CS 60050
Machine Learning

Evaluation and Error analysis

Validation and Regularization

Some slides taken from course materials of Andrew Ng

How to evaluate a model?

- Regression
  - Some measure of how close are predicted values (by a model) to the actual values
- Classification
  - Whether predicted classes match the actual classes

Evaluation metrics for Regression

- Mean Squared Error (MSE)
  - For every data point, compute error (distance between predicted value and actual value)
  - Sum squares of these errors, and take average
  - More popular variant: RMSE (square root of MSE)
- R2 or R-squared
  - A naïve Simple Average Model (SAM): for every point, predict the average of all points
  - R2: 1 – (error of model / error of SAM)
  - Best possible R2 is 1; can be negative for a really bad model

R2 or R-squared

- Dataset has n instances <x_i , y_i>, i=1..N
- Predicted values: f_i, i=1..N
- Mean of actual values: $\bar{y}$

$$R^2 \equiv 1 - \frac{SS_{\rm res}}{SS_{\rm tot}}$$

$$SS_{\rm res} = \sum_i (y_i - f_i)^2$$

Residual sum of squares

$$SS_{\rm tot} = \sum_i (y_i - \bar{y})^2$$

Total sum of squares
(proportional to variance)

Evaluation metrics for classification

- Let y = actual class, h = predicted class for an example

- Accuracy: Out of all examples, for what fraction is h = y?

- But accuracy is often not sufficient to indicate performance in practice

Skewed classes

- Often the class of interest is a rare class ($y=1$)
  - Spam emails / social network accounts
  - Cancerous cells
  - Fraud credit card transactions

Skewed classes

- Often the class of interest is a rare class ($y=1$)
  - Spam emails / social network accounts
  - Cancerous cells
  - Fraud credit card transactions
- Precision: Out of all examples for which model predicted $h=1$, for what fraction is $y=1$?
- Recall: Of all examples for which $y=1$, for what fraction did model correctly predict $h=1$?

Precision vs. Recall: tradeoff

- Predict y=1 if h > some threshold
- Predict y=1 only if highly confident: high precision, lower recall
- Avoid missing too many cases with y=1: high recall, lower precision

- F-score: harmonic mean of Precision and Recall

$$2\frac{PR}{P+R}$$

Confusion Matrix

		Predicted Label	
		h = 1	h = -1
True Label	$y = 1$	True positive	False negative
	$y = -1$	False positive	True negative

Precision: (True positive) / (True positive + False positive)

Recall: (True positive) / (True positive + False negative)

Another format of confusion matrix

		y	
		$+1$	-1
h	$+1$	no error	*false accept*
	-1	*false reject*	no error

- Two types of errors:
  - False positive/accept: hypothesis +1, true label -1
  - False negative/reject: hypothesis -1, true label +1

Two types of errors

- How do we penalize the two types of errors?
- Which is more important – higher Precision or higher Recall?
- Depends on the specific application

Example: Fingerprint verification

- Input fingerprint, classify as known identity or intruder
- Application 1: Supermarket verifies customers for giving a discount
- Application 2: For entering into RAW, GoI

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		y	
		$+1$	-1
h	$+1$	0	1
	-1	10	0

Example: Fingerprint verification

- Input fingerprint, classify as known identity or intruder

- Application 1: Supermarket verifies customers for giving a discount

		y	
		$+1$	-1
h	$+1$	0	1
	-1	10	0

- Application 2: For entering into RAW, GoI

		y	
		$+1$	-1
h	$+1$	0	1000
	-1	1	0

On what data to measure precision, recall, error rate, ..?

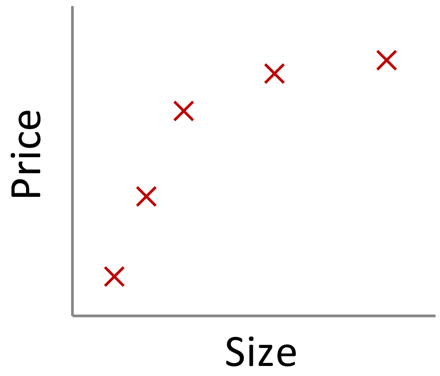
- Option 1: training set
- Option 2: some other set of examples that was unknown at the time of training (test set)

- Motivation for ML: learn a model that performs well (generalizes well) to unknown examples
- Option 2 gives better guarantees for generalization of a learnt model

Error Analysis

Bias and Variance

Example: Linear regression (housing prices)

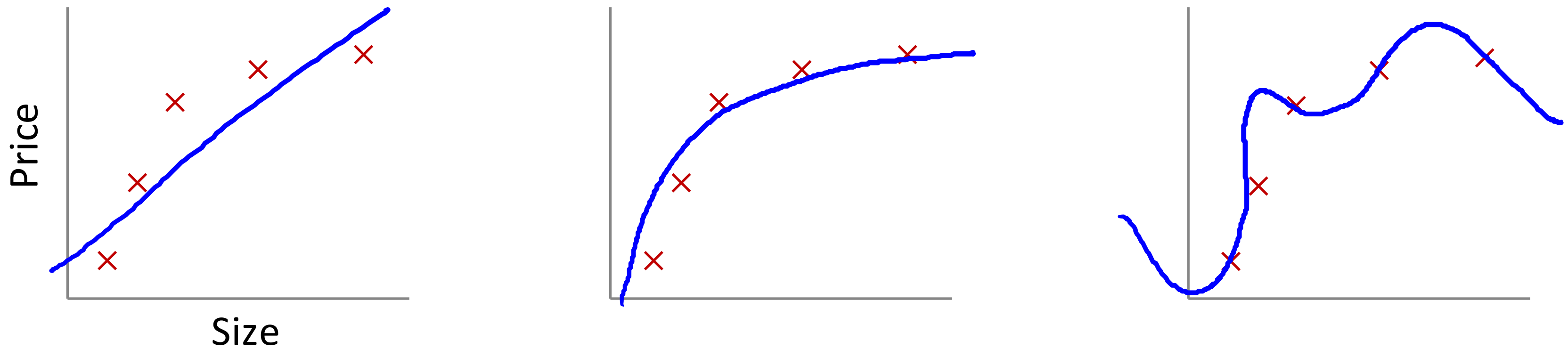


$$\theta_0 + \theta_1 x$$ Fitting a linear function

$$\theta_0 + \theta_1 x + \theta_2 x^2$$ Fitting a quadratic function

$$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$ Fitting a higher order function

Bias vs. variance in linear regression



$d=1$

$\theta_0 + \theta_1 x$

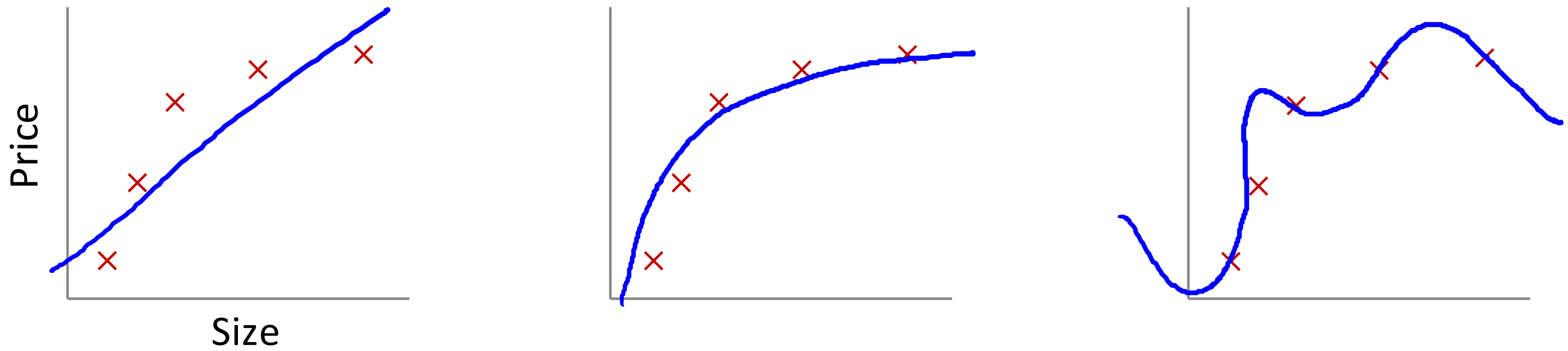
$d=2$

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

$d=4$

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

Bias vs. variance in linear regression



High bias
(underfitting)

$d=1$

$$\theta_0 + \theta_1 x$$

"Just right"

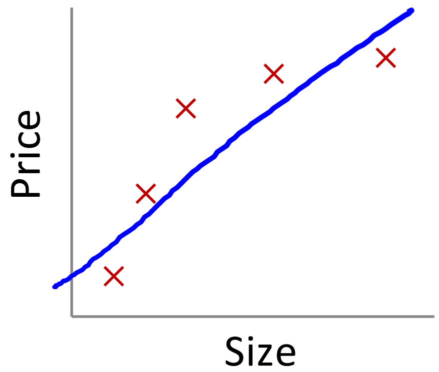
$d=2$

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

$d=4$

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

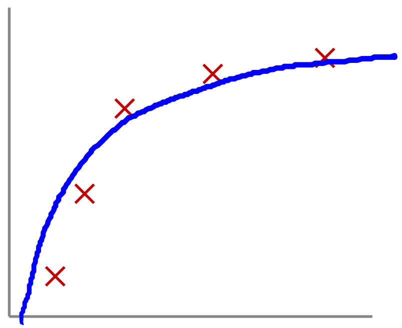
Bias vs. variance in linear regression



High bias
(underfitting)

d=1

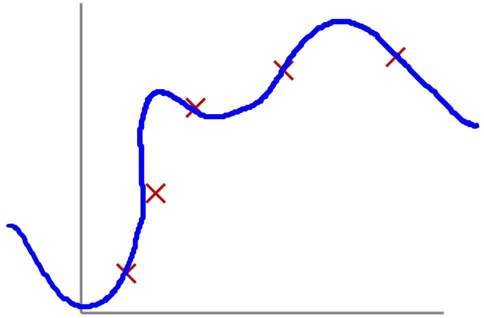
$$\theta_0 + \theta_1 x$$



"Just right"

d=2

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



High variance
(overfitting)

d=4

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

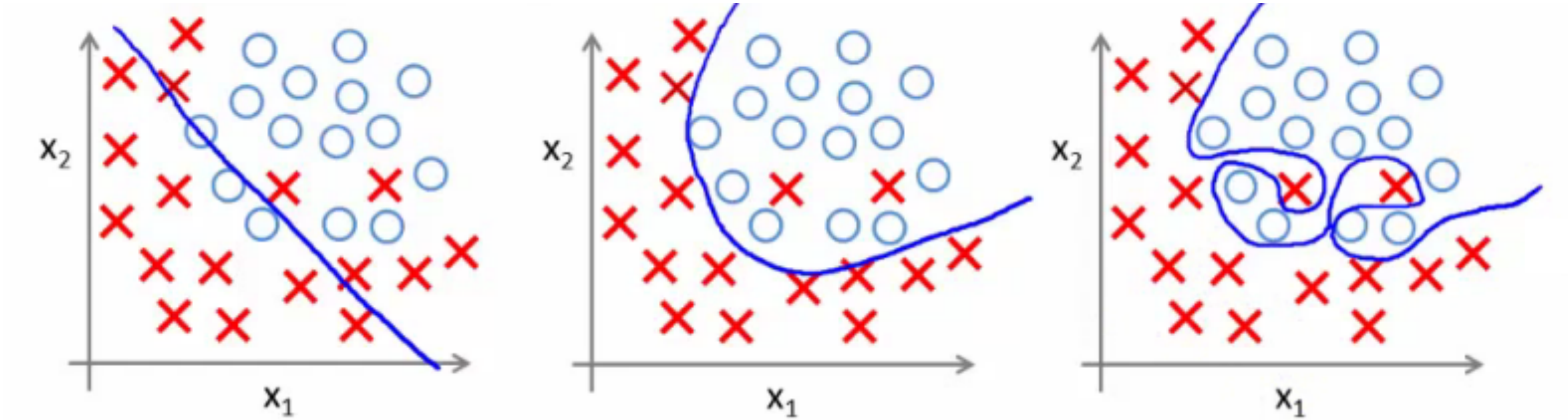
Overfitting

If we have too many features, the learned hypothesis may fit the training set very well

but fail to generalize to new examples.

Bias vs. variance in logistic regression

Example: Logistic regression



$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$ (g = sigmoid function)	$g(\theta_0 + \theta_1 x_1 + \theta_2 x_2$ $+\theta_3 x_1^2 + \theta_4 x_2^2$ $+\theta_5 x_1 x_2)$	$g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2$ $+\theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2$ $+\theta_5 x_1^2 x_2^3 + \theta_6 x_1^3 x_2 + \ldots$
UNDERFITTING **(high bias)**		**OVERFITTING** **(high variance)**

Sources of noise and error

- While learning a target function using a training set
- Two sources of noise
  - Some training points may not come exactly from the target function: stochastic noise
  - The target function may be too complex to capture using the chosen hypothesis set: deterministic noise

- Generalization error: Model tries to fit the noise in the training data, which gets extrapolated to the test set

Ways to handle noise

- Validation
  - Check performance on data other than training data, and tune model accordingly
- Regularization
  - Constraint the model so that the noise cannot be learnt too well

Validation

Validation

- Divide given data into train set and test set
  - E.g., 80% train and 20% test
  - Better to select randomly
- Learn parameters using training set
- Check performance (validate the model) on test set, using measures such as accuracy, misclassification rate, etc.
- Trade-off: more data for training vs. validation

An example: model selection

- Which order polynomial will best fit a given data? Polynomials available: h_1, h_2, …, h_{10}
- As if an extra parameter - degree of the polynomial - is to be learned
- Approach
  - Divide into train and test set
  - Train each hypothesis on train set, measure error on test set
  - Select the hypothesis with minimum test set error

An example: model selection

- Problem with the previous approach
  - The test set error we computed is not a true estimate of generalization error
  - Since our extra parameter (order of polynomial) is fit to the test set

An example: model selection

- Approach 2
  - Divide data into train set (60%), validation set (20%) and test set (20%)
  - Select that hypothesis which gives lowest error on validation set
  - Use test set to estimate generalization error

- Note: Test set not at all seen during training

Popular methods of evaluating a classifier

- Holdout method
  - Split data into train and test set (usually 2/3 for train and 1/3 for test). Learn model using train set and measure performance over test set
  - Usually used when there is sufficiently large data, since both train and test data will be a part

Popular methods of evaluating a classifier

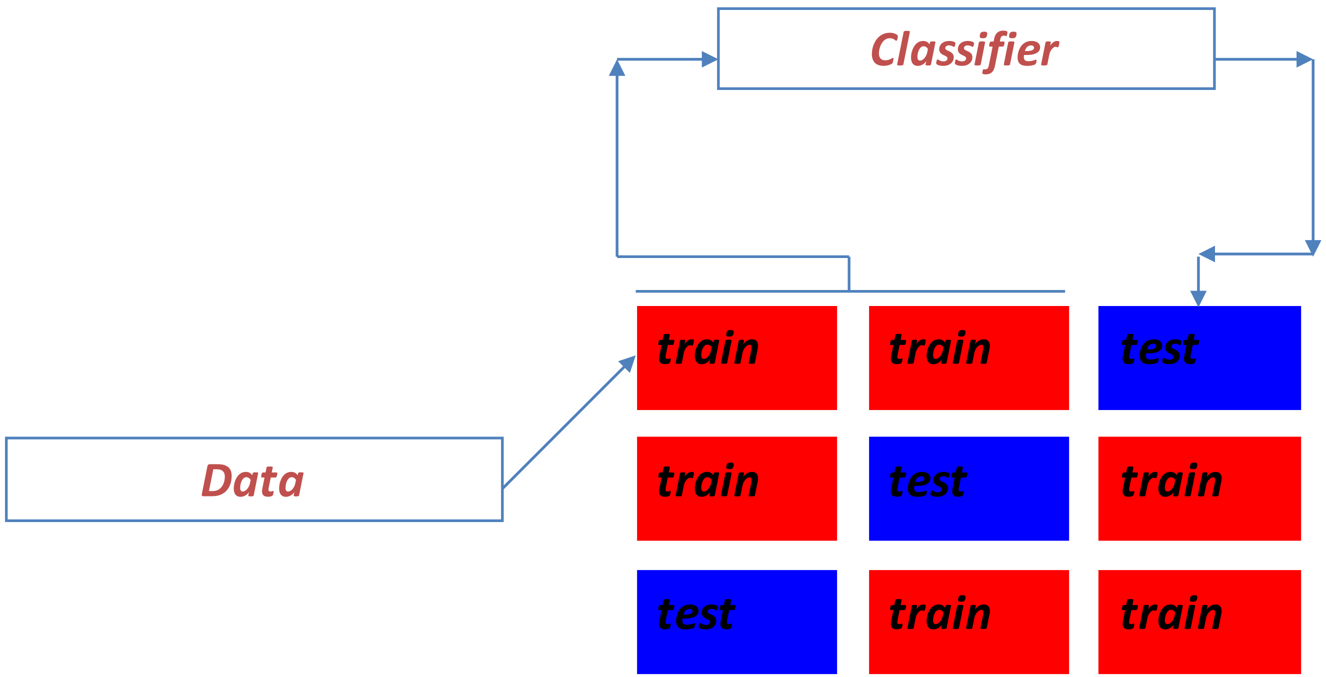
- Repeated Holdout method
  - Repeat the Holdout method multiple times with different subsets used for train/test
  - In each iteration, a certain portion of data is randomly selected for training, rest for testing
  - The error rates on the different iterations are averaged to yield an overall error rate
  - More reliable than simple Holdout

Popular methods of evaluating a classifier

- k-fold cross-validation
  - *First step*: data is split into *k* subsets of equal size;
  - *Second step*: each subset in turn is used for testing and the remainder for training
  - Performance measures averaged over all folds

- Popular choice for k: 10 or 5
- Advantage: all available data points being used to train as well test model

k-fold cross validation (shown for k=3)



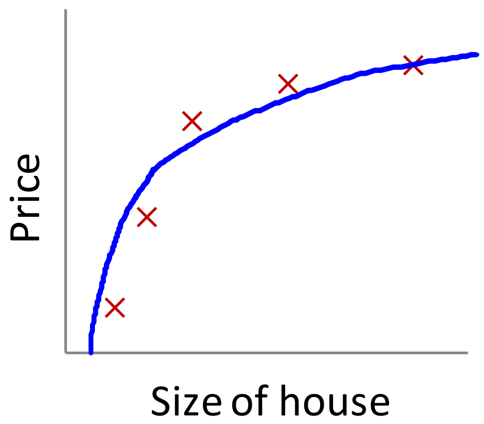
Regularization

Addressing overfitting: Two ways

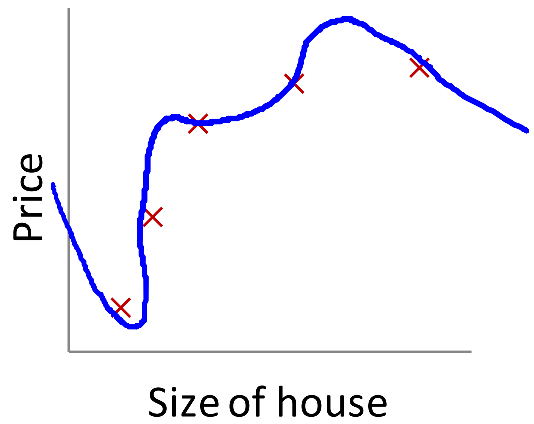
1. Reduce number of features
   - Manually select which features to keep
   - Problem: loss of some information (discarded features)

2. Regularization
   - 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

Intuition of regularization



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



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

Suppose we penalize and make θ_3, θ_4 really small.

$$\min_\theta \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 \quad + K\,\Theta_3^2 + K\,\Theta_4^2$$

Regularization for linear regression

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

$$\min_\theta J(\theta)$$

By convention, regularization is not applied on θ_0 (makes little difference to the solution)

λ: Regularization parameter

Smaller values of parameters lead to more generalizable models, less overfitting

Regularization for linear regression

In regularized linear regression, we choose θ to minimize

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

Regularization parameter λ

- Controls trade-off between our two goals
- (1) fitting the training data well
- (2) keeping values of parameters small

- What if λ is too large? Underfitting

L1 and L2 regularization

- What we are discussing is called L2 regularization or “ridge” regularization
  - adds *squared magnitude* of parameters as penalty term

- Look up L1 or “Lasso” regularization
  - adds *absolute value of magnitude* of parameters as penalty term

Regularized linear regression

Gradient Descent for ordinary linear regression

Repeat $\{$

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

$$(j = \cancel{0}, 1, 2, 3, \ldots, n)$$

$\}$

Regularized linear regression

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$$\min_\theta J(\theta)$$

Gradient Descent for Regularized Linear Regression

Repeat $\{$

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

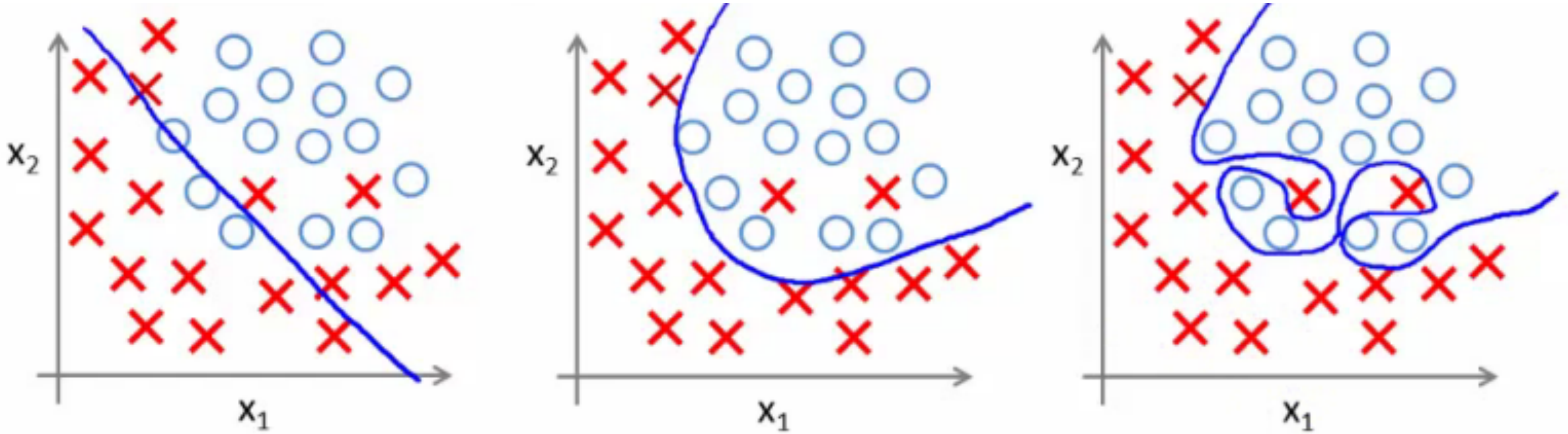
$$\theta_j := \theta_j (1 - \alpha \frac{\lambda}{m}) - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

$$(j = \cancel{0}, 1, 2, 3, \ldots, n)$$

$\}$

Regularized logistic regression

Example: Logistic regression



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(g = sigmoid function)

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UNDERFITTING
(high bias)

OVERFITTING
(high variance)

Gradient descent for ordinary logistic regression

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

Repeat $\{$

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

$$(j = \cancel{0}, 1, 2, 3, \dots, n)$$

$\}$

Gradient Descent for Regularized Logistic Regression

$$J(\theta) = -\frac{1}{m}[\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_\theta(x^{(i)}))]$$

$$+ \frac{\lambda}{2m} \sum_{j=1}^{n} \theta_j^2$$

Gradient Descent for Regularized Logistic Regression

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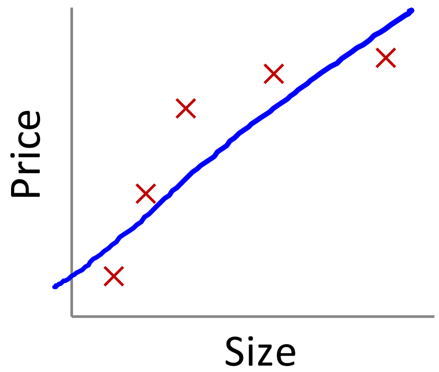
$$\theta_j := \theta_j (1 - \alpha \frac{\lambda}{m}) - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

$$(j = \cancel{0}, 1, 2, 3, \ldots, n)$$

$\}$

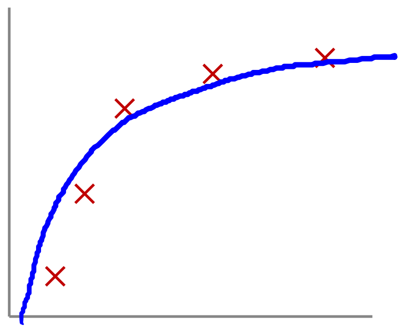
Bias vs. Variance
A closer look

Example: Linear regression



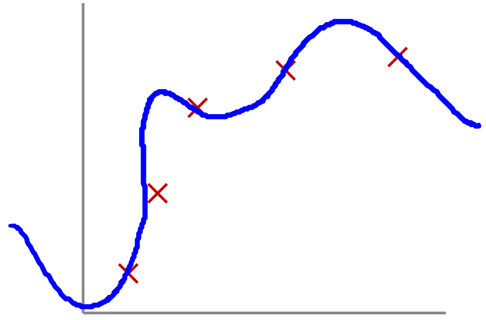
High bias
(underfit)

$d=1$



"Just right"

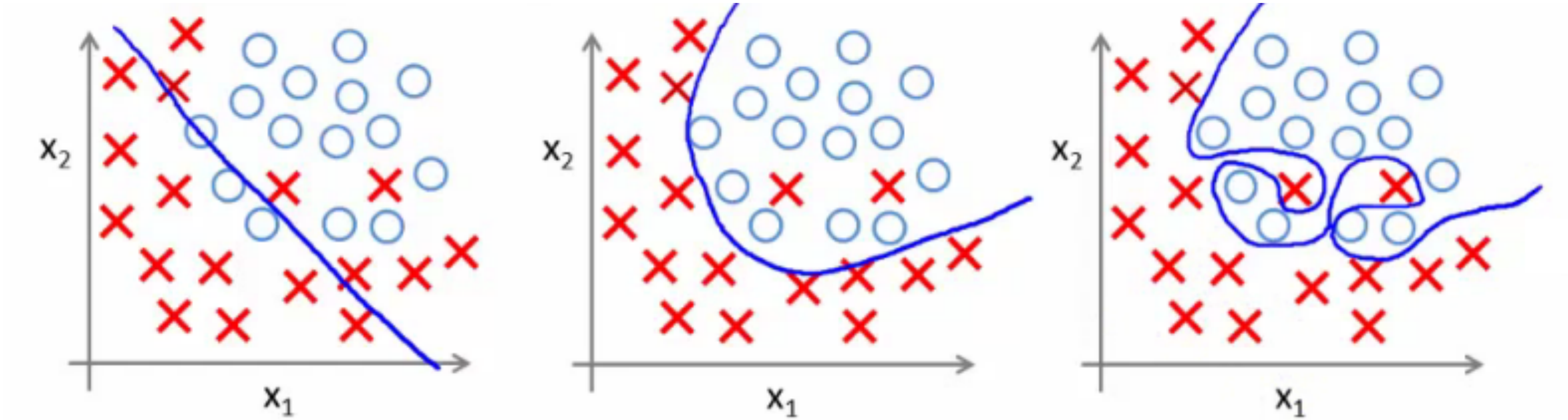
$d=2$



High variance
(overfit)

$d=4$

Example: Logistic regression



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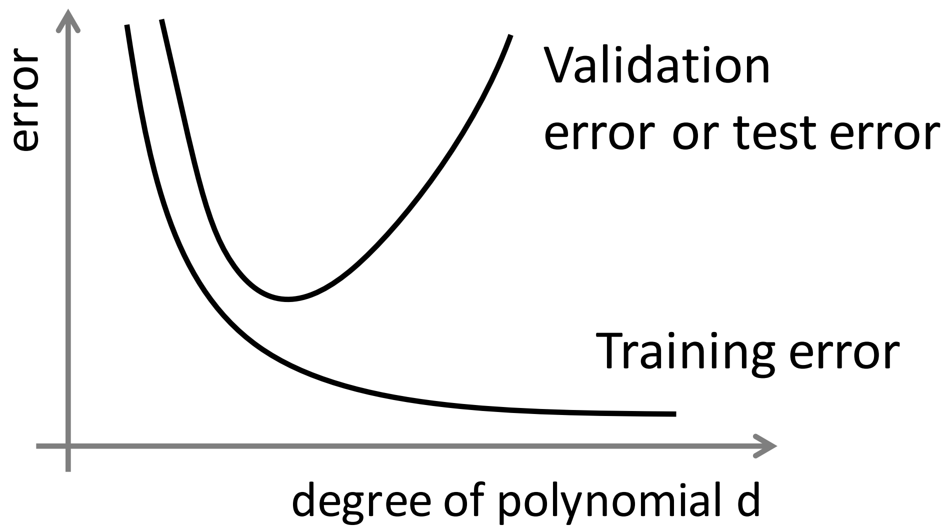
UNDERFITTING
(high bias)

OVERFITTING
(high variance)

Analysing bias vs. variance

- Suppose your model is not performing as well as expected. Is it a bias problem or a variance problem?



Bias (underfit):
Both training error and validation / test error are high

Variance (overfit):
Low training error
High validation / test error

Bias vs. Variance

- Bias and variance both contribute to the error of classifier
- Variance is error due to randomness in how the training data was selected (variance of an estimate refers to how much the estimate will vary from sample to sample)
- Bias is error due to something systematic, not random

Will more training data help?

- A learnt model is not performing as well as expected. Will having more training data help?

- Note that there can be substantial cost for getting more training data.

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- A learnt model is not performing as well as expected. Will having more training data help?

- Note that there can be substantial cost for getting more training data.

- If model is suffering from high bias, getting more training data will not (by itself) help much.
- If model is suffering from high variance, getting more training data is likely to help

Practical approach

- Divide data into training set and validation set
- Start with simple algorithm, train on different amounts of training data, test performance on validation set
- Plot learning curves to decide if more training data, more features likely to help
- Error analysis: Manually examine the examples (in validation set) where algorithm made errors. Any systematic trend in what type of examples it is making errors on?

Learning curves

- How do training error (in-sample error) and test or validation error (out-of-sample error) generally vary with number of training points?