Model Selection and Train/Validation/Test Sets

Evaluating a Learning Algorithm

Advice for Applying Machine Learning

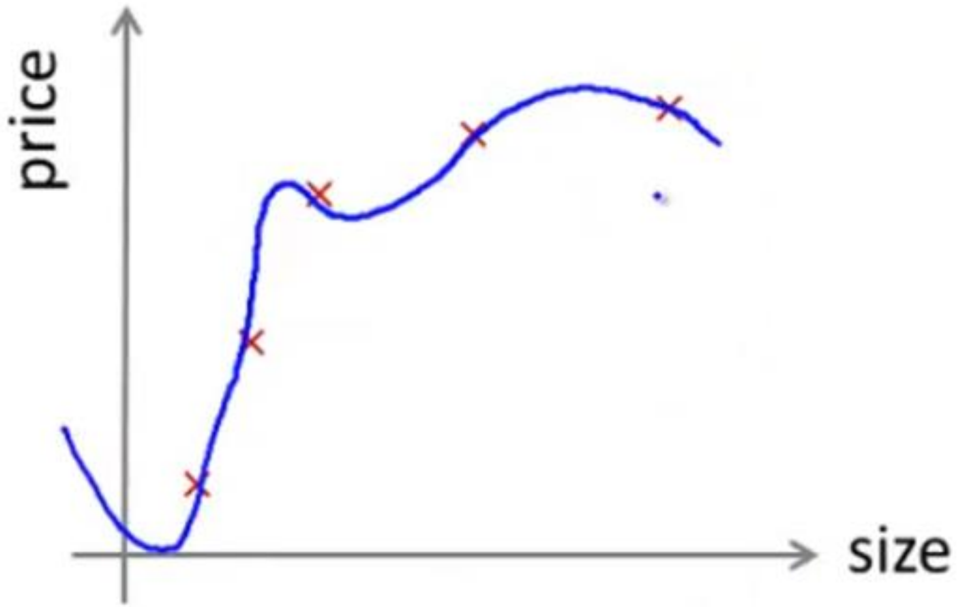
Introduction

- Suppose you are left to decide what degree of polynomial to fit to a data set.
- So that what features to include that gives you a learning algorithm.
- Or suppose you'd like to choose the regularization parameter lambda for learning algorithm
- These are called model selection problems.

Introduction

- We've already seen a lot of times the problem of overfitting, in which just because a learning algorithm fits a training set well, that doesn't mean it's a good hypothesis.
- More generally, this is why the training set's error is not a good predictor for how well the hypothesis will do on new example.

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

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. $h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_{10} x^{10}$

d = degree of polynomial

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. $h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_{10} x^{10}$

d = degree of polynomial

Model selection

$d=1$ 1. $\rightarrow h_\theta(x) = \theta_0 + \theta_1 x$

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

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

$\vdots$ $\quad\vdots$

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

d = degree of polynomial

Model selection

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

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

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

$\vdots$ $\quad\vdots$

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

d = degree of polynomial

Model selection

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

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

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

$\vdots$ $\qquad \vdots$ $\qquad \vdots$

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

d = degree of polynomial

Model selection

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

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

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

$\vdots$ $\vdots$ $\vdots$

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

Choose $\theta_0 + \ldots \theta_5 x^5 \longleftarrow$

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

d = degree of polynomial

Model selection

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

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

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

$\vdots$ $\vdots$ $\vdots$

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

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.

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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

Evaluating your hypothesis

Dataset:

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

Evaluating your hypothesis

Dataset:

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

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

60% Training set

20% Cross validation set (CV)

20% test set

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

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

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:

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

$J(\theta)$

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

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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. $h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_{10} x^{10}$

Model selection

1. $h_\theta(x) = \theta_0 + \theta_1 x \longrightarrow \min_\theta J(\theta) \rightarrow \Theta^{(1)}$
2. $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 \longrightarrow \Theta^{(2)}$
3. $h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_3 x^3 \longrightarrow \Theta^{(3)}$

$\vdots$

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

Find theta's using the test set, i.e., find theta that minimizes the error of the test set.

Model selection

1. $h_\theta(x) = \theta_0 + \theta_1 x \longrightarrow \min_\theta J(\theta) \rightarrow \Theta^{(1)} \rightarrow J_{cv}(\Theta^{(1)})$
2. $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 \longrightarrow \Theta^{(2)} \rightarrow J_{cv}(\Theta^{(2)})$
3. $h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_3 x^3 \longrightarrow \Theta^{(3)}$

$\vdots$

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

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

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

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

$\vdots$

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

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

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

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

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

$\vdots$

$d=10$ 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 $\theta_0 + \theta_1 x_1 + \cdots + \theta_4 x^4 \Leftarrow$

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

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- Consider the model selection procedure where we choose the degree of polynomial using a cross validation set. For the final model (with parameters θ), we might generally expect $\mathrm{J}_{\mathrm{CV}}(\theta)$ to be lower than $\mathrm{J}_{\mathrm{test}}(\theta)$
    - An extra parameter (d, the degree of the polynomial) has been fit to the cross validation set.
    - An extra parameter (d, the degree of the polynomial) has been fit to the test set.
    - The cross validation set is usually smaller than the test set.
    - The cross validation set is usually larger than the test set.