



Northeastern University
Khoury College of
Computer Sciences

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

Recap

Derivative of the Sigmoid Function

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

Let $f(x) = 1 + e^{-x}$ 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

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

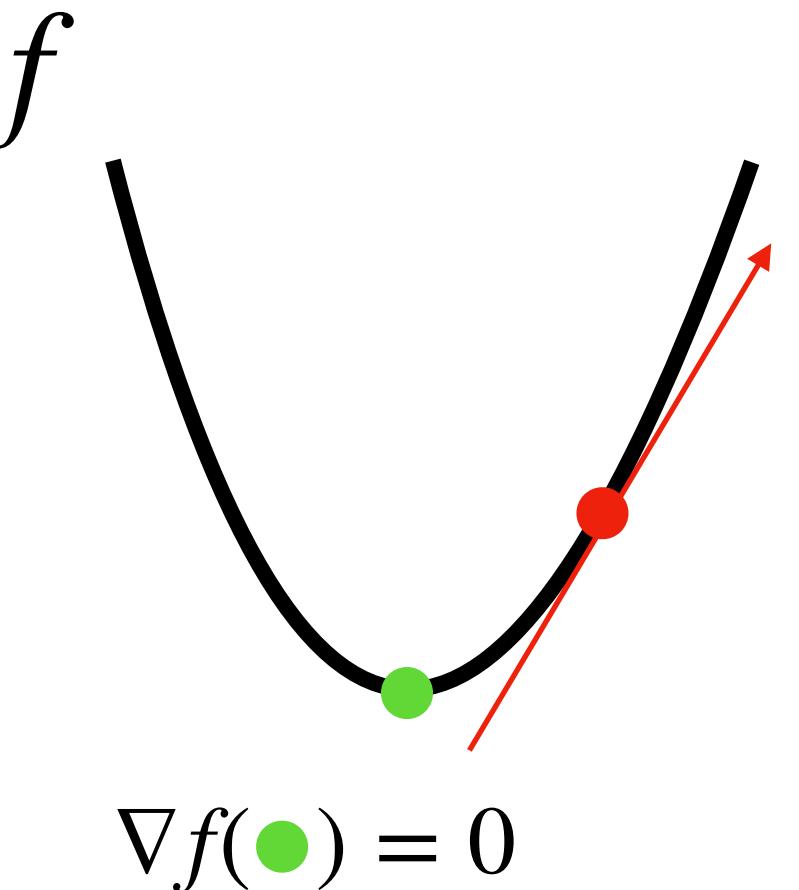
$$L(\theta) = \frac{1}{m} \sum_{i=1}^m [\theta_0 + \theta_1 \cdot x_i - y_i]^2$$

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

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

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

Recap

Linear Regression Derivation - Matrix Form

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

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

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

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

Recap

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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

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

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

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

Recap

Linear Regression Derivation - Matrix Form

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

Recap

Linear Regression Derivation - Matrix Form

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

Each of these is a vector

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

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

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

Recap

Linear Regression Derivation - Matrix Form

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

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

These two representations are now similar

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

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

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

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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

Linear Regression Derivation - Matrix Form

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

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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

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

Recap

Matrix Form - Derivative

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

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

Recap

Matrix Form - Derivative

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

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

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

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

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

Recap

Matrix Form - Derivative

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

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

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

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

The derivative rule we had:

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

Recap

Matrix Form - Derivative

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For any vector A

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

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So we have

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

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

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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 - Rough rule of thumb is that this is an 80-20 split

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

20% of the entire dataset is set aside
to test the models

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:
$$\theta = (X^T X)^{-1} X^T Y$$
Simple Detection:
If correlation between features ≥ 0.8
- $X^T X$ 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

Quick Aside

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

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

m : Number of training examples

n : Number of parameters in the model

When else is this not going to be invertible?

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

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

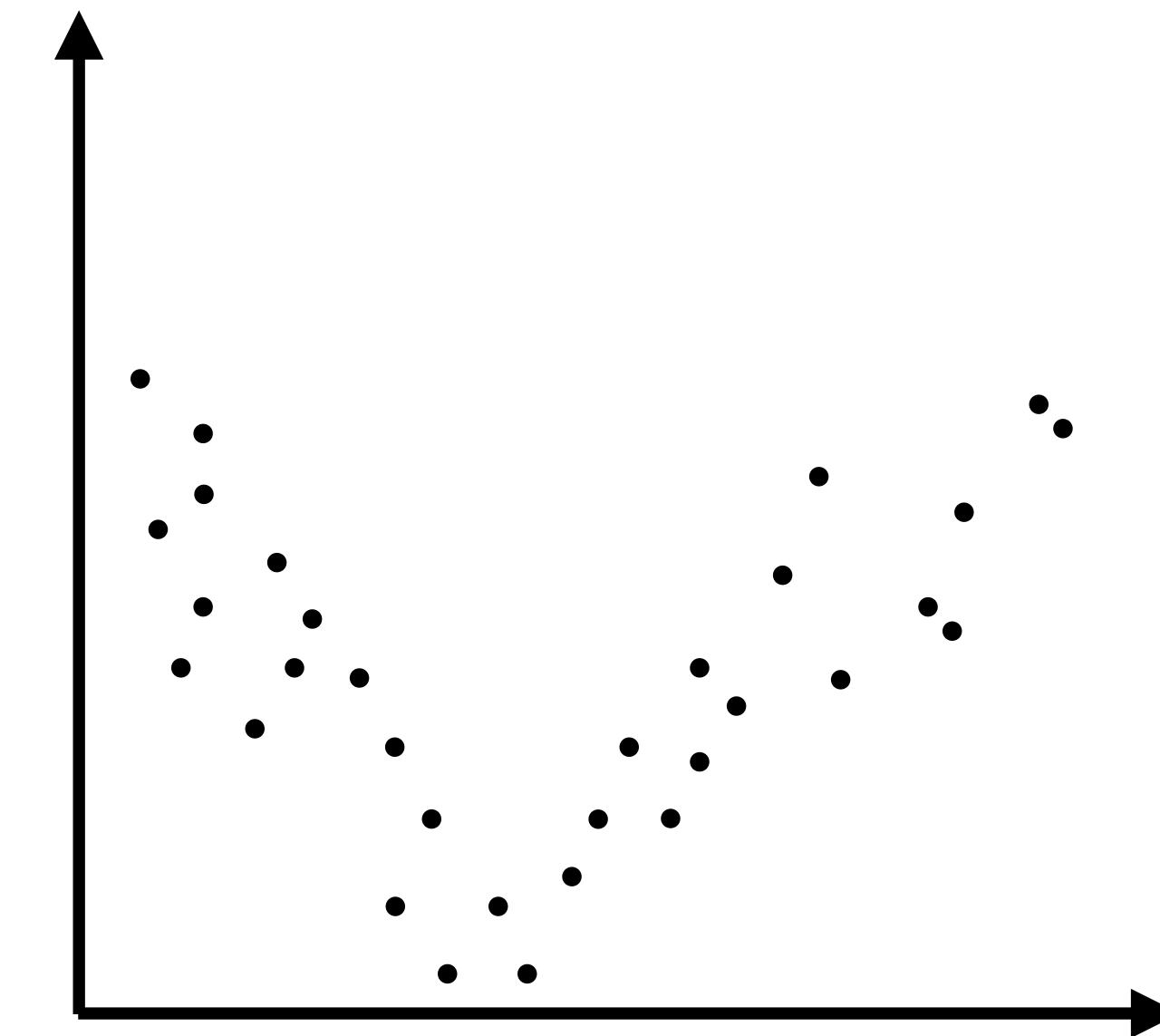
m : Number of training examples

n : Number of parameters in the model

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

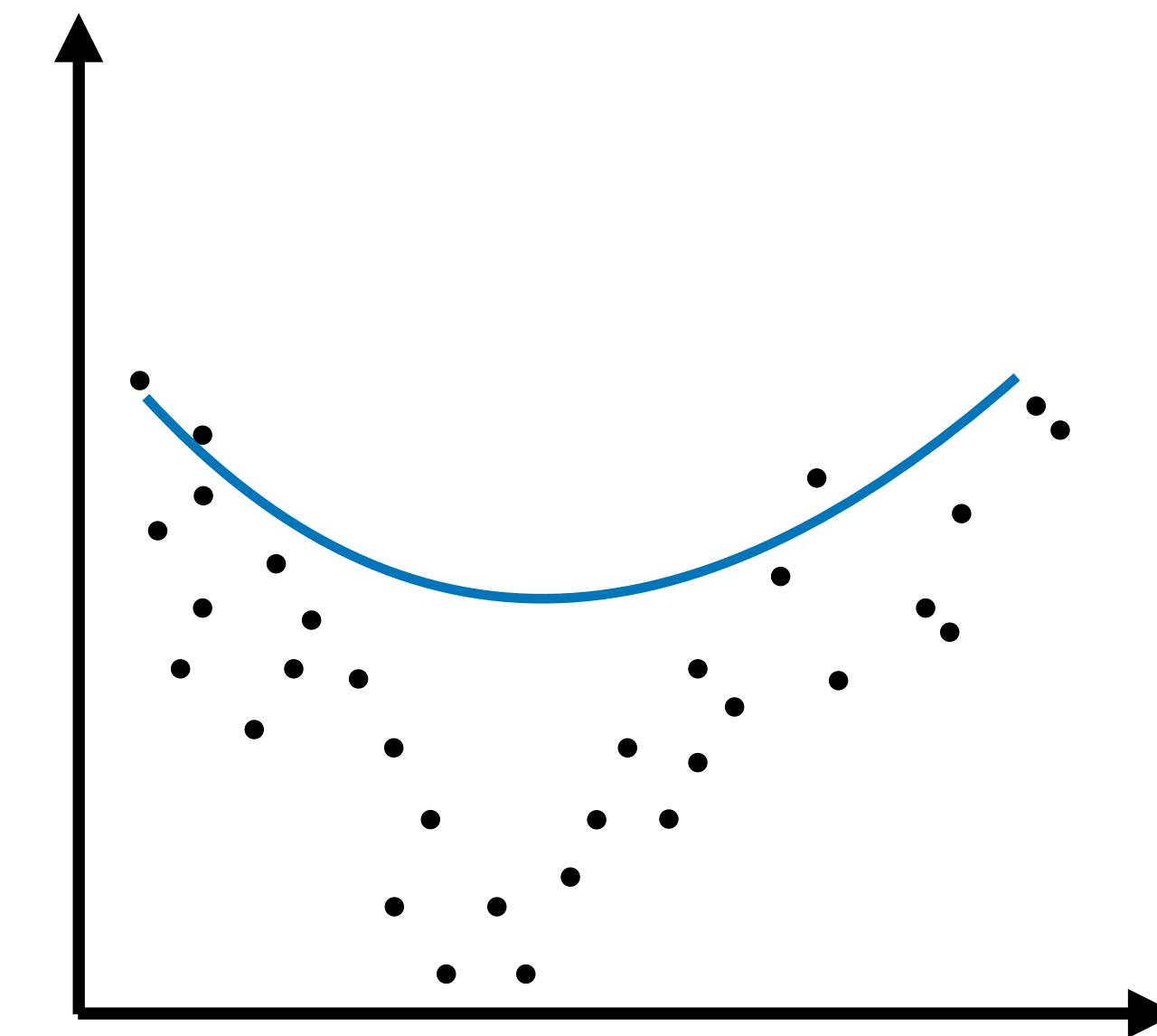
Practical Issues in Linear Regression

Overfitting vs Underfitting



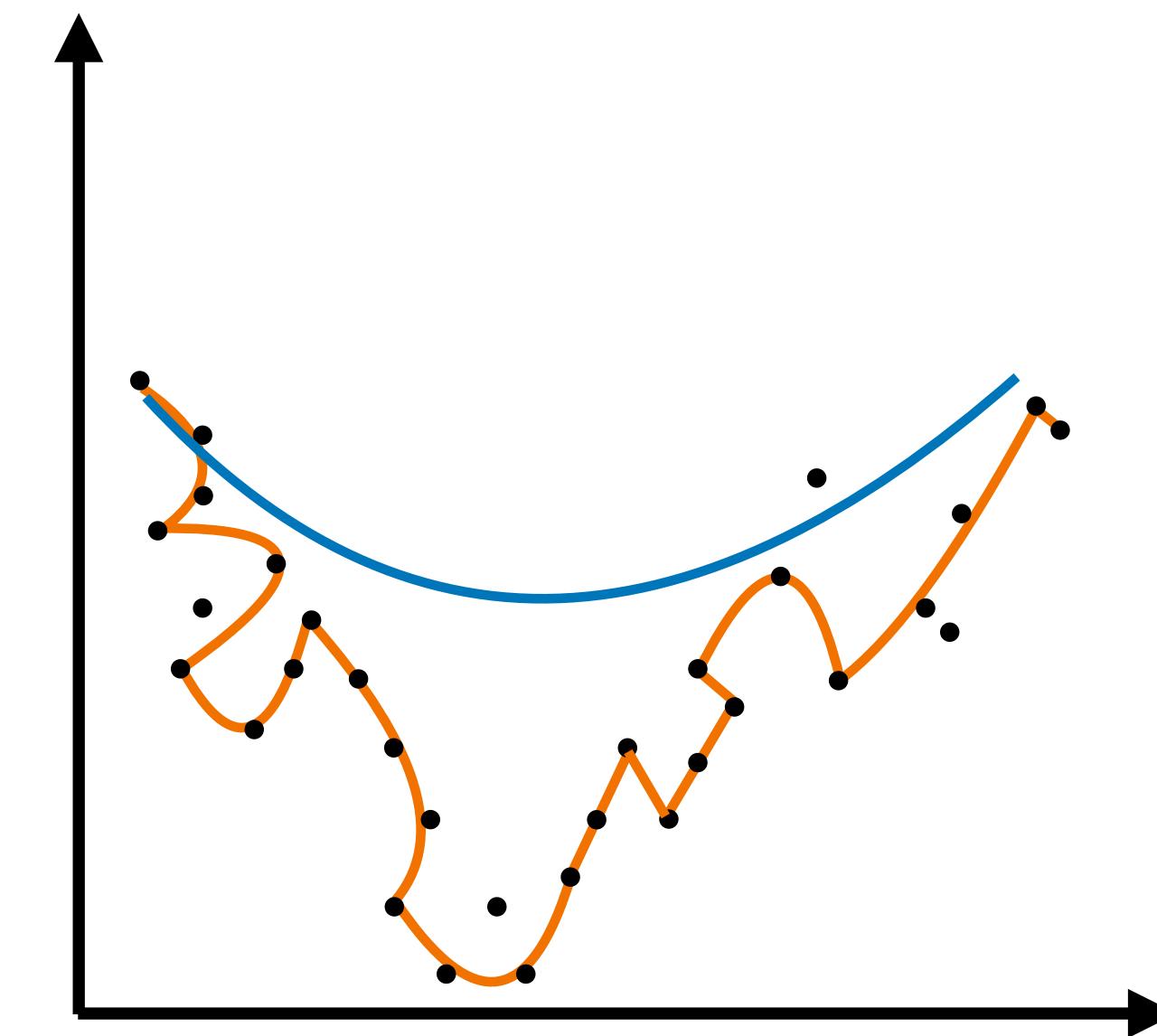
Practical Issues in Linear Regression

Overfitting vs Underfitting



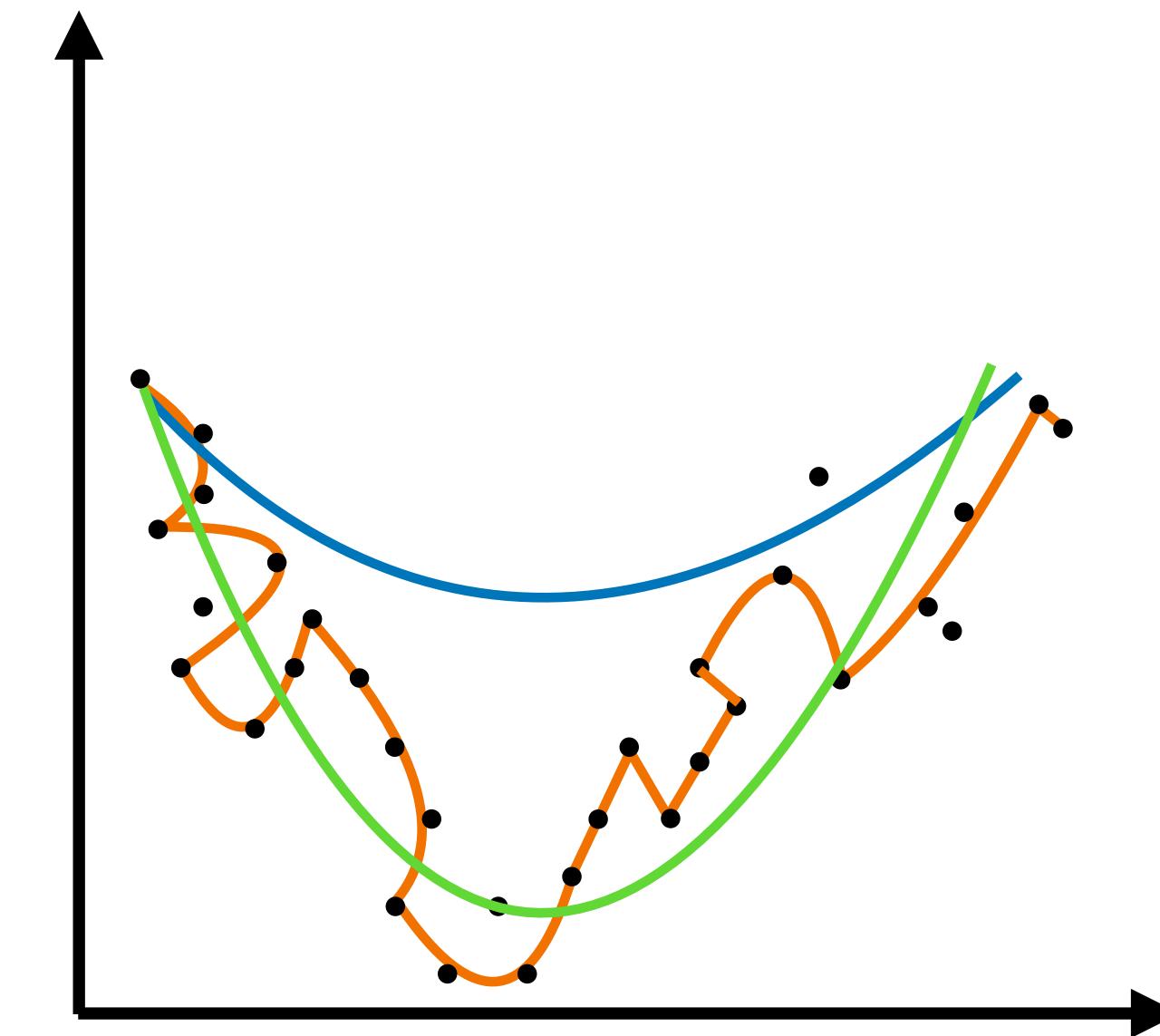
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Practical Issues in Linear Regression

Overfitting vs Underfitting



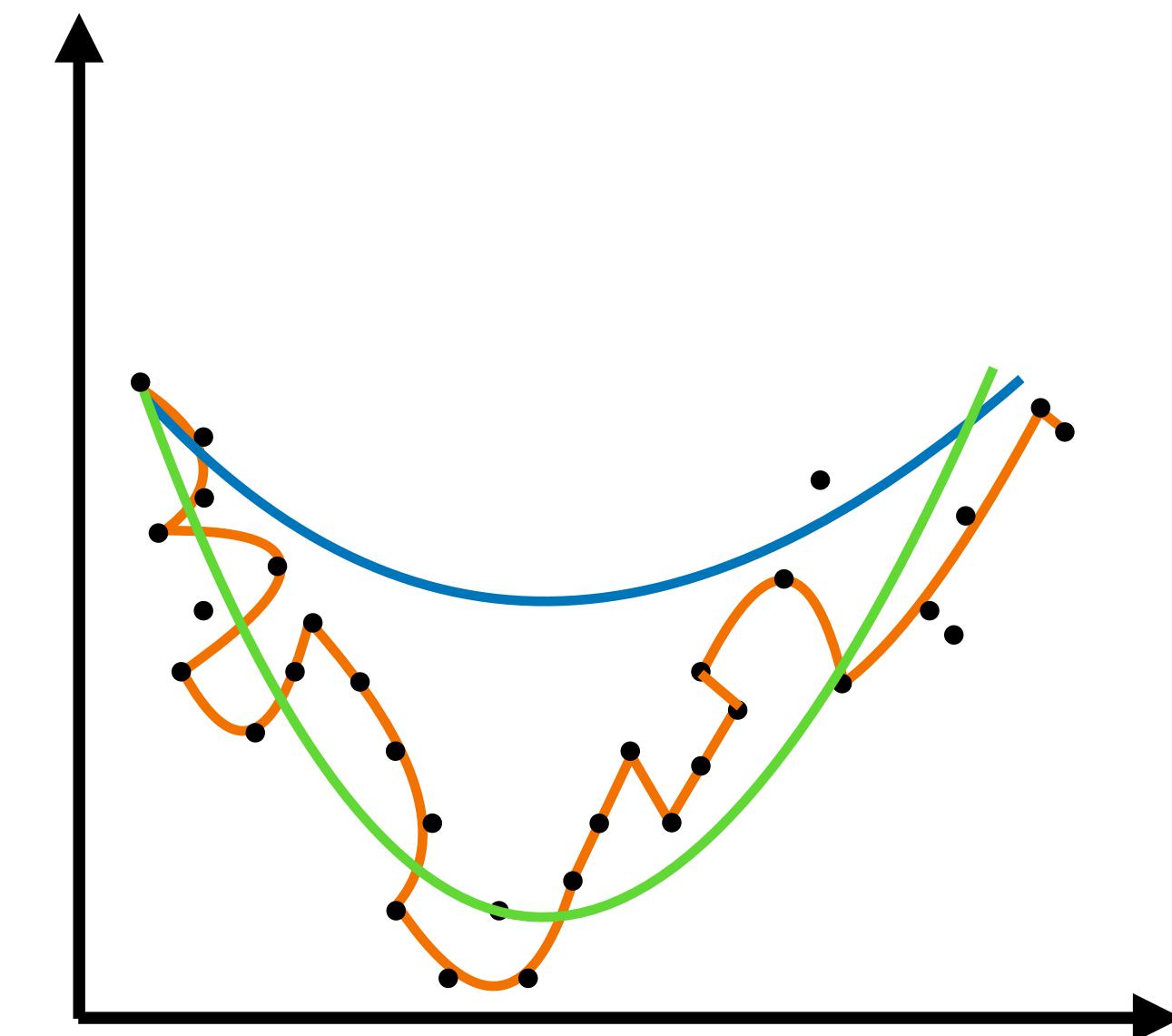
Practical Issues in Linear Regression

Overfitting vs Underfitting

The blue model is **underfitting** the data

The orange model is **overfitting** the data

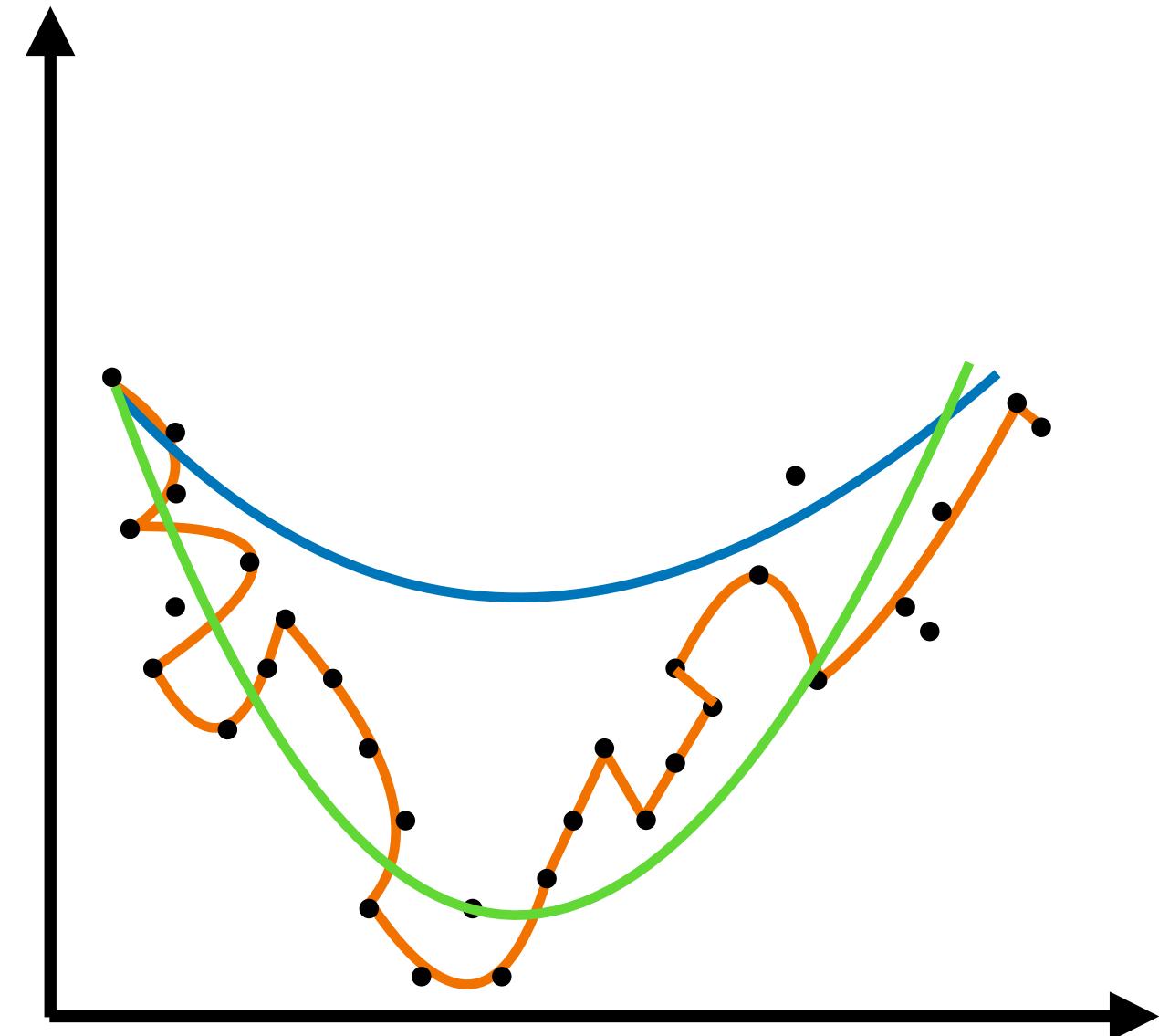
The green model is a good fit of the data



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



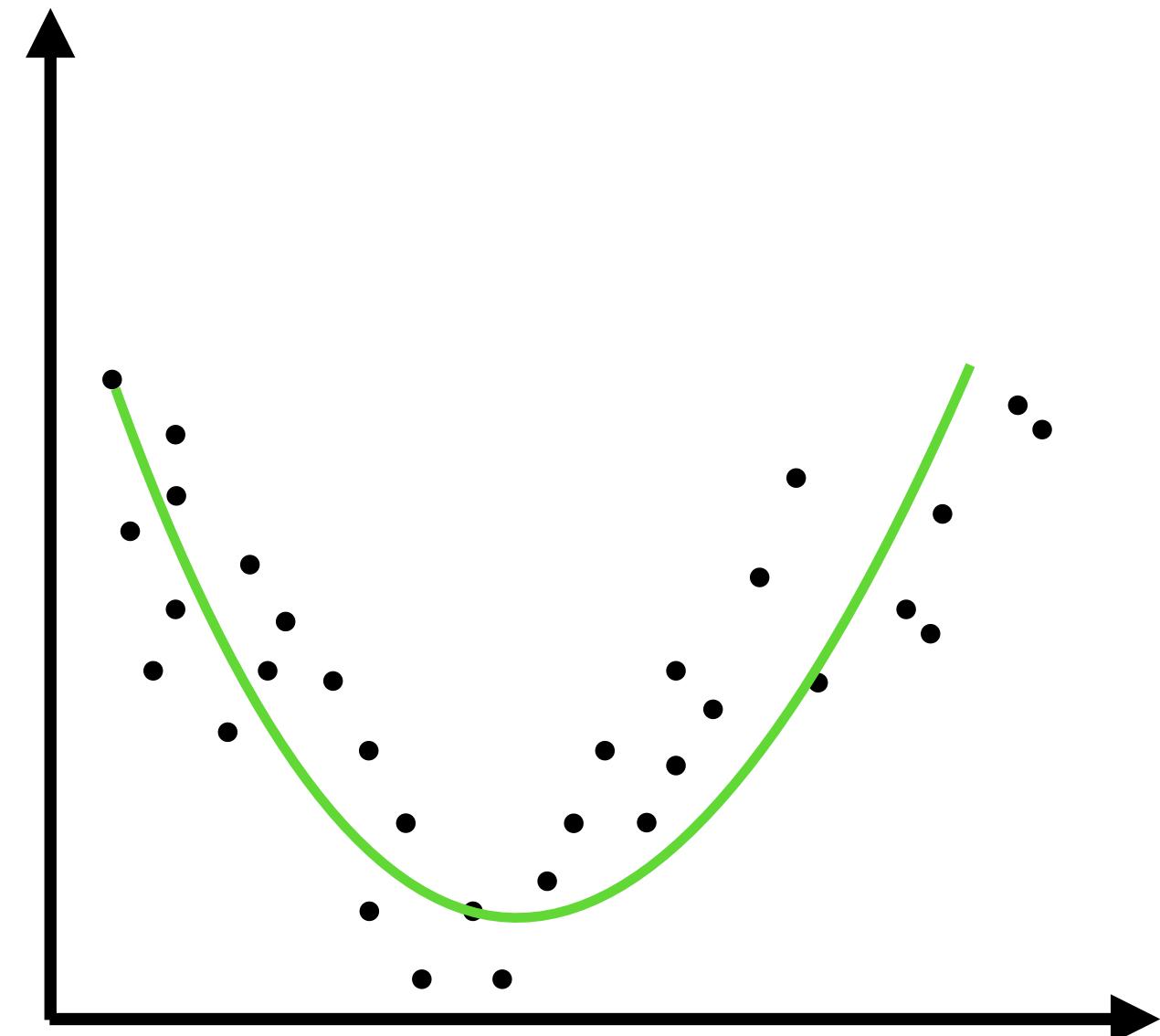
Practical Issues in Linear Regression

Quick Aside

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

$$f_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_1^2$$

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



Practical Issues in Linear Regression

Quick Aside

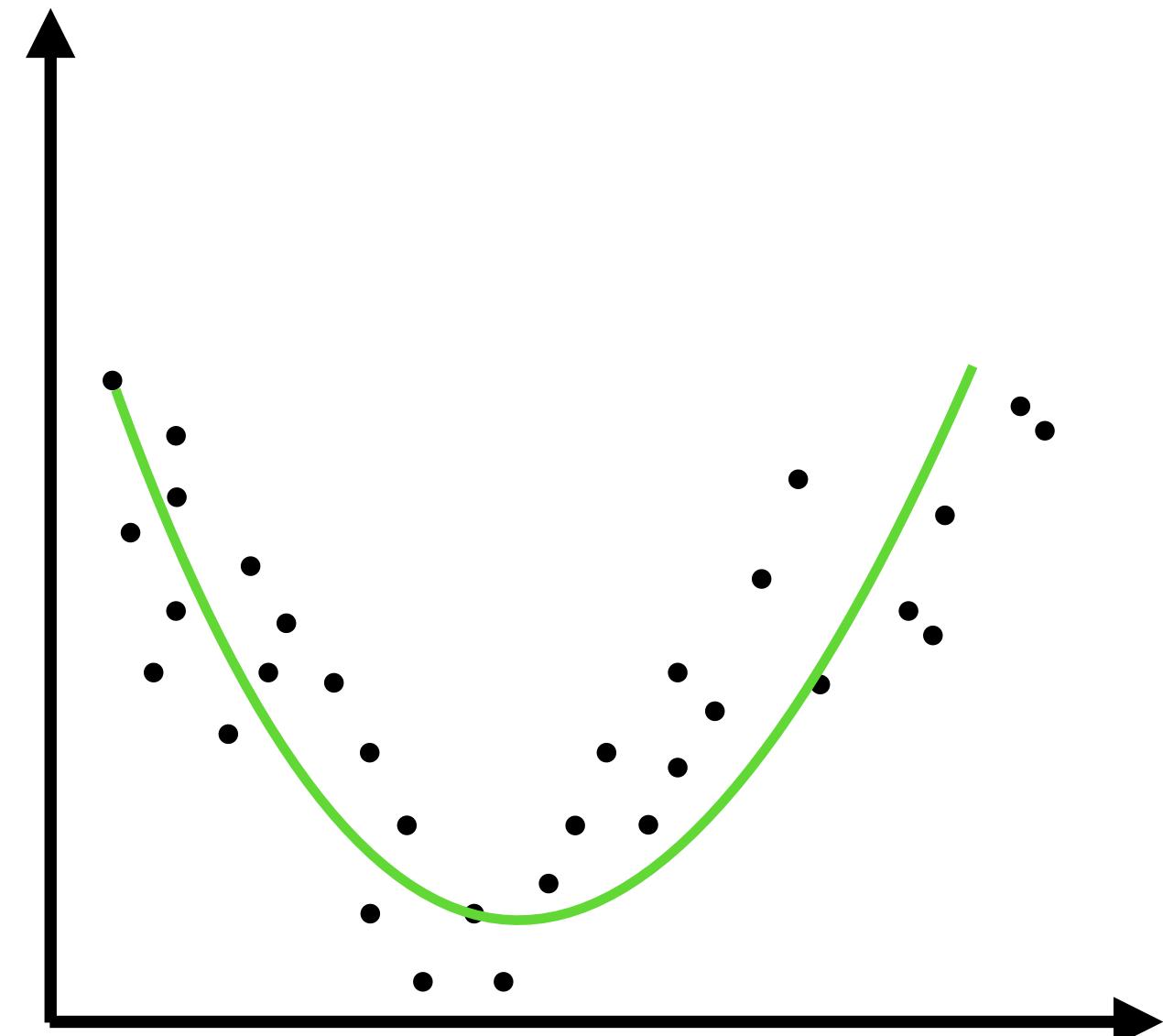
- Add polynomial features ($x_1^2, x_2^2, x_1x_2, \dots$)

$$f_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_1^2$$

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

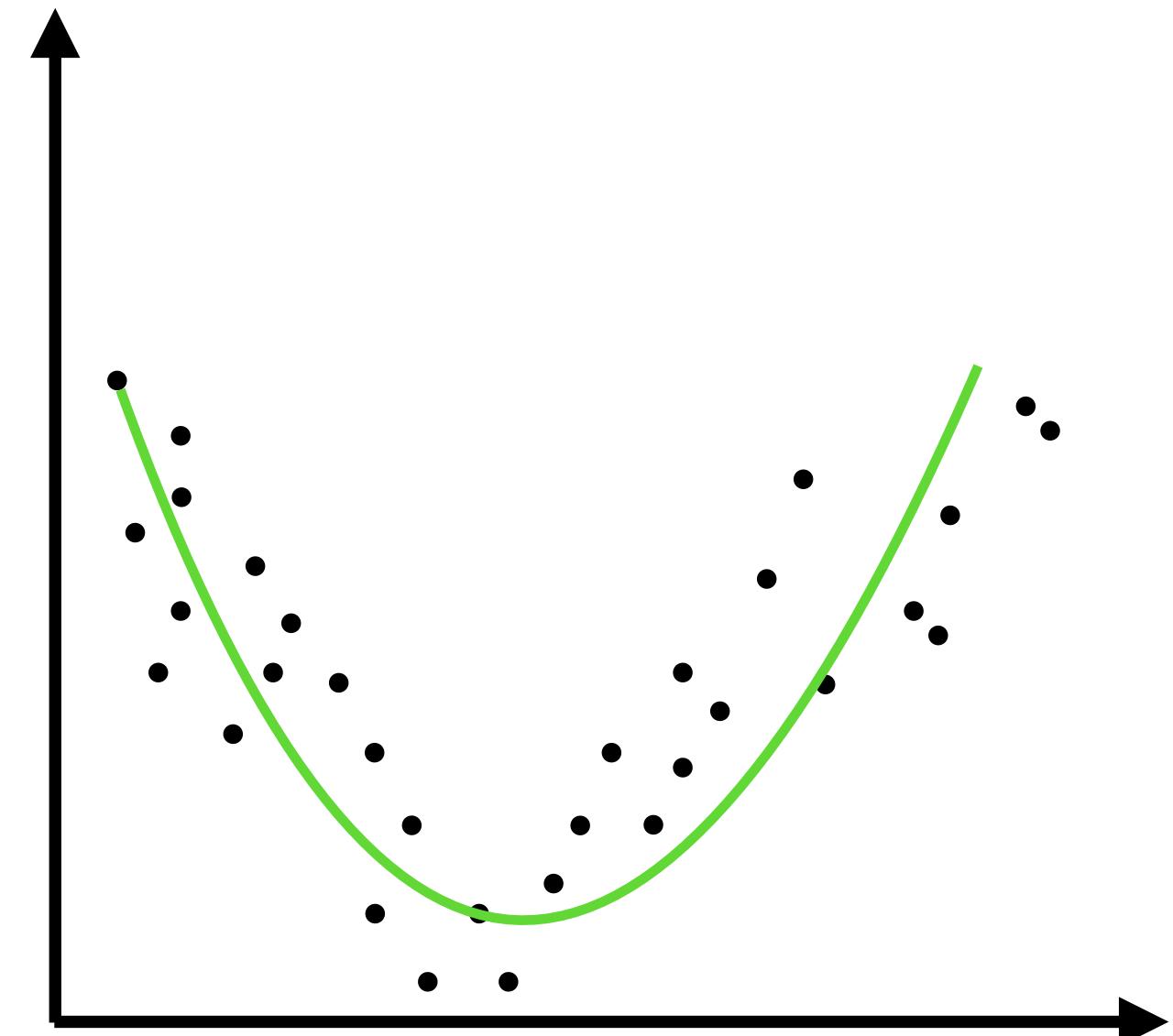
- Add polynomial features ($x_1^2, x_2^2, x_1x_2, \dots$)

$$f_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_1^2$$

What about these models?

$$f_{\theta}(x) = \theta_1 e^{x_1} + \theta_2 \sin(x_2)$$

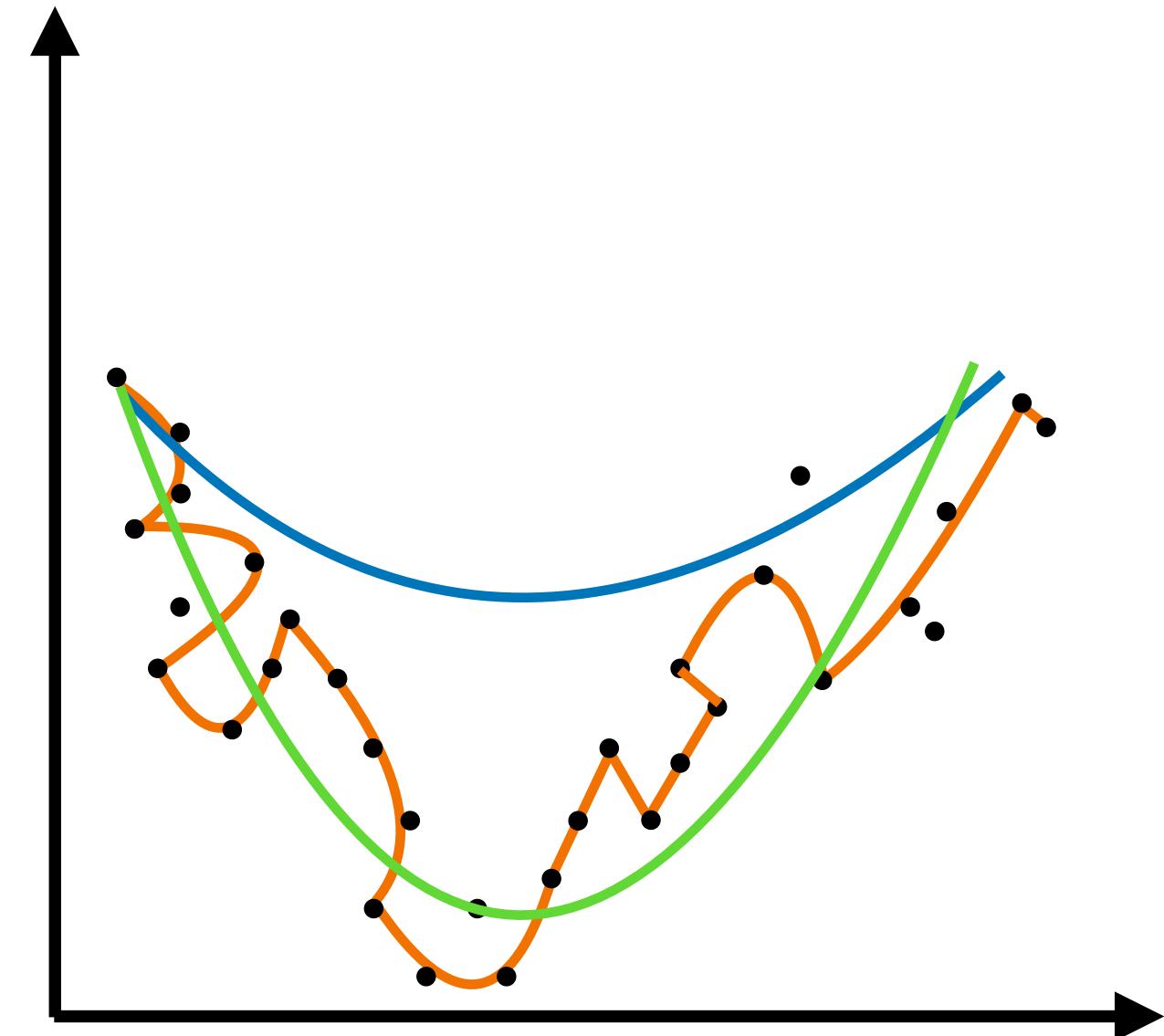
$$f_{\theta}(x) = \sin(\theta_1 x_1 + \theta_2 x_1^2) + \theta_2$$



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

A more mathematical look - Bias / Variance Tradeoff

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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

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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:

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

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

Practical Issues in Linear Regression

A more mathematical look - Bias / Variance Tradeoff

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How far is the average prediction from the true labels?

Practical Issues in Linear Regression

A more mathematical look - Bias / Variance Tradeoff

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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

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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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| Too Simple | High | Low | High | High |
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Practical Issues in Linear Regression

Bias / Variance Tradeoff

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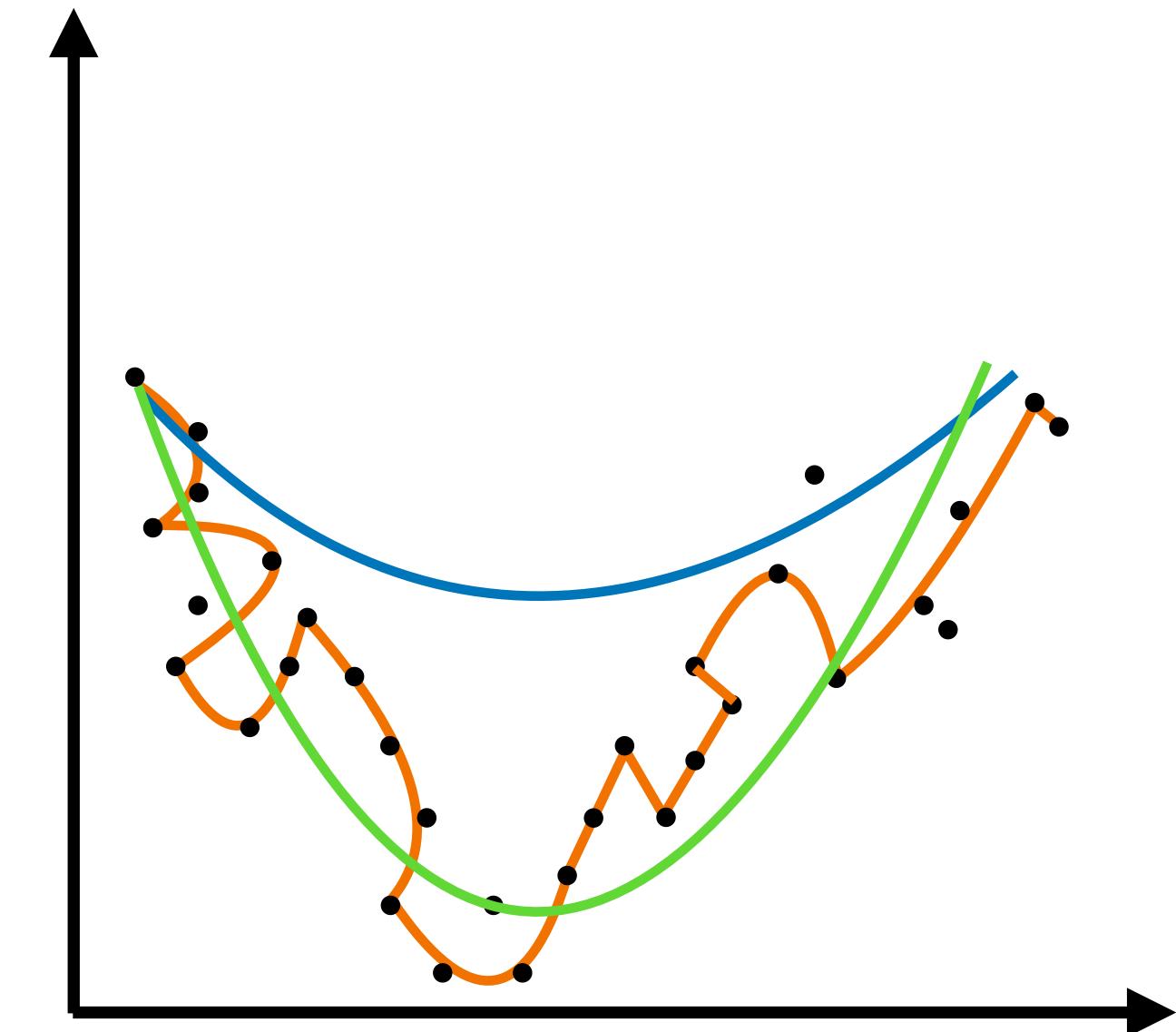
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|------------------|--------|----------|-------------|------------|
| Too Simple | High | Low | High | High |
| Sweet Spot | Medium | Medium | Medium | Medium |
| Too Complex | Low | High | Low | High |

Practical Issues in Linear Regression

Regularization

- Regularization explicitly trades bias for variance.

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



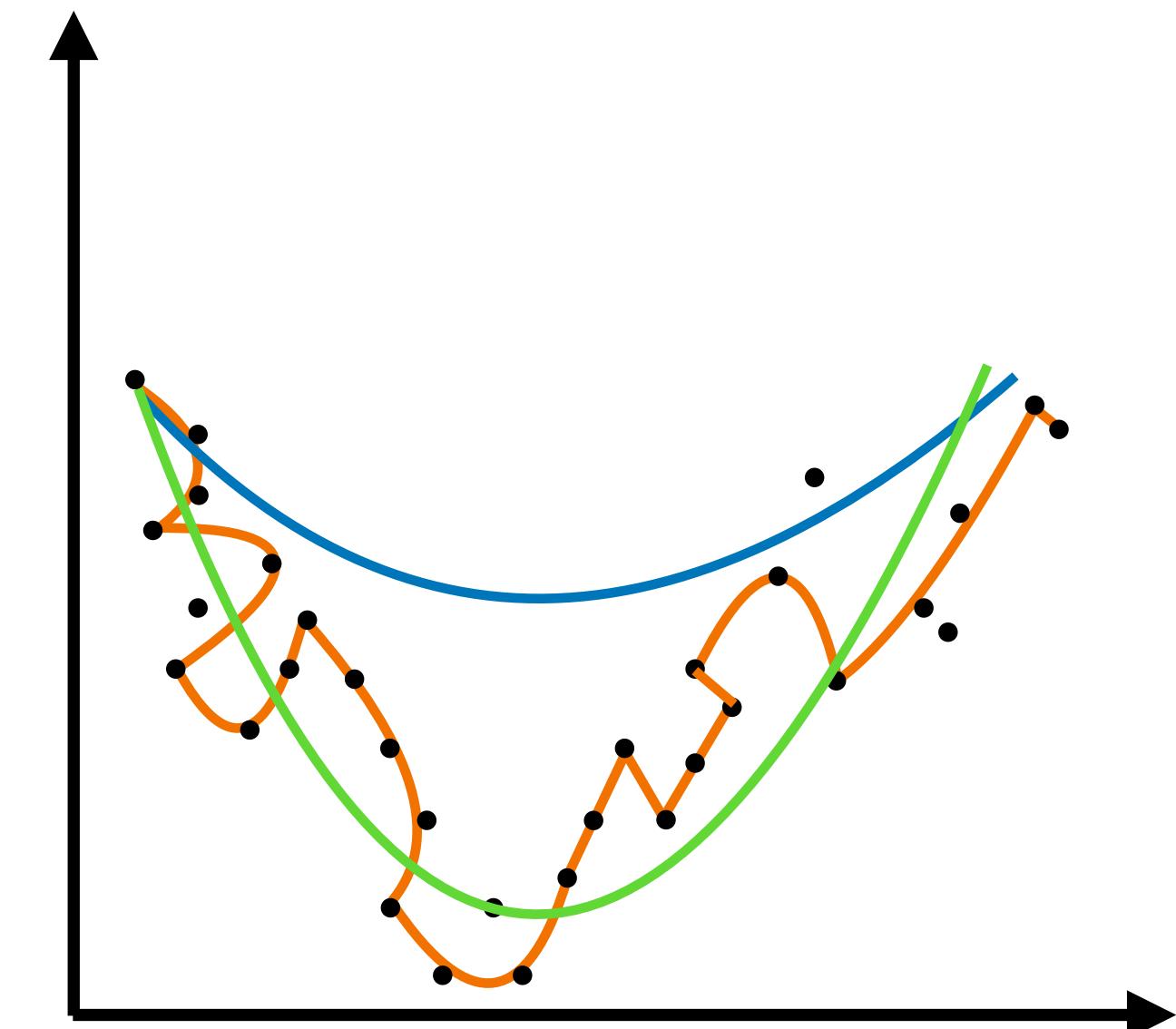
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Practical Issues in Linear Regression

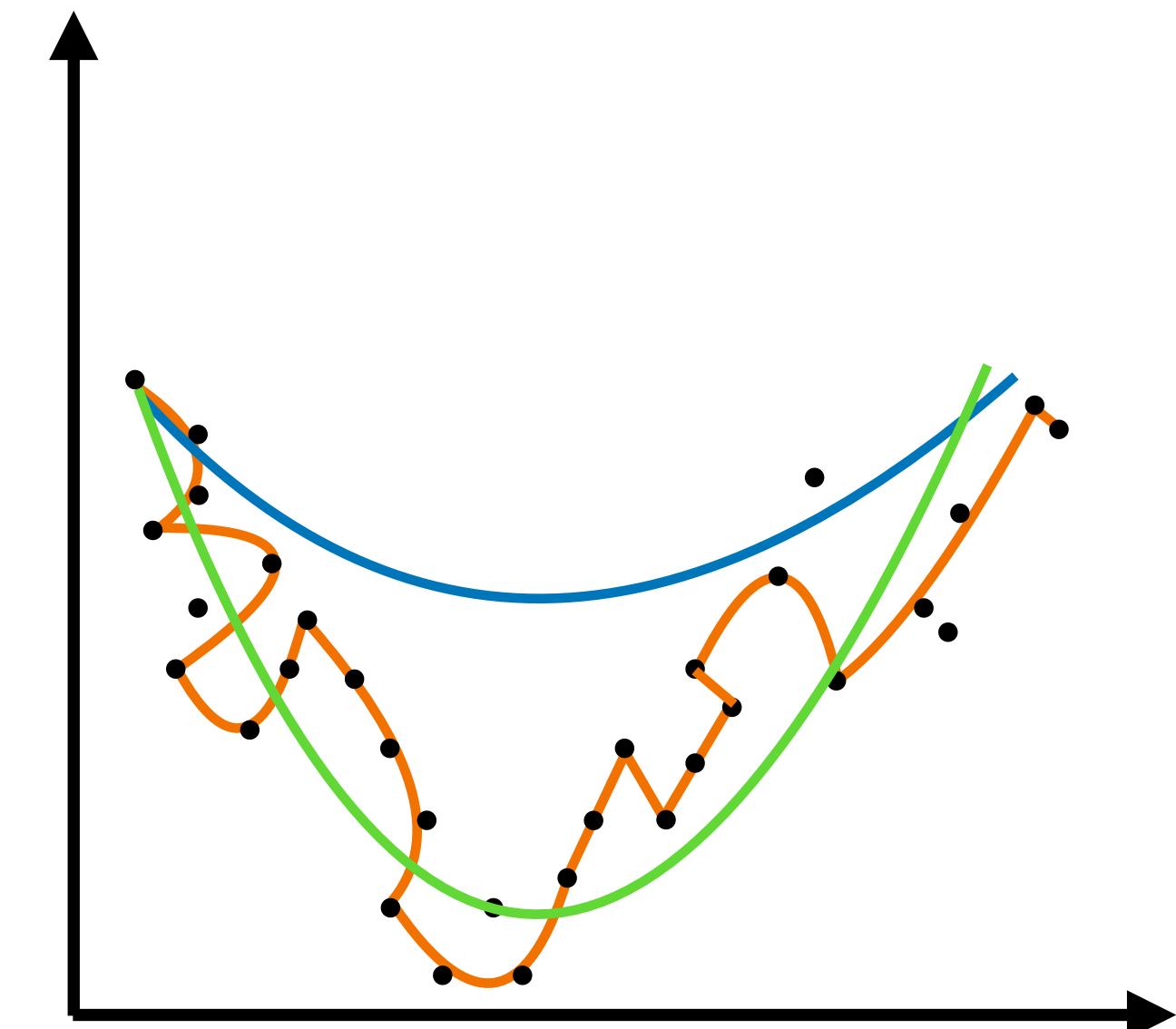
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Practical Issues in Linear Regression

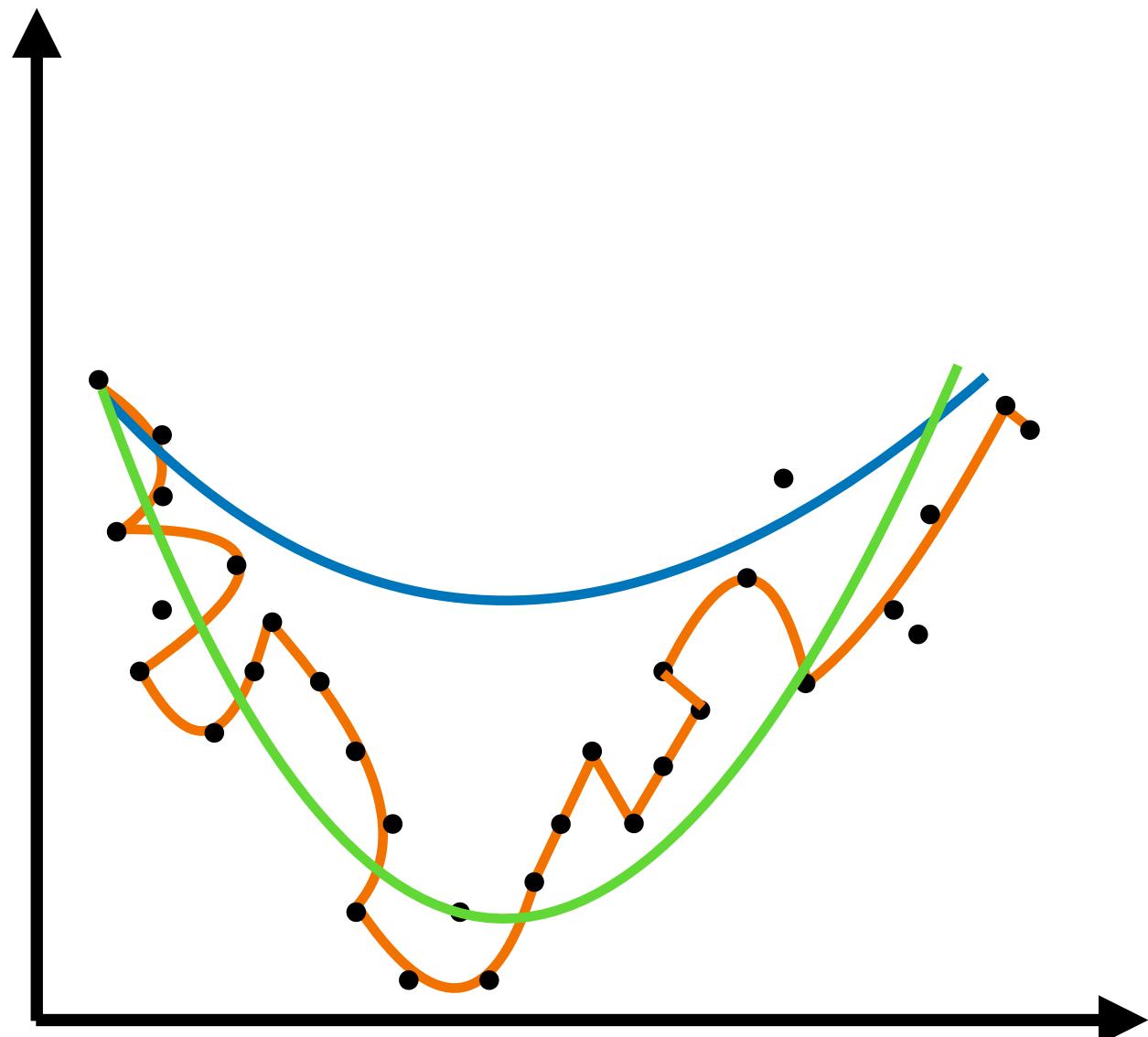
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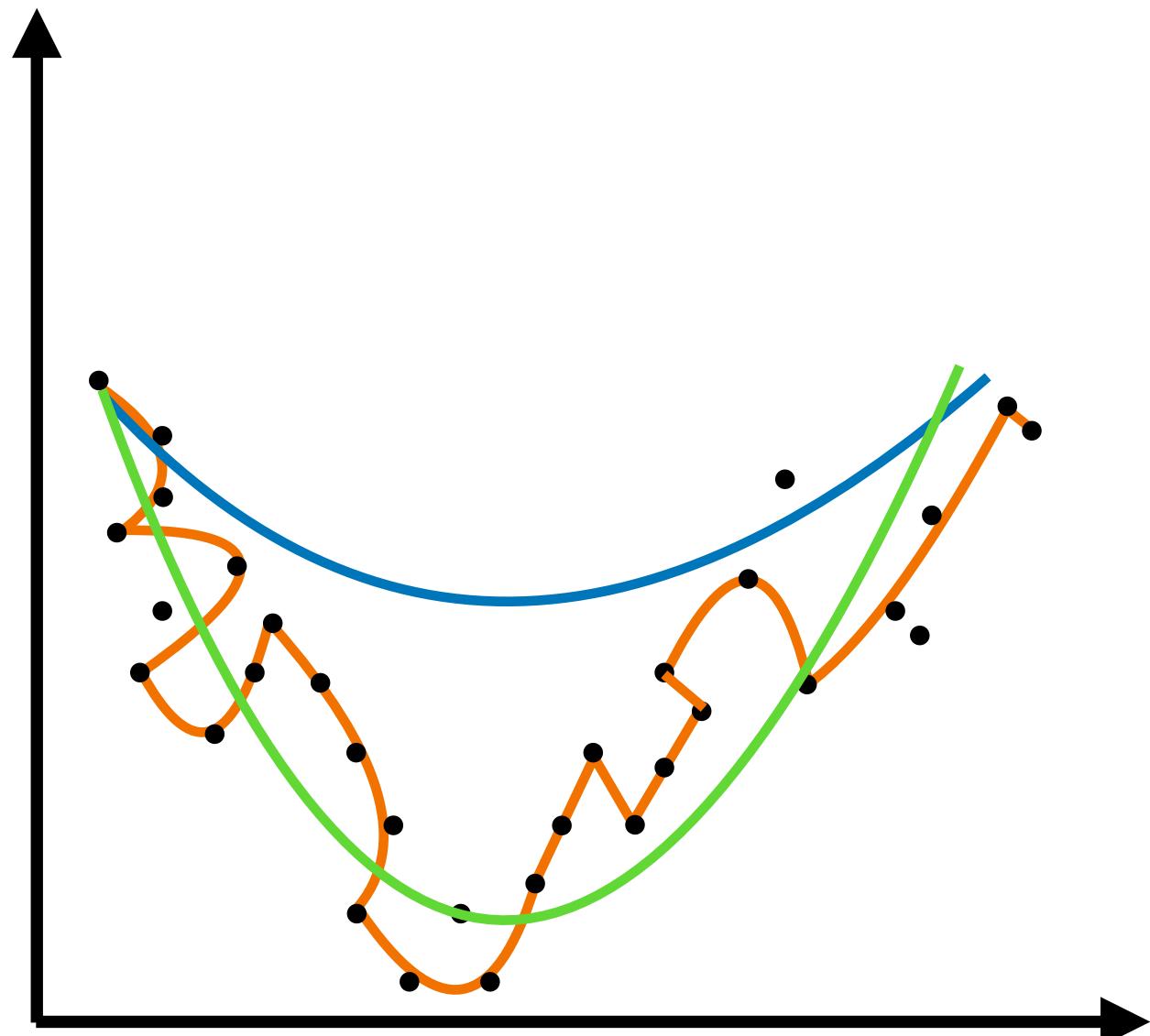
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These sort of parameters
are usually called
hyper-parameters

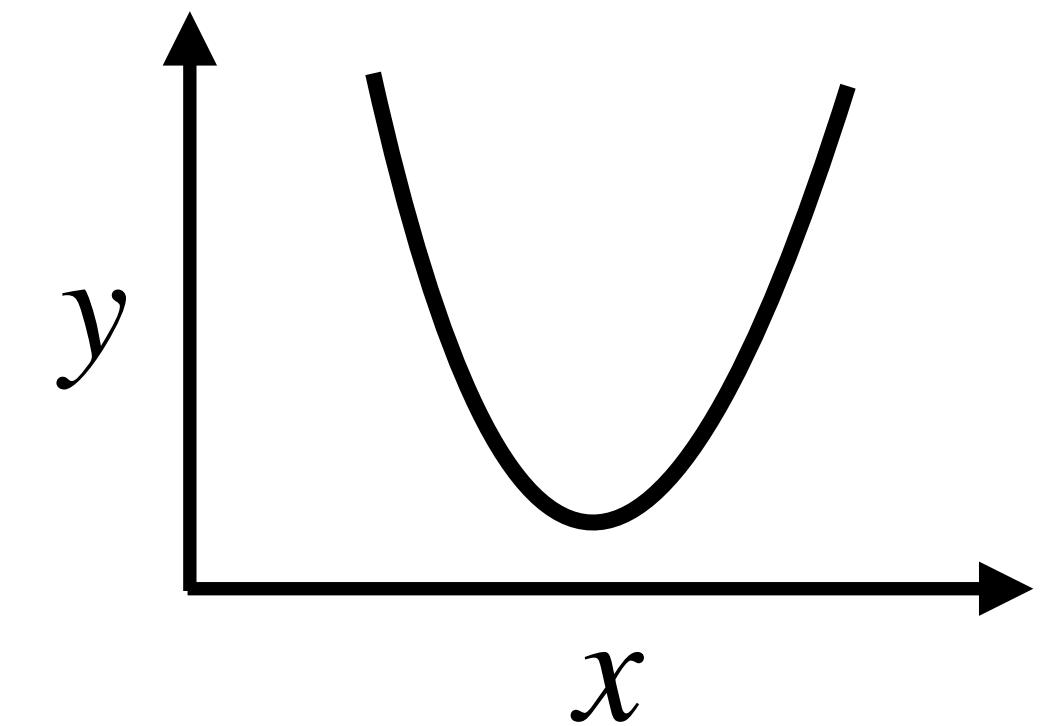
They are **not learnable**
but are human defined



Practical Issues in Linear Regression

Non-Linearity

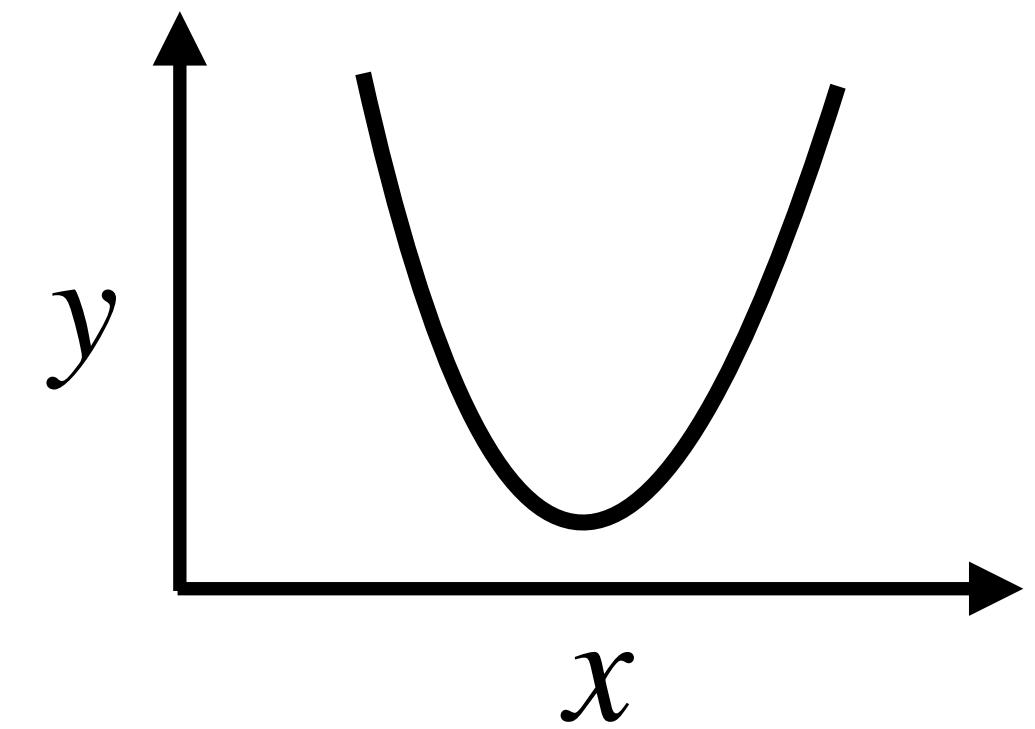
- True relationship between x and y is not linear



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

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
 - This is particular relevant to gradient descent

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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

Indicator Variables and One-Hot Encoding

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Feature Normalization

Indicator Variables and One-Hot Encoding

- For a variable like “Student” that takes True/False values:
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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

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

- 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