Linear Models

Geometric Algorithms
Lecture 24

CAS CS 132

Practice Problem

$$A = \begin{array}{ccc} \vec{a}_1 & \vec{a}_2 & \vec{a}_3 \\ \end{array}$$

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

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

<u>hint:</u> $\vec{a}_2 - \vec{a}_1 = \vec{a}_3$

Answer

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

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

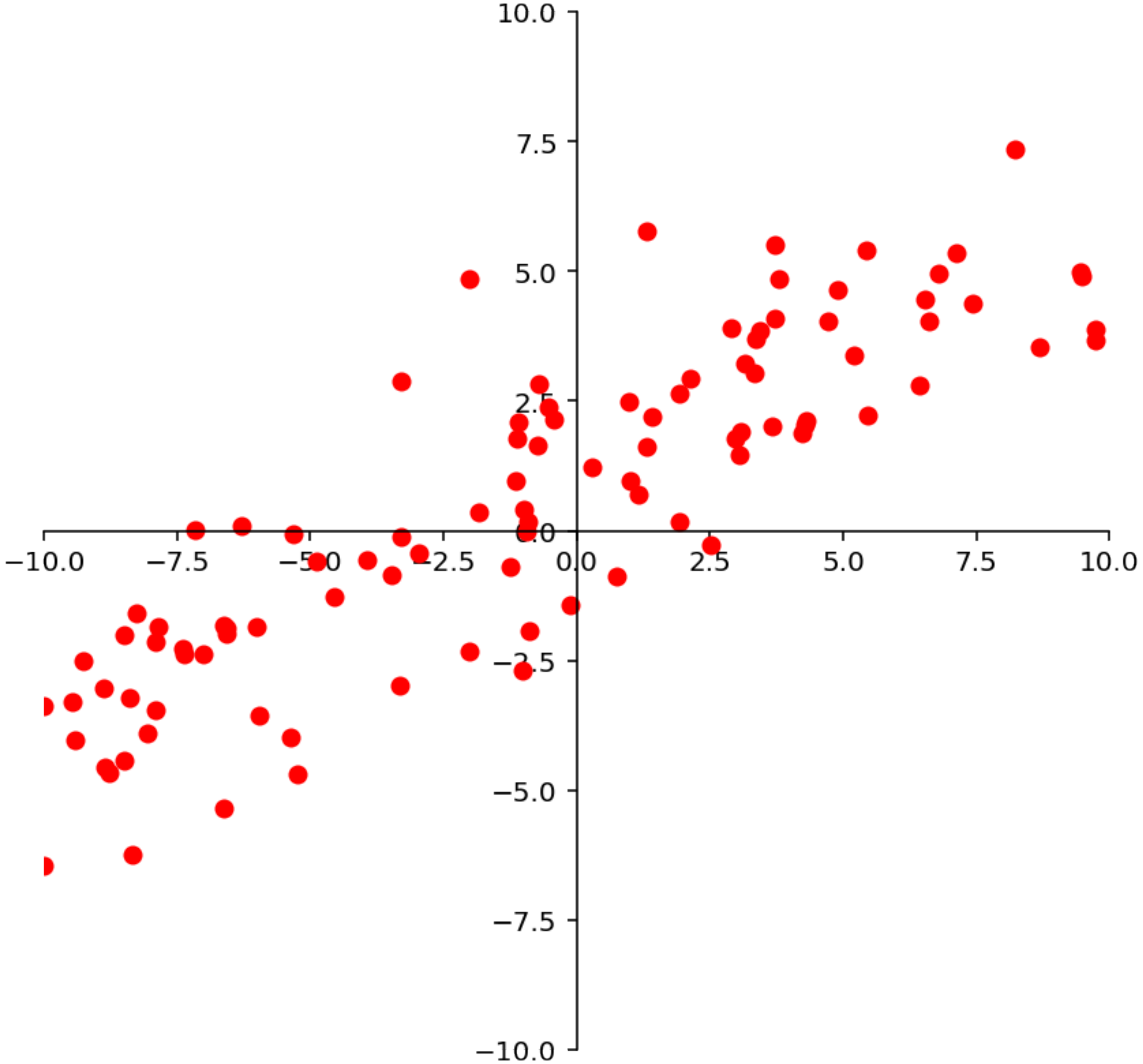
model fitting

model parameters

design matrices

Warm-up: Line of Best Fit

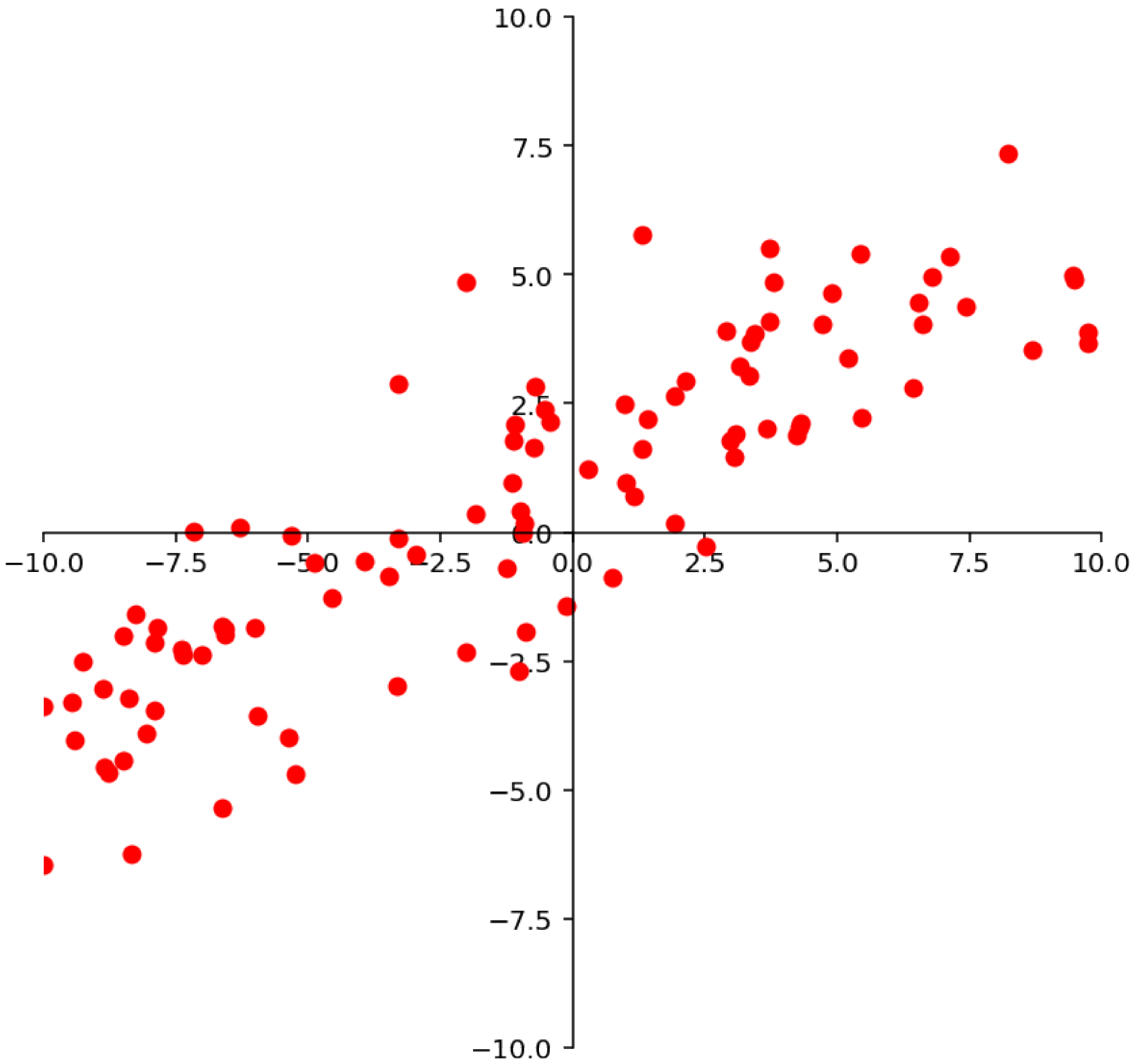
The Setup



The Setup

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

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



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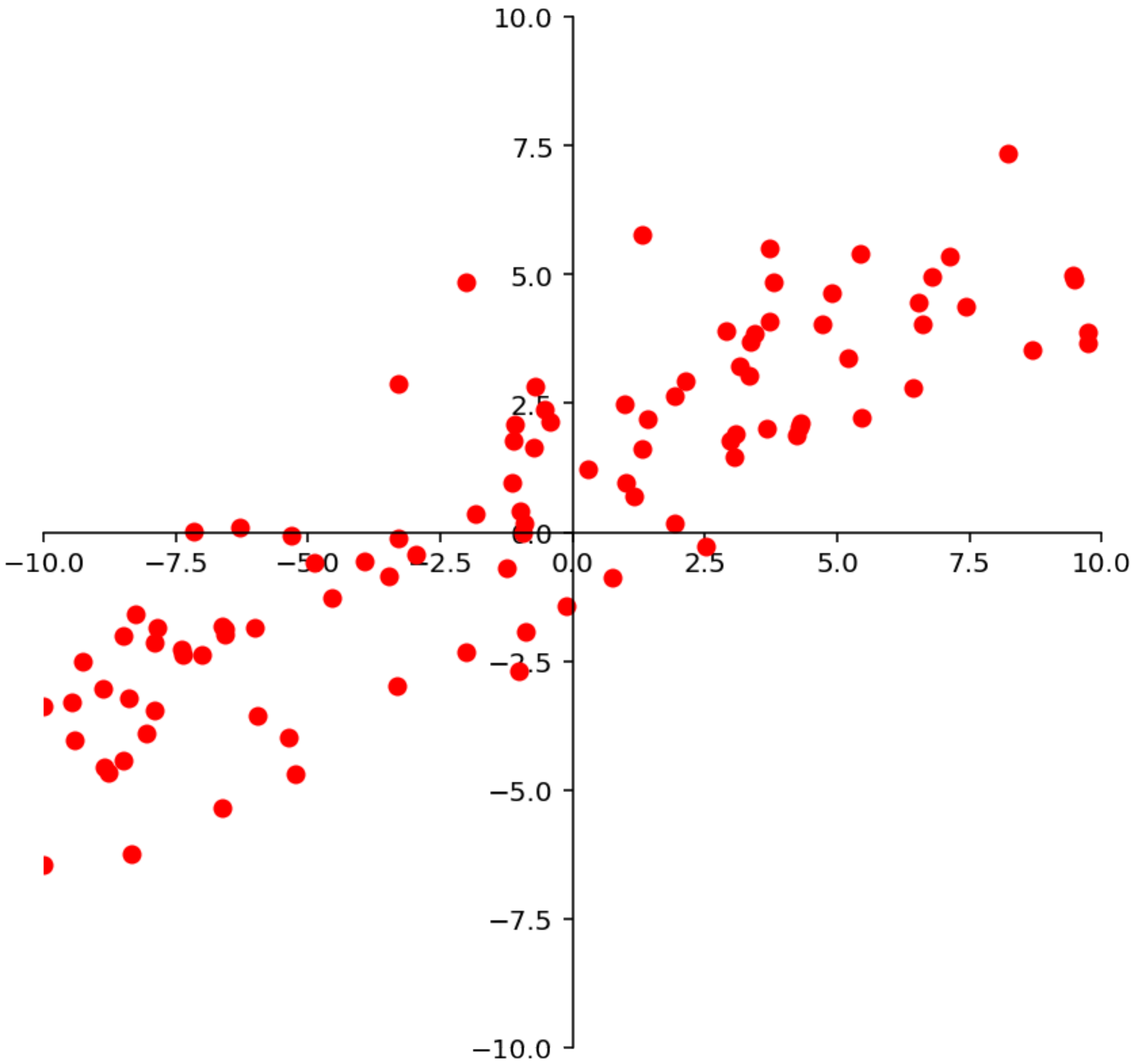
Example. You collect (height, weight) data for a population.



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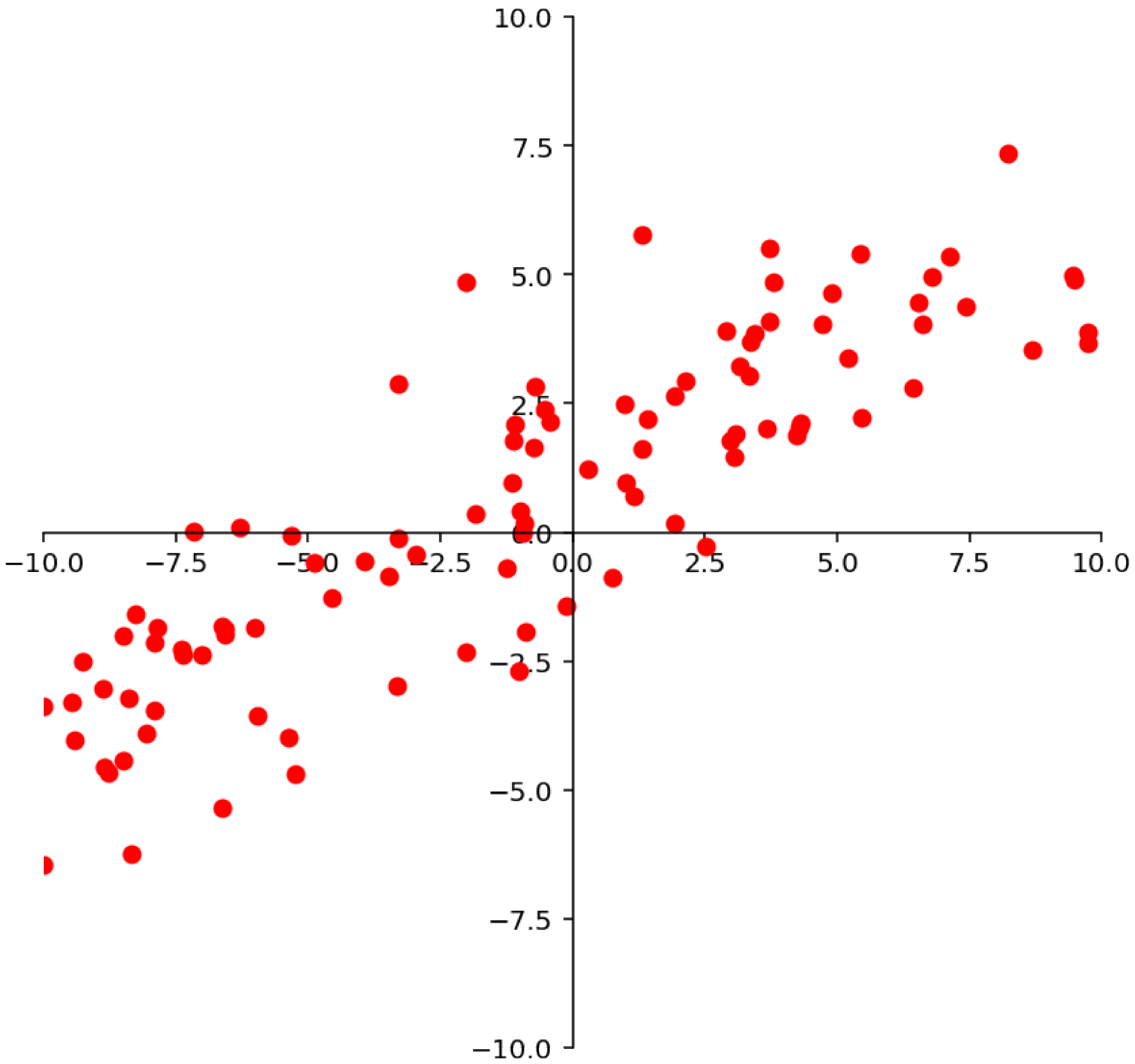
You notice they *kind of* trend as a line.



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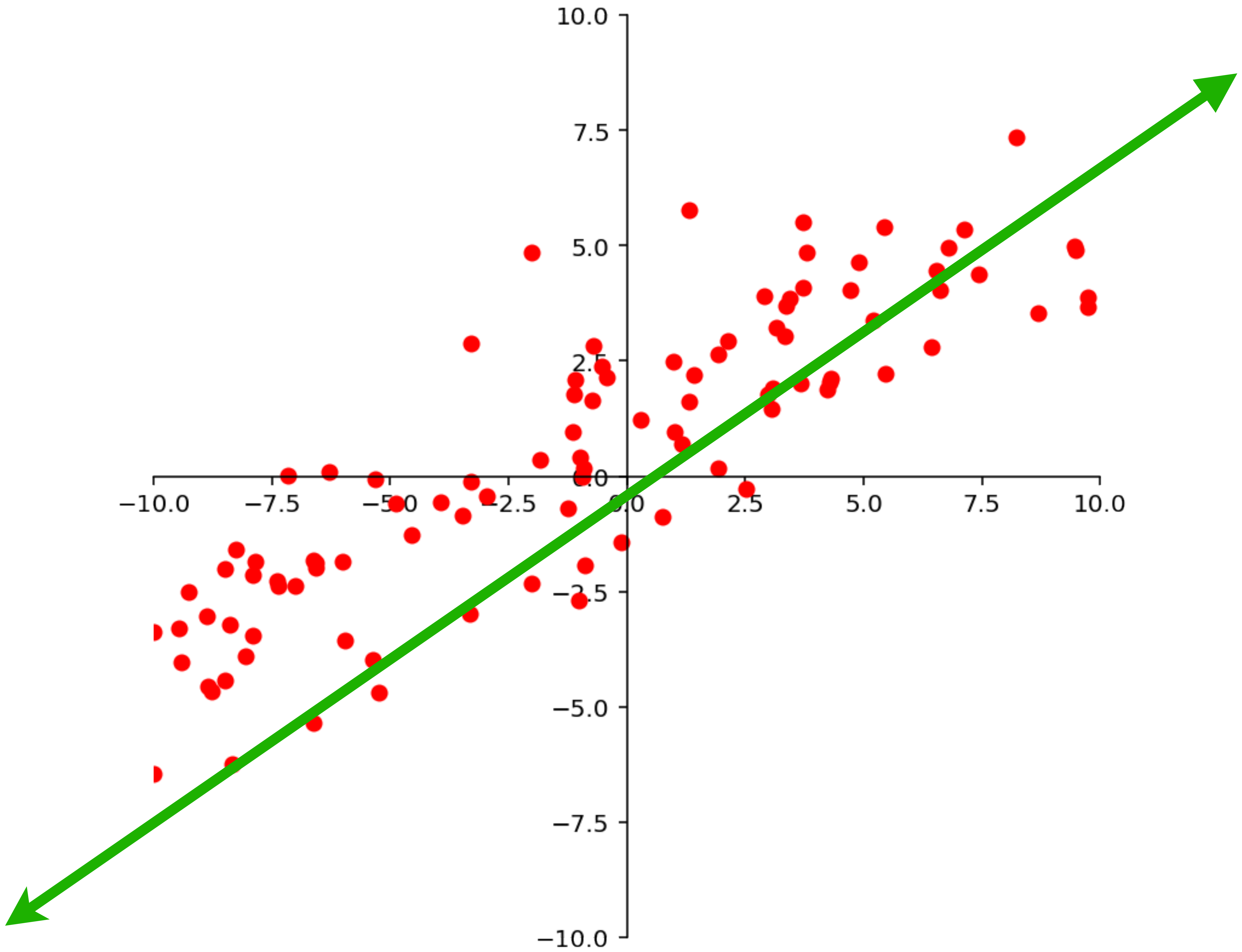

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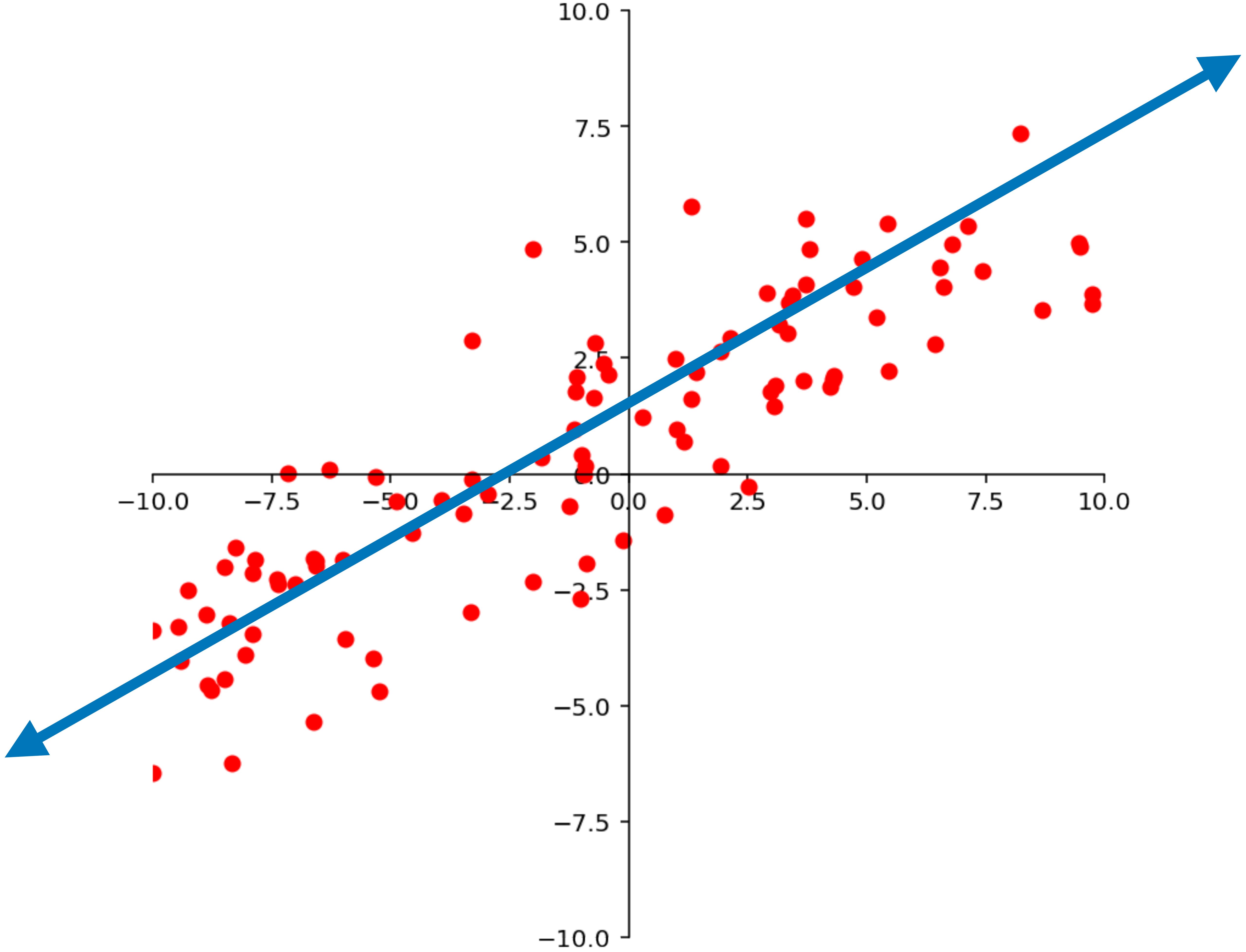
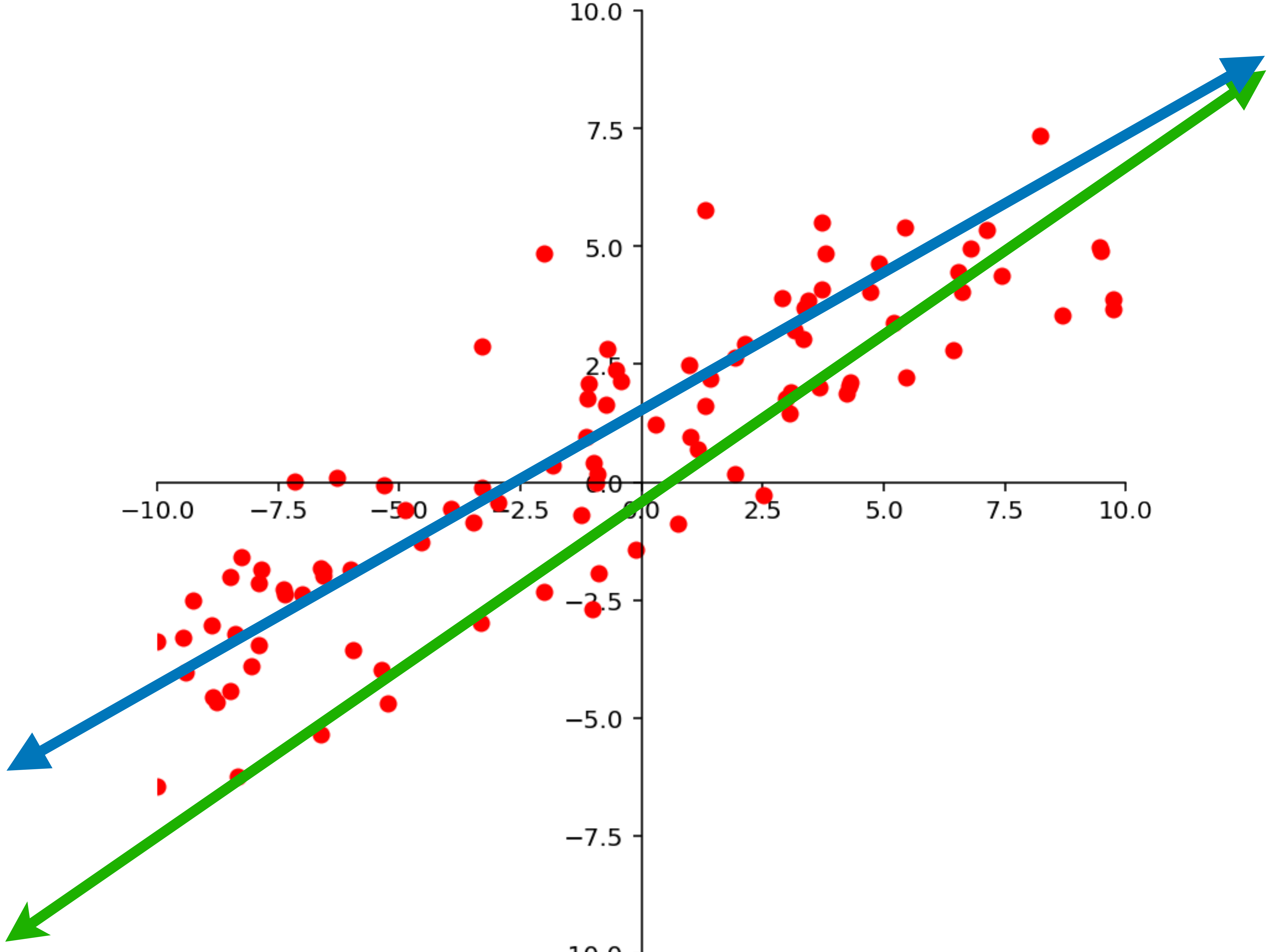


The Setup

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

Which one *best models* the dataset?



Two Important Questions

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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 $\{(x_1, y_1), \ldots, (x_n, y_n)\}$, 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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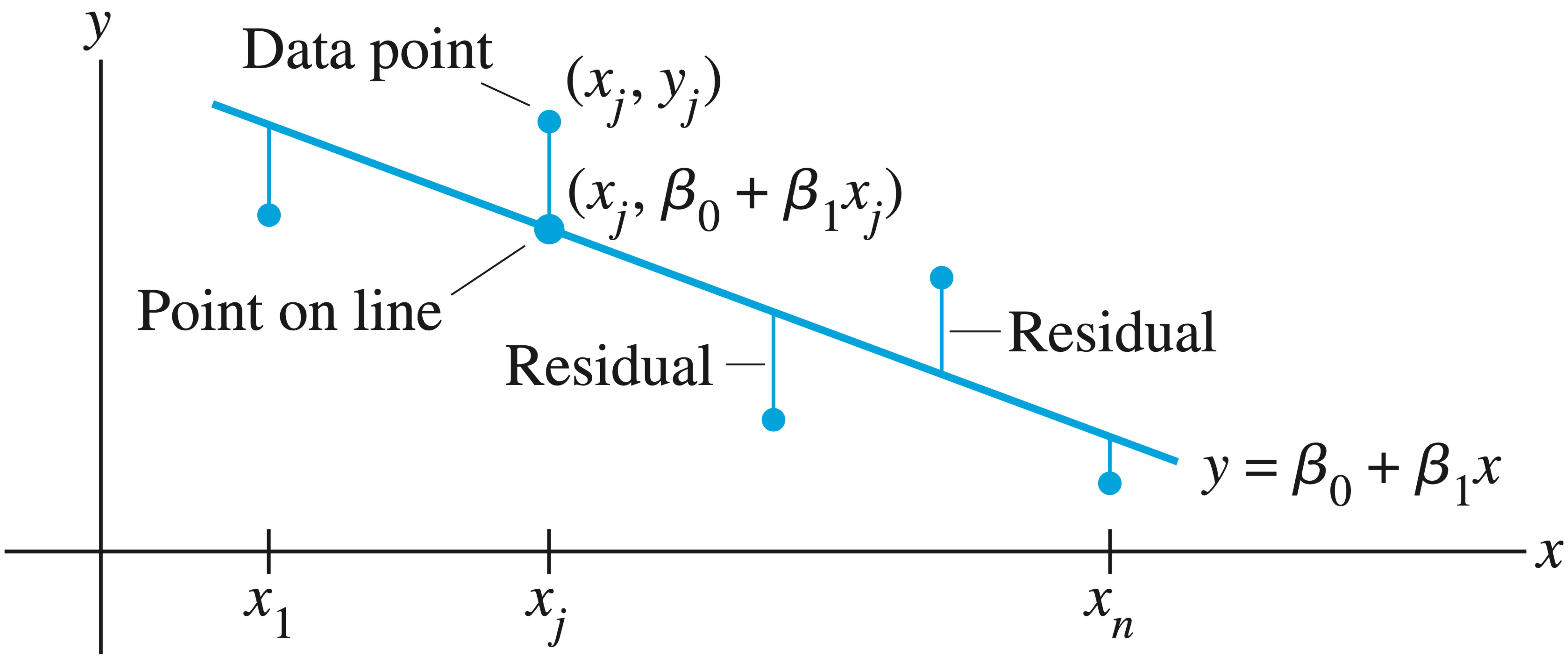
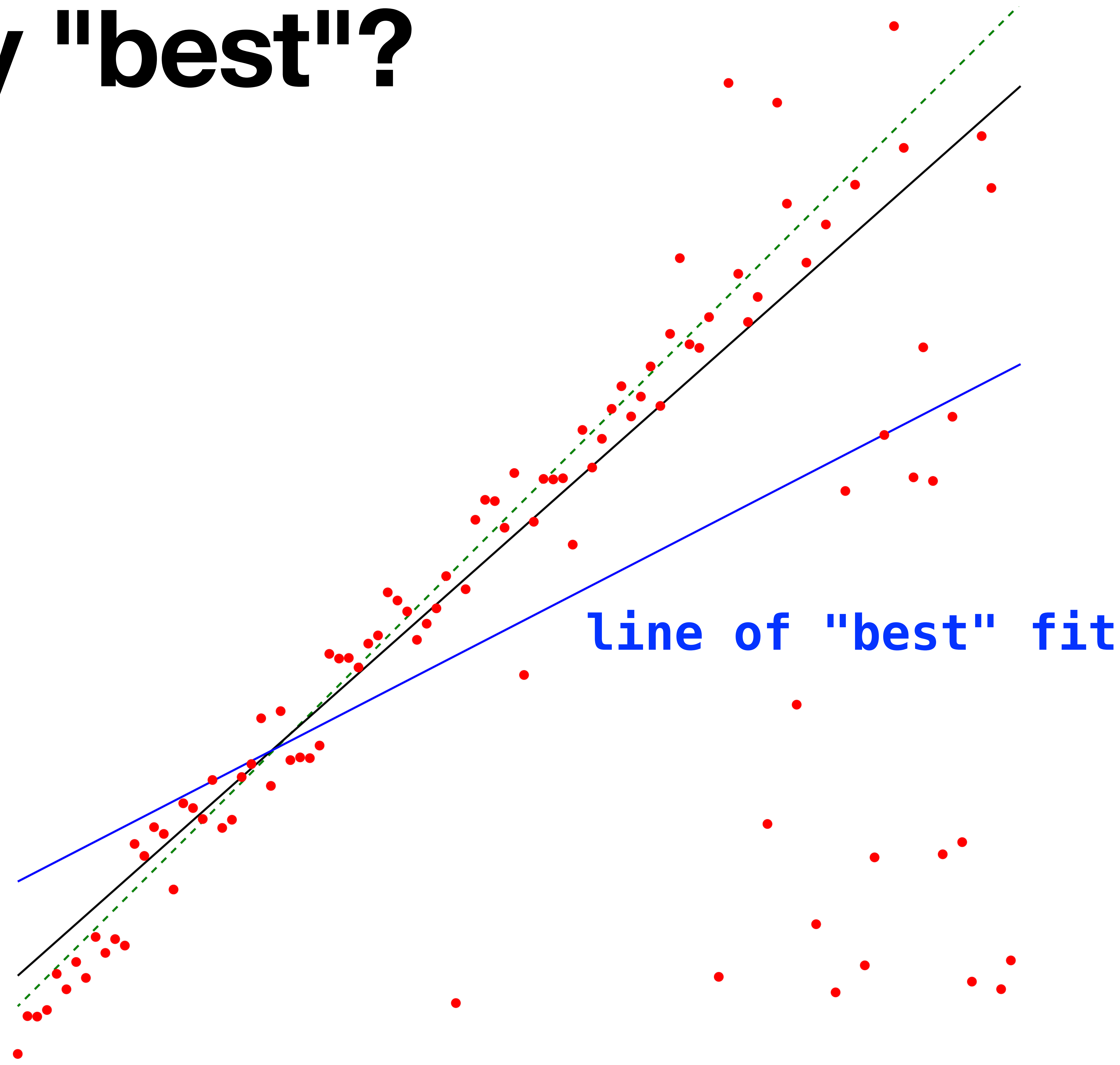
The "best" line minimizes the *sum of squares of differences.*

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"?



https://commons.wikimedia.org/wiki/File:Thiel-Sen_estimator.svg

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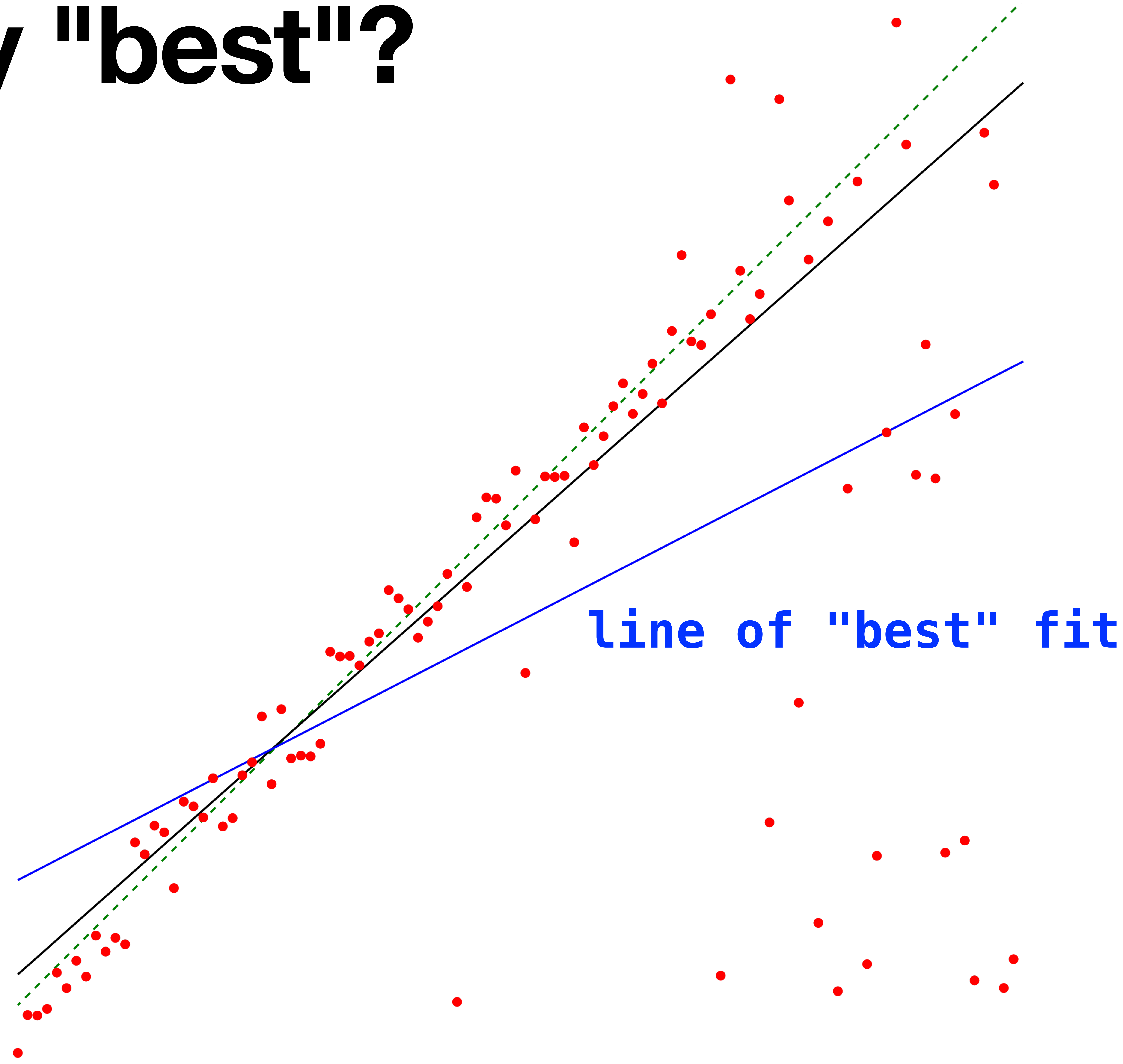

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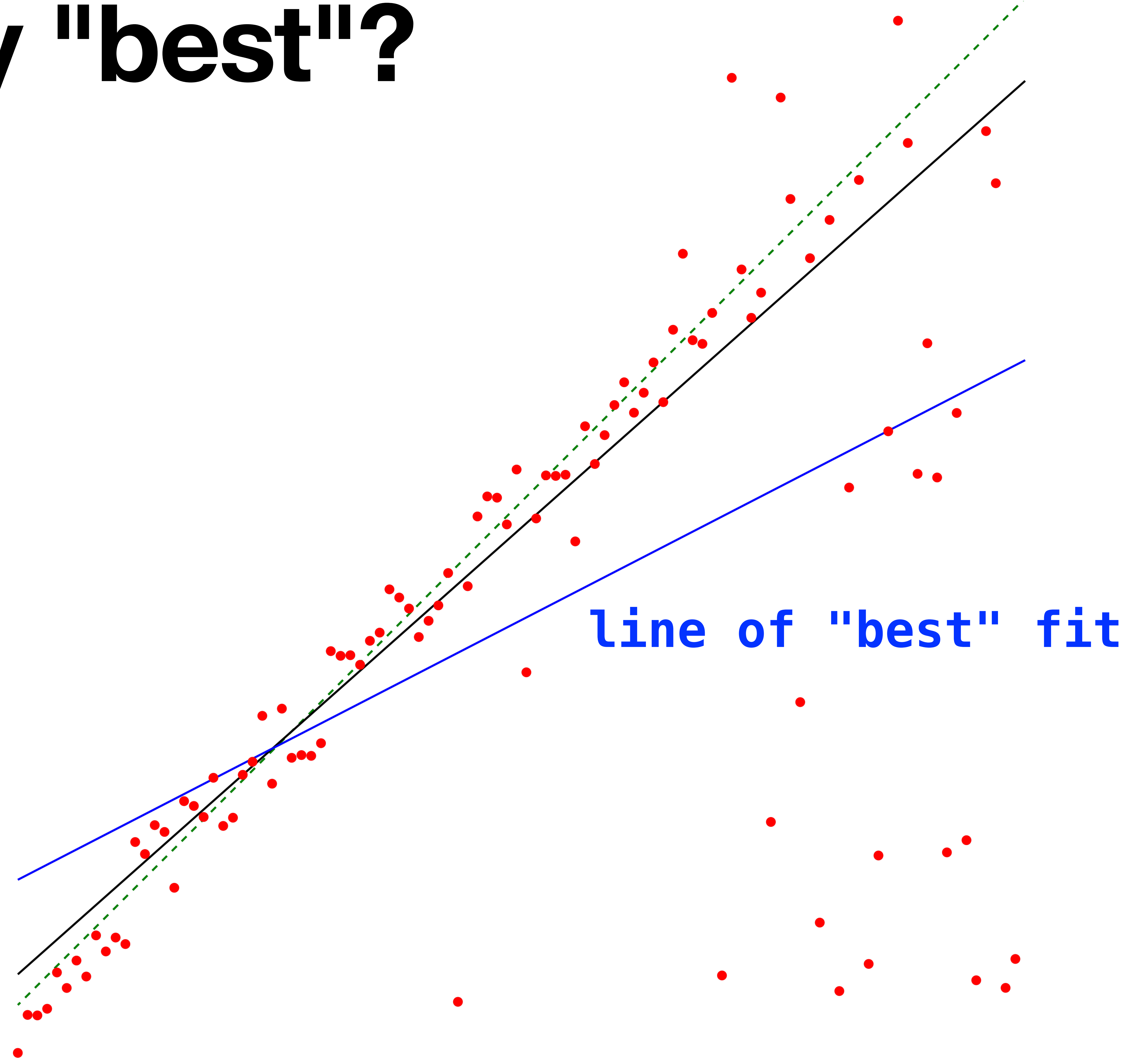
It depends on the data, on the application domain, etc.



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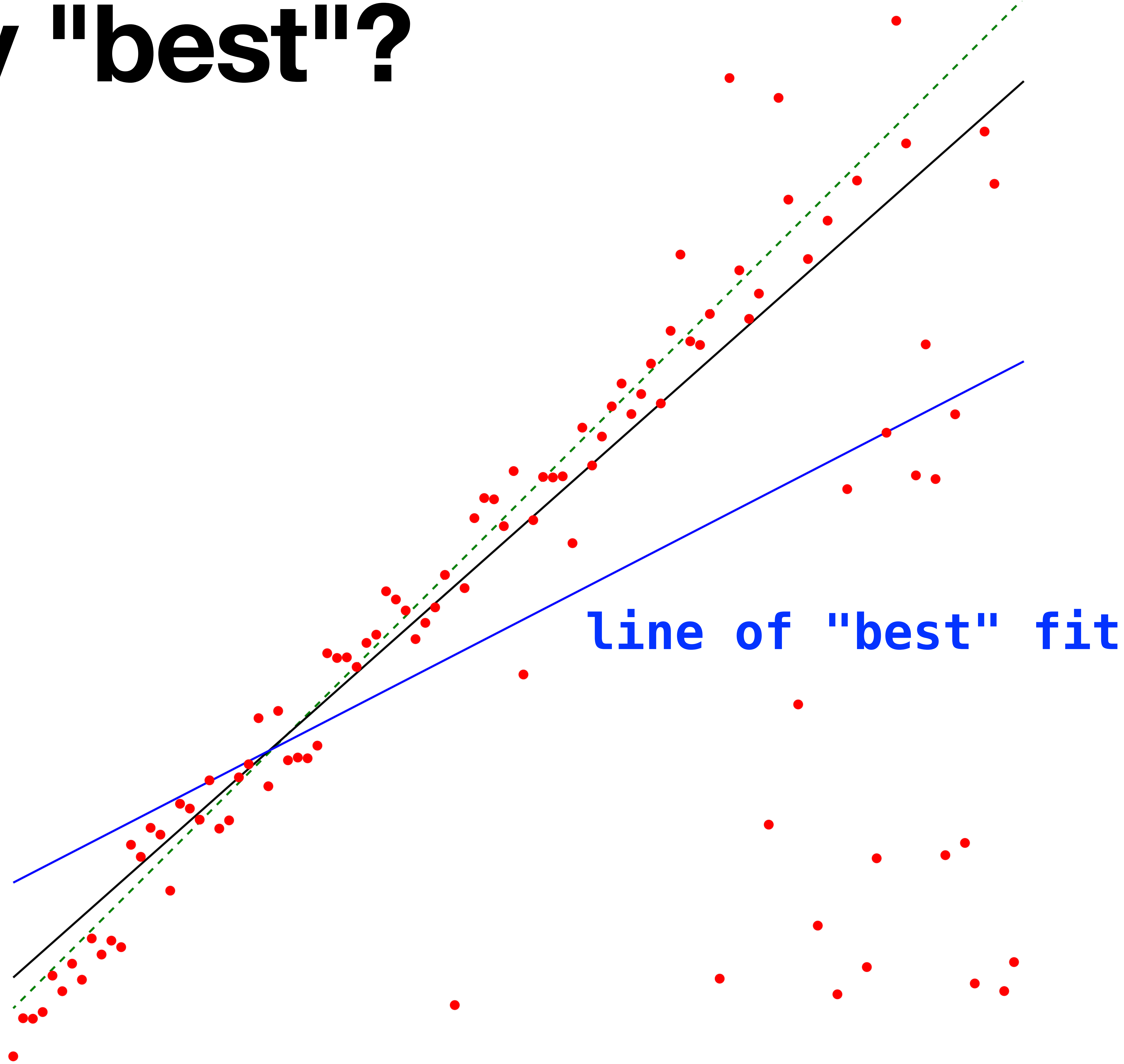
Who's to say...

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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dataset

$$(x_i, y_i)$$

Terminology: Datasets

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dataset

independent variable
(feature)

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Terminology: Datasets

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dataset

independent variable
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dependent variable
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Terminology: Models

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

Terminology: Models

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

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

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

residual

Terminology: Least-Squares Error

observation

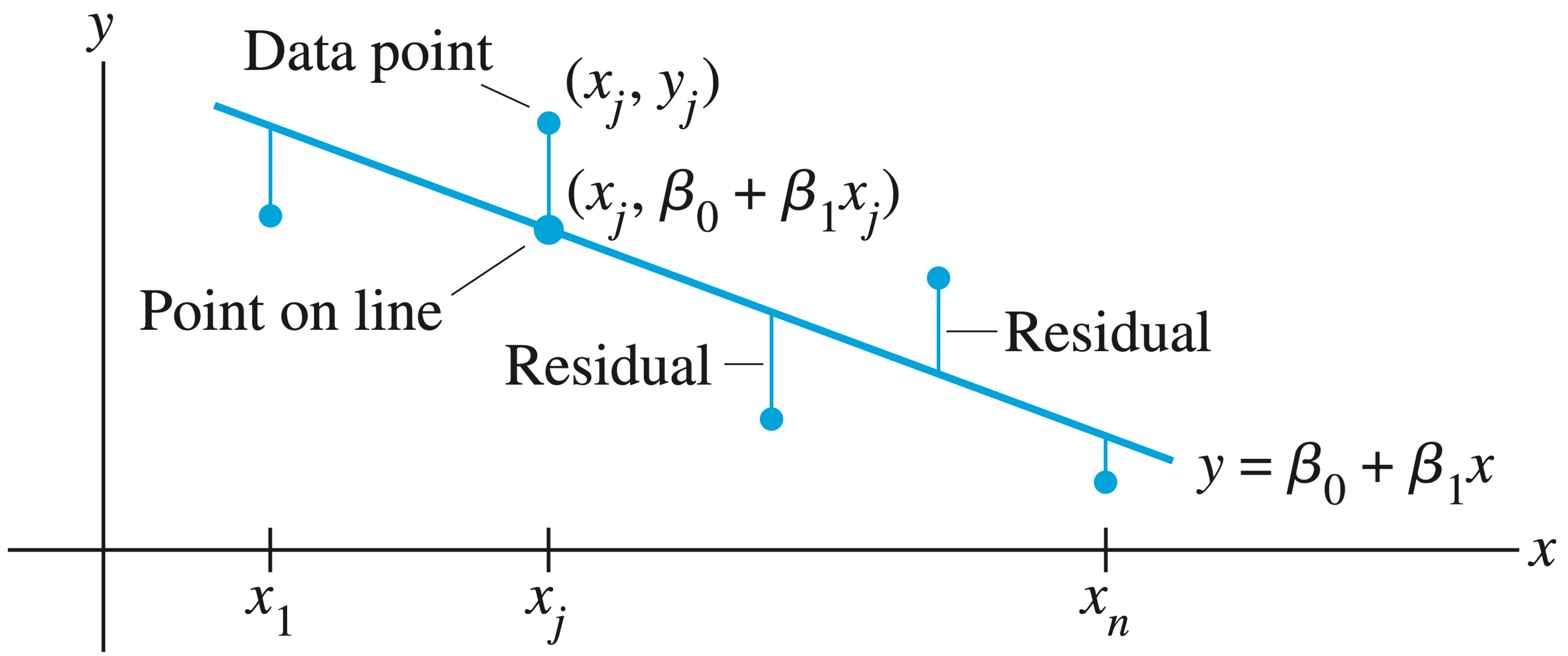
residual

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

Terminology: Least-Squares Error

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

Terminology



data point

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

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observation

residual

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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.

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An Observation

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

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

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minimize for least-squares line

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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.**

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

A Least Squares Problem

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$$\beta_0 + \beta_1 x_1 = y_1$$
$$\beta_0 + \beta_1 x_2 = y_2$$
$$\vdots$$
$$\beta_0 + \beta_1 x_n = y_n$$

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,
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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

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

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

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 $\mathbf{y}$.

A Least Squares Problem

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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

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

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

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

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

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

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

Just for Fun

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

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

`Let's derive it:`

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

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

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

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

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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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.

Question

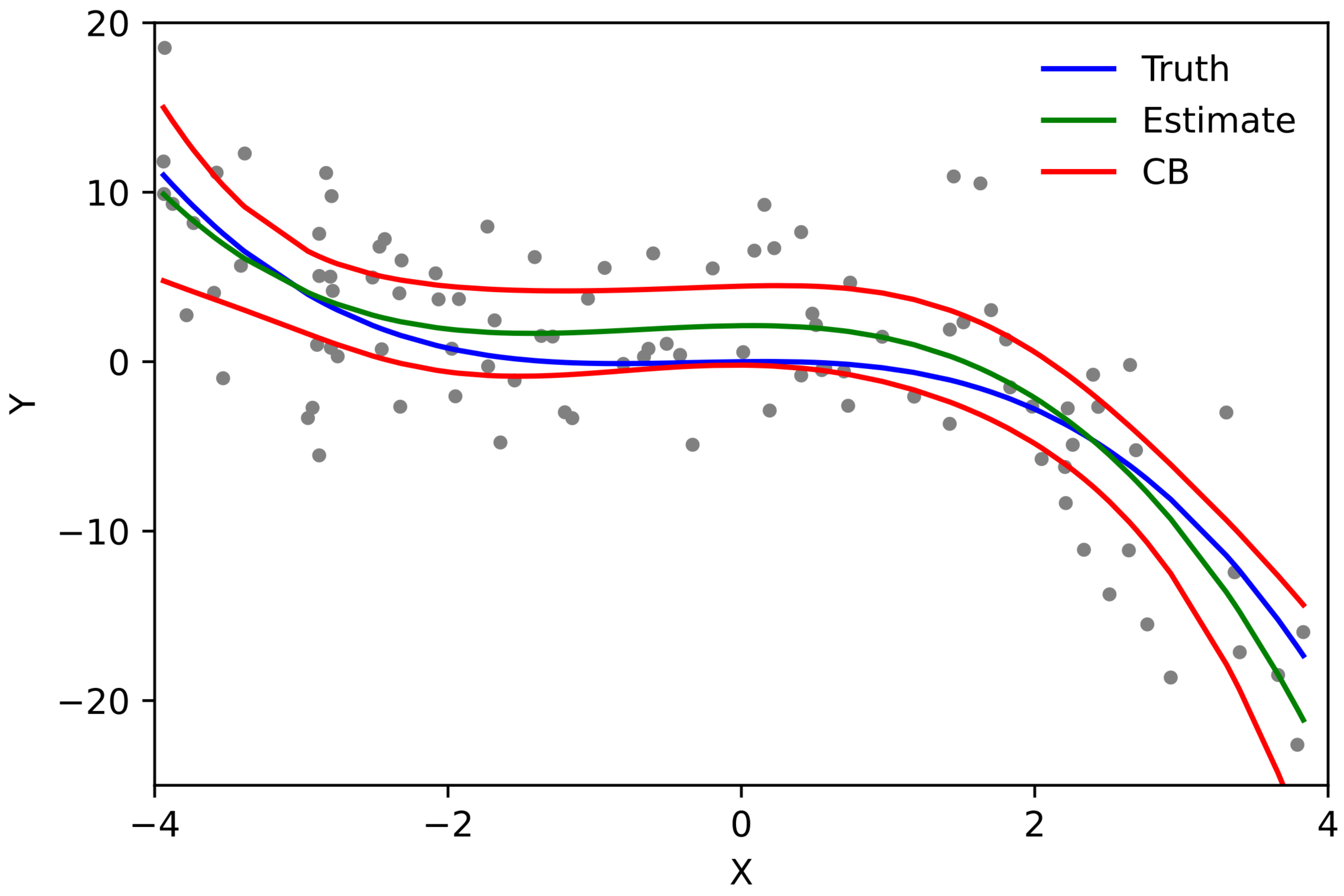
Find the line of best fit for the dataset

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

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.

General Regression



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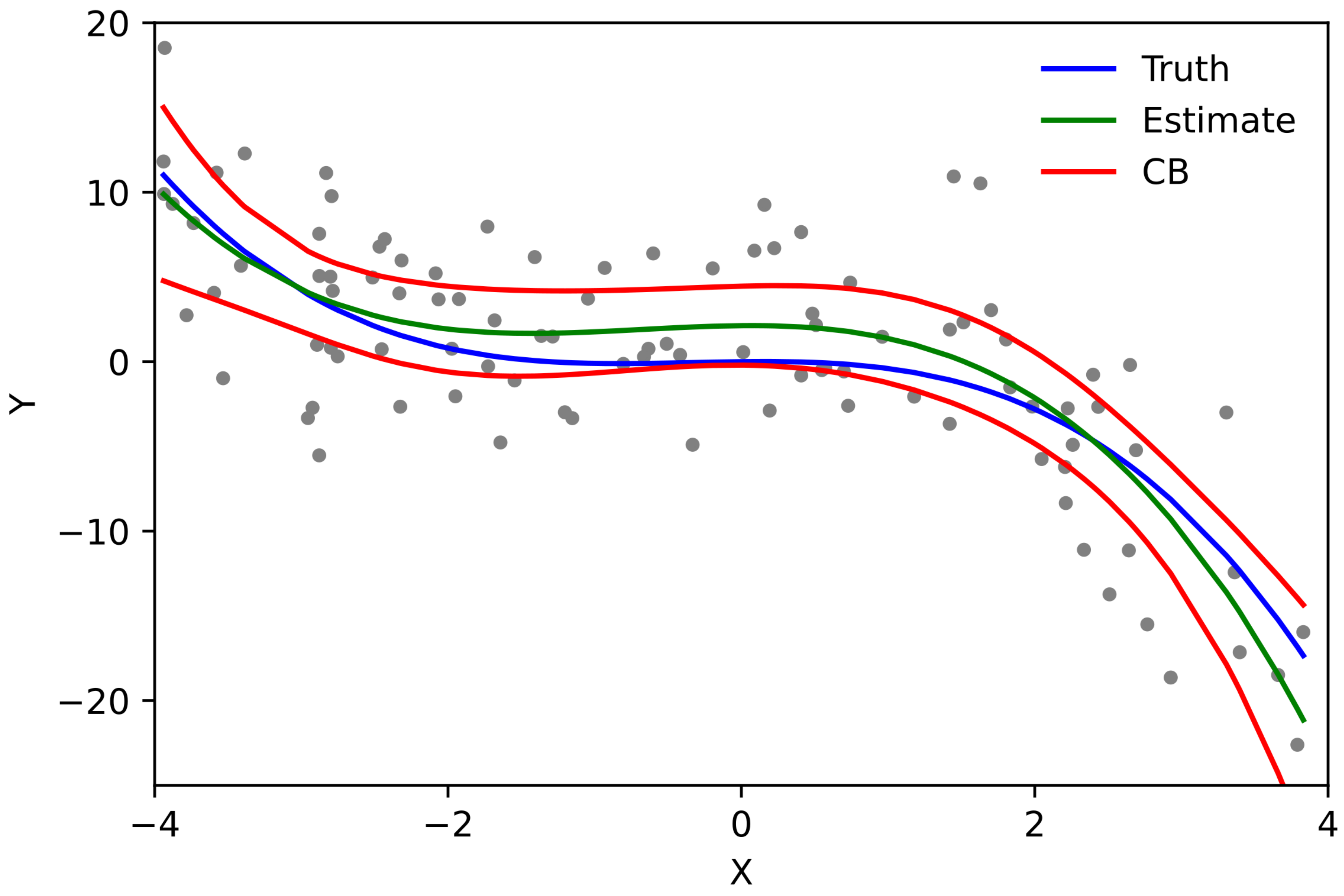
General Regression

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



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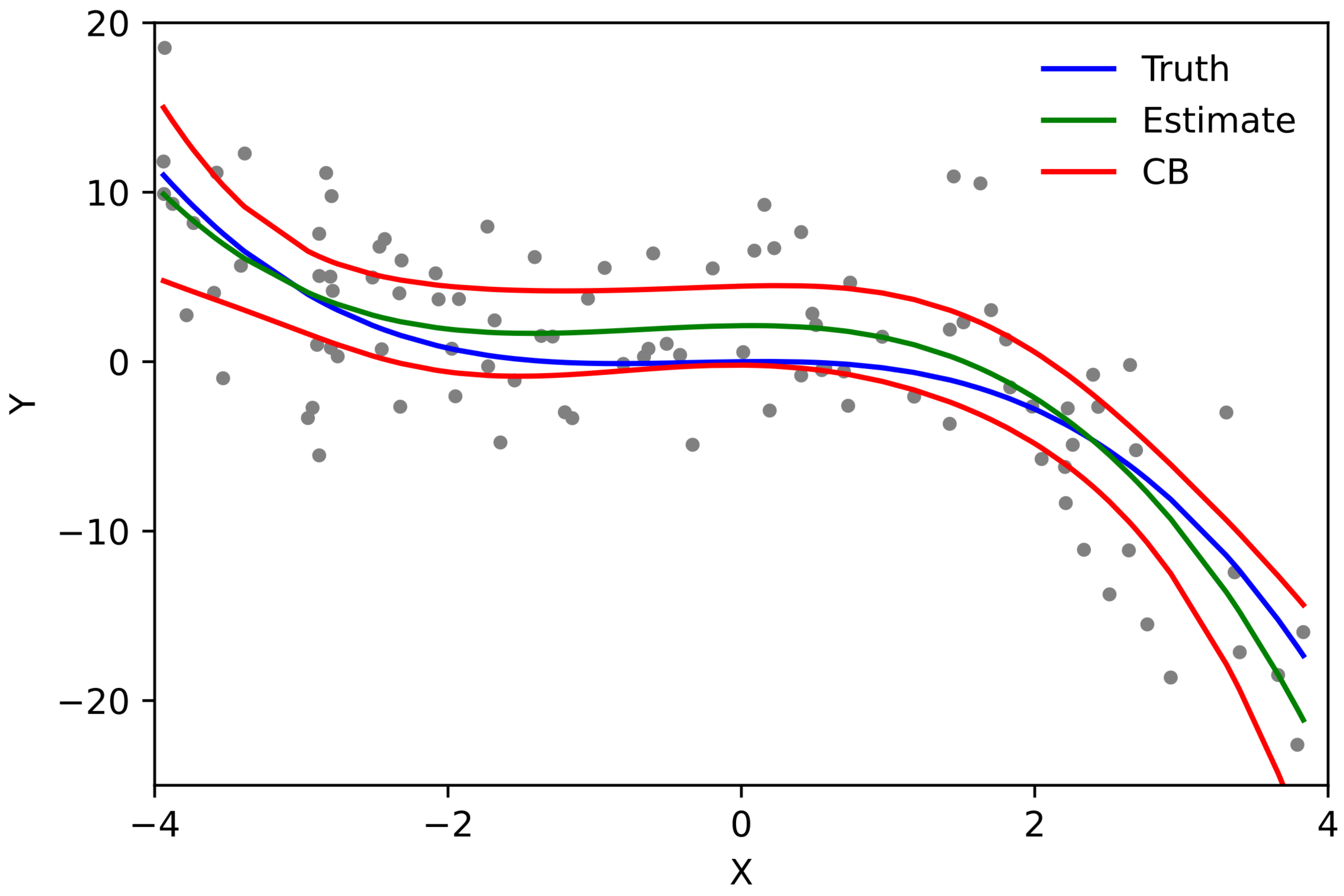

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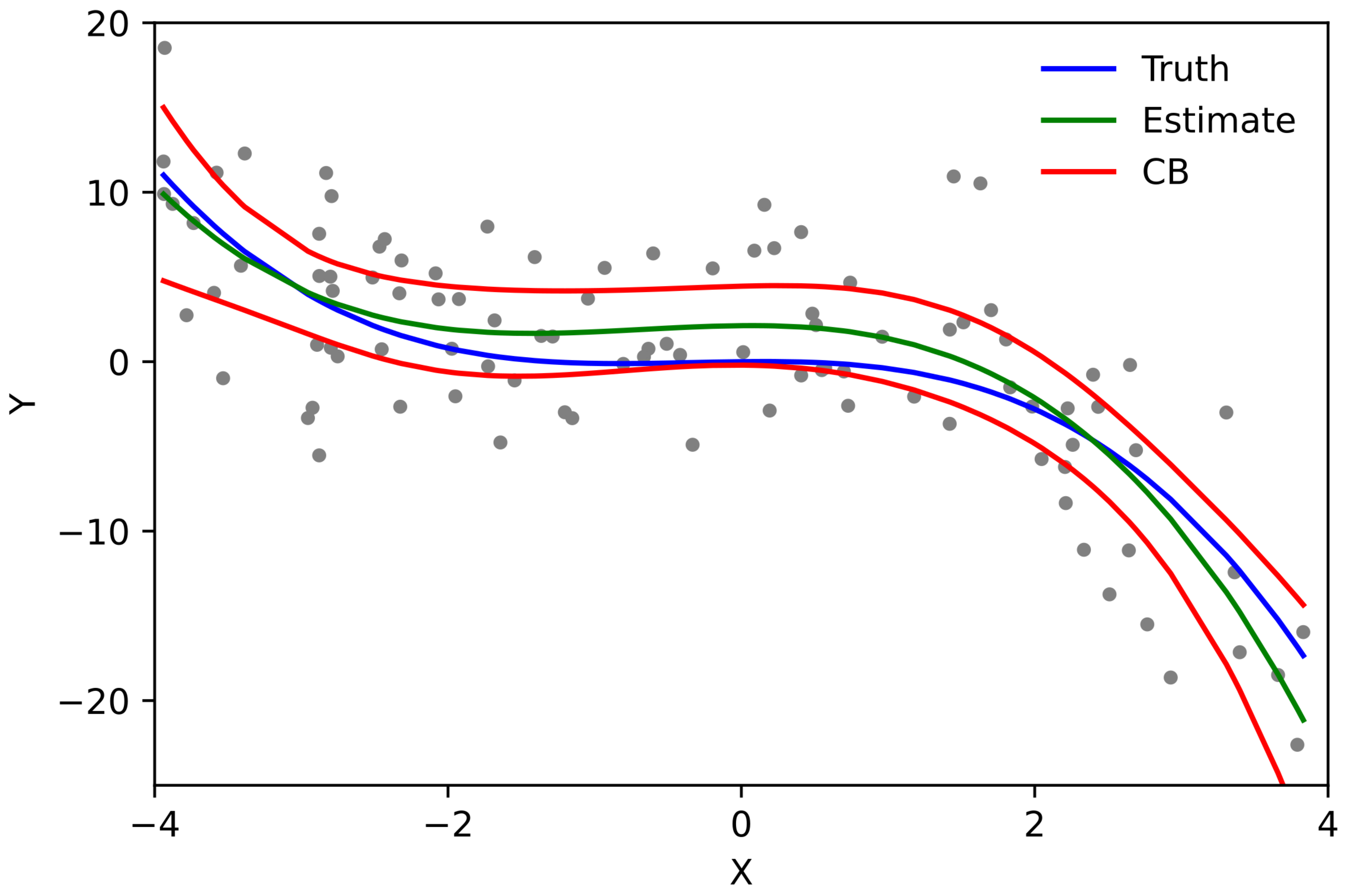
Regression is the process of estimating the relationships independent and dependent variables in a dataset.

What we are estimating is a mathematical function

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



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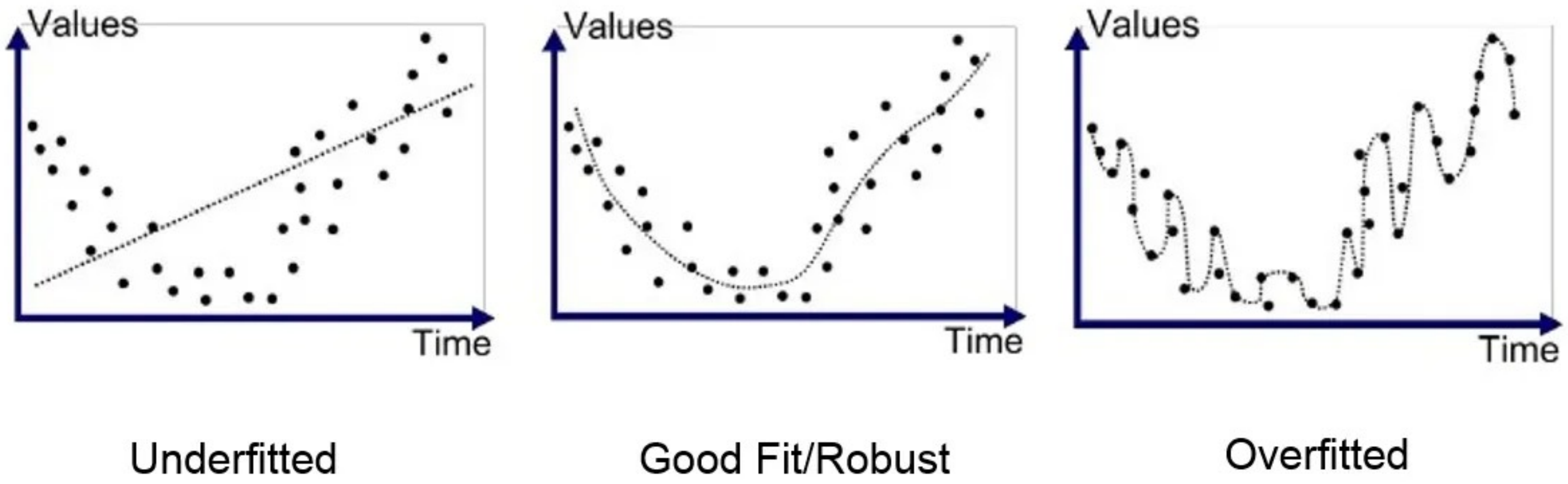
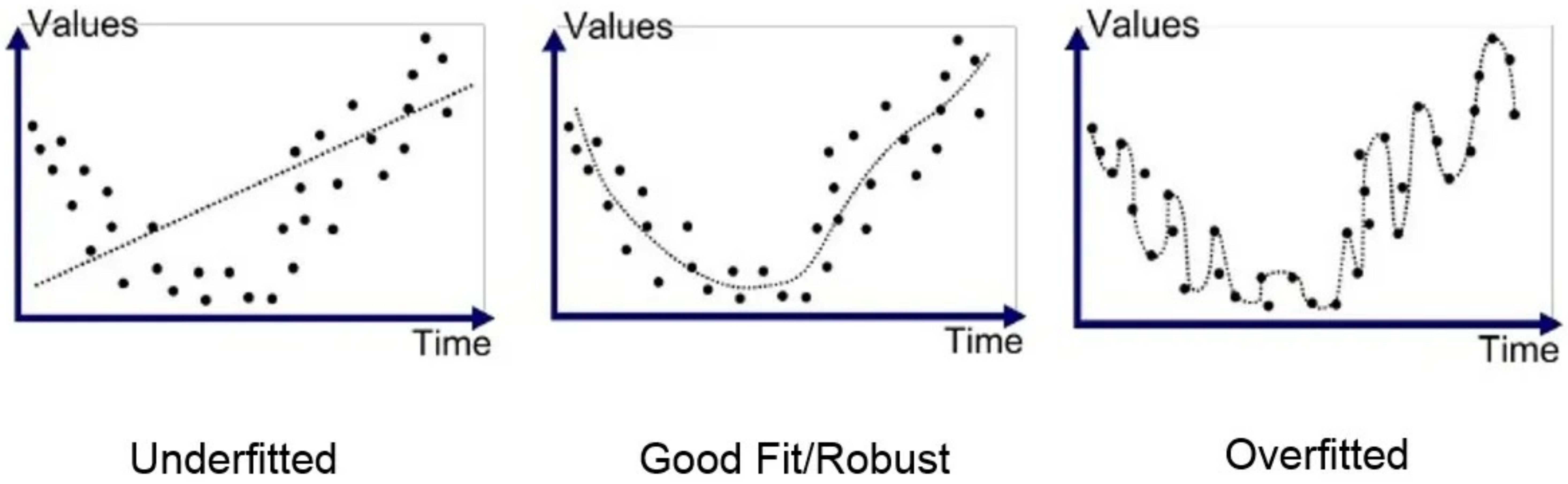
Models



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

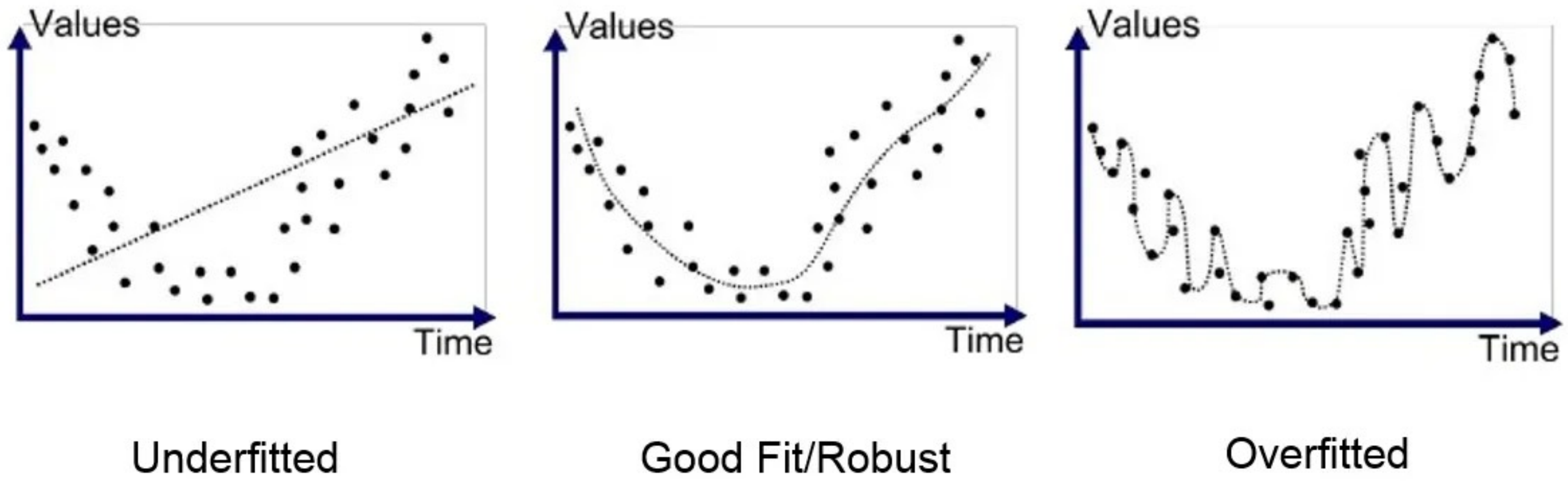
Models



Therefore, a *model* is a mathematical function.

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

Models



Therefore, a *model* is a mathematical function.

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

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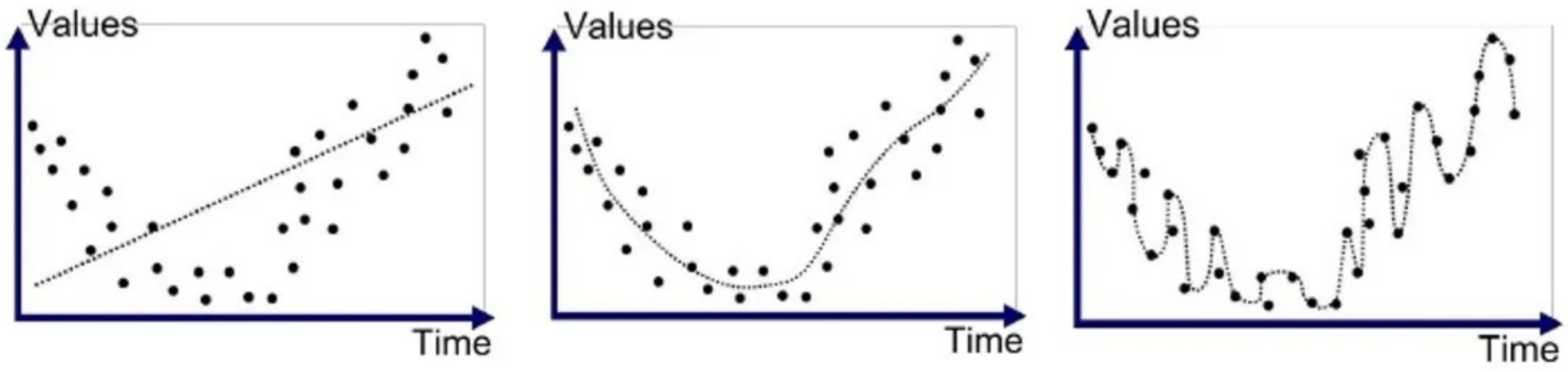

Underfitted Good Fit/Robust Overfitted

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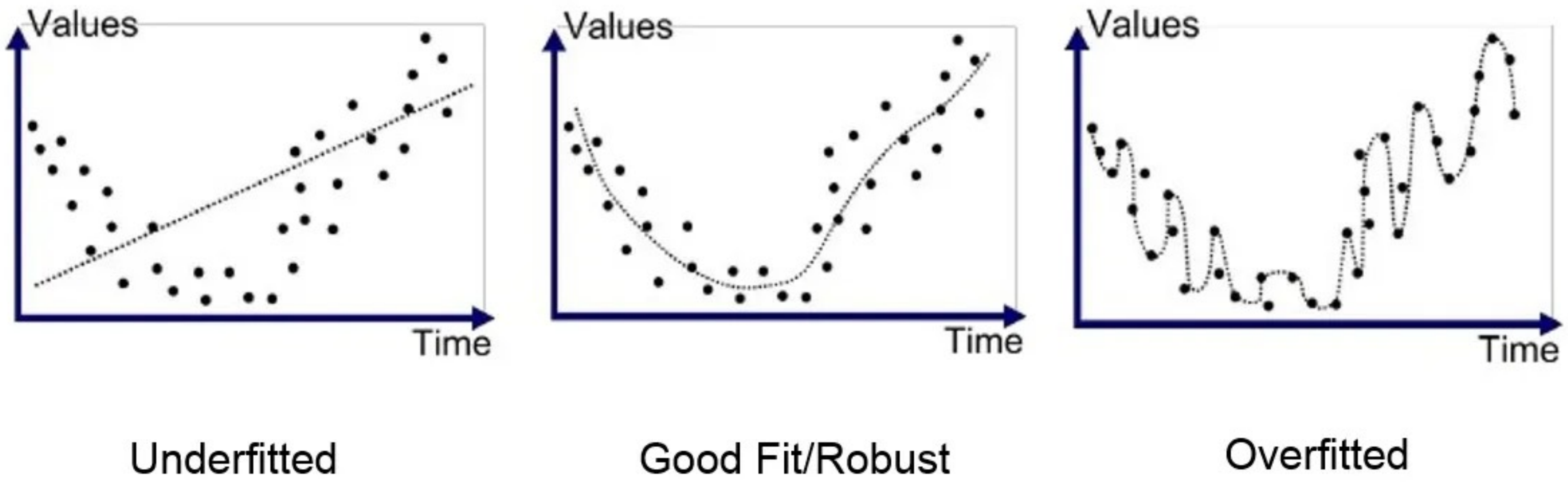

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But this would a bit boring if we *just* wanted to model data we've seen.

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

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How To: Prediction

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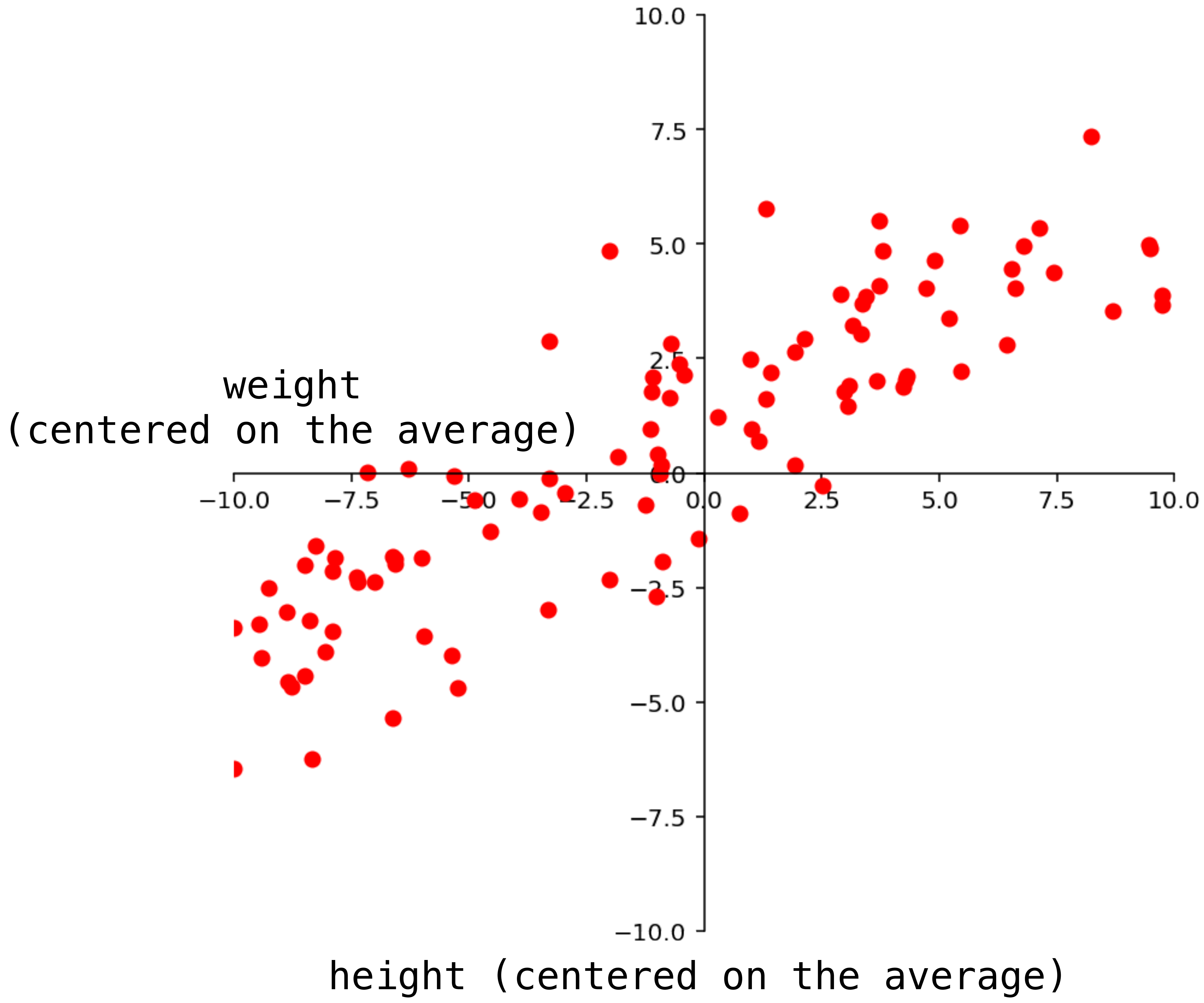
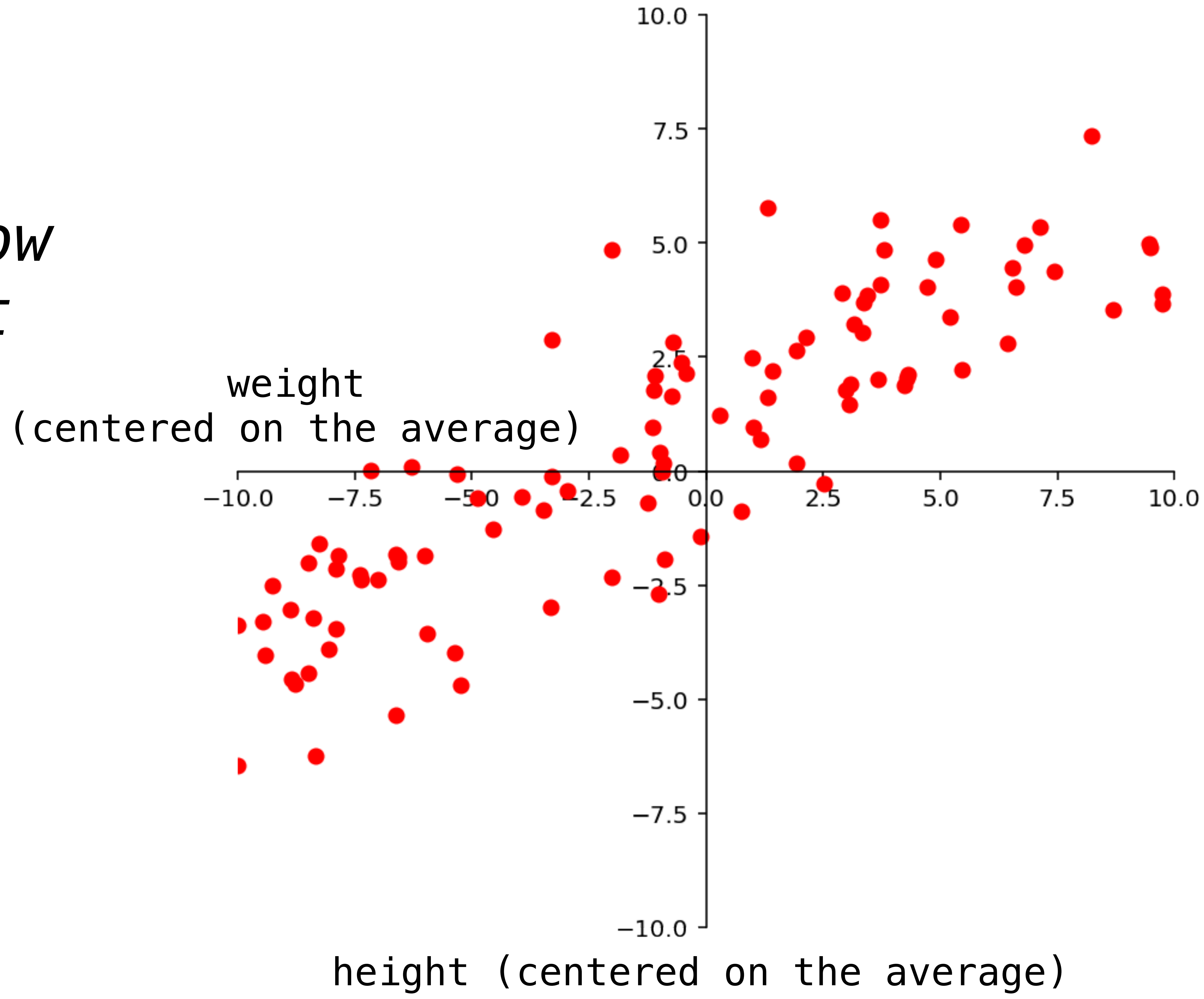
This generalizes to any model fitting problem

Example: Height from Weight



Example: Height from Weight

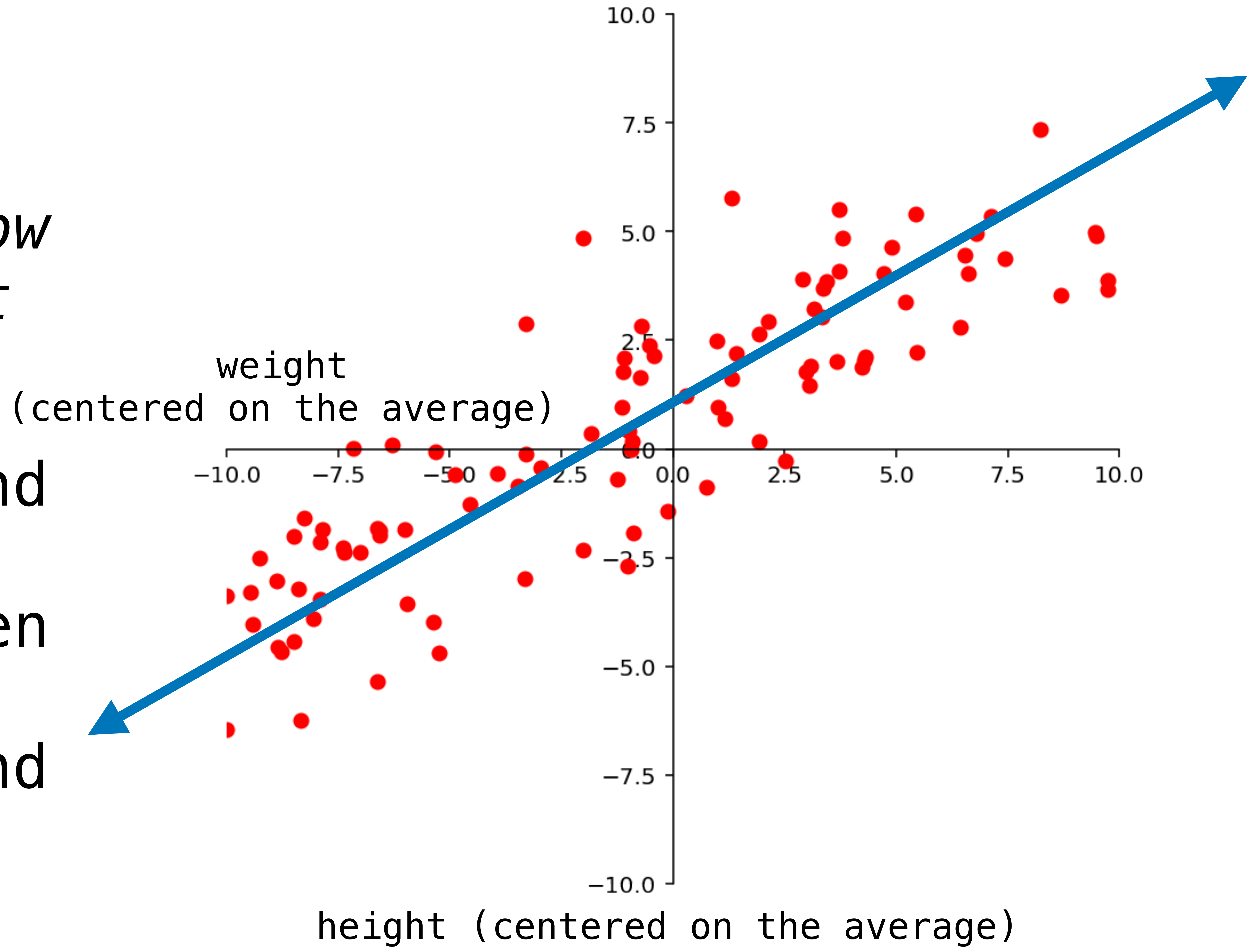
Suppose we know that person X weighs 150lb. *How would we guess the height of person X?*



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.



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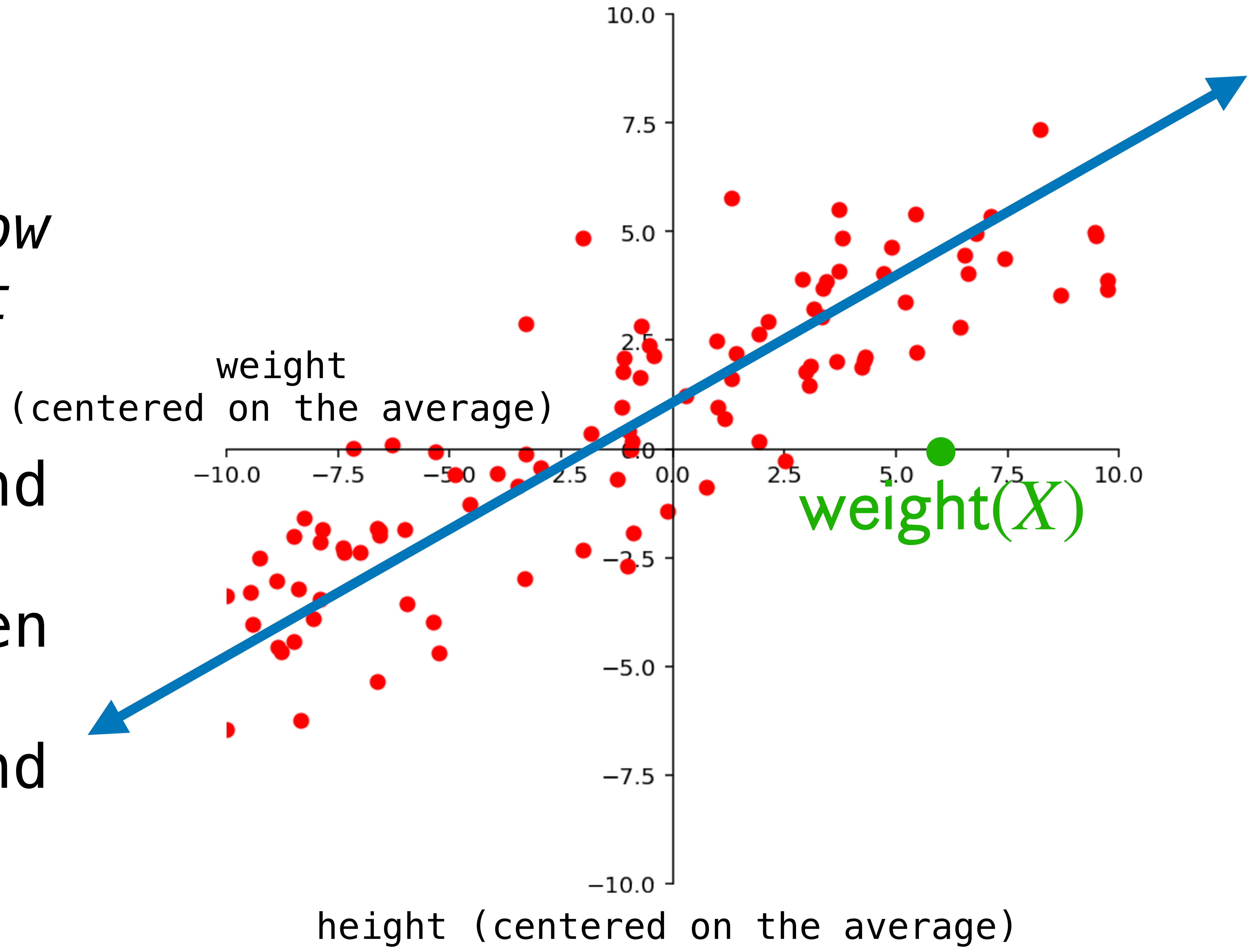

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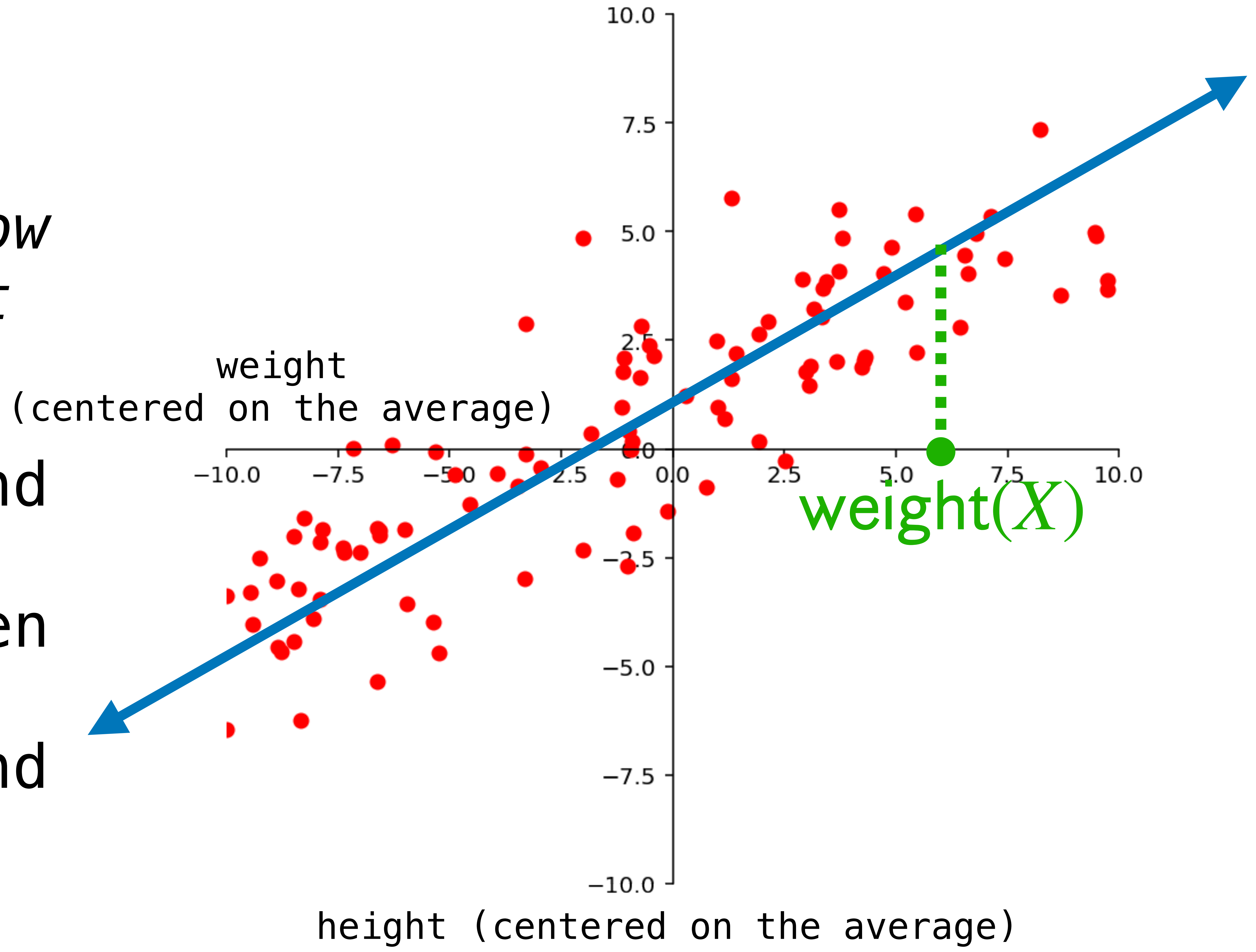

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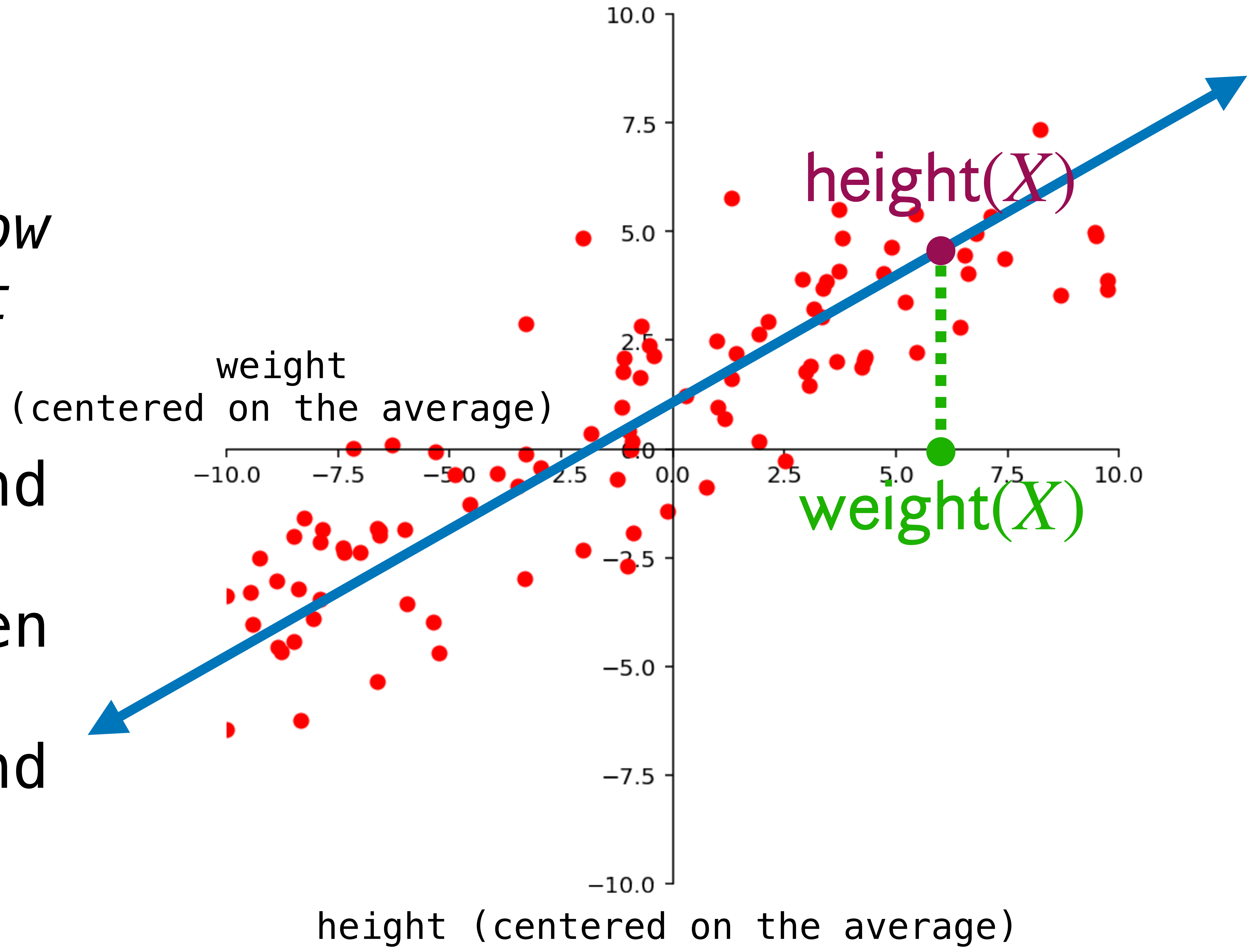

Question

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

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

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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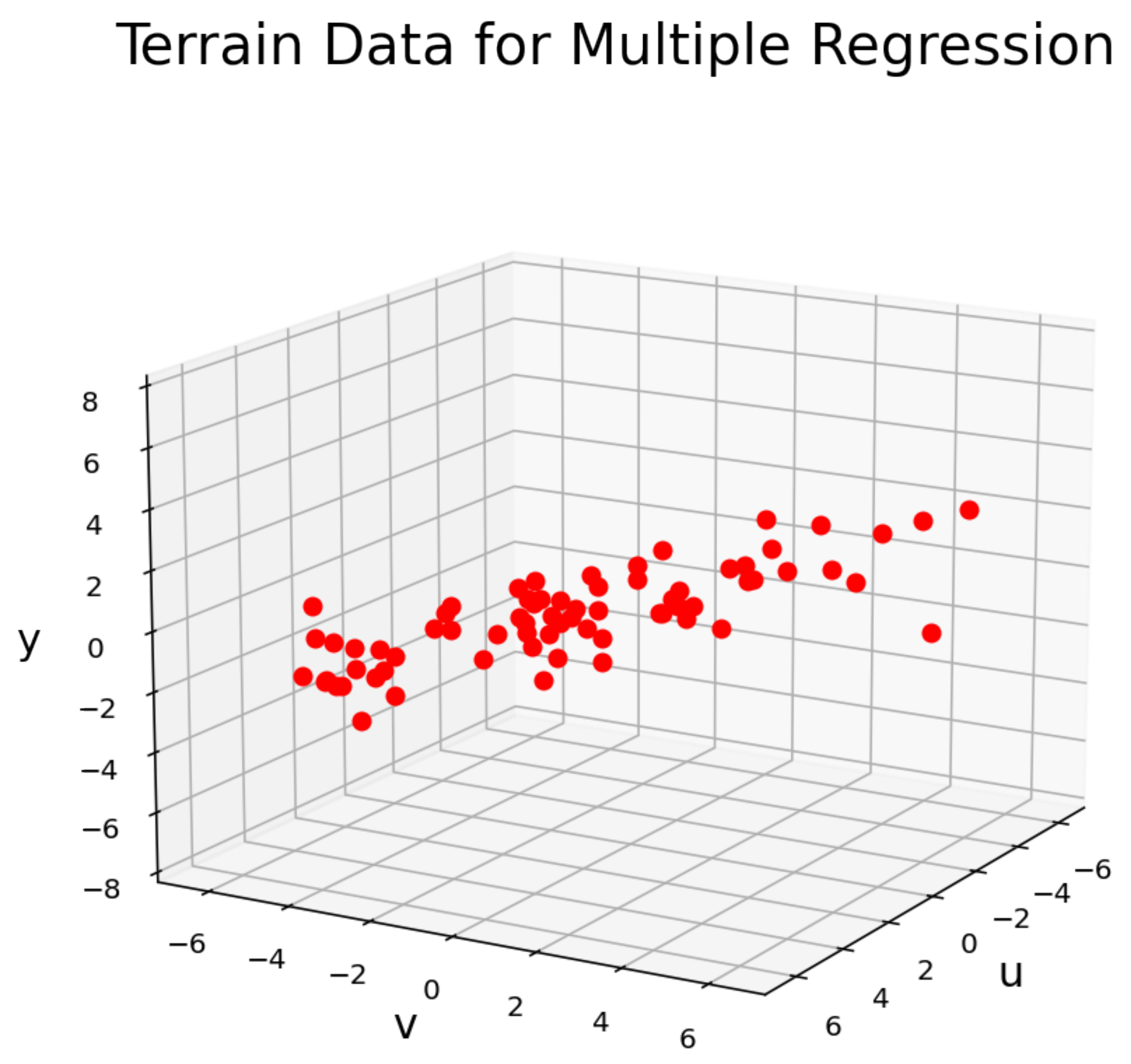
Example: Terrain Data

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

Figure 23.1



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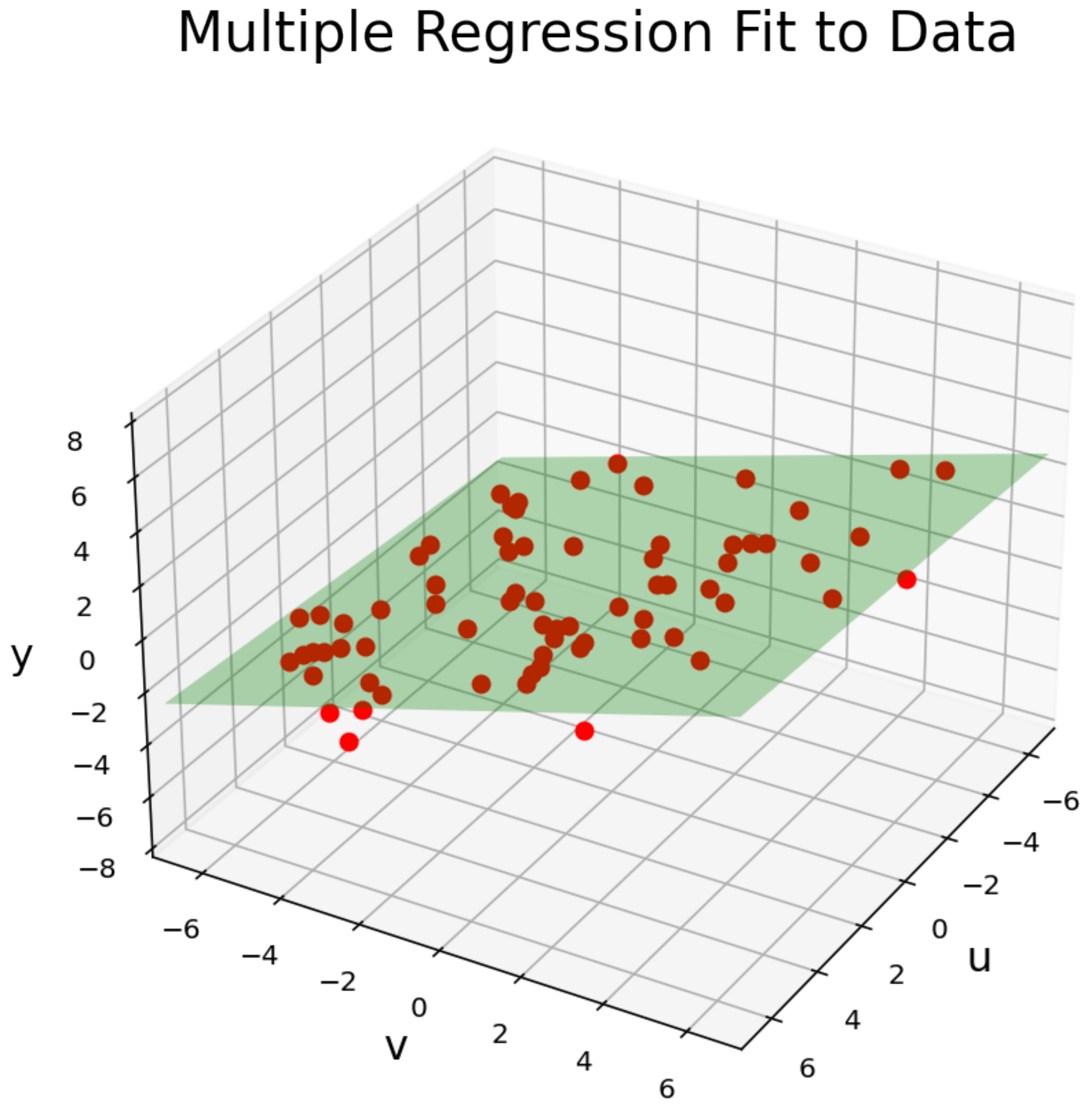
Problem: Find $\beta_0, \beta_1, \beta_2$ such that

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

which minimizes

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

Figure 23.2



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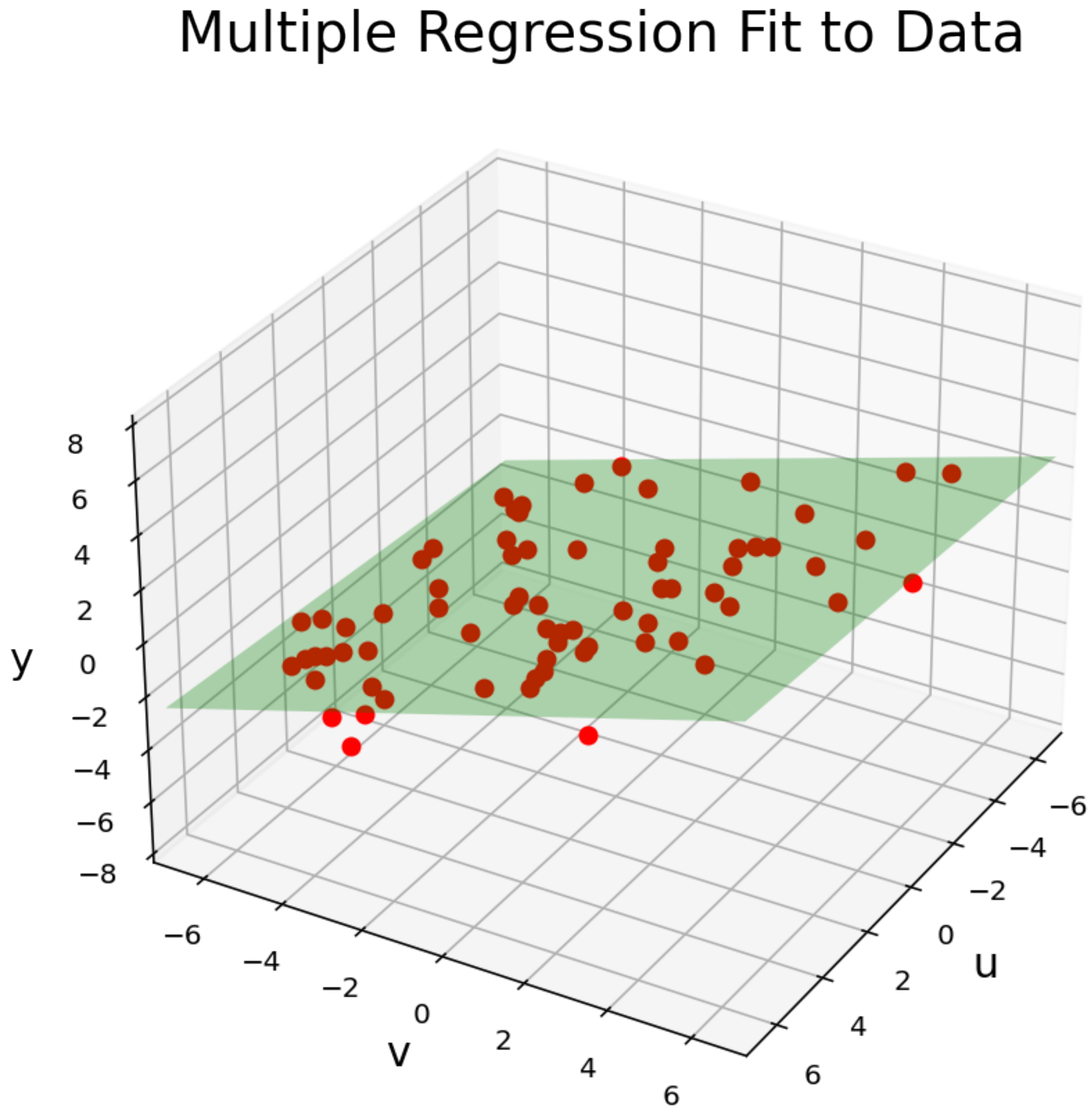

$f(x, y)$ is a good approximation of the altitude.

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recall: planes are given by linear equations

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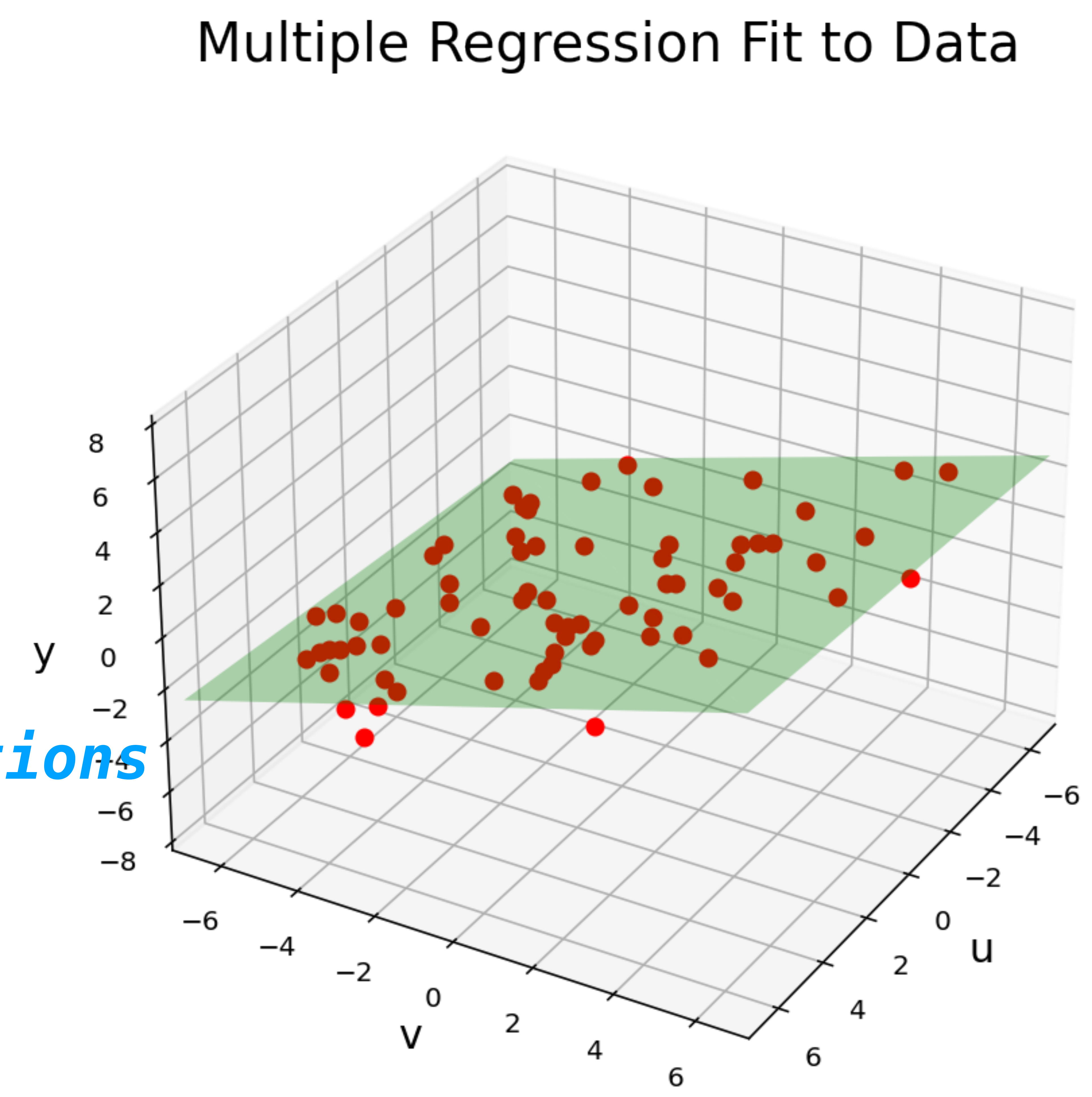

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$$\overset{X}{\begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ \vdots & \vdots & \vdots \\ 1 & x_k & y_k \end{bmatrix}} \overset{\vec{\beta}}{\begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}} = \overset{\mathbf{z}}{\begin{bmatrix} z_1 \\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

Step 2: Rewrite the system as a matrix equation.

Example: Terrain Data

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

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

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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.

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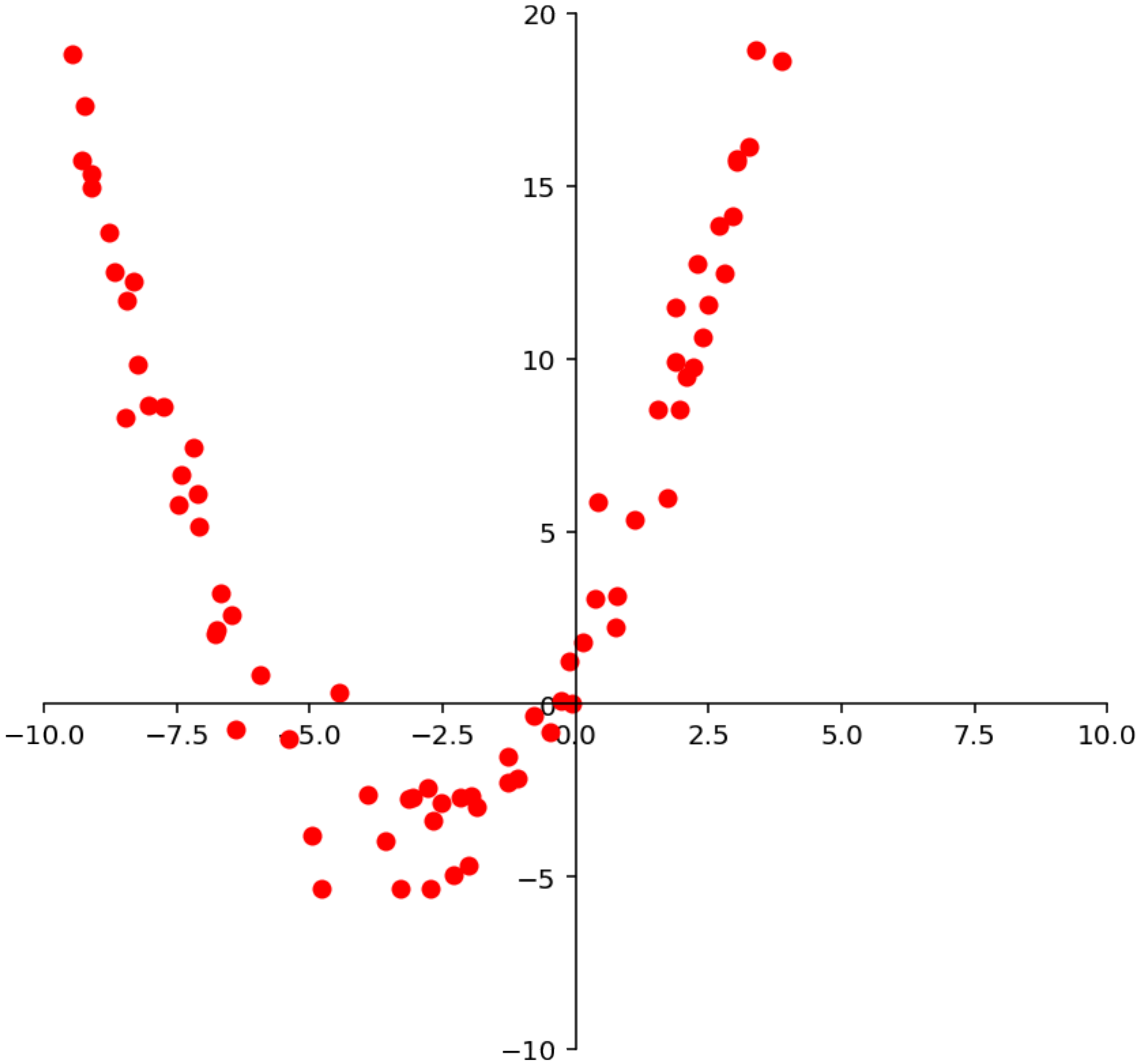

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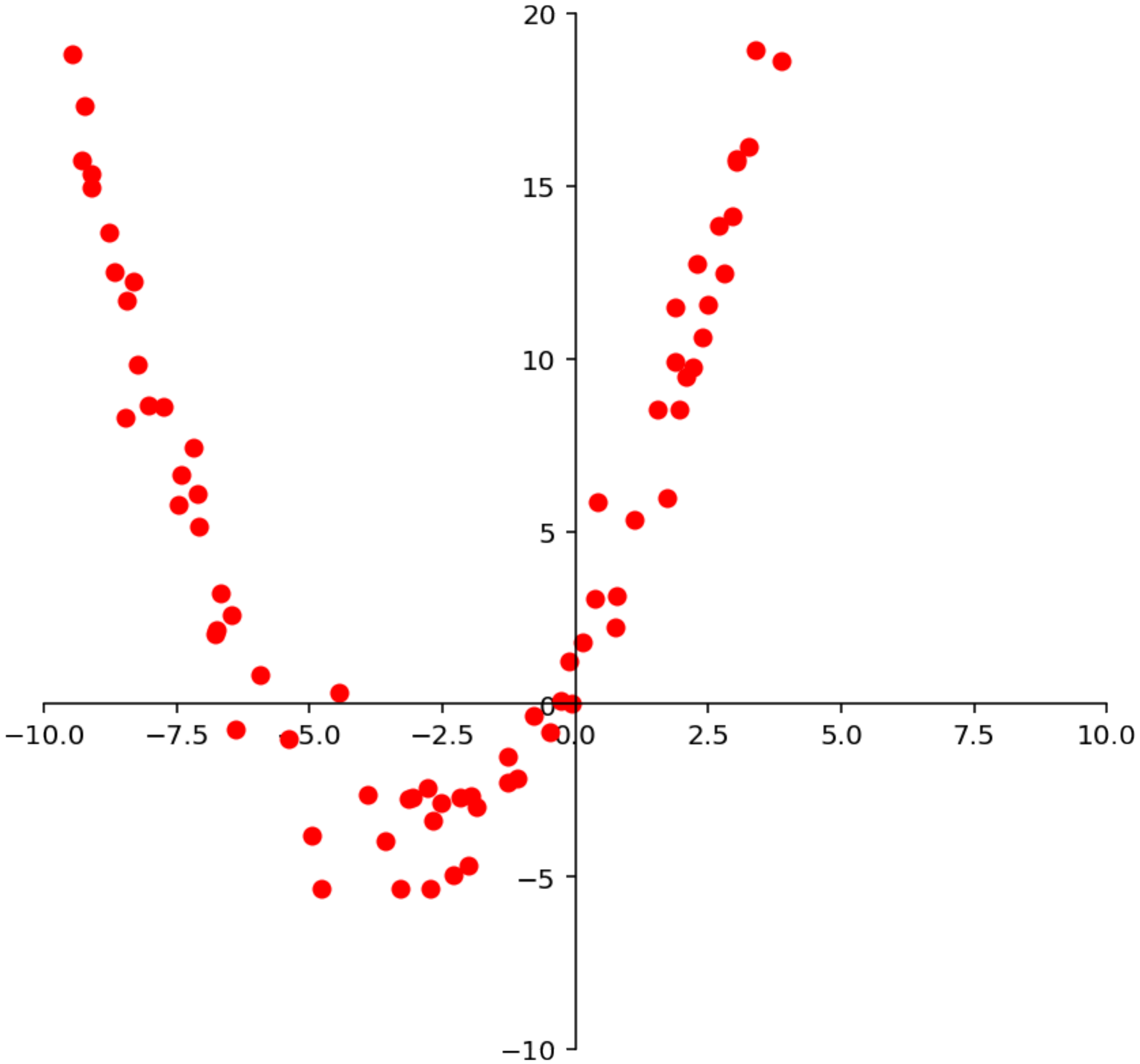
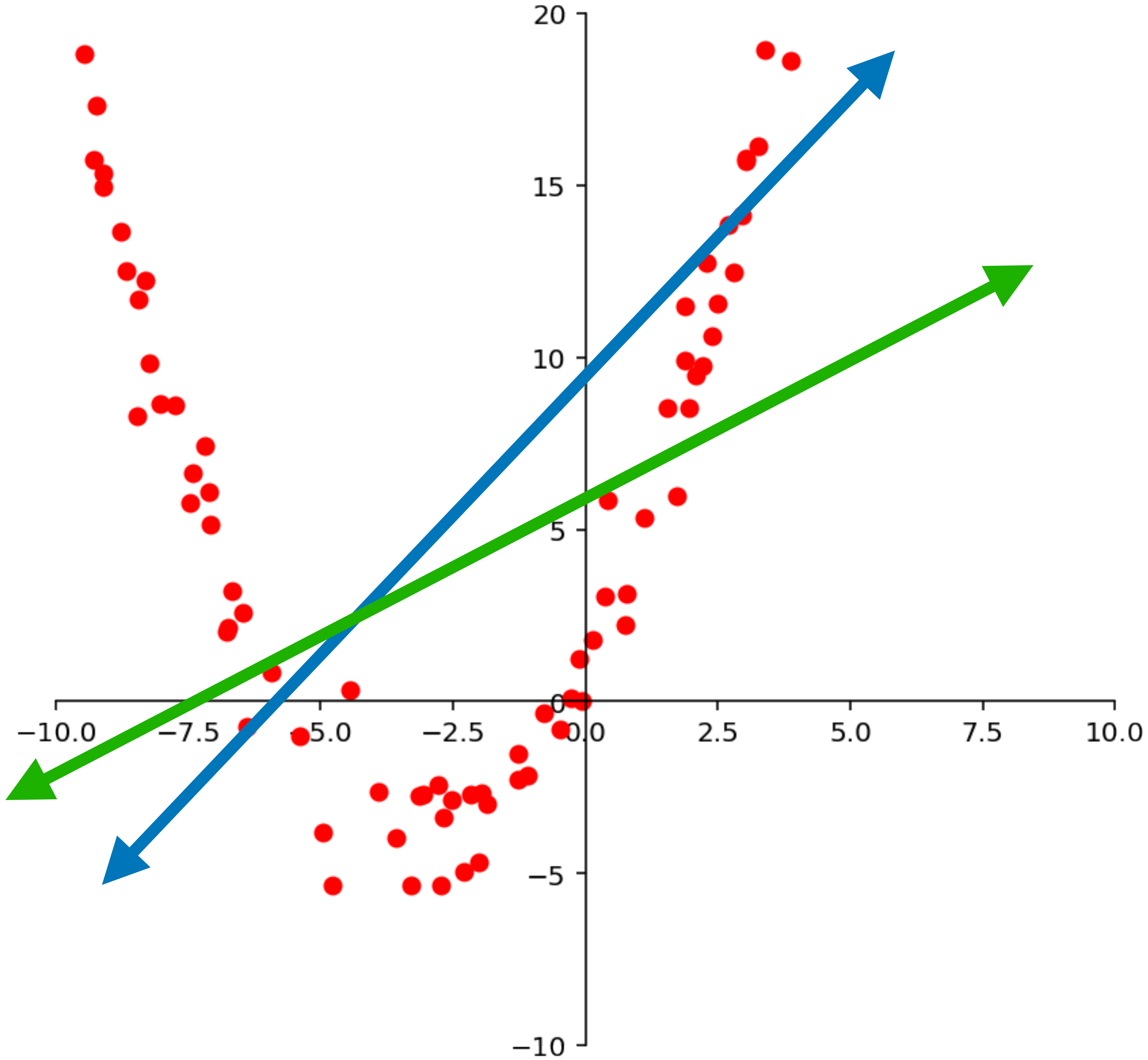
Dataset: $\{(x_1, y_1), \ldots, (x_k, y_k)\}$



Example: Best Fit Quadratic

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

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



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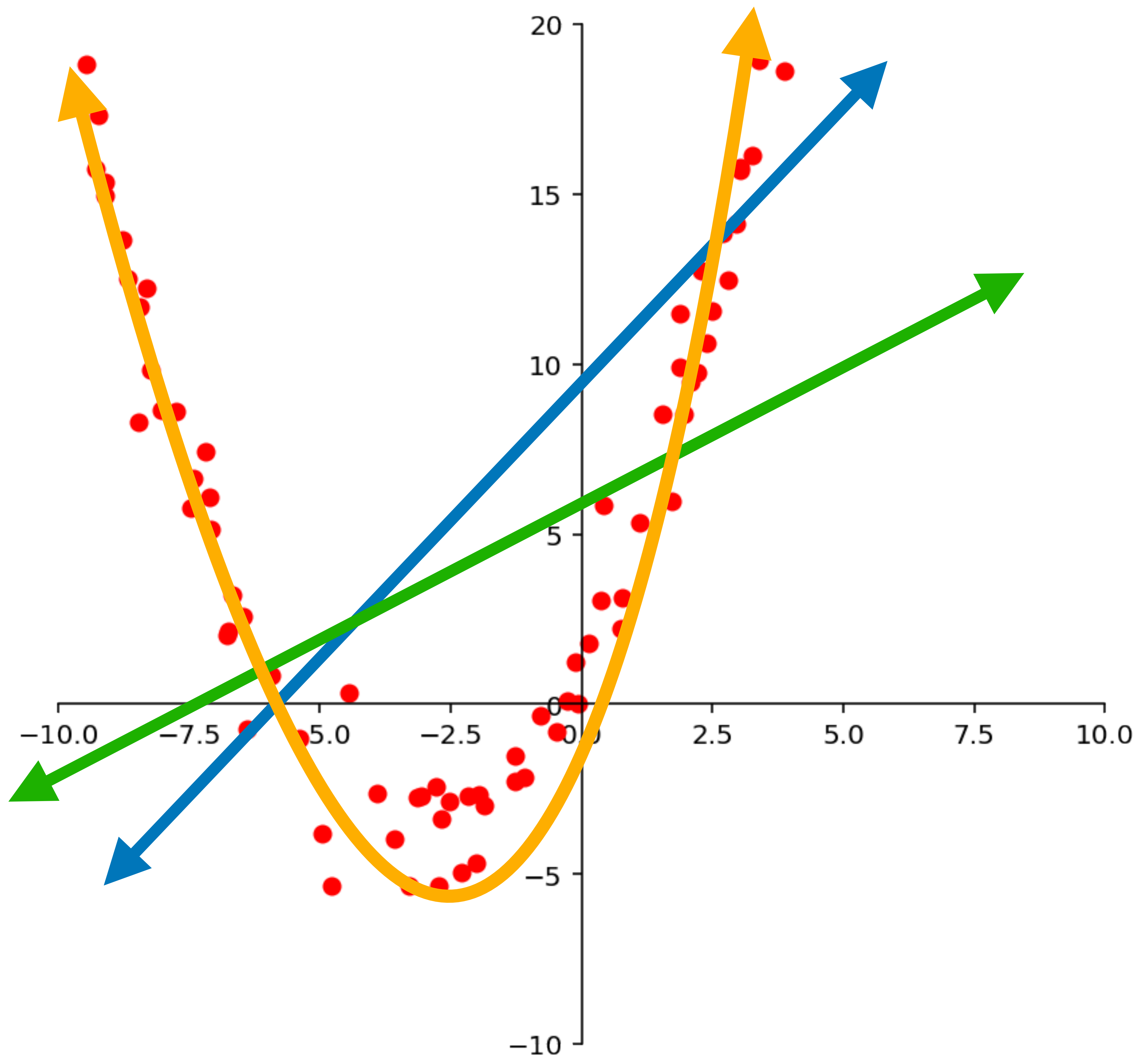
What about a parabola?



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minimizes

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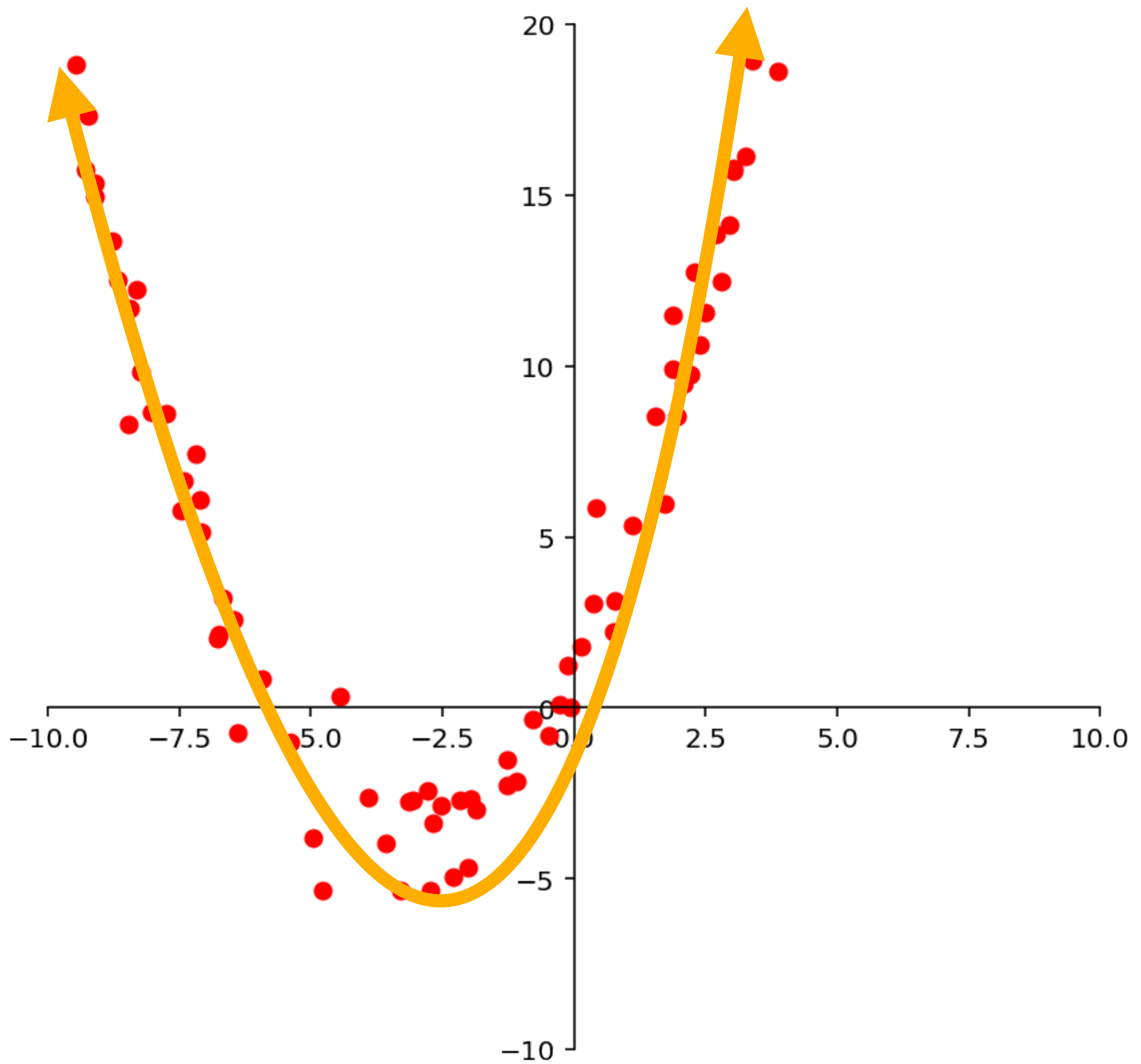

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\vdots \\
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\end{gathered}$$

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

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

The Takeaway

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

Linear in Parameters

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:

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

General Linear Regression

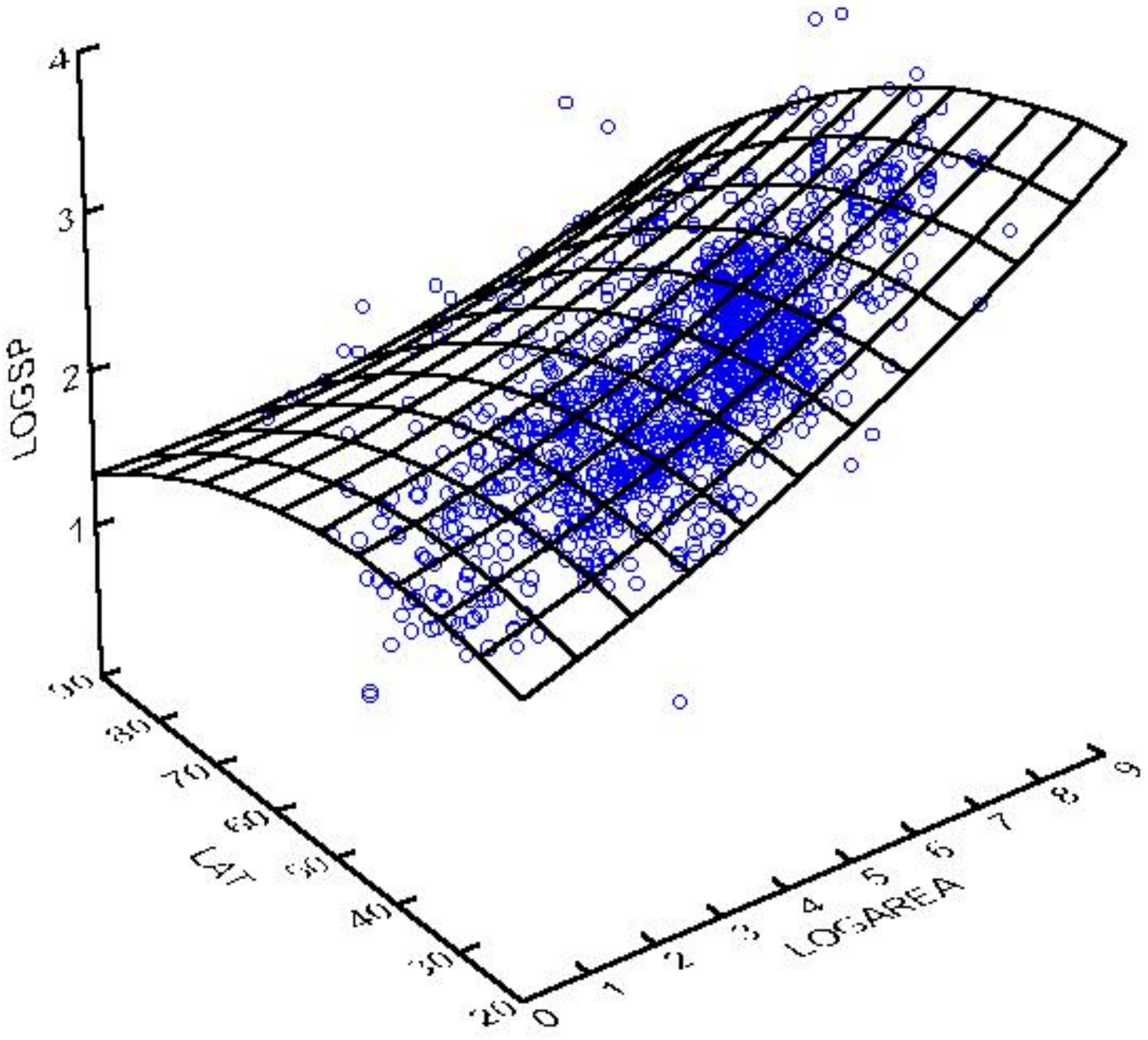
dataset: $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$ where $\mathbf{x}_i \in \mathbb{R}^n$ and $y_i \in \mathbb{R}$

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

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$$\begin{aligned}
\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 \\
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design matrix

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

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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

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

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

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

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

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.