Linear Models

Geometric Algorithms
Lecture 24

CAS CS 132

Introduction

Recap Problem

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

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

Answer

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

Question

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

Answer

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

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

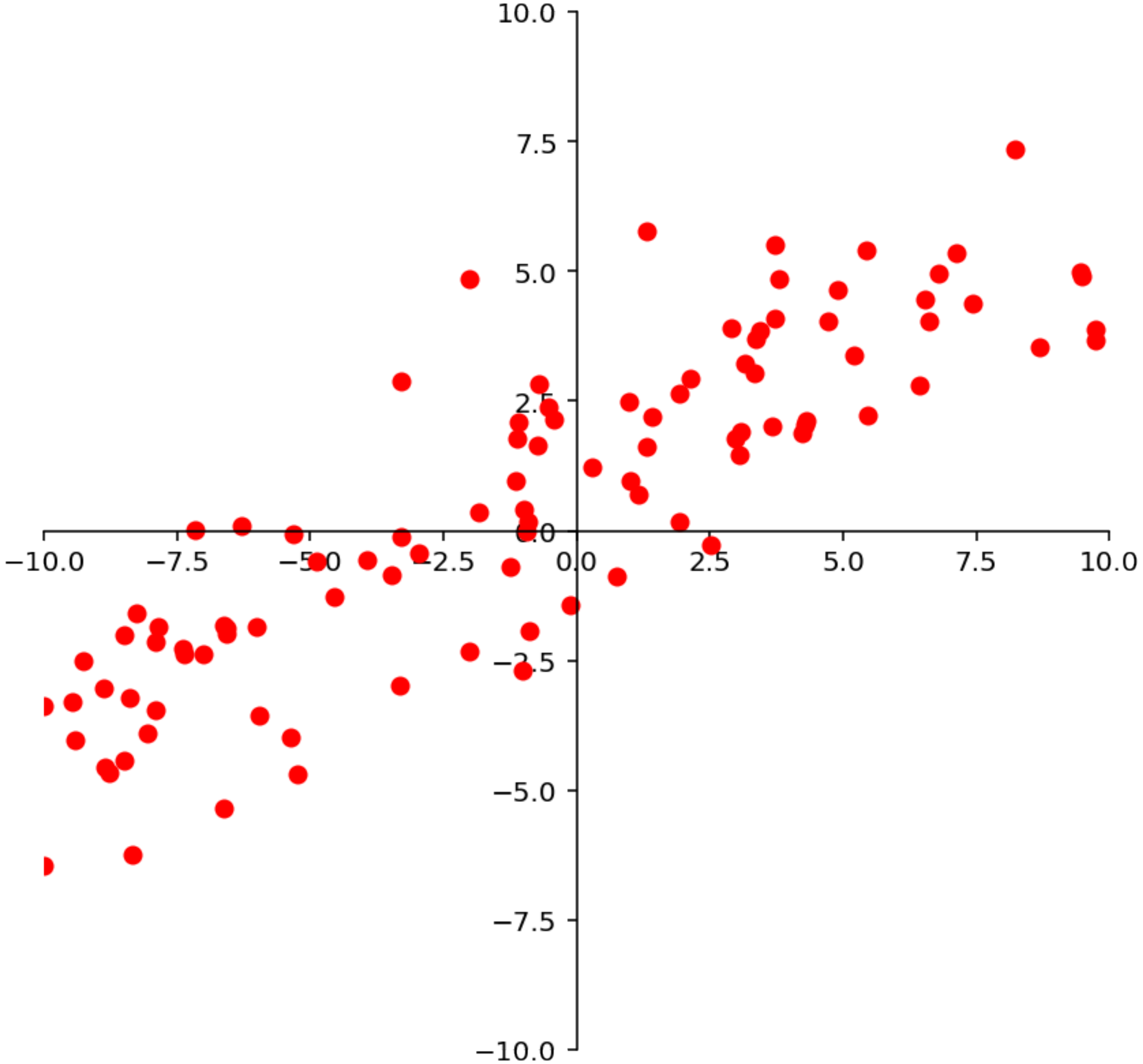
model fitting

model parameters

design matrices

A Warmup: Line of Best Fit

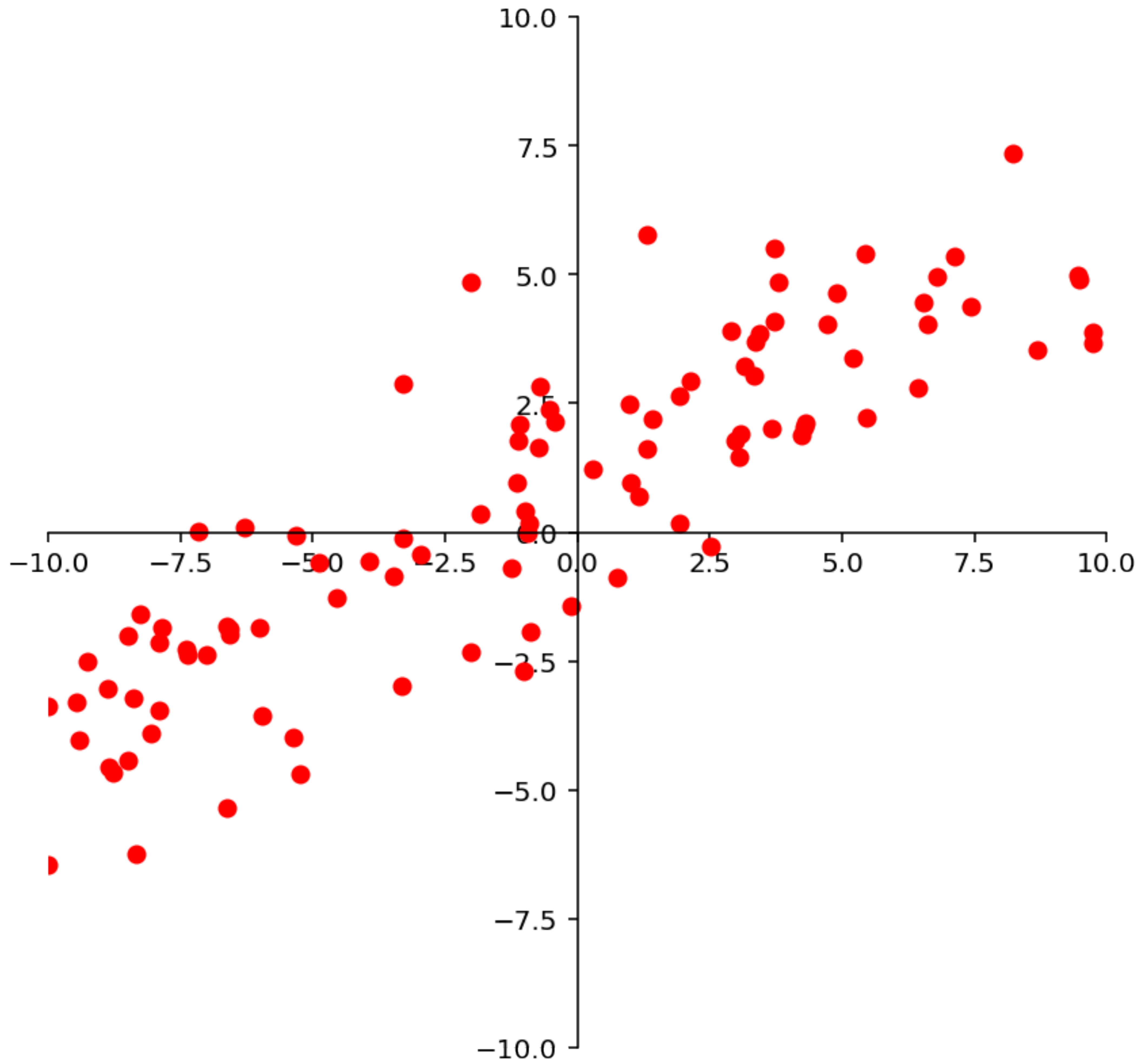
The Setup



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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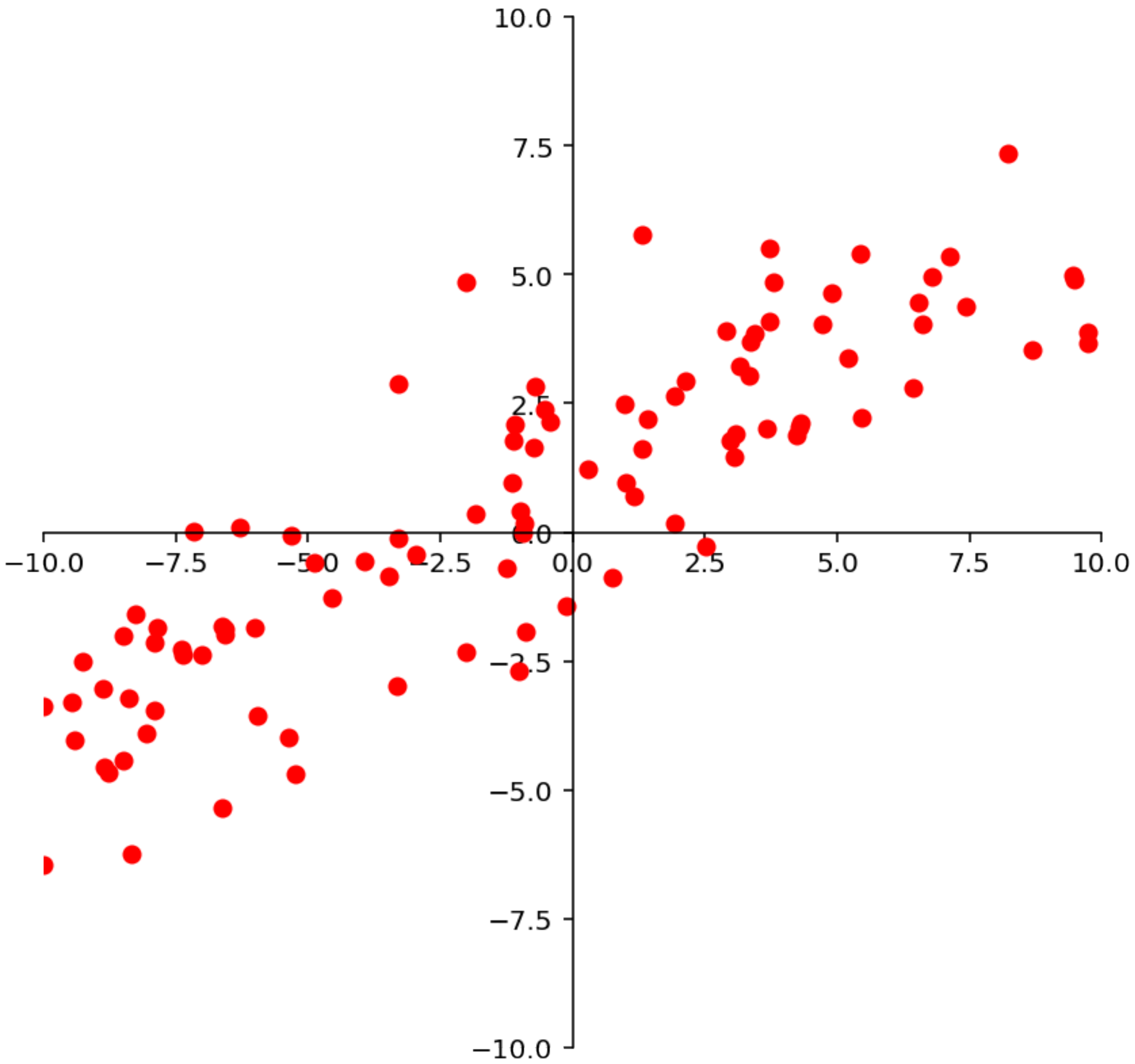

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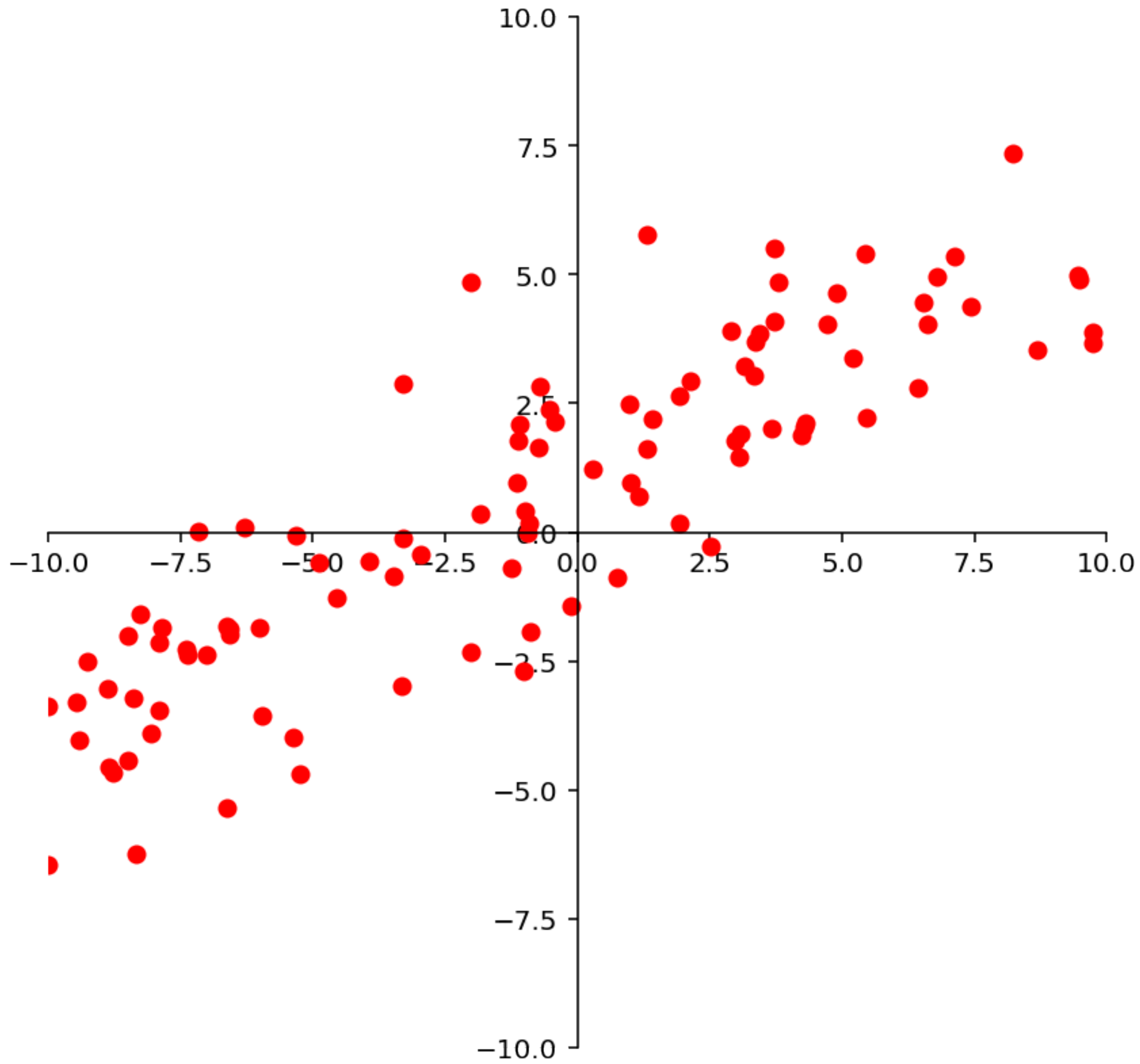

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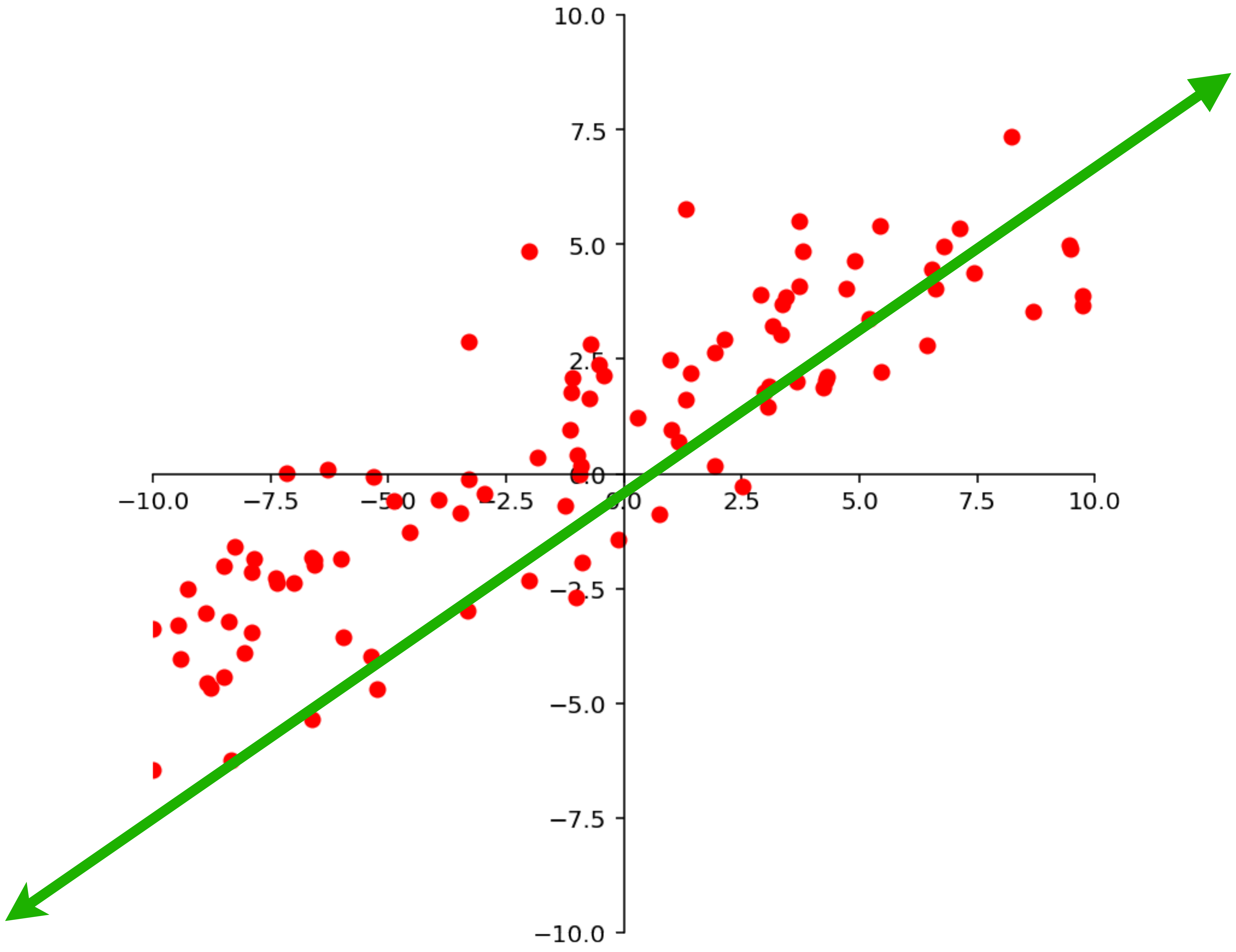

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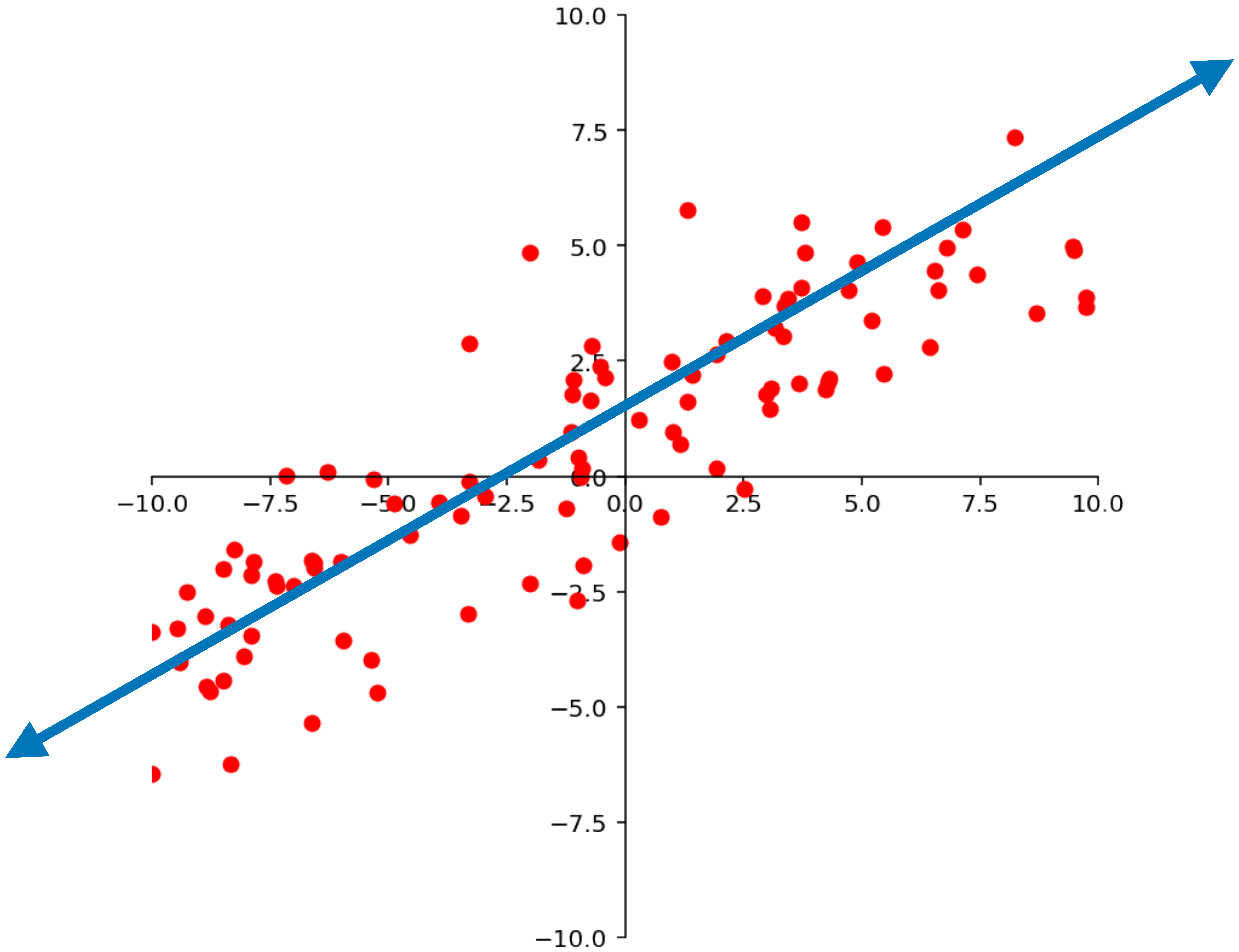
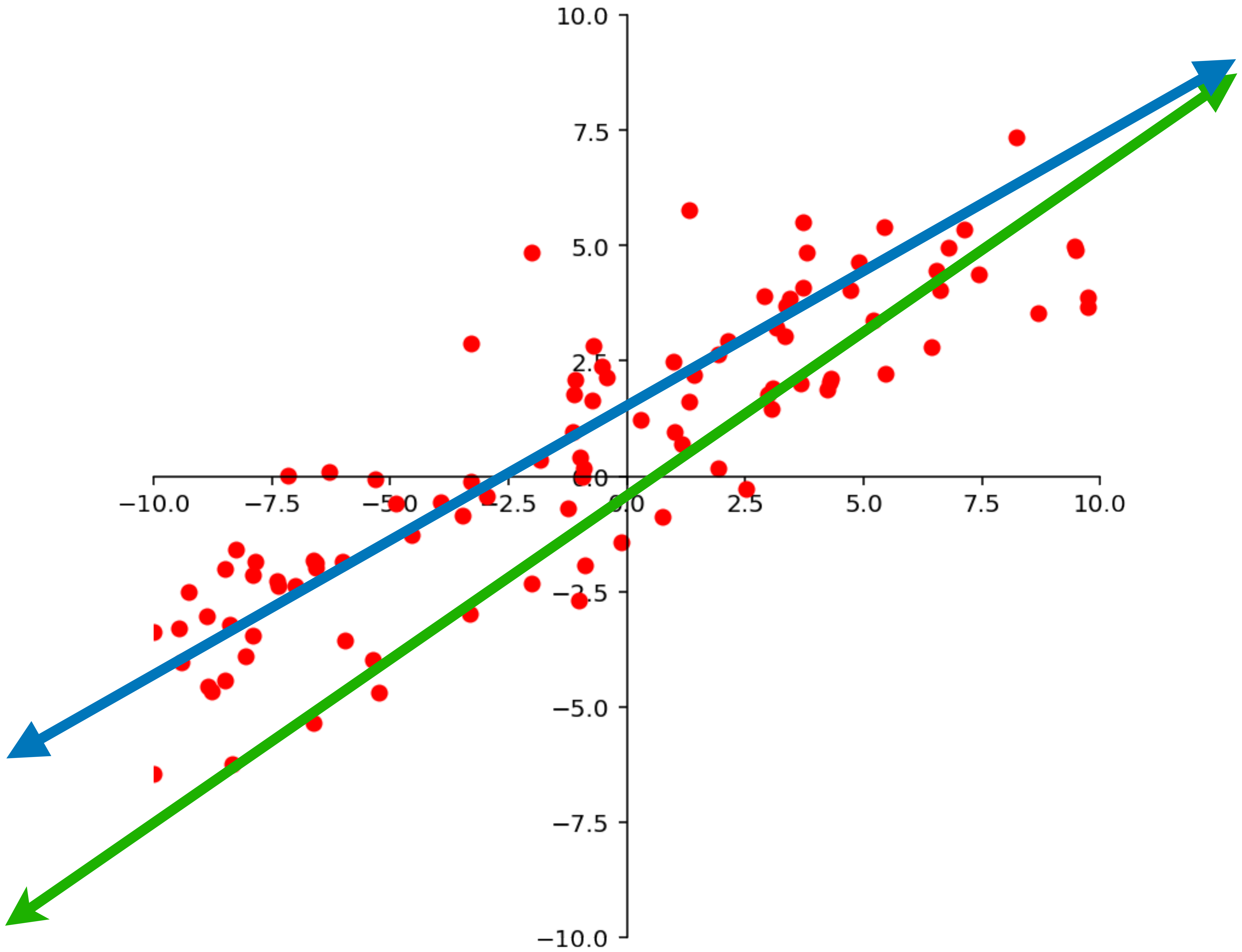


The Setup

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

Which one *best models* the dataset?



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1. What is a model?

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    `We'll come back to this...`

Two Important Questions

1. What is a model?

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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 minimizes

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

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which <u>minimizes</u>

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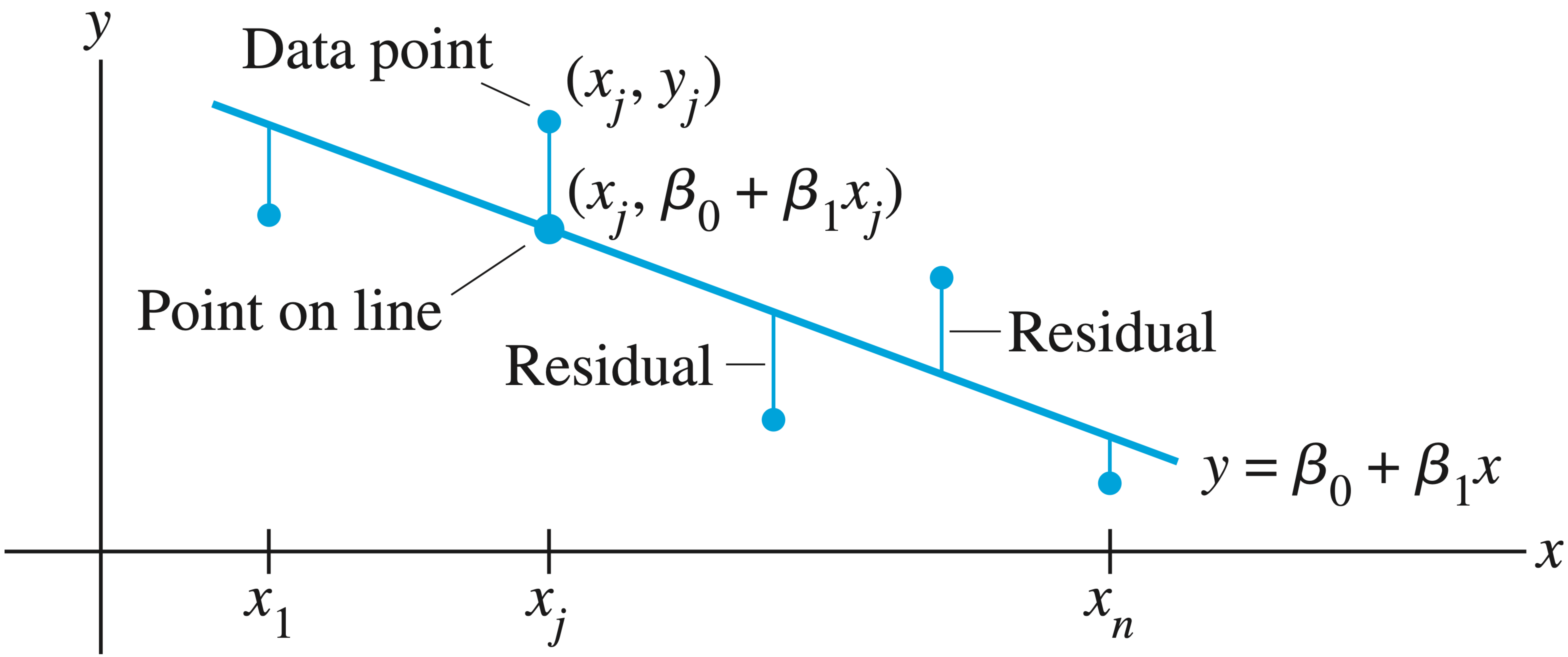
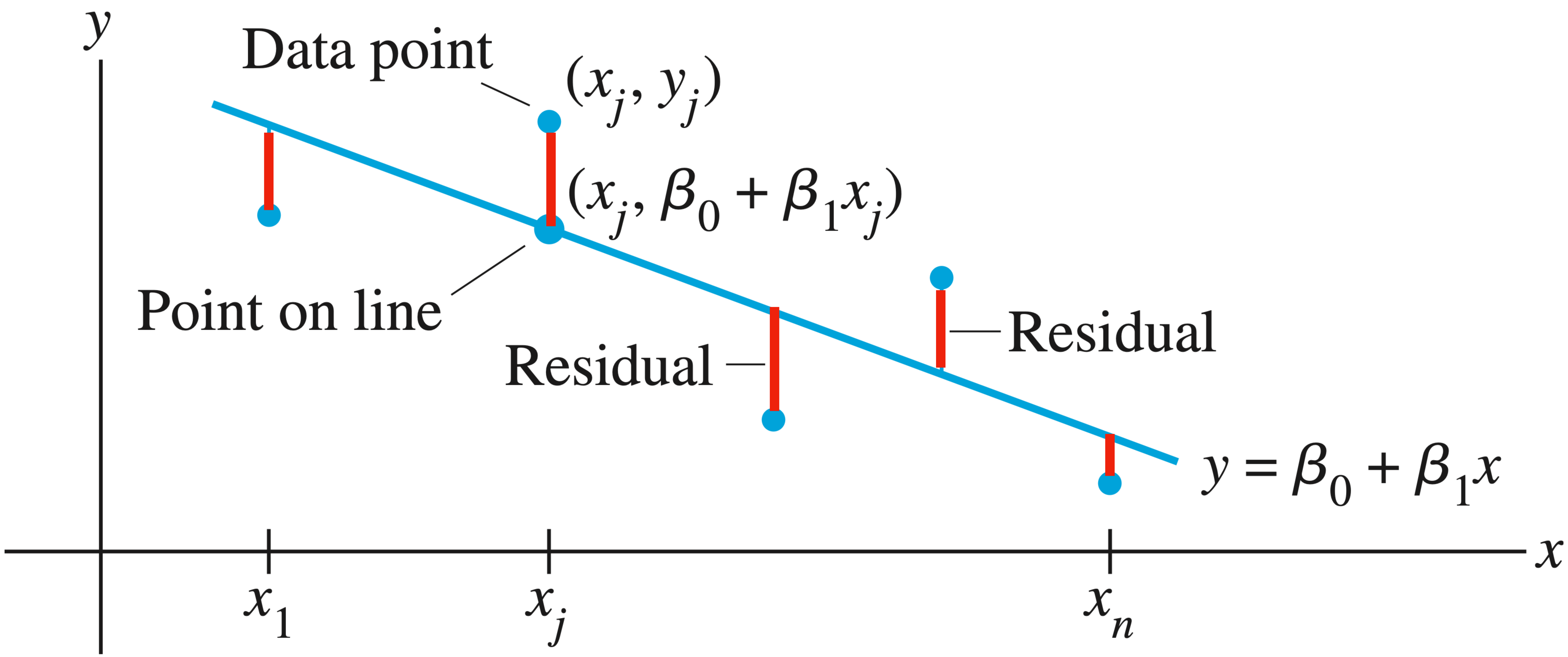
The "best" line minimizes the *sum of squares of differences.*

The Picture



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

The Picture



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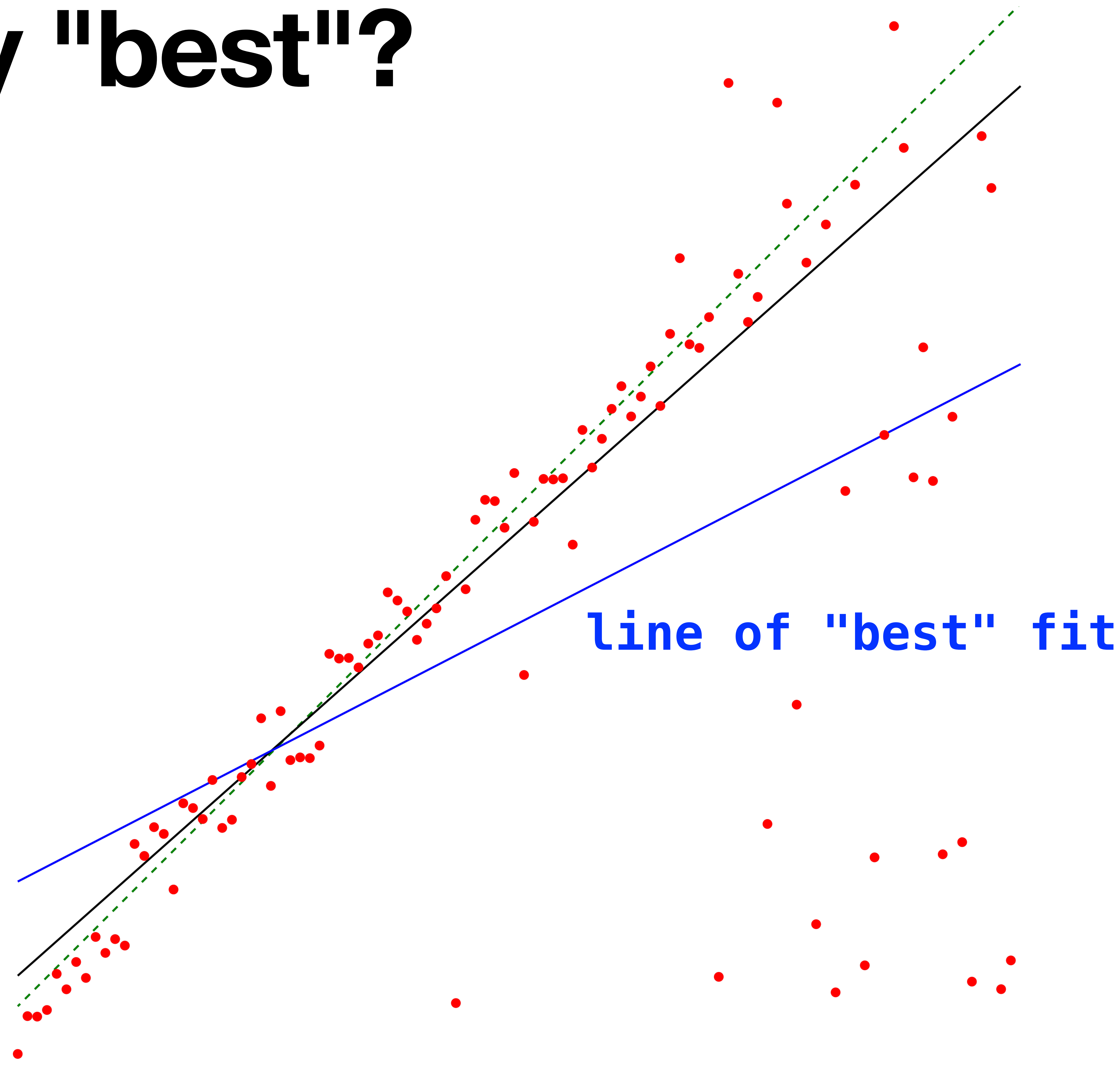
An Aside: Is this really "best"?



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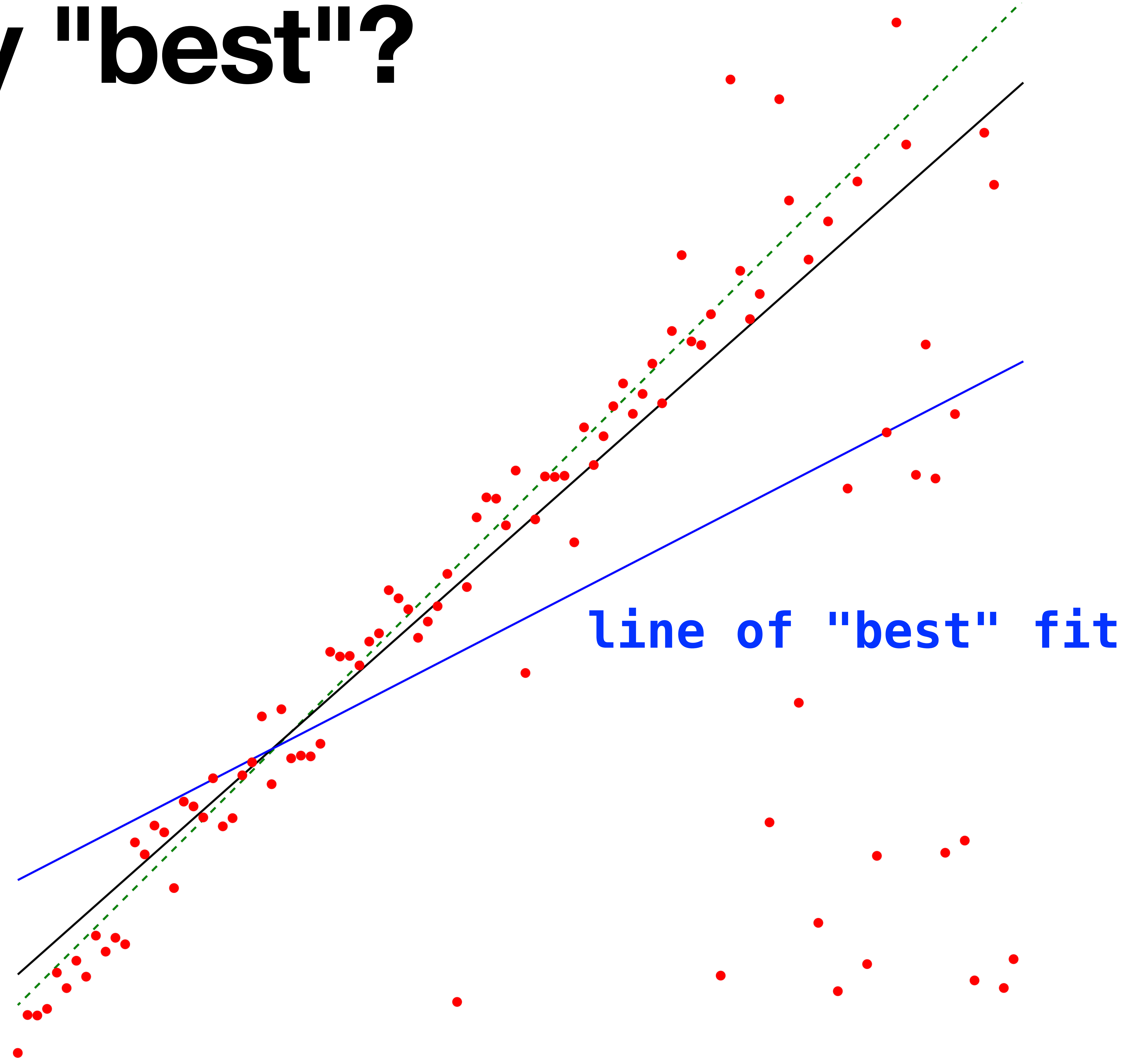

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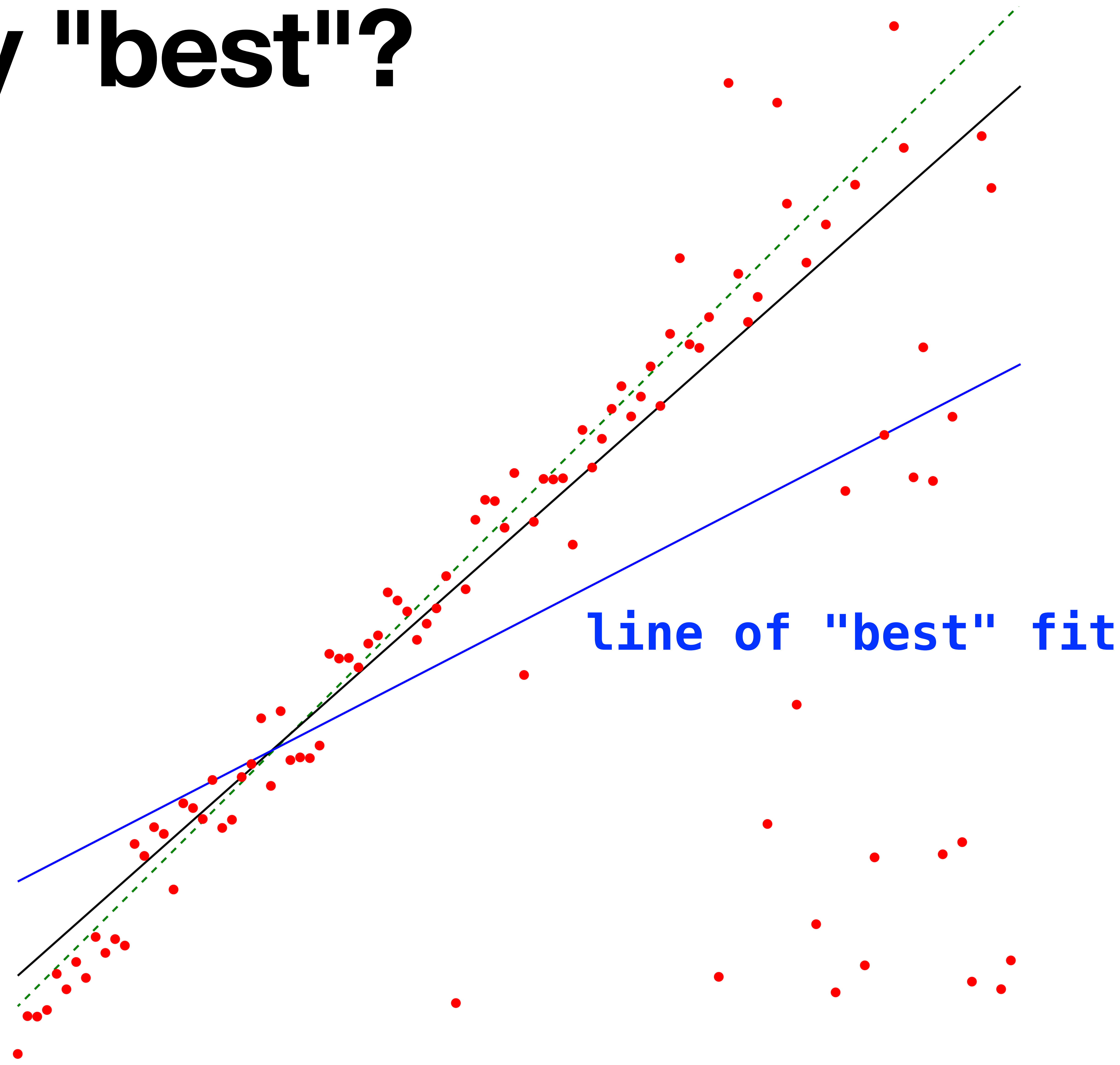

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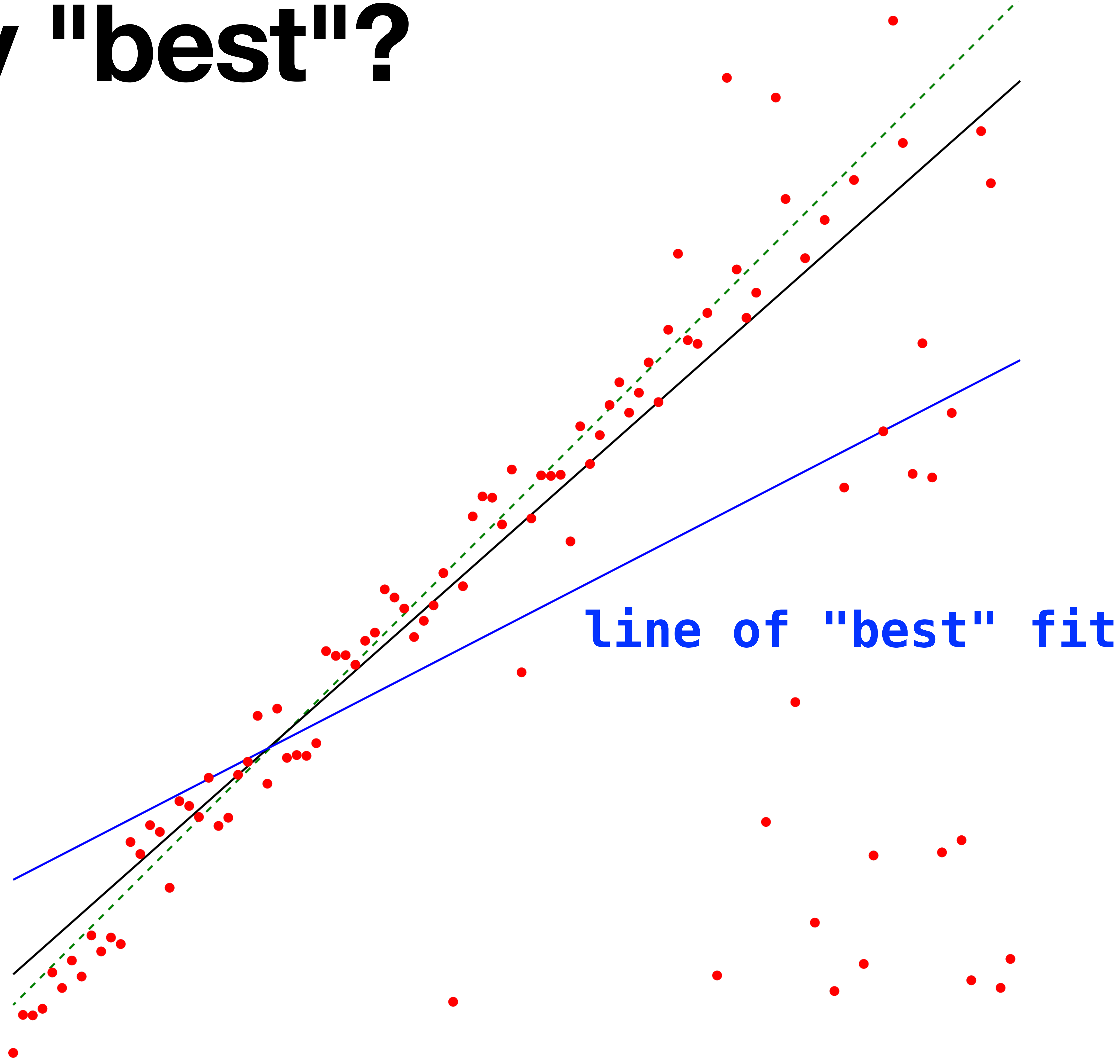
The point. We fix our notion of "best" first, and then we do calculations and derivations from there.



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Terminology: Datasets

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

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data point

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$$(x_i, y_i)$$

Terminology: Datasets

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dataset

independent variable (feature)

$$(x_i, y_i)$$

Terminology: Datasets

data point

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

dataset

independent variable
(feature)

$$(x_i, y_i)$$

dependent variable
(label)

Terminology: Models

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

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model

Terminology: Models

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

model

Terminology: Least-Squares Error

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

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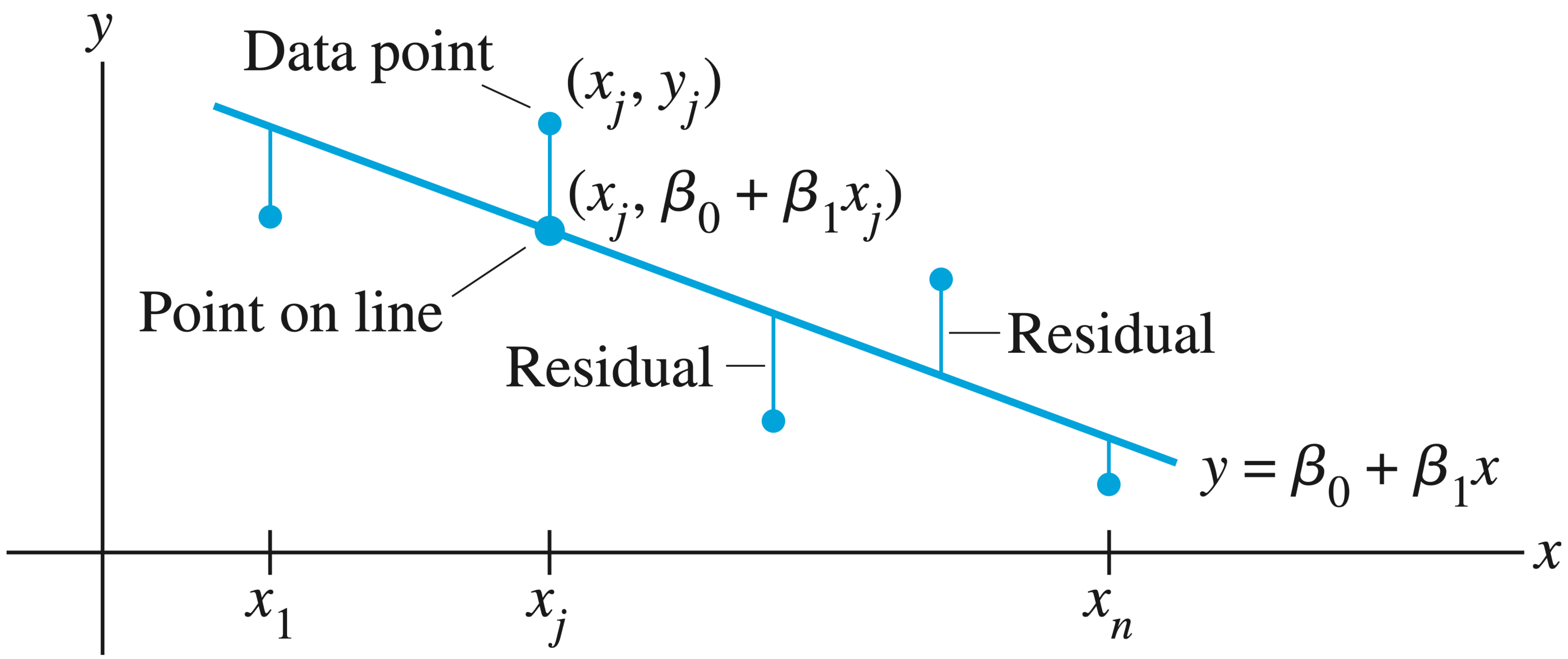
prediction

Terminology



data point

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$$(x_i, y_i)$$

independent variable

dependent variable
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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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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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These expressions look very similar.

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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.

$$
\begin{aligned}
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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
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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

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

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

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 $\mathbf{y}$.

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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:`

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

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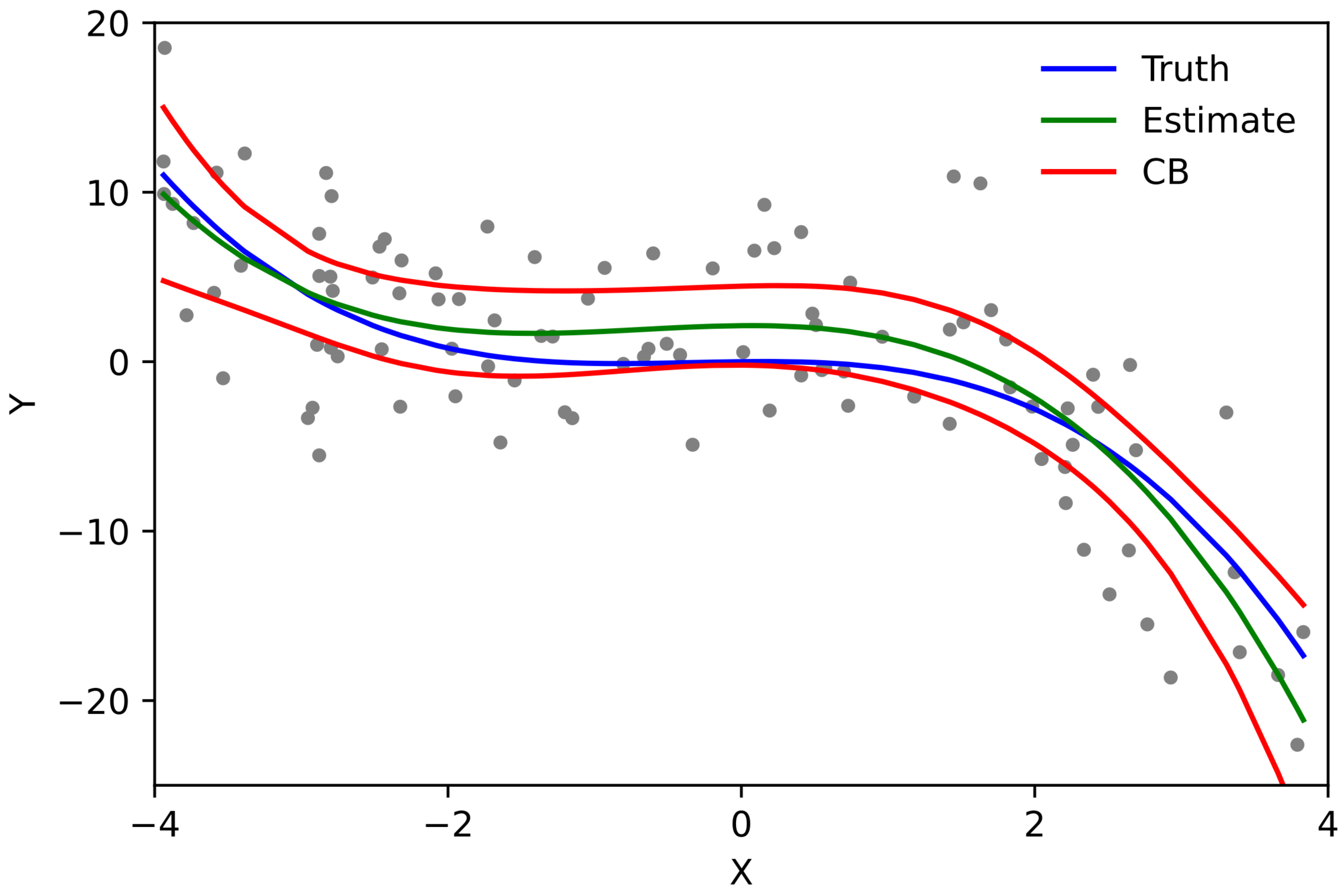
Problem. Find the least squares line for the dataset $\{(x_1, y_1), \ldots, (x_n, y_n)\}$.

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

General Regression



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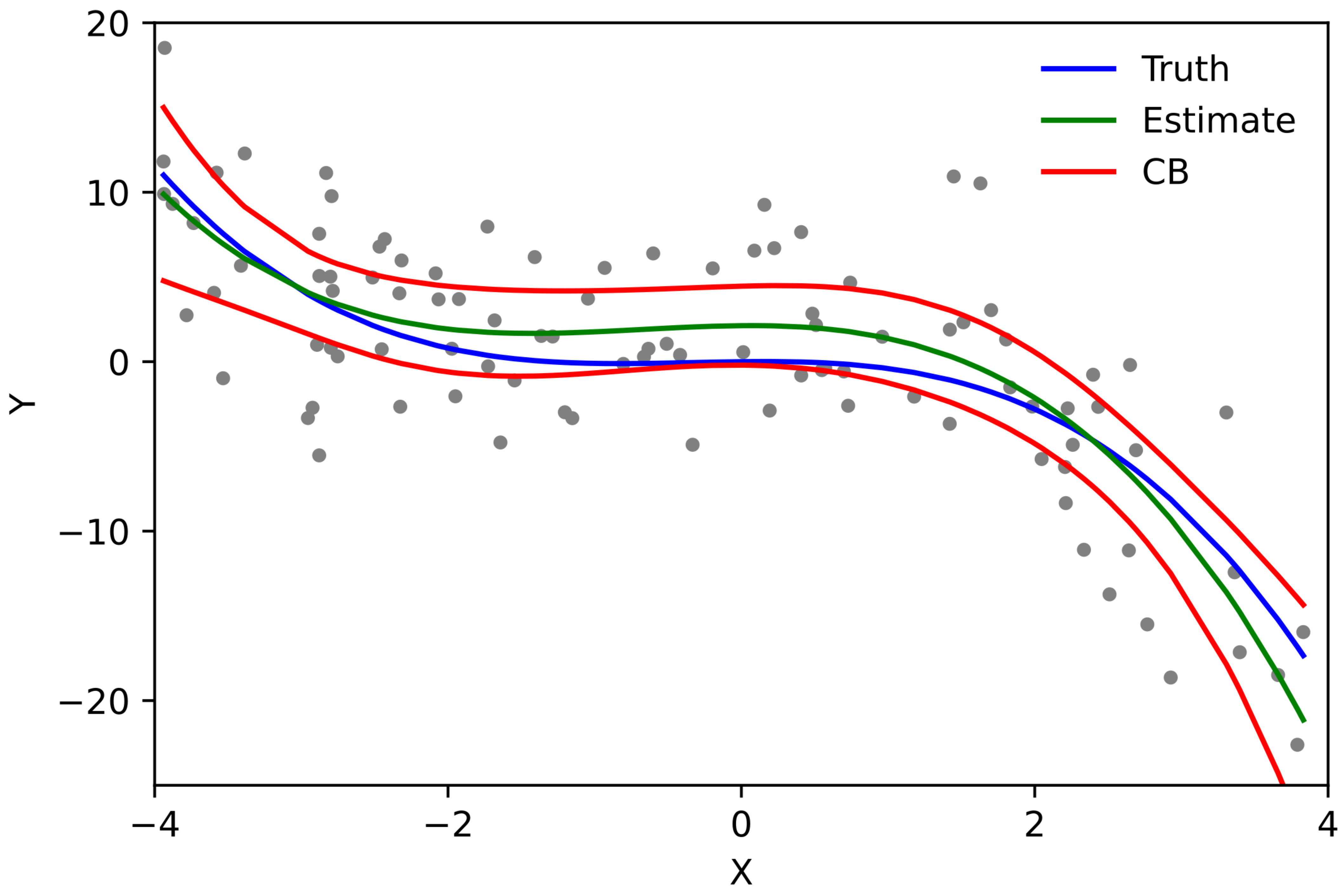
General Regression

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



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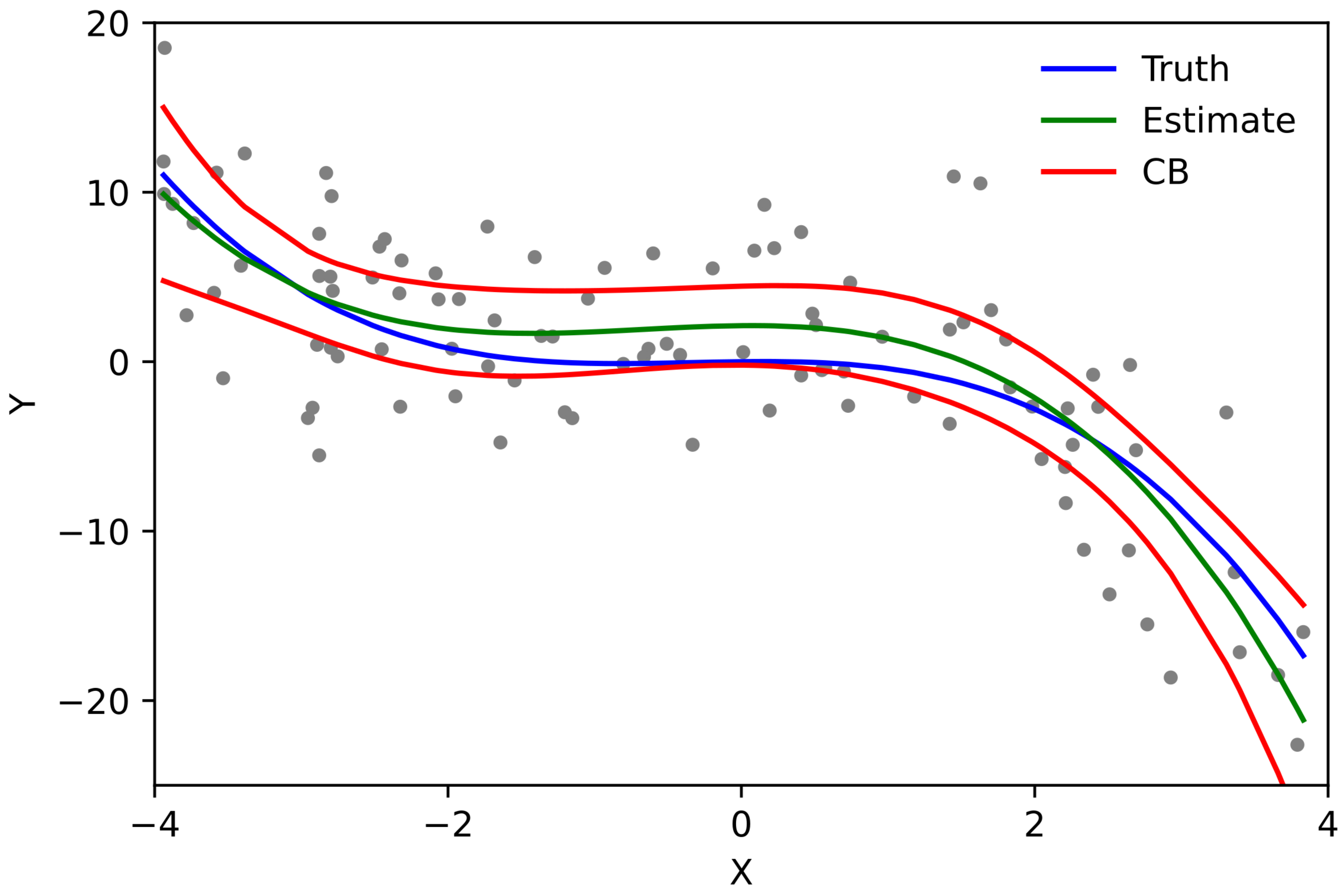

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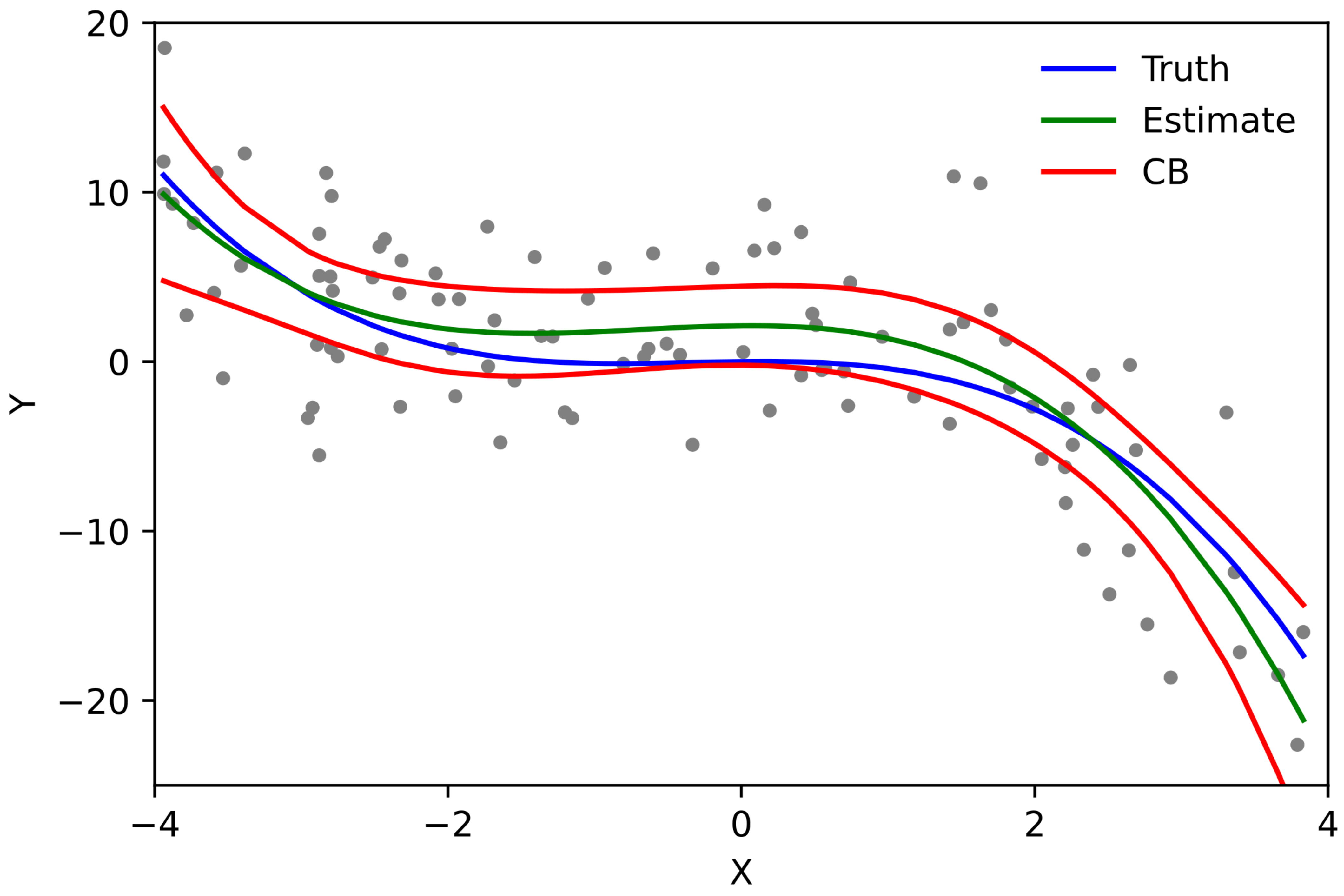
We think of the environment has providing us a function from our independent variables to our dependent variables.



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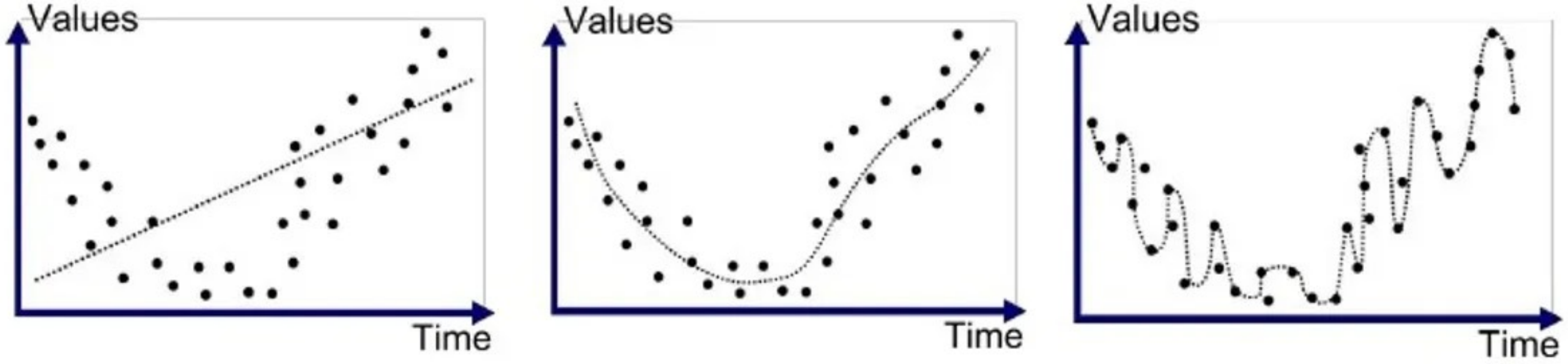
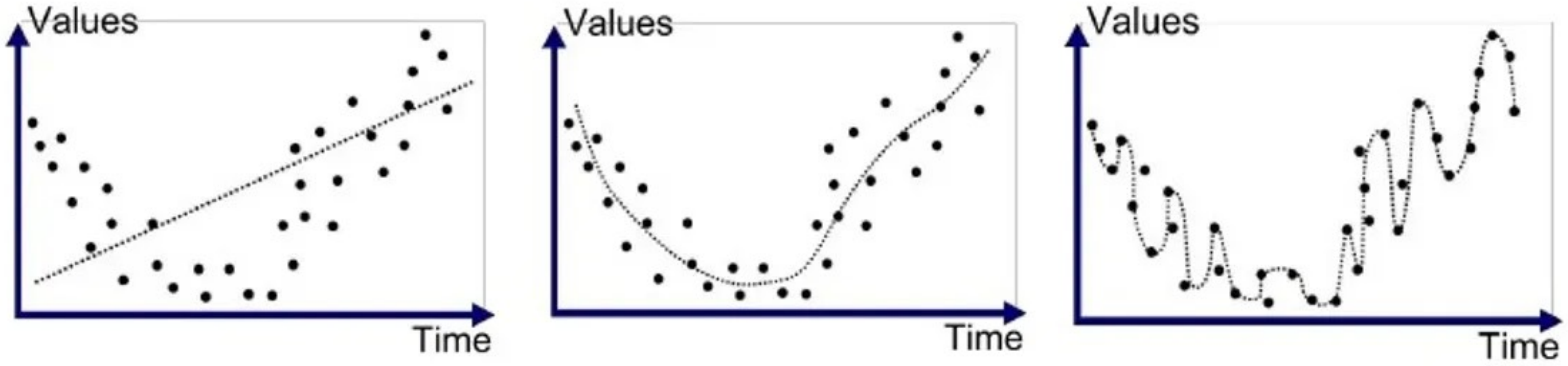
Models



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



Underfitted Good Fit/Robust Overfitted

Therefore, a *model* is a mathematical function.

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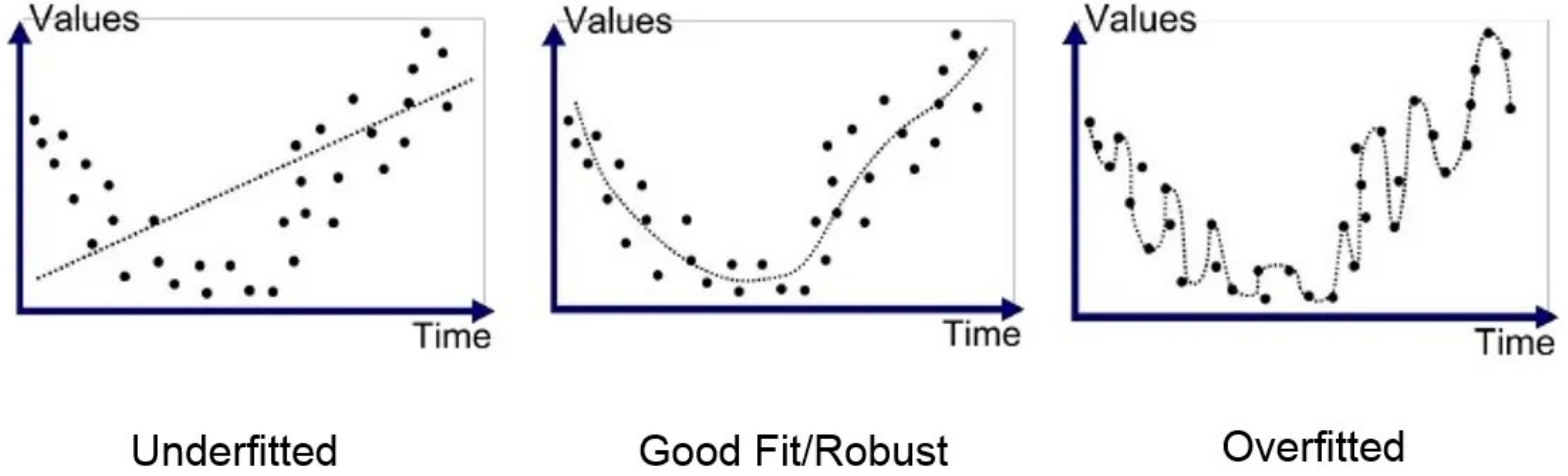
Models



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

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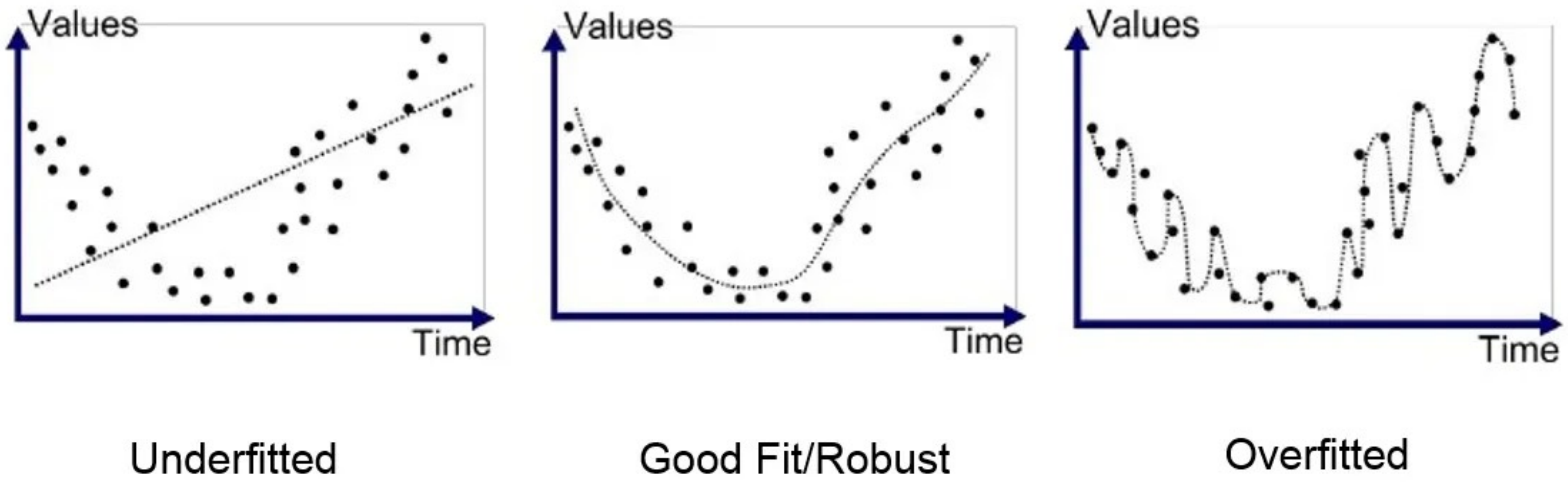

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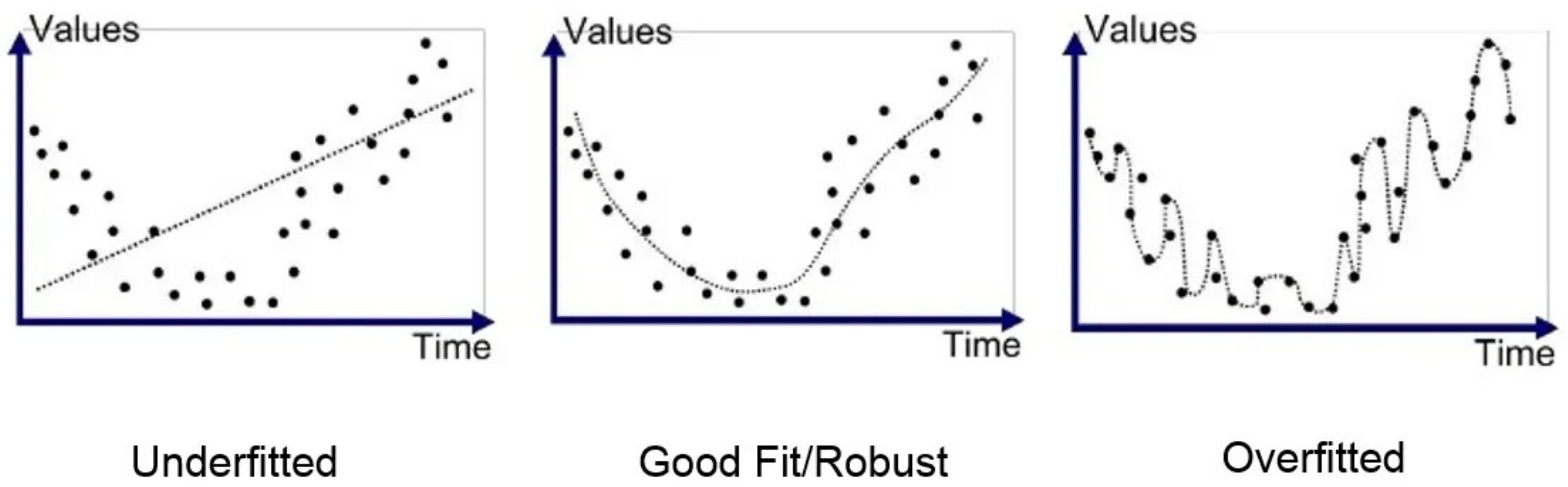

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*(Advanced) We pick models from weaker classes of functions so that they are more robust when we **predict** values using the model.*

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How To: Prediction

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

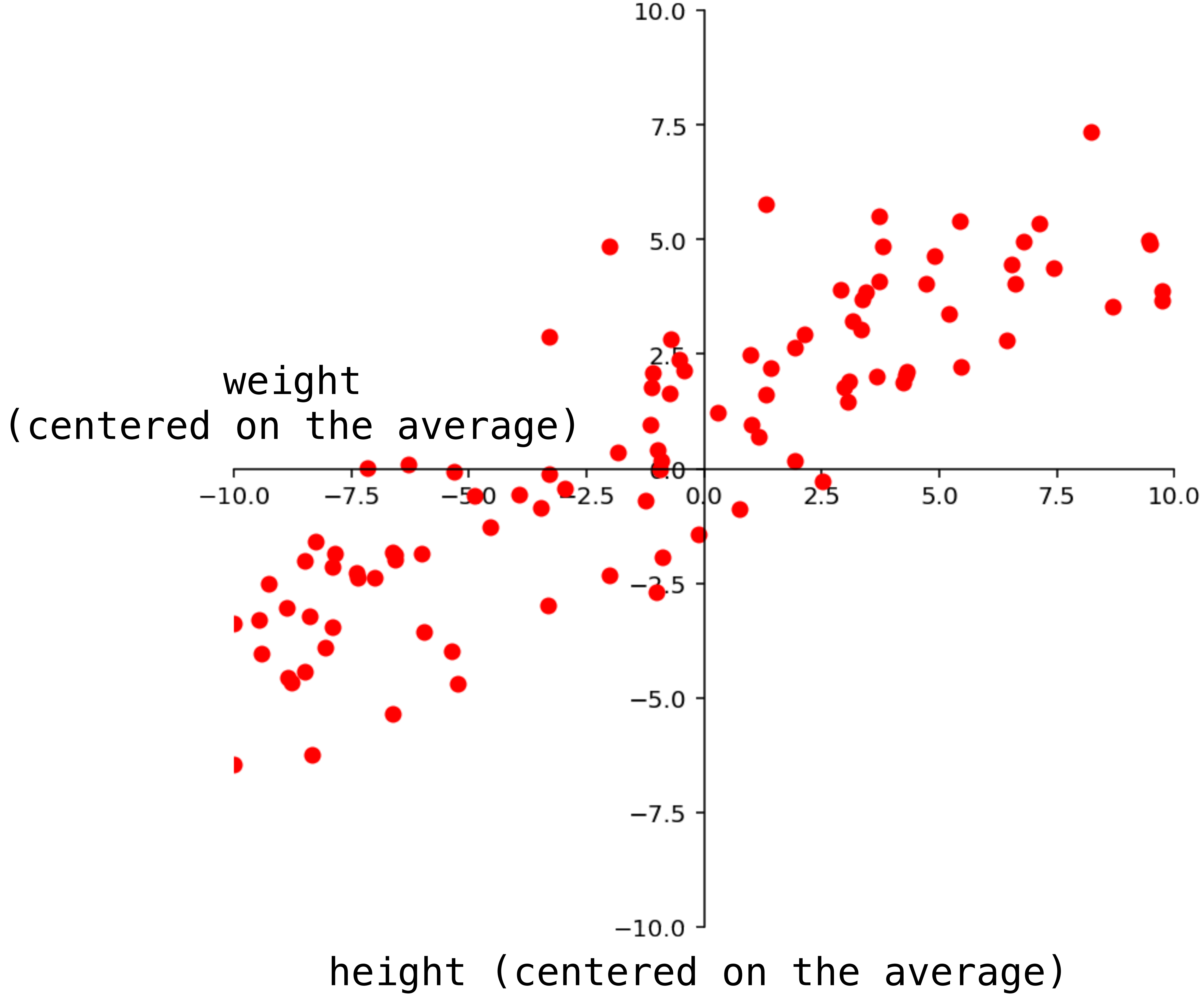
How To: Prediction

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

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

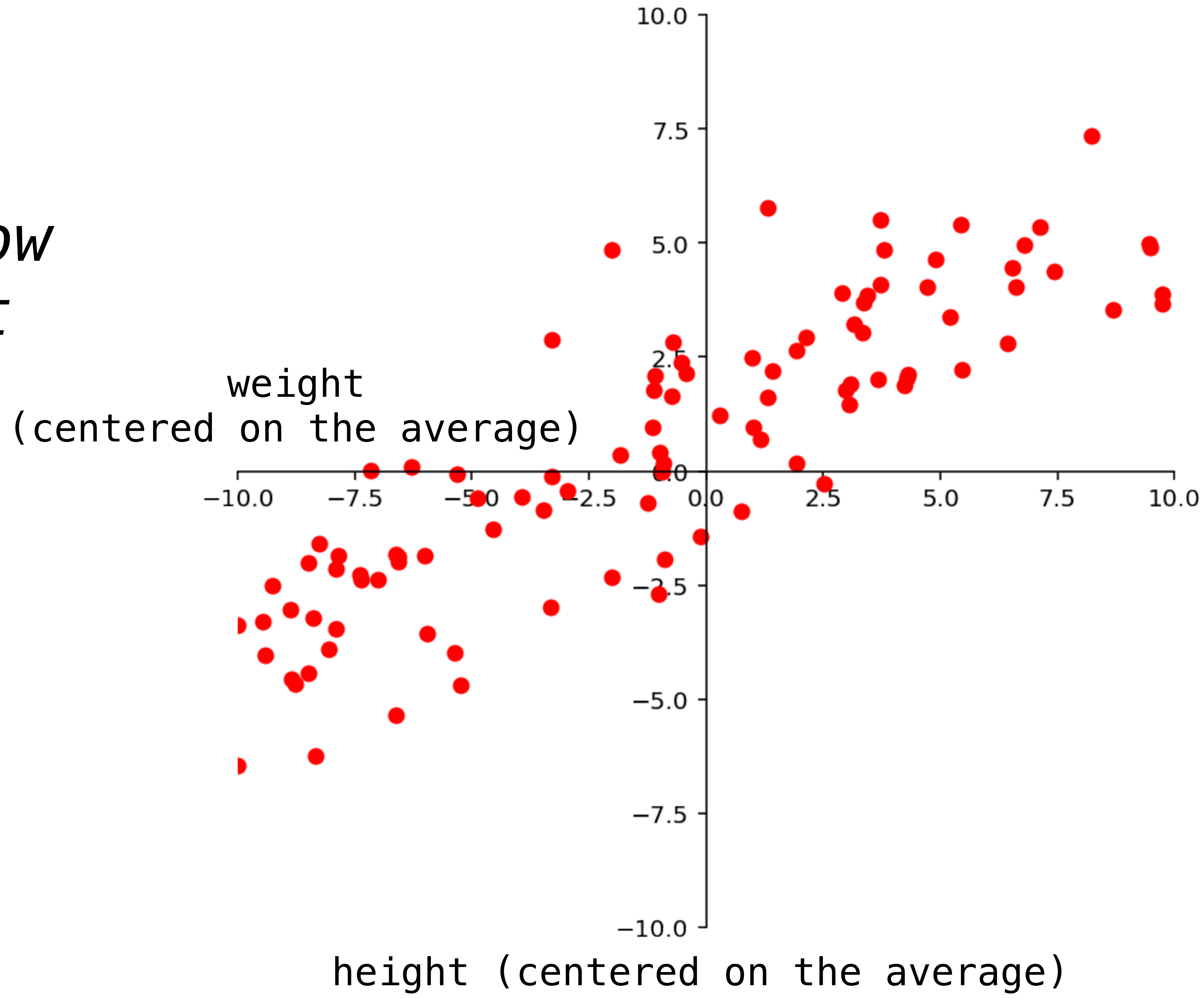
This generalizes to any model fitting problem

Example: Height from Weight



Example: Height from Weight

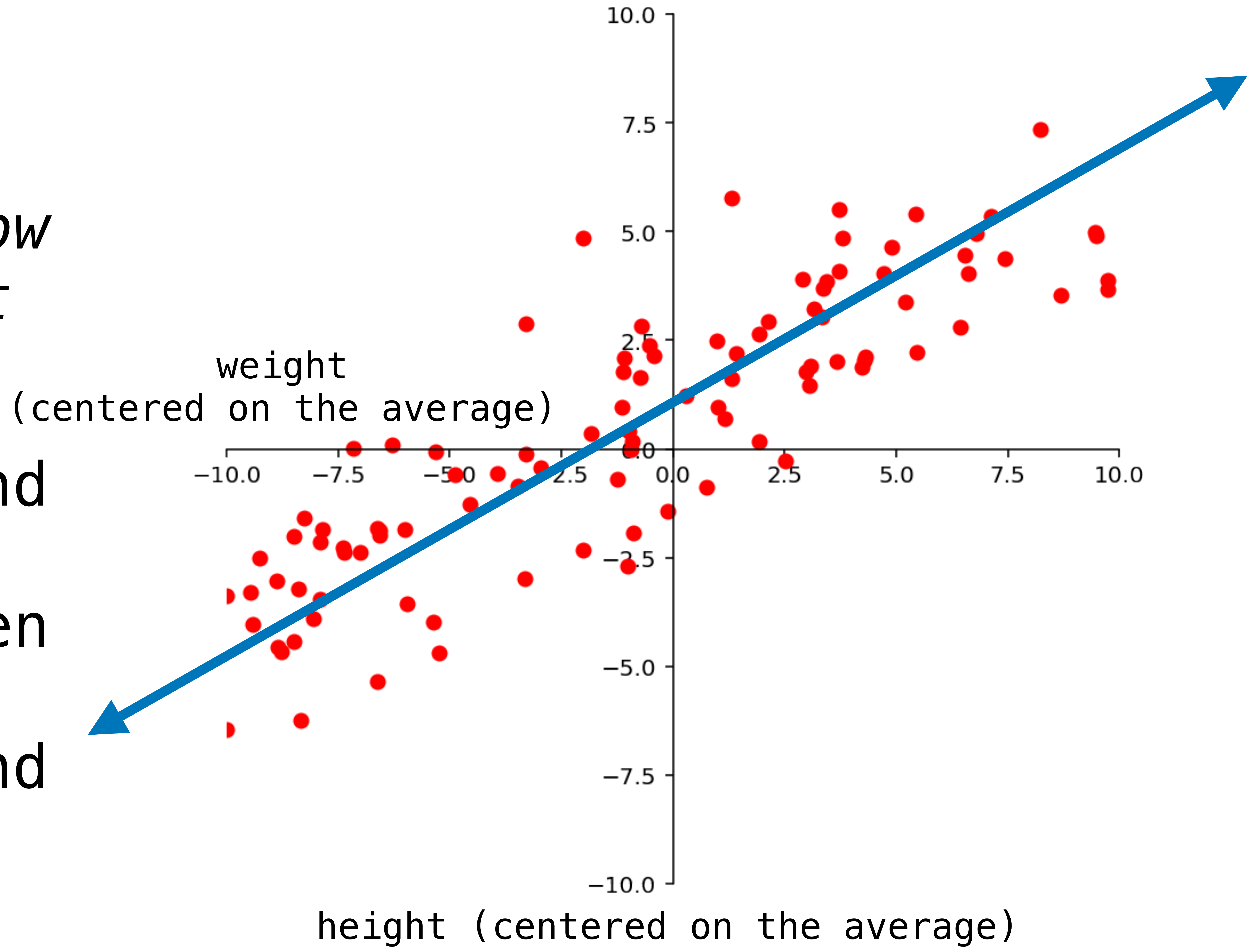
Suppose we know that person X weighs 150lb. *How would we guess the height of person X?*



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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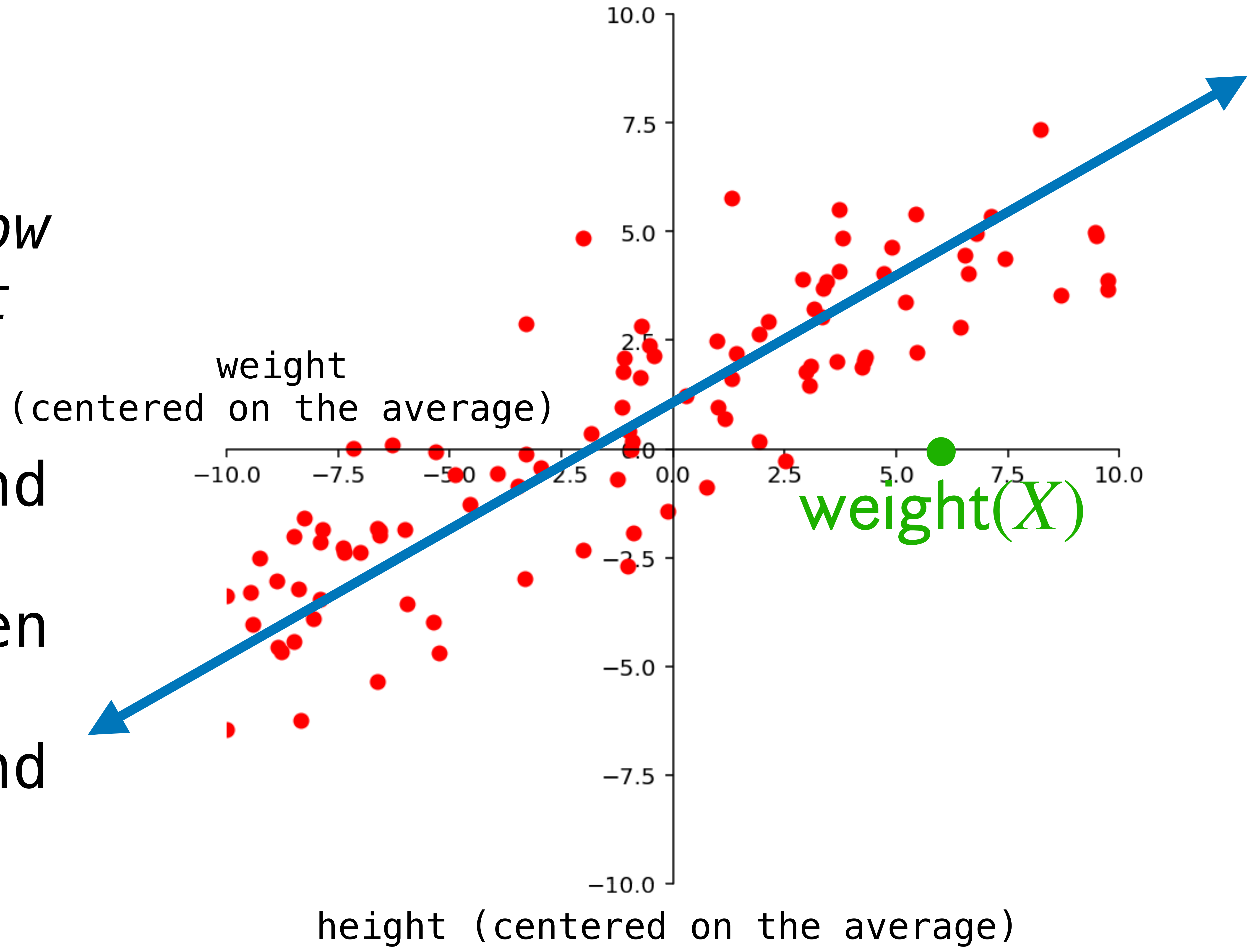

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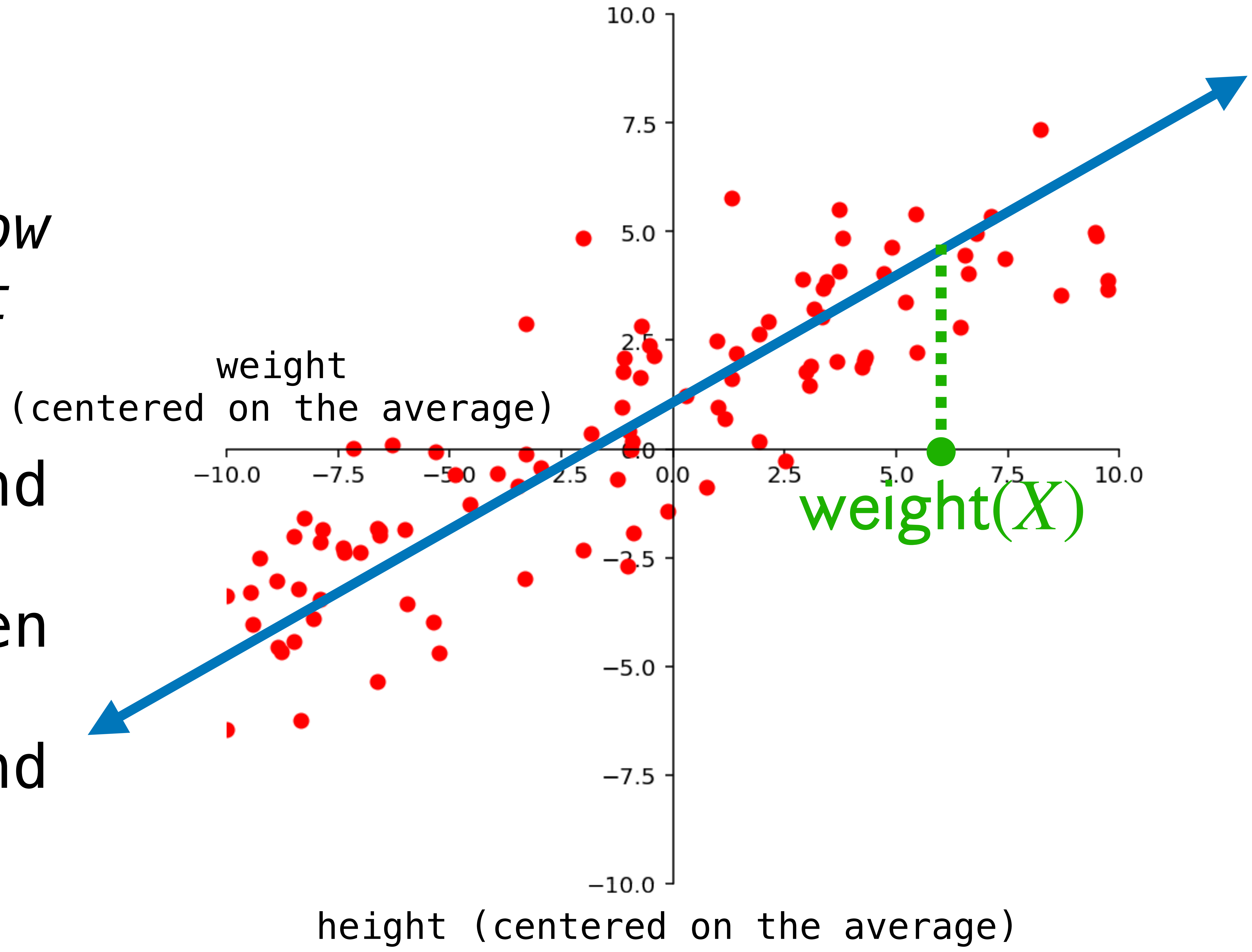

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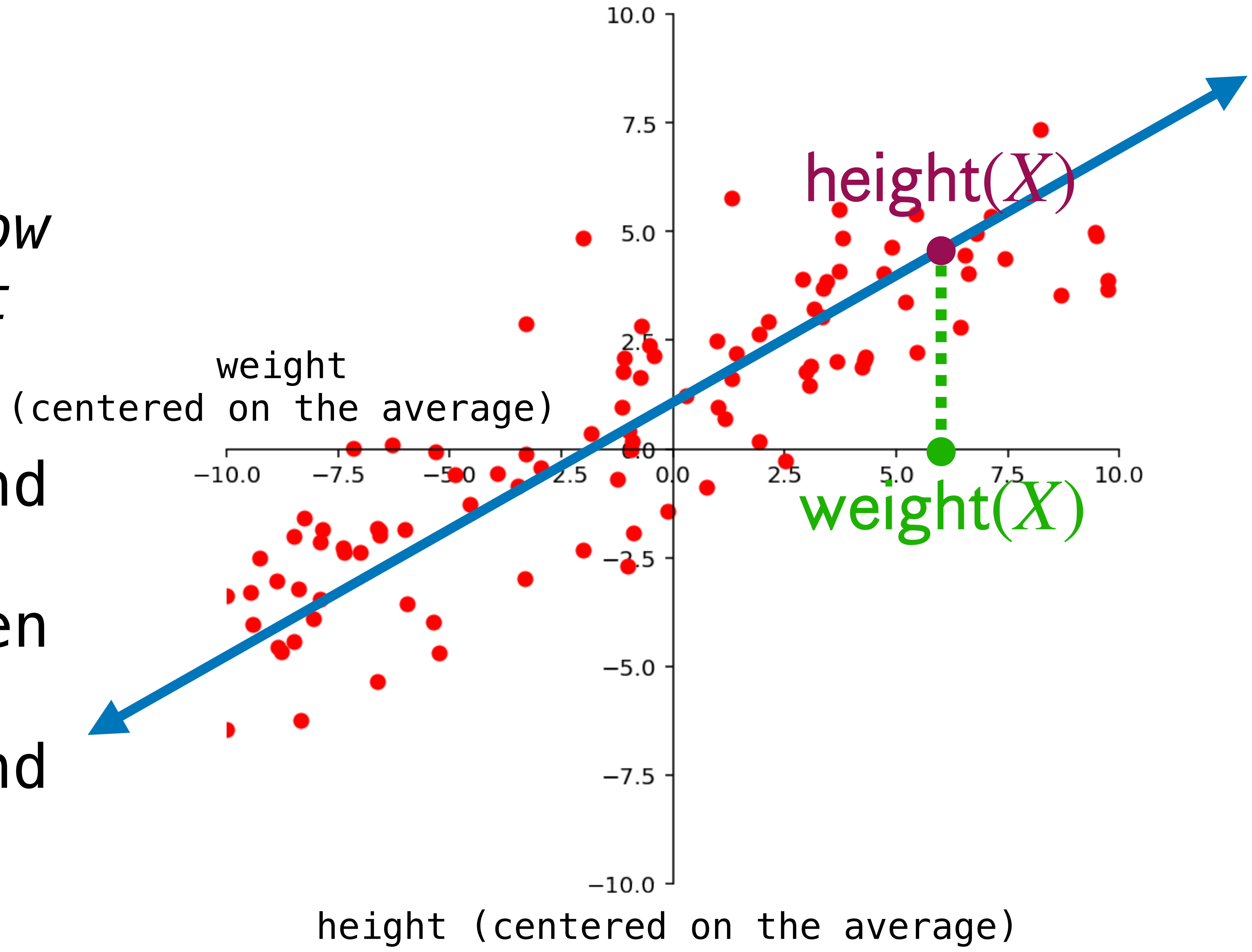

Question

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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multiple regression, (hyper)plane of best fit

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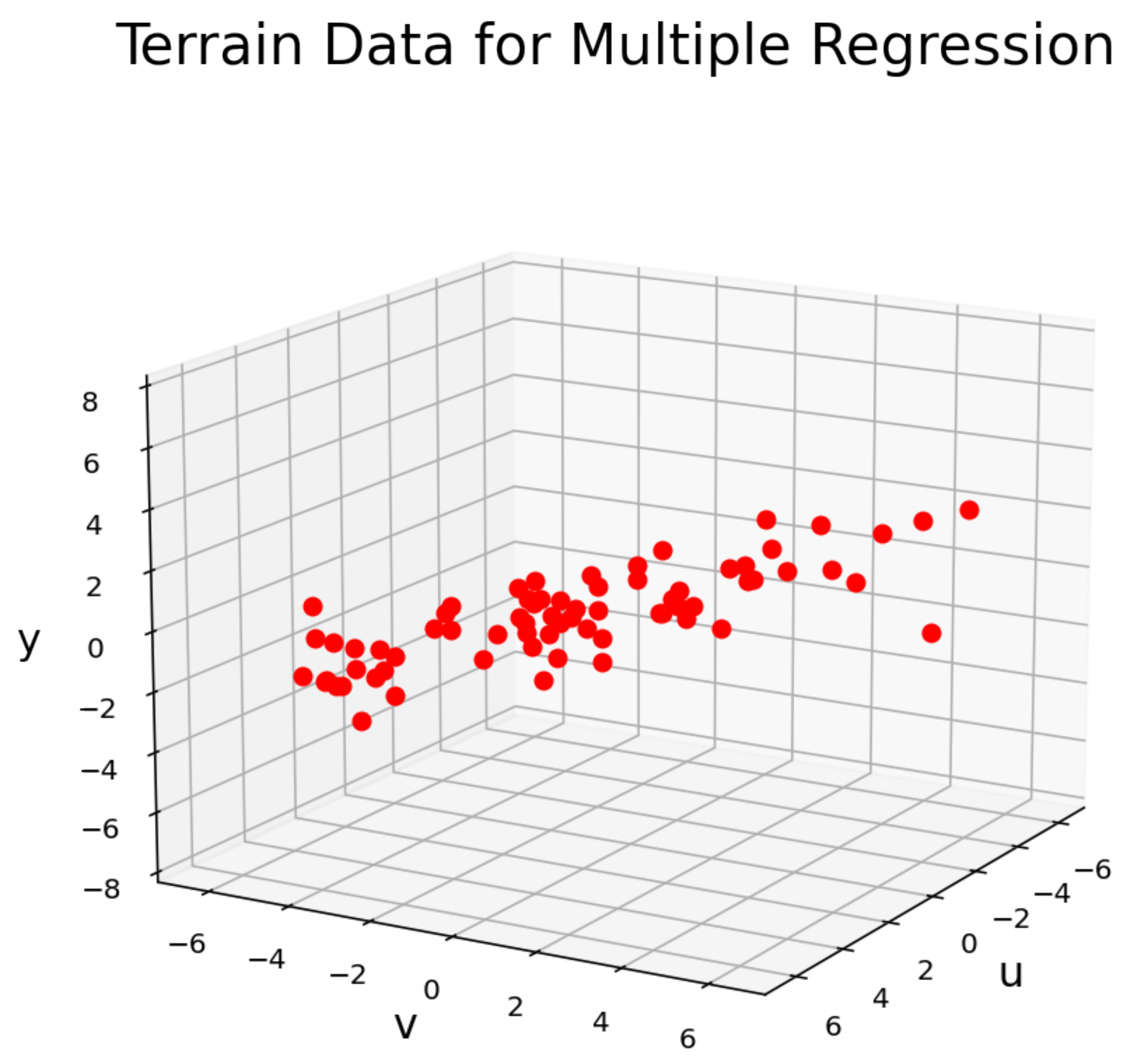
Example: Terrain Data

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

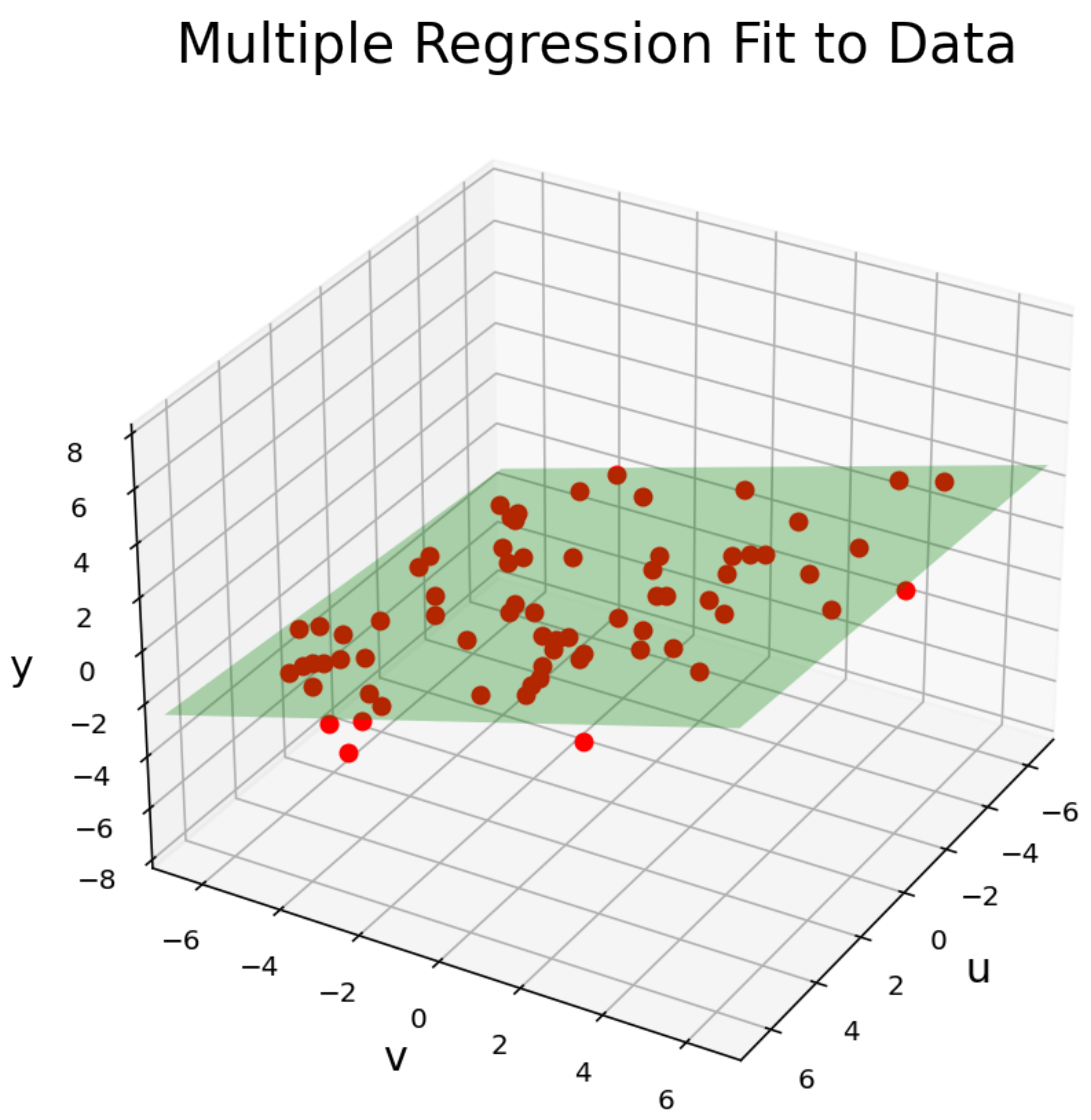

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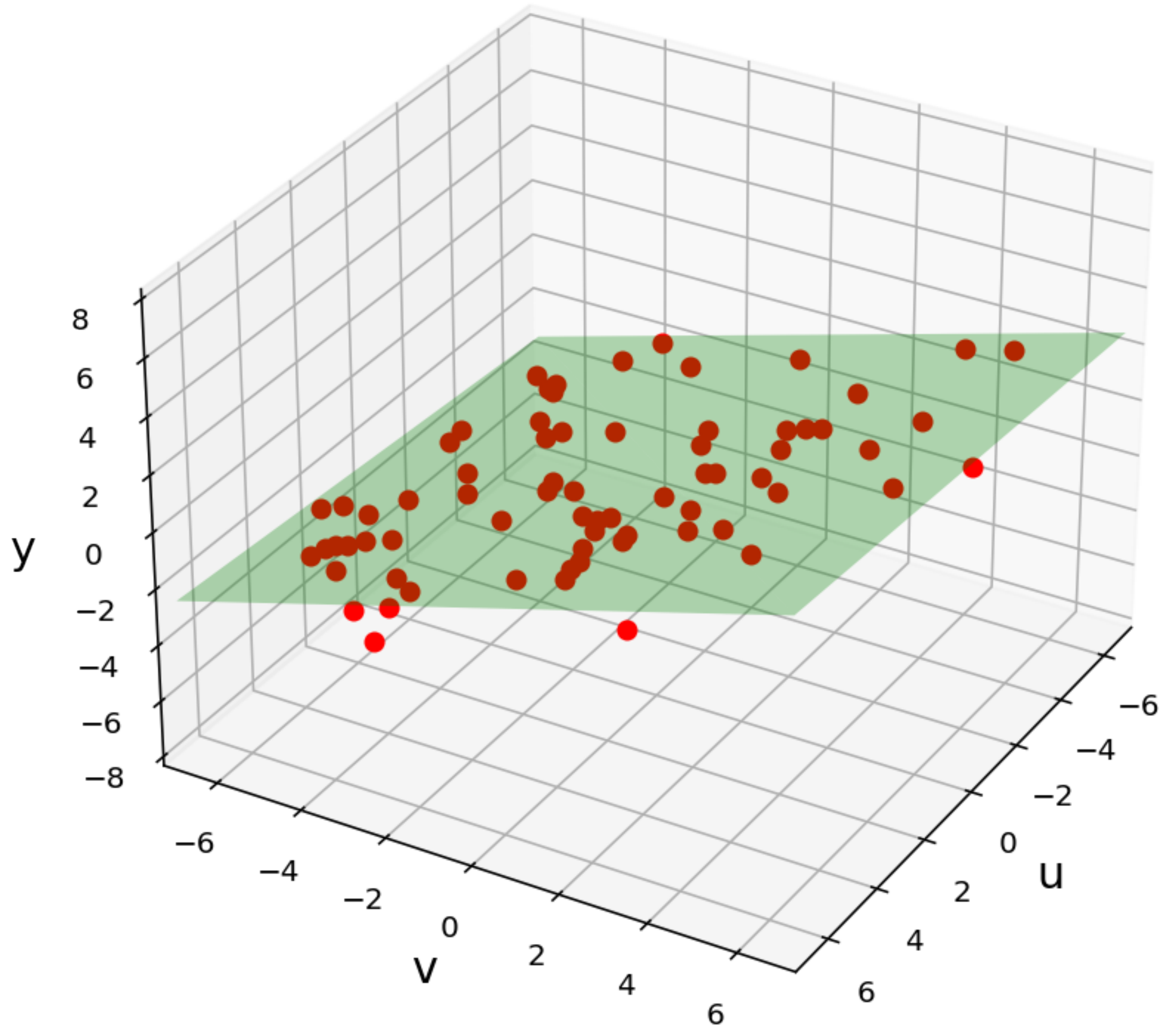
Figure 23.2

Multiple Regression Fit to Data



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

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

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

recall: planes are given by linear equations

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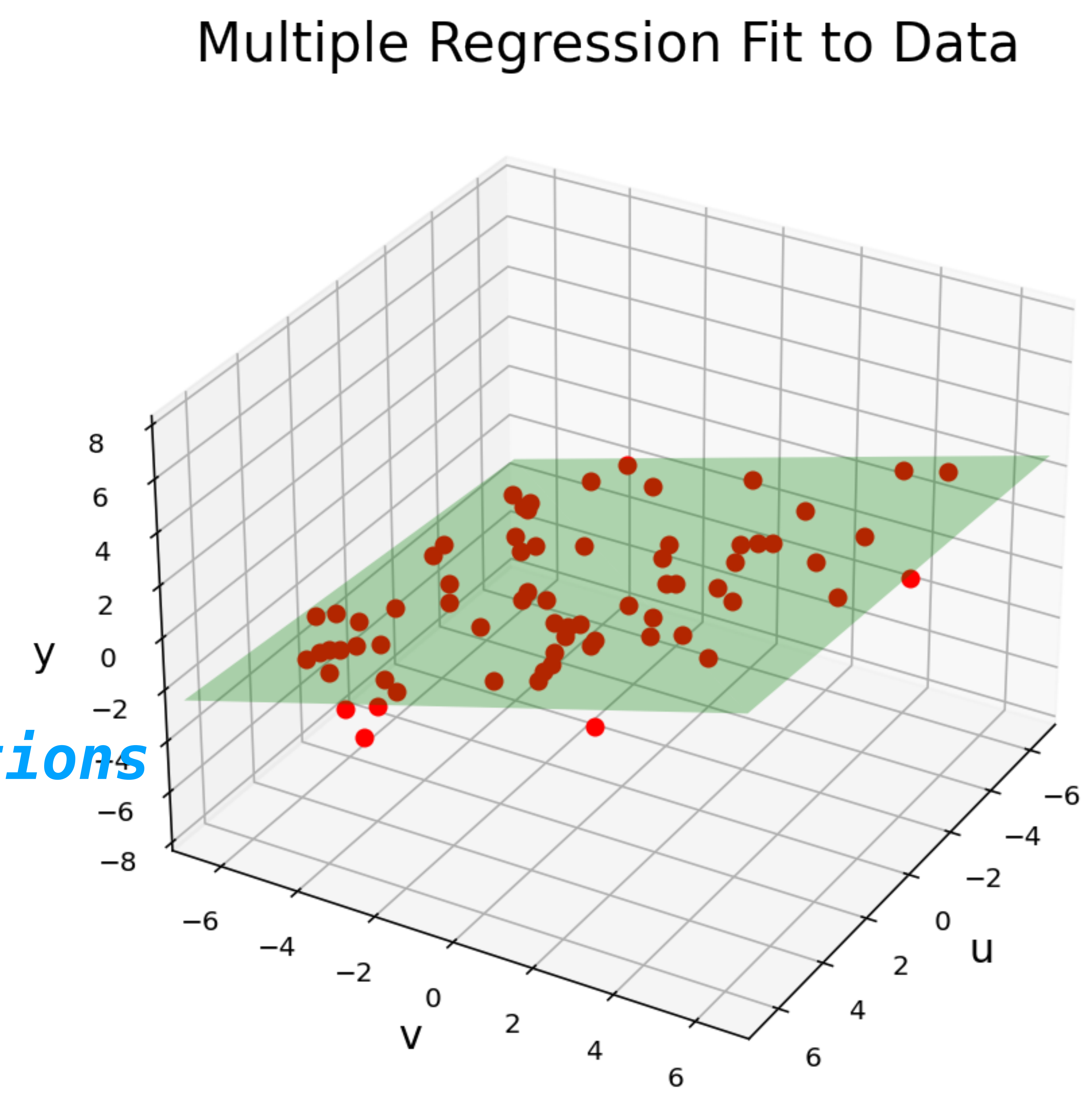
$f(x, y)$ ***is a good approximation of the altitude.***

Figure 23.2



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This is still linear in the β's

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

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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

Answer

```
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.

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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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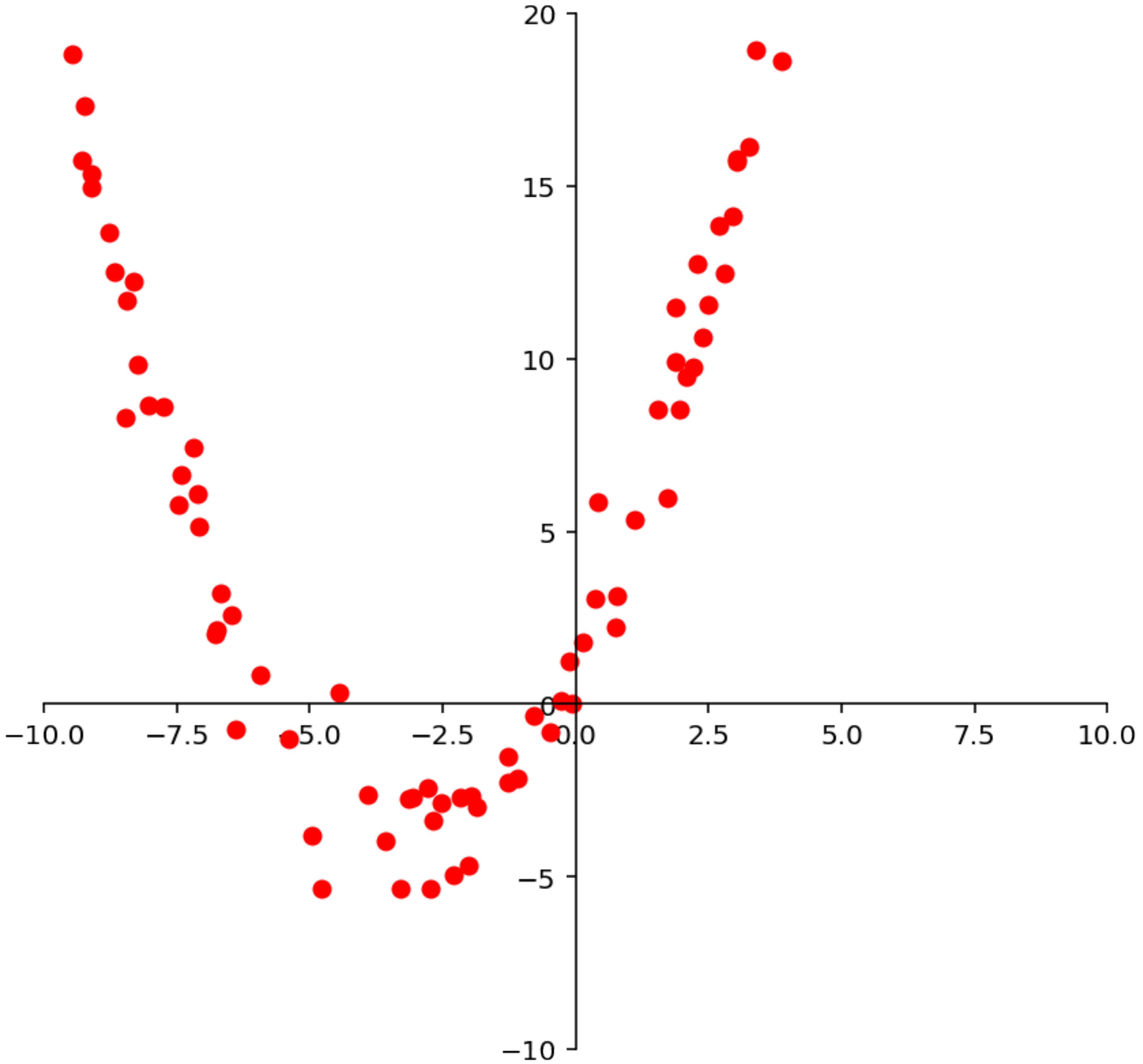
Example: Best Fit Quadratic



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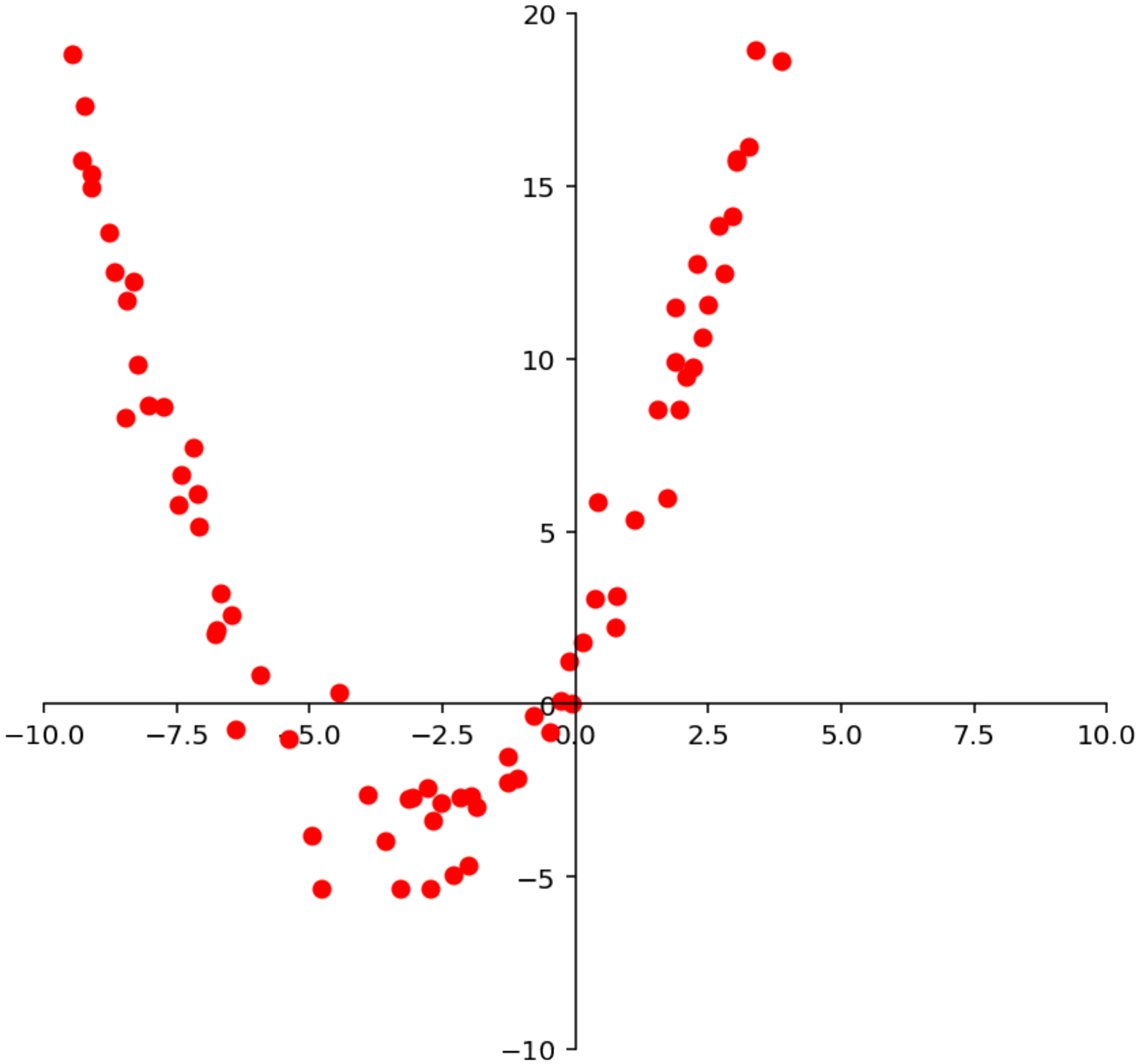

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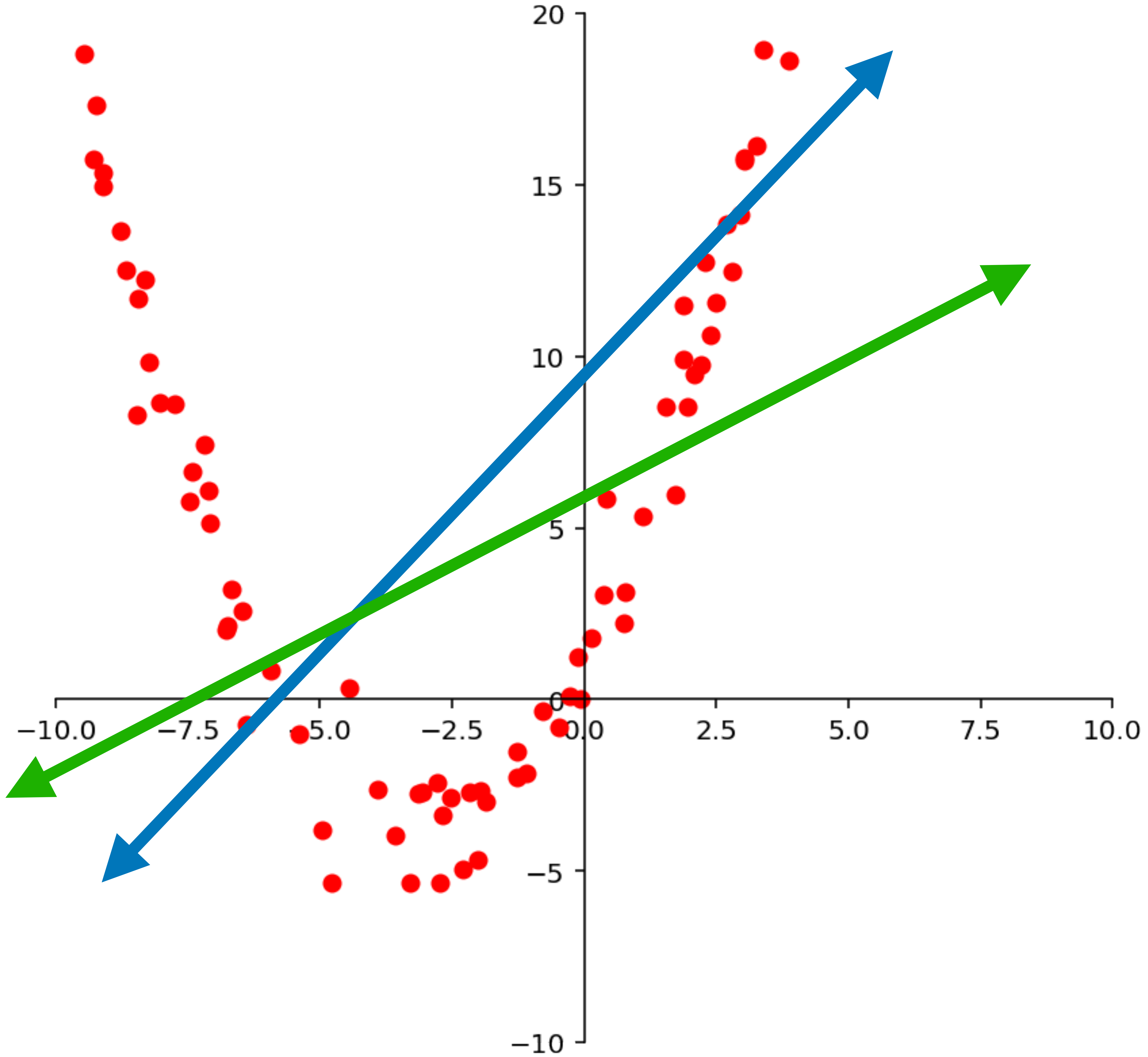
The issue: There is no good line to approximate this data.



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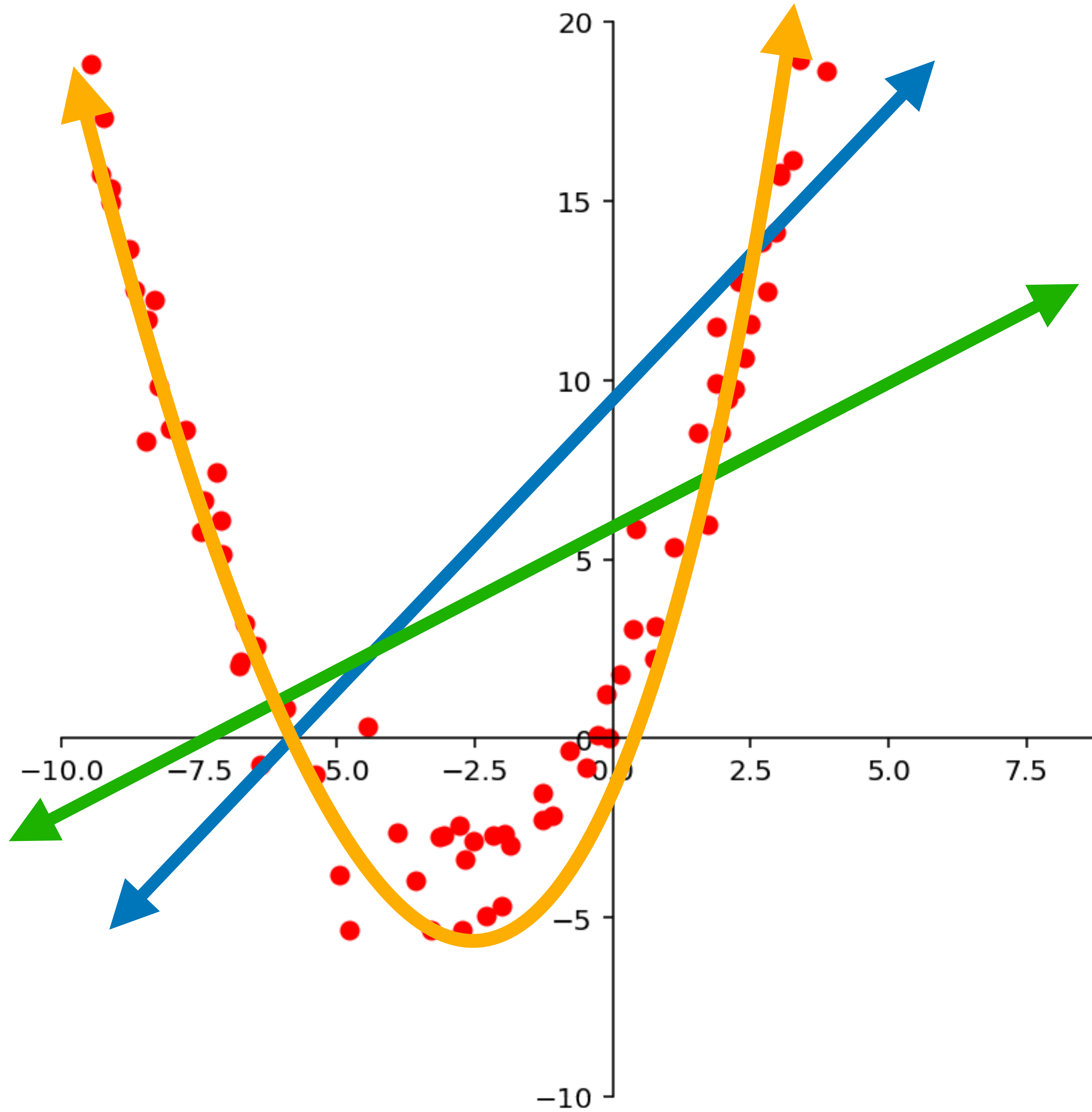
What about a parabola?



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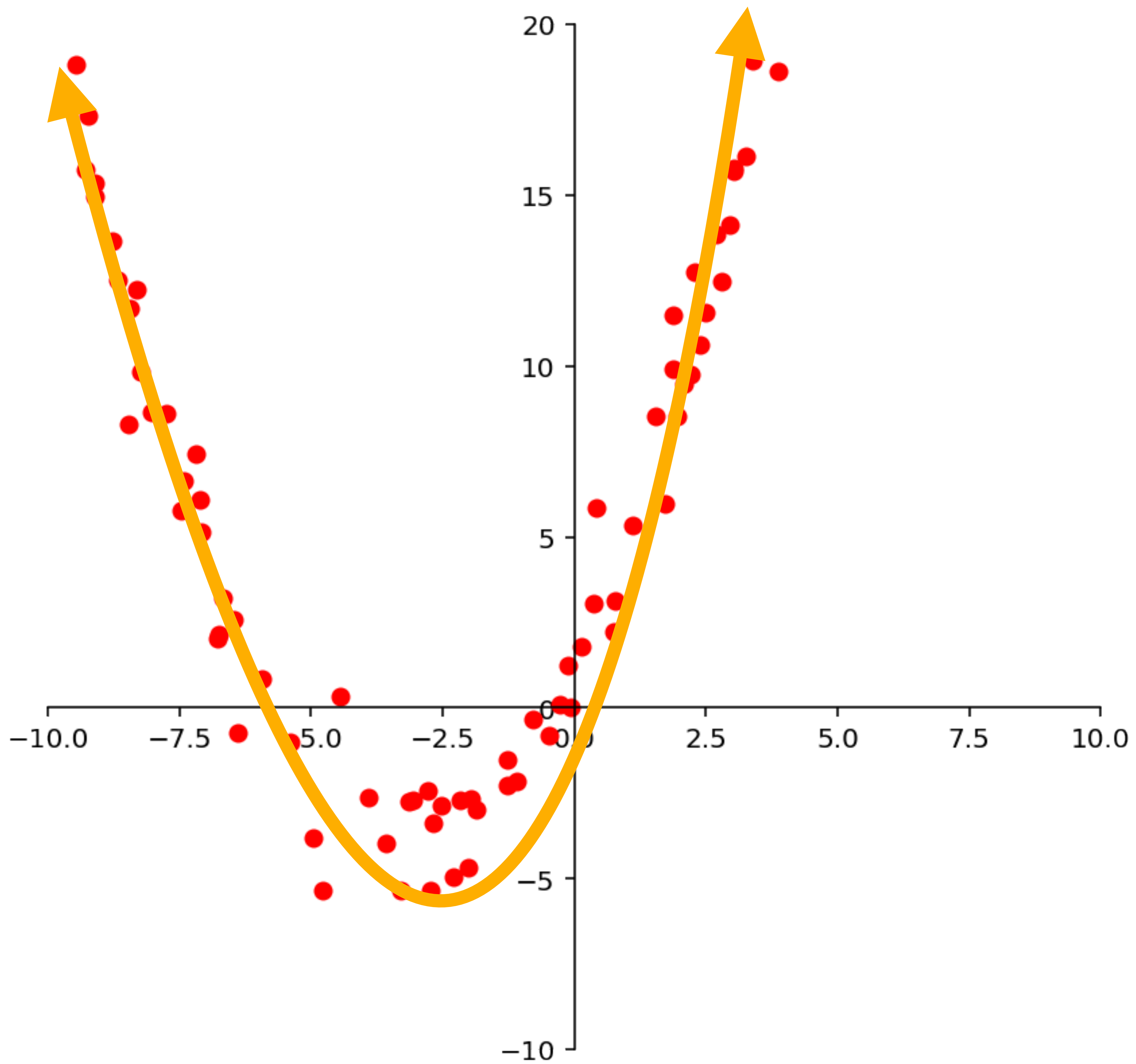

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This is still linear in the β's

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

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

Question

Find the <u>parabola</u> 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

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:

An Aside: Statistical Models (Another view)

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

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

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It is also common to *make the system consistent* by adding error terms (the ϵ's).

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

An Aside: Statistical Models (Another view)

design matrix

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

It is also common to *make the system consistent* by adding error terms (the ϵ's).

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

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

General Linear Regression

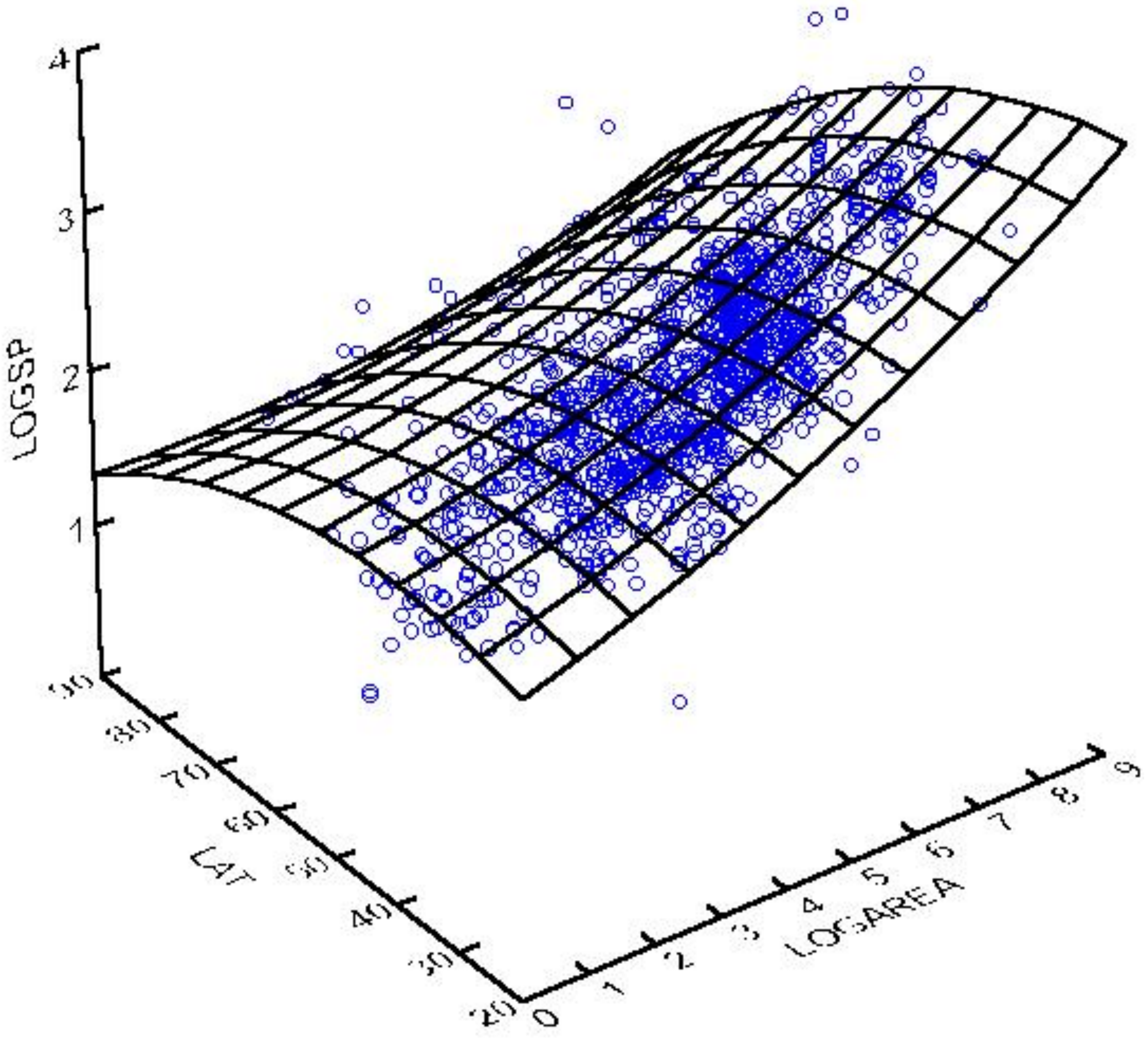
dataset: $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$ where $\mathbf{x}_i \in \mathbb{R}^n$ and $y_i \in \mathbb{R}$

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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$$\begin{aligned}\beta_1\phi_1(\mathbf{x}_1) + \ldots + \beta_k\phi_k(\mathbf{x}_1) &= y_1\\ \beta_1\phi_1(\mathbf{x}_2) + \ldots + \beta_k\phi_k(\mathbf{x}_2) &= y_2\\ &\vdots\\ \beta_1\phi_1(\mathbf{x}_2) + \ldots + \beta_k\phi_k(\mathbf{x}_2) &= y_2\end{aligned}$$

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General Linear Regression

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.

General Linear Regression

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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 $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$.

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 $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$.

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.