

# **Practical Issues and Feature Normalization**

## **DS 4400 | Machine Learning and Data Mining I**

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# Today's Outline

1. Recap
2. Practical Issues in Linear Regression
3. Feature Pre-processing and Normalization

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1. **Recap**
2. Practical Issues in Linear Regression
3. Feature Pre-processing and Normalization

# Recap

## Derivative of the Sigmoid Function

- Sigmoid:  $\sigma(x) = \frac{1}{1 + e^{-x}}$

$$\text{Let } f(x) = 1 + e^{-x} \text{ and } g(x) = \frac{1}{x} = x^{-1}$$

$$\sigma(x) = g(f(x))$$

$$\sigma(x) = (1 + e^{-x})^{-1}$$

$$\sigma'(x) = -1 \cdot (1 + e^{-x})^{-2} \cdot -e^{-x}$$

$$\sigma'(x) = \frac{e^{-x}}{(1 + e^{-x})^2}$$

$$\sigma'(x) = \sigma(x) \cdot \frac{e^{-x}}{1 + e^{-x}}$$

$$\sigma'(x) = \sigma(x) \cdot (1 - \sigma(x))$$

# Recap

## Linear Regression Derivation

$$L(\theta) = \frac{1}{m} \sum_{i=1}^m [f_{\theta}(x_i) - y_i]^2$$

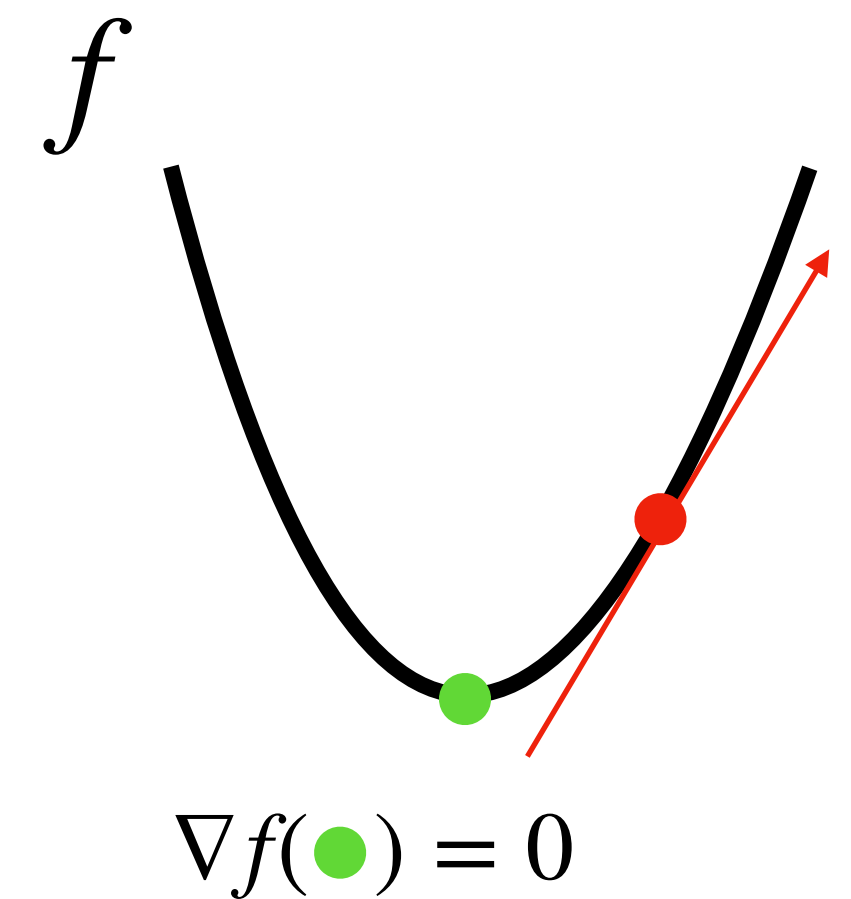
$$L(\theta) = \frac{1}{m} \sum_{i=1}^m [\theta_0 + \theta_1 \cdot x_i - y_i]^2$$

Find the point where  $\nabla L(\theta) = 0$

$$\frac{\partial L(\theta)}{\partial \theta_0} = \frac{2}{m} \sum_{i=1}^m (\theta_0 + \theta_1 x_i - y_i) = 0$$

$$\frac{\partial L(\theta)}{\partial \theta_1} = \frac{2}{m} \sum_{i=1}^m x_i \cdot (\theta_0 + \theta_1 x_i - y_i) = 0$$

$\nabla f(\bullet)$  points in direction of steepest ascent



# Recap

## Linear Regression Derivation

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$$\theta_0 = \bar{y} - \theta_1 \bar{x}$$

$$\theta_1 = \frac{Cov(x, y)}{Var(x)}$$

# Recap

## Linear Regression Derivation - Matrix Form

$$L(\theta) = \frac{1}{m} \sum (Y - X\theta)^2$$

$$Y \in \mathbb{R}^{m \times 1}$$

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

$$\theta \in \mathbb{R}^{n \times 1}$$

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$$\vec{u} = \begin{bmatrix} 5 \\ 7 \\ 9 \end{bmatrix} \quad \vec{u}^2 = \begin{bmatrix} 25 \\ 49 \\ 81 \end{bmatrix}$$

# Recap

## Linear Regression Derivation - Matrix Form

$$L(\theta) = \frac{1}{m} \sum (Y - X\theta)^2$$

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$$u^T u = [5 \ 7 \ 9] \cdot \begin{bmatrix} 5 \\ 7 \\ 9 \end{bmatrix} = [5 \cdot 5 + 7 \cdot 7 + 9 \cdot 9] = [155]$$

# Recap

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$$u^T u = [u_1^2 + u_2^2 + u_3^2 + \cdots u_n^2] = \sum_i^n u_i^2$$

# Recap

## Linear Regression Derivation - Matrix Form

$$L(\theta) = \frac{1}{m} \sum (Y - X\theta)^2$$

Each of these is a vector

$$\vec{u} = \begin{bmatrix} 5 \\ 7 \\ 9 \end{bmatrix} \quad \vec{u}^2 = \begin{bmatrix} 25 \\ 49 \\ 81 \end{bmatrix}$$

$$u^T u = [5 \ 7 \ 9] \cdot \begin{bmatrix} 5 \\ 7 \\ 9 \end{bmatrix} = [5 \cdot 5 + 7 \cdot 7 + 9 \cdot 9] = [155]$$

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# Recap

## Linear Regression Derivation - Matrix Form

$$L(\theta) = \frac{1}{m} \sum (Y - X\theta)^2$$

This whole thing is then also a vector

$$\vec{u} = \begin{bmatrix} 5 \\ 7 \\ 9 \end{bmatrix} \quad \vec{u}^2 = \begin{bmatrix} 25 \\ 49 \\ 81 \end{bmatrix}$$

$$u^T u = [5 \ 7 \ 9] \cdot \begin{bmatrix} 5 \\ 7 \\ 9 \end{bmatrix} = [5 \cdot 5 + 7 \cdot 7 + 9 \cdot 9] = [155]$$

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# Recap

## Linear Regression Derivation - Matrix Form

$$L(\theta) = \frac{1}{m} \sum (Y - X\theta)^2$$

These two representations are now similar

$$\vec{u} = \begin{bmatrix} 5 \\ 7 \\ 9 \end{bmatrix} \quad \vec{u}^2 = \begin{bmatrix} 25 \\ 49 \\ 81 \end{bmatrix}$$

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# Recap

## Linear Regression Derivation - Matrix Form

$$L(\theta) = \frac{1}{m} \sum (Y - X\theta)^2$$

So we can replace this with  $(Y - X\theta)^T(Y - X\theta)$

$$\vec{u} = \begin{bmatrix} 5 \\ 7 \\ 9 \end{bmatrix} \quad \vec{u}^2 = \begin{bmatrix} 25 \\ 49 \\ 81 \end{bmatrix}$$

$$u^T u = [5 \ 7 \ 9] \cdot \begin{bmatrix} 5 \\ 7 \\ 9 \end{bmatrix} = [5 \cdot 5 + 7 \cdot 7 + 9 \cdot 9] = [155]$$

$$u^T u = [u_1^2 + u_2^2 + u_3^2 + \cdots u_n^2] = \sum_i^n u_i^2$$

# Recap

## Linear Regression Derivation - Matrix Form

$$L(\theta) = \frac{1}{m} \sum (Y - X\theta)^2$$

$$L(\theta) = (Y - X\theta)^T (Y - X\theta)$$

(why is this true?)

$$L(\theta) = (Y^T - \theta^T X^T)(Y - X\theta)$$

(Take the transpose inside. And then, because  $(AB)^T = B^T A^T$ )

$$L(\theta) = Y^T Y - Y^T X\theta - \theta^T X^T Y + \theta^T X^T X\theta$$

(the two terms in the centre are equivalent, why?)

$$L(\theta) = Y^T Y - 2\theta^T X^T Y + \theta^T X^T X\theta$$



# Recap

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# Recap

## Linear Regression Derivation - Matrix Form

$$Y^T X \theta \in \mathbb{R}^{1 \times m} \cdot \mathbb{R}^{m \times n} \cdot \mathbb{R}^{n \times 1}$$

Which means

$$Y^T X \theta \in \mathbb{R}^{1 \times 1}$$

Which means

$Y^T X \theta$  is **symmetric**

Which is why

$$Y^T X \theta = (Y^T X \theta)^T = \theta^T X^T Y$$

# Recap

## Linear Regression Derivation - Matrix Form

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# Recap

## Matrix Form - Derivative

$$L(\theta) = Y^T Y - 2\theta^T X^T Y + \theta^T X^T X \theta$$

For any vector  $A$

$$\nabla_A (B^T A) = B$$

For any symmetric matrix  $B$

$$\nabla_A (A^T B A) = 2BA$$

So we have

$$\nabla L(\theta) = -2X^T Y + 2X^T X \theta$$

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$X^T Y \in \mathbb{R}^{n \times 1}$  - This is a vector.

# Recap

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$$\theta^T B \text{ where } B = X^T Y \in \mathbb{R}^{n \times 1}$$



# Recap

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We know this is symmetric because the result is  $\in \mathbb{R}^{1 \times 1}$

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Lets look at  $\theta^T X^T Y$

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$$\theta^T B = (\theta^T B)^T = B^T \theta$$

The derivative rule we had:

$$\nabla_A (B^T A) = B$$

# Recap

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$$L(\theta) = Y^T Y - 2\theta^T X^T Y + \theta^T X^T X \theta$$

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# Recap

## Matrix Form - Derivative

Is  $X^T X$  symmetric?

$$(X^T X)^T = X^T \cdot (X^T)^T = X^T X$$

$X^T X$  is **always** symmetric

$$L(\theta) = Y^T Y - 2\theta^T X^T Y + \theta^T X^T X \theta$$

For any vector  $A$

$$\nabla_A (B^T A) = B$$

For any **symmetric** matrix  $B$

$$\nabla_A (A^T B A) = 2BA$$

So we have

$$\nabla L(\theta) = -2X^T Y + 2X^T X \theta$$

# Recap

## Solution

We want to find the minimum so set gradient to zero

$$\nabla L(\theta) = -2X^T Y + 2X^T X \theta = 0$$

$$2X^T X \theta = 2X^T Y$$

$$X^T X \theta = X^T Y$$

If  $X^T X$  is invertible, then

$$\theta = (X^T X)^{-1} X^T Y$$

# Practical Example

[https://zohairshafi.github.io/pages/lectures/Lecture\\_2\\_Notebook.ipynb](https://zohairshafi.github.io/pages/lectures/Lecture_2_Notebook.ipynb)



# Today's Outline

1. Recap
- 2. Practical Issues in Linear Regression**
3. Feature Pre-processing and Normalization

# Train / Test Splits

- Generally data is split into a training dataset and a testing data
- Rough rule of thumb is that this is an 80-20 split

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[illegible]

# Train / Test Splits

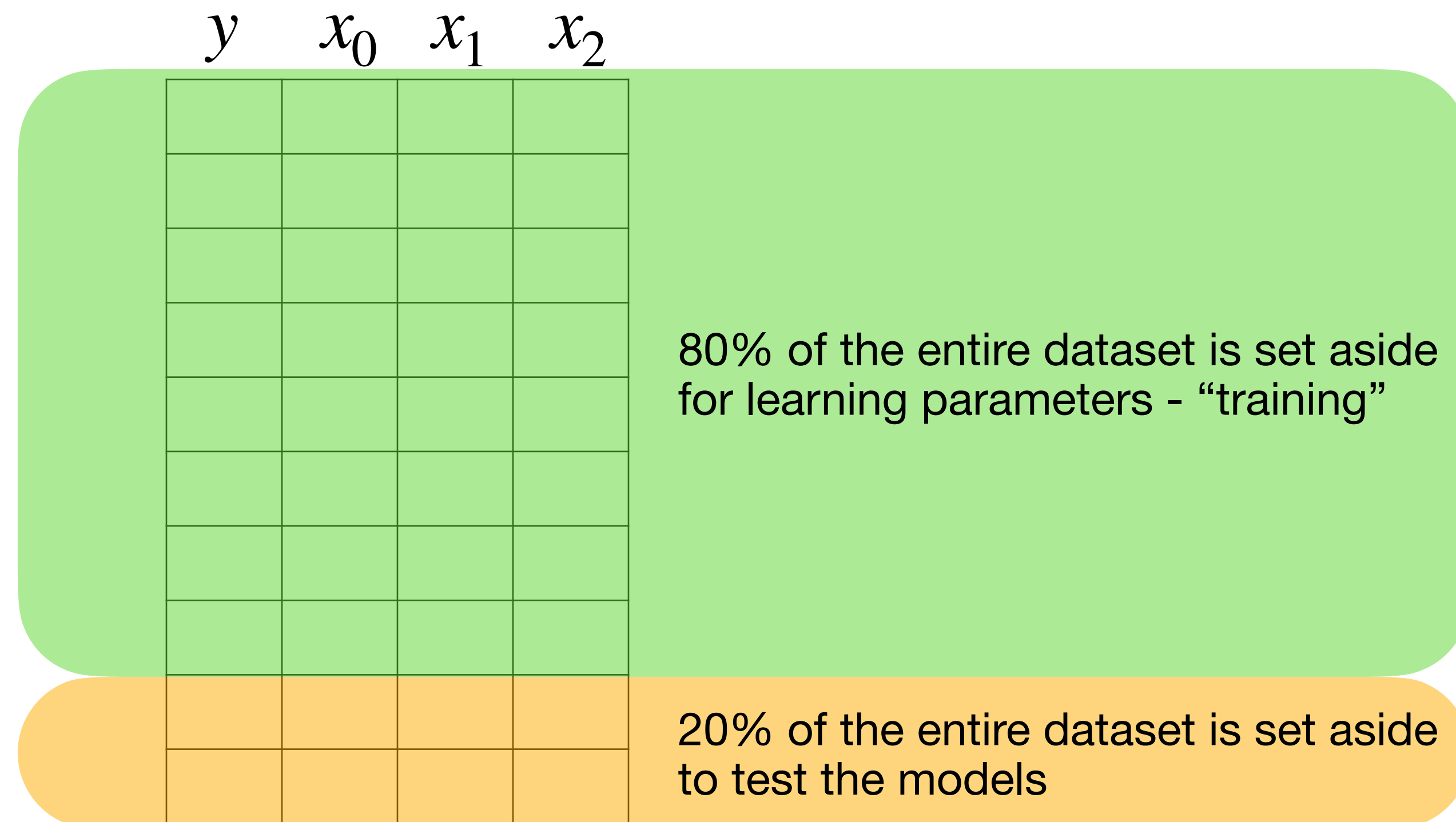
- Generally data is split into a training dataset and a testing data
- Rough rule of thumb is that this is an 80-20 split

$y$	$x_0$	$x_1$	$x_2$

80% of the entire dataset is set aside for learning parameters - "training"

# Train / Test Splits

- Generally data is split into a training dataset and a testing data
- Rough rule of thumb is that this is an 80-20 split



This is **unseen** data and tells you if the model can generalize well

# Train / Test Splits

- However, in practice, if you are given only one train and test set, its easy to accidentally pick model architectures that work well on the test set, even though test set data is unseen
- To counter this, we use two unseen datasets - “validation” set and “test” set
- The split is generally of the form 80-10-10 where 80% is training data, 10% is validation data and 10% is test data

# Practical Issues in Linear Regression

## Multicollinearity

- When two features are highly correlated or are linearly dependent on each other

# Practical Issues in Linear Regression

## Multicollinearity

- When two features are highly correlated or are linearly dependent on each other
- Why it's a problem:  $\theta = (X^T X)^{-1} X^T Y$ 
  - $X^T X$  becomes nearly singular (ill-conditioned)
  - Small changes in data cause huge changes in coefficients
  - Coefficients become unreliable and hard to interpret
  - Standard errors blow up



# Practical Issues in Linear Regression

## Multicollinearity

- When two features are highly correlated or are linearly dependent on each other
  - Why it's a problem:  $\theta = (X^T X)^{-1} X^T Y$ 
    - $X^T X$  becomes nearly singular (ill-conditioned)
    - Small changes in data cause huge changes in coefficients
    - Coefficients become unreliable and hard to interpret
    - Standard errors blow up
- Simple Detection:  
If correlation between features  $\geq 0.8$

# Practical Issues in Linear Regression

## Quick Aside

$$\theta = (X^T X)^{-1} X^T Y$$

When else is this not going to be invertible?

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

$m$ : Number of training examples

$n$ : Number of parameters in the model

# Practical Issues in Linear Regression

## Quick Aside

$$\theta = (X^T X)^{-1} X^T Y$$

When else is this not going to be invertible?

If  $m < n$ , then  $\text{rank}(X) \leq m$ , so need **more** data points than number of parameters to get a unique set of parameters

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

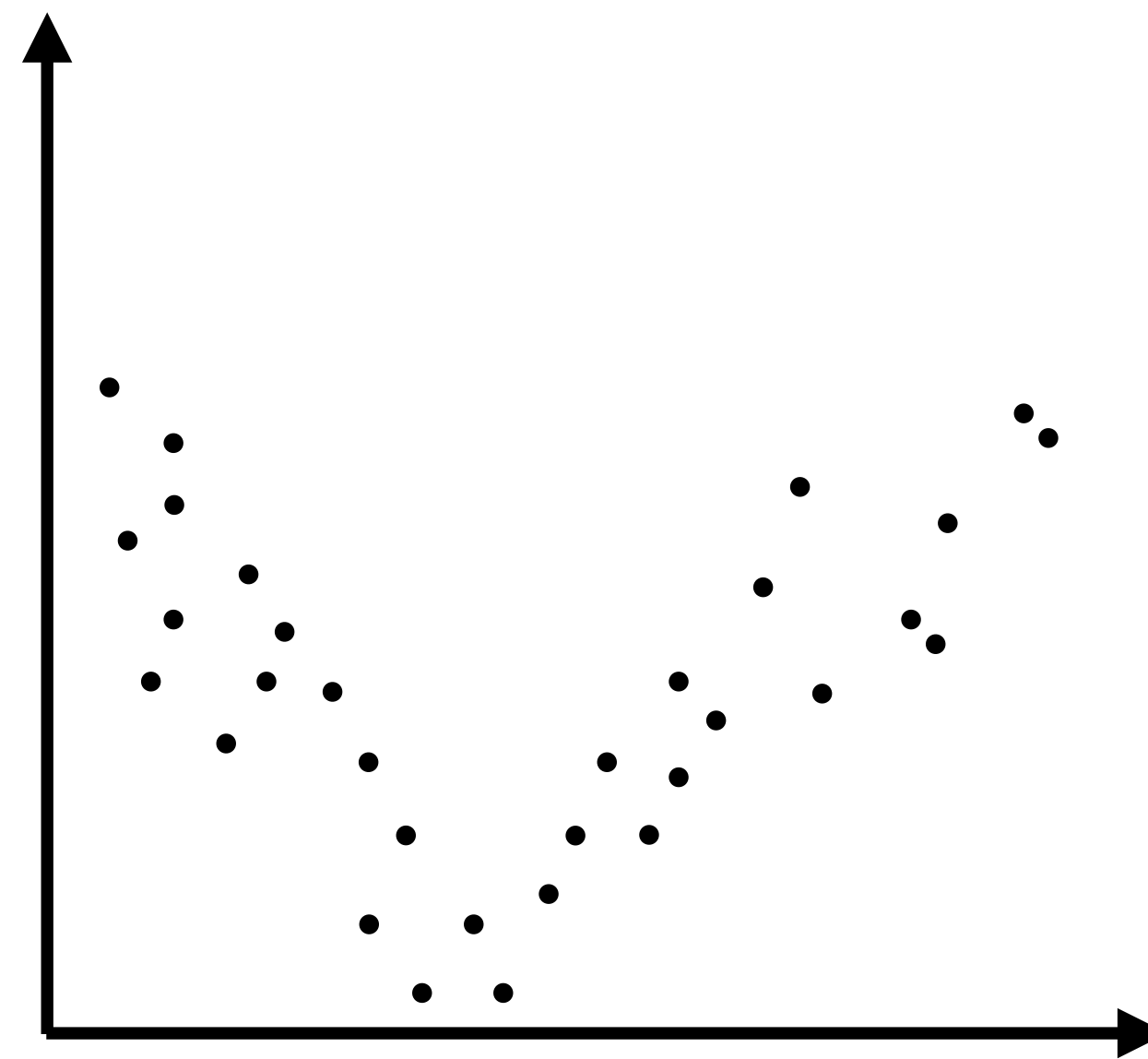
$m$ : Number of training examples

$n$ : Number of parameters in the model

$$\text{rank}(X) = \min(m, n)$$

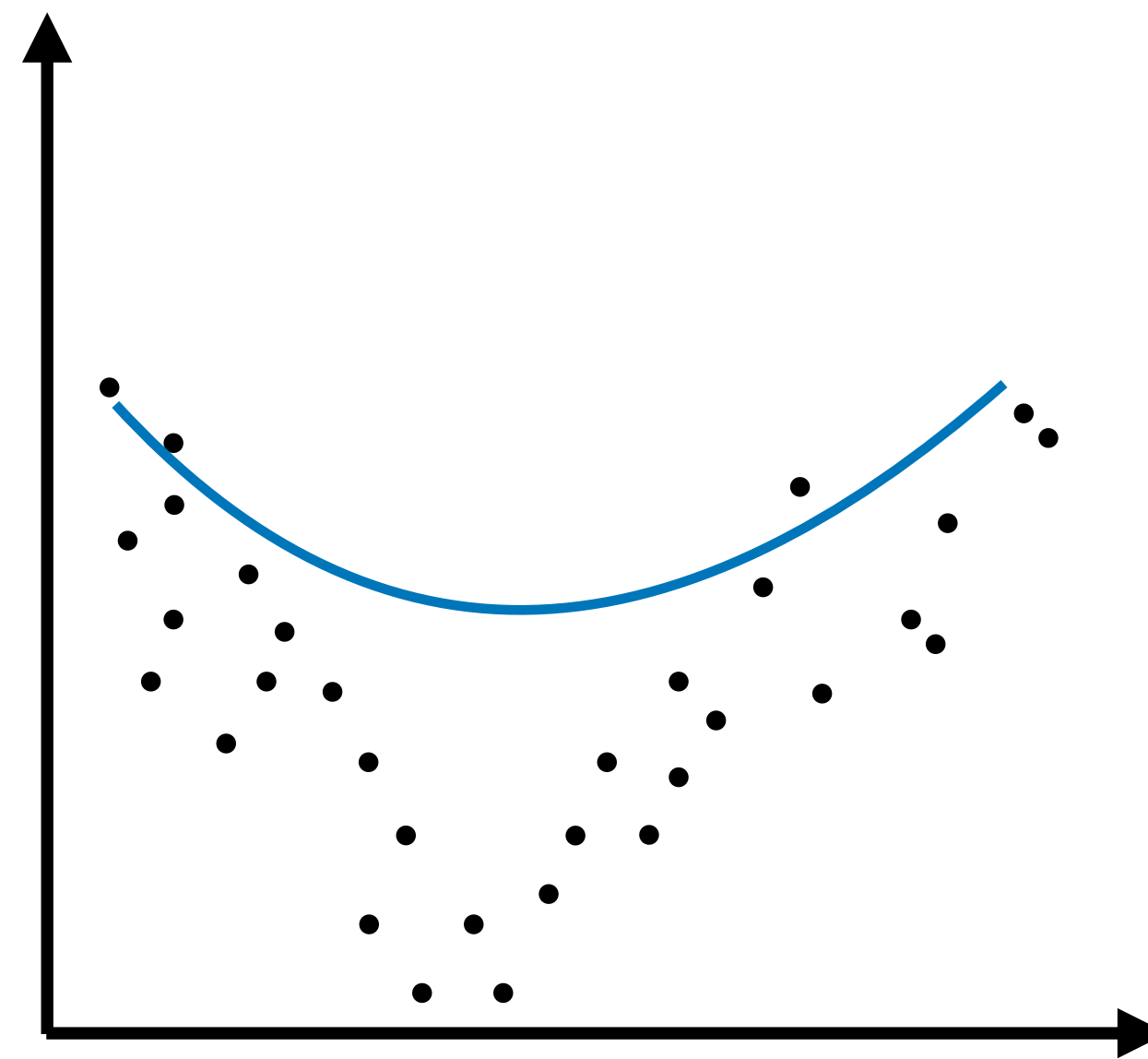
# Practical Issues in Linear Regression

## Overfitting vs Underfitting



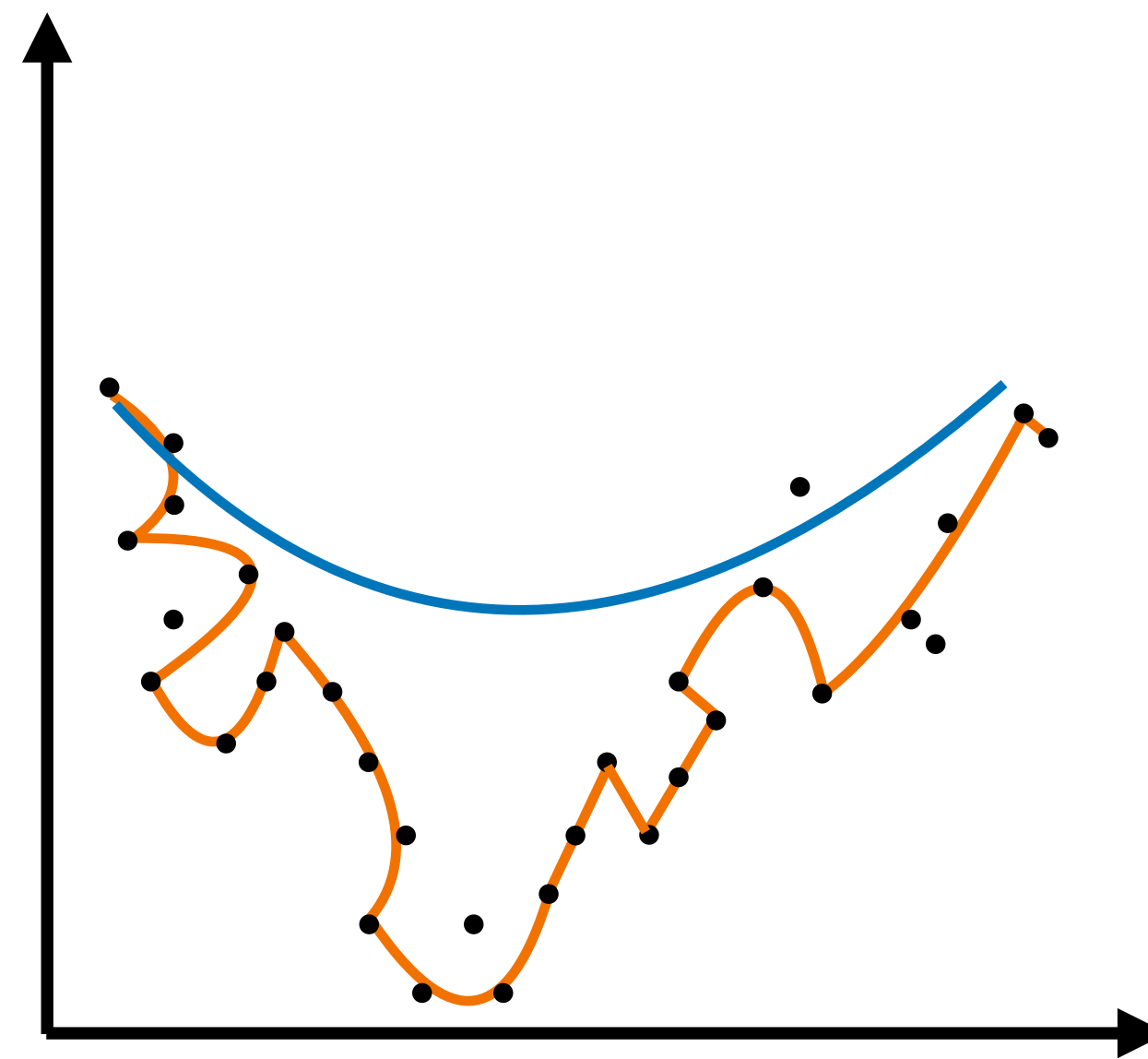
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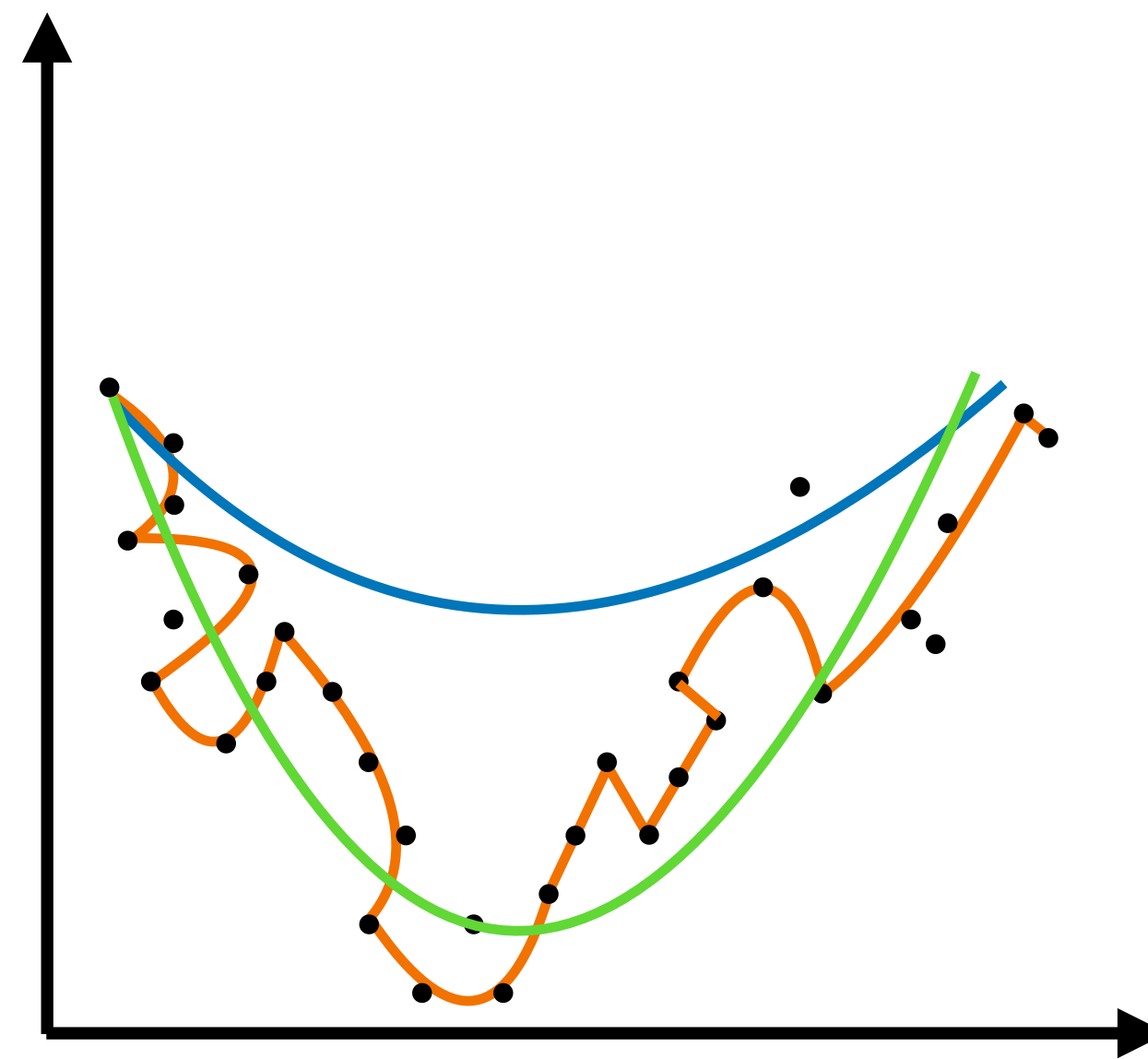
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# Practical Issues in Linear Regression

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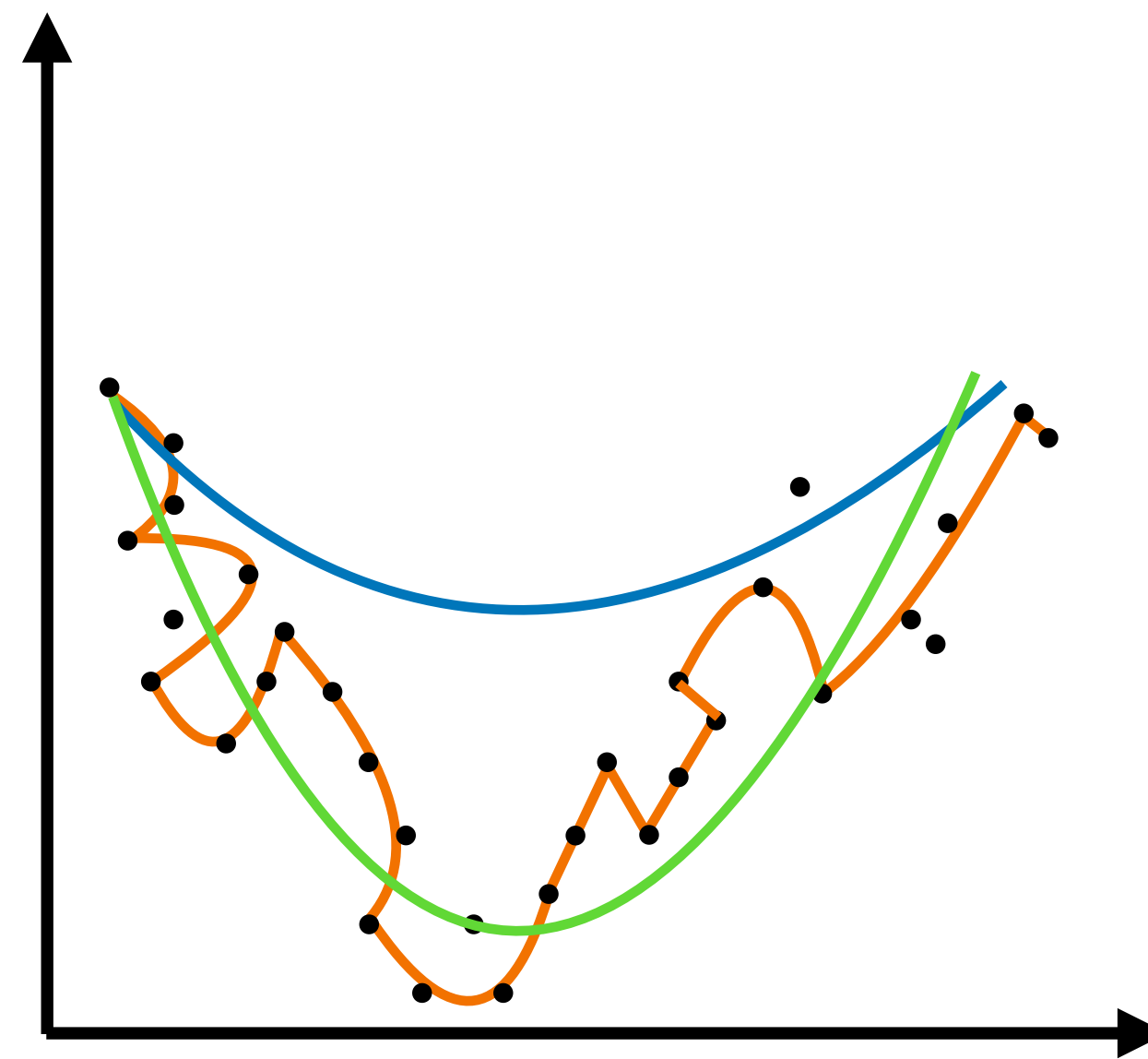
# Practical Issues in Linear Regression

## Overfitting vs Underfitting

The blue model is **underfitting** the data

The orange model is **overfitting** the data

The green model is a good fit of the data

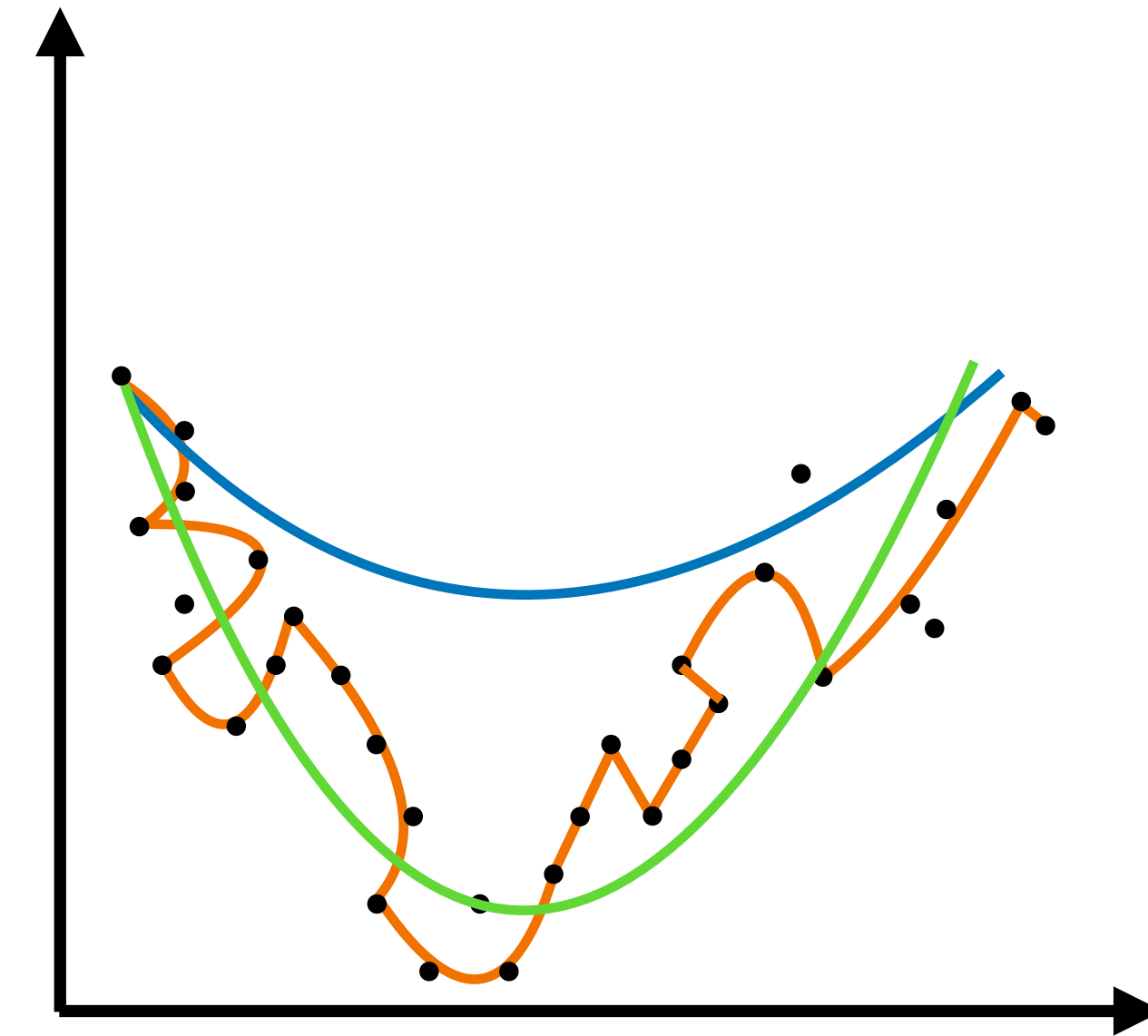




# Practical Issues in Linear Regression

## Underfitting

- What is happening?
  - The model is too simple to be able to capture the data
- How do you identify it?
  - Training loss is **high**
  - Test loss is **high**
- Solutions
  - Add more features
  - Add polynomial features ( $x_1^2, x_2^2, x_1x_2, \dots$ )
  - Use a more complex model



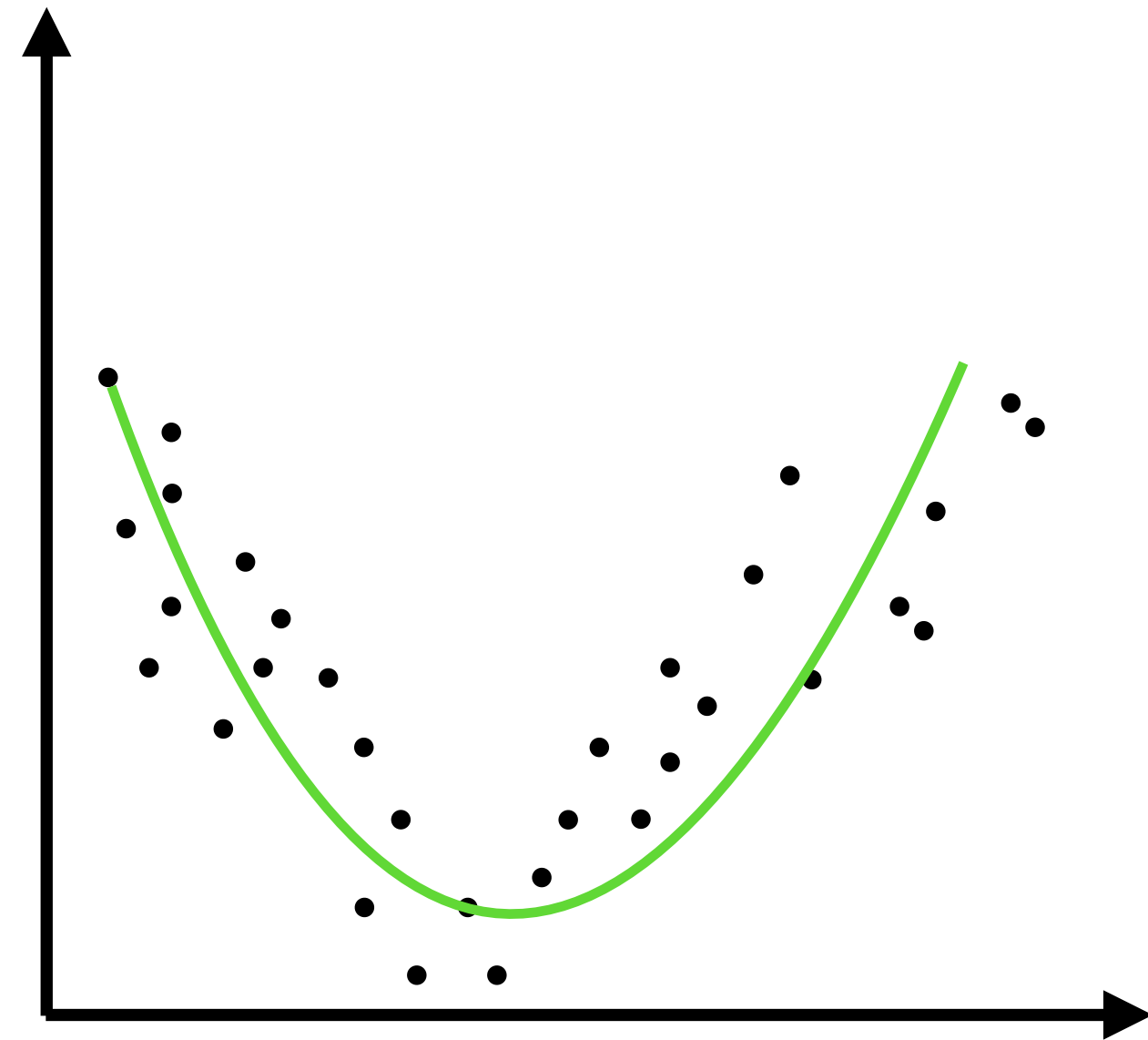
# Practical Issues in Linear Regression

## Quick Aside

- Add polynomial features ( $x_1^2, x_2^2, x_1x_2, \dots$ )

$$f_{\theta}(x) = \theta_0 + \theta_1x_1 + \theta_2x_1^2$$

**Question:** If the output looks like the curve in **green**, is this still **linear** regression?



# Practical Issues in Linear Regression

## Quick Aside

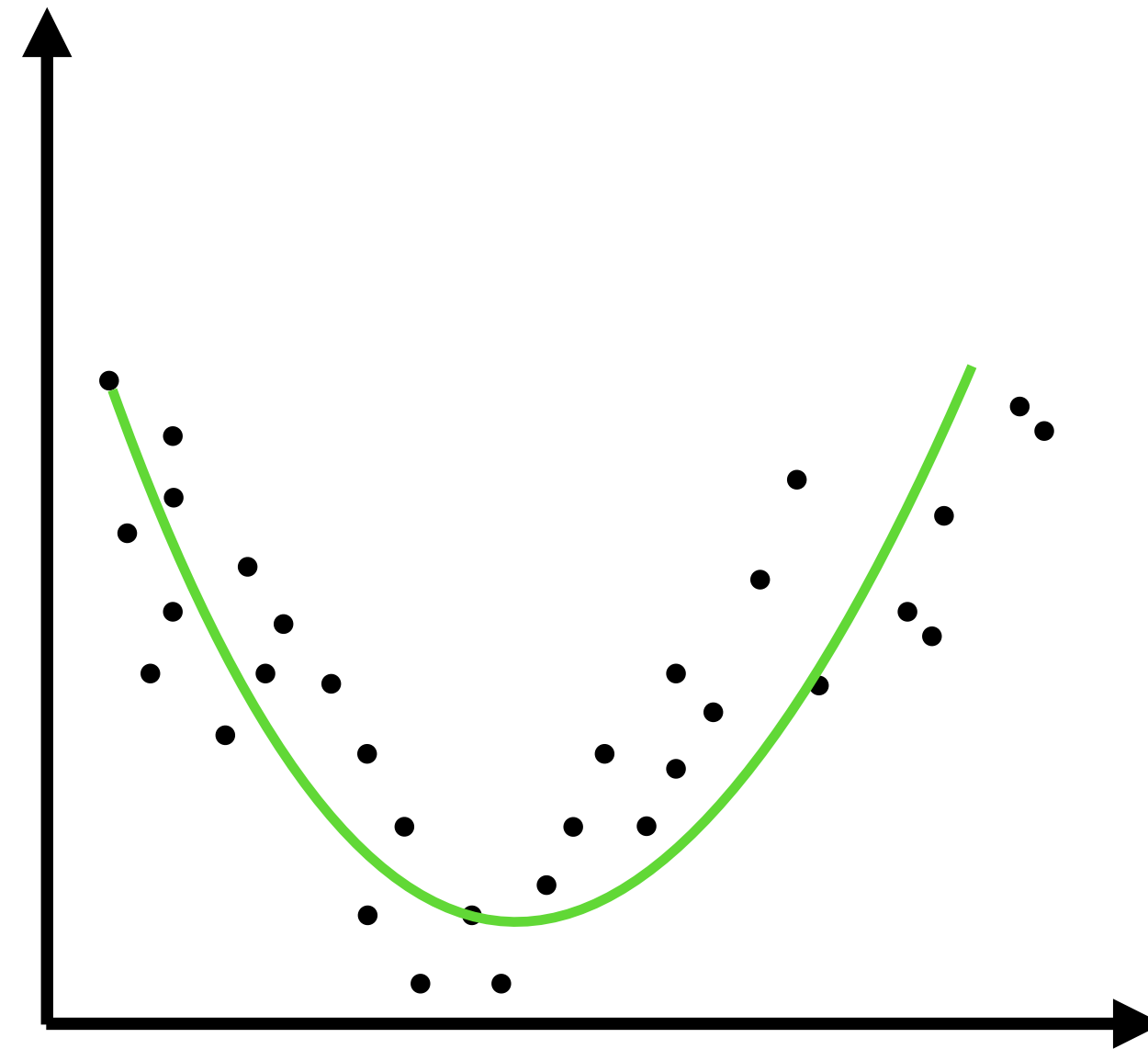
- Add polynomial features ( $x_1^2, x_2^2, x_1x_2, \dots$ )

$$f_{\theta}(x) = \theta_0 + \theta_1x_1 + \theta_2x_1^2$$

**Question:** If the output looks like the curve in **green**, is this still **linear** regression?

Yes, the model  $f_{\theta}(x)$  is still **linear** in its parameters, but just not in its inputs.

A model like  $f_{\theta}(x) = \theta_0 + x_1^{\theta_1}$  would however **not** classify as linear regression



# Practical Issues in Linear Regression

## Quick Aside

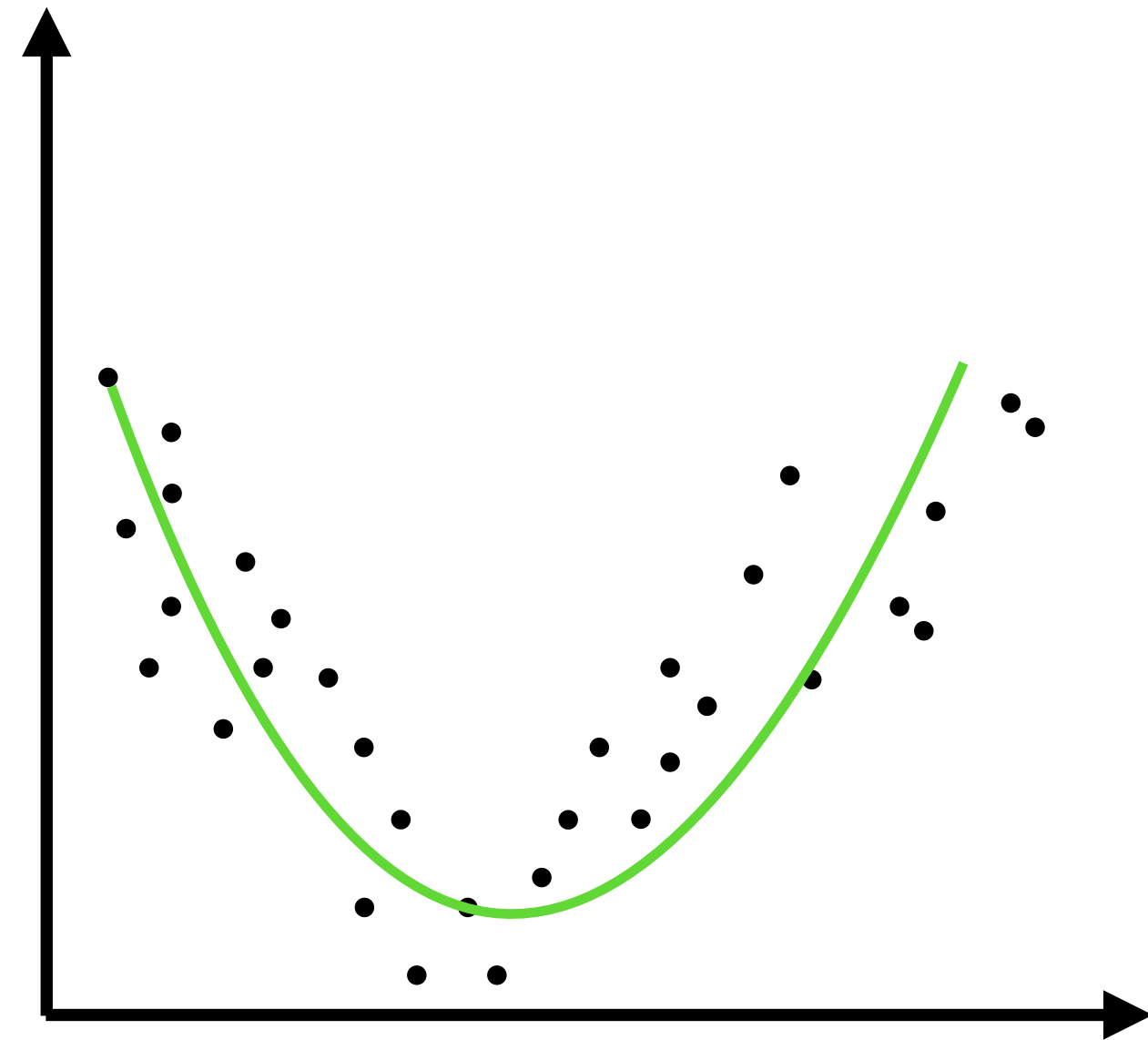
- Add polynomial features ( $x_1^2, x_2^2, x_1x_2, \dots$ )

$$f_{\theta}(x) = \theta_0 + \theta_1x_1 + \theta_2x_1^2$$

What about these models?

$$f_{\theta}(x) = \theta_1e^{x_1} + \theta_2\sin(x_2)$$

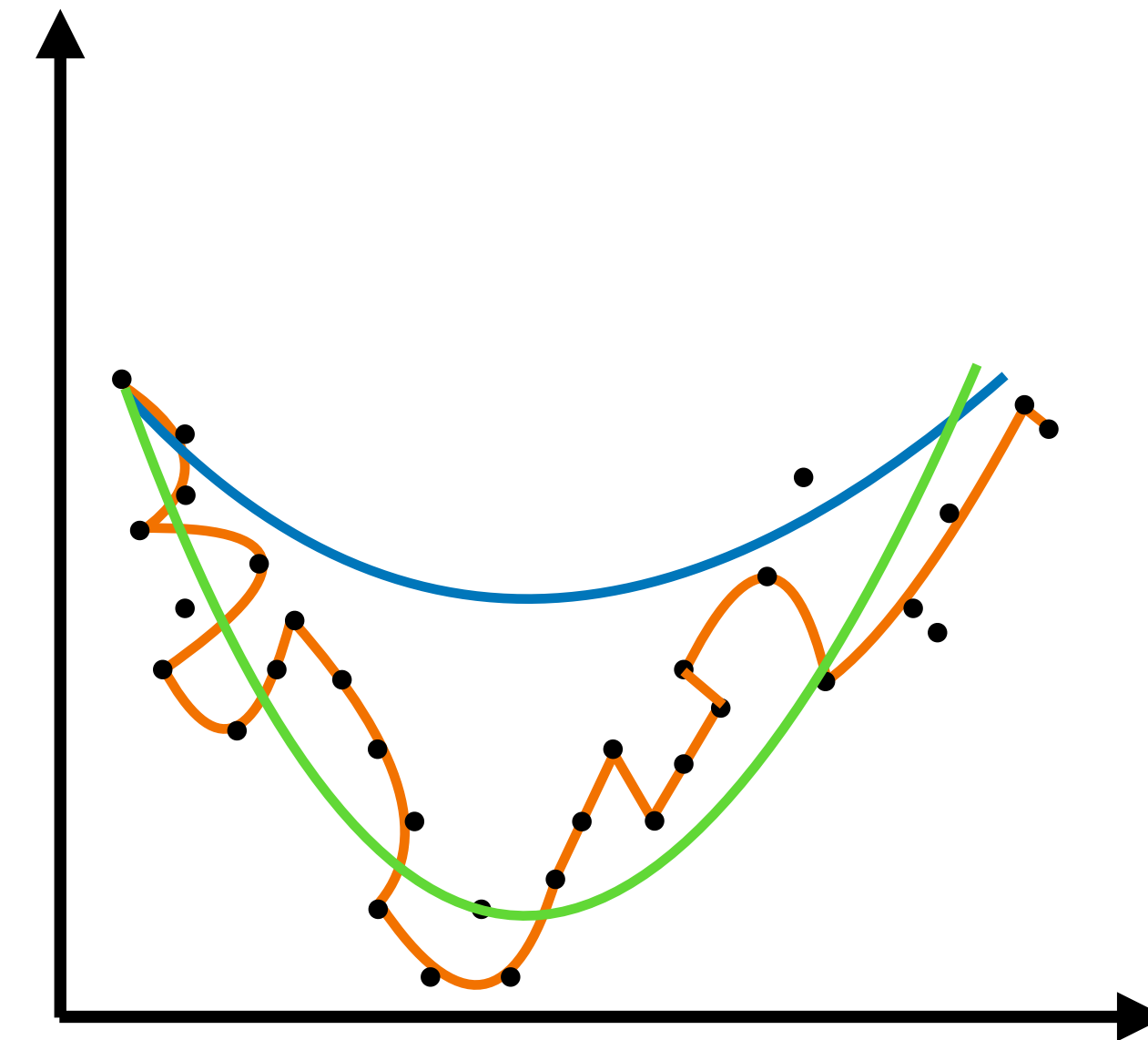
$$f_{\theta}(x) = \sin(\theta_1x_1 + \theta_2x_1^2) + \theta_2$$



# Practical Issues in Linear Regression

## Overfitting

- What is happening?
  - The model is too complex, so it learns the noise distribution and outliers and hence does not generalize well to new data points
- How do you identify it?
  - Training loss is **low**
  - Test loss is **high**
  - Coefficients have **large** magnitudes
- Solutions
  - Regularization ( $L_1, L_2$ )
  - Cross-validation for model selection
  - Reduce number of features
  - Get more training data



# Practical Issues in Linear Regression

## A more mathematical look - Bias / Variance Tradeoff

Every model's prediction error/loss can be decomposed into three parts:

$$\text{Expected Loss} = \text{Bias}^2 + \text{Variance} + \text{Irreducible Noise}$$

# Practical Issues in Linear Regression

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Every model's prediction error/loss can be decomposed into three parts:

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Error from wrong assumptions due to the model being too simple

# Practical Issues in Linear Regression

## A more mathematical look - Bias / Variance Tradeoff

Every model's prediction error/loss can be decomposed into three parts:

$$\text{Expected Loss} = \text{Bias}^2 + \text{Variance} + \text{Irreducible Noise}$$

Error from high sensitivity to each data point and noise due to the model being too complex



# Practical Issues in Linear Regression

## A more mathematical look - Bias / Variance Tradeoff

Every model's prediction error/loss can be decomposed into three parts:

$$\text{Expected Loss} = \text{Bias}^2 + \text{Variance} + \text{Irreducible Noise}$$

Inherent randomness in data. Cannot be removed.

# Practical Issues in Linear Regression

## A more mathematical look - Bias / Variance Tradeoff

Every model's prediction error/loss can be decomposed into three parts:

Expected Loss = Bias<sup>2</sup> + Variance + Irreducible Noise

$$\mathbb{E}[(Y - \hat{Y})^2] = (\mathbb{E}[\hat{Y}] - Y)^2 + \mathbb{E}[(\hat{Y} - \mathbb{E}[\hat{Y}])^2] + \sigma^2$$

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Expected Loss = Bias<sup>2</sup> + Variance + Irreducible Noise

$$\mathbb{E}[(Y - \hat{Y})^2] = (\mathbb{E}[\hat{Y}] - Y)^2 + \mathbb{E}[(\hat{Y} - \mathbb{E}[\hat{Y}])^2] + \sigma^2$$

How far is the average prediction from the true labels?

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If we use different training datasets, how much does  $\hat{Y}$  vary?

# Practical Issues in Linear Regression

## A more mathematical look - Bias / Variance Tradeoff

Every model's prediction error/loss can be decomposed into three parts:

Expected Loss = Bias<sup>2</sup> + Variance + Irreducible Noise

$$\mathbb{E}[(Y - \hat{Y})^2] = (\mathbb{E}[\hat{Y}] - Y)^2 + \mathbb{E}[(\hat{Y} - \mathbb{E}[\hat{Y}])^2] + \sigma^2$$

This is not the Sigmoid function. This is just irreducible noise in the true data  $Y$

# Practical Issues in Linear Regression

## Bias / Variance Tradeoff

Why is it called a **tradeoff**?

# Practical Issues in Linear Regression

## Bias / Variance Tradeoff

Why is it called a **tradeoff**?

Model Complexity	Bias	Variance	Train Error	Test Error
Too Simple	High	Low	High	High

# Practical Issues in Linear Regression

## Bias / Variance Tradeoff

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# Practical Issues in Linear Regression

## Bias / Variance Tradeoff

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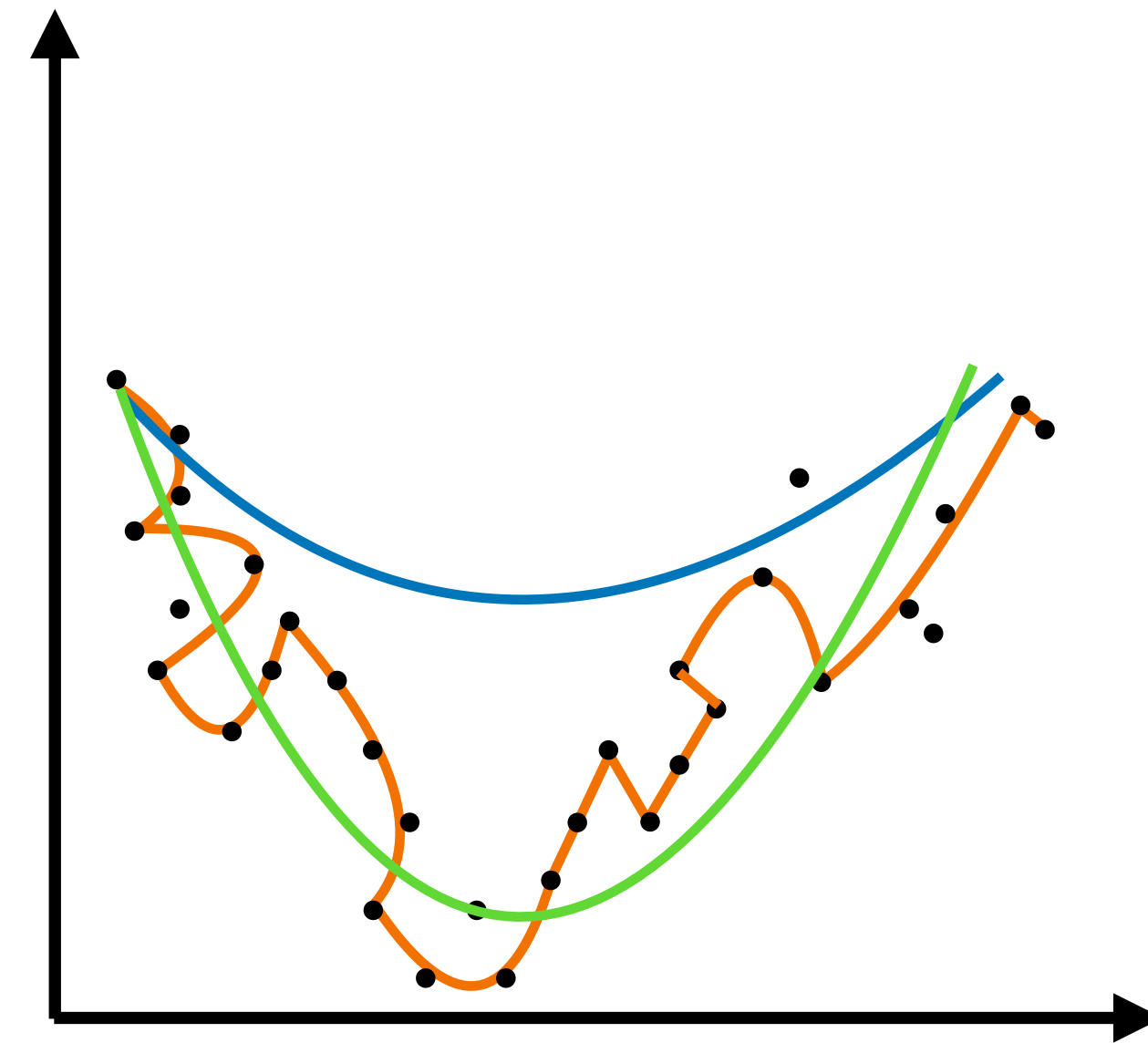
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Sweet Spot	Medium	Medium	Medium	Medium
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# Practical Issues in Linear Regression

## Regularization

- Regularization explicitly trades bias for variance.

$$L(\theta) = \frac{1}{m} \sum (Y - X\theta)^2$$



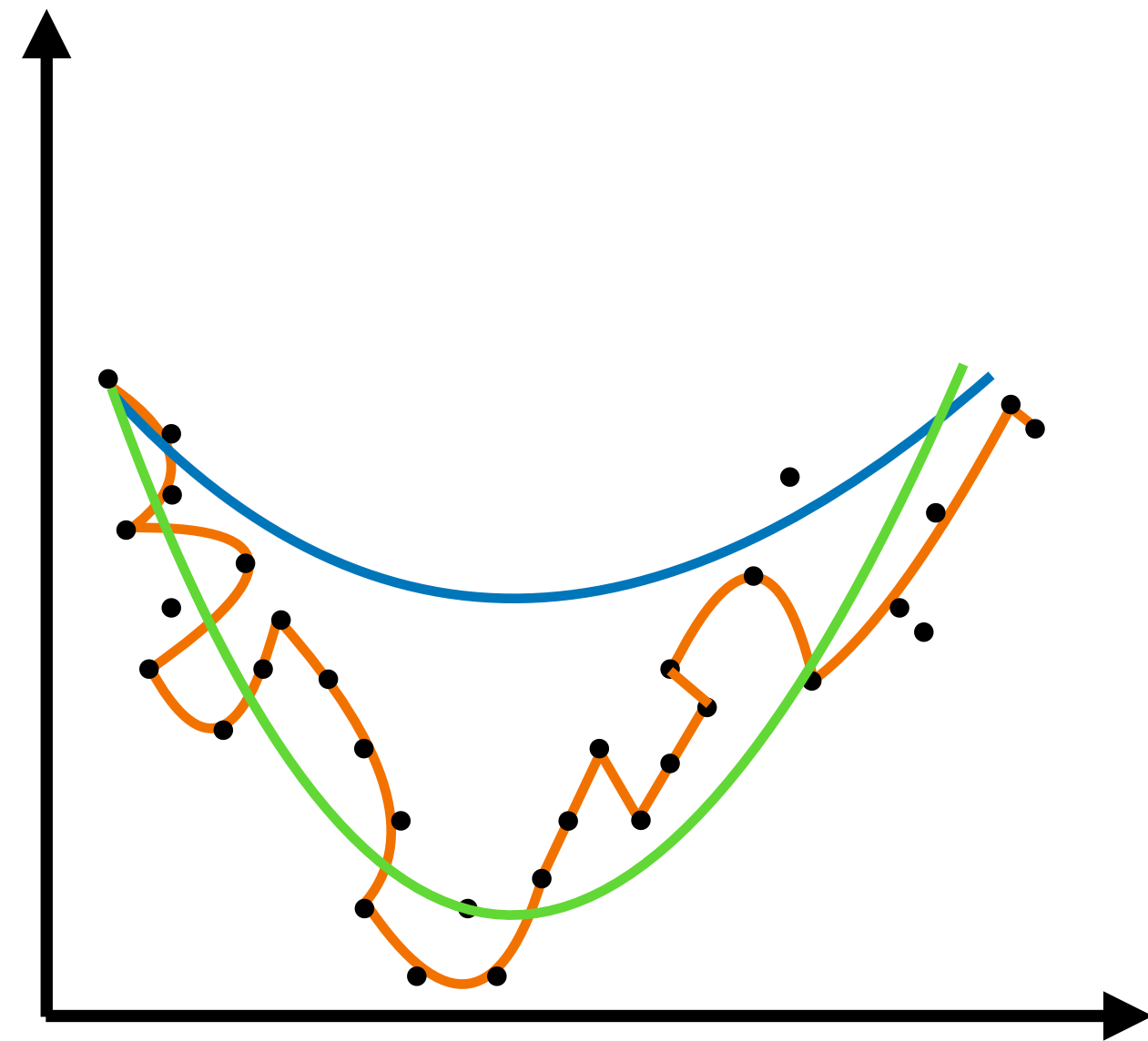
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# Practical Issues in Linear Regression

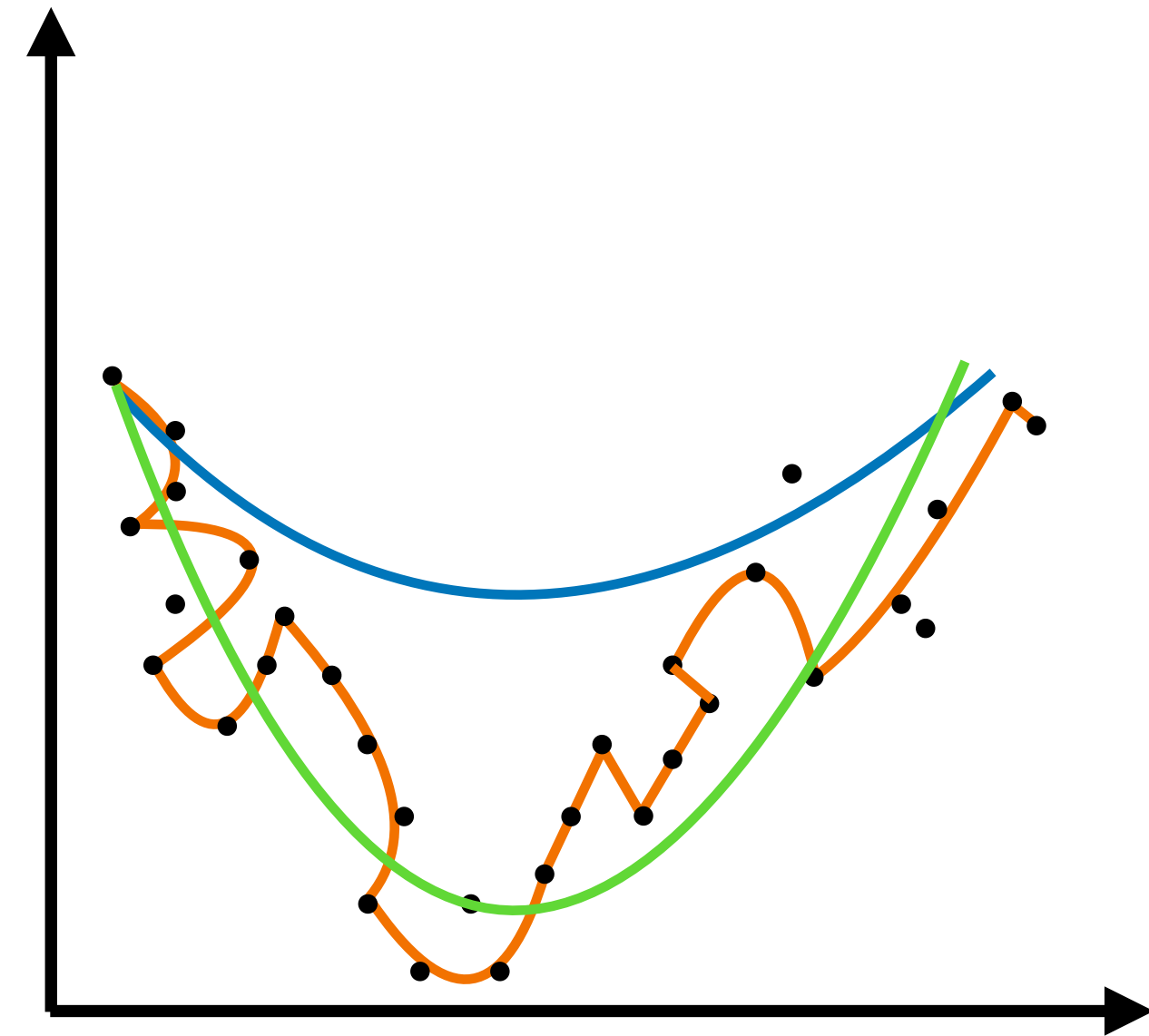
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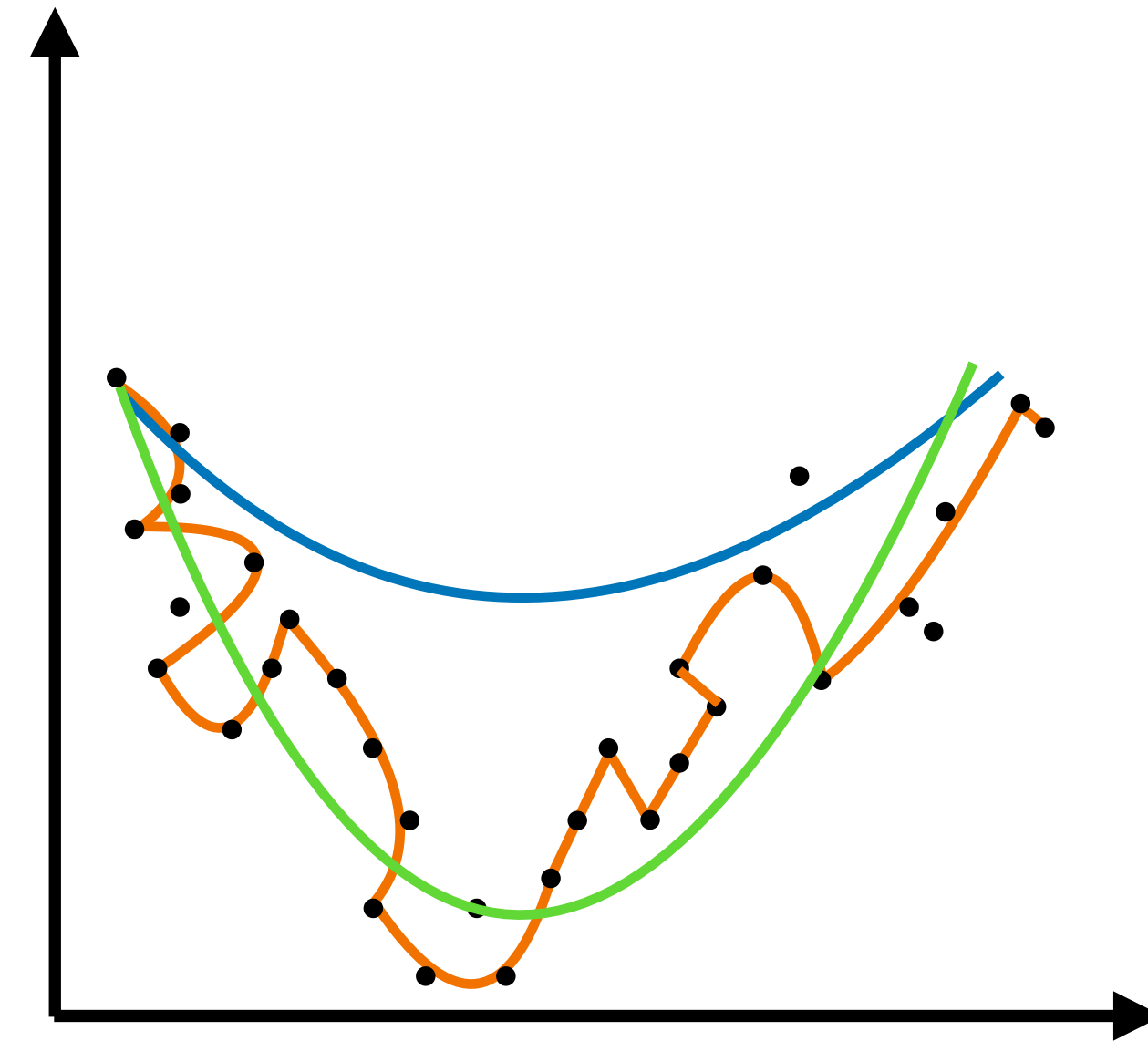
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  - Coefficients shrink toward zero
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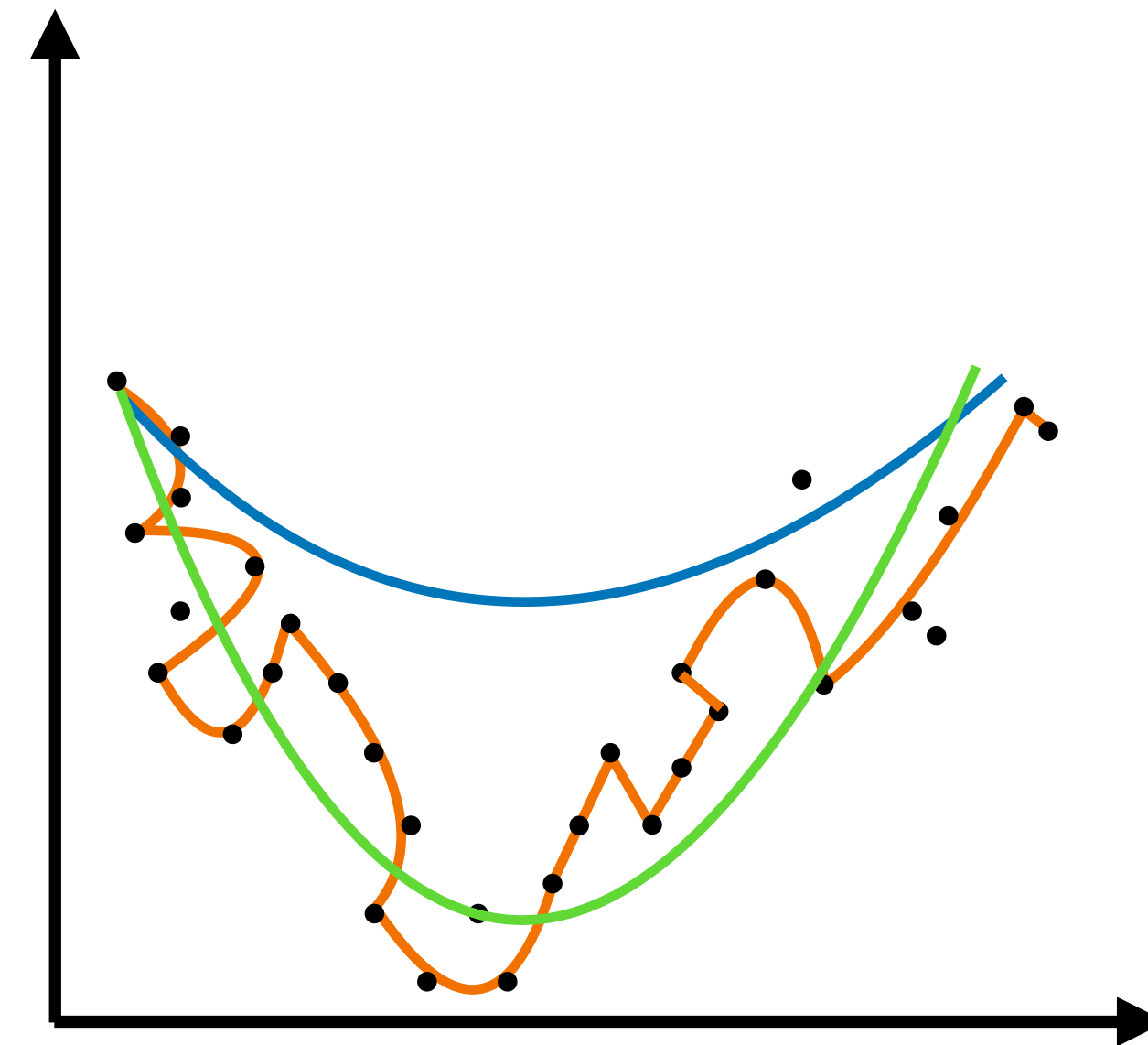
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These sort of parameters are usually called **hyper-parameters**

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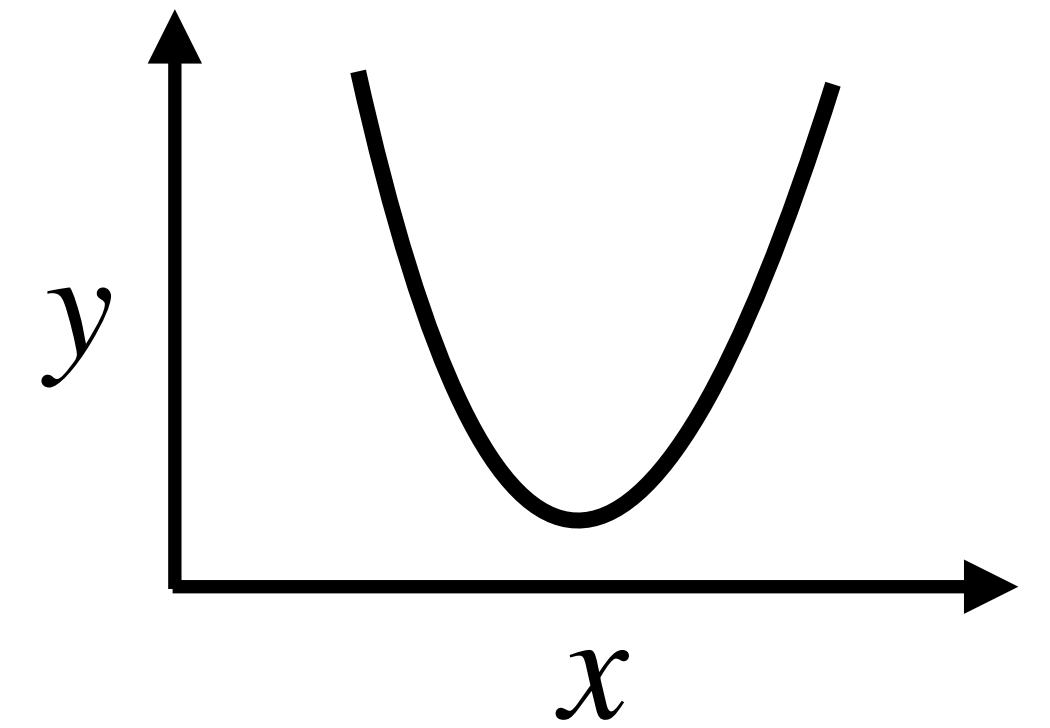
They are **not learnable** but are human defined



# Practical Issues in Linear Regression

## Non-Linearity

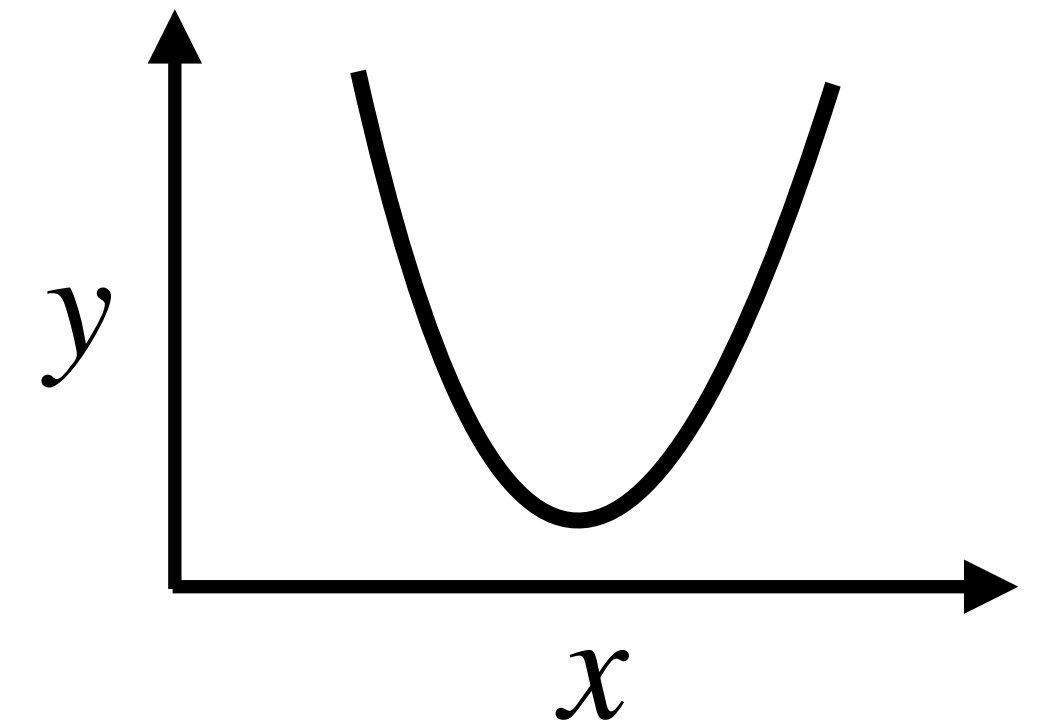
- True relationship between  $x$  and  $y$  is not linear



# Practical Issues in Linear Regression

## Non-Linearity

- True relationship between  $x$  and  $y$  is not linear
- Solutions:
  - Add polynomial terms like  $x^2, x^3$ , etc..
  - Add interaction terms like  $x_1 \cdot x_2$
  - Transform input features like  $\log(x), \sqrt{x}$
  - Use a non-linear model





# Today's Outline

1. Recap
2. Practical Issues in Linear Regression
3. Feature Pre-processing and Normalization

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# Feature Normalization

## Why Normalize?

- If feature  $x_1$  ranges from 0 to 1 and feature  $x_2$  ranges from 0 to 1,000,000, this could lead to numerical instability in the solving process
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- Regularization unfairness
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  - The regularization penalty then affects features unequally based on arbitrary scale choices.
- Distance-based algorithms

# Feature Normalization

## Categorical vs Continuous Features

- Predict credit card balance
  - Age
  - Income
  - Number of cards
  - Credit limit
  - Credit rating
- Categorical variables
  - Student (Yes/No)
  - State (50 different states)

# Feature Normalization

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# Feature Normalization

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- For a variable like “State” which in the US can take 50 values, we use something called One-Hot encoding
  - $state = [x_{NY}, x_{MA}, x_{NJ}, x_{WA}, x_{CA}, \dots x_{RI}]$
  - If the particular data point is from MA, that element of the vector is set to 1 and everything else 0
    - $state = [0, 1, 0, 0, 0, \dots 0]$



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A key disadvantage of one-hot encoding is that the feature space grows extremely large

# Feature Normalization

## Normalization Methods

1. Min-Max Normalization
2. Mean-Variance Normalization
3. Max-Absolute Normalization
4. Robust Normalization

# Feature Normalization

## Min-Max Normalization

- For every column in the input data, i.e., for each  $x_0, x_1, x_2, x_4$  etc., this normalization method will scale each column to 0 and 1

$$x' = \frac{x - \min(x)}{\max(x) - \min(x)}$$

- This method preserves zero entries in sparse data
- But is very sensitive to **outliers**

# Feature Normalization

## Mean-Variance Normalization

- For every column in the input data, i.e., for each  $x_0, x_1, x_2, x_4$  etc., this normalization method will scale to have mean 0 and standard deviation 1

$$x' = \frac{x - \mu(x)}{\sigma(x)}$$

- Most common in practice
- Less sensitive to outliers than min-max
- Does not bound the range to 0 and 1

# Feature Normalization

## Max-Absolute Normalization

- For every column in the input data, i.e., for each  $x_0, x_1, x_2, x_4$  etc., this normalization method will scale each column to -1 and 1

$$x' = \frac{x}{| \max(x) |}$$

- Good for sparse data since it preserves sparsity (zeros stay zero)

# Feature Normalization

## Robust Normalization

- For every column in the input data, i.e., for each  $x_0, x_1, x_2, x_4$  etc., this normalization method will scale each column as

$$x' = \frac{x - \text{median}(x)}{IQR(x)}$$

- Robust to outliers
- Use when data has many outliers

# Feature Normalization

## Robust Normalization

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This is just the second quartile  $Q_2$

- Robust to outliers
- Use when data has many outliers

Inter-quartile range  $Q_3 - Q_1$



# Conclusion

- We saw practical issues and considerations in linear regression like
  - Train/test splits
  - Multicollinearity
  - Overfitting and Underfitting
  - Bias-Variance tradeoffs
  - Regularization
- Feature pre-processing
  - One-hot encoding
- Normalization methods