Machine Learning and Data Analytics
ME 5013- Fall 2019

Lectures 13

- Regularization

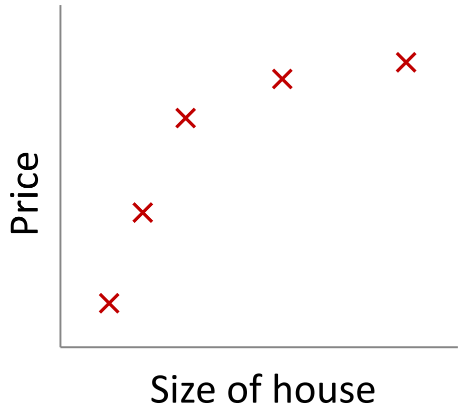
UTSA
The University of Texas at San Antonio™

Adel Alaeddini, PhD
Associate Professor of Mechanical Engineering
Advanced Data Engineering Lab
adel.alaeddini@utsa.edu

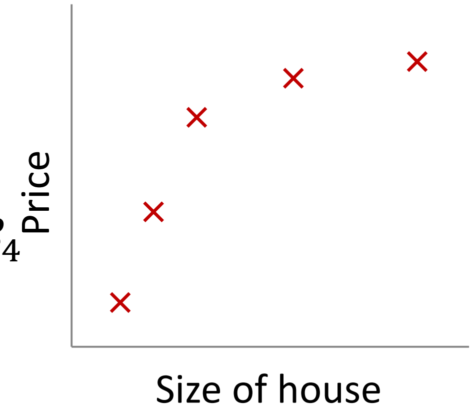
Disclosure: the slides are adopted from various online resources

Keep all the features, but reduce magnitude/values of parameters

Works well when we have a lot of features, each of which contributes a bit to predicting



$$h_\beta(x) = \beta_0 + \beta_1 x + \beta_2 x^2$$



β_3, β_4

$$h_\beta(x) = \beta_0 + \beta_1 x + \cdots + \beta_4 x^4$$

Suppose we penalize and make β_3, β_4 really small.

$$\min_\beta \frac{1}{2n} \sum_{i=1}^{n} \left(y^{(i)} - h_\beta\left(x^{(i)}\right)\right)^2$$

Regularization

Small values for parameters $\beta_0, \beta_4, \ldots, \beta_p$

- "Simpler" hypothesis
- Less prone to overfitting

Housing:

- Features: $x_1, x_2, \ldots, x_{100}$
- Parameters: $\beta_0, \beta_4, \ldots, \beta_{100}$

Regression Problem

$$J(\beta) = \frac{1}{2n}\sum_{i=1}^{n}\left(y^{(i)} - h_\beta\left(x^{(i)}\right)\right)^2$$

$$J(\beta) = \frac{1}{2n}\left[\sum_{i=1}^{n}\left(y^{(i)} - h_\beta\left(x^{(i)}\right)\right)^2 + \lambda \underbrace{\sum_{j=1}^{p}\beta_j^2}_{\text{Regularization term}}\right]$$

$$\min_{\beta} J(\beta)$$

Regularization/Tuning parameter

Multiple Linear Regression

$$\mathrm{RSS} = \sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2$$

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}\beta_j^2 = \mathrm{RSS} + \lambda\sum_{j=1}^{p}\beta_j^2.$$

The tuning parameter serves to control the relative impact of the two terms on the regression coefficient estimates.

Regularized linear regression

Hypothesis: $h_\beta(x) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$

Cost Function: $J(\beta) = \frac{1}{2n}\left[\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_1^{(i)} - \cdots - \beta_p x_p^{(i)})^2 + \lambda \sum_{j=1}^{p} \beta_{j=1}^2\right]$

Parameters: $\beta_0, \beta_1, \ldots, \beta_p$

$\min_\beta \mathrm{J}(\beta)$

Gradient descent:

Repeat until convergence{

$\beta_0 := \beta_0 + \alpha \frac{1}{n}\left[\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_1^{(i)} - \cdots - \beta_p x_p^{(i)})\right]$

$\beta_1 := \beta_1 + \alpha \frac{1}{n}\left[\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_1^{(i)} - \cdots - \beta_p x_p^{(i)})\, x_1^{(i)} - \lambda\beta_1\right]$

…

$\beta_p := \beta_p + \alpha \frac{1}{n}\left[\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_1^{(i)} - \cdots - \beta_p x_p^{(i)})\, x_p^{(i)} - \lambda\beta_p\right]$

}

NOTE:

$$\beta_p := \beta_p\left(1 - \alpha\frac{\lambda}{n}\right) + \alpha\frac{1}{n}\left[\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_1^{(i)} - \cdots - \beta_p x_p^{(i)})\, x_p^{(i)}\right]$$

Normal equation

$$\boxed{\mathbf{y} = \mathbf{X}\beta + \epsilon}$$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1\ p} \\ 1 & x_{21} & x_{22} & \cdots & x_{2\ p} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{n\ p} \end{bmatrix} \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{p+1} \end{bmatrix} \quad \epsilon = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

Multiple linear regression: $\beta = (X'X)^{-1}X'y$

Regularized multiple linear regression: $\beta = (X'X + \lambda I)^{-1}X'y$

where $I = \begin{bmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{bmatrix}_{(p+1)\times(p+1)}$

Non-invertibility

Suppose n<=p

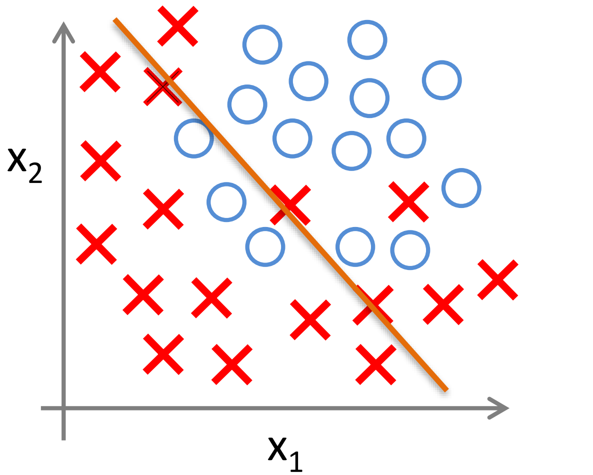
(#examples) (#features)

$$\beta = (X^T X)^{-1} X^T y$$

If $\lambda > 0$,

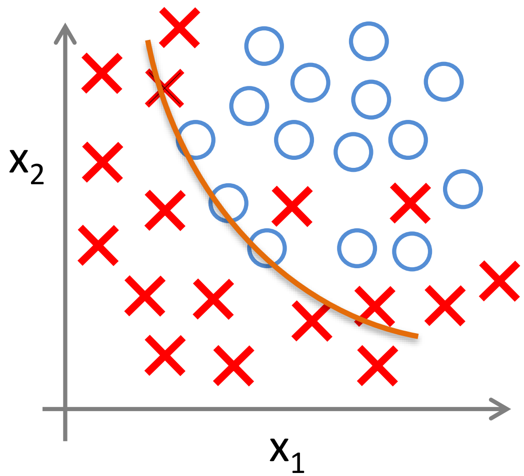
$$\beta = \left(X^T X + \lambda \begin{bmatrix} 0 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix} \right)^{-1} X^T y$$

Logistic regression

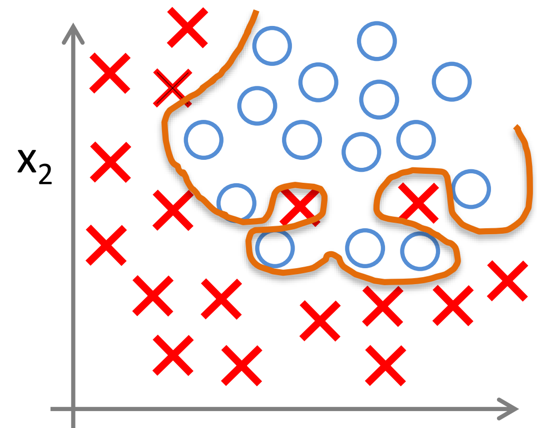


$$h_\beta(x) = g(\beta_0 + \beta_1 x_1 + \beta_2 x_2)$$

(g = sigmoid function)

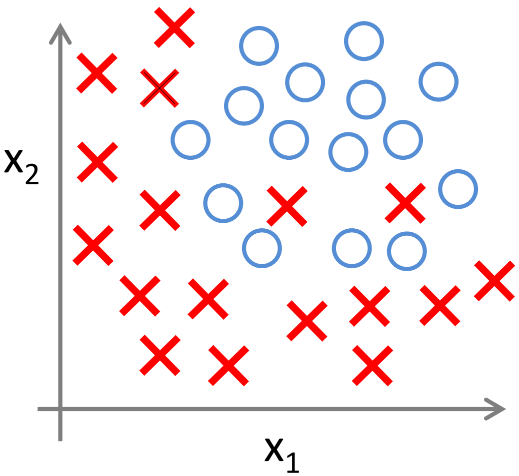


$$h_\beta(x)$$
$$= g(\beta_0 + \beta_1 x_1 + \beta_2 x_2$$



$$h_\beta(x)$$
$$= g(\beta_0 + \beta_1 x_1 + \beta_2 x_2$$
$$+ \beta_3 x_1^2 + \beta_4\, x_2^2$$

Regularized logistic regression.



Cost function:

$$J(\beta) = -\frac{1}{n}\left[\sum_{i=1}^{n} y^{(i)} \log h_\beta\left(x^{(i)}\right) + (1-y^{(i)}) \log\left(1 - h_\beta\left(x^{(i)}\right)\right)\right] + \frac{\lambda}{n}\sum_{j=1}^{p} \beta_j^2$$

Gradient Descent

$$J(\beta) = -\frac{1}{n}\left[\sum_{i=1}^{n} y^{(i)} \log h_\beta\left(x^{(i)}\right) + (1-y^{(i)}) \log\left(1-h_\beta\left(x^{(i)}\right)\right)\right] + \frac{\lambda}{n}\sum_{j=1}^{p} \beta_j^2$$

Want $\min_{\beta} J(\beta)$:

Repeat {

$$\beta_j := \beta_j - \alpha \frac{\partial}{\partial \beta_j} J(\beta_0, \beta_1) \quad \text{(for } j=0 \text{ and } j=1\text{)}$$

} (simultaneously update all parameters)

Closed form formula of the gradients

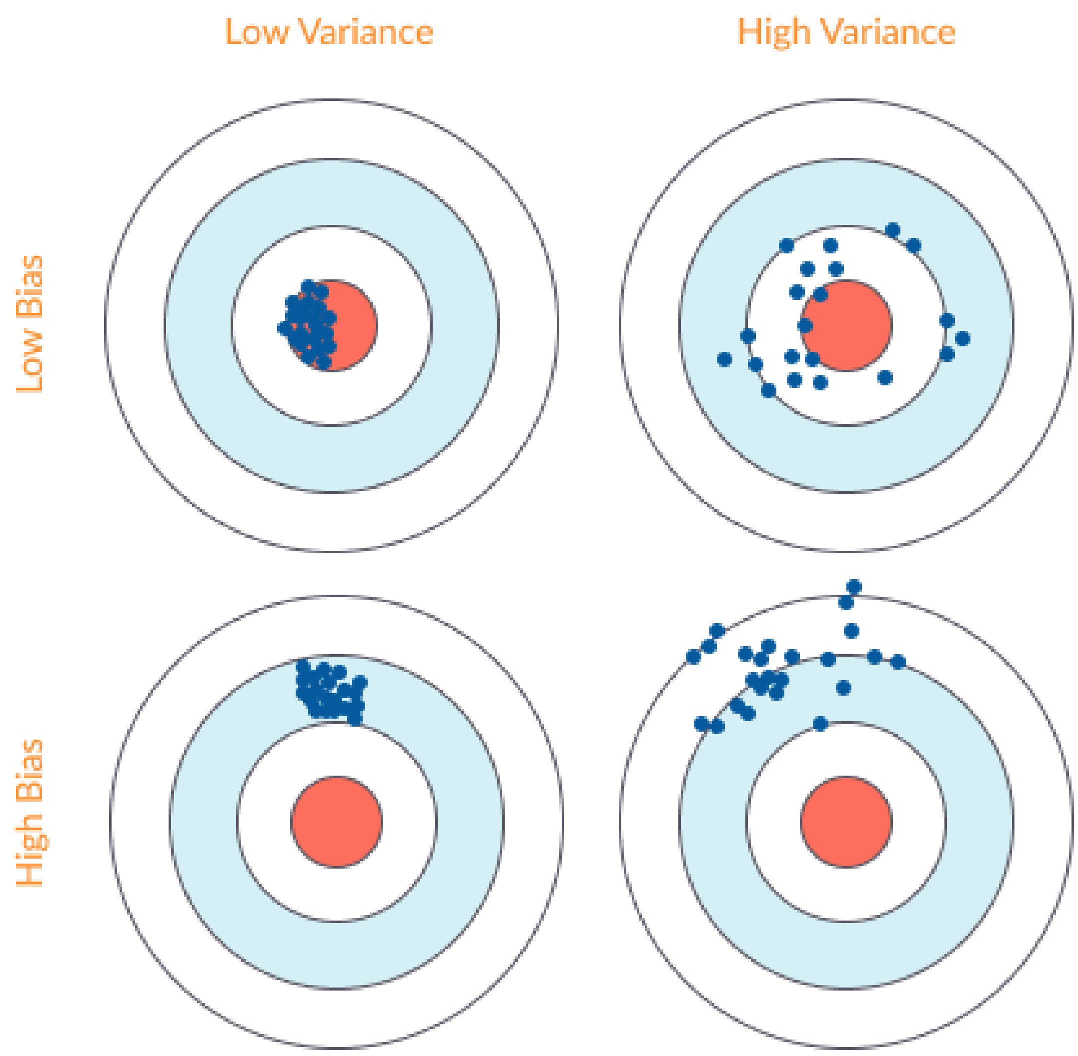
$$\beta_0 := \beta_0 + \alpha \frac{1}{n} \sum_{i=1}^{n} \left(y^{(i)} - h_\beta\left(x^{(i)}\right)\right) x^{(i)}$$

$$\beta_{j \neq 0} := \beta_j + \alpha \frac{1}{n} \sum_{i=1}^{n} \left(y^{(i)} - h_\beta\left(x^{(i)}\right)\right) x^{(i)} - \frac{\lambda}{n}\beta_j$$

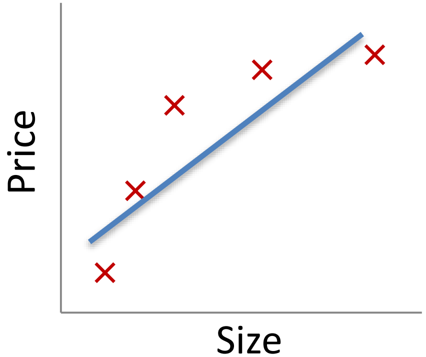
$$h_\beta(x) = \frac{1}{1+e^{-x\beta}}$$

$$x = [x_0 = 1 \quad x_1 \quad \ldots]$$

Bias vs. Variance

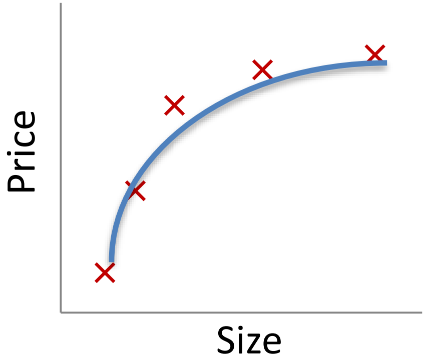


Bias/variance



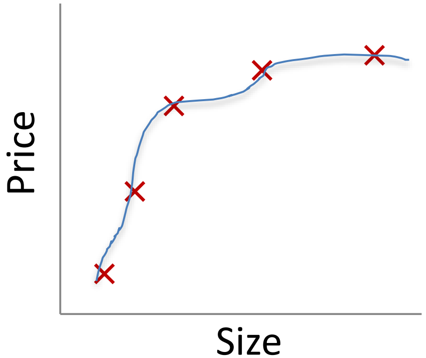
$$h_\beta(x) = \beta_0 + \beta_1 x$$

High bias
(underfit)



$$h_\beta(x) = \beta_0 + \beta_1 x + \beta_2 x^2$$

"Just right"



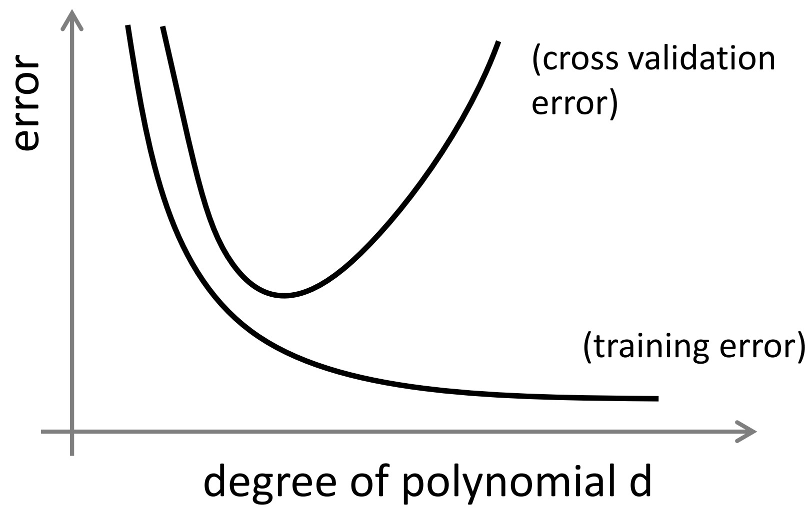
$$h_\beta(x) = \beta_0 + \beta_1 x + \cdots + \beta_4 x^4$$

High variance
(overfit)

Fail to generalize to new examples

Bias vs. Variance

Suppose your learning algorithm is performing less well than you were hoping. Is it a bias problem or a variance problem?



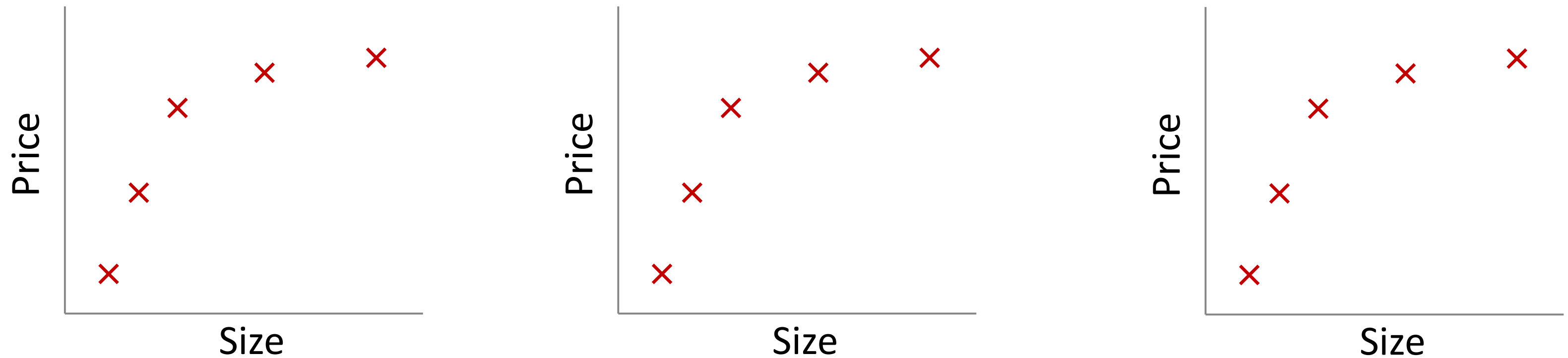
Bias (underfit):

Variance (overfit):

Regularization and bias/variance

Linear regression with regularization

$$J(\beta) = \frac{1}{2n}\left[\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_1^{(i)} - \cdots - \beta_p x_p^{(i)})^2 + \lambda \sum_{j=1}^{p} \beta_{j=1}^2\right]$$



Large λ
High bias (underfit)

Intermediate λ
"Just right"

Small λ
High variance (overfit)

Choosing the regularization parameter

$$h_\beta(x) = \beta_0 + \beta_1 x + \cdots + \beta_4 x^4$$

$$J(\beta) = \frac{1}{2n}\left[\sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_1^{(i)} - \cdots - \beta_p x_p^{(i)})^2 + \lambda \sum_{j=1}^{p} \beta_j^2\right]$$

$$J_{train}(\beta) = \frac{1}{2n_{train}} \sum_{i=1}^{n_{train}} (y_i - \beta_0 - \beta_1 x_1^{(i)} - \cdots - \beta_p x_p^{(i)})^2$$

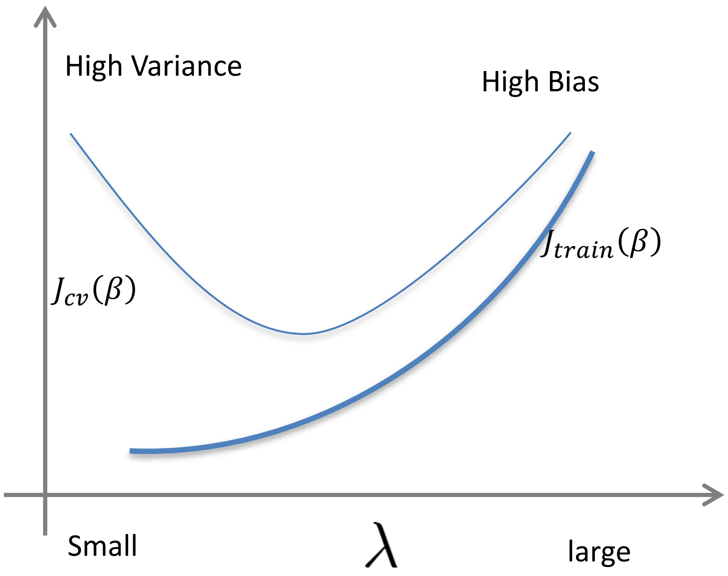
$$J_{cv}(\beta) = \frac{1}{2n_{cv}} \sum_{i=1}^{n_{cv}} (y_i - \beta_0 - \beta_1 x_1^{(i)} - \cdots - \beta_p x_p^{(i)})^2$$

$$J_{test}(\beta) = \frac{1}{2n_{test}} \sum_{i=1}^{n_{test}} (y_i - \beta_0 - \beta_1 x_1^{(i)} - \cdots - \beta_p x_p^{(i)})^2$$

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 $\lambda = 10$

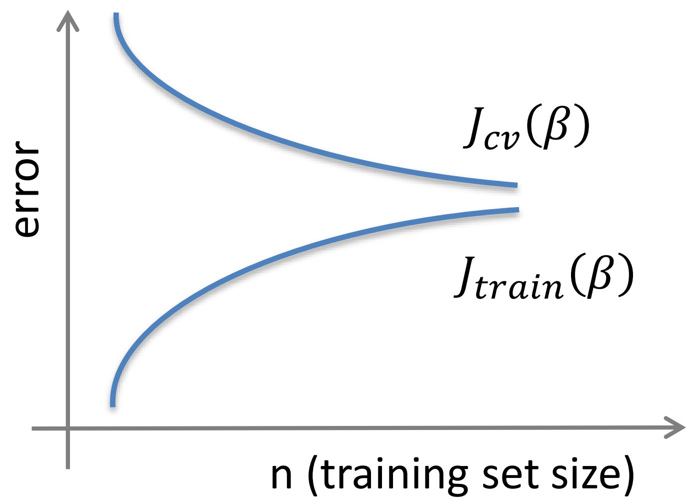


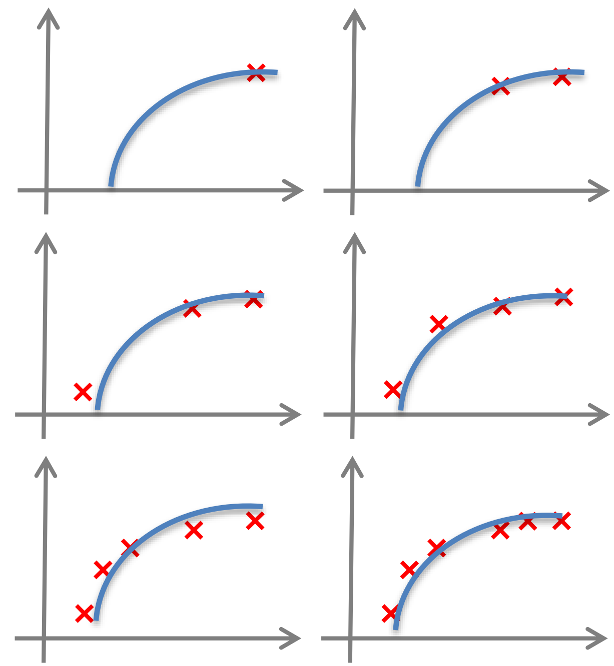
Learning curves

$$J_{train}(\beta) = \frac{1}{2n_{train}} \sum_{i=1}^{n_{train}} (y_i - \beta_0 - \beta_1 x_1^{(i)} - \cdots - \beta_2 x_2^{(i)})^2$$

$$J_{cv}(\beta) = \frac{1}{2n_{cv}} \sum_{i=1}^{n_{cv}} (y_i - \beta_0 - \beta_1 x_1^{(i)} - \cdots - \beta_2 x_2^{(i)})^2$$

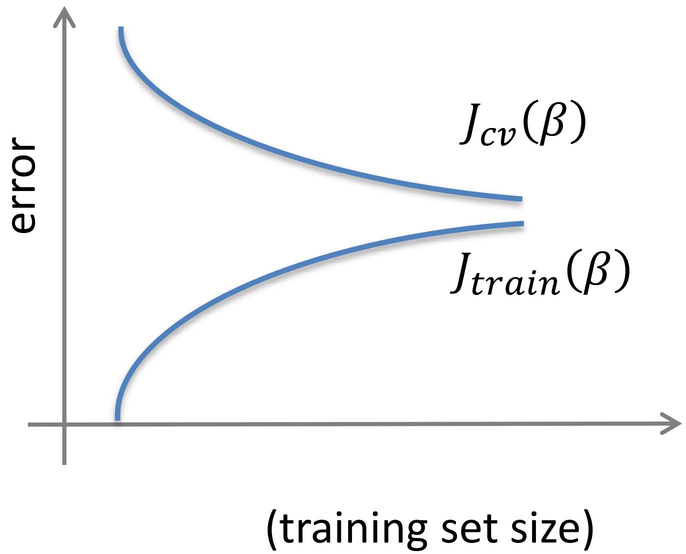
$$h_\beta(x) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$$





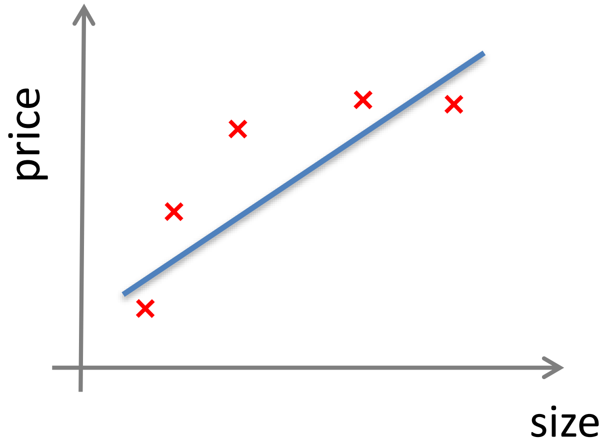
High bias

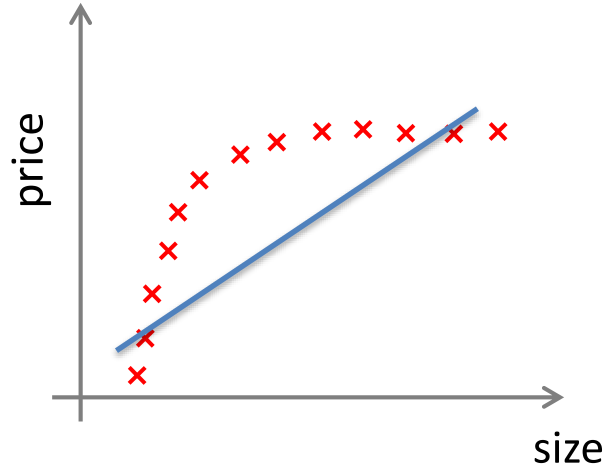
High bias



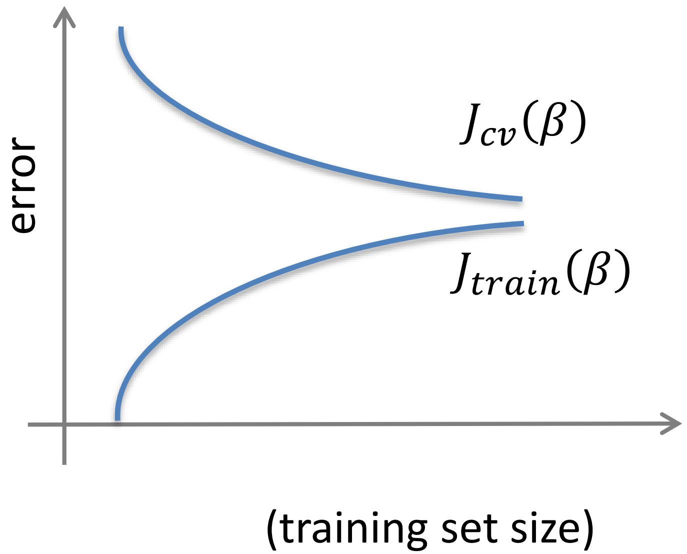
If a learning algorithm is suffering from high bias, getting more training data will not (by itself) help much.

$$h_\beta(x) = \beta_0 + \beta_1 x$$



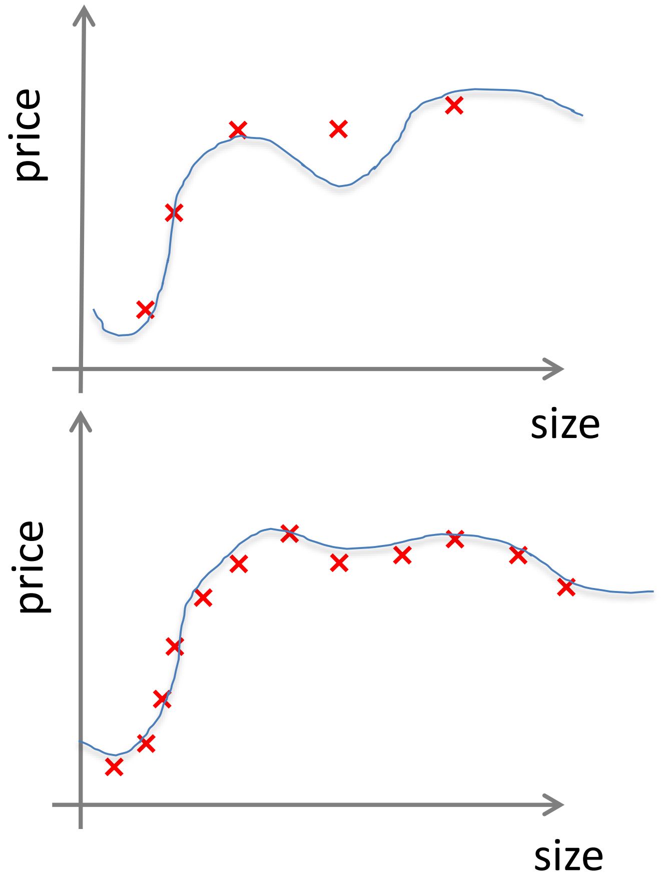


High variance



$$h_\beta(x) = \beta_0 + \beta_1 x + \cdots + \beta_4 x^4$$

(and small λ)



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

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
- Try smaller sets of features
- Try getting additional features
- Try adding polynomial features $(x_1^2, x_2^2, x_1 x_2, \text{etc})$
- Try decreasing λ
- Try increasing λ