Regularization

Machine Learning and Pattern Recognition

(Largely based on slides from Andrew Ng)

Prof. Sandra Avila
Institute of Computing (IC/Unicamp)

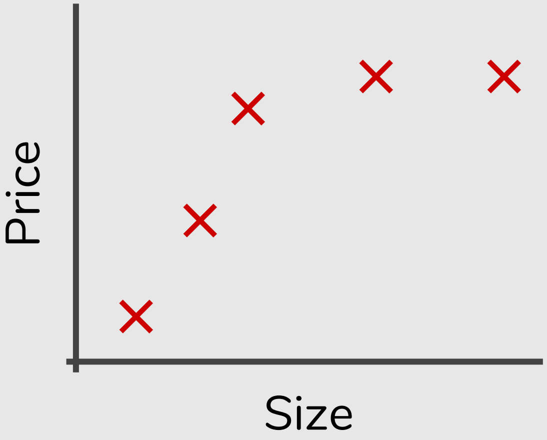
MC886/MO444, August 25, 2017

Today's Agenda

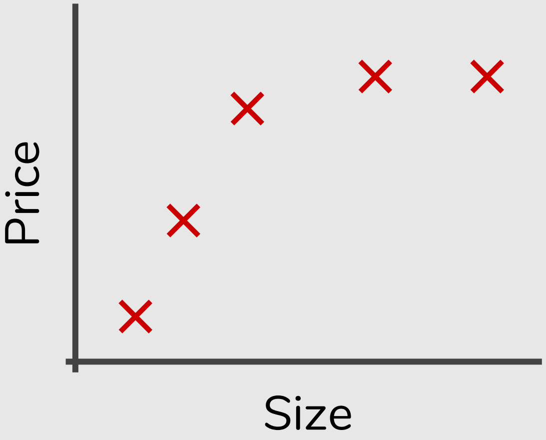
- Regularization
    - The Problem of Overfitting
    - Diagnosing Bias vs. Variance
    - Cost Function
    - Regularized Linear Regression
    - Regularized Logistic Regression

The Problem of Overfitting

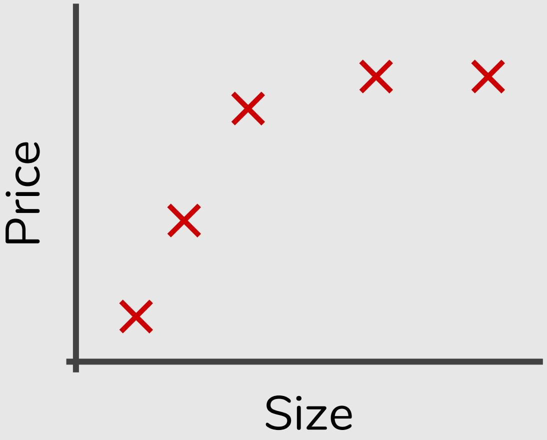
Example: Linear Regression



$\theta_0 + \theta_1 x$

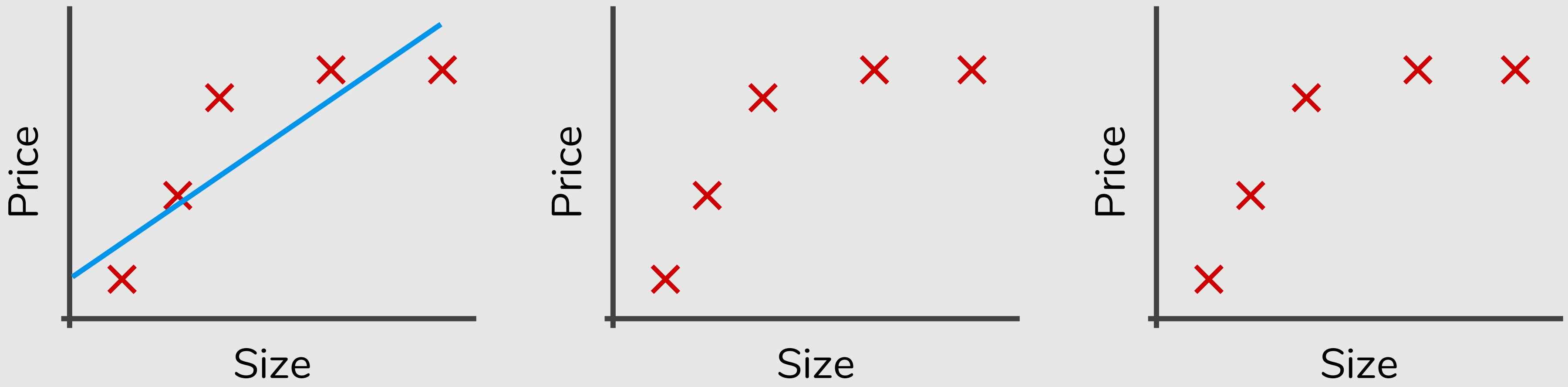


$\theta_0 + \theta_1 x + \theta_2 x^2$



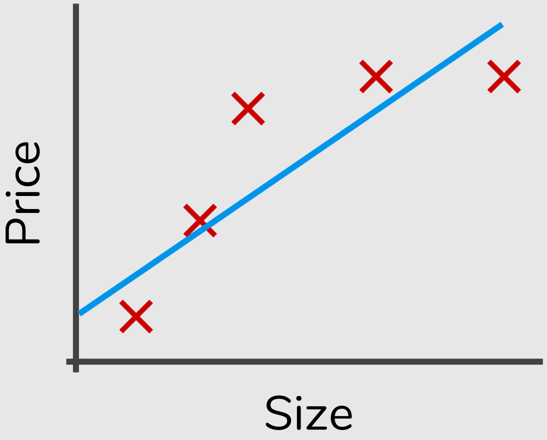
$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

Example: Linear Regression



$\theta_0 + \theta_1 x$ $\quad$ $\theta_0 + \theta_1 x + \theta_2 x^2$ $\quad$ $\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

Example: Linear Regression



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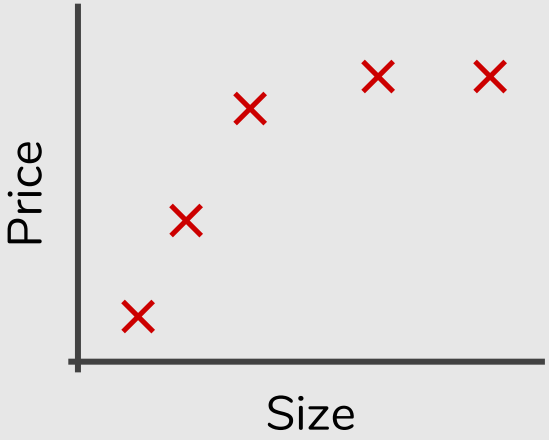

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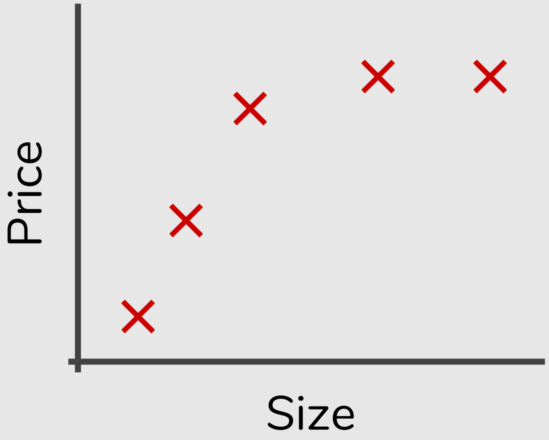
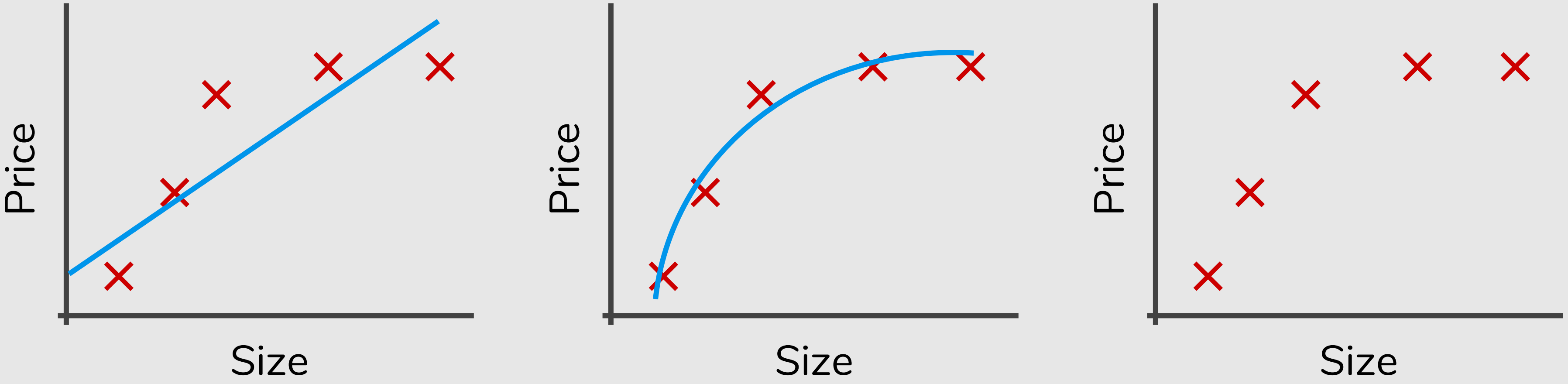


$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

Underfitting

High bias

Example: Linear Regression



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Underfitting

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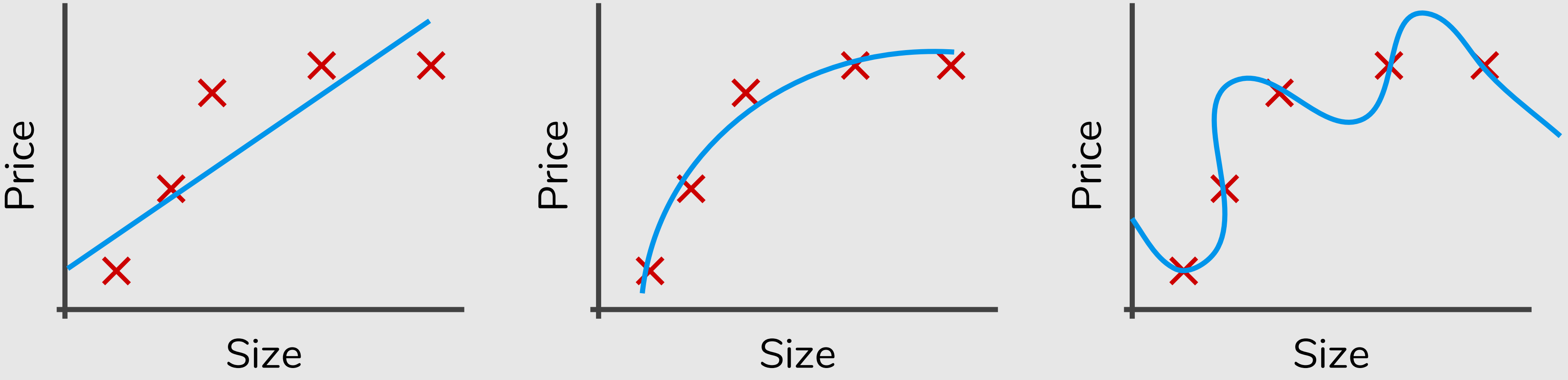

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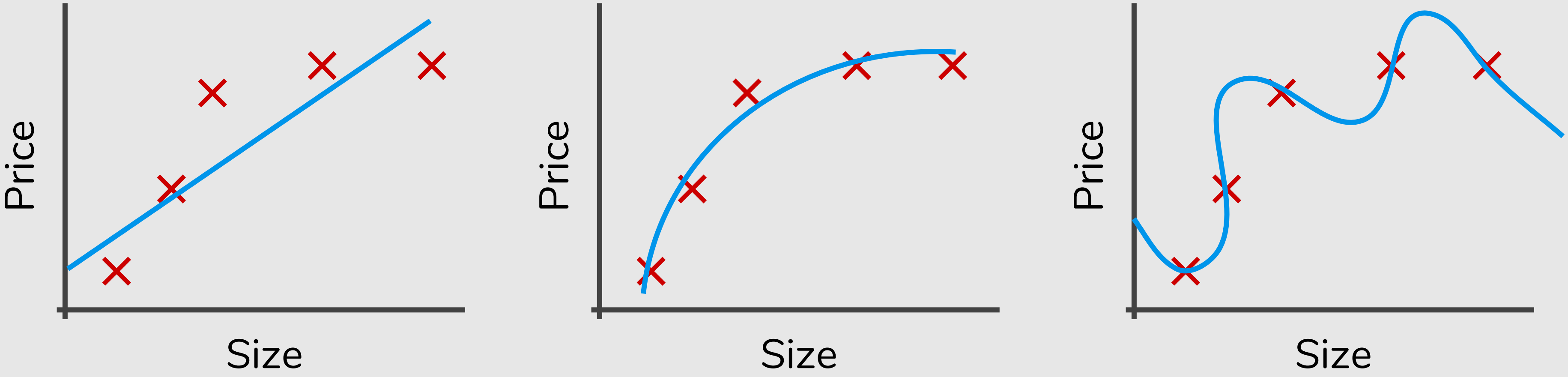

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Underfitting
High bias

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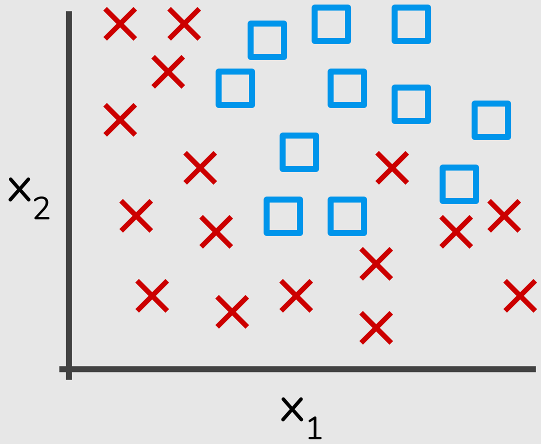
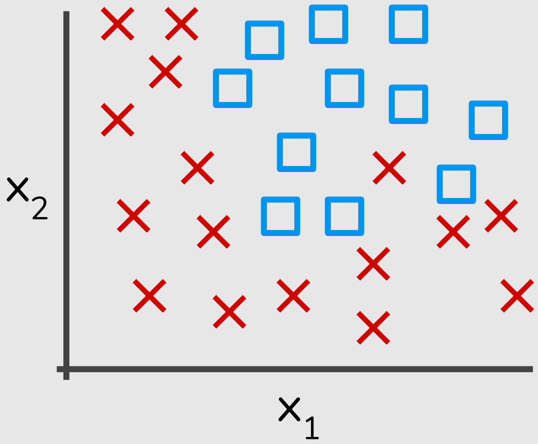
$$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$

Overfitting
High variance

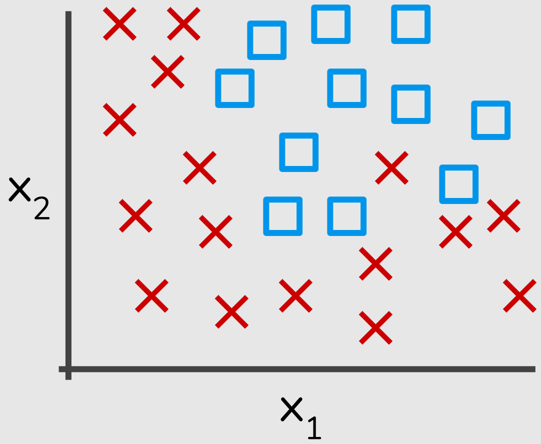
Example: Logistic Regression



$$g(\theta_0+\theta_1 x_1+\theta_2 x_2)$$



$$g(\theta_0+\theta_1 x_1+\theta_2 x_2+\theta_3 x_1^2+ \\ +\theta_4 x_2^2+\theta_5 x_1 x_2)$$



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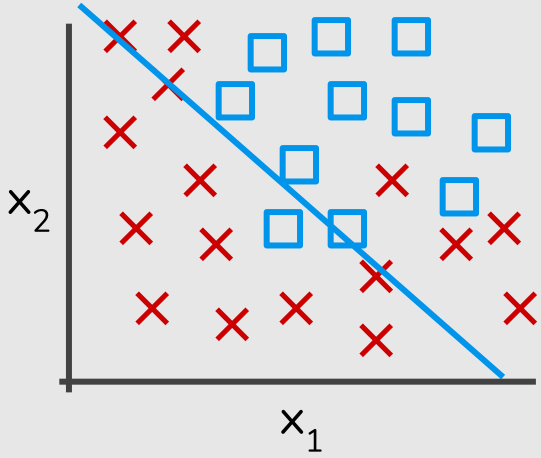
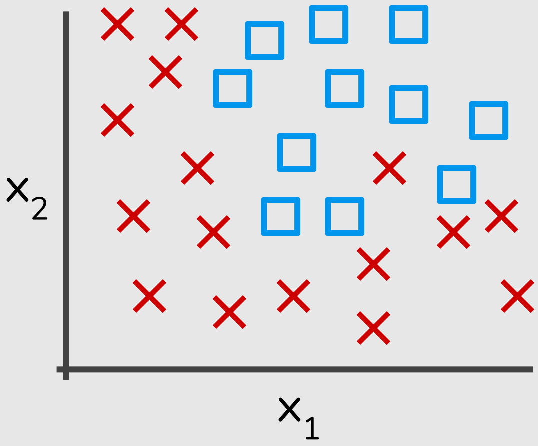
Example: Logistic Regression



$$g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$$

Underfitting

High bias



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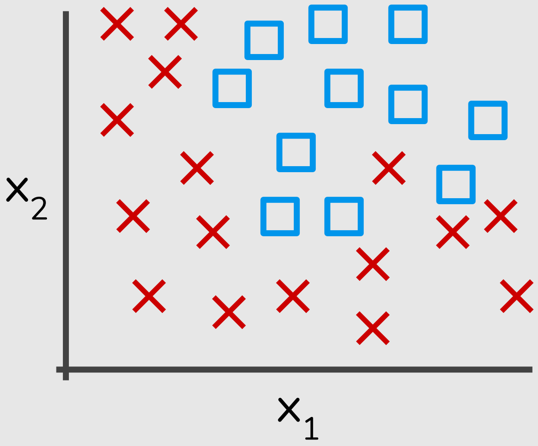

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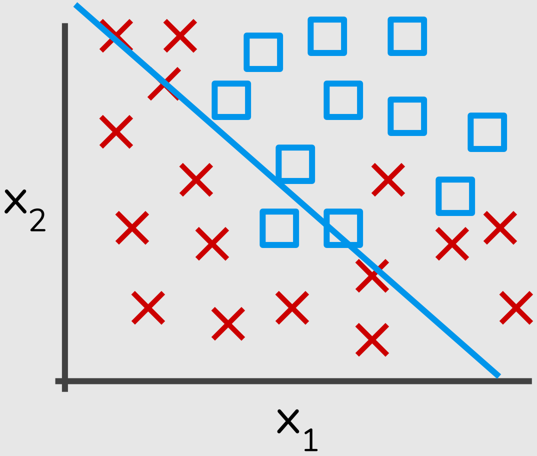

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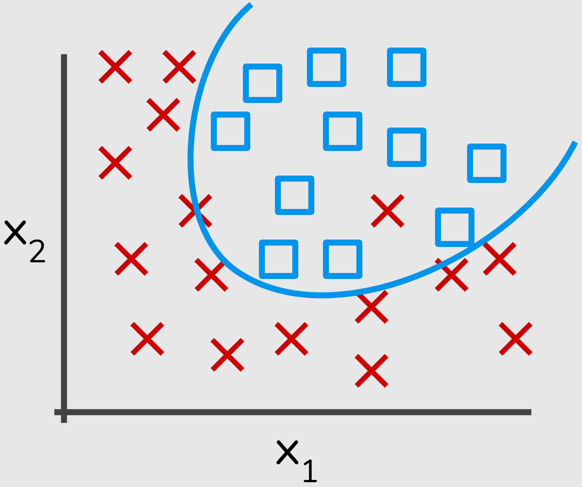
Underfitting
High bias



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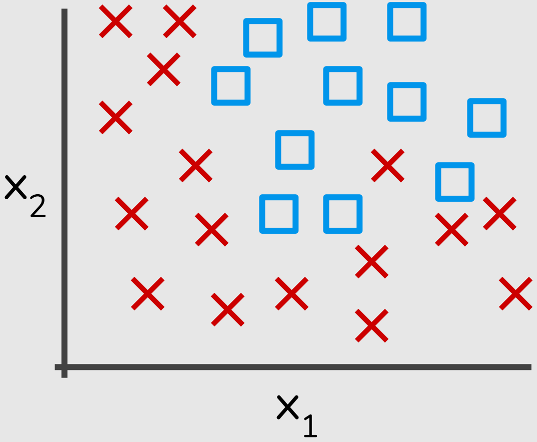

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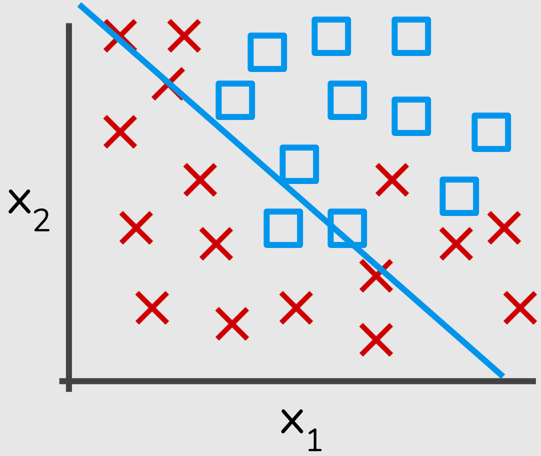
Example: Logistic Regression



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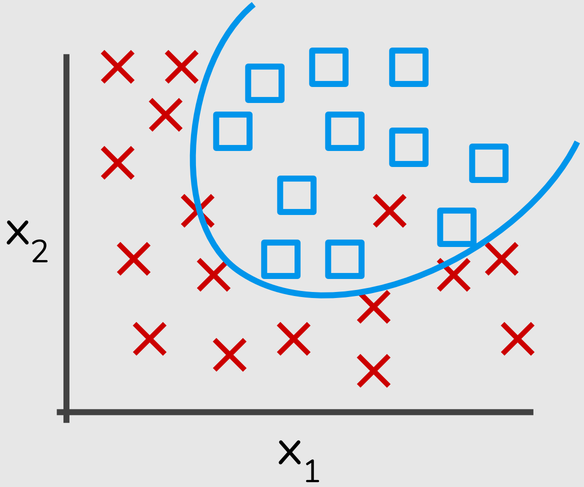
Underfitting

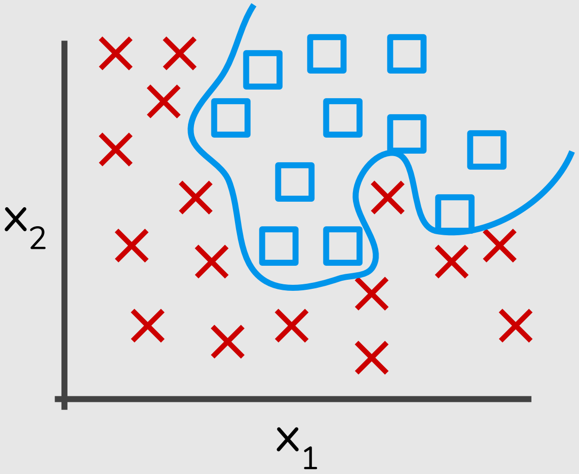
High bias



$$g(\theta_0+\theta_1 x_1+\theta_2 x_2+\theta_3 x_1^2+ \\ +\theta_4 x_2^2+\theta_5 x_1 x_2)$$

Overfitting

High variance



$$g(\theta_0+\theta_1 x_1+\theta_2 x_1^2+ \\ +\theta_3 x_1^2 x_2+\theta_4 x_1^2 x_2^2+ \\ +\theta_5 x_1^2 x_2^3+\ldots)$$

The Bias/Variance Tradeoff

A model's generalization error can be expressed as the sum of **three** very different errors:

- Bias
- Variance
- Irreducible error

The Bias/Variance Tradeoff

A model's generalization error can be expressed as the sum of **three** very different errors:

- **Bias**
  - Due to wrong assumptions, such as assuming that the data is linear when it is actually quadratic.
  - A **high-bias** model is most likely to **underfit** the training data.
- Variance
- Irreducible error

The Bias/Variance Tradeoff

A model's generalization error can be expressed as the sum of **three** very different errors:

- Bias
- **Variance**
  - Due to the model's excessive sensitivity to small variations in the training data.
  - A model with many degrees of freedom is likely to have **high variance**, and thus to **overfit** the training data.
- Irreducible error

The Bias/Variance Tradeoff

A model's generalization error can be expressed as the sum of **three** very different errors:

- Bias
- Variance
- **Irreducible error**
    - Due to the noisiness of the data itself.
    - The only way to reduce this part of the error is to clean up the data.

The Bias/Variance Tradeoff

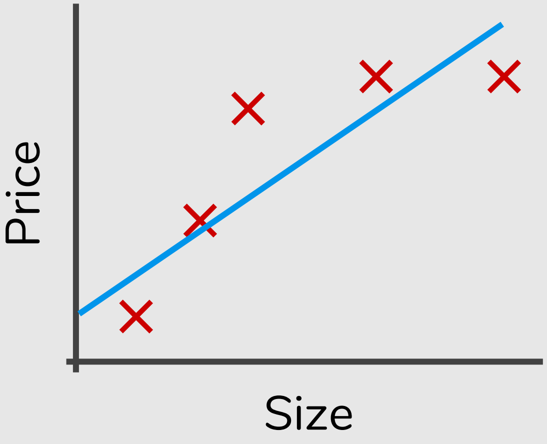
Increasing a model's complexity will typically increase its variance and reduce its bias.

Reducing a model's complexity increases its bias and reduces its variance.

This is why it is called a **tradeoff**.

Diagnosing
Bias vs. Variance

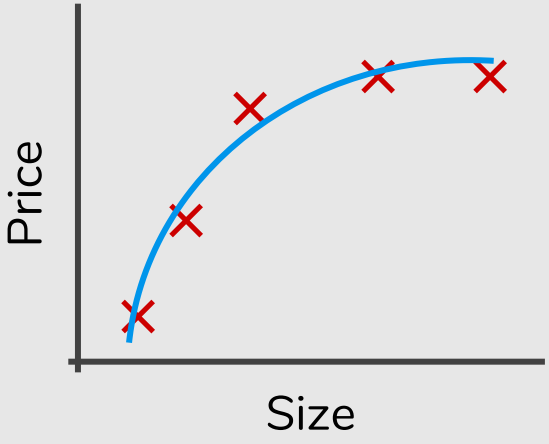
Bias/Variance



$$\theta_0 + \theta_1 x$$

Underfitting

High bias



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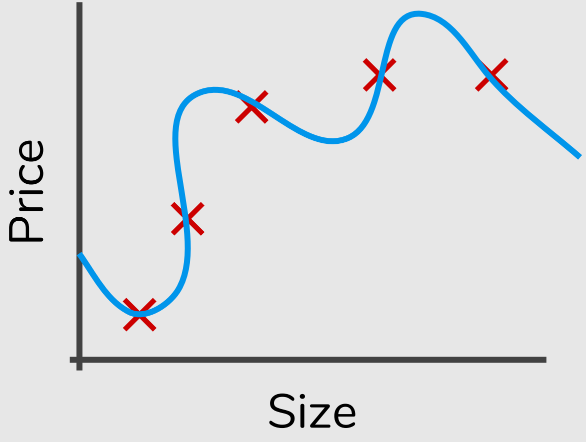

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Overfitting

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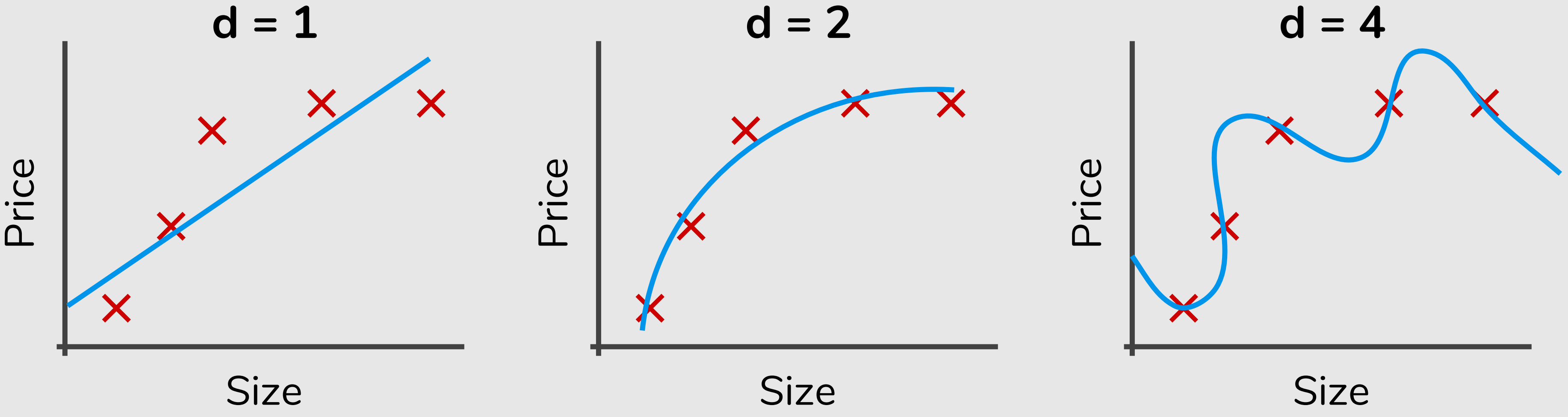
Bias/Variance



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Underfitting

High bias

Overfitting

High variance

Bias/Variance

Training error: $J_{train}(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$

Cross-validation error: $J_{cv}(\theta) = \frac{1}{2m_{cv}} \sum_{i=1}^{m_{cv}} (h_\theta(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$

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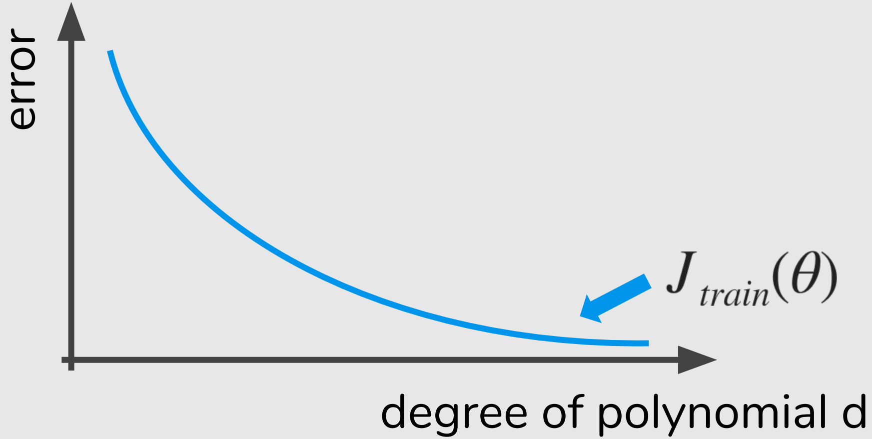

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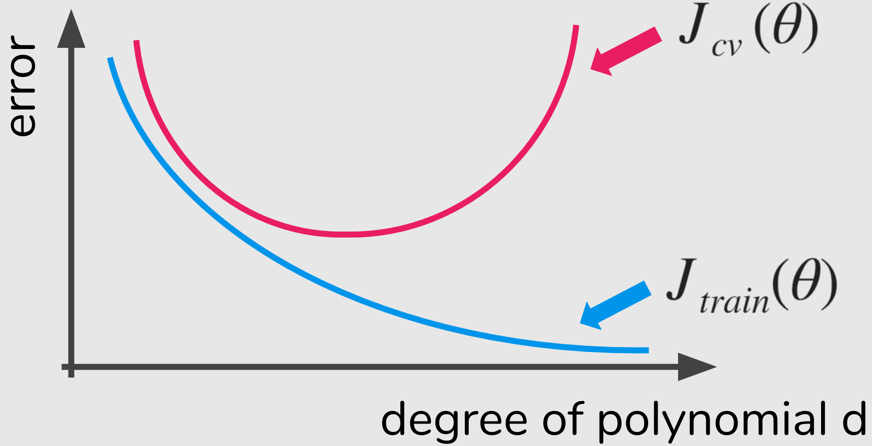
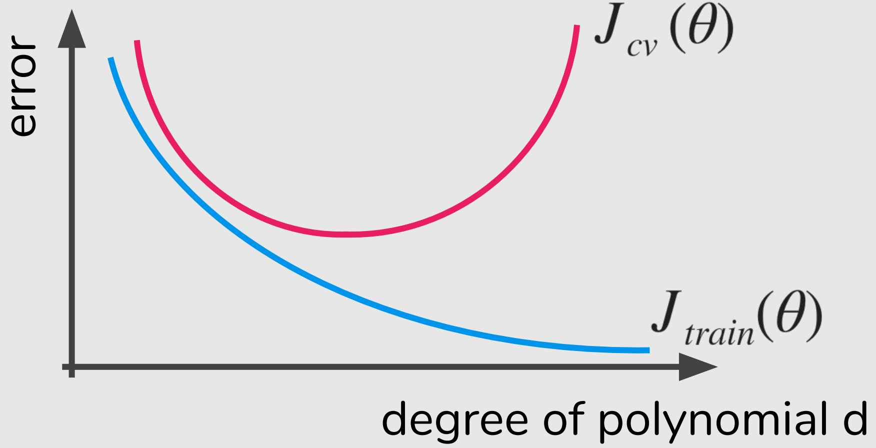


Diagnosing Bias vs. Variance

Suppose your learning algorithm is performing less well than you were hoping: $J_{cv}(\theta)$ is high. Is it a bias problem or a variance problem?



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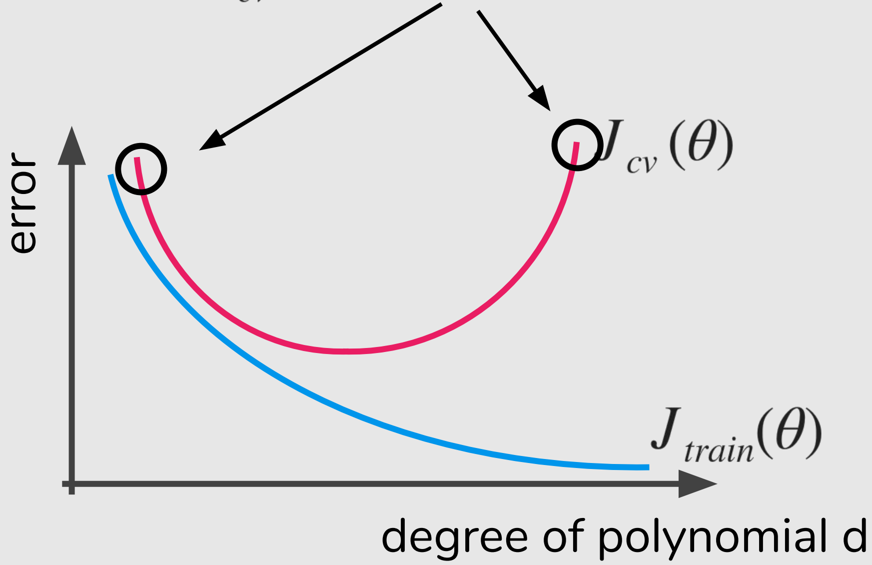

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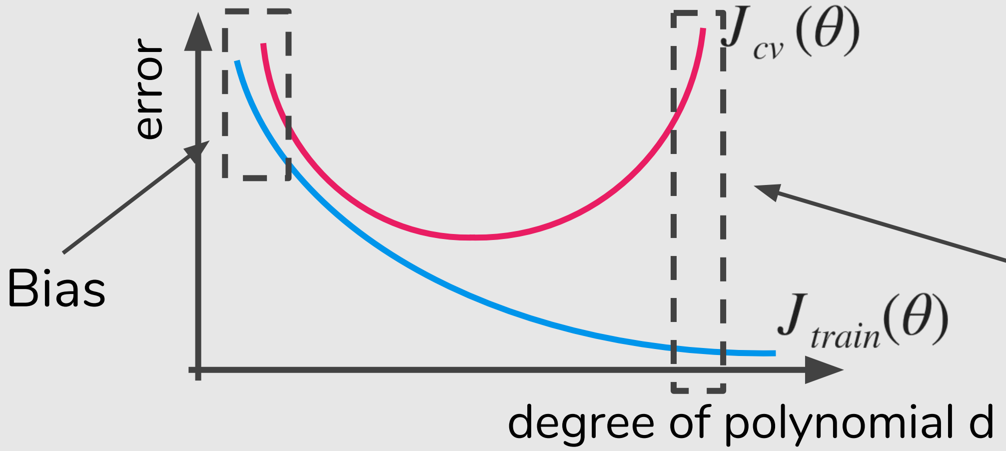

Bias (underfit):

Variance (overfit):

Diagnosing Bias vs. Variance

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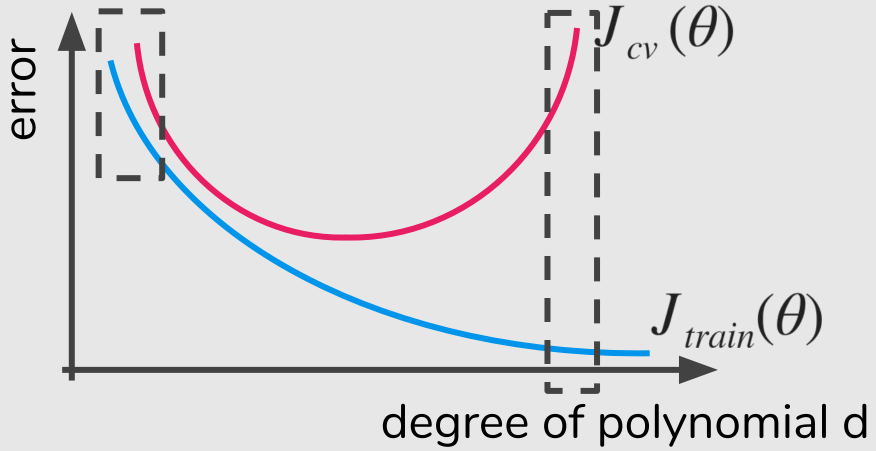

Bias (underfit):

$J_{train}(\theta)$ will be high

$J_{cv}(\theta) \approx J_{train}(\theta)$

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Diagnosing Bias vs. Variance

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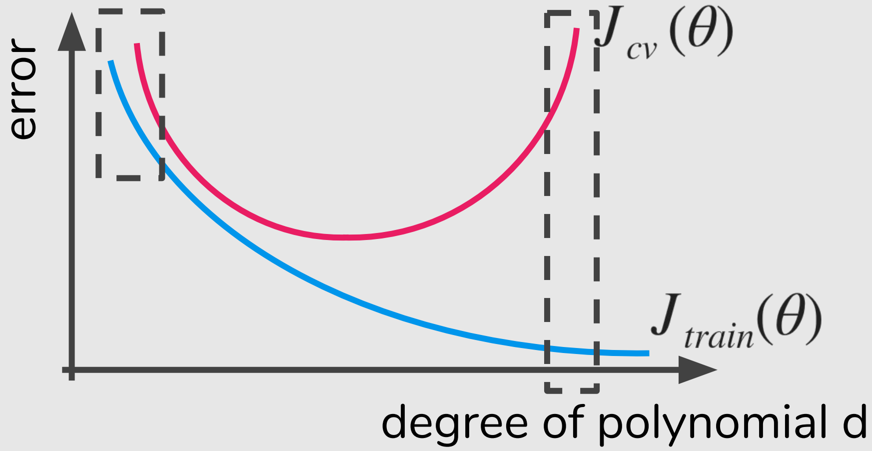


Bias (underfit):

$J_{train}(\theta)$ will be high

$J_{cv}(\theta) \approx J_{train}(\theta)$

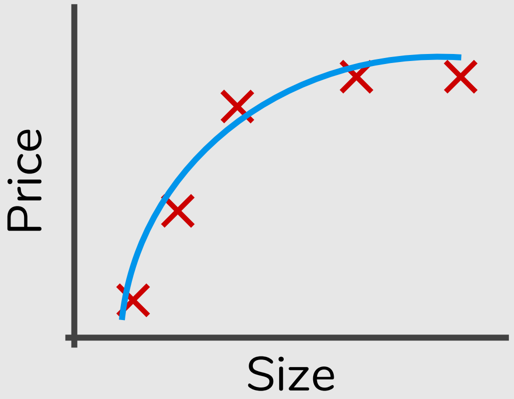
Variance (overfit):

$J_{train}(\theta)$ will be low

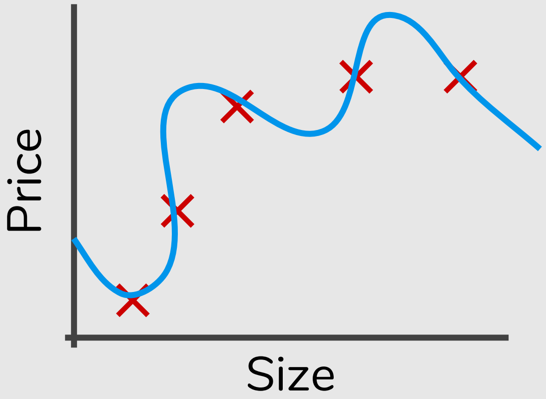
$J_{cv}(\theta) \gg J_{train}(\theta)$

Cost Function

Intuition



$$\theta_0 + \theta_1 x + \theta_2 x^2$$



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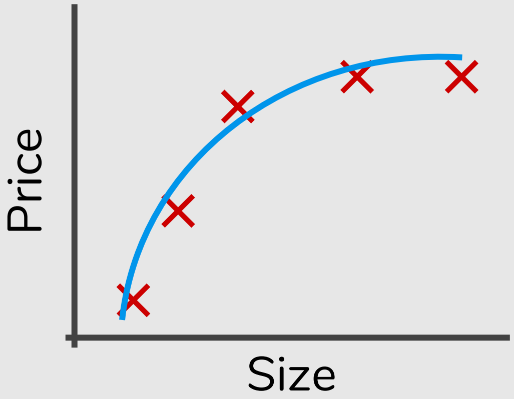
Intuition



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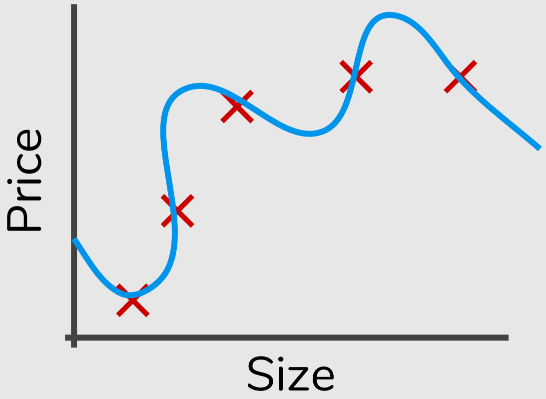
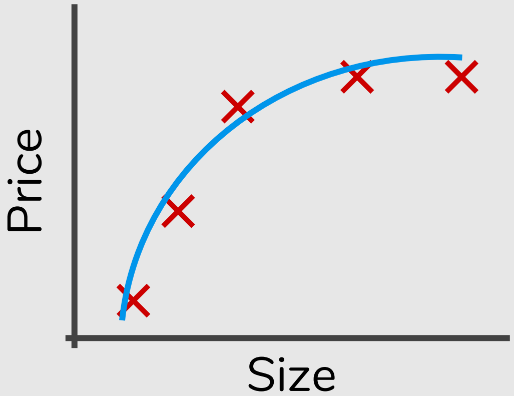


$$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$

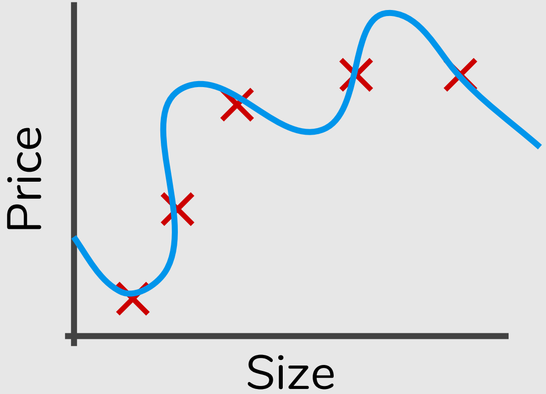
Suppose we penalize and make θ_3, θ_4 really small.

$$\min_{\theta} \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

Intuition



$\theta_0 + \theta_1 x + \theta_2 x^2$

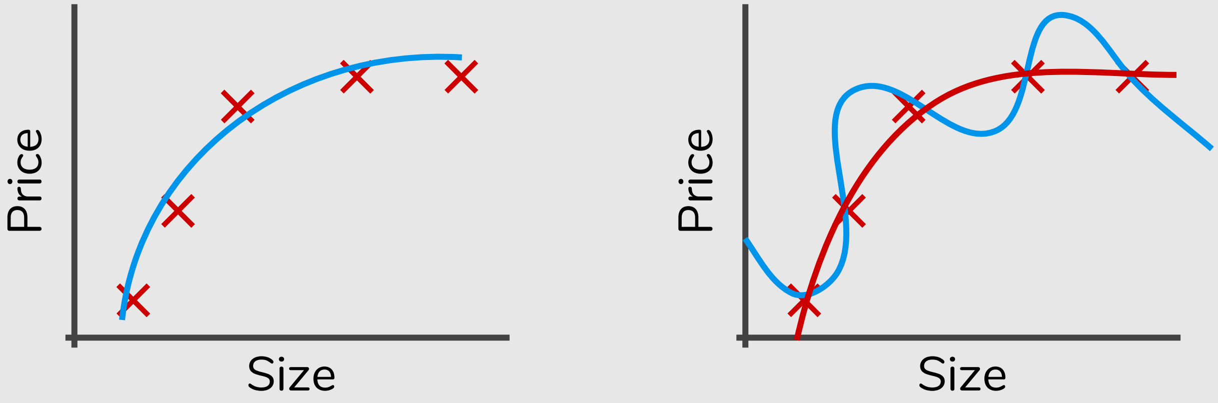


$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

Suppose we penalize and make θ_3, θ_4 really small.

$$\min_{\theta} \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 + 1000\ \theta_3^2 + 1000\ \theta_4^2$$

Intuition



$\theta_0 + \theta_1 x + \theta_2 x^2$

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$\theta_3 \approx 0$

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Regularization

Small values for parameters $\theta_0, \theta_1, \ldots, \theta_n$

- "Simpler" hypothesis
- Less prone to overfitting

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Housing

- Features: $x_0, x_1, \ldots, x_{100}$
- Parameters: $\theta_0, \theta_1, \theta_2, \ldots, \theta_{100}$

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

Regularization

Small values for parameters $\theta_0, \theta_1, \ldots, \theta_n$

- "Simpler" hypothesis
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Housing

- Features: $x_0, x_1, \ldots, x_{100}$
- Parameters: $\theta_0, \theta_1, \theta_2, \ldots, \theta_{100}$

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n} \theta_j^2 \right]$$

Regularization

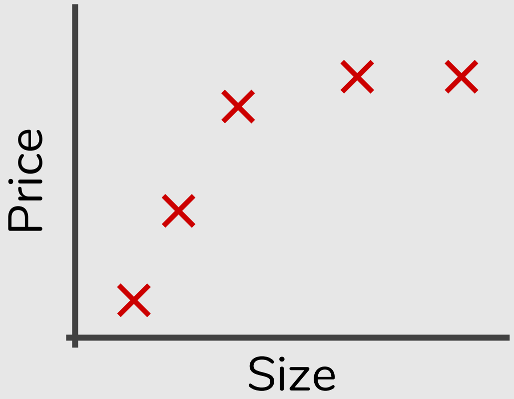
Regularization parameter

$$J(\theta) = \frac{1}{2m}\left[\underbrace{\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2}_{\text{to fit the training data well}} + \boxed{\lambda} \underbrace{\sum_{j=1}^{n}\theta_j^2}_{\text{to keep the parameters small}} \right]$$

In regularized linear regression, we choose θ to minimize

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda\sum_{j=1}^{n}\theta_j^2\right]$$

What if λ is set to an extremely large value (perhaps for too large for our problem, say $\lambda = 10^{10}$)?



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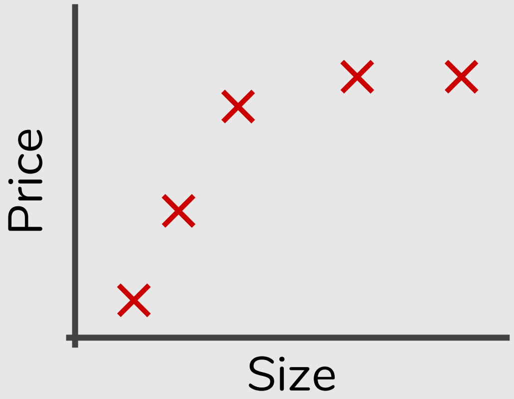
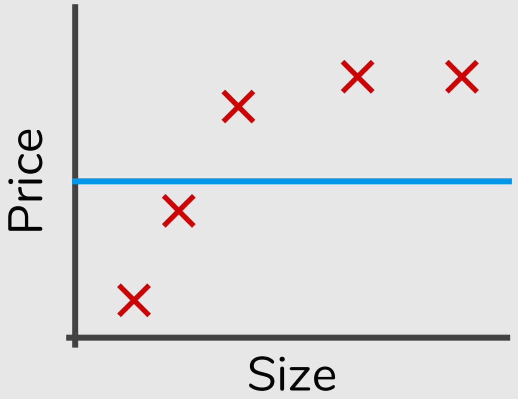


$$\theta_0 + \cancel{\theta_1 x} + \cancel{\theta_2 x^2} + \cancel{\theta_3 x^3} + \cancel{\theta_4 x^4}$$

In regularized linear regression, we choose θ to minimize

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2 + \lambda\sum_{j=1}^{n}\theta_j^2\right]$$

What if λ is set to an extremely large value (perhaps for too large for our problem, say $\lambda = 10^{10}$)?



$\theta_0 + \cdots + \cdots + \cdots + \cdots$

Regularized Linear Function

Gradient Descent

repeat {

$$\theta_j := \theta_j - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

(simultaneously update θ_j for $j = 0, 1, \ldots, n$)

}

Gradient Descent

repeat {

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

} (simultaneously update θ_j for $j = \cancel{0}\ 1, \ldots, n$)

Gradient Descent

repeat {

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \left[\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} \boxed{+ \frac{\lambda}{m} \theta_j} \right]$$

} (simultaneously update θ_j for $j = \cancel{0,}\ 1, \ldots, n$)

Gradient Descent

repeat {

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \left[\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j \right]$$

} (simultaneously update θ_j for $j = 1, \ldots, n$)

$$\theta_j := \theta_j (1 - \alpha \frac{\lambda}{m}) - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

Gradient Descent

repeat {

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \left[\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j \right]$$

} (simultaneously update θ_j for $j = \cancel{0},\ 1,\ \ldots,\ n$)

$$\theta_j := \theta_j \boxed{(1 - \alpha \frac{\lambda}{m})} - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

Normal Equation

$$X = \begin{bmatrix} \text{——} & (x^{(1)})^{\mathrm{T}} & \text{——} \\ \text{——} & (x^{(2)})^{\mathrm{T}} & \text{——} \\ \text{——} & \vdots & \text{——} \\ \text{——} & (x^{(m)})^{\mathrm{T}} & \text{——} \end{bmatrix} \qquad y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix} \qquad \theta = (X^T X)^{-1} X^T y$$

Normal Equation

$$X = \begin{bmatrix} \text{—} & (x^{(1)})^{\mathrm{T}} & \text{—} \\ \text{—} & (x^{(2)})^{\mathrm{T}} & \text{—} \\ \text{—} & \vdots & \text{—} \\ \text{—} & (x^{(m)})^{\mathrm{T}} & \text{—} \end{bmatrix} \quad y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix} \quad \theta = (X^T X)^{-1} X^T y$$

$$\theta = \left(X^T X \qquad\qquad\qquad \right)^{-1} X^T y$$

Normal Equation

$$X = \begin{bmatrix} \text{---} & (x^{(1)})^{\mathrm{T}} & \text{---} \\ \text{---} & (x^{(2)})^{\mathrm{T}} & \text{---} \\ \text{---} & \vdots & \text{---} \\ \text{---} & (x^{(m)})^{\mathrm{T}} & \text{---} \end{bmatrix} \quad y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix} \quad \theta = (X^T X)^{-1} X^T y$$

$$\theta = \left(X^T X + \lambda \begin{bmatrix} 0 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix} \right)^{-1} X^T y$$

Regularized Logistic Function

Gradient Descent

repeat {

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \left[\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j \right]$$

} (simultaneously update θ_j for $j = \cancel{0}\ 1, \ldots, n$)

$$\theta_j := \theta_j (1 - \alpha \frac{\lambda}{m}) - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

Gradient Descent

$$h_\theta(x) = \theta^T x \quad \Rightarrow \quad h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}$$

repeat {

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \left[\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j \right]$$

} (simultaneously update θ_j for $j = \cancel{0}, 1, \ldots, n$)

$$\theta_j := \theta_j (1 - \alpha \frac{\lambda}{m}) - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

References

Machine Learning Books

- Hands-On Machine Learning with Scikit-Learn and TensorFlow, Chap. 4
- Pattern Recognition and Machine Learning, Chap. 3

Machine Learning Courses

- https://www.coursera.org/learn/machine-learning, Week 3 & 6