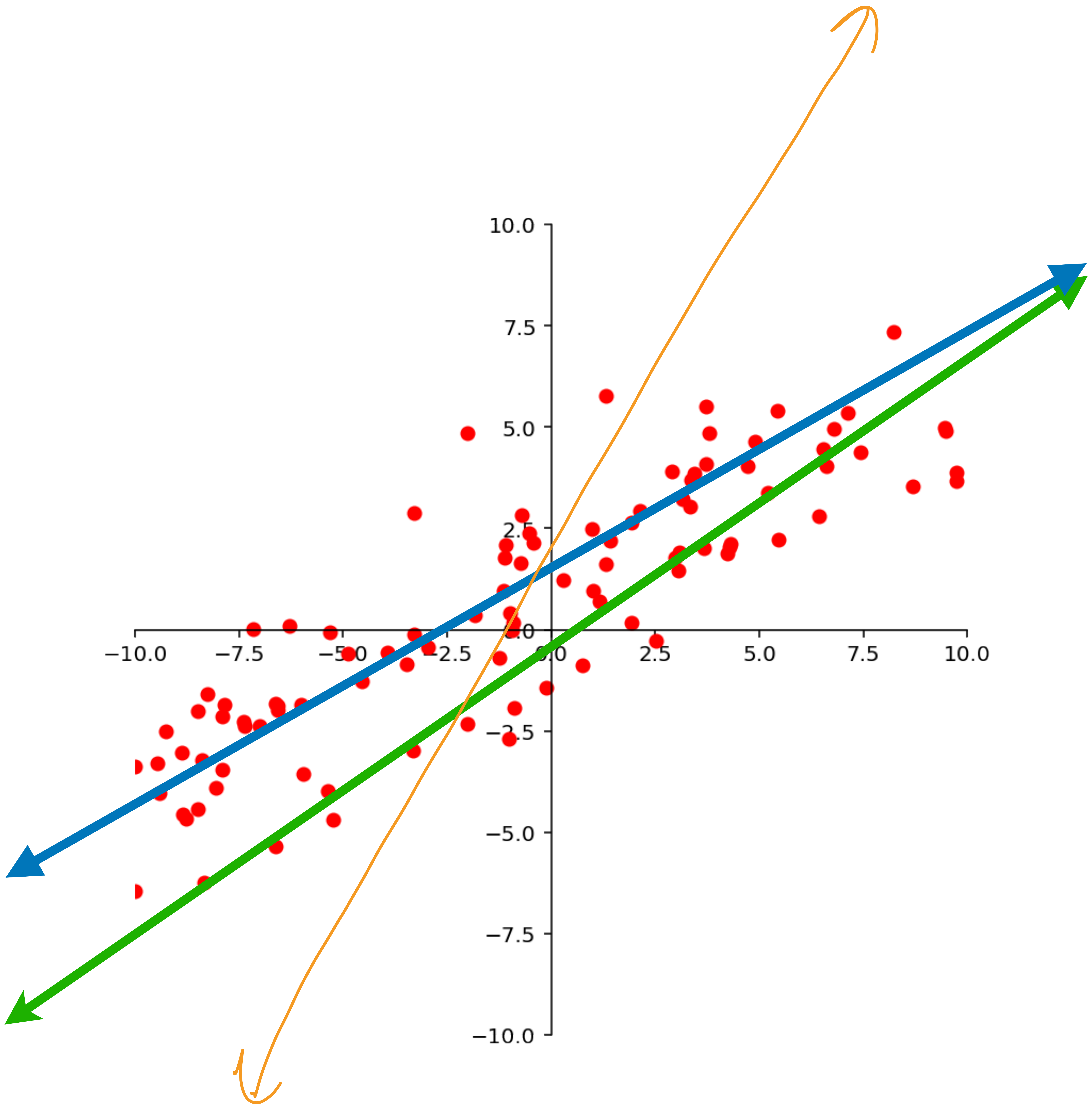


The Setup

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

Which one *best models* the dataset?



Two Important Questions

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

slope

$$f(x) = \boxed{\beta_0} + \boxed{\beta_1} x$$

y-intercept

which minimizes

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

Least Squares Simple Linear Regression

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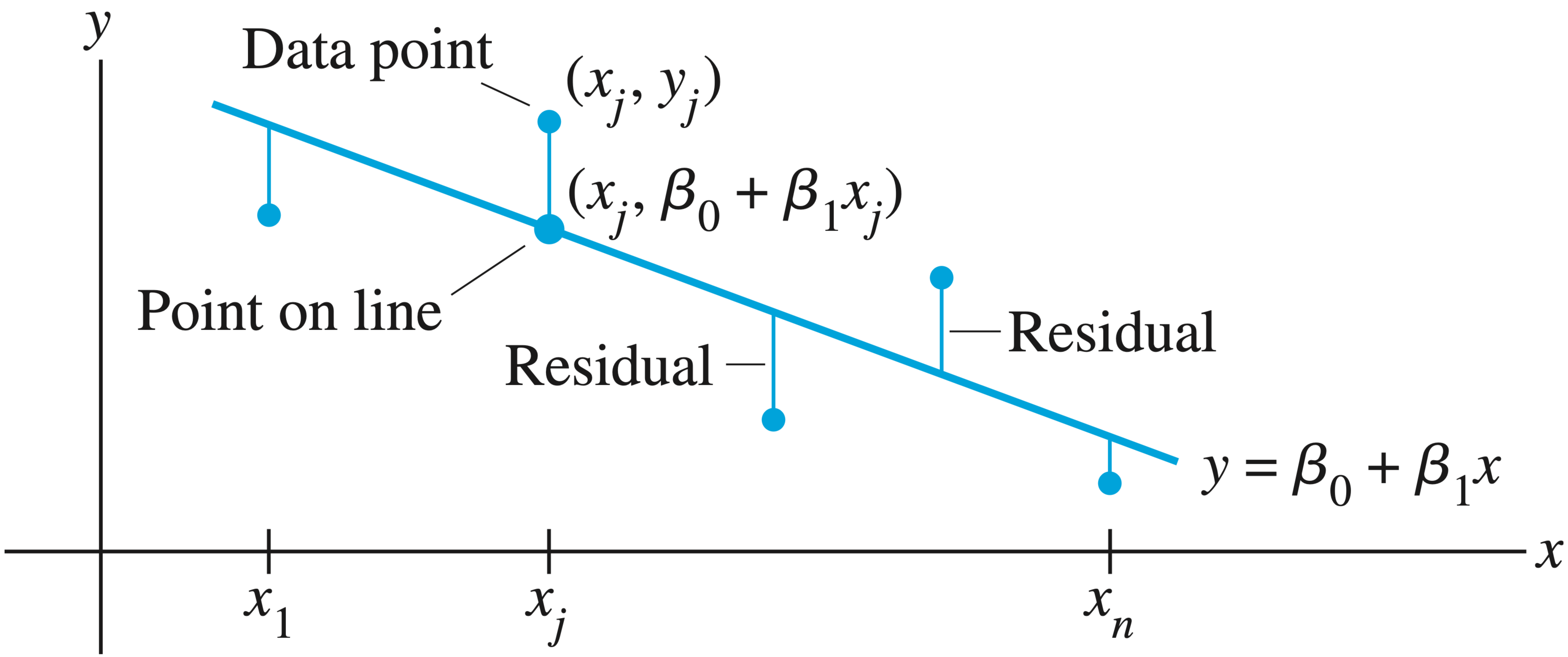
$$f(x) = \beta_0 + \beta_1 x$$

which <u>minimizes</u>

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

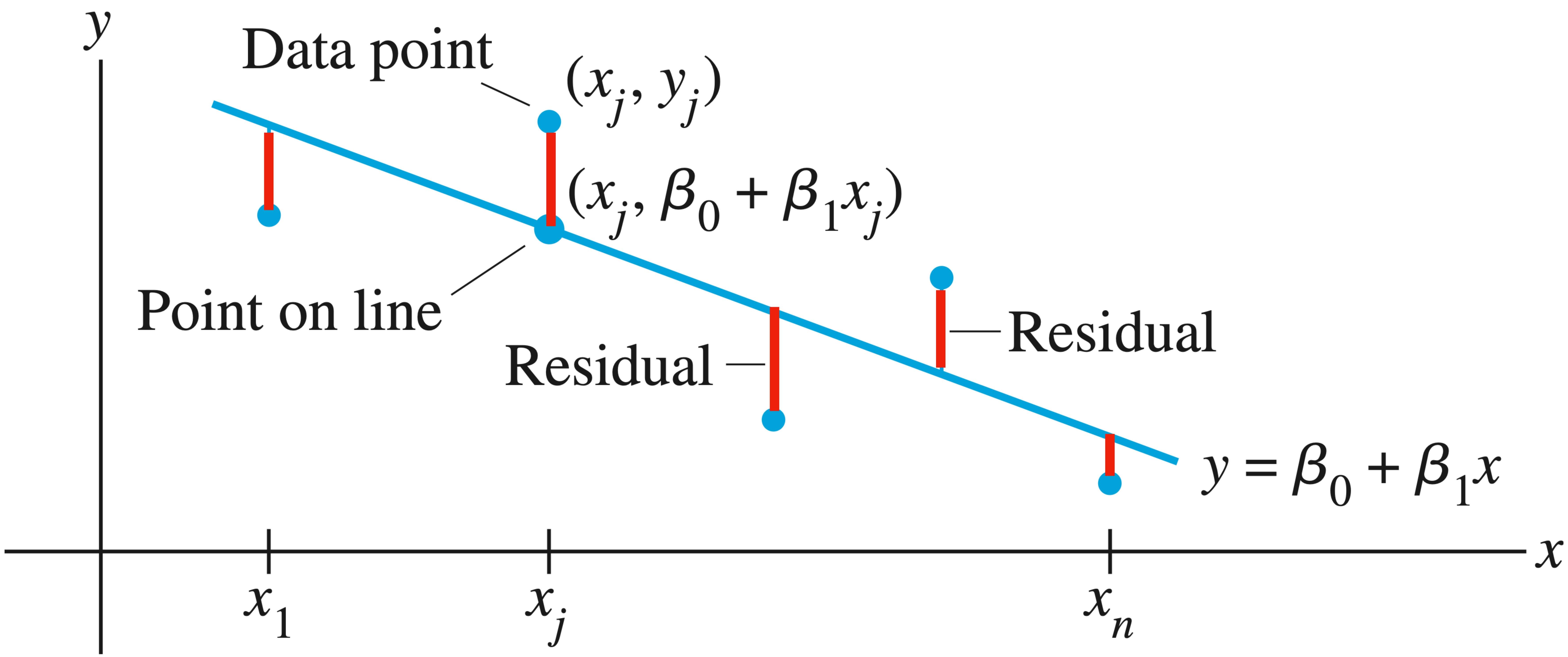
The "best" line minimizes the *sum of squares of differences.*

The Picture



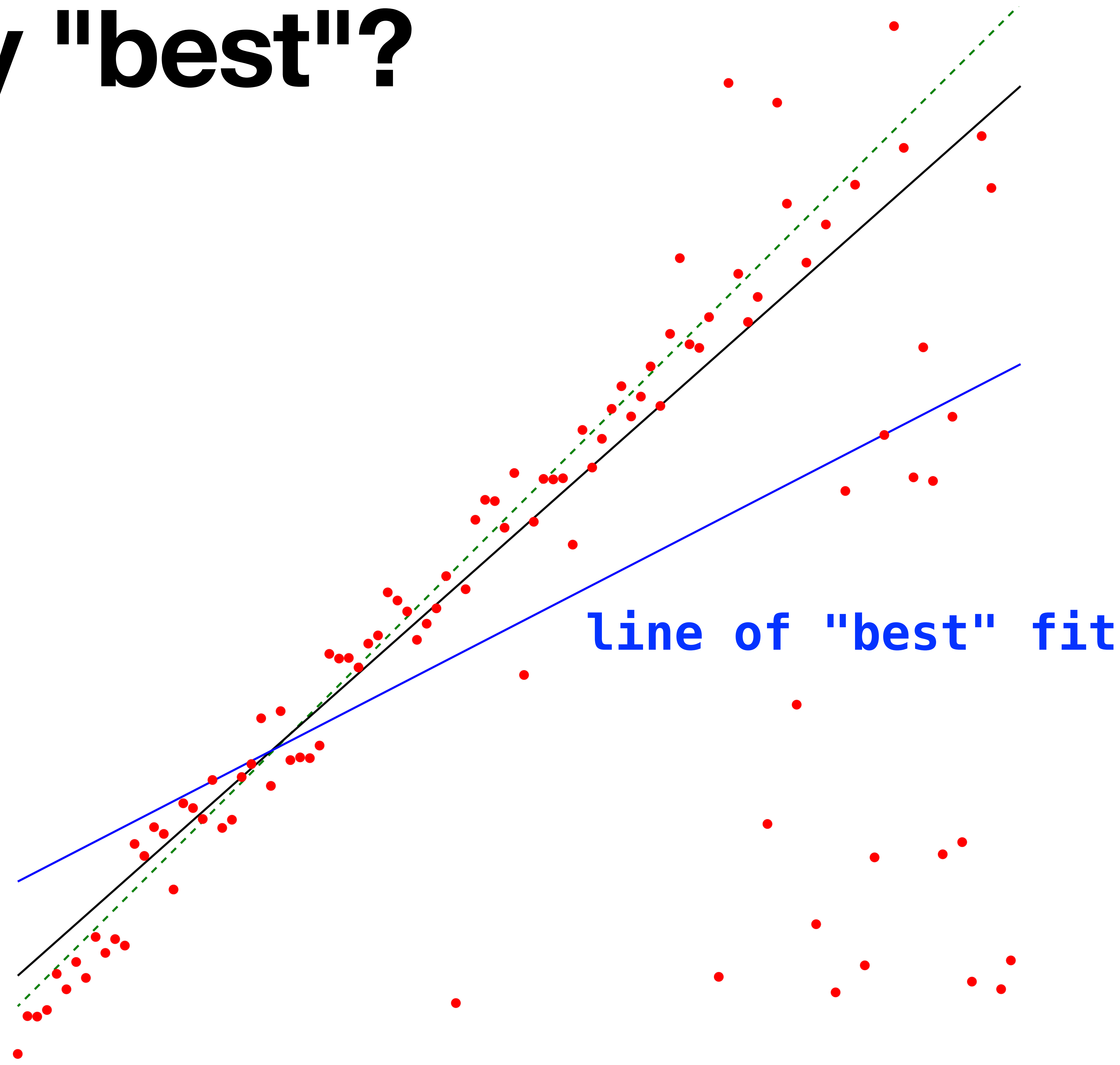
We want to find the line which makes the sum of these differences *as small as possible*.

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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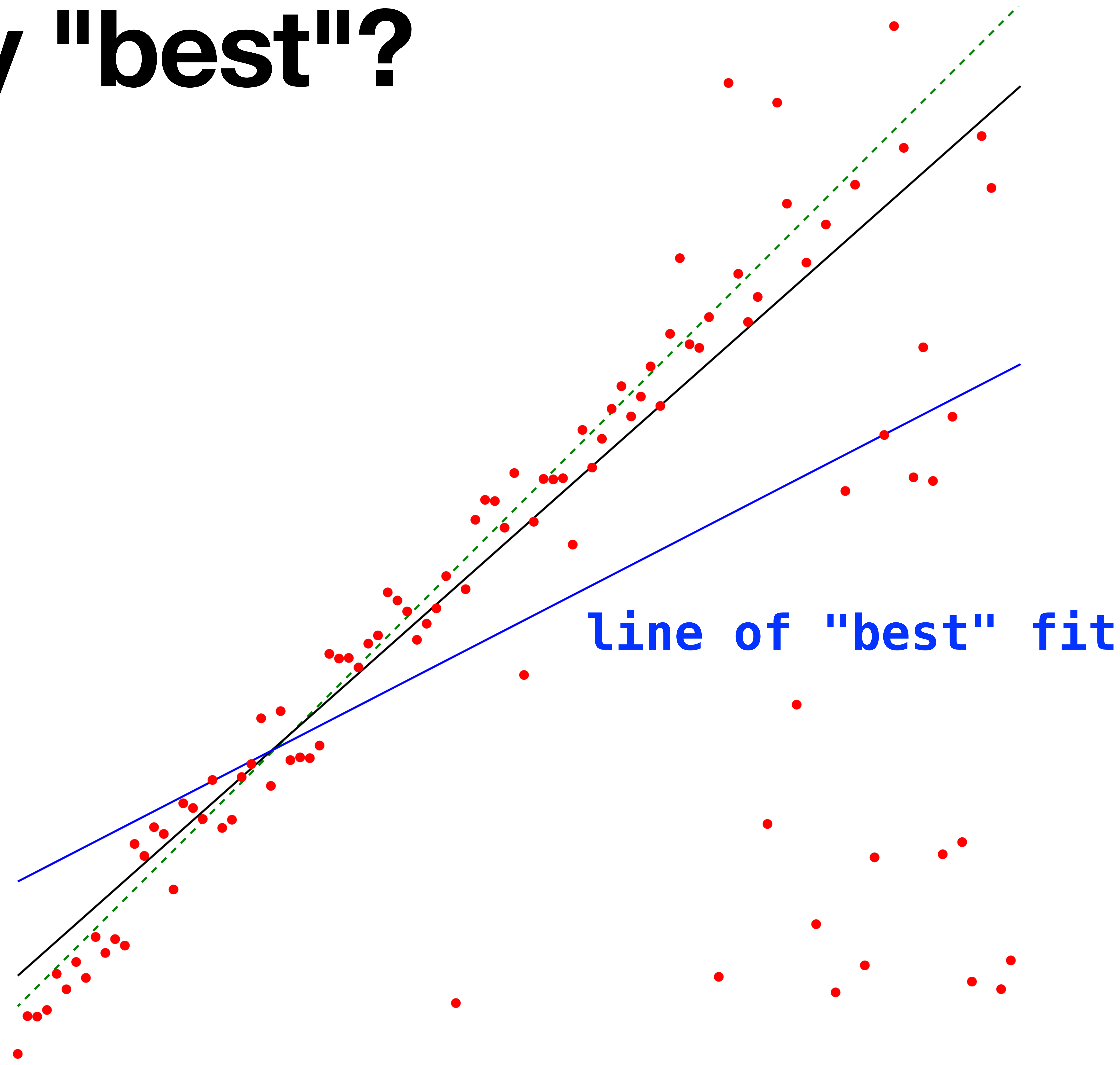
An Aside: Is this really "best"?

Who's to say...



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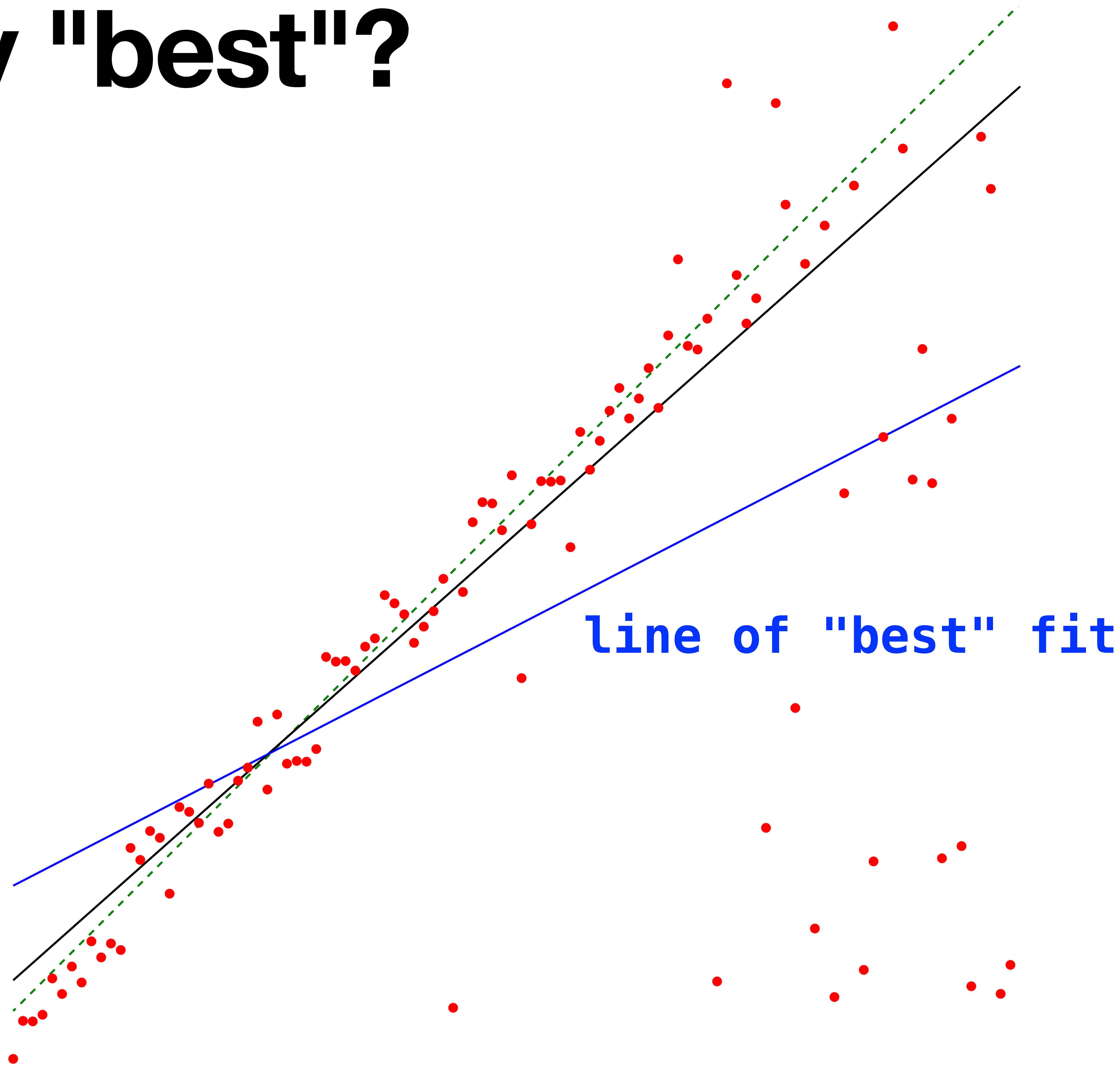

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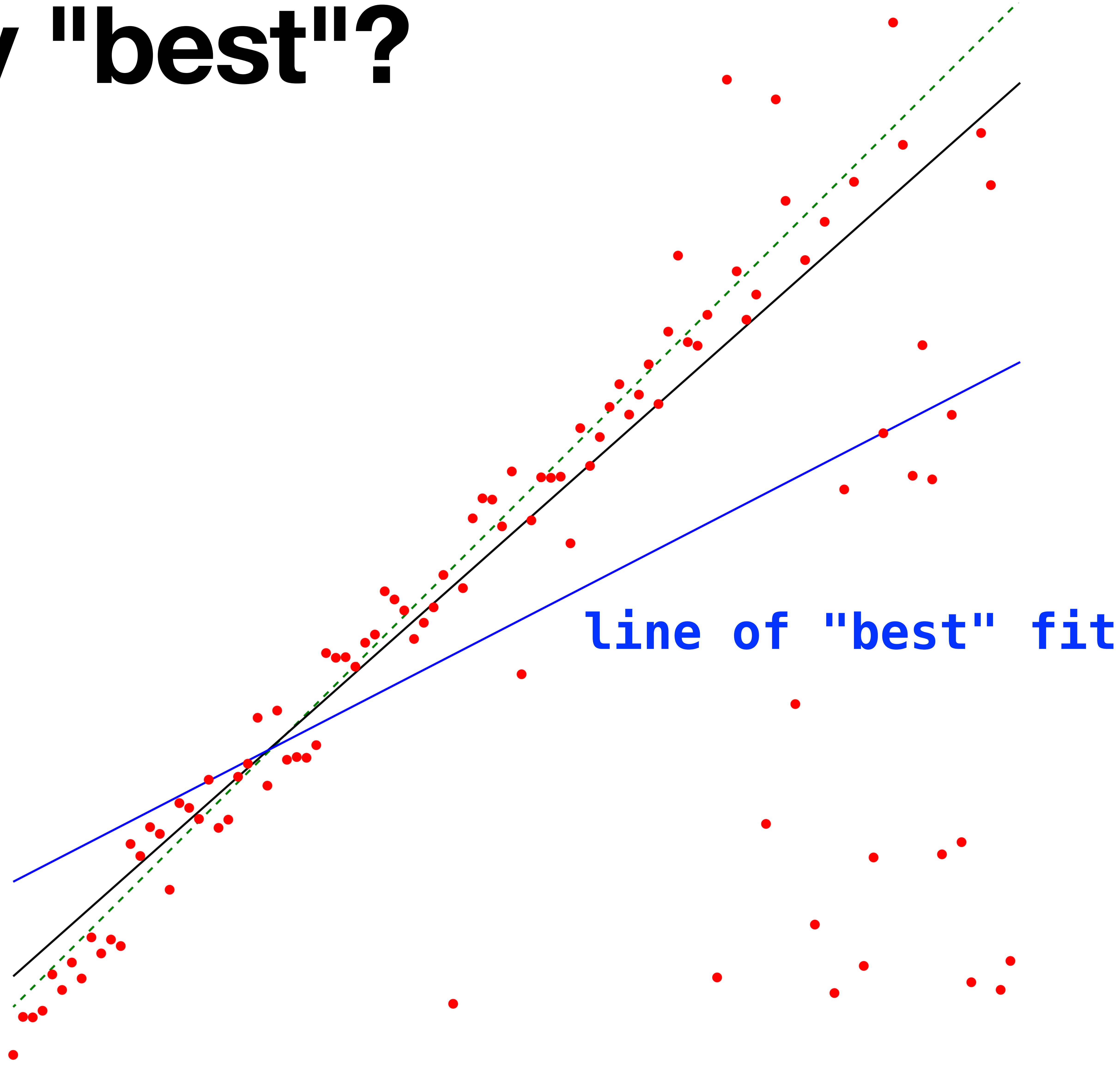
Who's to say...

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.



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Terminology: Datasets

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

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dataset

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data point

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Terminology: Datasets

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dataset

independent variable
(feature)

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Terminology: Datasets

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$$(x_i, y_i)$$

dependent variable
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Terminology: Models

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

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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

observation

residual

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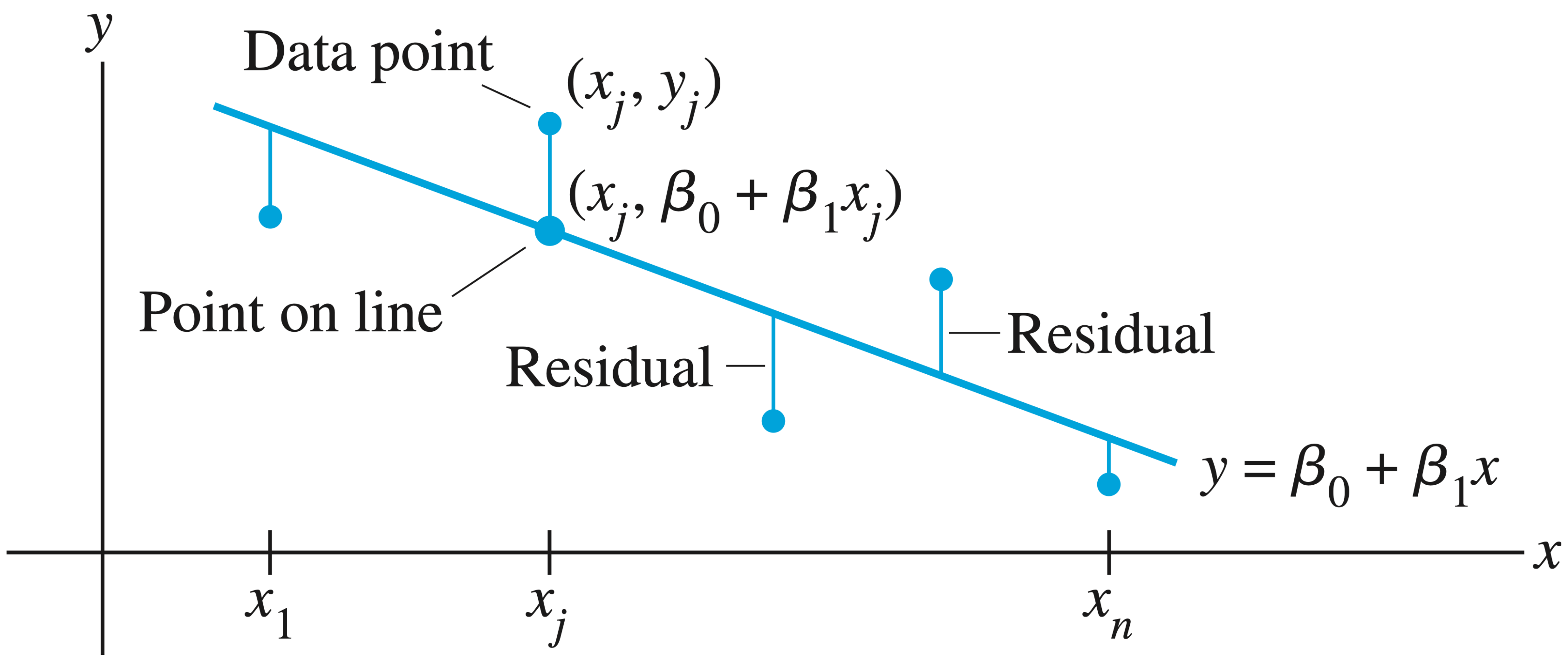
observation

residual

prediction

Terminology



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independent variable

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observation

residual

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

prediction

How to: Finding the Least Squares Line

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

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

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

How to: Finding the Least Squares Line

Don't memorize these.

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

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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

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

minimize for least-squares method

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These expressions look very similar.

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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

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

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

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

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

This is a linear system in the variables β_0 and β_1

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.**

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

A Least Squares Problem

$$\overbrace{\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}}^{X} \overbrace{\begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}}^{\vec{\beta}} = \overbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}}^{\mathbf{y}}$$

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

A Least Squares Problem

$$\overset{\color{red}{X}}{\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}} \overset{\color{red}{\vec{\beta}}}{\begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}} = \overset{\color{red}{\mathbf{y}}}{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}}$$

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

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

A Least Squares Problem

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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.

Just for Fun

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

Let's derive it:

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

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

$$A^T \vec{y}$$

$$(X^T X)^{-1} = \frac{1}{n(x \cdot x) - (1 \cdot x)^2} \begin{bmatrix} x \cdot x & -1 \cdot x \\ -x \cdot 1 & 1 \cdot 1 \end{bmatrix}$$

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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How To: Least Squares Line

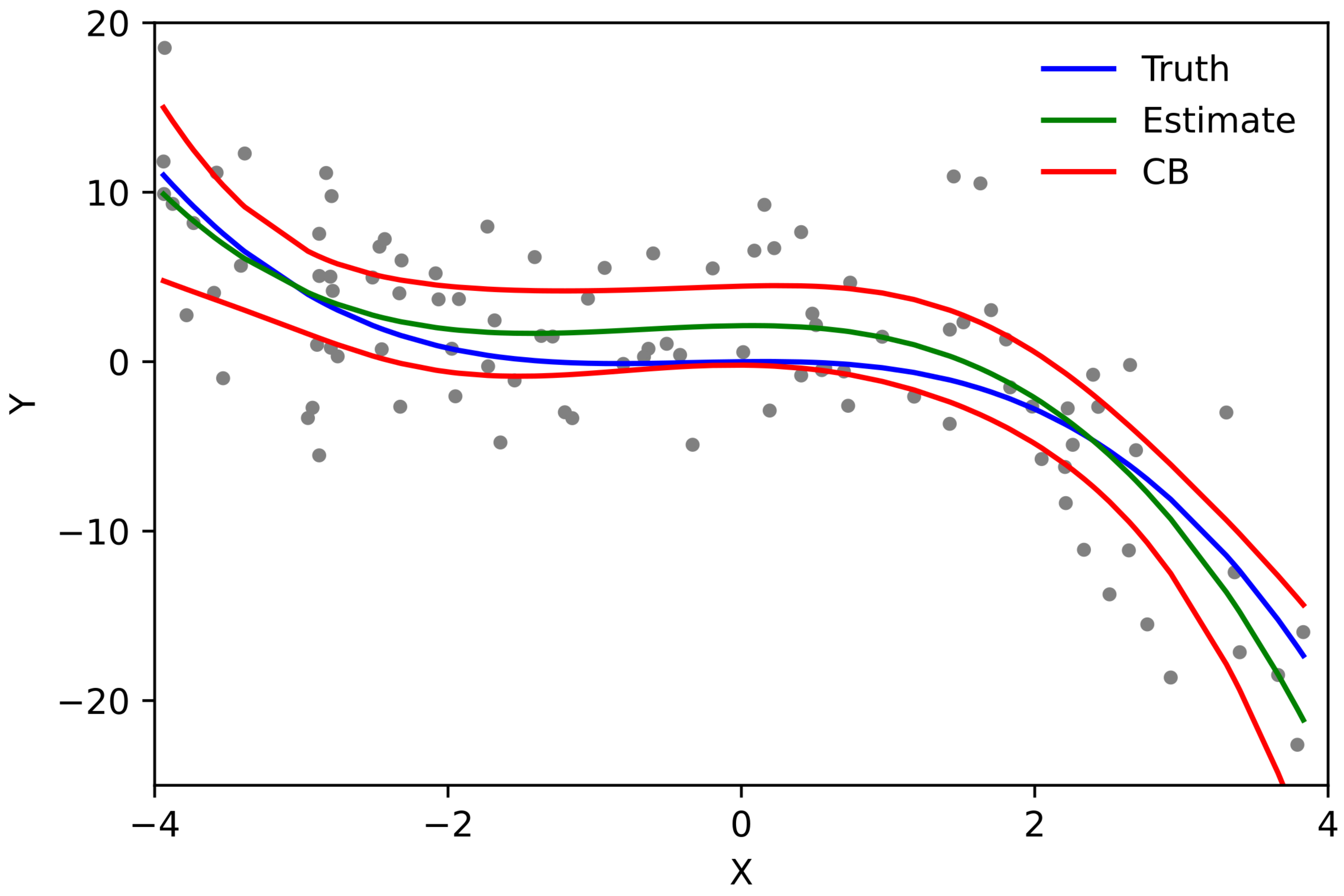
$$\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

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

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

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

General Regression



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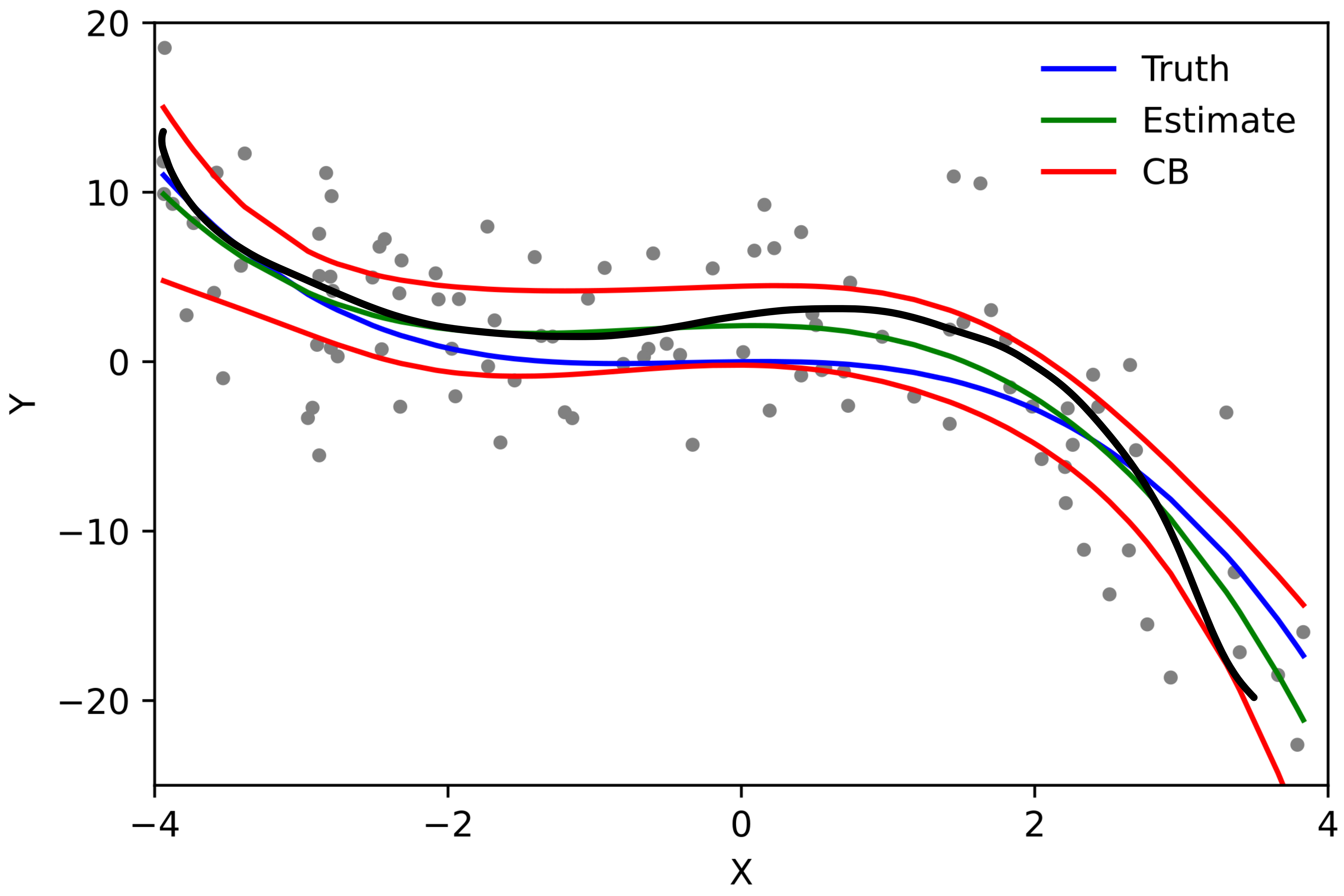
General Regression

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



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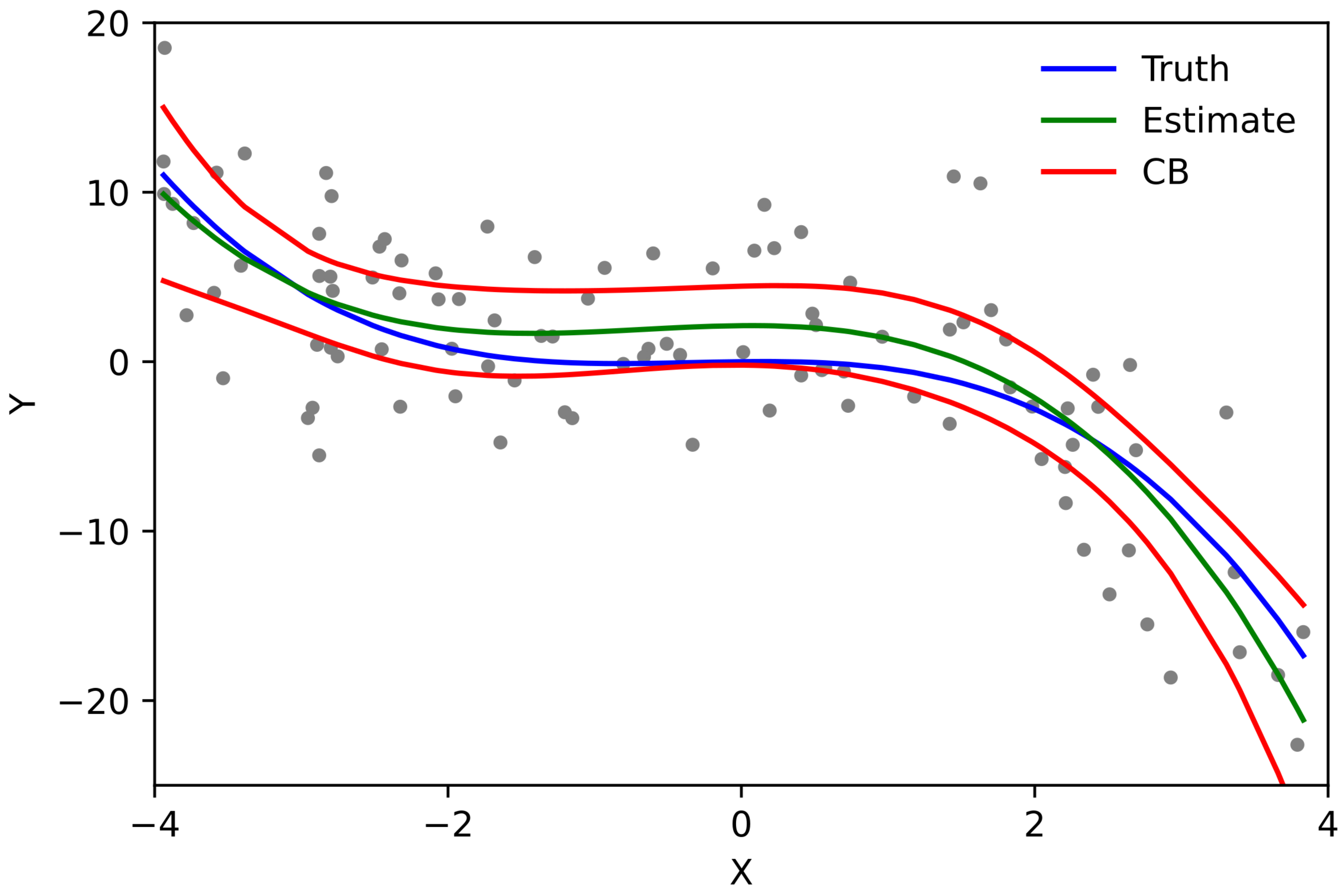
What we are estimating is a <u>mathematical function</u>



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General Regression

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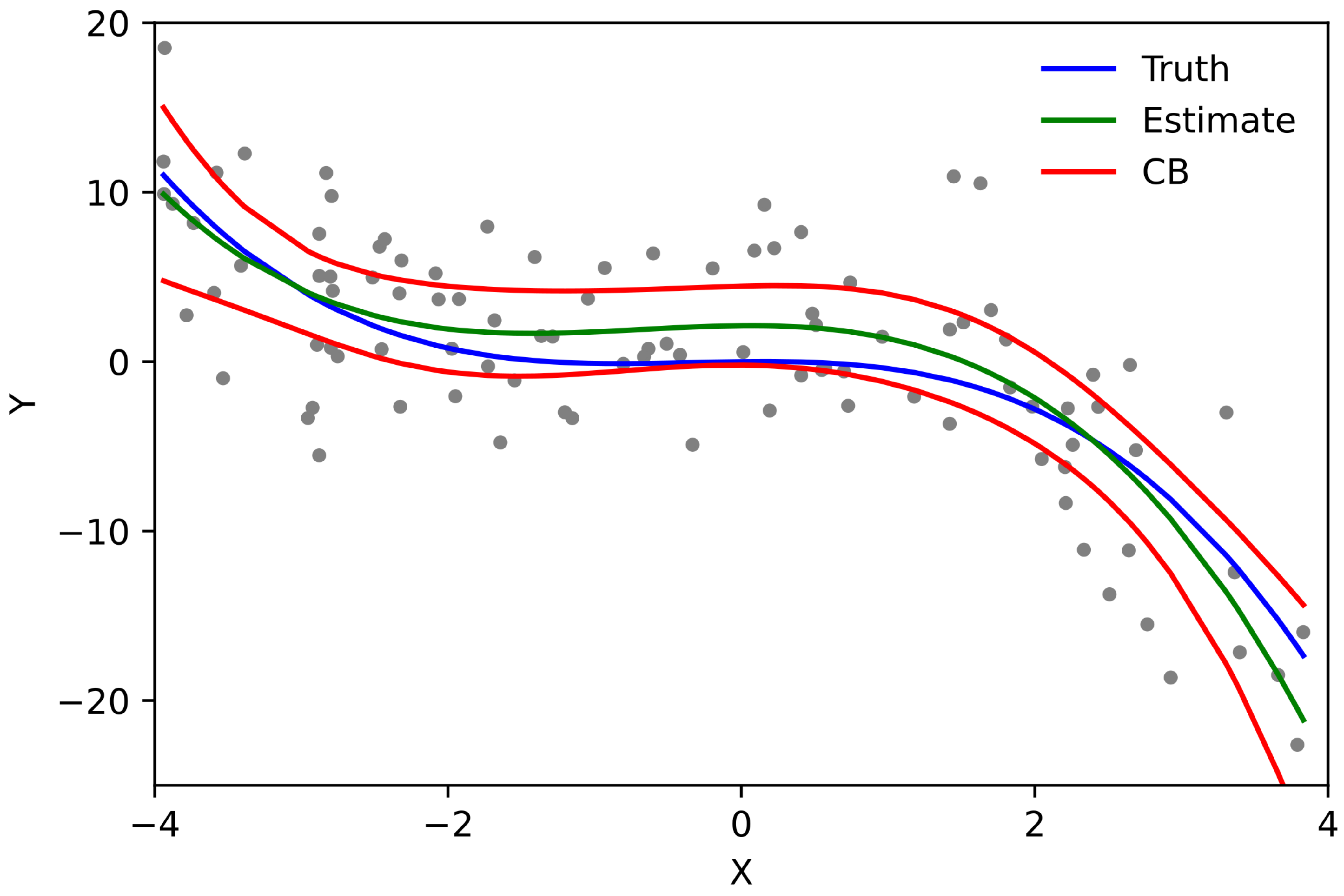
What we are estimating is a <u>mathematical function</u>

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



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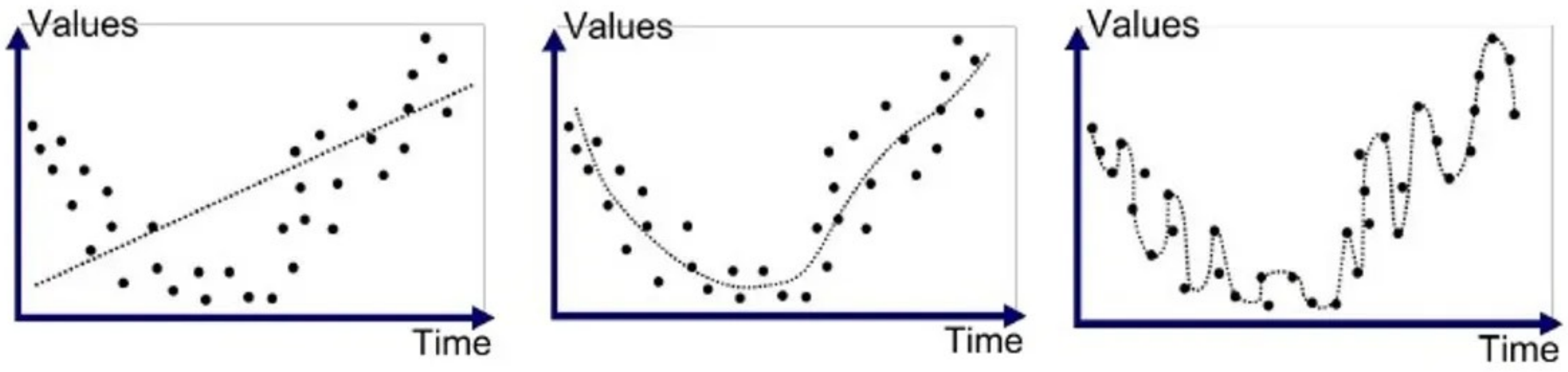
Models



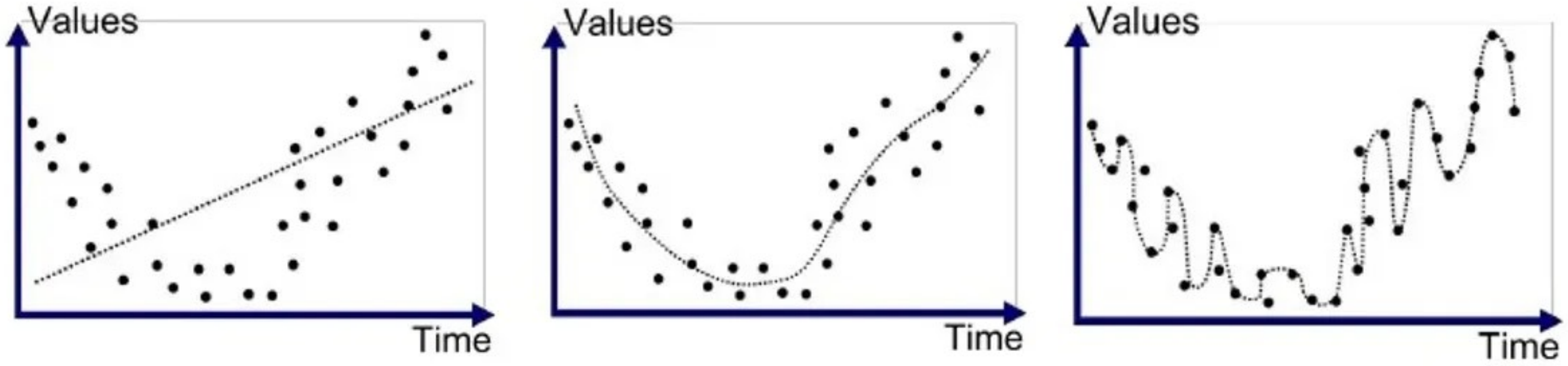
Underfitted

Good Fit/Robust

Overfitted

https://medium.com/greyatom/what-is-underfitting-and-overfitting-in-machine-learning-and-how-to-deal-with-it-6803a989c76

Models



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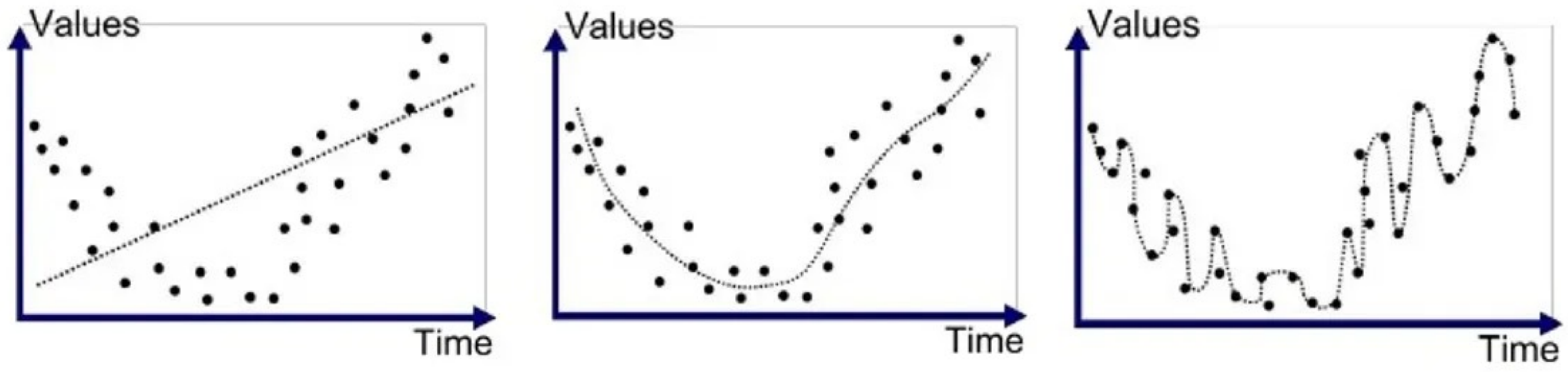

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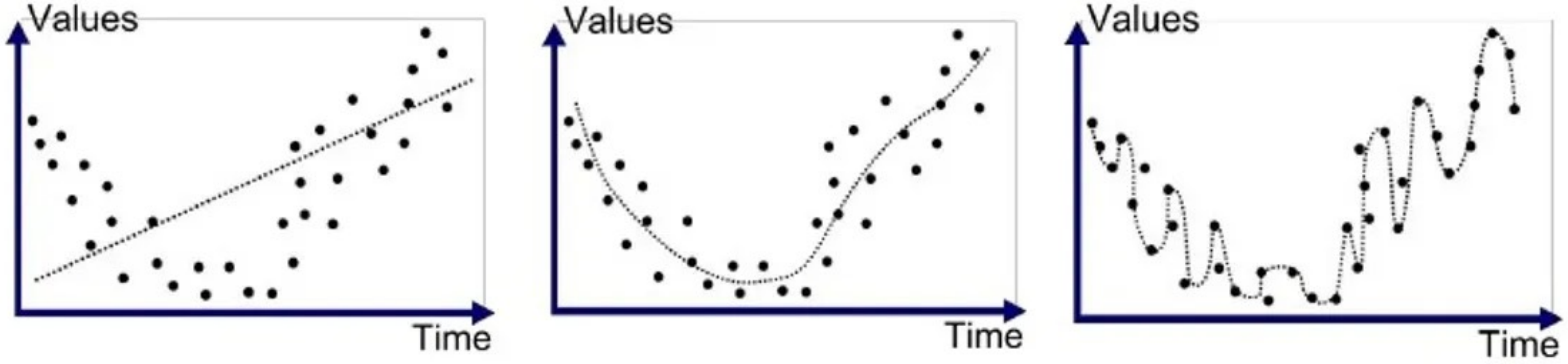

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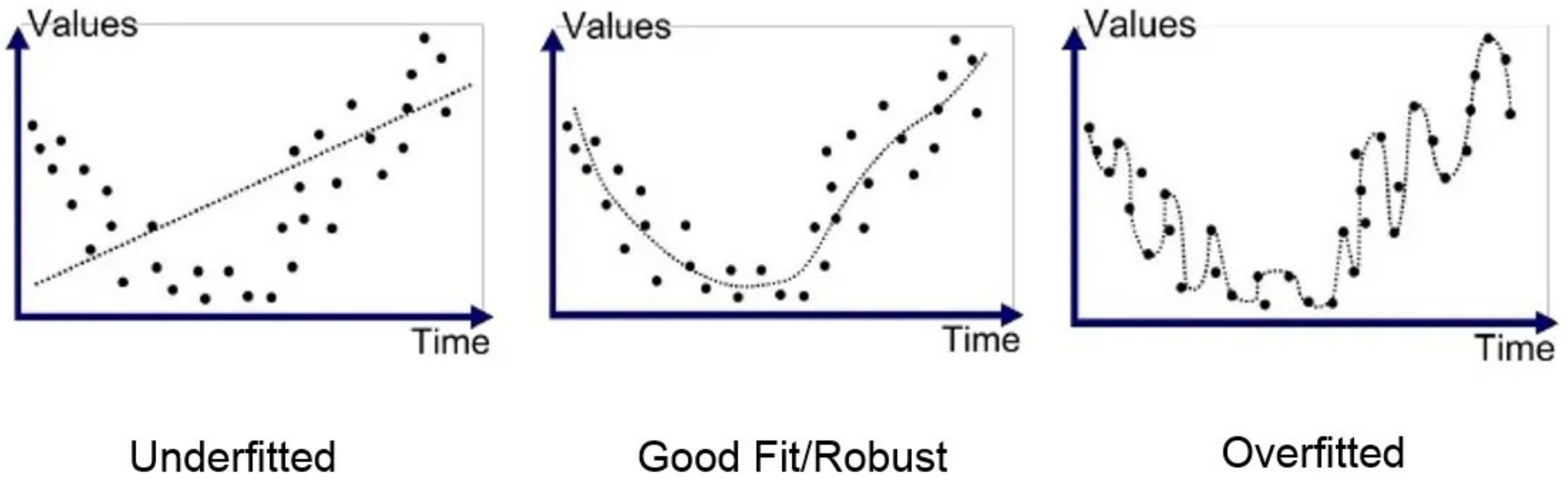

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We're interested in finding mathematical functions that "correctly" model the data we've seen.

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.*

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How To: Prediction

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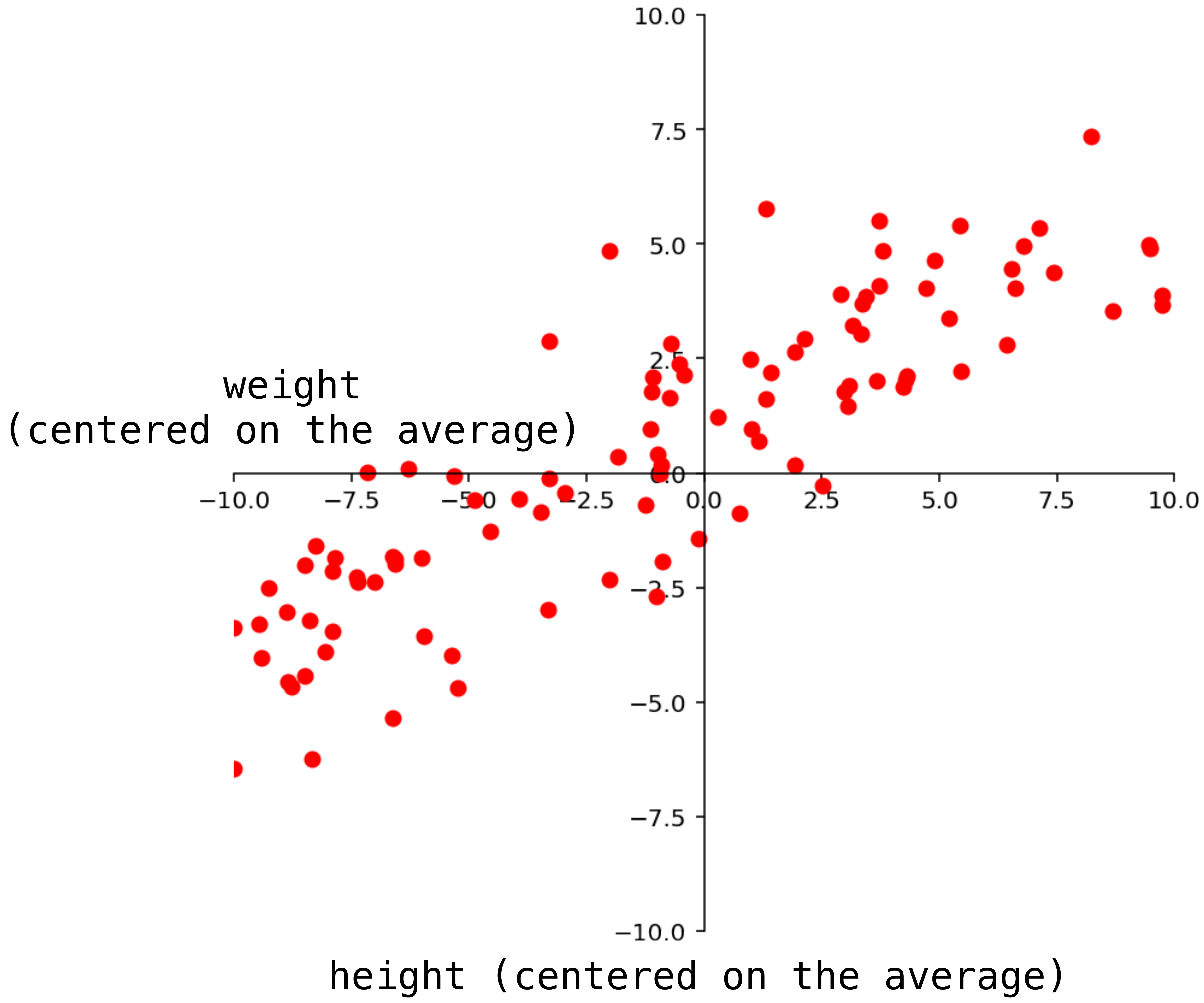
This generalizes to any model fitting problem

Example: Height from Weight



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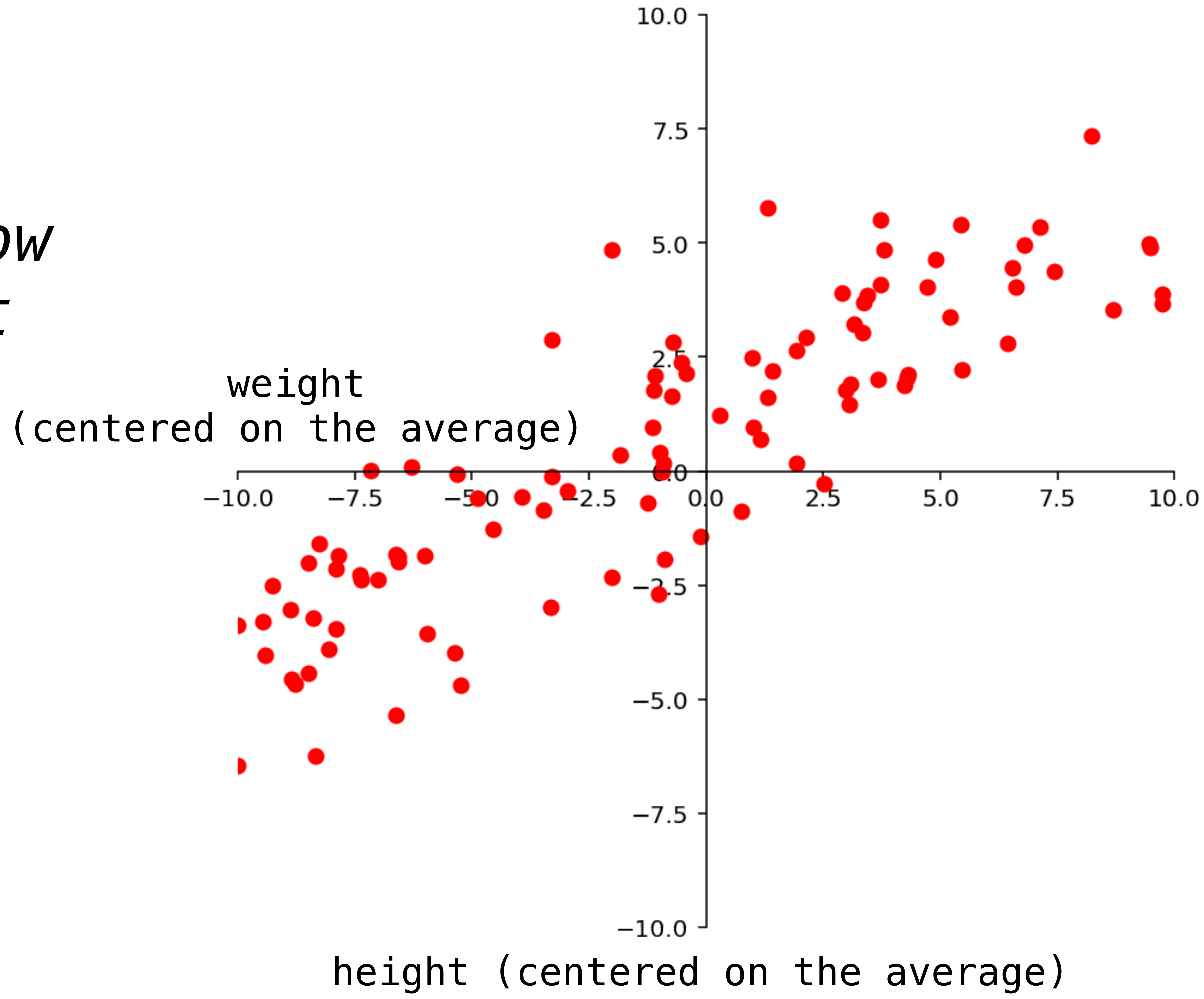

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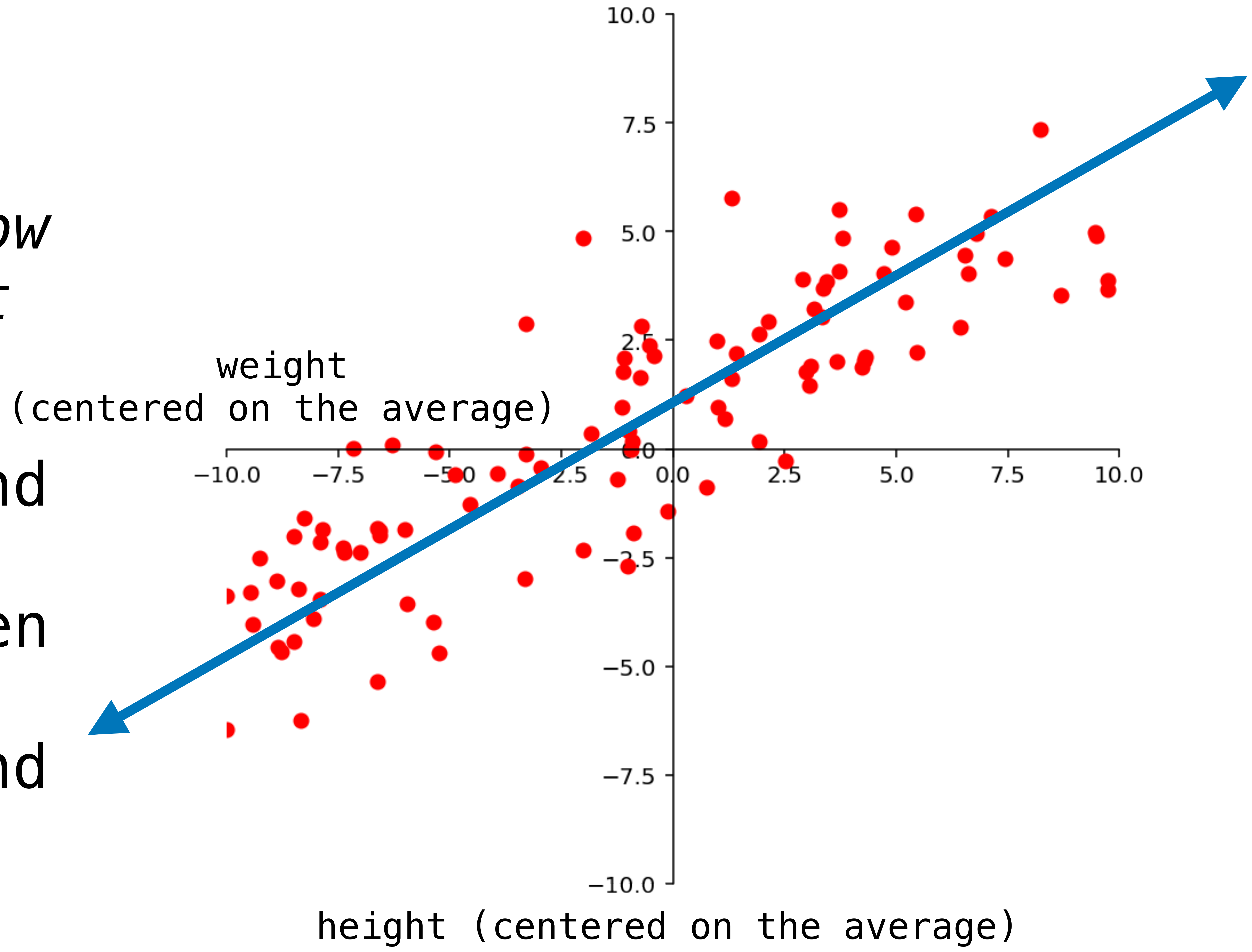
If we know the heights and weights of a population (from which X comes), then we can **find the line of best fit for that data** and then use that function.



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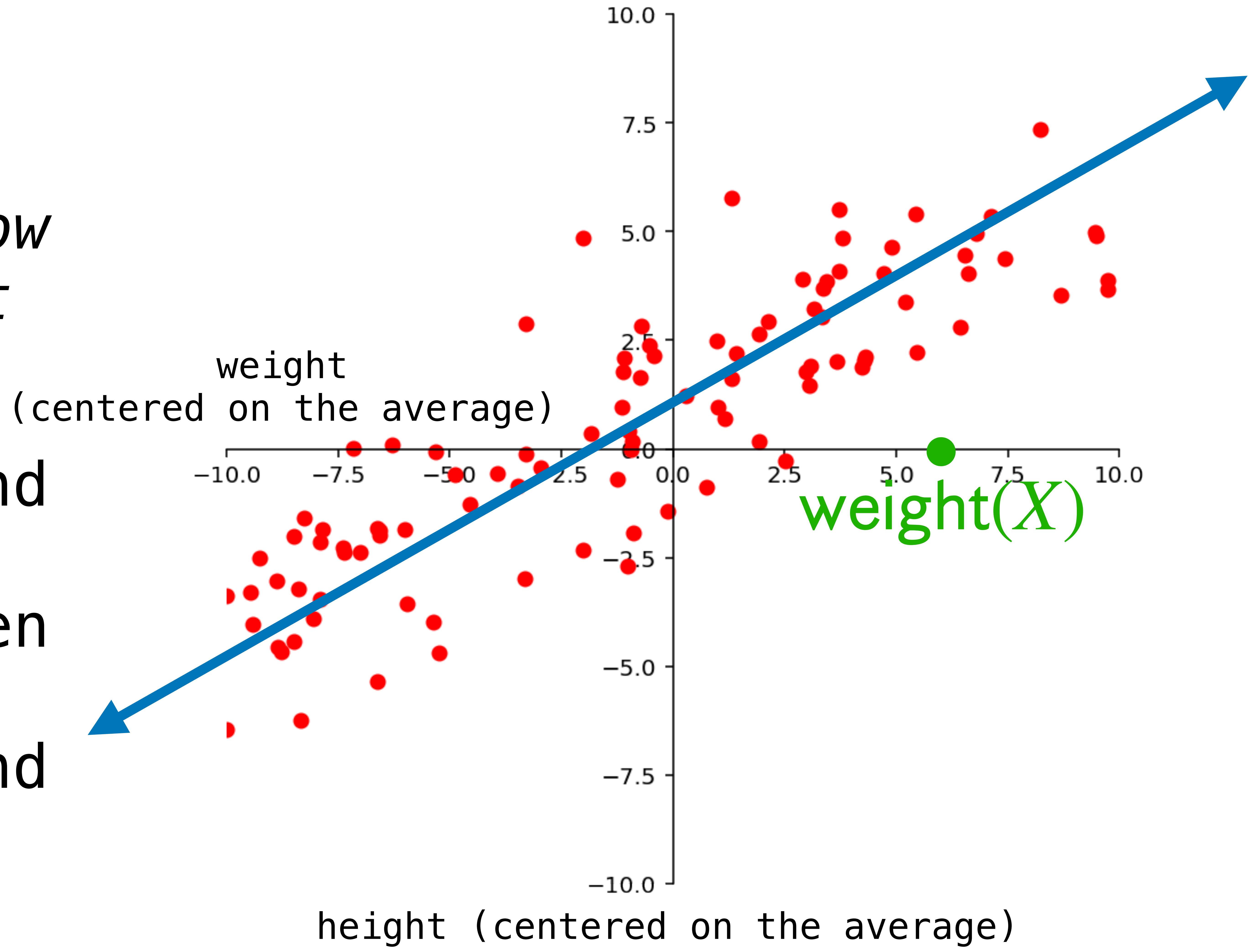

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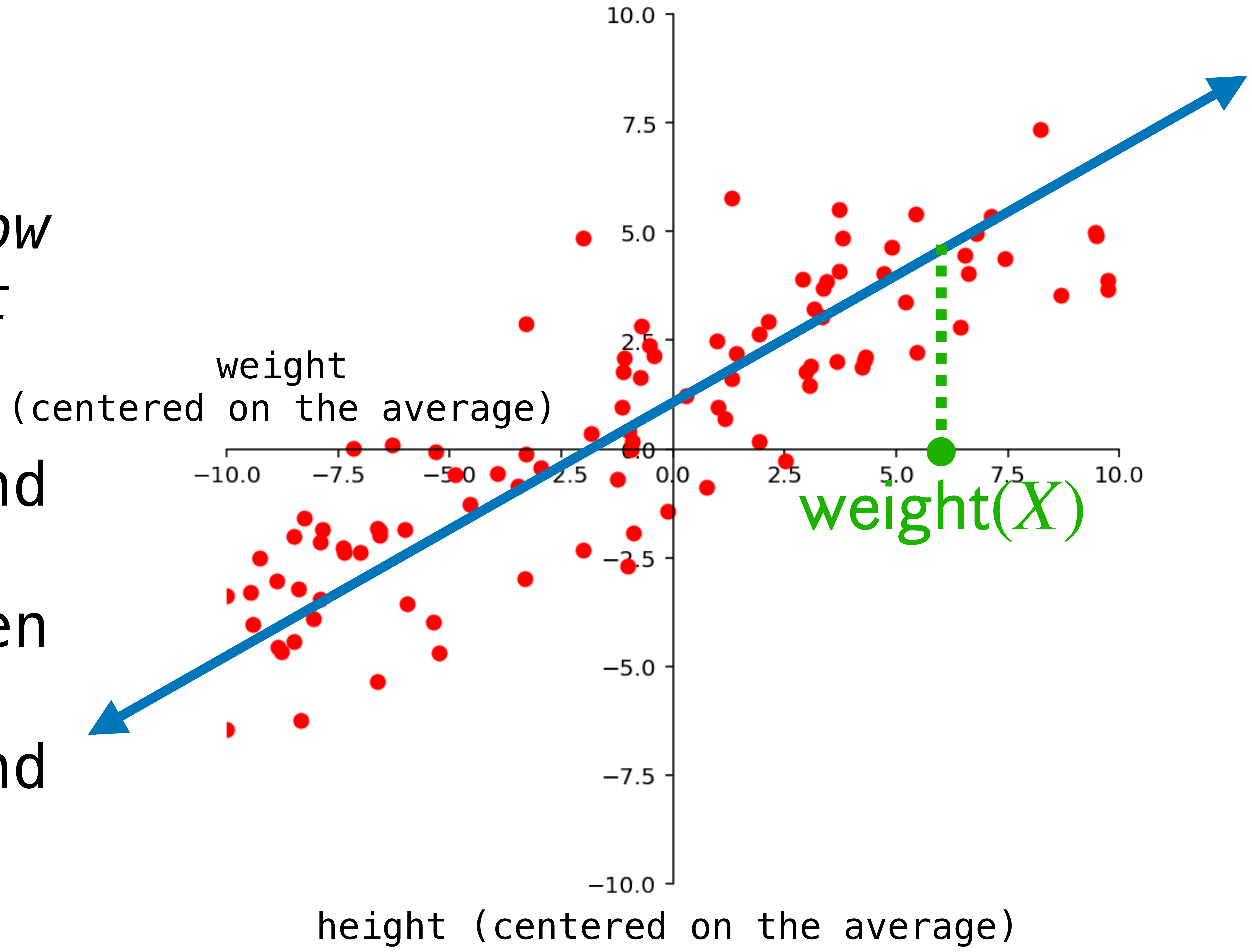

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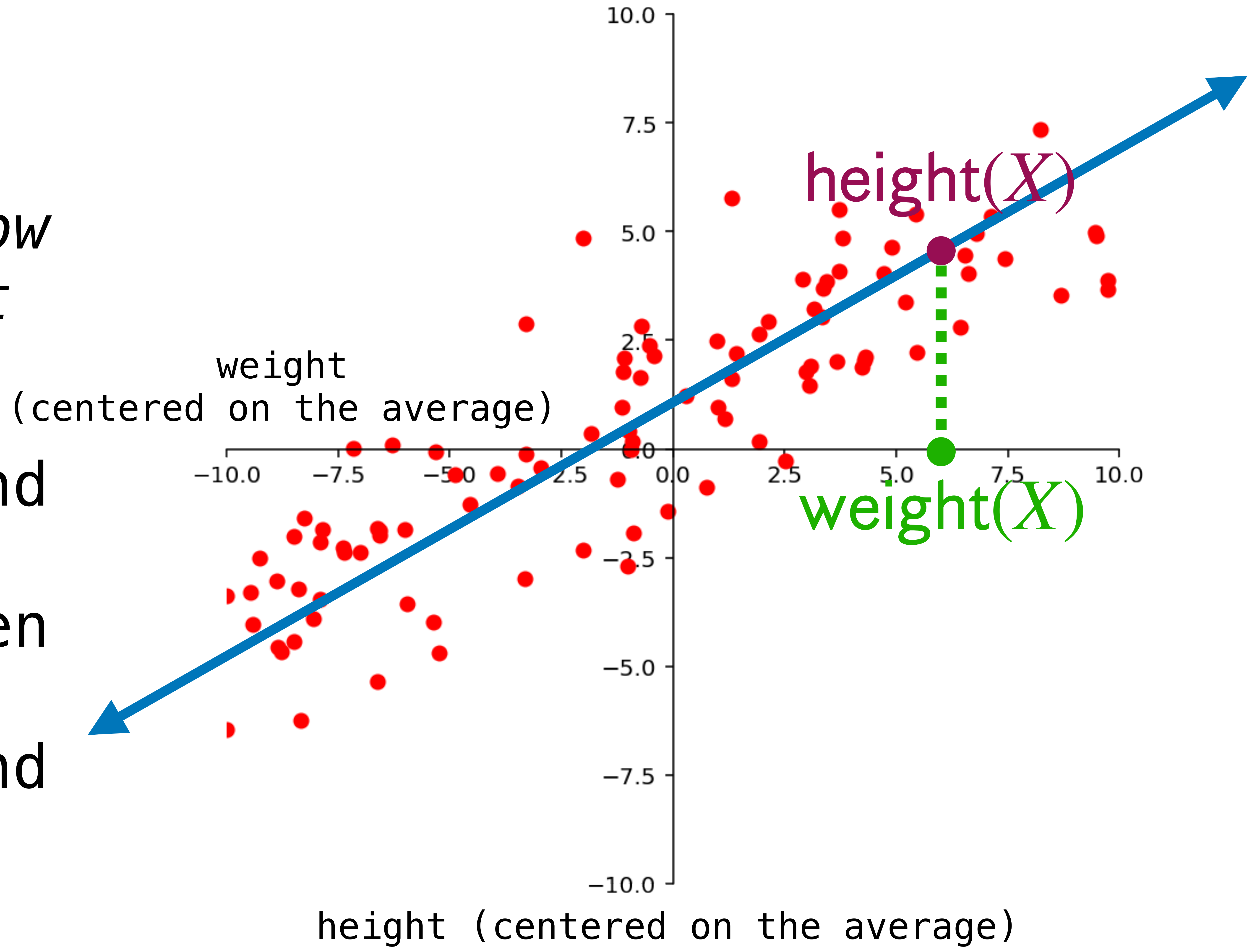


Question

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*.*

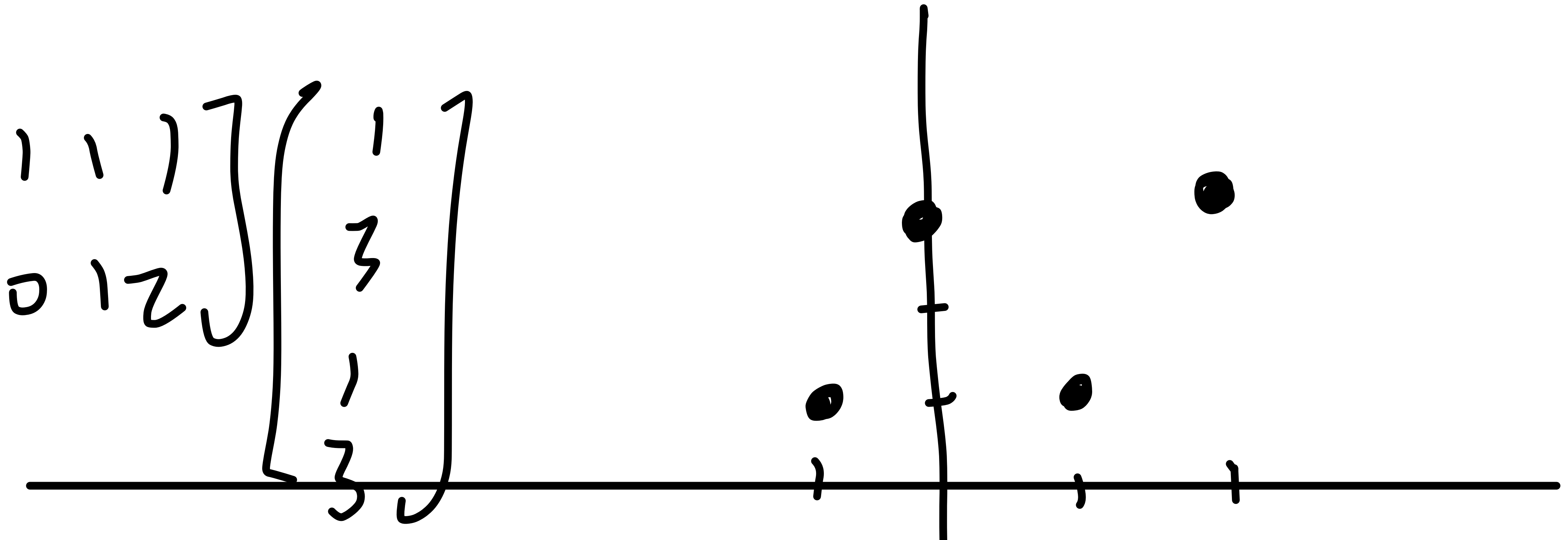
Answer

$$\begin{bmatrix}\beta_0\\ \beta_1\end{bmatrix} = \frac{1}{20}\begin{bmatrix}6 & 2\\ -2 & 4\end{bmatrix}\begin{bmatrix}8\\ 6\end{bmatrix}$$

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

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

$$X^T\vec{y} = \begin{bmatrix}1 & 1 & 1 & 1\\ -1 & 0 & 1 & 2\end{bmatrix}\begin{bmatrix}1\\ 3\\ 1\\ 3\end{bmatrix} = \begin{bmatrix}8\\ 6\end{bmatrix}$$



$$\vec{y} = \begin{bmatrix}1\\ 3\\ 1\\ 3\end{bmatrix}$$

$$\begin{bmatrix}4 & 2\\ 2 & 6\end{bmatrix}\begin{bmatrix}\beta_0\\ \beta_1\end{bmatrix} = \begin{bmatrix}8\\ 6\end{bmatrix}$$

$$X^TX = \begin{bmatrix}1 & 1 & 1 & 1\\ -1 & 0 & 1 & 2\end{bmatrix}\begin{bmatrix}1 & -1\\ 1 & 0\\ 1 & 1\\ 1 & 2\end{bmatrix} = \begin{bmatrix}4 & 2\\ 2 & 6\end{bmatrix}$$

Linear Models and Least Squares Regression

"Vectors" of Generalization

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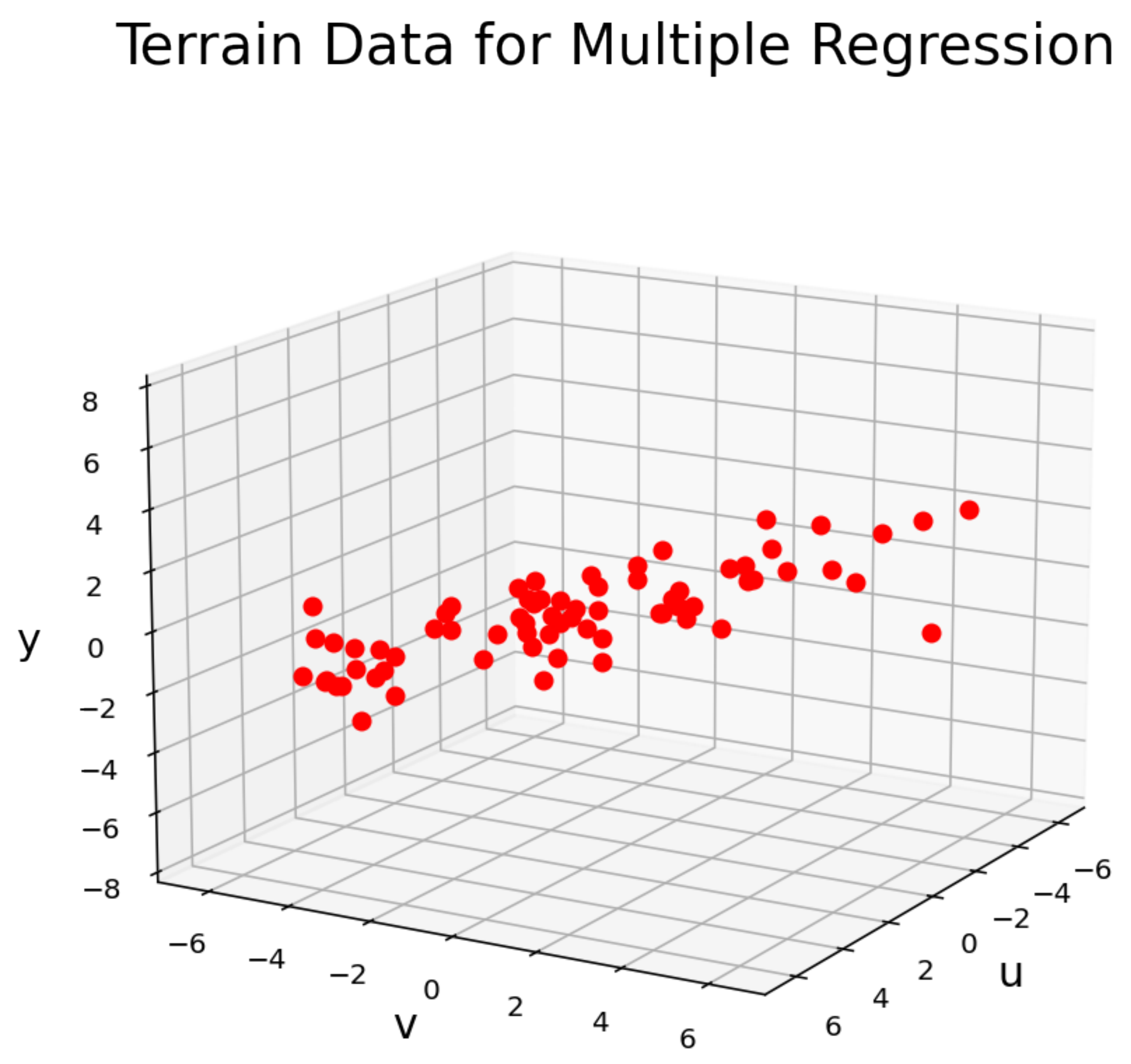
Example: Terrain Data

Figure 23.1



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

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

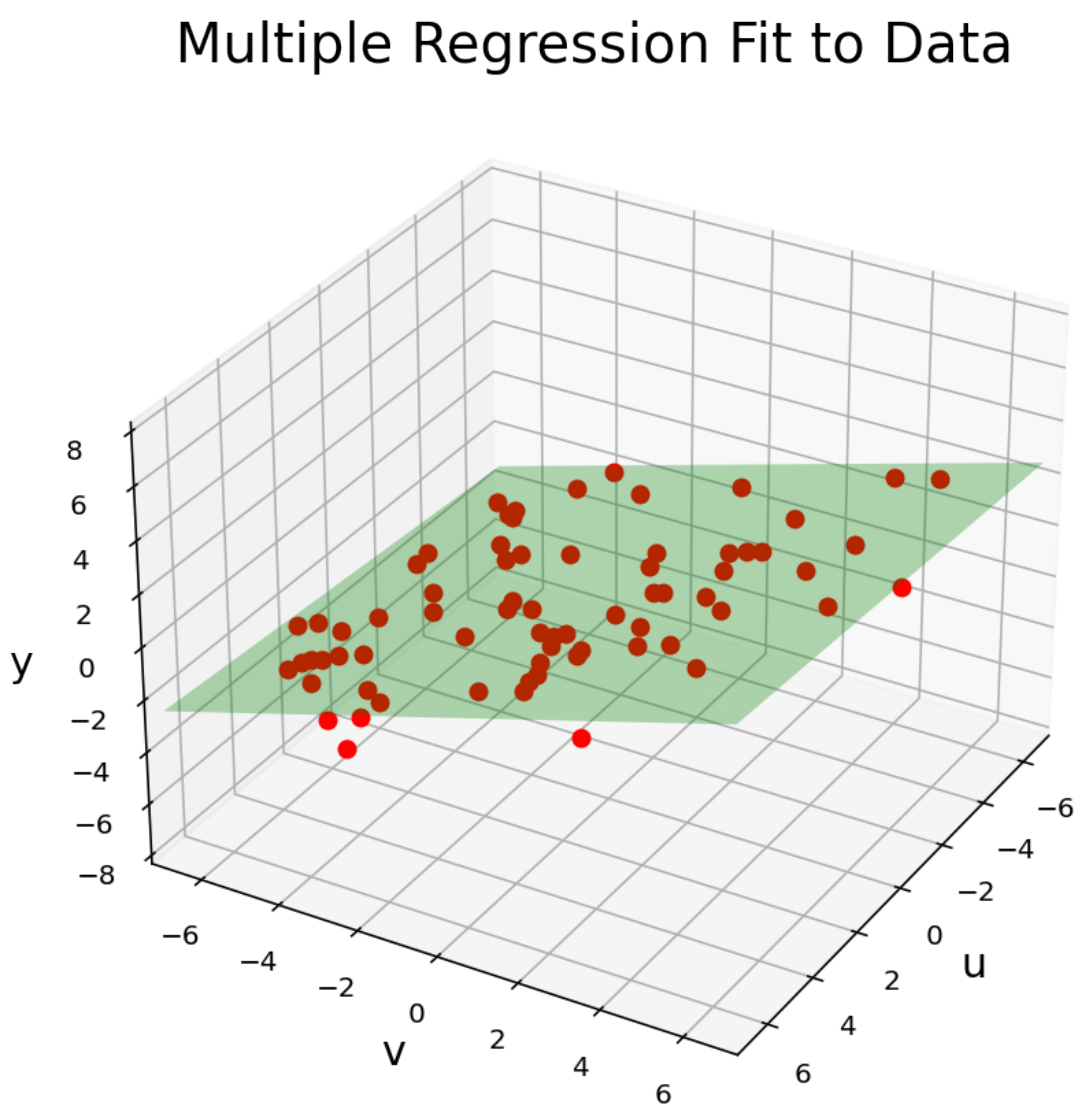
Problem: Find $\beta_0, \beta_1, \beta_2$ such that

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

which minimizes

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

Figure 23.2



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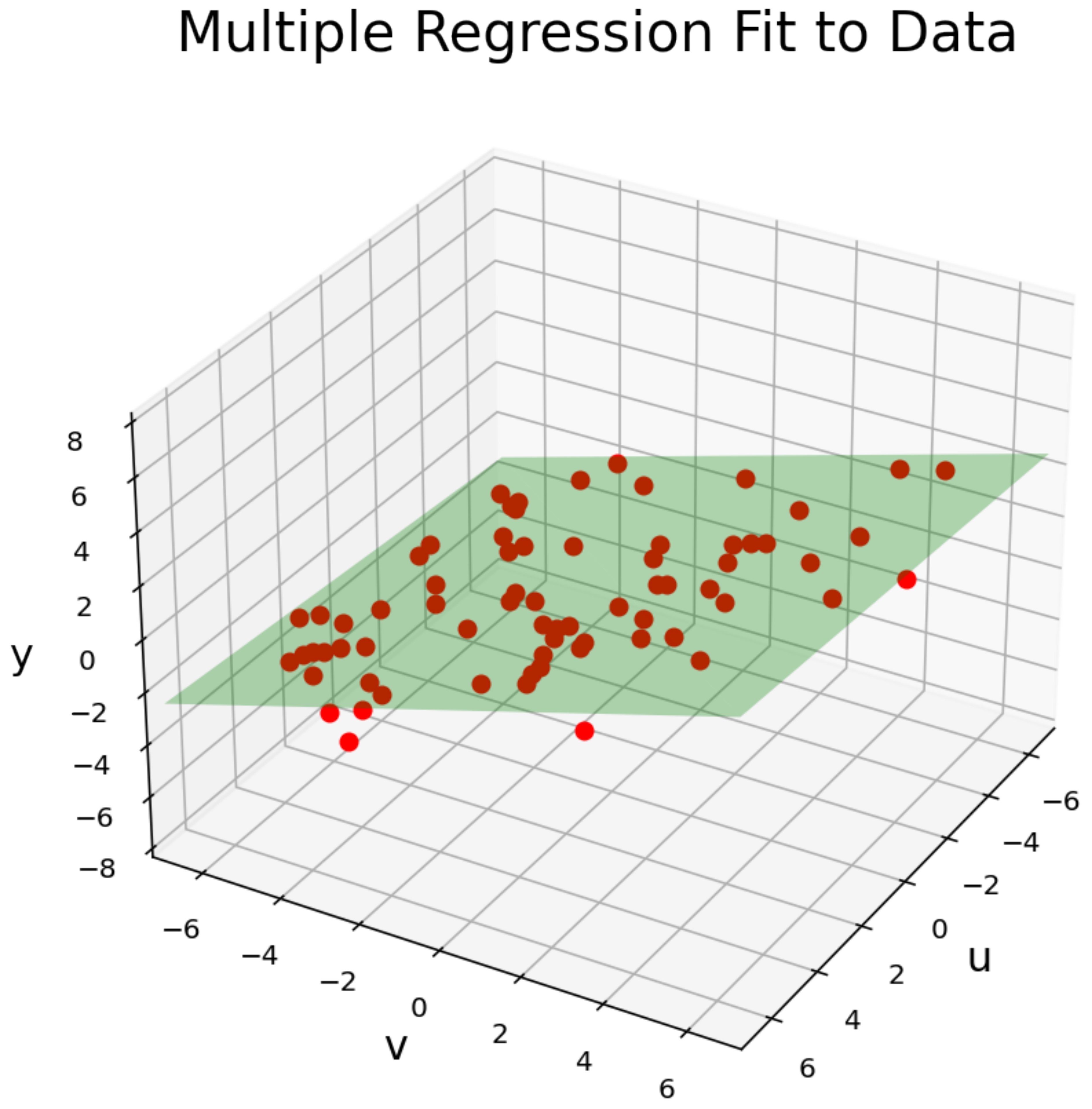

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recall: planes are given by linear equations

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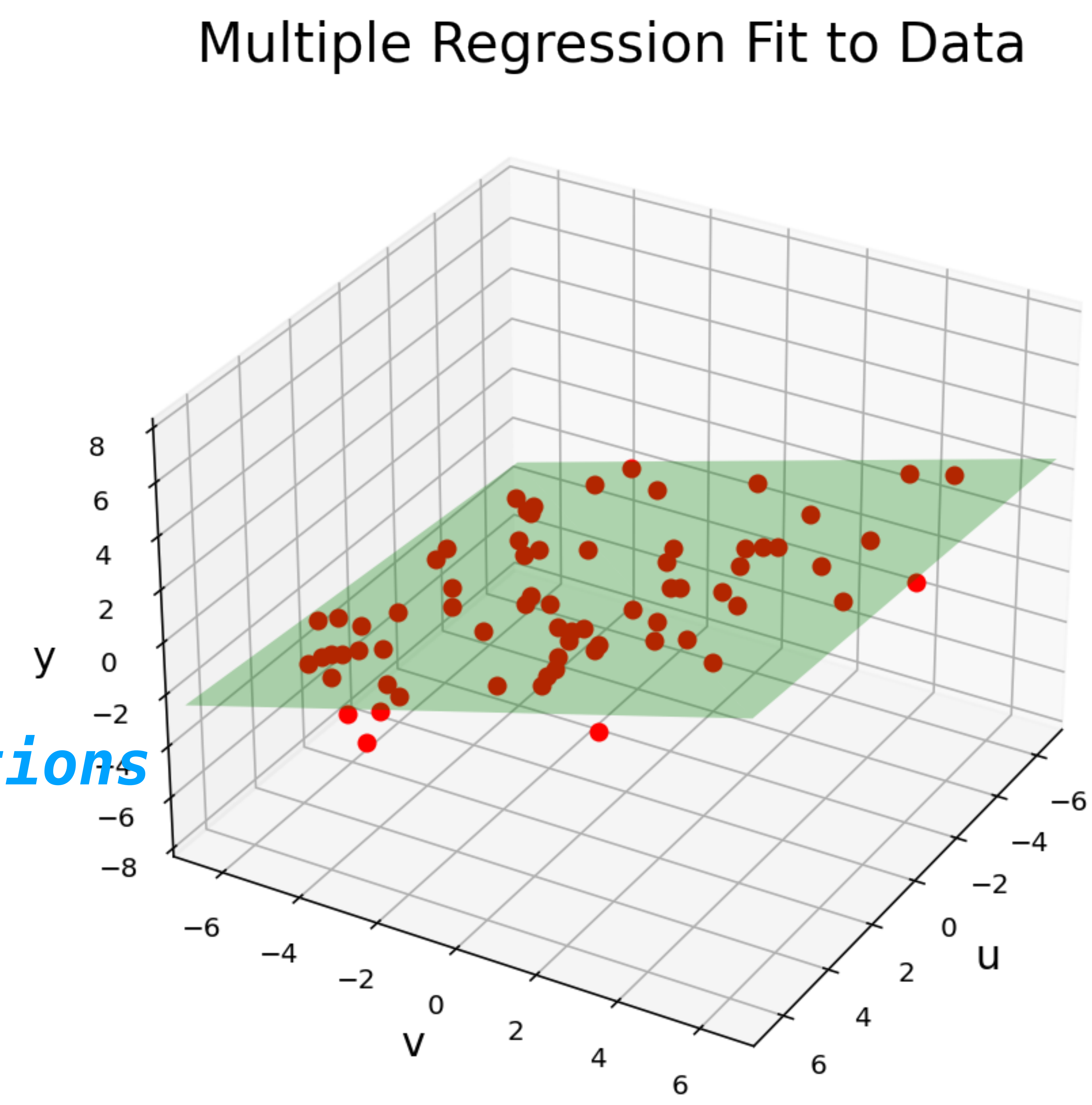

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$$\overset{X}{\begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ \vdots & \vdots & \vdots \\ 1 & x_k & y_k \end{bmatrix}} \overset{\vec{\beta}}{\begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}} = \overset{\mathbf{z}}{\begin{bmatrix} z_1 \\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

Step 2: Rewrite the system as a matrix equation.

Example: Terrain Data

$$\vec{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}$$

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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
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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.

"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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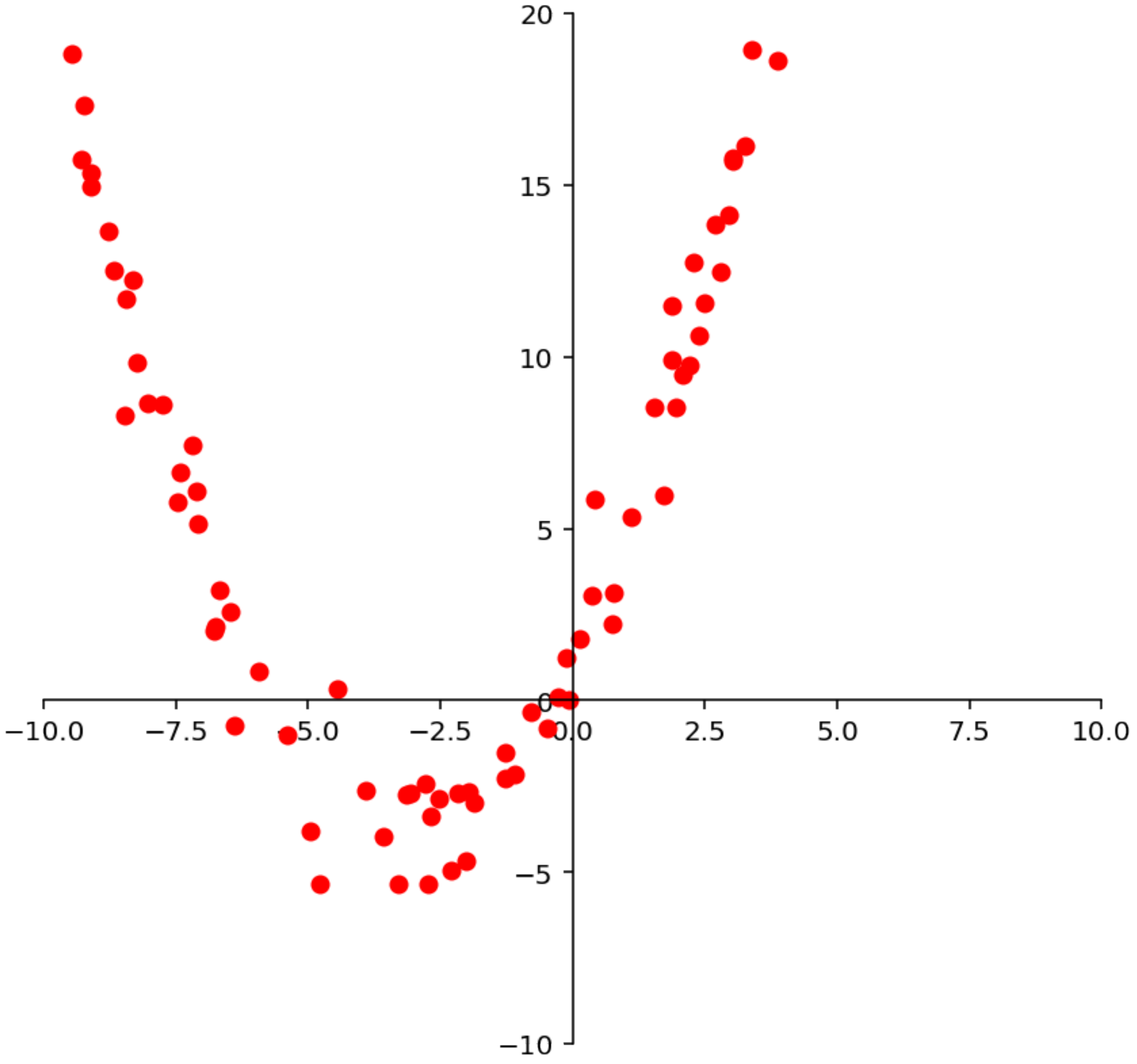

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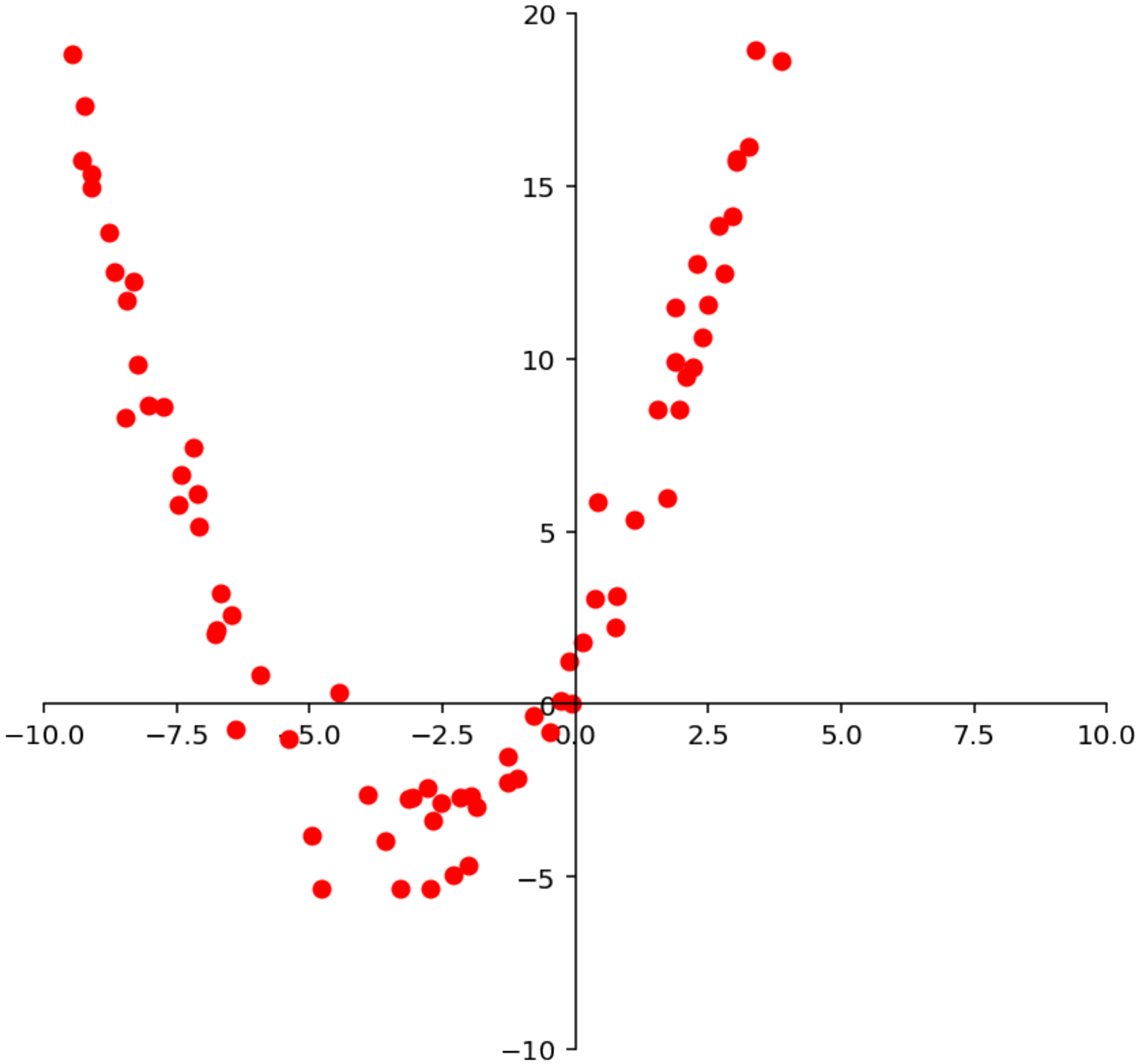

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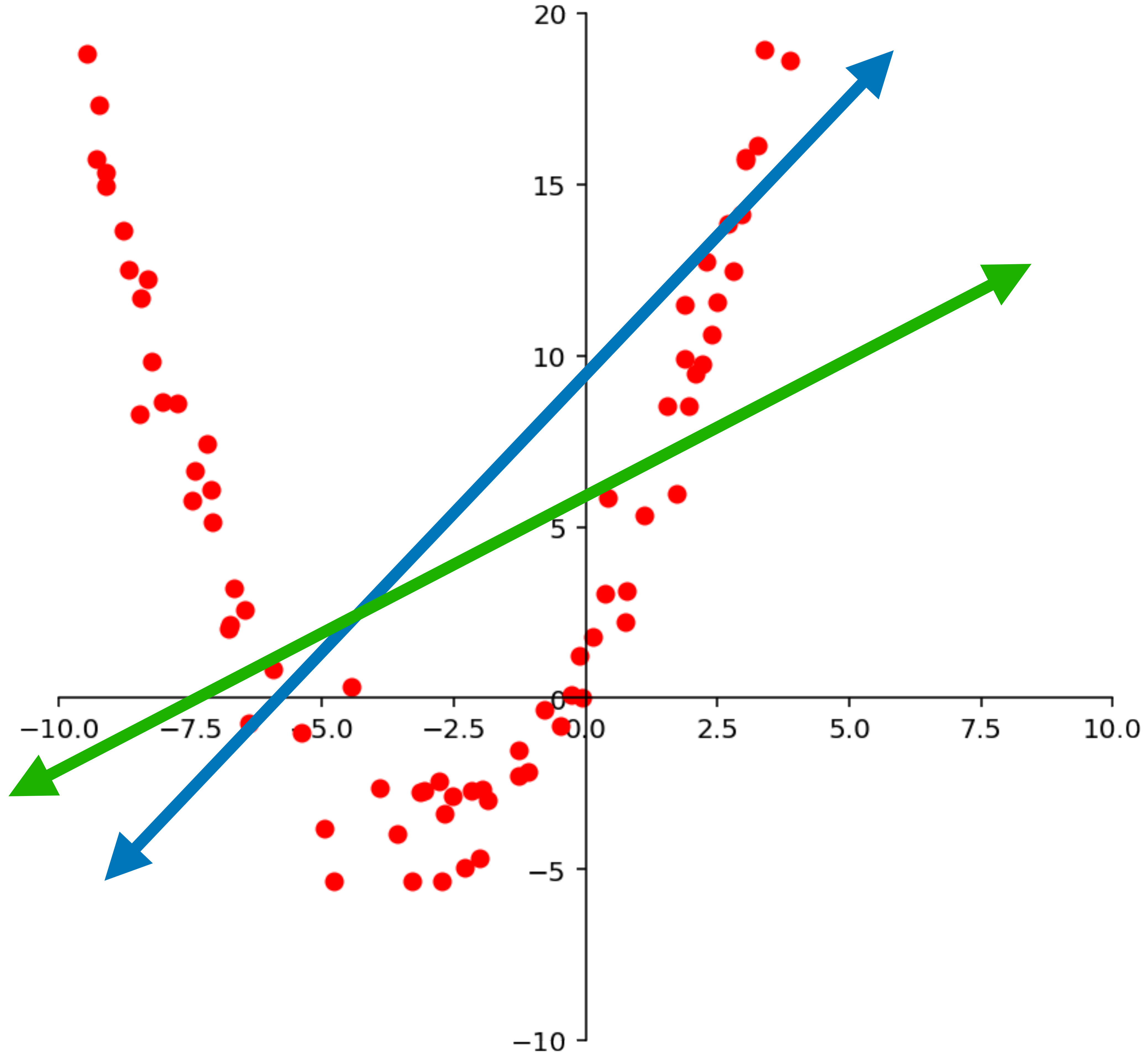
The issue: There is no good line to approximate this data.



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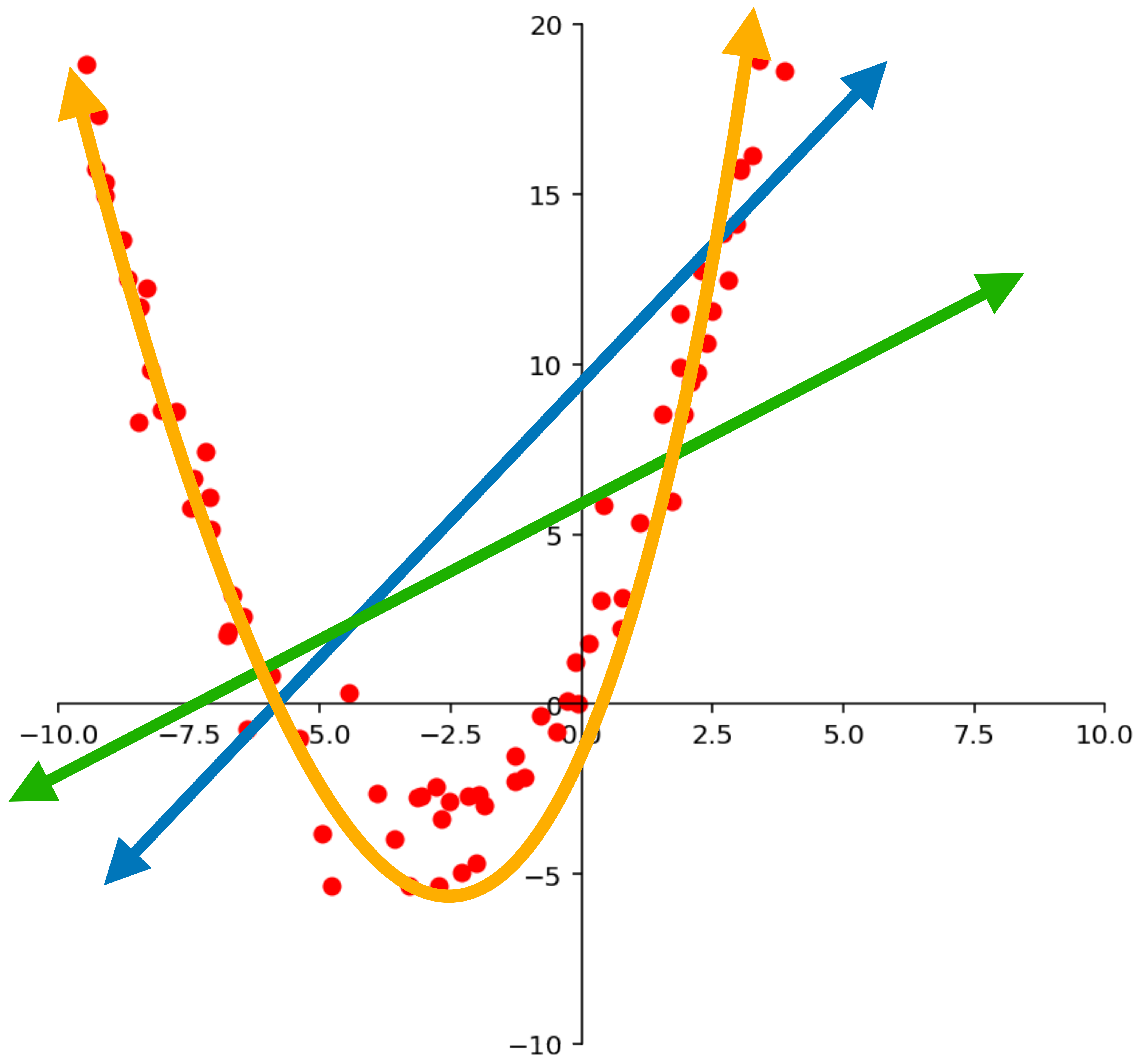
What about a parabola?



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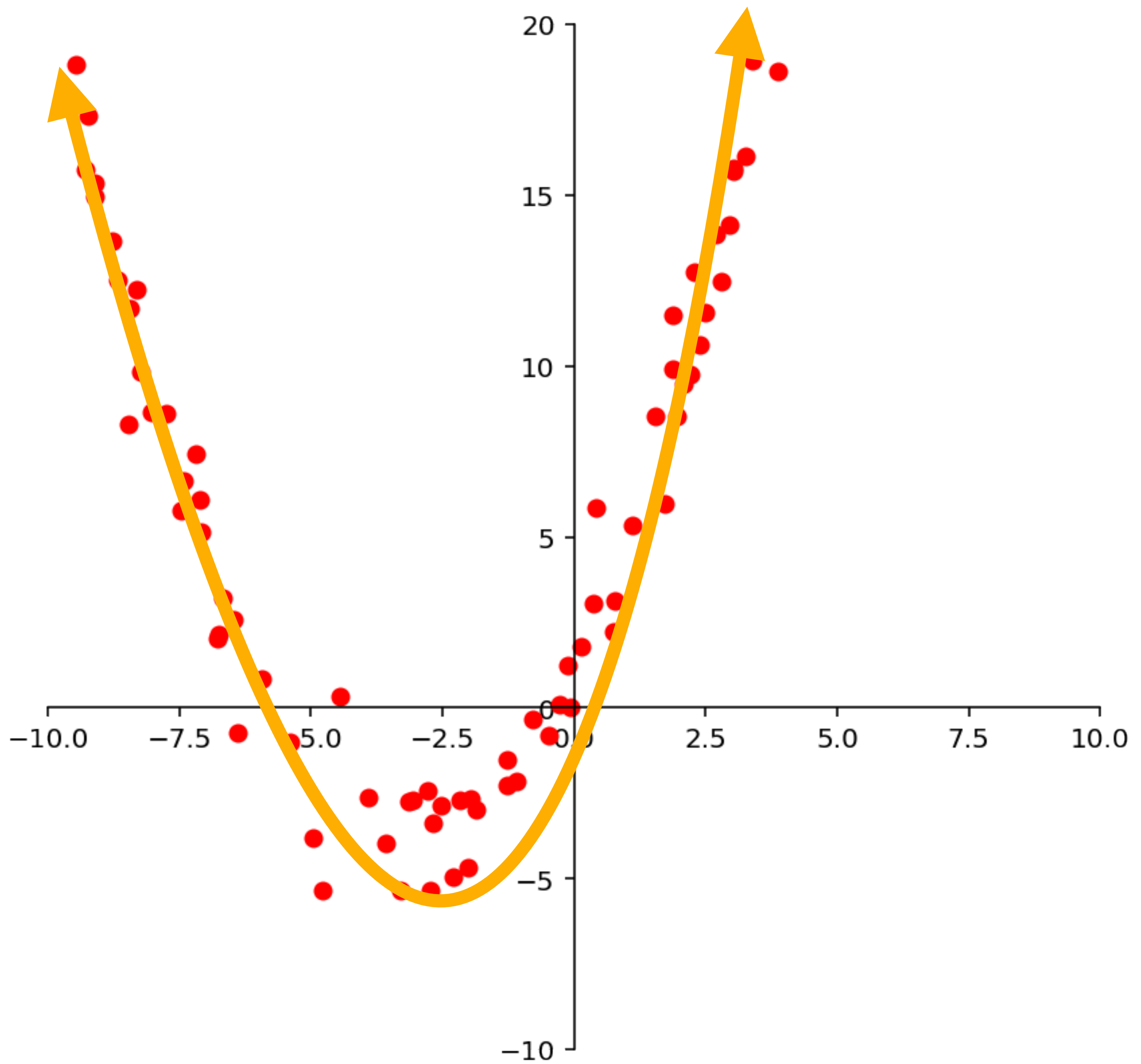

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Question

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 linear in the parameters.

Linear in Parameters

Non example

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \mapsto \beta_1 \beta_2 x_1$$

or $\mapsto e^{\beta_1 x_1}$

Definition. A function $f : \mathbb{R}^n \to \mathbb{R}$ is **linear in the parameters** $\beta_1, \ldots, \beta_k$ if it can be written as

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

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

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

An Aside: Statistical Models (Another view)

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

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design matrix

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

General Linear Regression

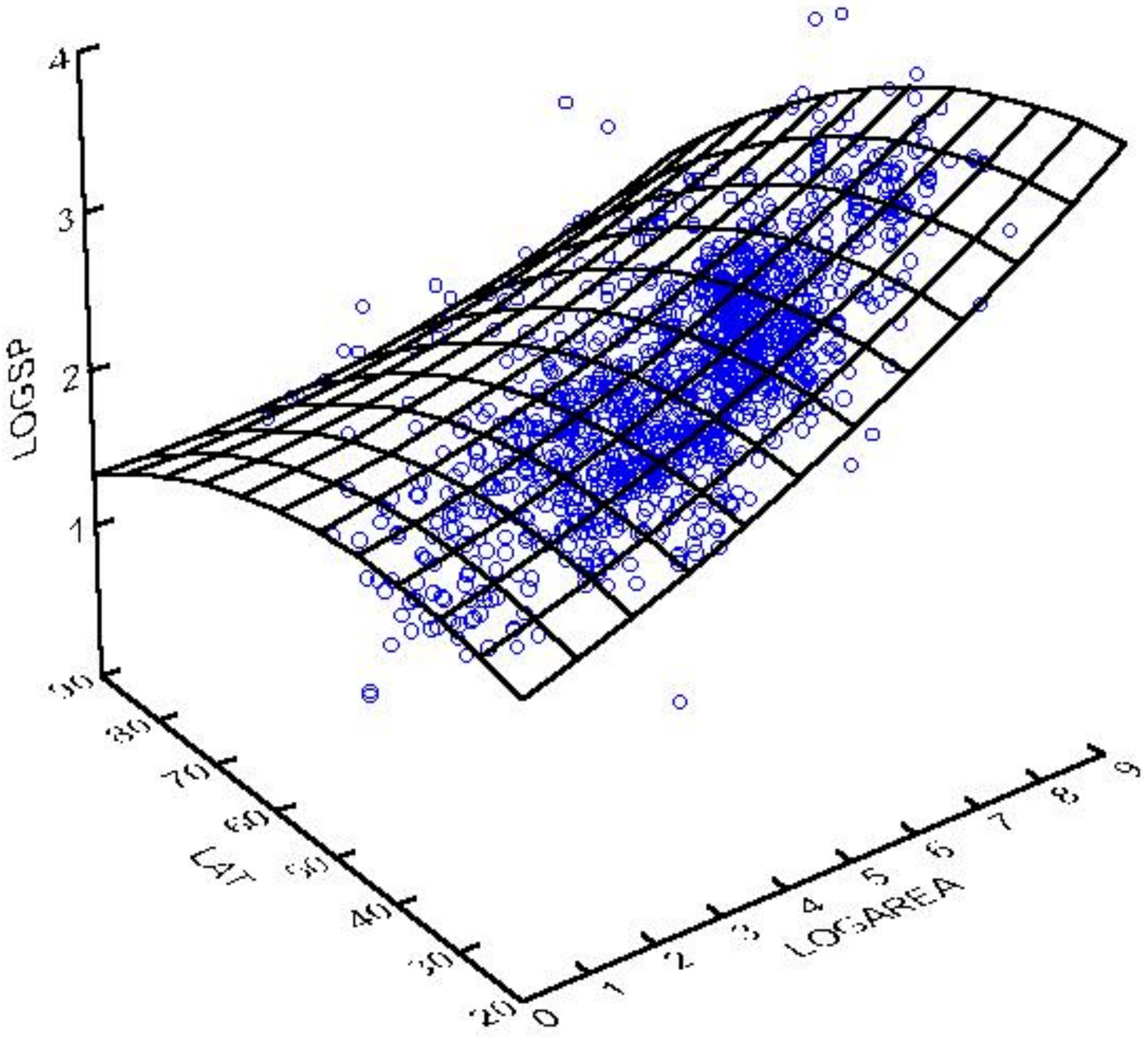
dataset: $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$ where $\mathbf{x}_i \in \mathbb{R}^n$ and $y_i \in \mathbb{R}$

Problem. Given a function

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

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

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



https://ordination.okstate.edu/MULTIPLE.htm

General Linear Regression

dataset: $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$ 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* $\beta_1, \ldots \beta_k$, find values for $\beta_1, \ldots, \beta_k$ which minimize

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

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

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

$$\vdots$$

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

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

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This is still linear in the β's

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design matrix

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

Step 2: Rewrite the system as a matrix equation.

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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 $\beta_1, \beta_2, \ldots, \beta_k$ given the dataset $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$.

How To: Design Matrices

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

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

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

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

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

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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.