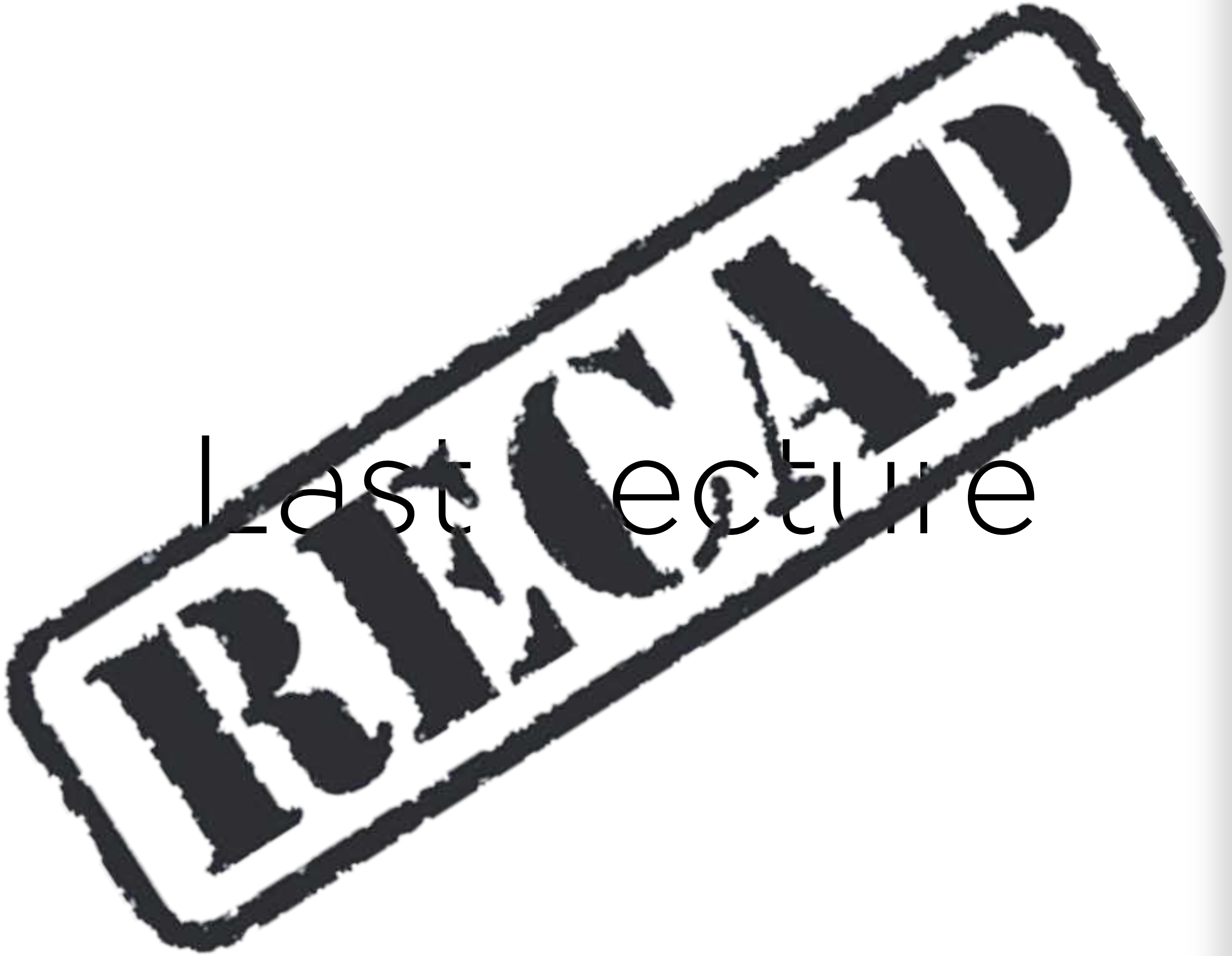
Machine Learning

Lecture 4 – Cost Function, Binary Classifier and Performance Measurement

Dr SHI Lei

Last Lecture



- Generalisation
- Training & Test Set
- Representation

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Generalisation

The big picture

- **Goal**: to predict well on new data drawn from (hidden) true distribution.
- **Issue**: we don't see the truth, but we only get to sample from it.
- If it fits current sample well, how can we trust it will predict well on other new samples?

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Generalisation

Three basic assumptions:

1. We draw examples independently and identically (i.i.d.) at random from the distribution.

2. The distribution is stationary - it doesn't change over time.

3. We always pull from the same distribution, including training, validation, and test sets.

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Training & Test Set

Divide into two sets:

- Training set
- Test set

Do not train on test data

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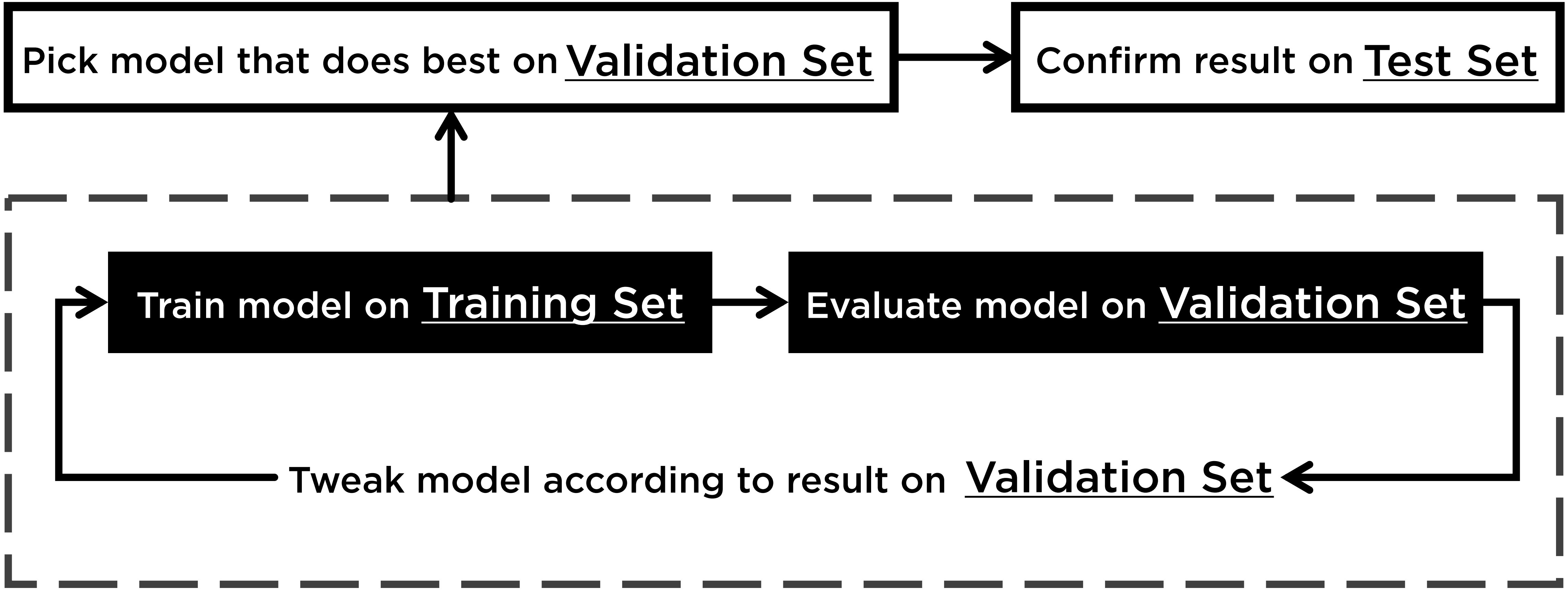
Training & Test Set

Better Workflow: Use a Validation Set



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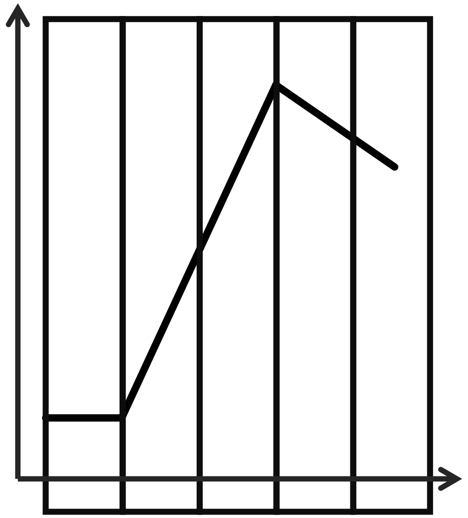
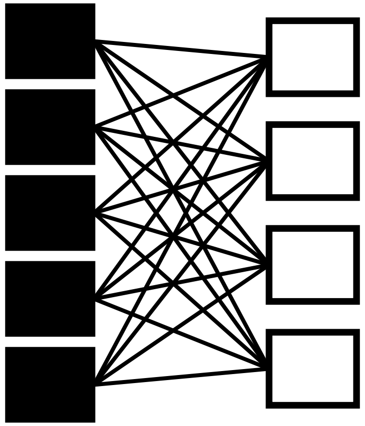
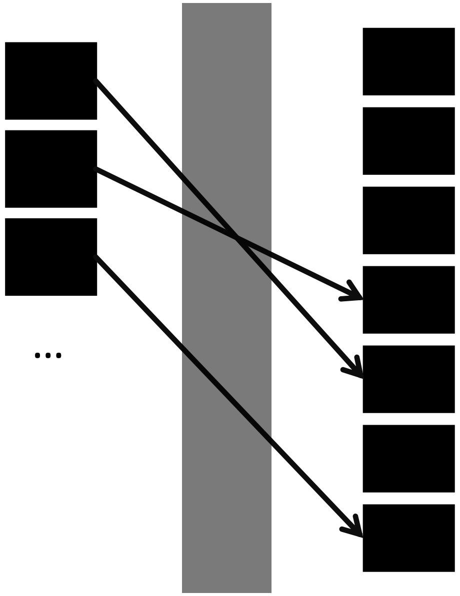
Representation



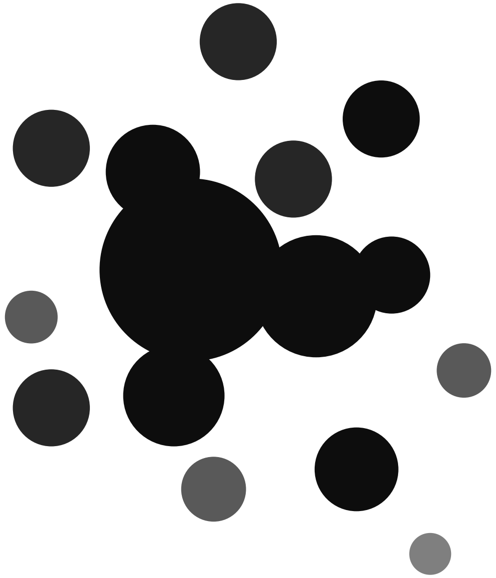
bucketing



crossing



hashing



embedding

Today

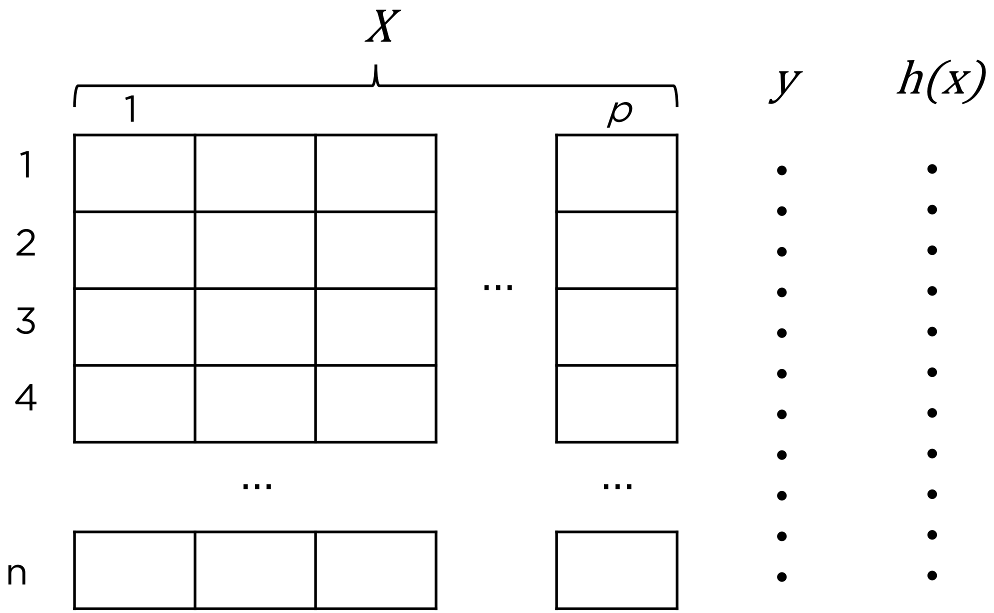
- Cost Functions
- Binary Classifier
- Performance Measures

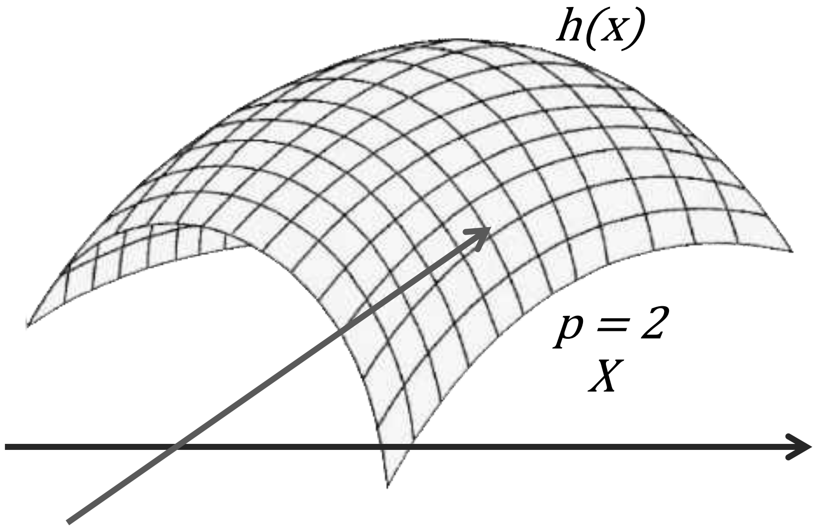
Cost Functions

Cost Functions

Supervised Learning Problem

- Collection of *n p*–dimensional feature vectors: $\{x_i\}, i = 1, n$
- Collection of observed responses: $\{y_i\}, i = 1, n$
- Aims to construct a response surface: $h(x)$



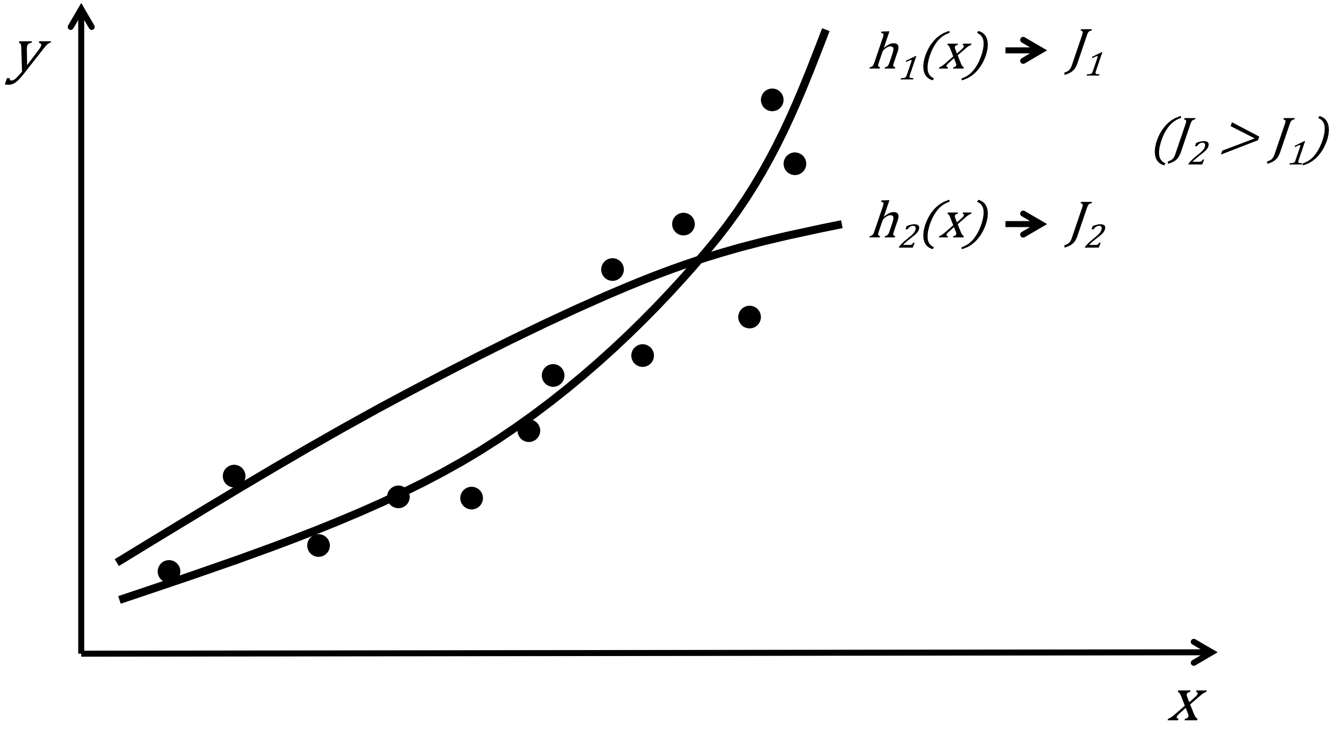


Cost Functions

- Describes how well the current response surface ***h(x)*** fits the available data (on a given data set):

$$J(y_i, h(x_i))$$

observed predicted



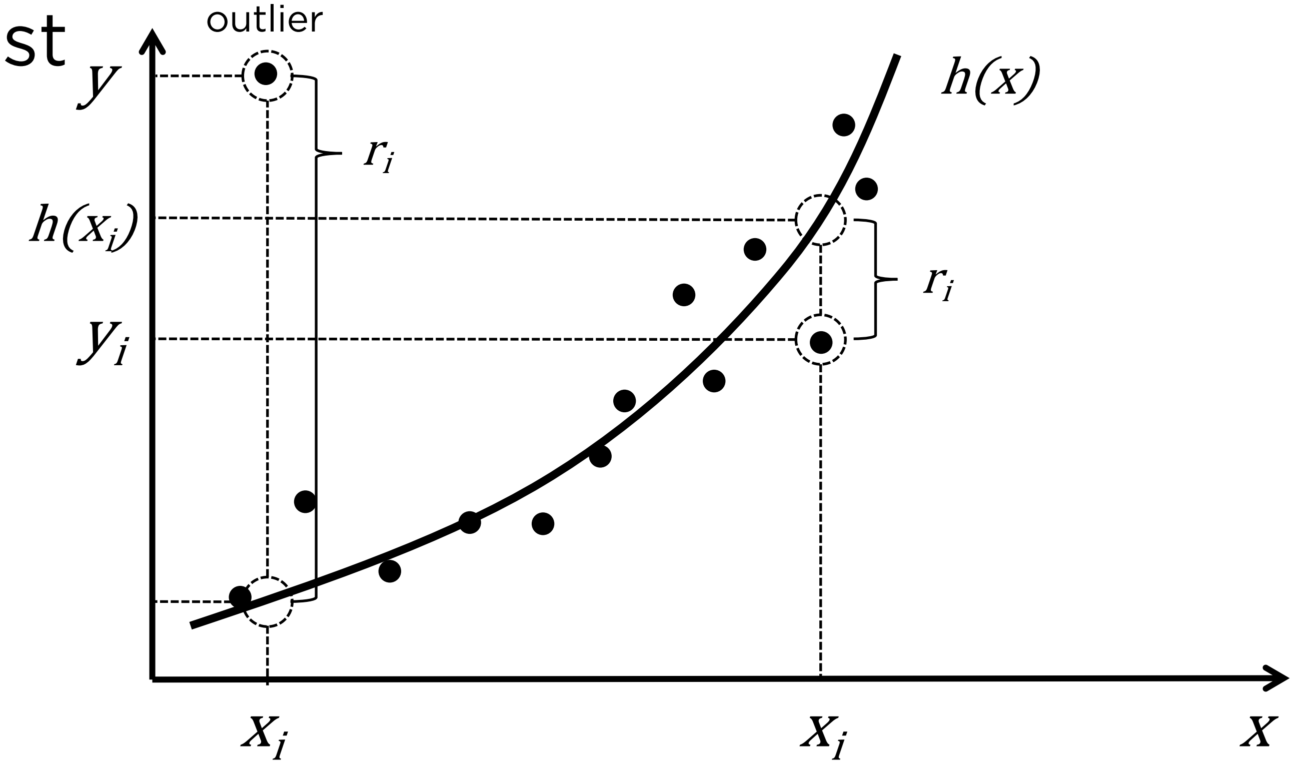
- Smaller values of the cost function correspond to a better fit.
- Machine learning goal: construct ***h(x)*** such that J is minimised.
- In regression, ***h(x)*** is usually directly interpretable as predicted response.

Cost Functions

Least Squares Deviation Cost

- Defined as

$$J(y_i, h(x_i)) = \boxed{\frac{1}{n}} \sum_{i=1}^{n} (\underbrace{y_i - h(x_i)}_{r_i \text{ (residual)}})^{\boxed{2}}$$



- Nice mathematical properties

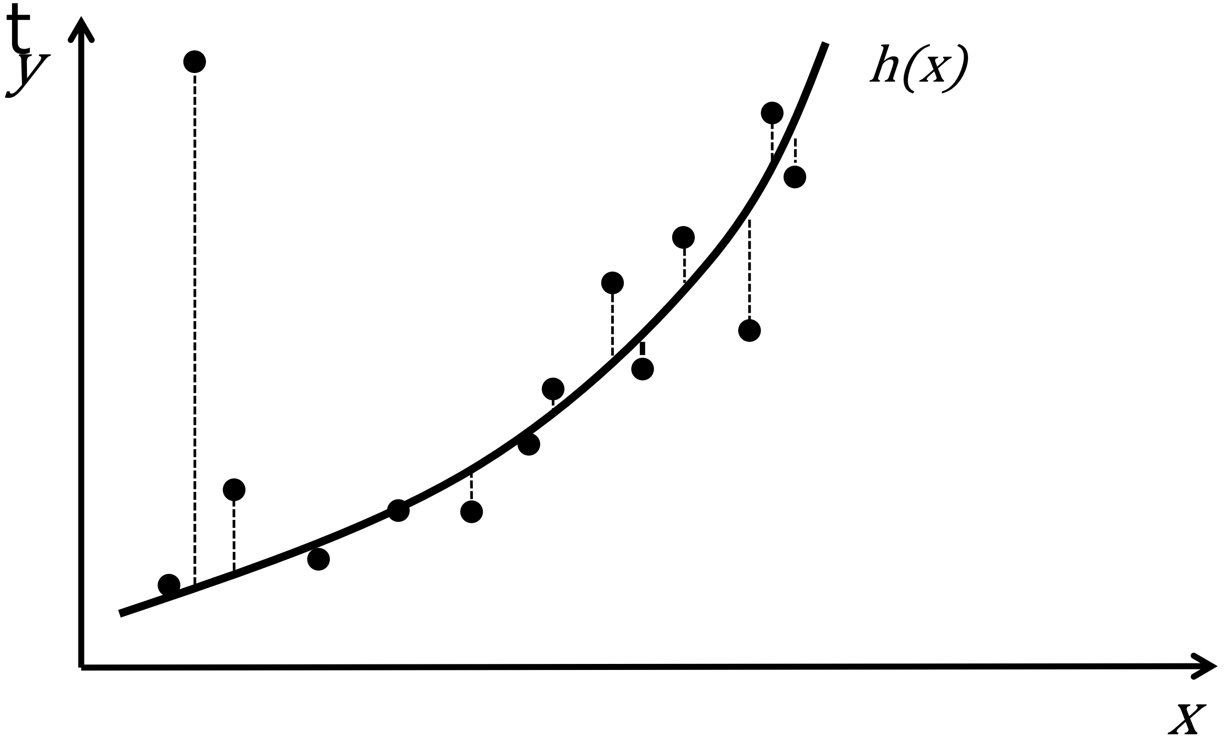
- Problem with outliers

Cost Functions

Least Absolute Deviation Cost

- Defined as

$$J(y_i, h(x_i)) = \boxed{\frac{1}{n}} \sum_{i=1}^{n} \underbrace{|y_i - h(x_i)|}_{r_i}{}^{\cancel{2}}$$



- More robust with respect to outliers

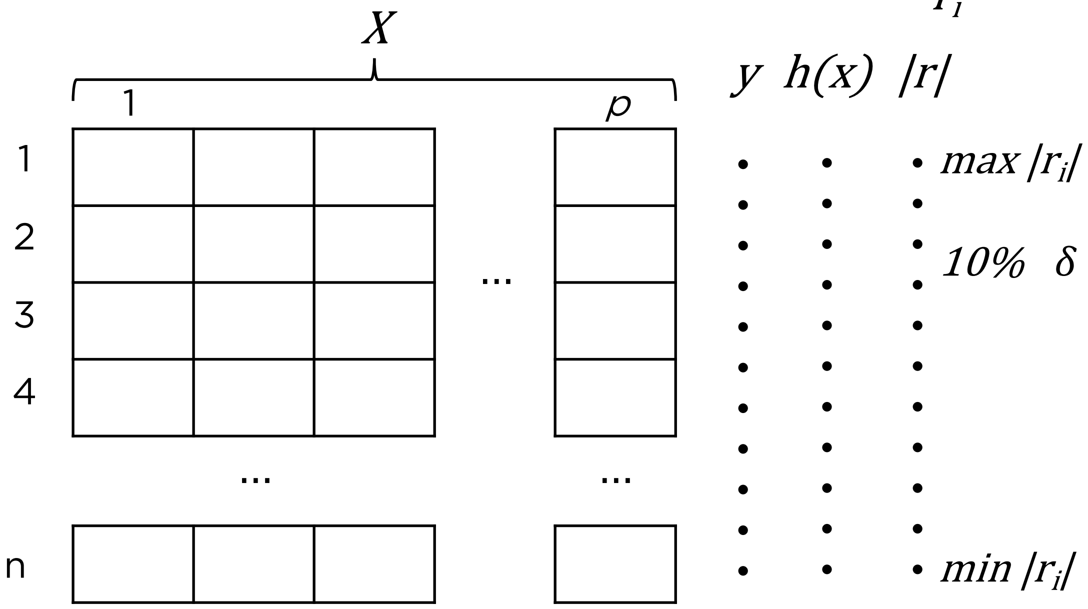
- May pose computational challenges

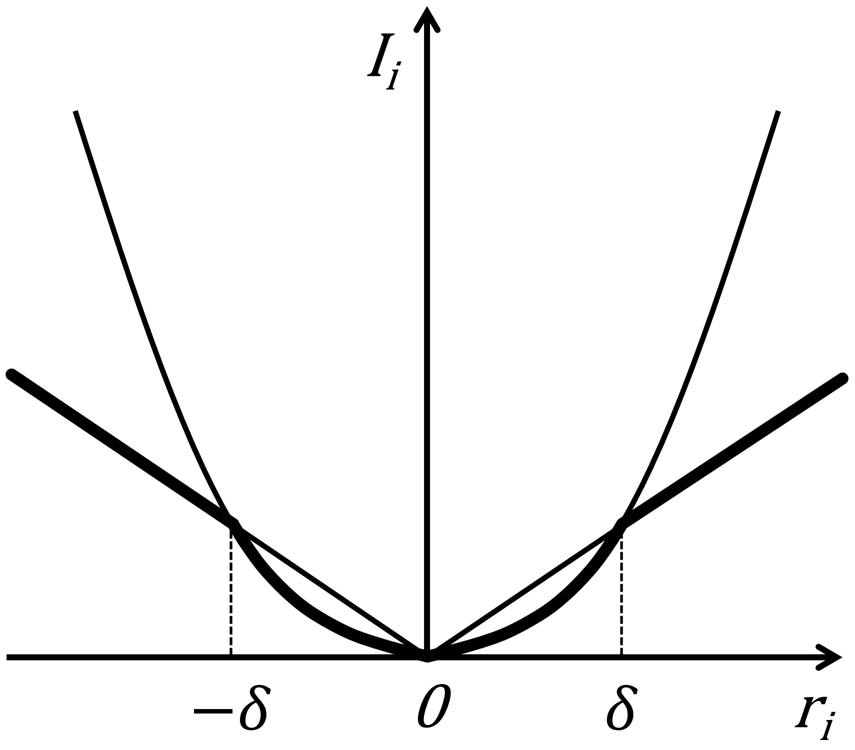
Cost Functions

Huber-M Cost

- Defined as

$$J(y_i, h(x_i)) = \frac{1}{n}\sum_{i=1}^{n} \overbrace{\begin{cases} 0.5(\underline{y_i - h(x_i)})^2, if\,|\underline{y_i - h(x_i)}| < \delta \\ \delta(|\underbrace{y_i - h(x_i)}_{r_i}| - 0.5\delta), otherwise \end{cases}}^{J_i}$$





- Combines the best qualities of the LS and LAD losses
- Parameter δ is usually set automatically to a specific percentile of absolute residuals

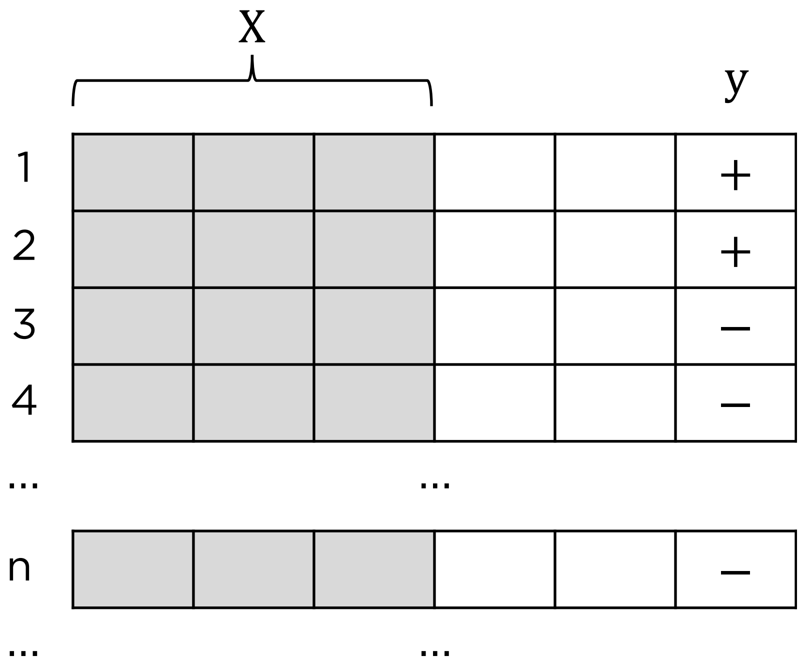
Today

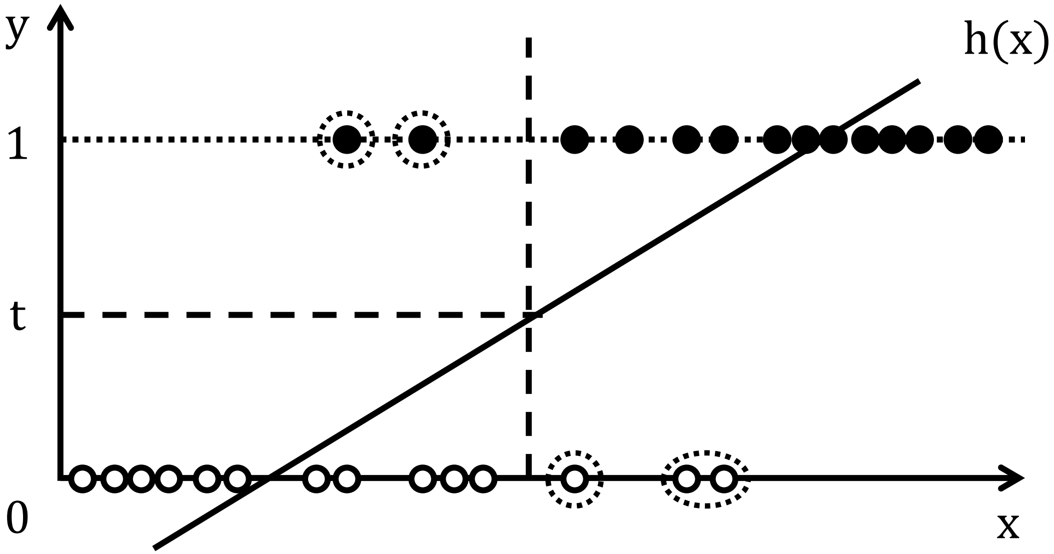
- Cost Functions
- Binary Classifier
- Performance Measures

Binary Classifier

Binary Classifier

- Observed response **y** takes only two possible values **+** and **–**
- Define relationship between ***h(x)*** and ***y***
- Use the decision rule: $\hat{y} = \begin{cases} +, & h(x) \geq t \\ -, & otherwise \end{cases}$





Performance Measures

Performance Measures

- Precision & Recall
- ROC Curve

Performance Measures - Precision & Recall

- How well did we capture the + group for the given threshold?

	y	$h(x)$	$\hat{y}$	
1	+	h_1	+	
2	+	h_2	−	
3	−	h_3	+	
4	−	h_4	−	
…		…		
n	−	h_n	+	
…		…		

Performance Measures - Precision & Recall

- How well did we capture the + group for the given threshold?

	y	h(x)	$\hat{y}$	
1	+	h_1	+	
2	+	h_2	−	
3	−	h_3	+	
4	−	h_4	−	
…		…		
n	−	h_n	+	
…		…		

		actual class	
		+	−
predicted class	+	true positives	false positives
	−	false negatives	true negatives

Prediction Success

(Confusion Matrix)

Performance Measures - Precision & Recall

- How well did we capture the + group for the given threshold?

predicted class \ actual class	+	–
+	tp	fp
–	fn	tn

Prediction Success

(Confusion Matrix)

- Precision $\dfrac{tp}{tp+fp} \gg 1$
- Recall (Sensitivity) $\dfrac{tp}{tp+fn} \gg 1$

Performance Measures - Precision & Recall

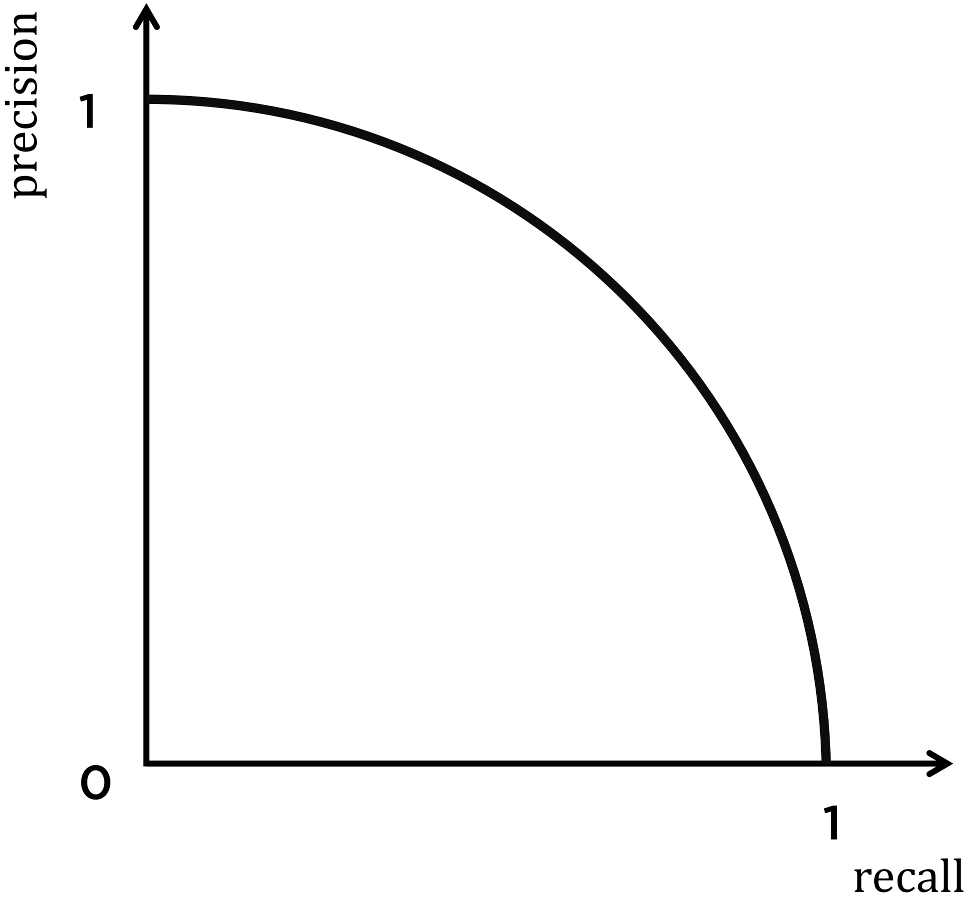
- How well did we capture the + group for the given threshold?

predicted class \ actual class	+	−
+	tp	fp
−	fn	tn

Prediction Success

(Confusion Matrix)

- Precision $\dfrac{tp}{tp + fp}$
- Recall (Sensitivity) $\dfrac{tp}{tp + fn}$



Performance Measures

- Precision & Recall
- ROC Curve

Performance Measures - ROC Curve

		actual class +	actual class –
predicted class	+	true positives	false positives
predicted class	–	false negatives	true negatives

- Recall (Sensitivity) $\frac{\boxed{tp}}{\boxed{tp + fn}}$
- Specificity $\frac{\boxed{tn}}{\boxed{tn + fp}}$

Performance Measures - ROC Curve

- Recall (Sensitivity) $\dfrac{tp}{tp + fn}$

- Specificity $\dfrac{tn}{tn + fp}$

y	h(x)	$\hat{y}$	
+	h_1		max
+	h_2		
−	h_3		
−	h_4		
+	h_5		
−	h_6		
+	h_7		
−	h_8		
−	h_9		min

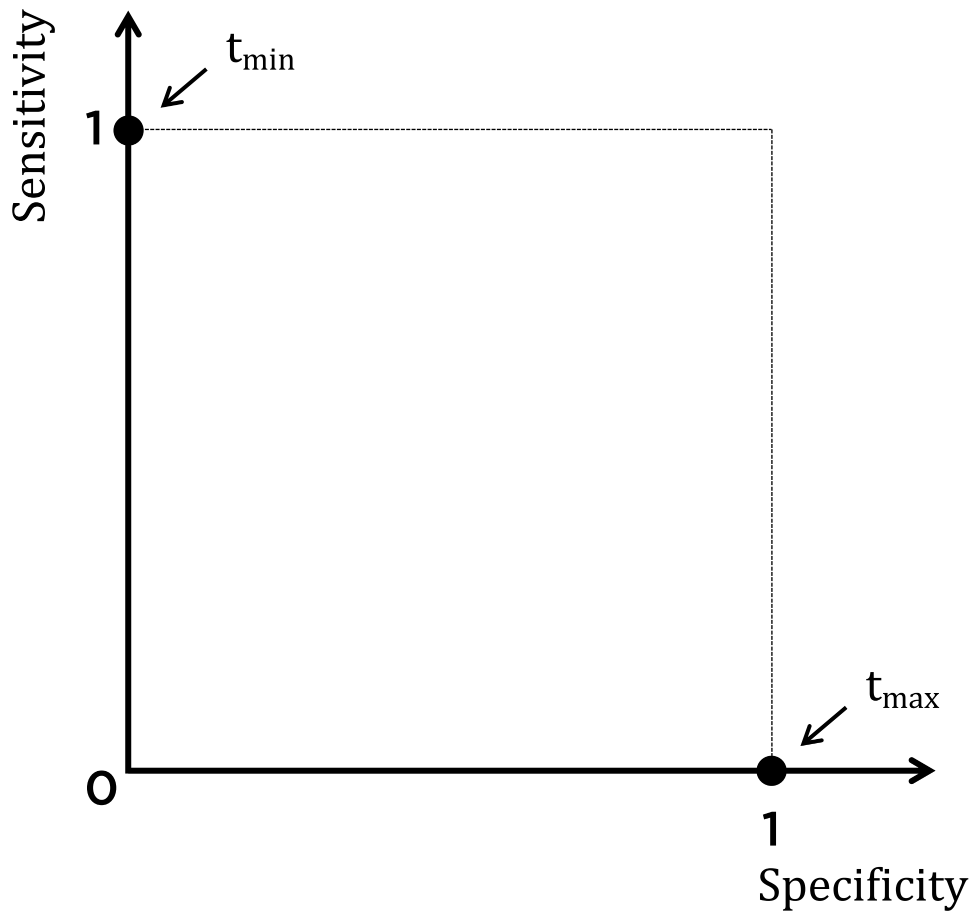
Performance Measures - ROC Curve

- Recall (Sensitivity) $\dfrac{tp}{tp + fn}$
- Specificity $\dfrac{tn}{tn + fp}$

$\leftarrow t_{max}$

y	h(x)	$\hat{y}$
+	h_1	+
+	h_2	+
−	h_3	+
−	h_4	+
+	h_5	+
−	h_6	+
+	h_7	+
−	h_8	+
−	h_9	+

$\leftarrow t_{min}$

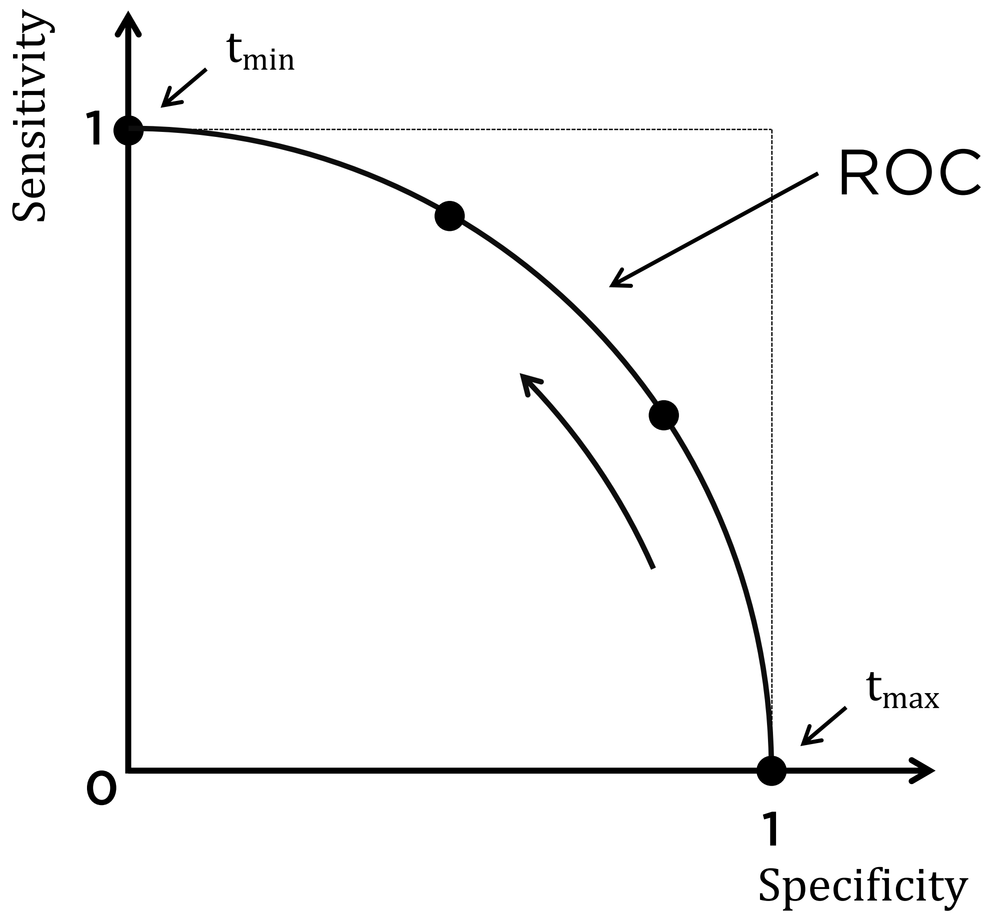


Performance Measures - ROC Curve

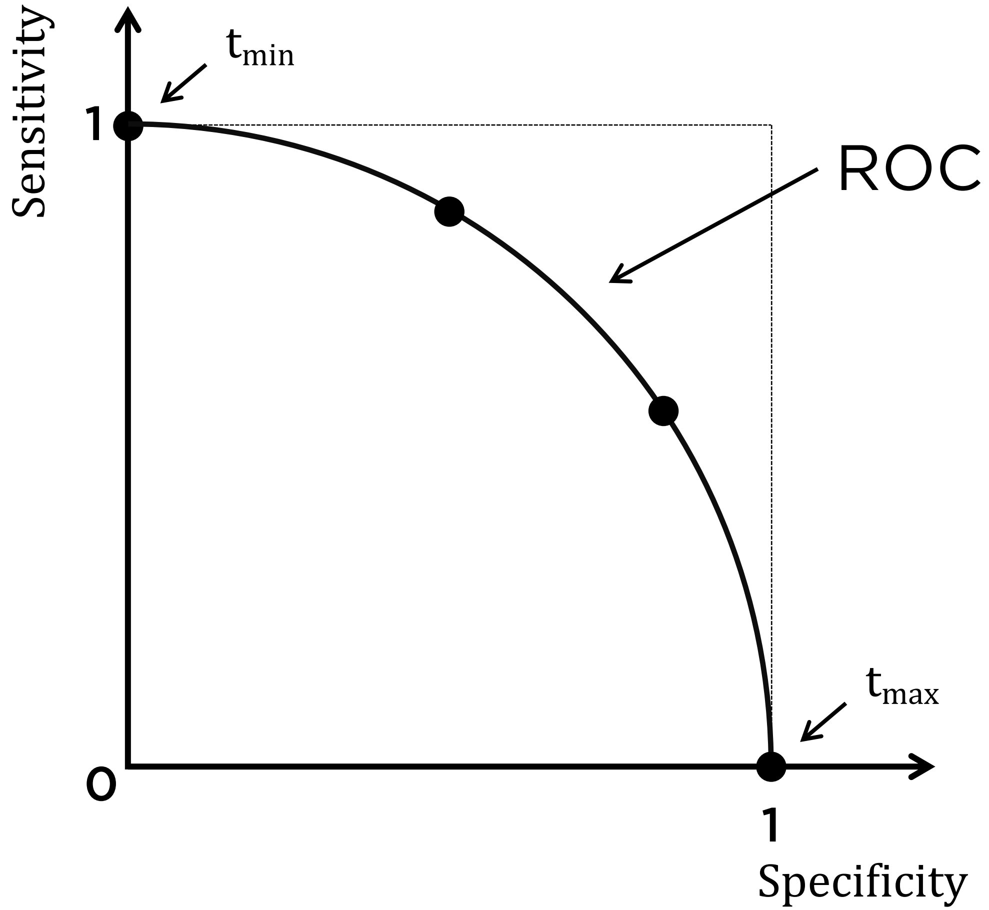
- Recall (Sensitivity) $\dfrac{tp}{tp + fn}$
- Specificity $\dfrac{tn}{tn + fp}$

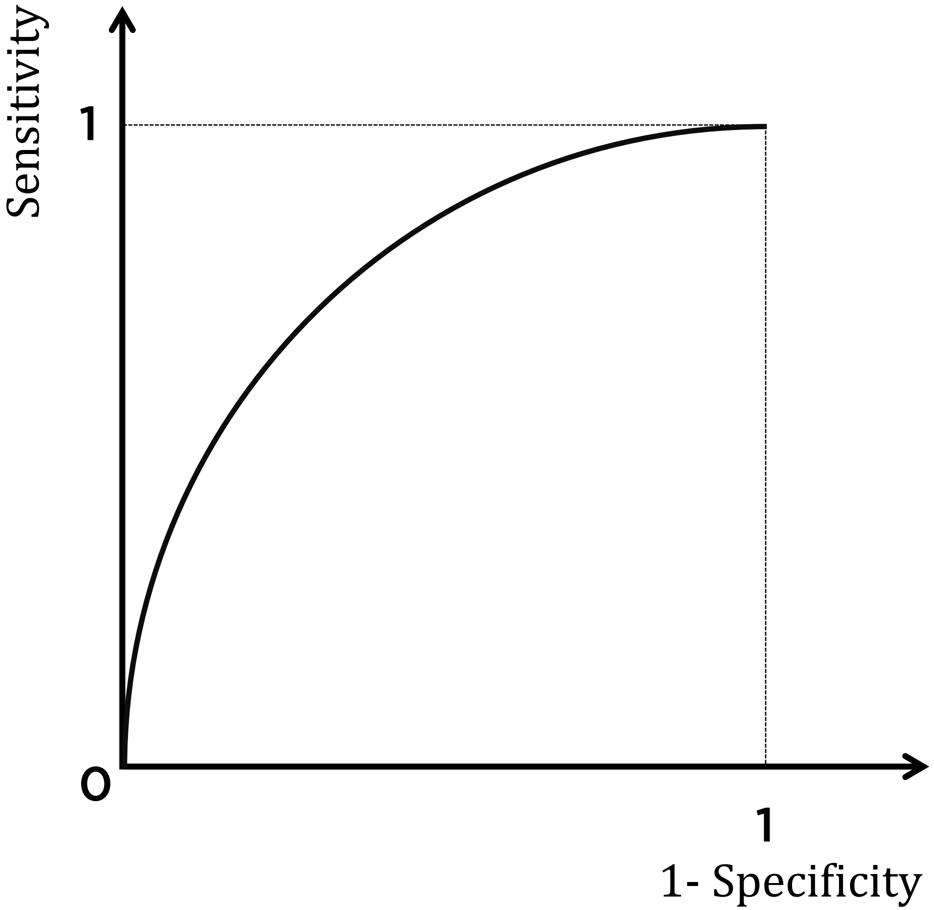
y	$h(x)$	$\hat{y}$
+	h_1	+
+	h_2	+
−	h_3	+
−	h_4	+
+	h_5	−
−	h_6	−
+	h_7	−
−	h_8	−
−	h_9	−

$\leftarrow t_{intermedia}$



Performance Measures - ROC Curve

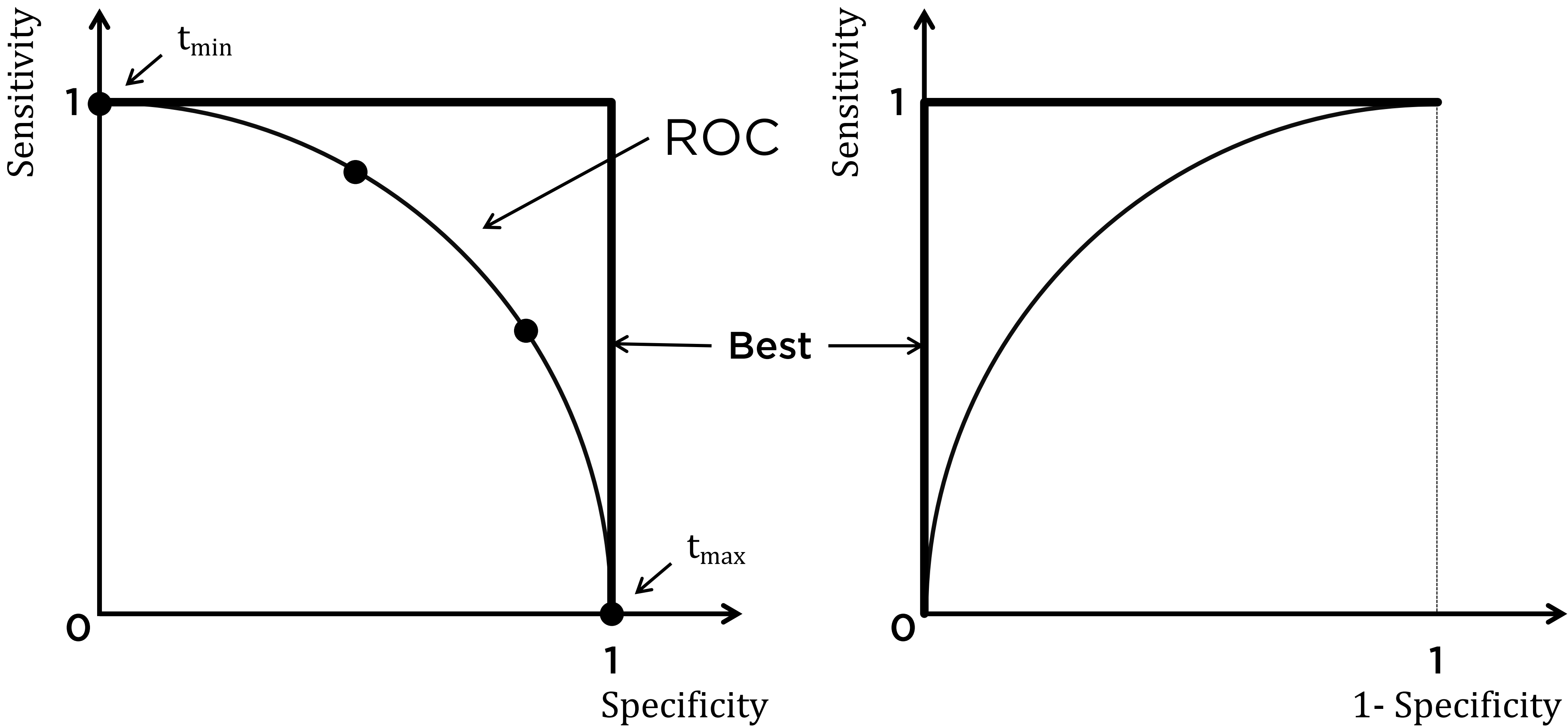




Performance Measures - ROC Curve

y	h(x)	$\hat{y}$
+	h_1	+
+	h_2	+
+	h_3	+
+	h_4	+
−	h_5	−
−	h_6	−
−	h_7	−
−	h_8	−
−	h_9	−

t_{max} t t t t t_{min}



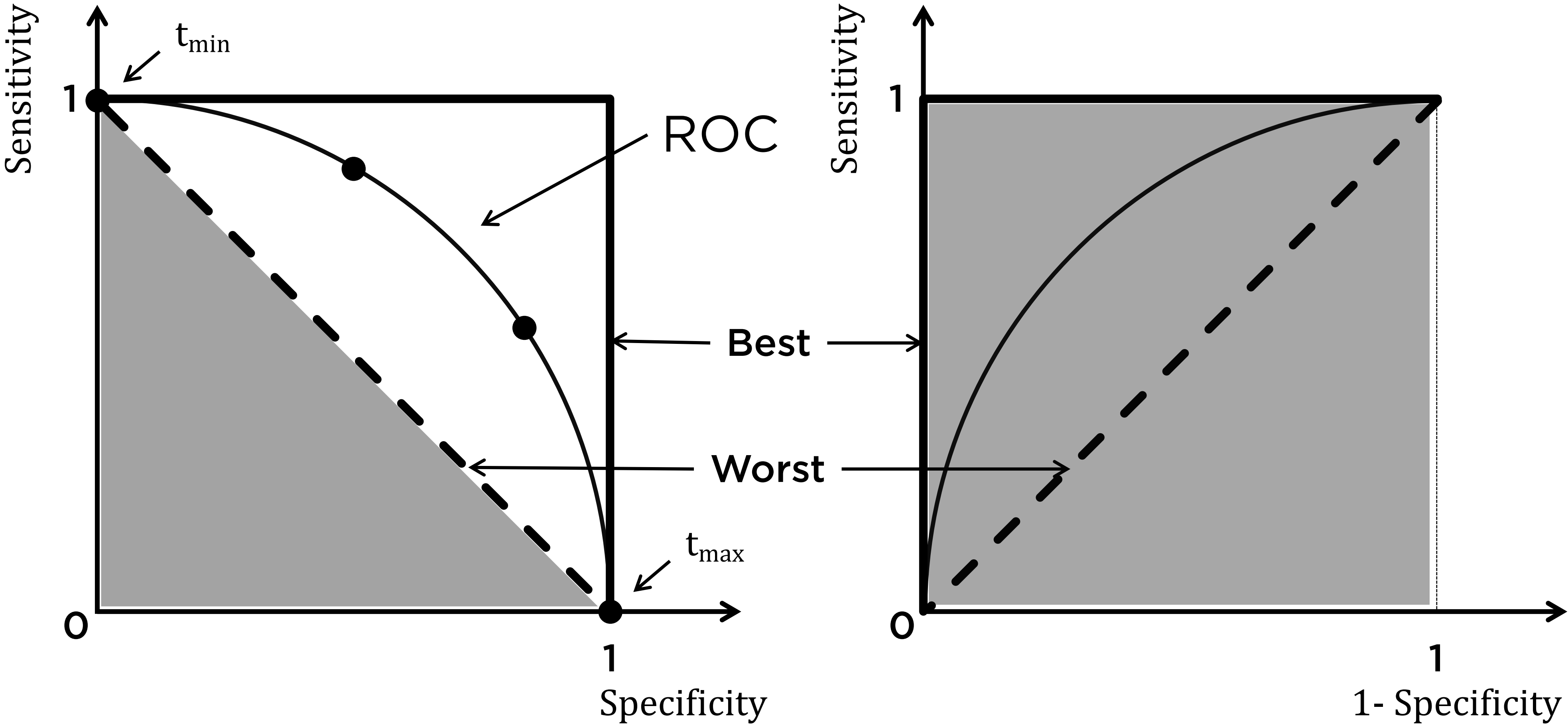
Performance Measures - ROC Curve

$$0.5 \leq AUC \leq 1.0$$

t_{max}

y	h(x)	$\hat{y}$
+	h_1	
−	h_2	
+	h_3	
+	h_4	
−	h_5	
+	h_6	
−	h_7	
+	h_8	
−	h_9	

t_{min}



No summary