Advice for applying machine learning

1 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

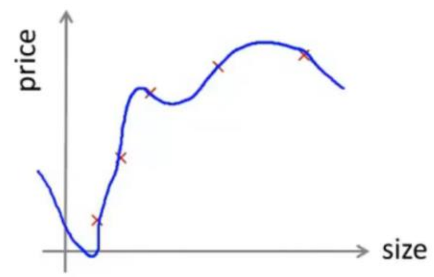
Machine learning diagnostic:

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.

2 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:

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

30% Test set → $(x^{(1)}_{test}, y^{(1)}_{test})$, $(x^{(2)}_{test}, y^{(2)}_{test})$, $\vdots$, $(x^{(m_{test})}_{test}, y^{(m_{test})}_{test})$

m_{test} = no. of test example

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

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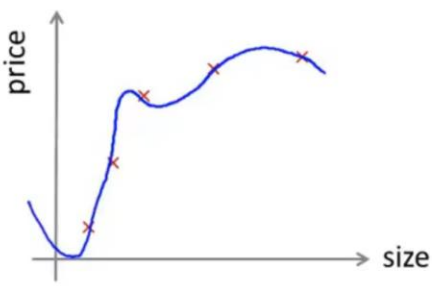
Training/testing procedure for linear regression

- Learn parameter θ from training data (minimizing training error $J(\theta)$) 70%
- Compute test set error:

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

3 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.

Model selection

d = degree of polynomial

$d=1$ 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.

Evaluating your hypothesis

Dataset:

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

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Train/validation/test error

Training error:

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

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:

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

Model selection

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

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

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

$\vdots$ $\quad J_{cv}(\Theta^{(4)})$

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

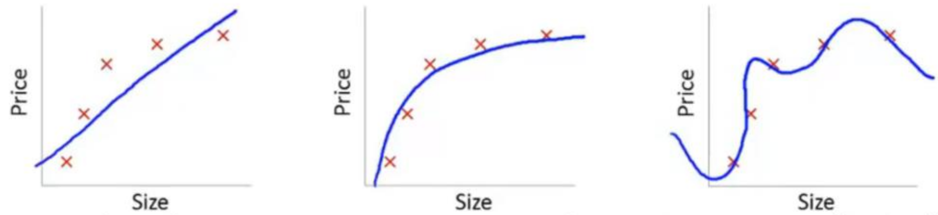
$\underline{d=4}$

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

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

4 Diagnosing bias vs. variance

Bias/variance

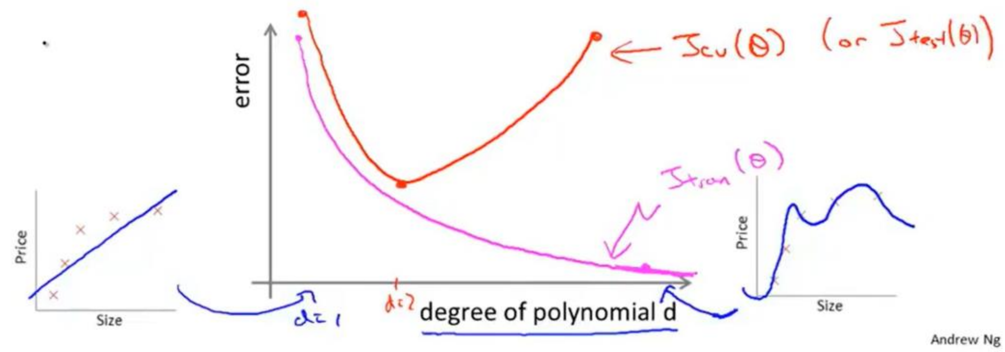


$\theta_0+\theta_1 x$	$\theta_0+\theta_1 x+\theta_2 x^2$	$\theta_0+\theta_1 x+\theta_2 x^2+\theta_3 x^3+\theta_4 x^4$
High bias (underfit)	"Just right"	High variance (overfit)
d=1	d=2	d=4

Bias/variance

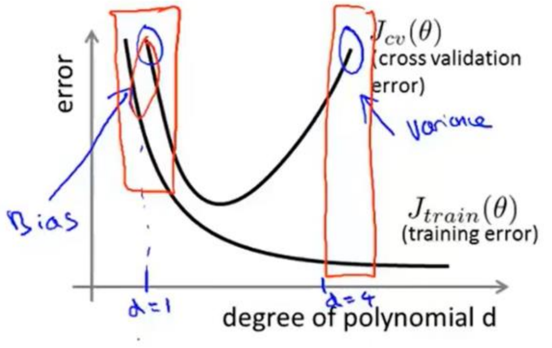
Training error: $\underline{J_{train}(\theta)}=\frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)})-y^{(i)})^2$

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



Bias (underfit):
→ $J_{train}(\theta)$ will be high
$J_{cv}(\theta) \approx J_{train}(\theta)$

Variance (overfit):
→ $J_{train}(\theta)$ will be low
$J_{cv}(\theta) \gg J_{train}(\theta)$

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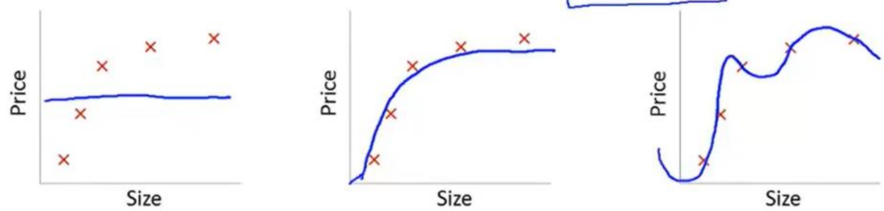
5 Regularization and bias/variance

Linear regression with regularization

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

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



Large λ ← | Intermediate λ ← | → Small λ

→ High bias (underfit) | "Just right" | High variance (overfit)

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

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

→ $\lambda = 0$

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Choosing the regularization parameter λ

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

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

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

J(θ)

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

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

Jtrain
Jcv
Jtest

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

⋮

12. Try $\lambda = 10$ → $\Theta^{(12)}$ → $J_{cv}(\Theta^{(12)})$

10.24

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

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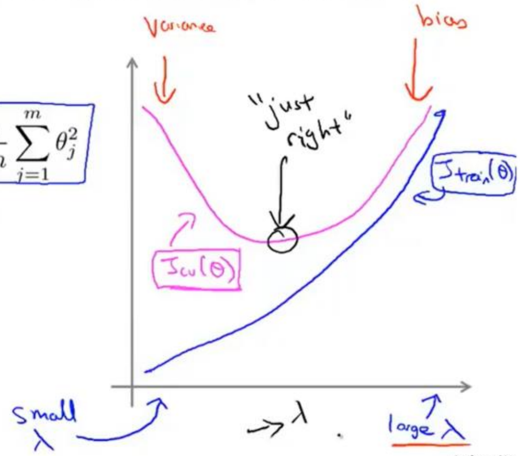
Bias/variance as a function of the regularization parameter λ

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

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

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



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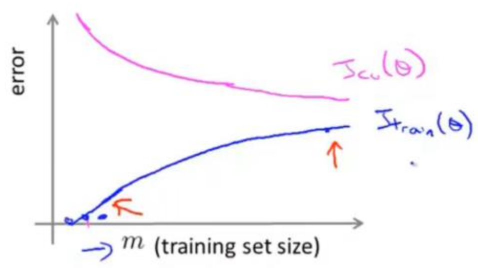
6 Learning curves

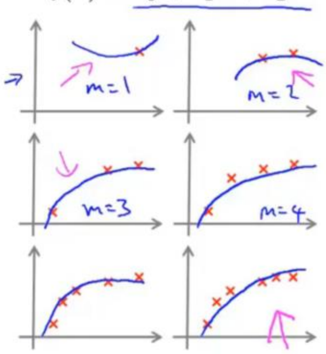
Learning curves

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

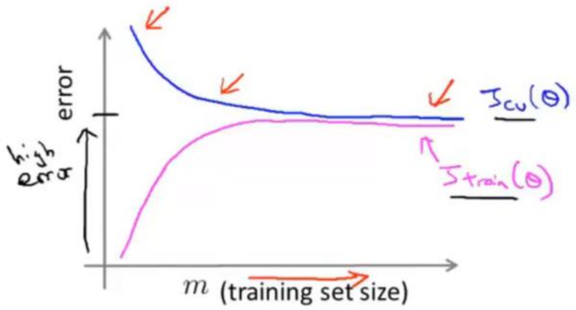
$$\to J_{cv}(\theta) = \frac{1}{2m_{cv}}\sum_{i=1}^{m_{cv}}(h_\theta(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$$



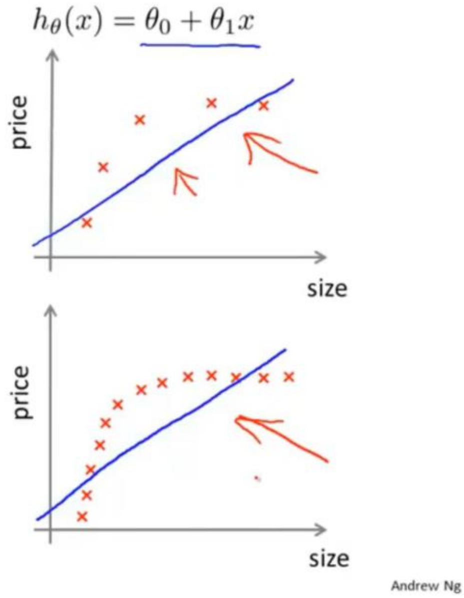
$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2$



High bias



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



7 Deciding what to try next(revisited)

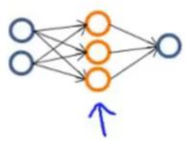
Debugging a learning algorithm:

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

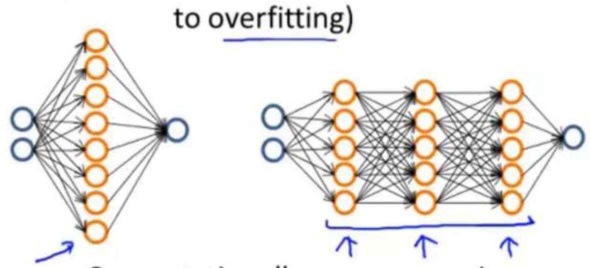
Neural networks and overfitting

→ "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.

$J_{cv}(\Theta)$