Diagnosing Bias vs Variance

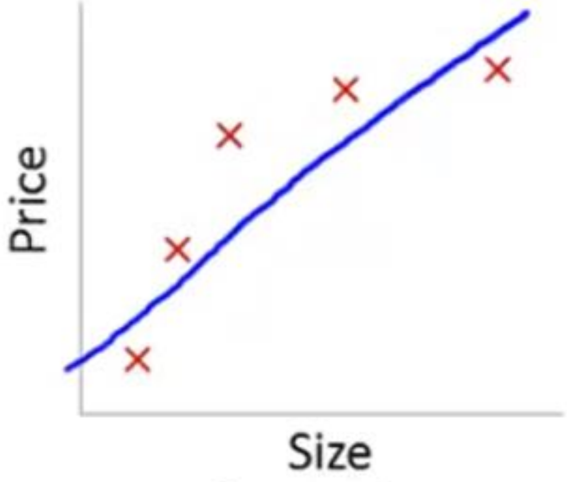
Bias and Variance

Advice for Applying Machine Learning

Introduction

- Most of the time you will have
  - High variance (overfitting)
  - High bias (underfitting)

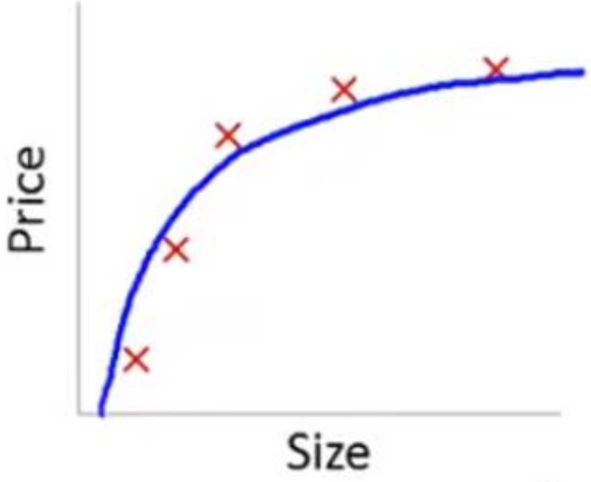
Bias/variance



$\theta_0 + \theta_1 x$

High bias
(underfit)

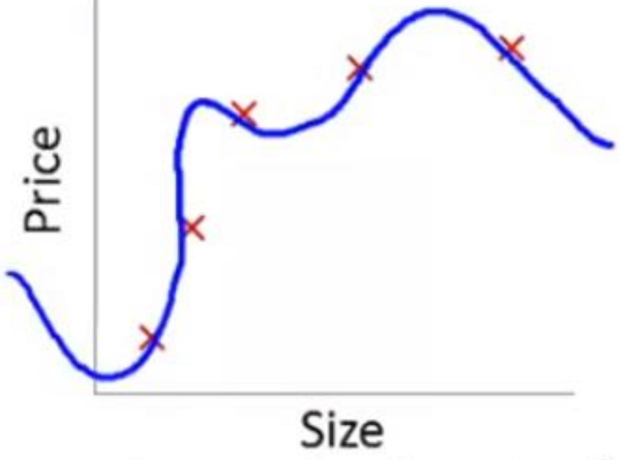
$d=1$



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

"Just right"

$d=2$



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

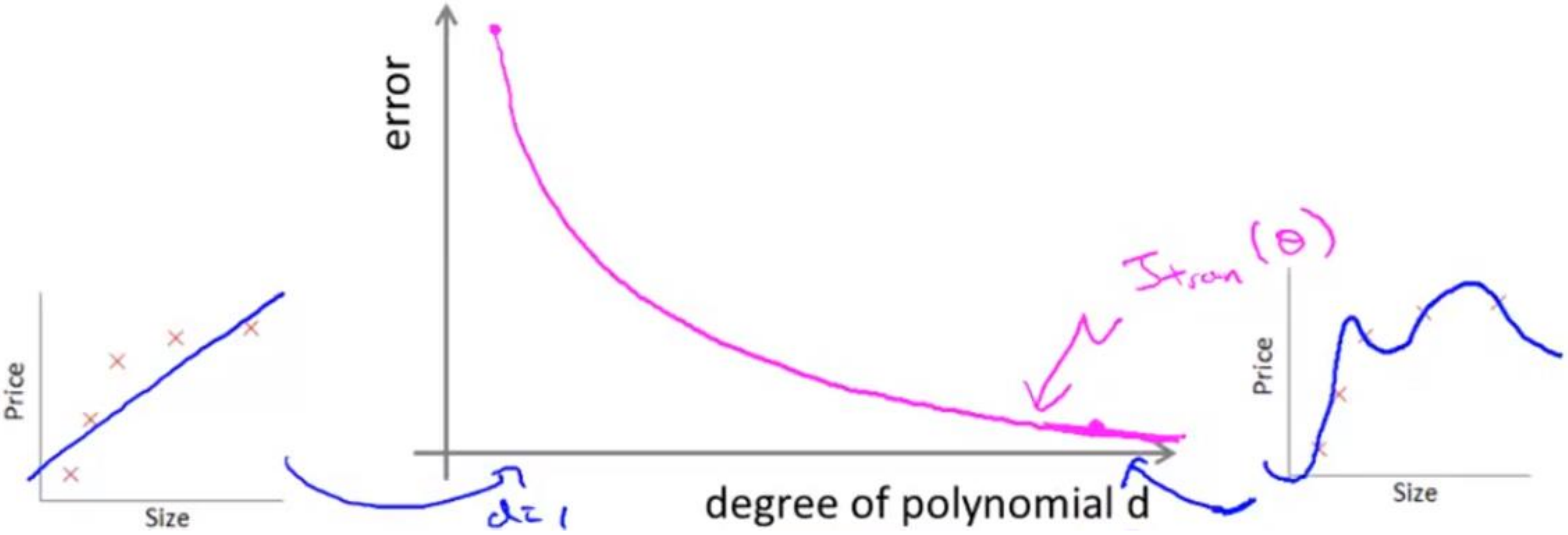
High variance
(overfit)

$d=4$

Bias/variance

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

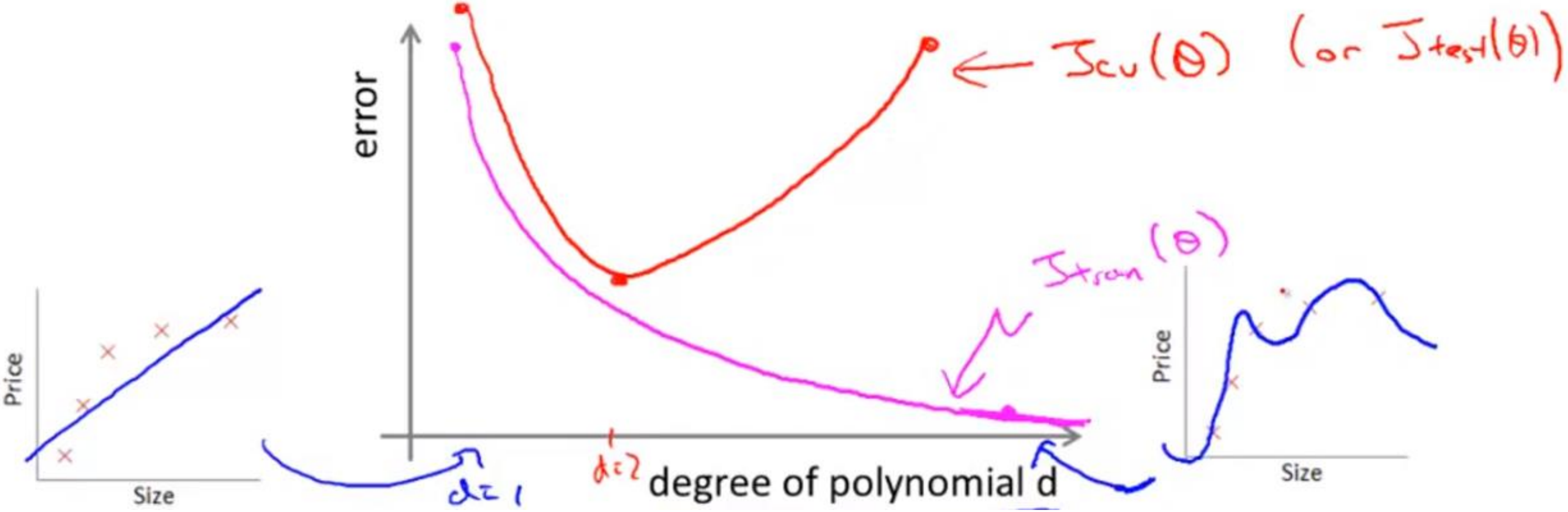
Cross validation error: $J_{cv}(\theta) = \frac{1}{2m_{cv}}\sum_{i=1}^{m_{cv}}(h_\theta(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$



Bias/variance

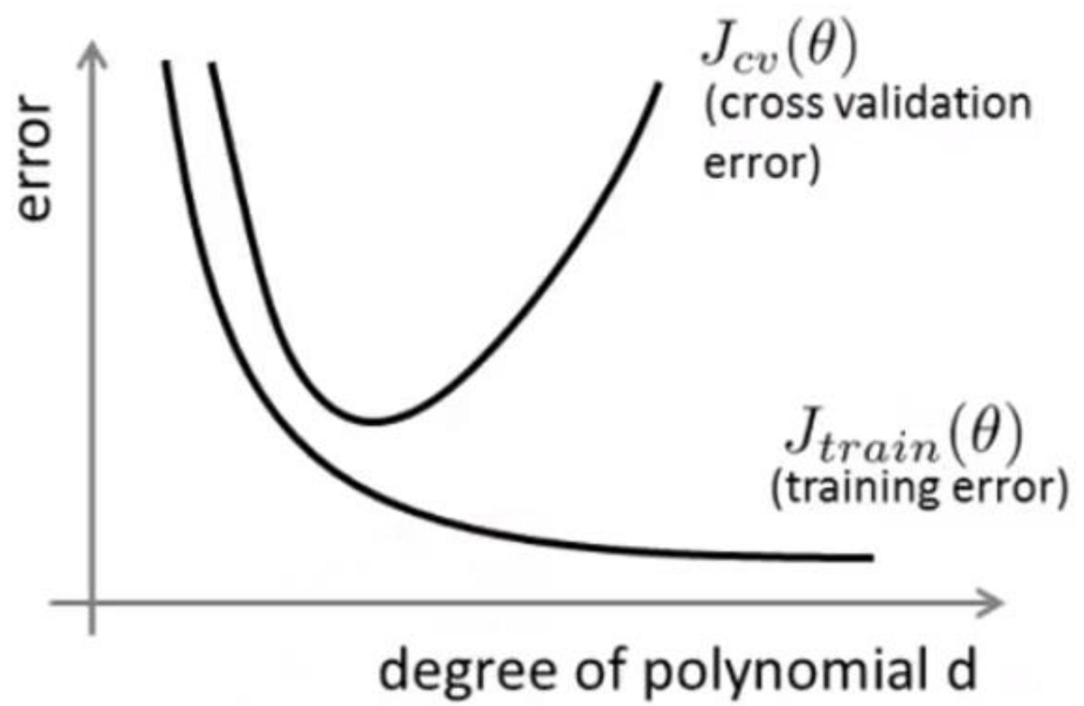
Training error: $J_{train}(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$

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



Diagnosing bias vs. variance

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



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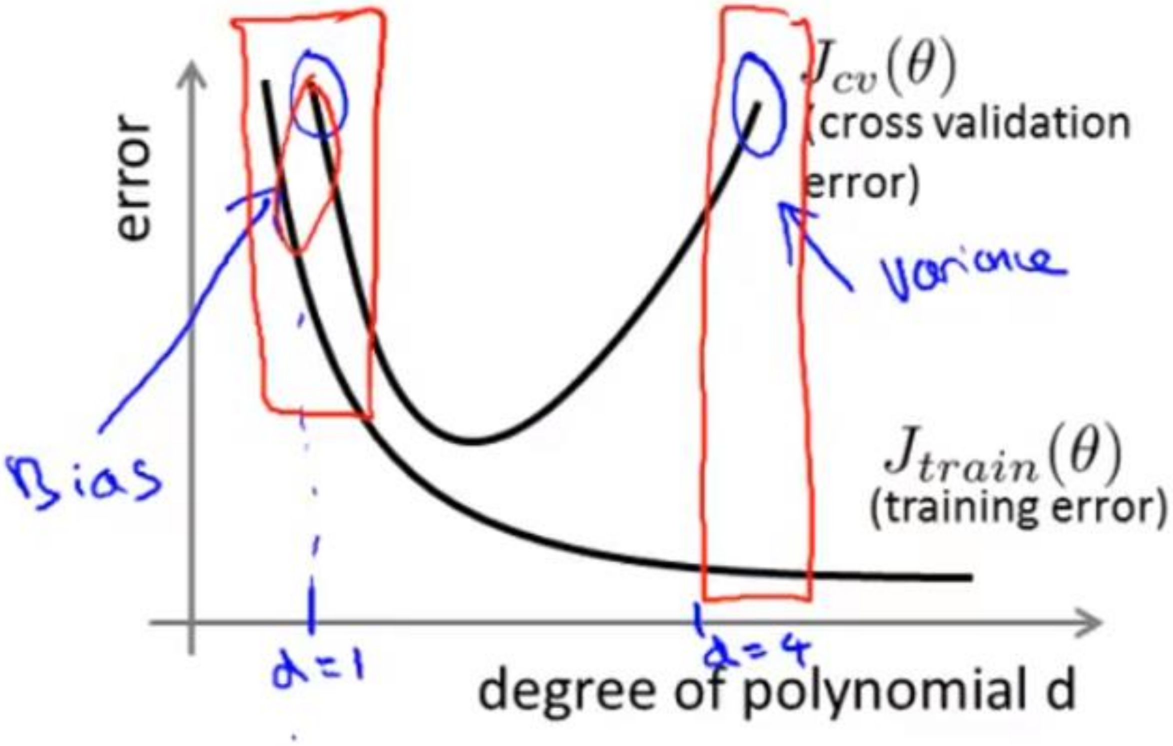


Bias (underfit):

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

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

Variance (overfit):

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

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

Exercise

- Suppose you have a classification problem. The (misclassification) error is defined as

$$\frac{1}{m}\sum_{i=1}^{m} err\left(h_\theta\left(x^{(i)}\right), y^{(i)}\right)$$

- and the cross validation (misclassification) error is similarly defined, using the cross validation examples $(x_{CV}^{(1)}, y_{CV}^{(1)}), \dots, (x_{CV}^{m_{cv}}, y_{CV}^{m_{cv}})$

- Suppose your training error is 0.10, and your cross validation error is 0.30. What problem is the algorithm most likely to be suffering from
    - High bias (overfitting)
    - High bias (underfitting)
    - High variance (overfitting)
    - High variance (underfitting)

Regularization and Bias/Variance

Bias and Variance

Advice for Applying Machine Learning

Introduction

- You've seen how regularization can help prevent over-fitting in previous lectures.
- In the lectures that we talked about today, there was no regularization…
- How does regularization affect the **bias** and **variances** of a learning algorithm?

Linear regression with regularization

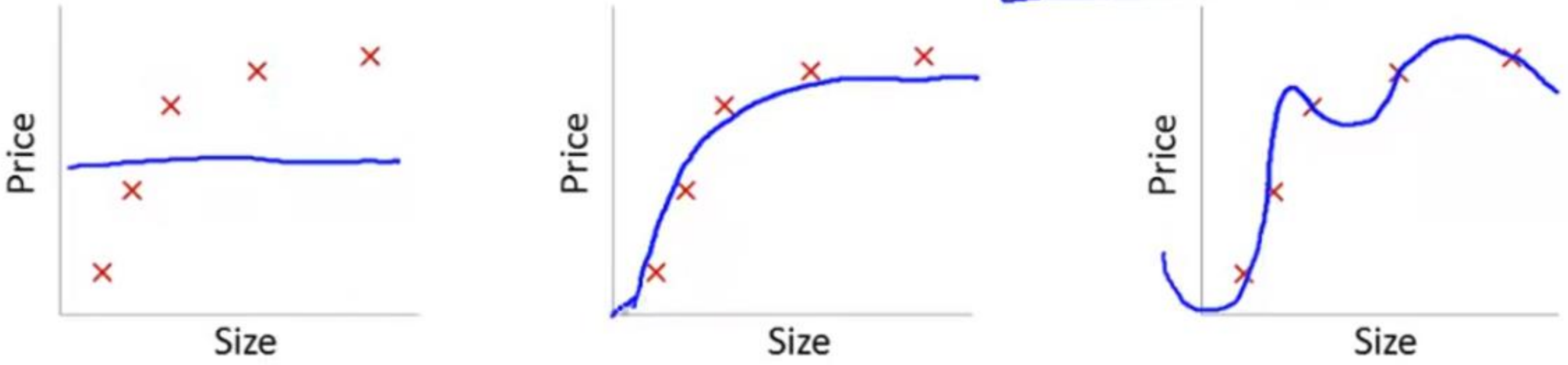
Model: $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

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

Linear regression with regularization

Model: $\boxed{h_\theta(x) = \theta_0} + \underline{\theta_1} x + \underline{\theta_2} x^2 + \underline{\theta_3} x^3 + \theta_4 x^4 \leftarrow$

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



Large λ $\leftarrow$	Intermediate λ $\leftarrow$	$\rightarrow$ Small λ
$\rightarrow$ High bias (underfit)	"Just right"	High variance (overfit)
$\rightarrow \lambda = 10000.\ \underline{\theta_1 \approx 0, \theta_2 \approx 0,} \ldots$ $h_\theta(x) \approx \theta_0$	**How to choose lambda??**	$\rightarrow \lambda = 0$

Choosing the regularization parameter λ

$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$

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

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

Choosing the regularization parameter λ

$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4 \leftarrow$$

$$J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \underline{\frac{\lambda}{2m}\sum_{j=1}^{m}\theta_j^2} \leftarrow$$

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

$J(\theta)$

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

$$J_{test}(\theta) = \frac{1}{2m_{test}}\sum_{i=1}^{m_{test}}(h_\theta(x_{test}^{(i)}) - y_{test}^{(i)})^2$$

Choosing the regularization parameter λ

$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$

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

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

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

$$J_{test}(\theta) = \frac{1}{2m_{test}}\sum_{i=1}^{m_{test}}(h_\theta(x_{test}^{(i)}) - y_{test}^{(i)})^2$$

$J(\theta)$

J_{train}

J_{cv}

J_{test}

Choosing the regularization parameter λ

Model: $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

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

1. Try $\lambda = 0$
2. Try $\lambda = 0.01$
3. Try $\lambda = 0.02$
4. Try $\lambda = 0.04$
5. Try $\lambda = 0.08$

$\vdots$

12. Try $\lambda = 10$

Choosing the regularization parameter λ

Model: $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

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

1. Try $\lambda = 0$ $\leftarrow$
2. Try $\lambda = \underline{0.01}$
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$\vdots$

12. Try $\lambda = 10$

10.24

Choosing the regularization parameter λ

Model: $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

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

1. Try $\lambda = 0$ $\longrightarrow \min_\theta J(\theta) \to \theta^{(1)} \to J_{cv}(\theta^{(1)})$
2. Try $\lambda = 0.01$ $\longrightarrow \min_\theta J(\theta) \to \theta^{(2)} \to J_{cv}(\theta^{(2)})$
3. Try $\lambda = 0.02$ $\longrightarrow \theta^{(3)} \to J_{cv}(\theta^{(3)})$
4. Try $\lambda = 0.04$
5. Try $\lambda = 0.08$ $\longrightarrow \theta^{(5)} \quad J_{cv}(\theta^{(5)})$

$\vdots$

12. Try $\lambda = 10$ $\longrightarrow \theta^{(12)} \to J_{cv}(\theta^{(12)})$

10.24

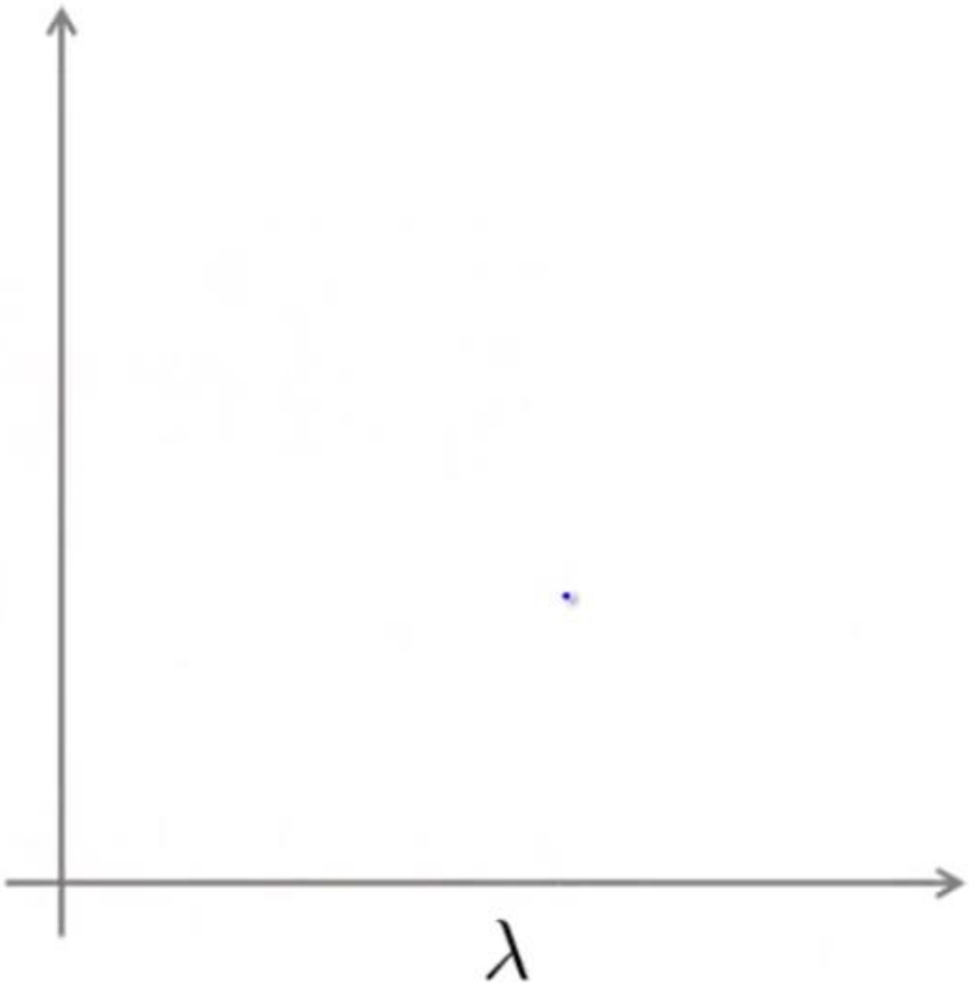
Pick (say) $\theta^{(5)}$. Test error: $J_{test}(\theta^{(5)})$

Bias/variance as a function of the regularization parameter λ

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

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

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

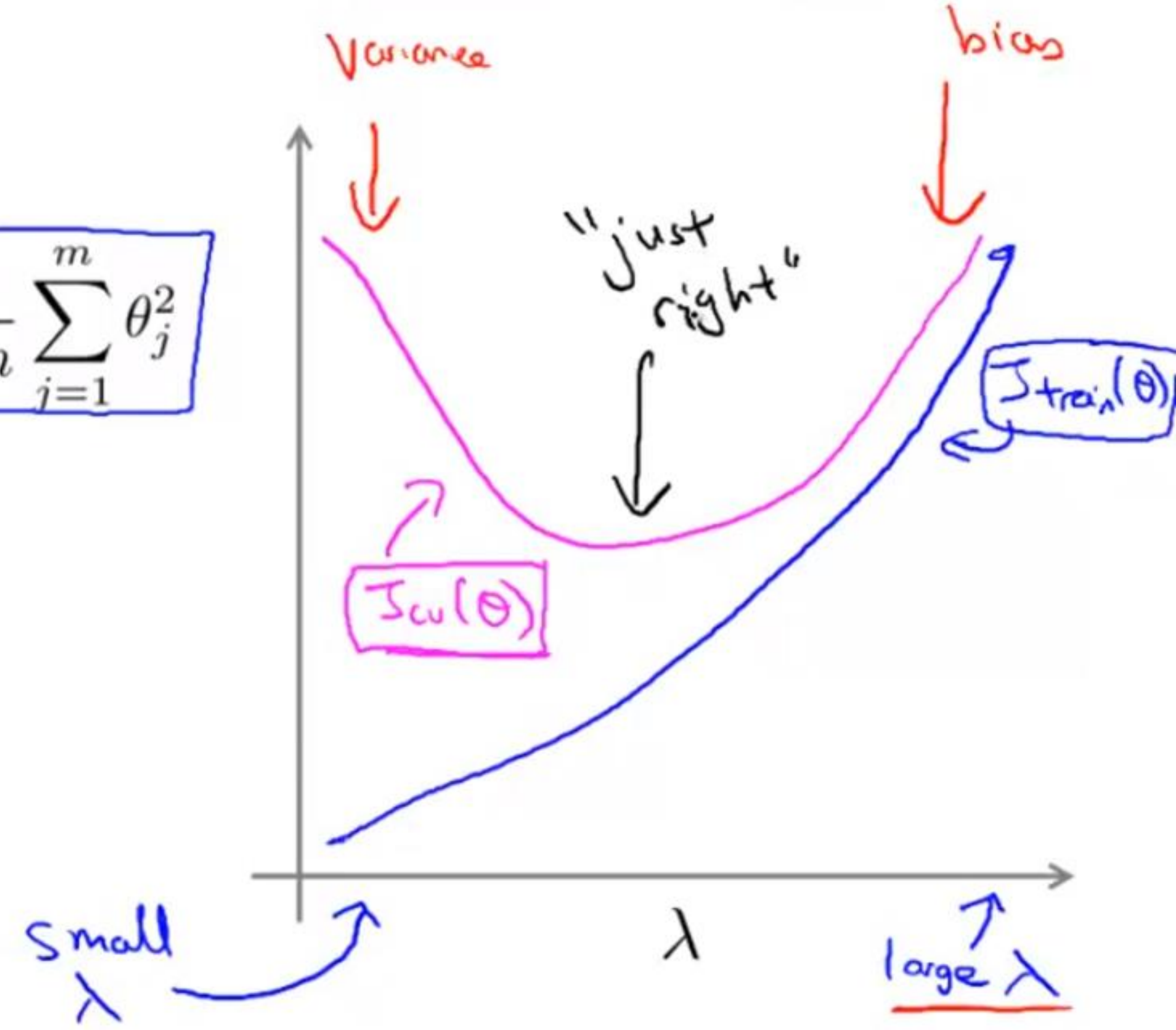


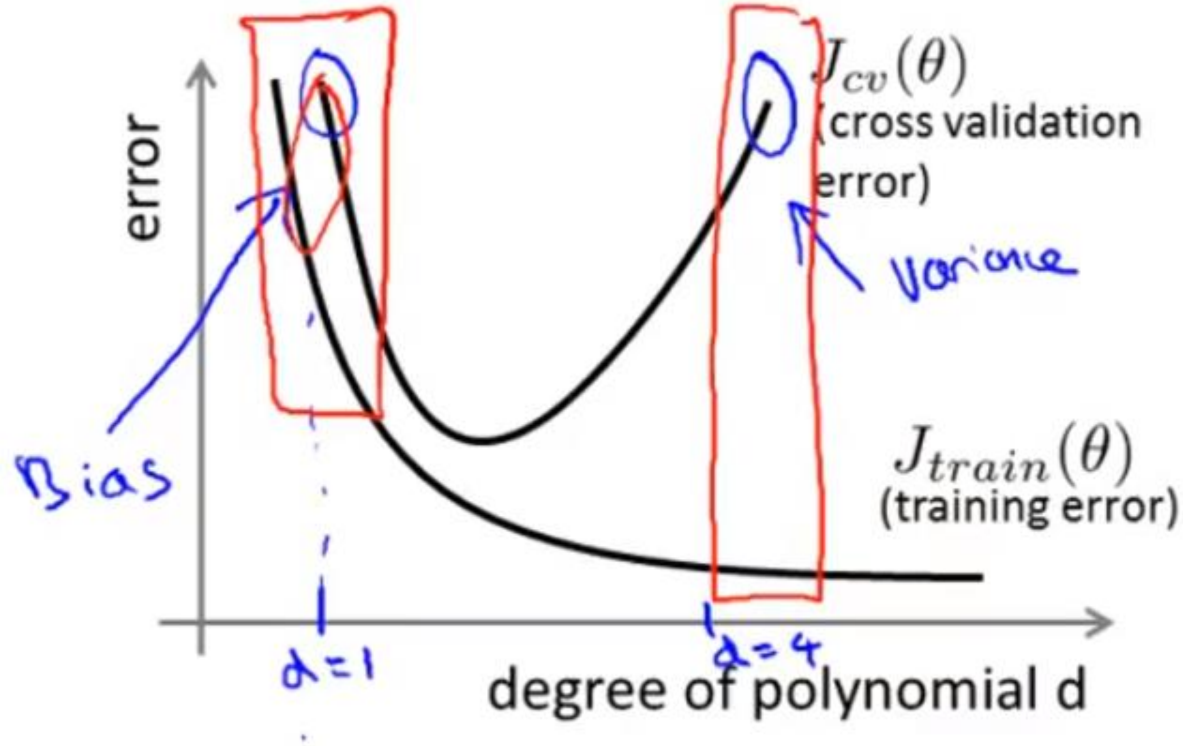
Bias/variance as a function of the regularization parameter λ

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

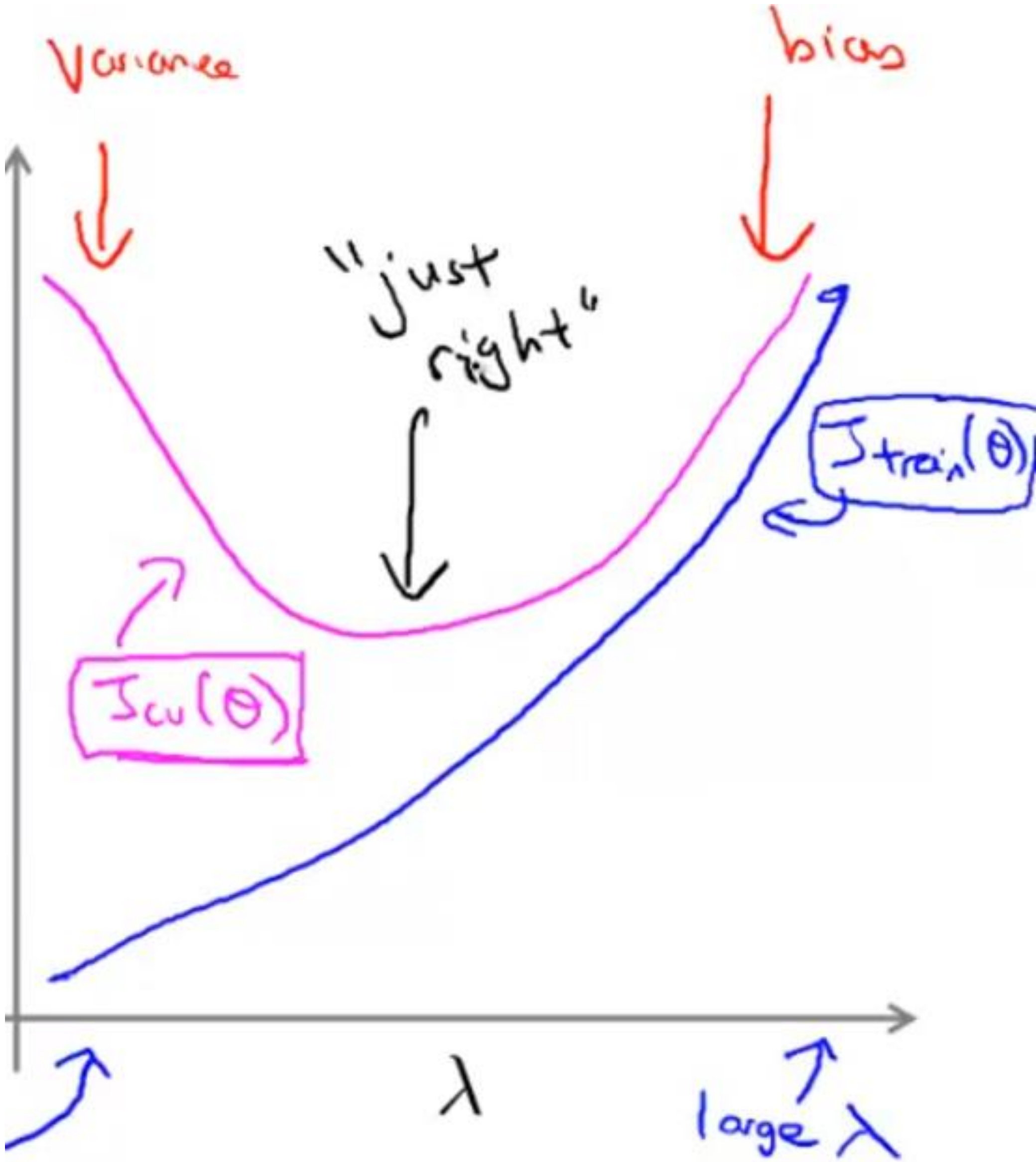
$$J_{train}(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

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





error
$J_{cv}(\theta)$
(cross validation error)
$J_{train}(\theta)$
(training error)
degree of polynomial d
Bias
variance
d=1
d=4



variance
bias
"just right"
$J_{cv}(\theta)$
$J_{train}(\theta)$
λ
large λ

Summary

- We understood that
  - as λ increases, our fit becomes more rigid.
  - as λ approaches 0, we tend to overfit the data.
- So how do we choose our parameter λ to get it 'just right' ?
- In order to choose the model and the regularization term λ, we need to:
  - Create a list of lambdas (i.e. $\lambda \in \{0,0.01,0.02,0.04,0.08,0.16,0.32,0.64,1.28,2.56,5.12,10.24\}$);
  - Create a set of models with different degrees or any other variants.
  - Iterate through the λs and for each λ go through all the models to learn some Θ.
  - Compute the cross validation error using the learned Θ (computed with λ) on the $J_{CV}(\Theta)$ **without** regularization or $\lambda = 0$.
  - Select the best combo that produces the lowest error on the cross validation set.
  - Using the best combo Θ and λ, apply it on $J_{test}(\Theta)$ to see if it has a *good generalization* of the problem.