

Machine Learning

Advice for applying machine learning

Deciding what to try next

Debugging a learning algorithm:

Suppose you have implemented regularized linear regression to predict housing prices.

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

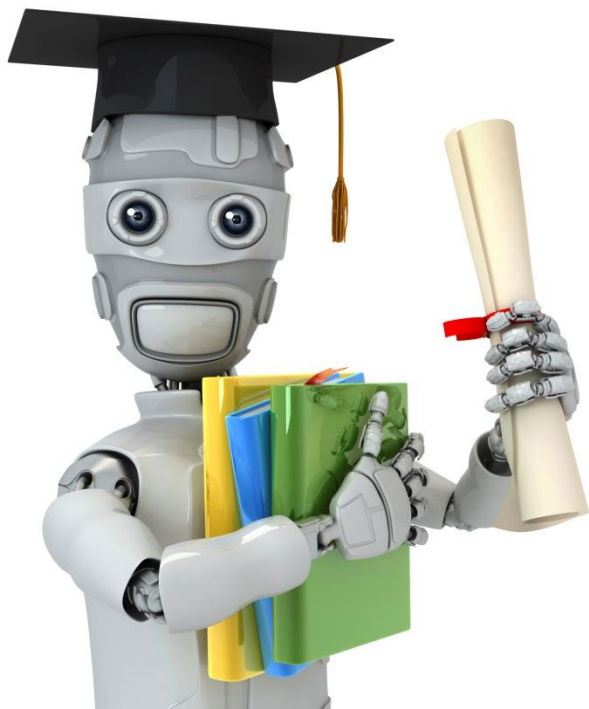
However, when you test your hypothesis on a new set of houses, you find that it makes unacceptably large errors in its predictions. What should you try next?

- Get more training examples
- Try smaller sets of features
- Try getting additional features
- Try adding polynomial features (x_1^2, x_2^2, x_1x_2 , etc.)
- Try decreasing λ
- Try increasing λ

Machine learning diagnostic:

Diagnostic: A test that you can run to gain insight what is/Isn't working with a learning algorithm, and gain guidance as to how best to improve its performance.

Diagnostics can take time to implement, but doing so can be a very good use of your time.

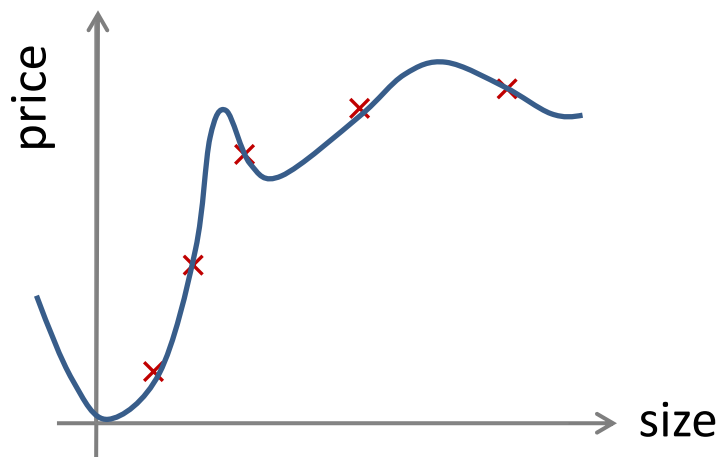


Machine Learning

Advice for applying machine learning

Evaluating a hypothesis

Evaluating your hypothesis



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

Fails to generalize to new examples not in training set.

x_1 = size of house

x_2 = no. of bedrooms

x_3 = no. of floors

x_4 = age of house

x_5 = average income in neighborhood

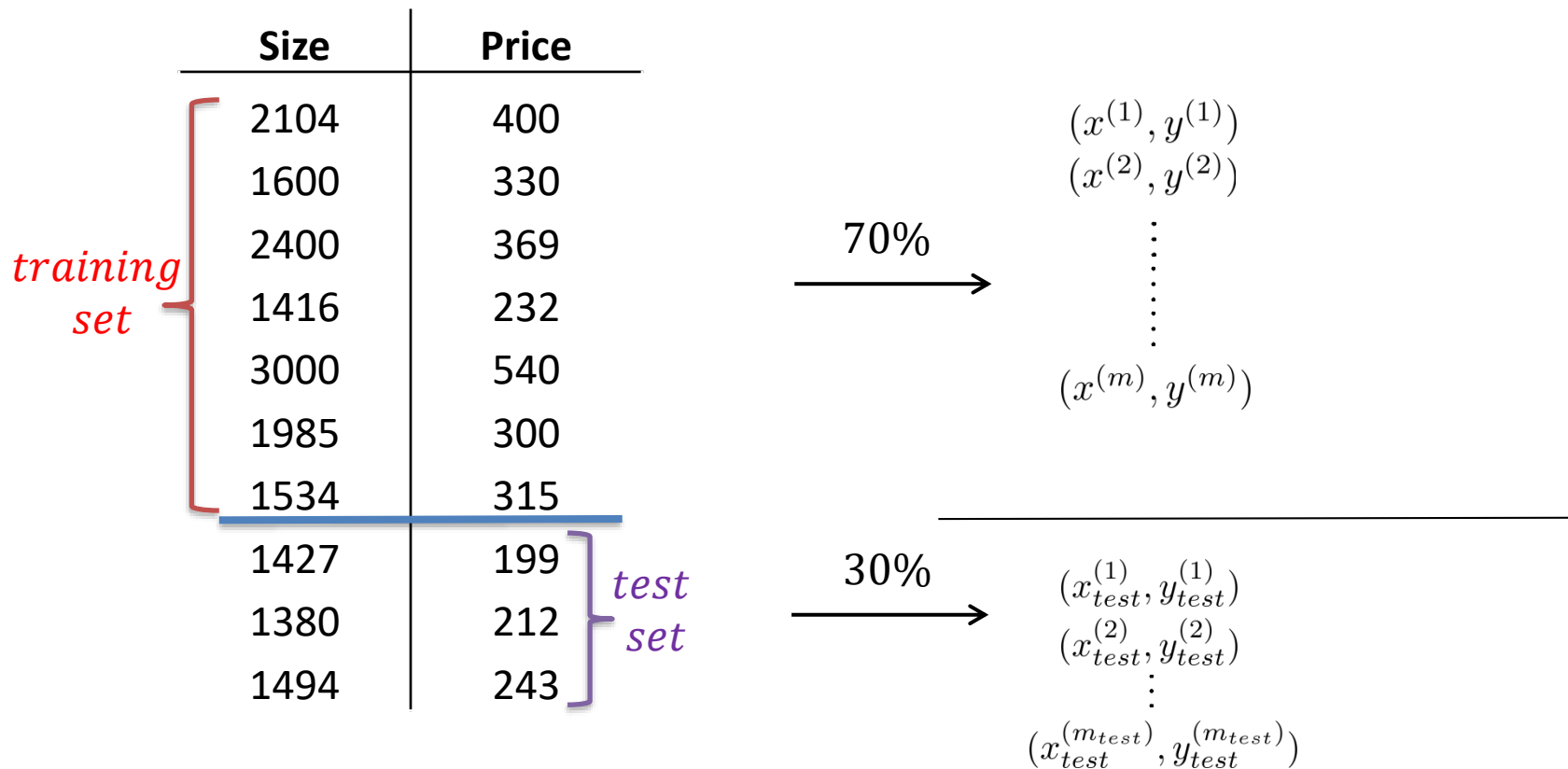
x_6 = kitchen size

\vdots

x_{100}

Evaluating your hypothesis

Dataset:



Training/testing procedure for linear regression

- Learn parameter θ from training data (minimizing training error $J(\theta)$)
- Compute test set error:

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

Training/testing procedure for logistic regression

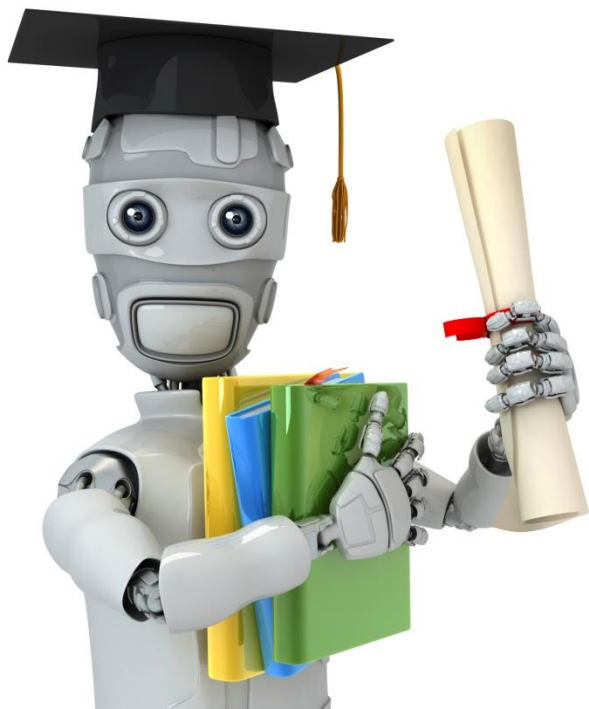
- Learn parameter θ from training data
- Compute test set error:

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

- Misclassification error (0/1 misclassification error):

$$\text{err}(h_{\theta}(x), y) = \begin{cases} 1 & \text{if } h_{\theta}(x) \geq 0.5, y = 0 \\ & \text{or if } h_{\theta}(x) < 0.5, y = 1 \\ 0 & \text{otherwise} \end{cases}$$

$$\text{Test error} = \frac{1}{m_{test}} \sum_{i=1}^{m_{test}} \text{err} \left(h_{\theta} \left(x_{test}^{(i)} \right), y_{test}^{(i)} \right)$$

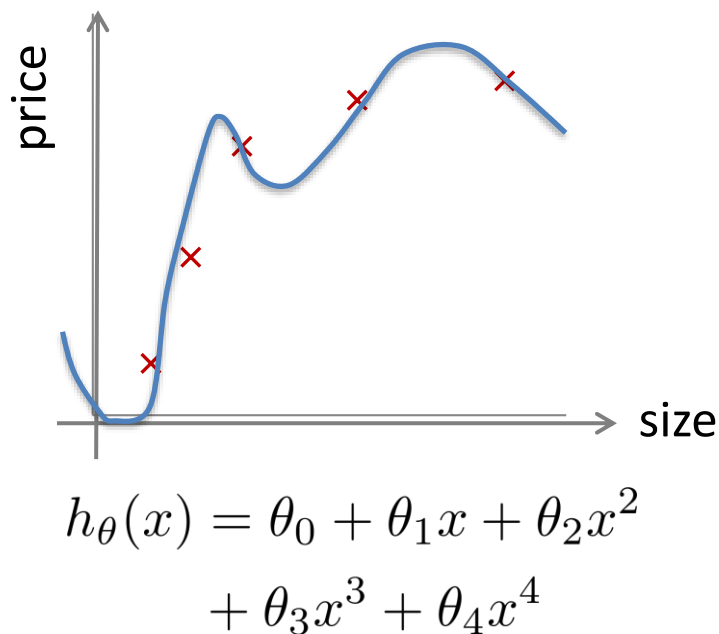


Machine Learning

Advice for applying machine learning

Model selection and
training/validation/test
sets

Overfitting example



Once parameters $\theta_0, \theta_1, \dots, \theta_4$ were fit to some set of data (training set), the error of the parameters as measured on that data (the training error $J(\theta)$) is likely to be lower than the actual generalization error.

Model selection

1. $h_{\theta}(x) = \theta_0 + \theta_1 x$
2. $h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2$
3. $h_{\theta}(x) = \theta_0 + \theta_1 x + \dots + \theta_3 x^3$
- \vdots
10. $h_{\theta}(x) = \theta_0 + \theta_1 x + \dots + \theta_{10} x^{10}$

Choose $\theta_0 + \dots + \theta_5 x^5$

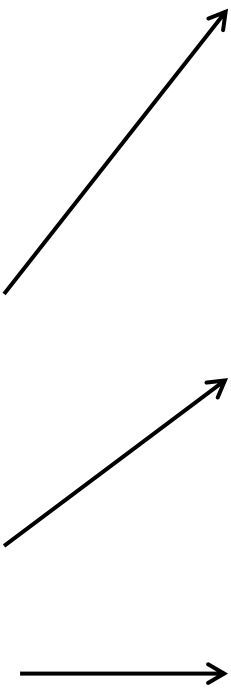
How well does the model generalize? Report test set error $J_{test}(\theta^{(5)})$.

Problem: $J_{test}(\theta^{(5)})$ is likely to be an optimistic estimate of generalization error. I.e. our extra parameter (d = degree of polynomial) is fit to test set.

Evaluating your hypothesis

Dataset:

	Size	Price	
	2104	400	
	1600	330	
	2400	369	
60%	1416	232	<i>training set</i>
	3000	540	
	1985	300	
	1534	315	<i>Cross validation set</i>
20%	1427	199	
	1380	212	<i>test set</i>
20%	1494	243	



$(x^{(1)}, y^{(1)})$
$(x^{(2)}, y^{(2)})$
\vdots
$(x^{(m)}, y^{(m)})$
$(x_{cv}^{(1)}, y_{cv}^{(1)})$
$(x_{cv}^{(2)}, y_{cv}^{(2)})$
\vdots
$(x_{cv}^{(m_{cv})}, y_{cv}^{(m_{cv})})$
$(x_{test}^{(1)}, y_{test}^{(1)})$
$(x_{test}^{(2)}, y_{test}^{(2)})$
\vdots
$(x_{test}^{(m_{test})}, y_{test}^{(m_{test})})$

Train/validation/test error

Training error:

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

Cross Validation error:

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

Test error:

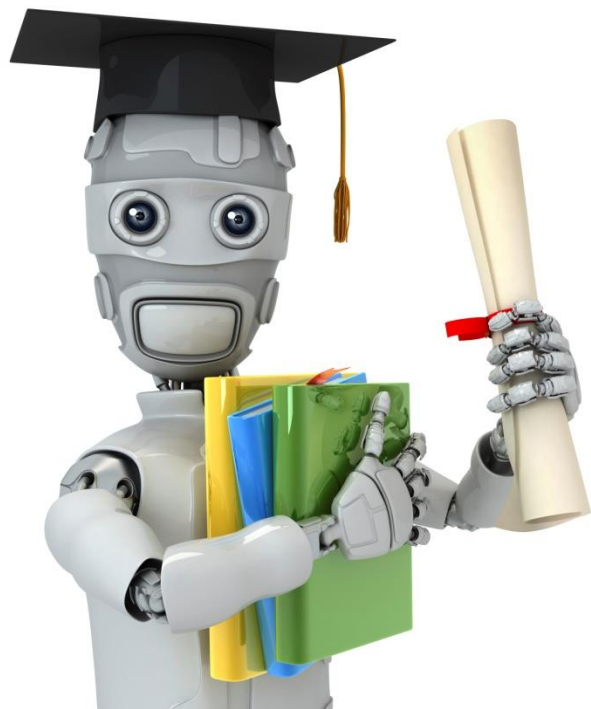
$$J_{test}(\theta) = \frac{1}{2m_{test}} \sum_{i=1}^{m_{test}} (h_{\theta}(x_{test}^{(i)}) - y_{test}^{(i)})^2$$

Model selection

1. $h_{\theta}(x) = \theta_0 + \theta_1 x$
2. $h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2$
3. $h_{\theta}(x) = \theta_0 + \theta_1 x + \cdots + \theta_3 x^3$
- \vdots
10. $h_{\theta}(x) = \theta_0 + \theta_1 x + \cdots + \theta_{10} x^{10}$

Pick $\theta_0 + \theta_1 x_1 + \cdots + \theta_4 x^4$

Estimate generalization error for test set $J_{test}(\theta^{(4)})$

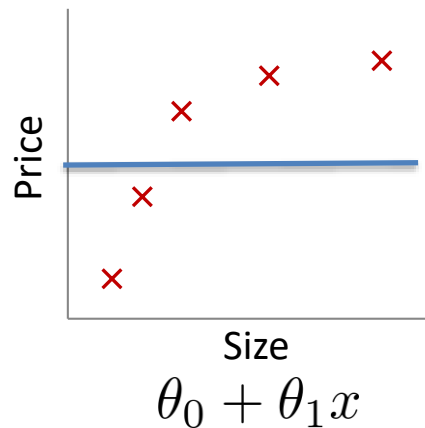


Machine Learning

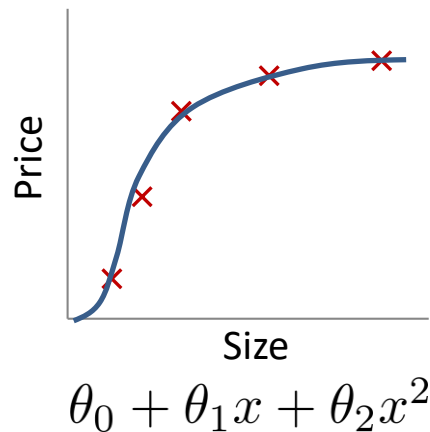
Advice for applying machine learning

Diagnosing bias vs. variance

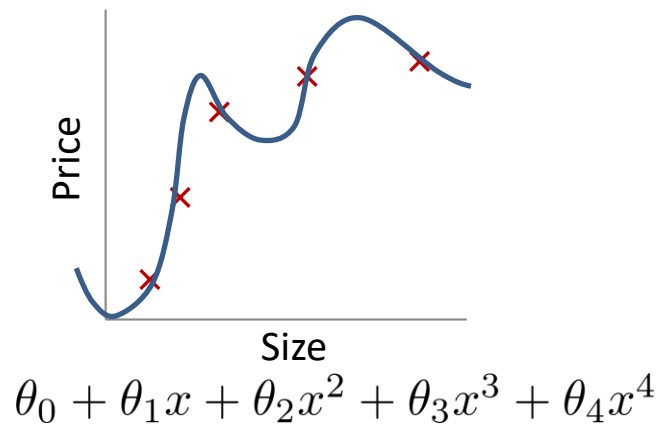
Bias/variance



High bias
(underfit)



“Just right”

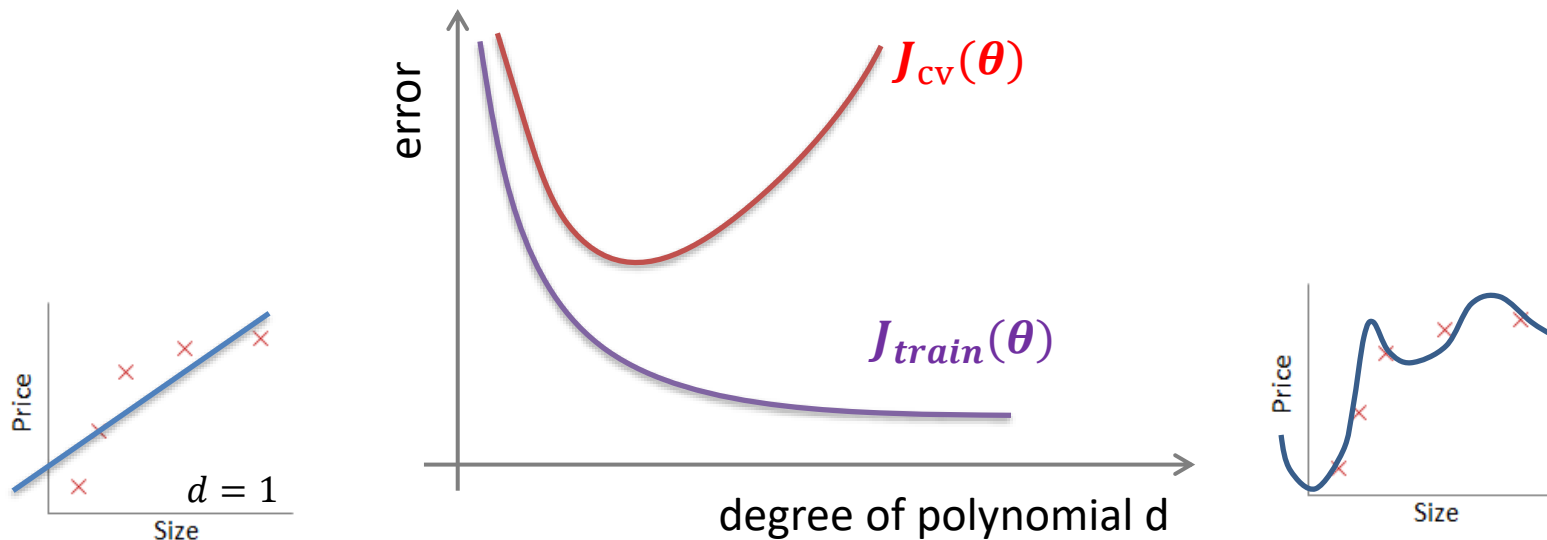


High variance
(overfit)

Bias/variance

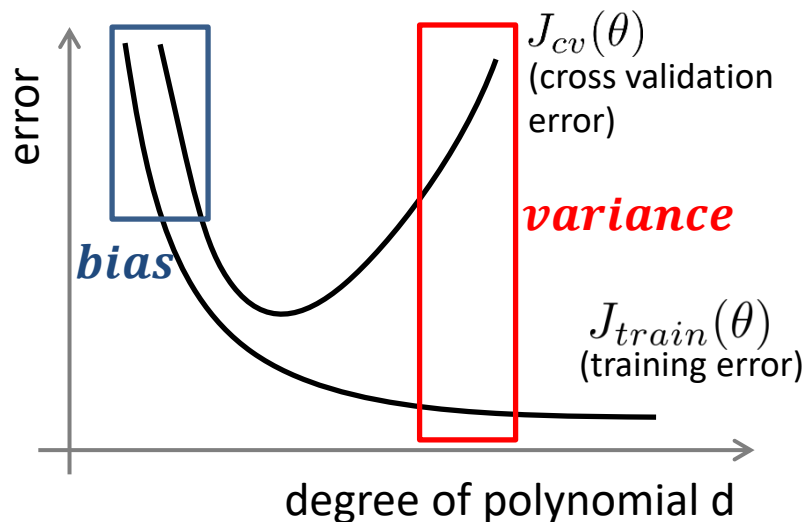
Training error: $J_{train}(\theta) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$

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



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?



Bias (underfit):

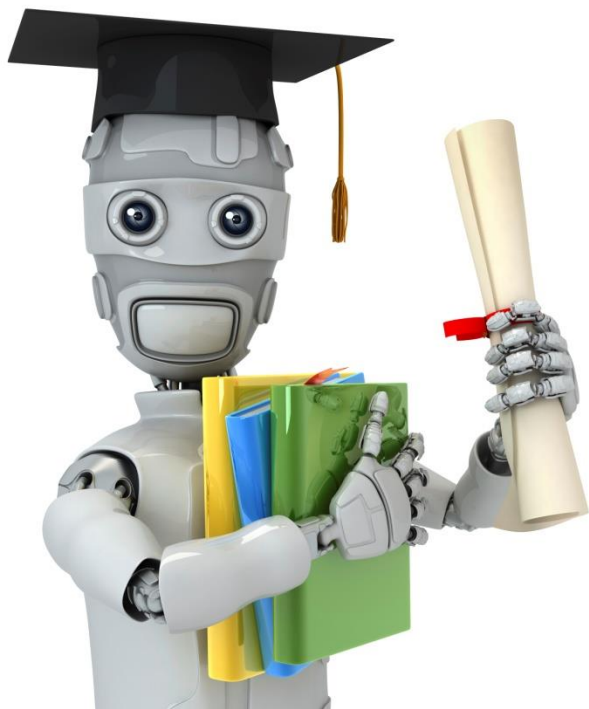
$J_{train}(\theta)$ will be high

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

Variance (overfit):

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

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



Machine Learning

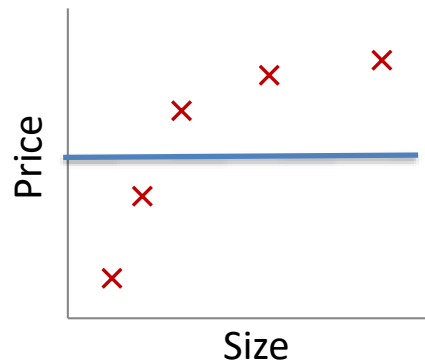
Advice for applying machine learning

Regularization and bias/variance

Linear regression with regularization

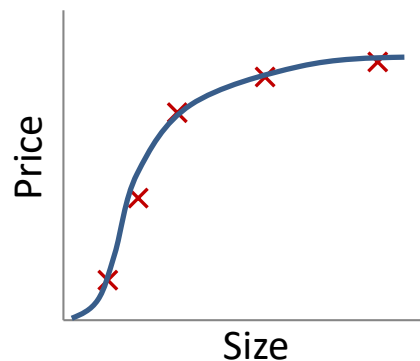
Model: $h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

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



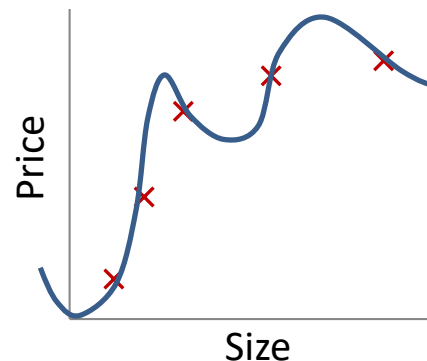
Large λ

High bias (underfit)



Intermediate λ

“Just right”



Small λ

High variance (overfit)

$\lambda = 10000$. $\theta_1 \approx 0, \theta_2 \approx 0, \dots$

$h_{\theta}(x) \approx \theta_0$

Choosing the regularization parameter λ

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

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

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

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

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

Choosing the regularization parameter λ

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 $\lambda = 10$

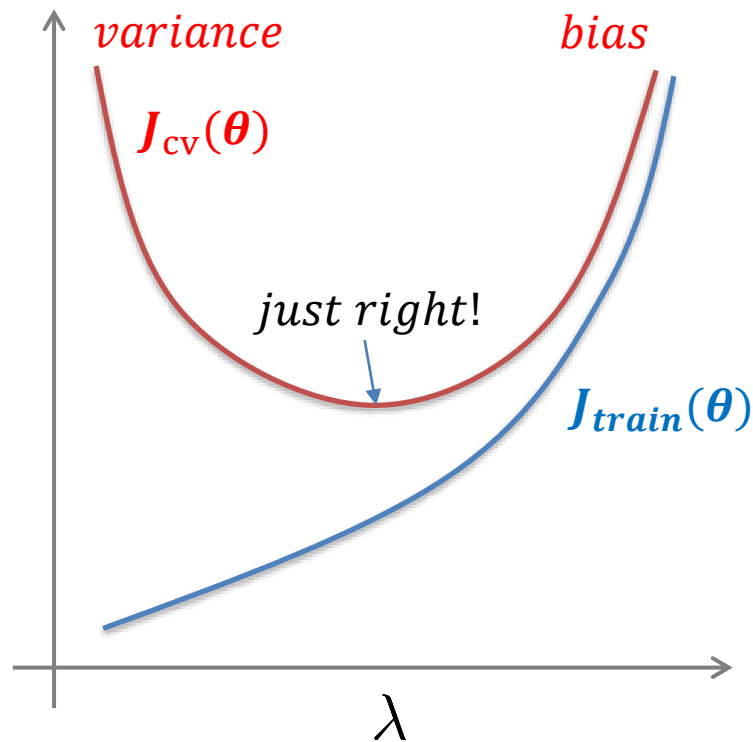
Pick (say) $\theta^{(5)}$. Test error:

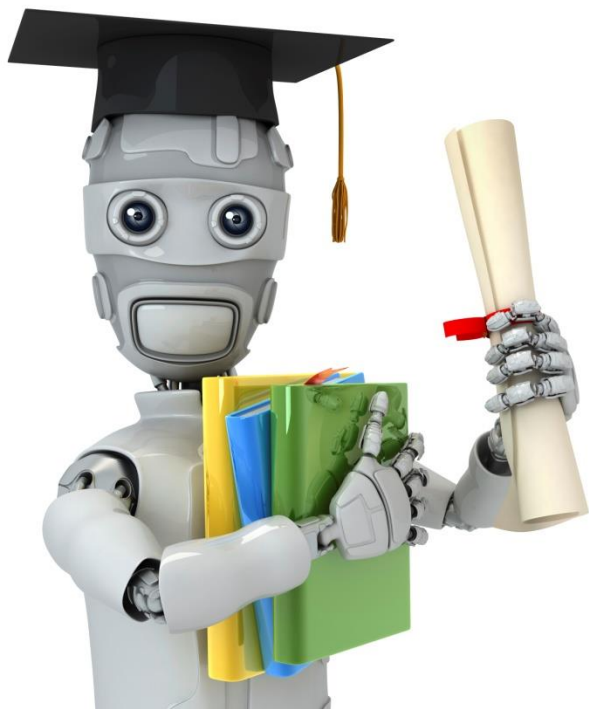
Bias/variance as a function of the regularization parameter λ

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

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

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





Machine Learning

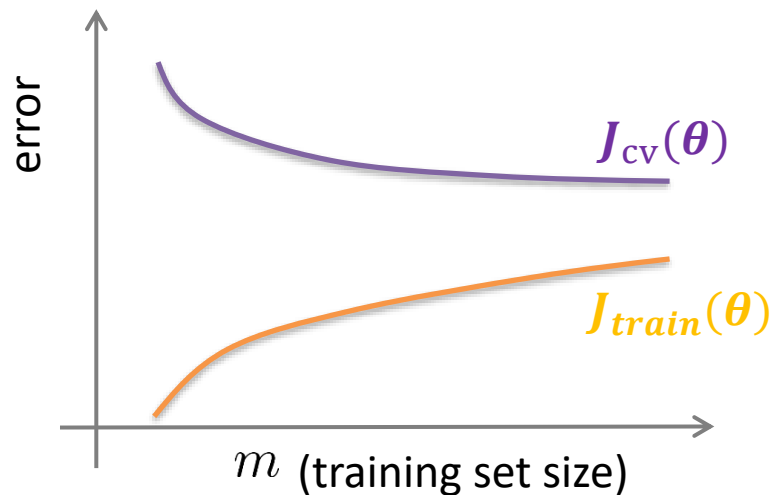
Advice for applying machine learning

Learning curves

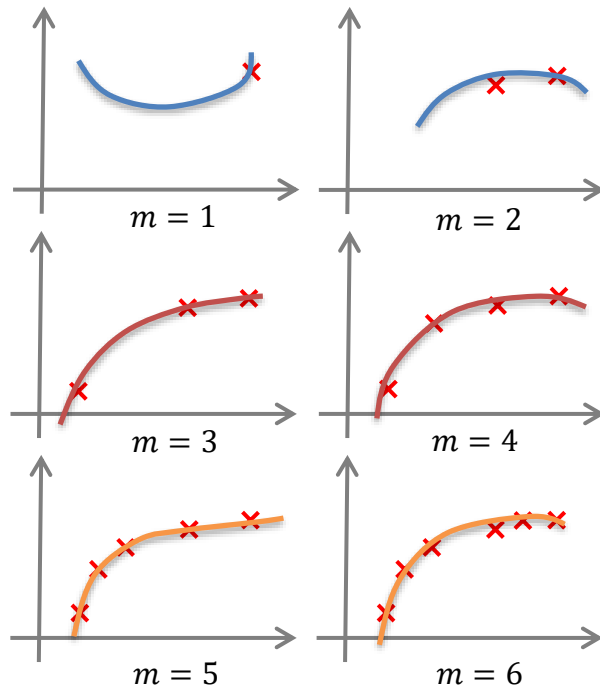
Learning curves

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

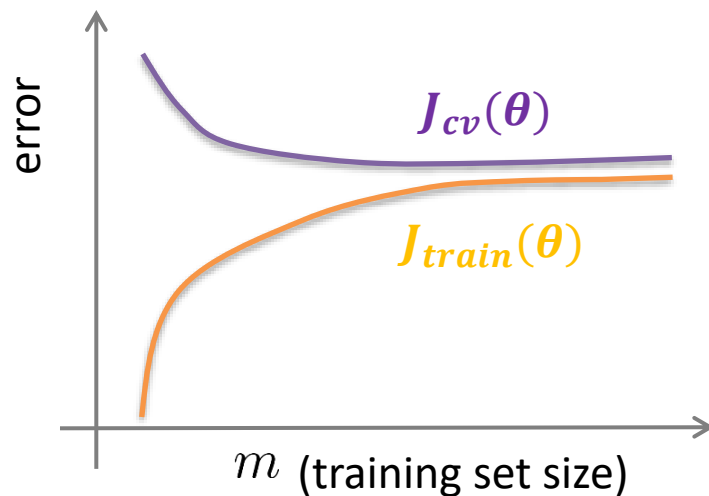
$$J_{cv}(\theta) = \frac{1}{2m_{cv}} \sum_{i=1}^{m_{cv}} (h_{\theta}(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$$



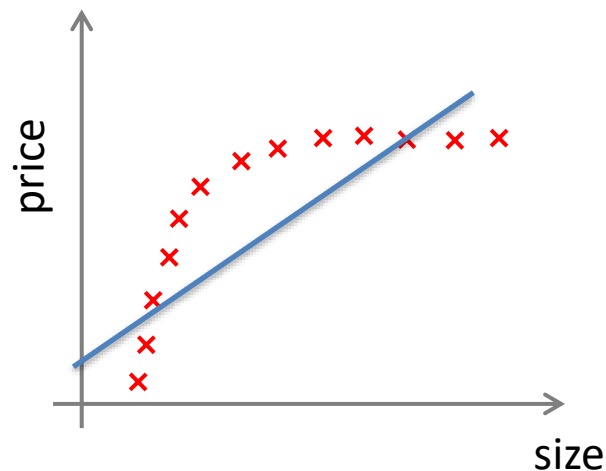
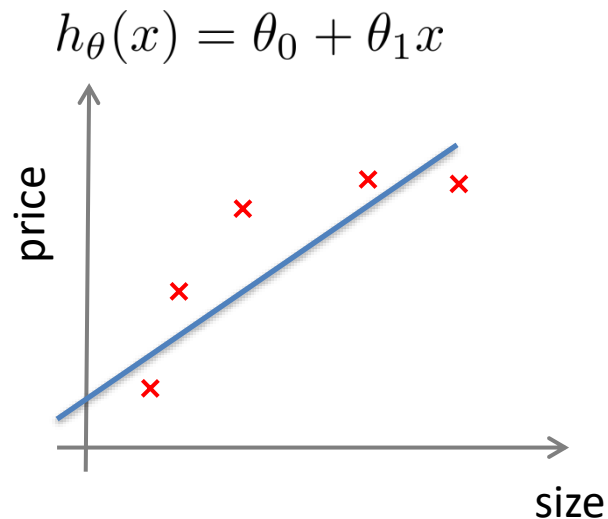
$$h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2$$



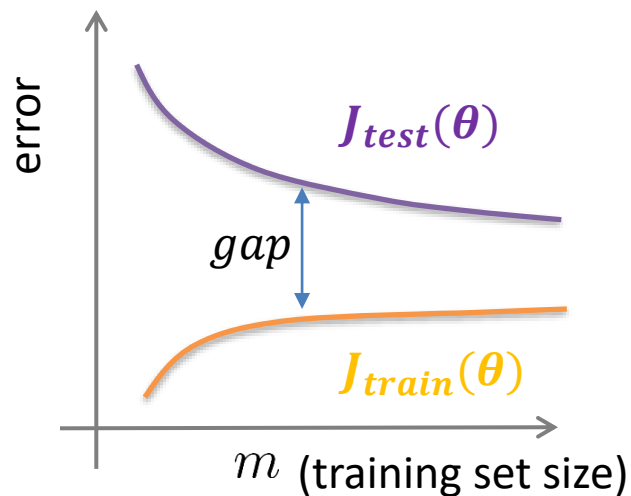
High bias



If a learning algorithm is suffering from high bias, getting more training data will not (by itself) help much.



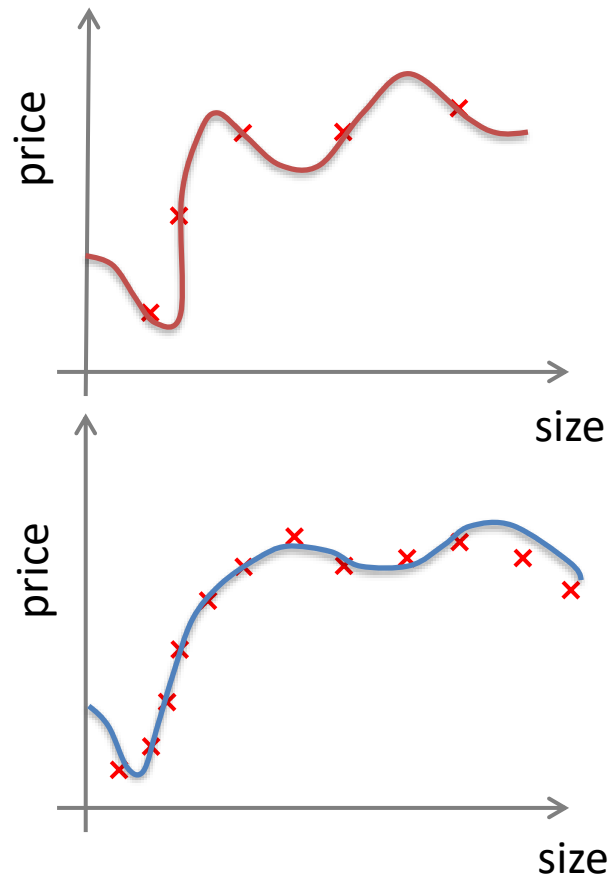
High variance



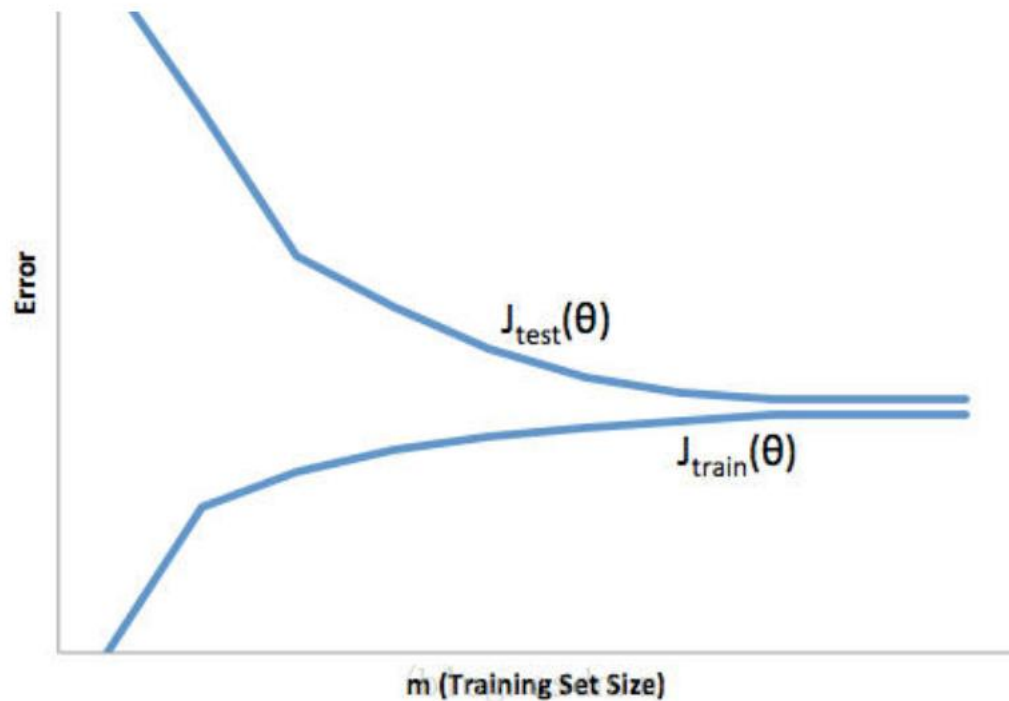
If a learning algorithm is suffering from high variance, getting more training data is likely to help.

$$h_{\theta}(x) = \theta_0 + \theta_1 x + \dots + \theta_{100} x^{100}$$

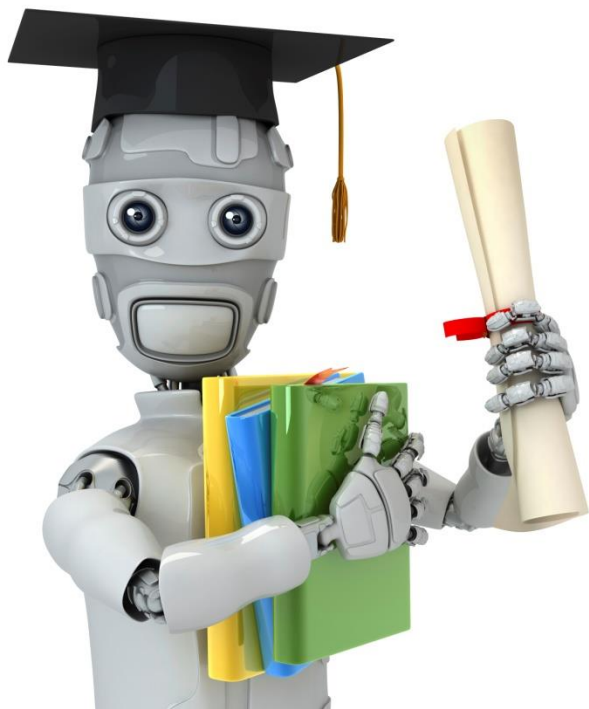
(and small λ)



你训练一个学习算法，发现它在测试集上的误差很高。绘制学习曲线，并获得下图。算法是否存在高偏差、高方差或两者都不存在？



A. 高偏差 B. 高方差 C. 两者都不



Machine Learning

Advice for applying machine learning

Deciding what to try next (revisited)

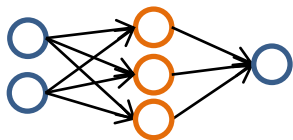
Debugging a learning algorithm:

Suppose you have implemented regularized linear regression to predict housing prices. However, when you test your hypothesis in a new set of houses, you find that it makes unacceptably large errors in its prediction. What should you try next?

- Get more training examples \rightarrow *fixes high variance*
- Try smaller sets of features \rightarrow *fixes high variance*
- Try getting additional features \rightarrow *fixes high bias*
- Try adding polynomial features (x_1^2, x_2^2, x_1x_2 , etc) \rightarrow *fixes high bias*
- Try decreasing λ \rightarrow *fixes high bias*
- Try increasing λ \rightarrow *fixes high variance*

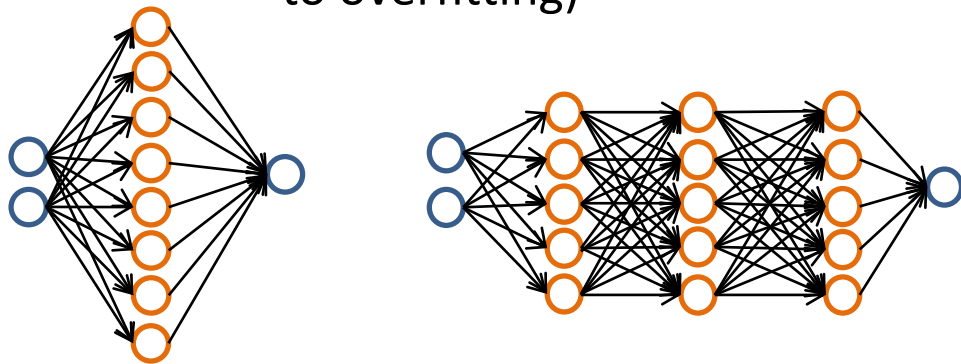
Neural networks and overfitting

“Small” neural network
(fewer parameters; more
prone to underfitting)



Computationally cheaper

“Large” neural network
(more parameters; more prone
to overfitting)



Computationally more expensive.

Use regularization (λ) to address overfitting.