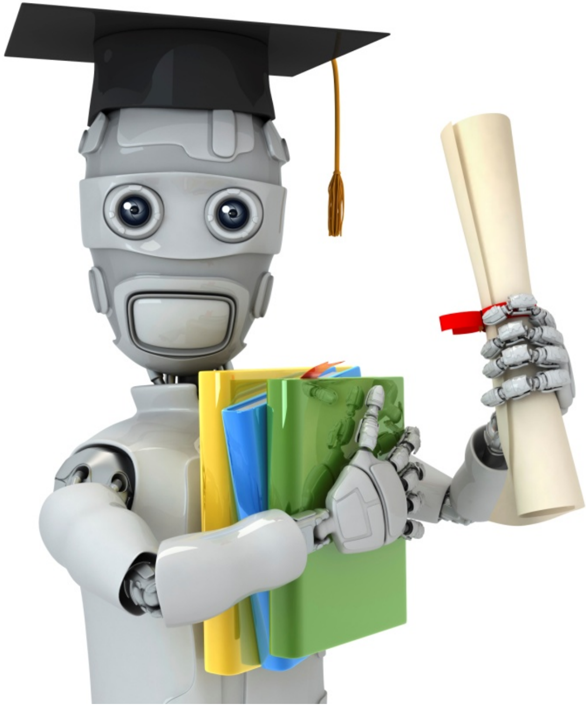


Machine Learning

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.

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

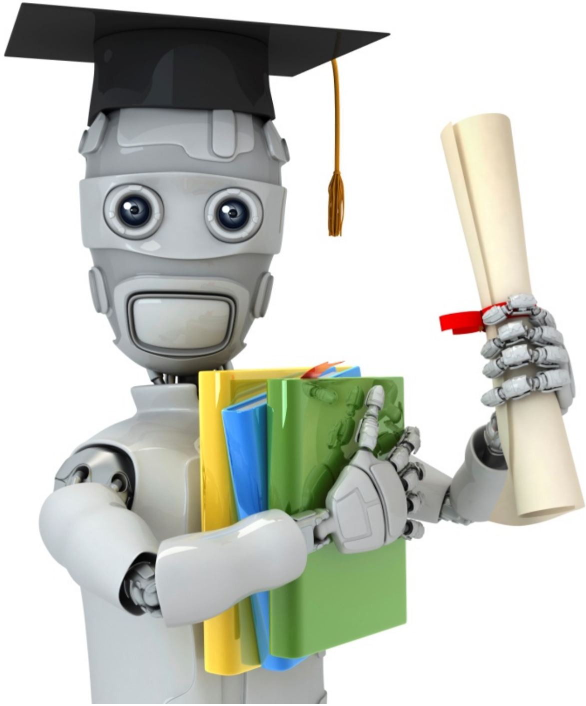
However, when you test your hypothesis on a new set of houses, you find that it makes unacceptably large errors in its predictions. What should you try next?

- Get more training examples
- Try smaller sets of features $x_1, x_2, x_3, \ldots, x_{100}$
- Try getting additional features
- Try adding polynomial features $(x_1^2, x_2^2, x_1x_2, \text{etc.})$
- 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.

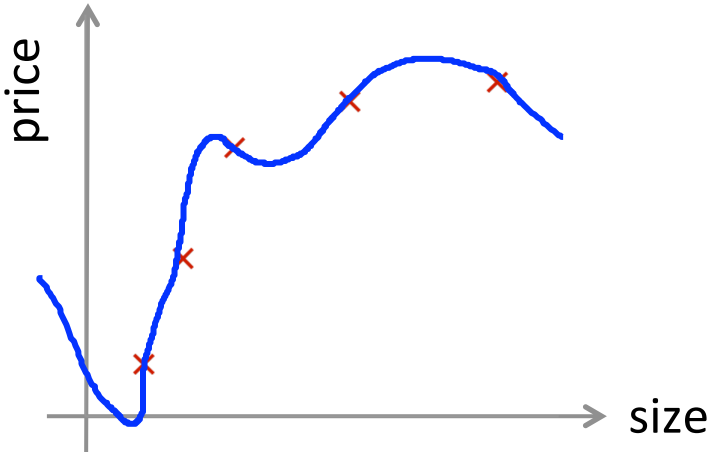


Machine Learning

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: best are randomly distributed

Size	Price
2104	400
1600	330
2400	369
1416	232
3000	540
1985	300
1534	315
1427	199
1380	212
1494	243

70%

Training set

30%

Test set

$$(x^{(1)}, y^{(1)})$$
$$(x^{(2)}, y^{(2)})$$
$$\vdots$$
$$(x^{(m)}, y^{(m)})$$

$$(x^{(1)}_{test}, y^{(1)}_{test})$$
$$(x^{(2)}_{test}, y^{(2)}_{test})$$
$$\vdots$$
$$(x^{(m_{test})}_{test}, y^{(m_{test})}_{test})$$

m_{test} = no. of test example

$(x^{(i)}_{test}, y^{(i)}_{test})$

Andrew Ng

Training/testing procedure for linear regression

- Learn parameter θ from training data (minimizing training error $J(\theta)$)

70%

- Compute test set error:

$$J_{test}(\theta) = \frac{1}{2m_{test}} \sum_{i=1}^{m_{test}} \left(h_\theta(x^{(i)}_{test}) - y^{(i)}_{test} \right)^2$$

Training/testing procedure for logistic regression

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

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

0: right model 1:wrong model

- Misclassification error (0/1 misclassification error):

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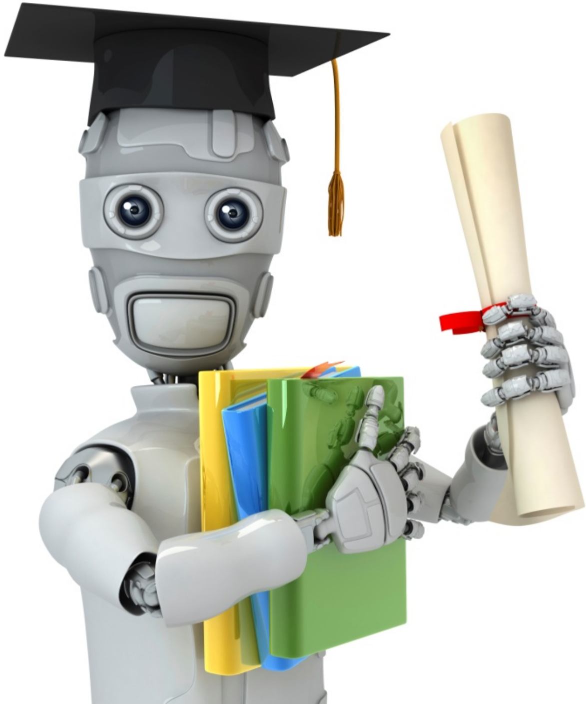
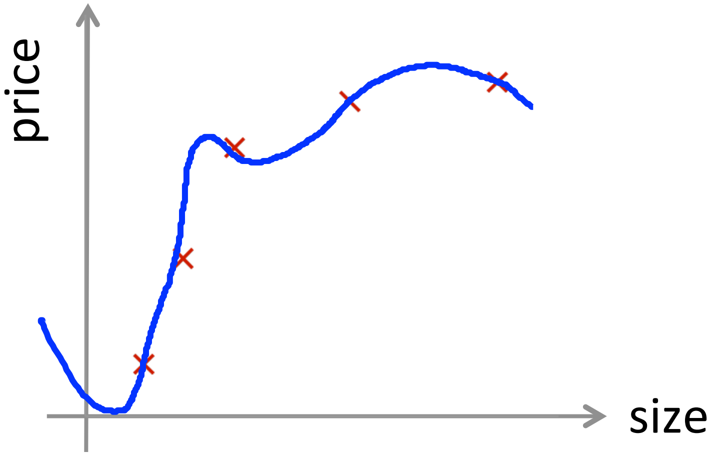


Machine Learning

Advice for applying machine learning

Model selection and training/validation/test sets

Overfitting example



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

Once parameters $\theta_0, \theta_1, \ldots, \theta_4$ 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.

d = degree of polynomial

Model selection

$d=1$ 1. $h_\theta(x) = \theta_0 + \theta_1 x$ $\rightarrow \Theta^{(1)} \rightarrow J_{test}(\Theta^{(1)})$

$d=2$ 2. $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2$ $\rightarrow \Theta^{(2)} \rightarrow J_{test}(\Theta^{(2)})$

$d=3$ 3. $h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_3 x^3$ $\rightarrow \Theta^{(3)} \rightarrow J_{test}(\Theta^{(3)})$

$\vdots$

$d=10$ 10. $h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_{10} x^{10}$ $\rightarrow \Theta^{(10)} \rightarrow J_{test}(\Theta^{(10)})$

Choose $\boxed{\theta_0 + \ldots \theta_5 x^5}$

$\boxed{\Theta_0, \Theta_1, \ldots}$

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

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.

Andrew Ng

Evaluating your hypothesis

Dataset:

Size	Price	
2104	400	Training set (60%)
1600	330	
2400	369	
1416	232	
3000	540	
1985	300	
1534	315	Cross validation set (CV) (20%)
1427	199	
1380	212	test set (20%)
1494	243	

$$(x^{(1)}, y^{(1)})$$
$$(x^{(2)}, y^{(2)})$$
$$\vdots$$
$$(x^{(m)}, y^{(m)})$$

$$(x_{cv}^{(1)}, y_{cv}^{(1)})$$
$$(x_{cv}^{(2)}, y_{cv}^{(2)})$$
$$\vdots$$
$$(x_{cv}^{(m_{cv})}, y_{cv}^{(m_{cv})})$$

m_{cv} = no. of cv example

$(x_{cv}^{(i)}, y_{cv}^{(i)})$

$$(x_{test}^{(1)}, y_{test}^{(1)})$$
$$(x_{test}^{(2)}, y_{test}^{(2)})$$
$$\vdots$$
$$(x_{test}^{(m_{test})}, y_{test}^{(m_{test})})$$

m_{test}

Train/validation/test error

One way to break down our dataset into the three sets is:

Training set: 60%
Cross validation set: 20%
Test set: 20%

Training error:

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

$J(\theta)$

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:

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

1. Optimize the parameters in theta using the training set for each polynomial degree.
2. Find the polynomial degree d with the least error using the cross validation set.
3. Estimate the generalization error using the test set with J_{test}(theta^{d}),(d = theta from polynomial with lower error);

Model selection according to the error of cross validation model

d=1 1. $h_\theta(x) = \theta_0 + \theta_1 x \longrightarrow \min_\theta J(\theta) \rightarrow \theta^{(1)} \rightarrow J_{cv}(\theta^{(1)})$

d=2 2. $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 \longrightarrow \theta^{(2)} \rightarrow J_{cv}(\theta^{(2)})$

d=3 3. $h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_3 x^3 \longrightarrow \theta^{(3)}$

$J_{cv}(\theta^{(4)})$

$\vdots$

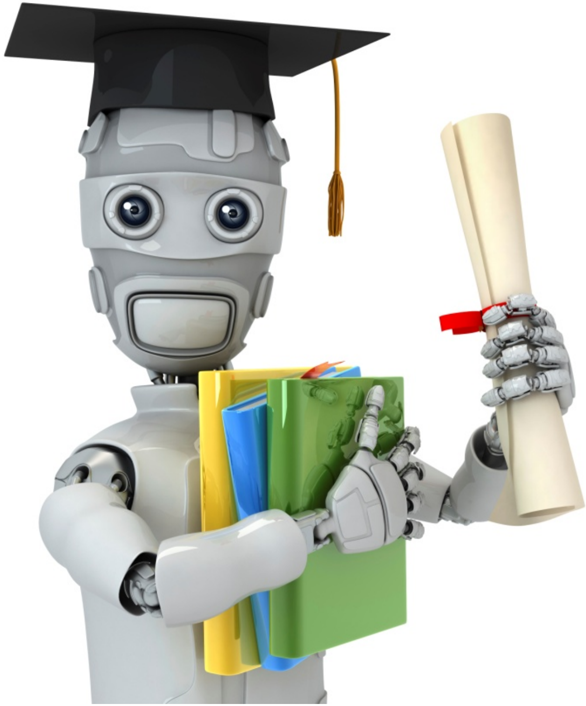
d=10 10. $h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_{10} x^{10} \longrightarrow \theta^{(10)} \rightarrow J_{cv}(\theta^{(10)})$

d=4

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

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

For the final model (with parameters \theta), we might generally expect J_{cv}(\theta) To be lower than J_{test}(\theta) because: An extra parameter (dd, the degree of the polynomial) has been fit to the cross validation set.



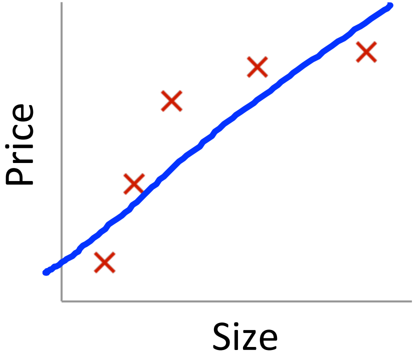
Machine Learning

Advice for applying machine learning

Diagnosing bias vs. variance

Bias/variance

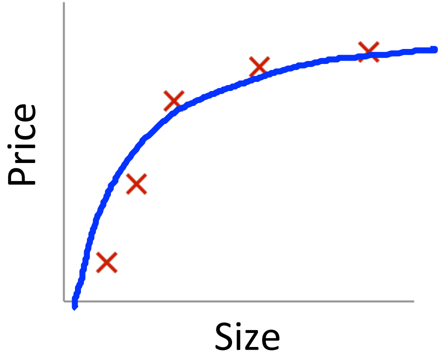
High bias is underfitting and high variance is overfitting.



$$\theta_0 + \theta_1 x$$

High bias
(underfit)

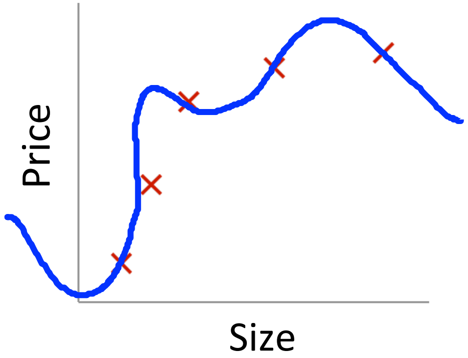
$d=1$



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

"Just right"

$d=2$



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

High variance
(overfit)

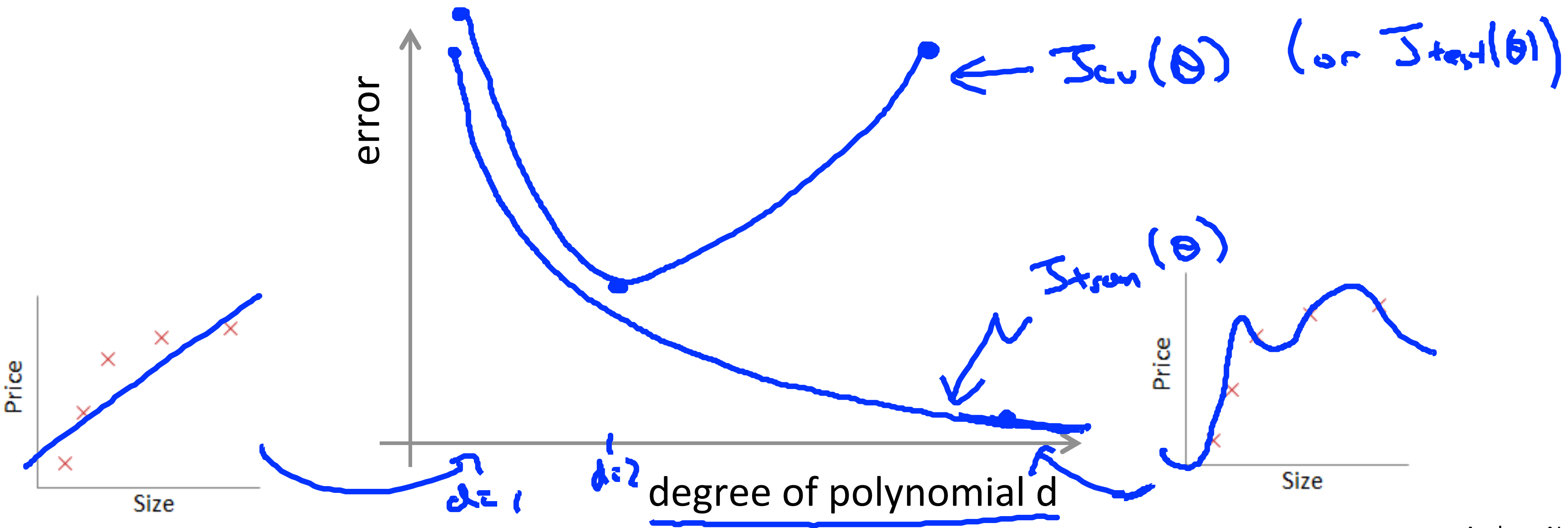
$d=4$

Bias/variance

The training error will tend to decrease as we increase the degree d of the polynomial.
At the same time, the cross validation error will tend to decrease as we increase d up to a point, and then it will increase as d is increased, forming a convex curve.

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 $J_{test}(\theta)$)



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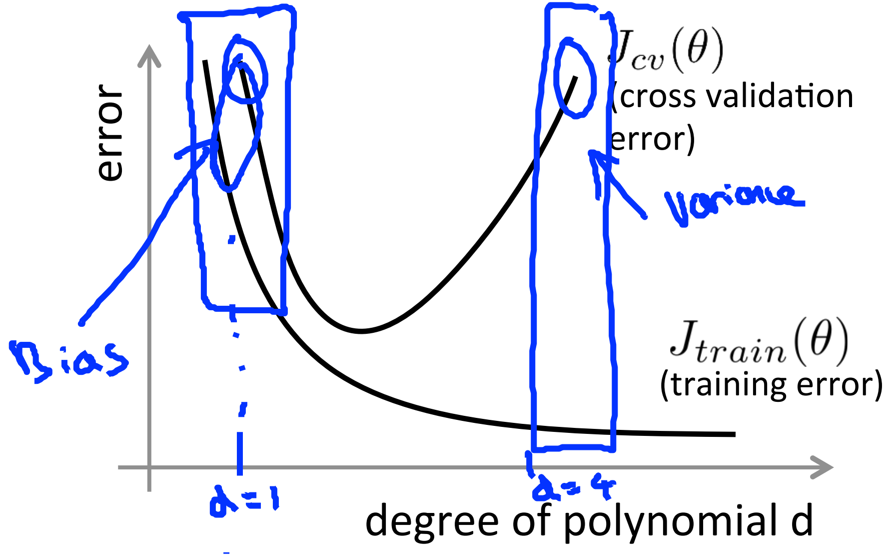
Diagnosing bias vs. variance

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

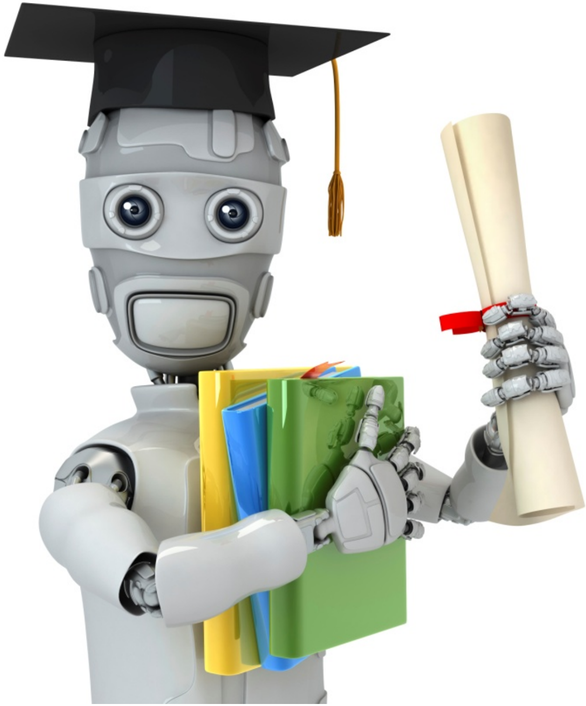
$J_{cv}(\theta) \approx J_{train}(\theta)$

Variance (overfit):

→ $J_{train}(\theta)$ will be low

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

$\gg$



Machine Learning

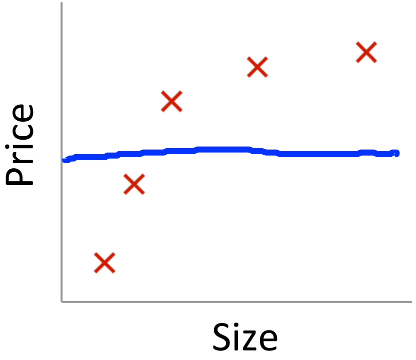
Advice for applying machine learning

Regularization and bias/variance

Linear regression with regularization

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

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

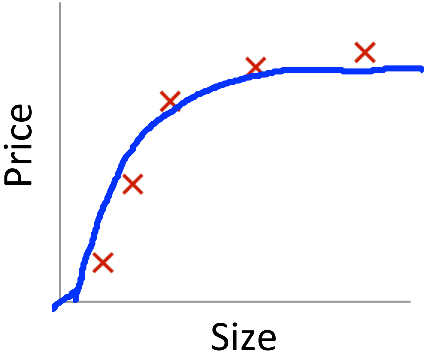


Large λ

High bias (underfit)

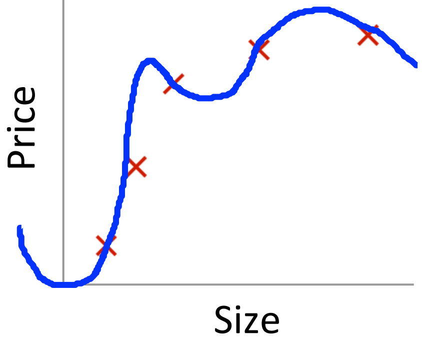
$\lambda = 10000.\ \theta_1 \approx 0, \theta_2 \approx 0, \ldots$

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



Intermediate λ

"Just right"



Small λ

High variance (overfit)

$\lambda = 0$

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Choosing the regularization parameter λ

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

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

$J(\theta)$

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

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

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

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

$\vdots$

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

0.24

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

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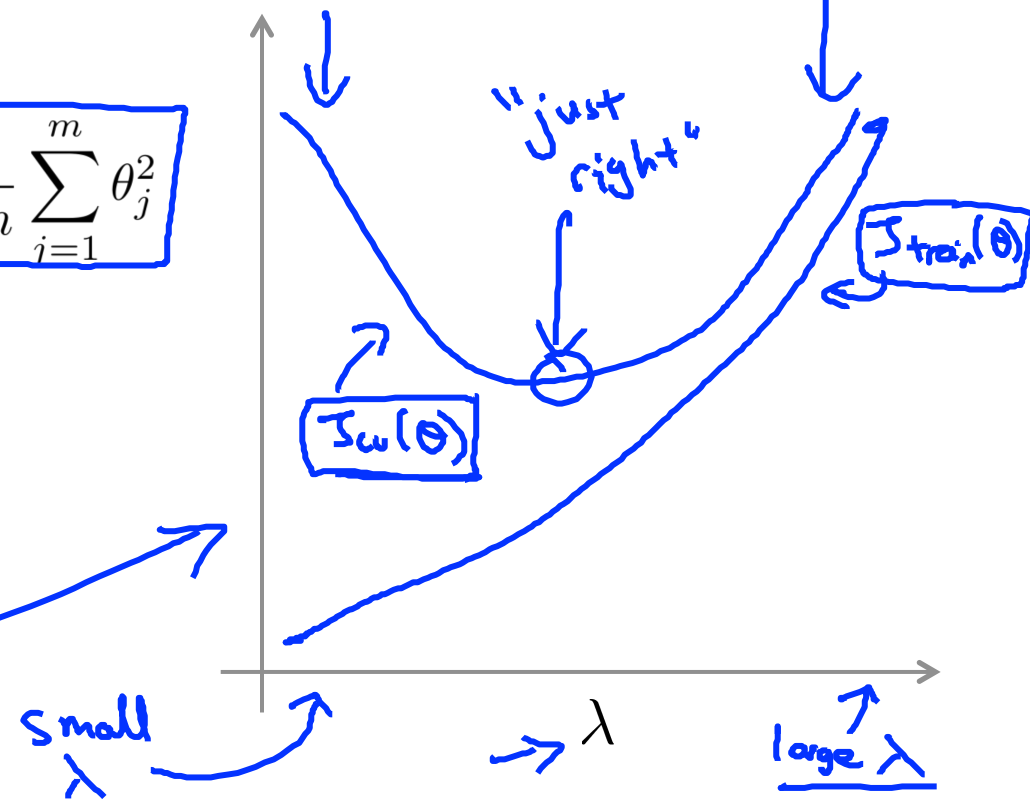
Bias/variance as a function of the regularization parameter λ

when lambda is small, cost function likely to cause overfit, so training error should be small, but cross validation error should be large.
when lambda is large, cost function likely to cause underfit, so training error should be large, but cross validation error should be also large.

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

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

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



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Machine Learning

Advice for applying machine learning

Learning curves

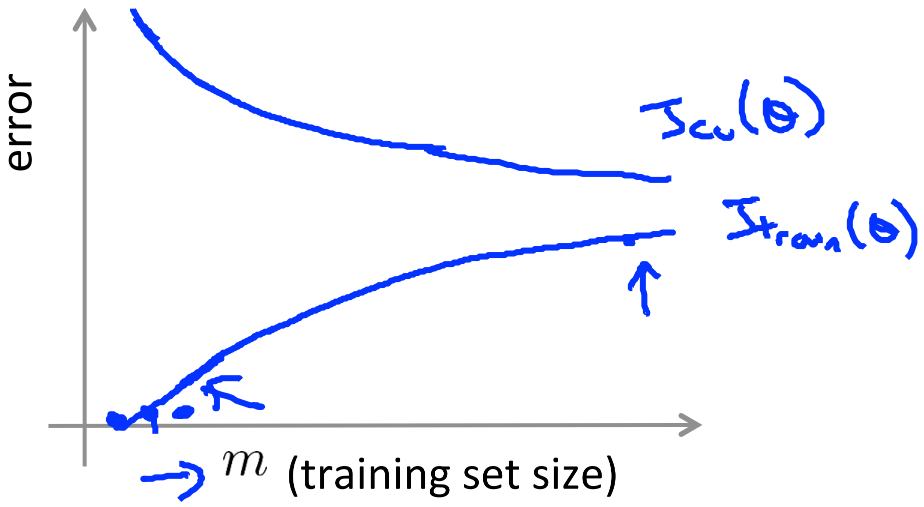
1. Lower-order polynomials (low model complexity) have high bias and low variance. In this case, the model fits poorly consistently.
2. Higher-order polynomials (high model complexity) fit the training data extremely well and the test data extremely poorly. These have low bias on the training data, but very high variance.
3. In reality, we would want to choose a model somewhere in between, that can generalize well but also fits the data reasonably well.

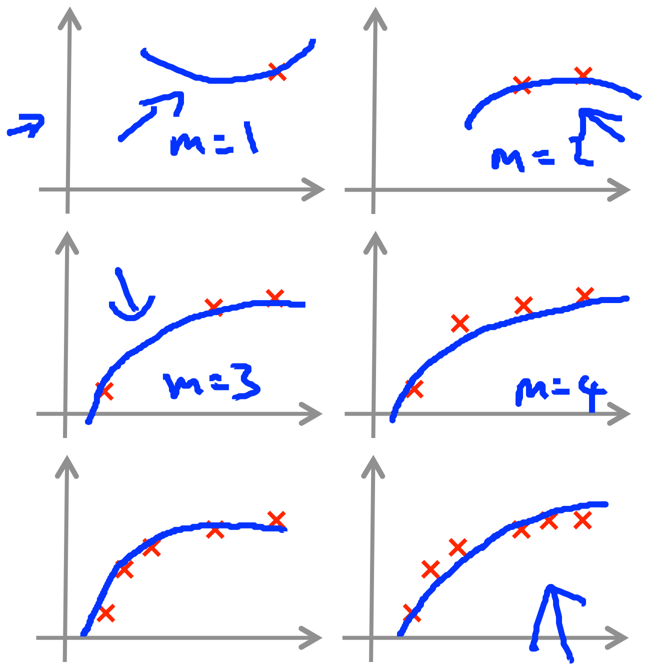
Learning curves

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

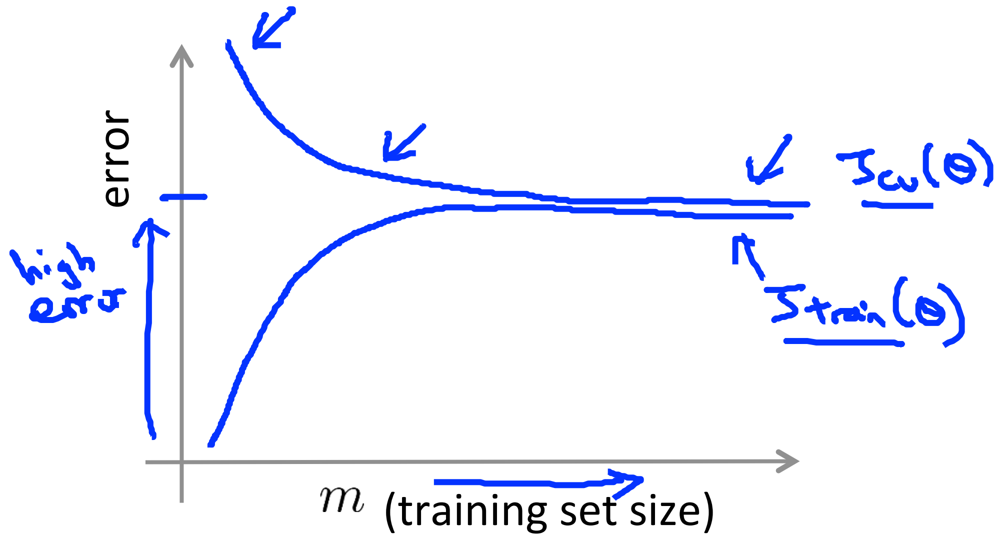
$$J_{train}(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

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



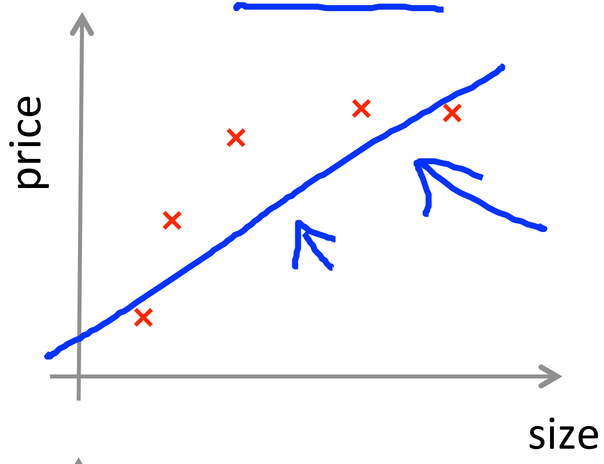


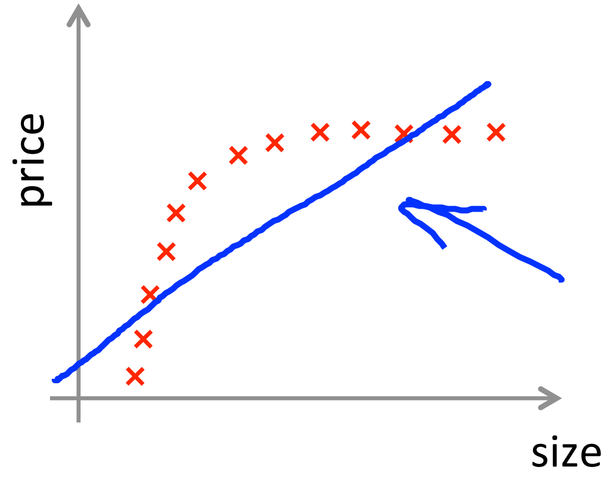
High bias underfit



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

$$h_\theta(x) = \theta_0 + \theta_1 x$$





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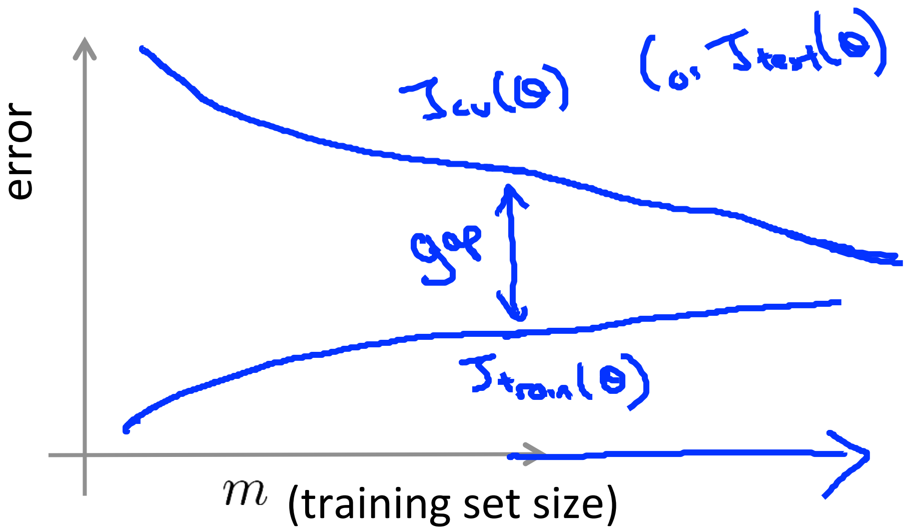
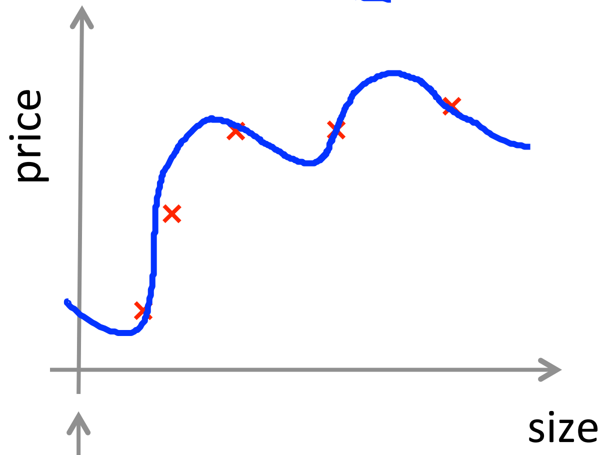
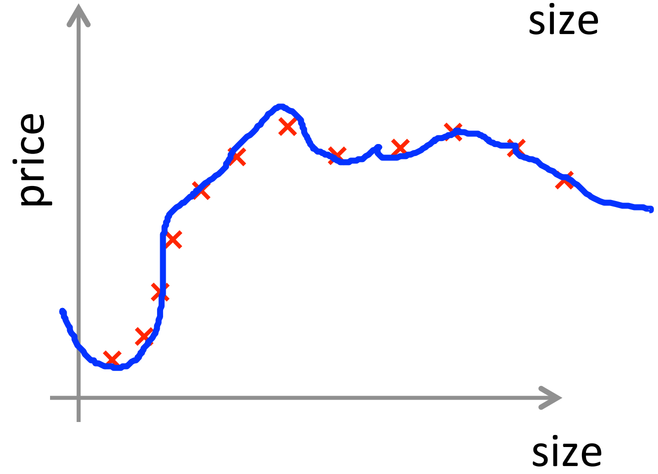
High variance overfit

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

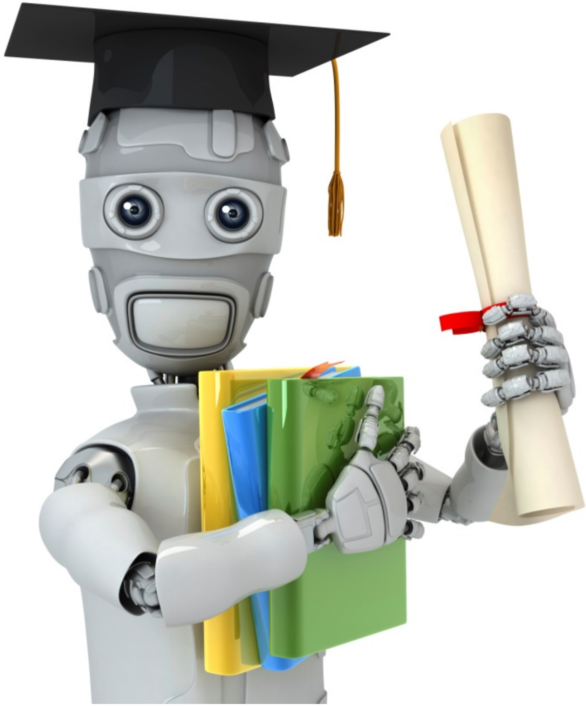
(and small λ)







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



Machine Learning

Advice for applying machine learning

Deciding what to try next (revisited)

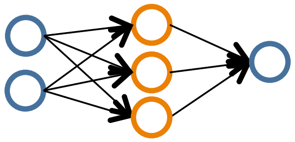
Debugging a learning algorithm:

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 → fixes high variance overfit
- Try smaller sets of features → fixes high variance overfit
- Try getting additional features → fixes high bias underfit
- Try adding polynomial features $(x_1^2, x_2^2, x_1x_2, \text{etc})$ → fixes high bias. underfit
- Try decreasing λ → fixes high bias underfit
- Try increasing λ → fixes high variance overfit

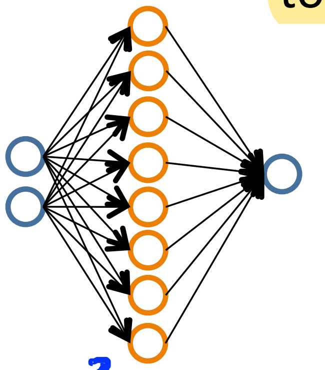
Neural networks and overfitting

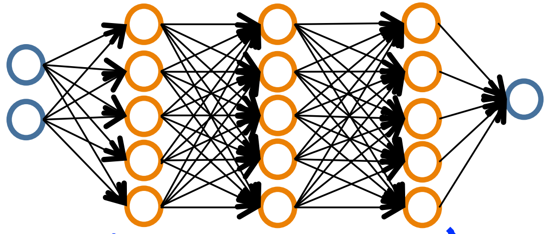
"Small" neural network
(fewer parameters; more prone to underfitting)



Computationally cheaper

"Large" neural network
(more parameters; more prone to overfitting)





Computationally more expensive.

Use regularization (λ) to address overfitting.

$J_{cv}(\Theta)$