DATA MINING 1

Classification Model Evaluation

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Revisited slides from Lecture Notes for Chapter 3 “Introduction to Data Mining”, 2nd Edition by Tan, Steinbach, Karpatne, Kumar

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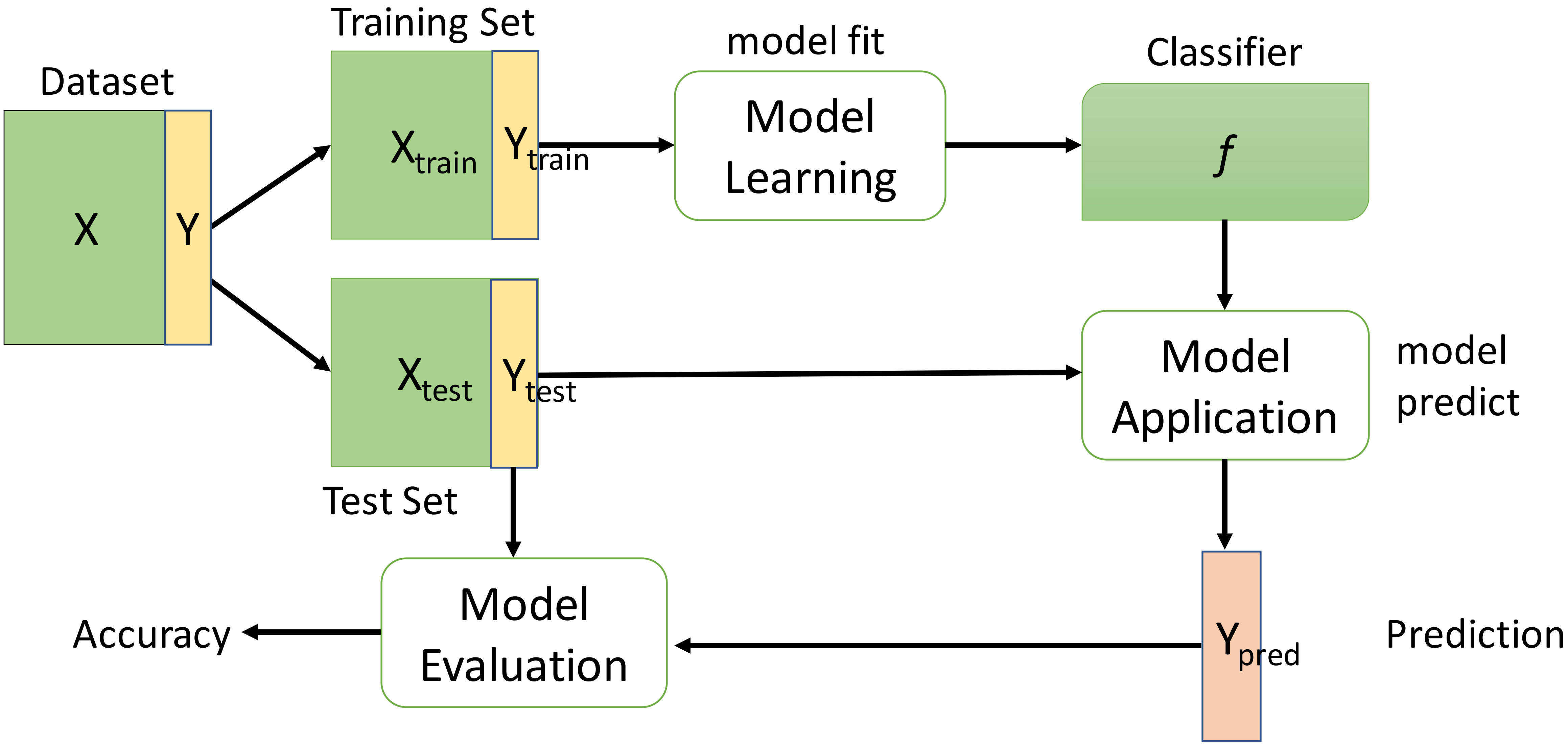
What is Classification?



Model Evaluation

Model Evaluation

- Metrics for Performance Evaluation
  - How to evaluate the performance of a model?
- Methods for Performance Evaluation
  - How to obtain reliable estimates?
- Methods for Model Comparison
  - How to compare the relative performance among competing models?

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Problem Setting

- Let suppose we have a vector y of actual/real class labels, i.e.,
- y = [0 0 0 1 1 1 0 1 0 1 0 1 1 1 0 0]

- Let name y' the vector returned by a trained model f, i.e.,
- y' = [0 0 1 1 1 0 0 1 0 1 1 1 0 0 0 0]

Metrics for Performance Evaluation

- Focus on the predictive capability of a model
  - Rather than how fast it takes to classify or build models, scalability, etc.
- **Confusion Matrix:**

	PREDICTED CLASS		
ACTUAL CLASS		Class=Yes	Class=No
	Class=Yes	a	b
	Class=No	c	d

a: TP (true positive)

b: FN (false negative)

c: FP (false positive)

d: TN (true negative)

Metrics for Performance Evaluation

- y = [0 0 0 1 1 1 0 1 0 1 0 1 1 1 0 0]
- y' = [0 0 1 1 1 0 0 1 0 1 1 1 0 0 0 0]
- TN FP FN TP

Metrics for Performance Evaluation…

	PREDICTED CLASS		
ACTUAL CLASS		Class=Yes	Class=No
	Class=Yes	a (TP)	b (FN)
	Class=No	c (FP)	d (TN)

Most widely-used metric:

$$\text{Accuracy} = \frac{a+d}{a+b+c+d} = \frac{TP+TN}{TP+TN+FP+FN}$$

Limitation of Accuracy

- Consider a 2-class problem
  - Number of Class 0 examples = 9990
  - Number of Class 1 examples = 10

- If model predicts everything to be class 0, accuracy is 9990/10000 = 99.9 %
- Accuracy is misleading because model does not detect any class 1 example

Cost-Sensitive Measures

$$\text{Precision (p)} = \frac{TP}{TP + FP}$$

$$\text{Recall (r)} = \frac{TP}{TP + FN}$$

$$\text{F-measure (F)} = \frac{2rp}{r + p} = \frac{2TP}{2TP + FN + FP}$$

- Precision is biased towards C(Yes|Yes) & C(Yes|No)
- Recall is biased towards C(Yes|Yes) & C(No|Yes)
- F-measure is biased towards all except C(No|No)

$$\text{Weighted Accuracy} = \frac{w_1 a + w_4 d}{w_1 a + w_2 b + w_3 c + w_4 d}$$

Cost Matrix

	PREDICTED CLASS		
ACTUAL CLASS	C(i|j)	**Class=Yes**	**Class=No**
	Class=Yes	C(Yes|Yes)	C(No|Yes)
	Class=No	C(Yes|No)	C(No|No)

C(i|j): Cost of misclassifying class j example as class i

Computing Cost of Classification

Cost Matrix	PREDICTED CLASS		
ACTUAL CLASS	C(i|j)	+	-
	+	-1	100
	-	1	0

Model M_1	PREDICTED CLASS		
ACTUAL CLASS		+	-
	+	150	40
	-	60	250

Model M_2	PREDICTED CLASS		
ACTUAL CLASS		+	-
	+	250	45
	-	5	200

Accuracy = 80%

Cost = 3910

Accuracy = 90%

Cost = 4255

Cost vs Accuracy

Count	PREDICTED CLASS		
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a	b
	Class=No	c	d

Cost	PREDICTED CLASS		
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	p	q
	Class=No	q	p

Accuracy is proportional to cost if

1. C(Yes|No)=C(No|Yes) = q
2. C(Yes|Yes)=C(No|No) = p

$N = a + b + c + d$

$\text{Accuracy} = (a + d)/N$

$$\begin{aligned}\text{Cost} &= p\,(a + d) + q\,(b + c)\\ &= p\,(a + d) + q\,(N - a - d)\\ &= q\,N - (q - p)(a + d)\\ &= N\,[q - (q-p) \times \text{Accuracy}]\end{aligned}$$

Binary vs Multiclass Evaluation

	PREDICTED CLASS		
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	TP	FN
	Class=No	FP	TN

	PREDICTED CLASS			
		Class=A	Class=B	Class=C
ACTUAL CLASS	Class=A	TP-A		
	Class=B		TP-B	
	Class=C			TP-C

Accuracy = TP+TN / (TP+TN+FN+FP) = # correct / N

Accuracy = # correct / N = (TP-A + TP-B + TP-C) / N

Multiclass Evaluation

	PREDICTED CLASS			
ACTUAL CLASS		Class=A	Class=B	Class=C
	Class=A	TP-A	a	b
	Class=B	c	TP-B	d
	Class=C	e	f	TP-C

$$\text{Precision (p)} = \frac{TP}{TP + FP}$$

$$\text{Recall (r)} = \frac{TP}{TP + FN}$$

$$\text{F-measure (F)} = \frac{2rp}{r + p} = \frac{2TP}{2TP + FN + FP}$$

A	PREDICTED CLASS		
ACTUAL CLASS		Class=A	Class=Not A
	Class=A	TP-A	a + b
	Class=Not A	c + e	TP-B + TP-C + d + f

B	PREDICTED CLASS		
ACTUAL CLASS		Class=B	Class=Not B
	Class=B	TP-B	c + d
	Class=Not B	a + f	TP-A + TP-C + b + e

C	PREDICTED CLASS		
ACTUAL CLASS		Class=C	Class=Not C
	Class=C	TP-C	e + f
	Class=Not C	b + d	TP-A + TP-B + a + c

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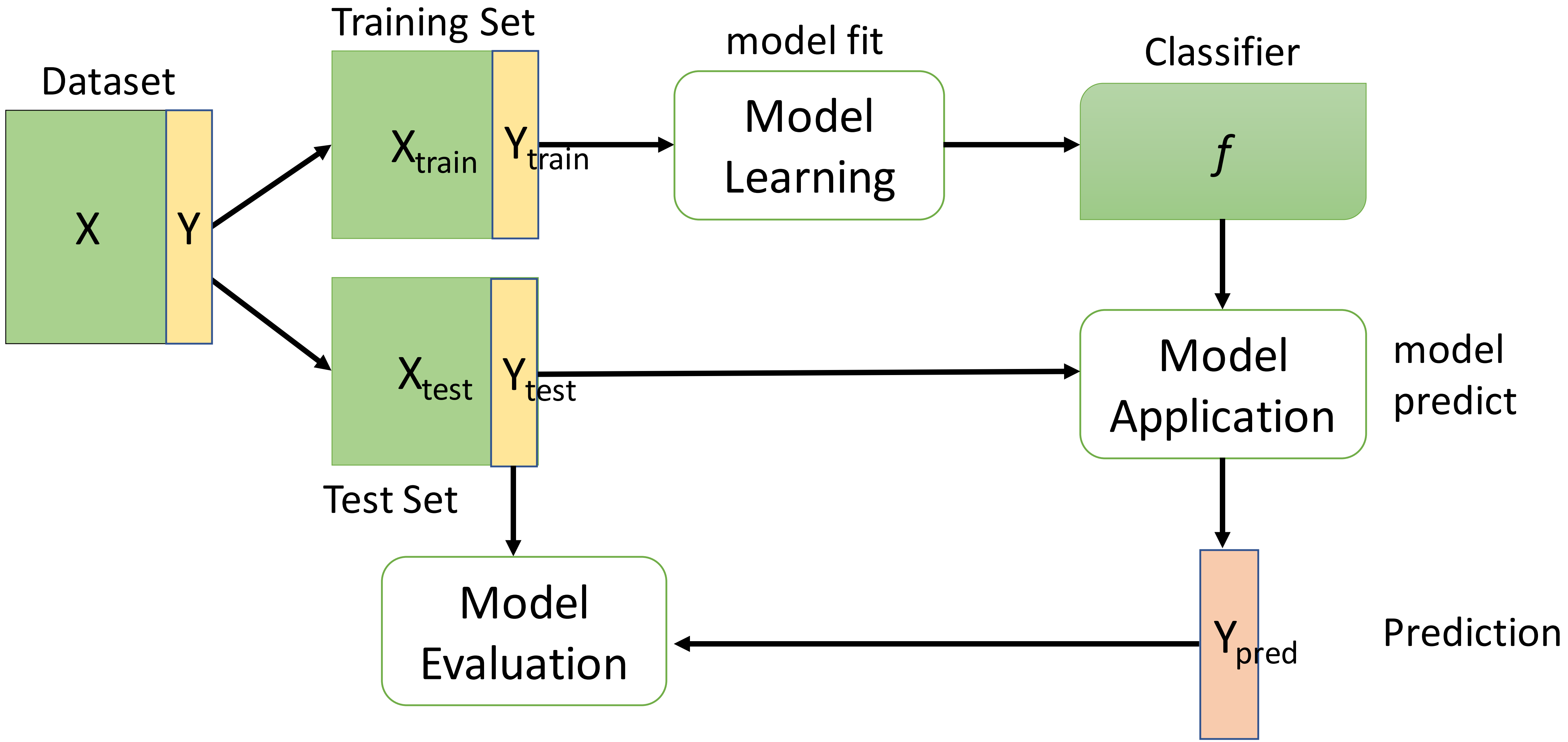
Methods for Evaluation



Parameter Tuning

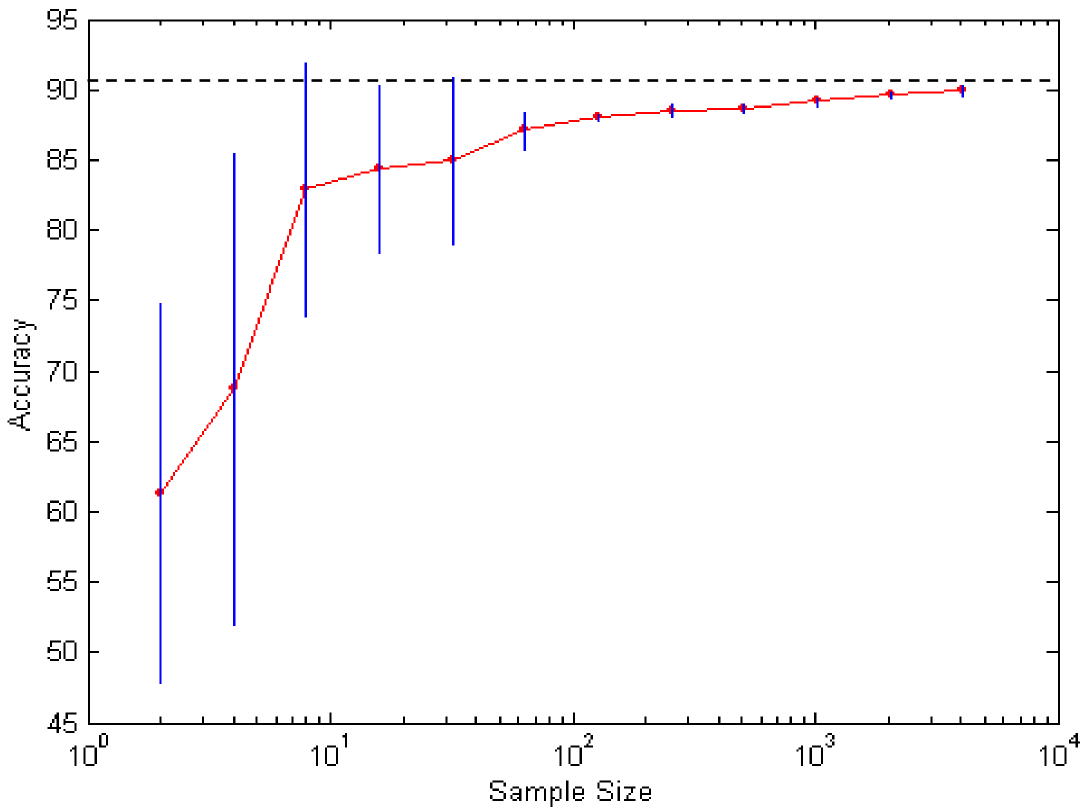
- It is important that the test data is not used in any way to create the classifier
- Some learning schemes operate in two stages:
    - **Stage 1**: builds the basic structure
    - **Stage 2**: optimizes parameter settings
    - **The test data can't be used for parameter tuning!**
    - Proper procedure uses three sets:
        - training data,
        - validation data,
        - test data
    - **Validation data is used to optimize parameters**
- Once evaluation is complete, all the data can be used to build the final classifier
- Generally, the larger the training data the better the classifier
- The larger the test data the more accurate the error estimate

Methods for Performance Evaluation

- How to obtain a reliable estimate of performance?

- Performance of a model may depend on other factors besides the learning algorithm:
  - Class distribution
  - Cost of misclassification
  - Size of training and test sets

Learning Curve



- Learning curve shows how accuracy changes with varying sample size
- Requires a sampling schedule for creating learning curve:

Effect of small sample size:

- Bias in the estimate
- Variance of estimate

1. How much a classification model benefits from adding more training data?

2. Does the model suffer from a variance error or a bias error?

Methods of Estimation

- Holdout
  - Reserve 2/3 for training and 1/3 for testing
- Random subsampling
  - Repeated holdout
- Cross validation
  - Partition data into k disjoint subsets
  - k-fold: train on k-1 partitions, test on the remaining one
  - Leave-one-out: k=n
- Stratified sampling
  - oversampling vs undersampling
- Bootstrap
  - Sampling with replacement

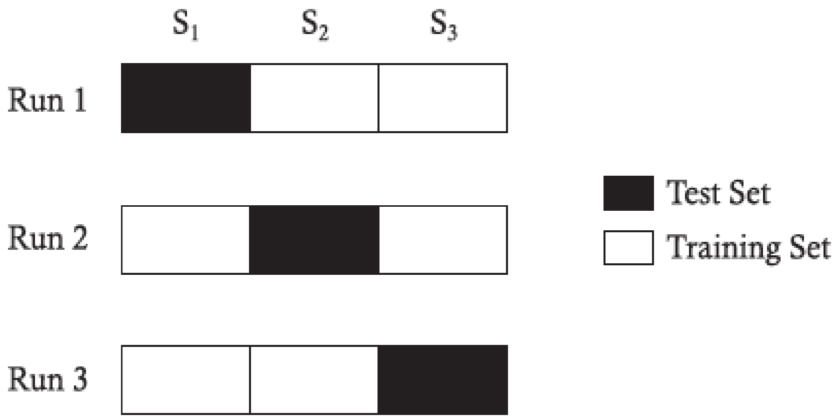
Holdout

- The holdout method reserves a certain amount for **testing** and uses the remainder for **training**
- Usually, **one third for testing**, the rest for training.
- Typical quantities are 60%-40%, 66%-34%, 70%-30%.
- For small or “unbalanced” datasets, **samples might not be representative**
  - For instance, few or none instances of some classes
- Stratified sample
  - **Balancing the data**
  - Make sure that each class is represented with approximately equal proportions in both subsets

Repeated Holdout

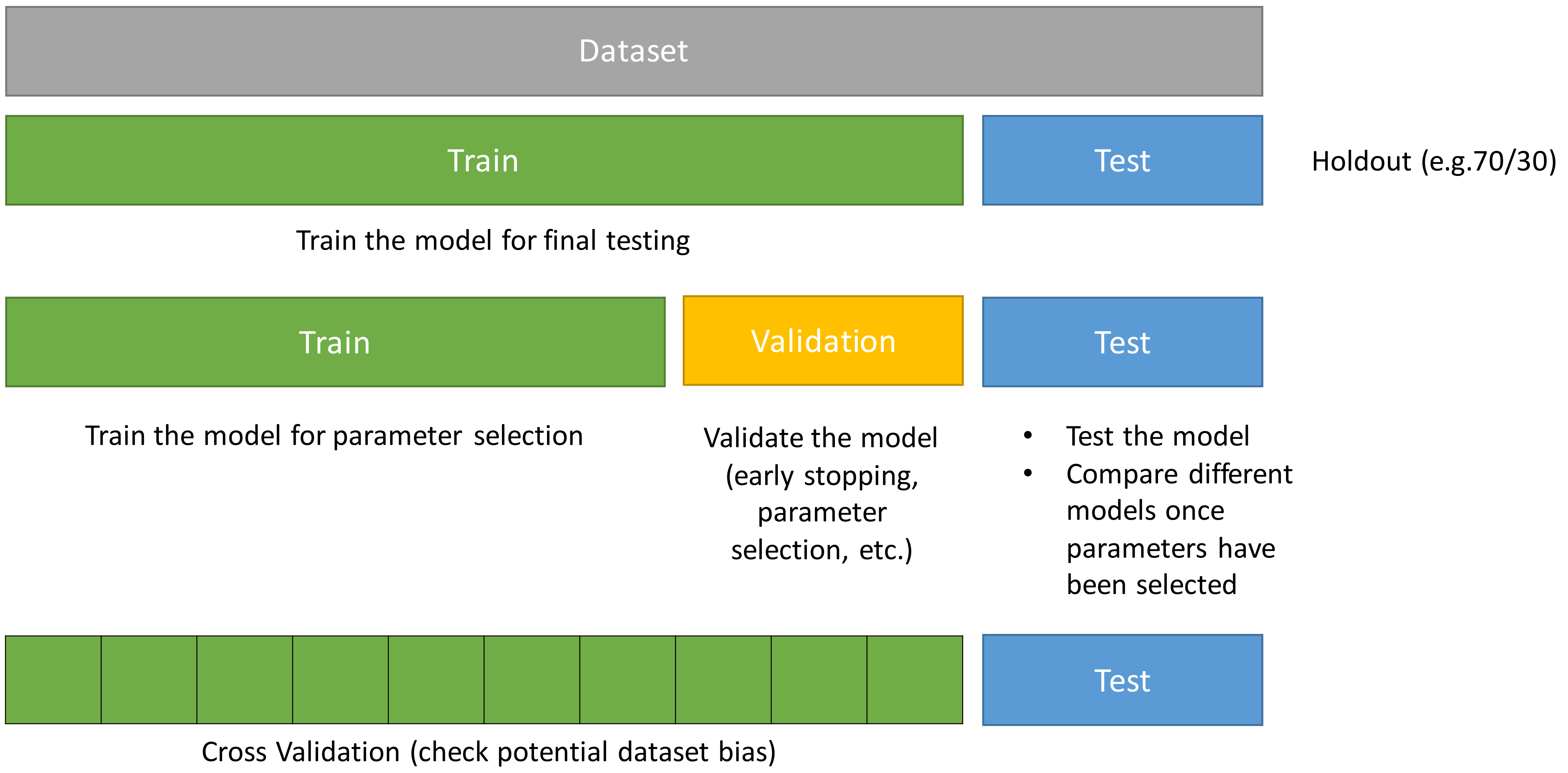
- Holdout estimate can be made more reliable by **repeating the process with different subsamples**
  - In each iteration, a certain proportion is **randomly selected for training** (possibly with stratification)
  - The error rates on the different iterations are **averaged** to yield an overall error rate
- This is called the **repeated holdout method**
- Still not optimum: the different test sets overlap

Cross Validation

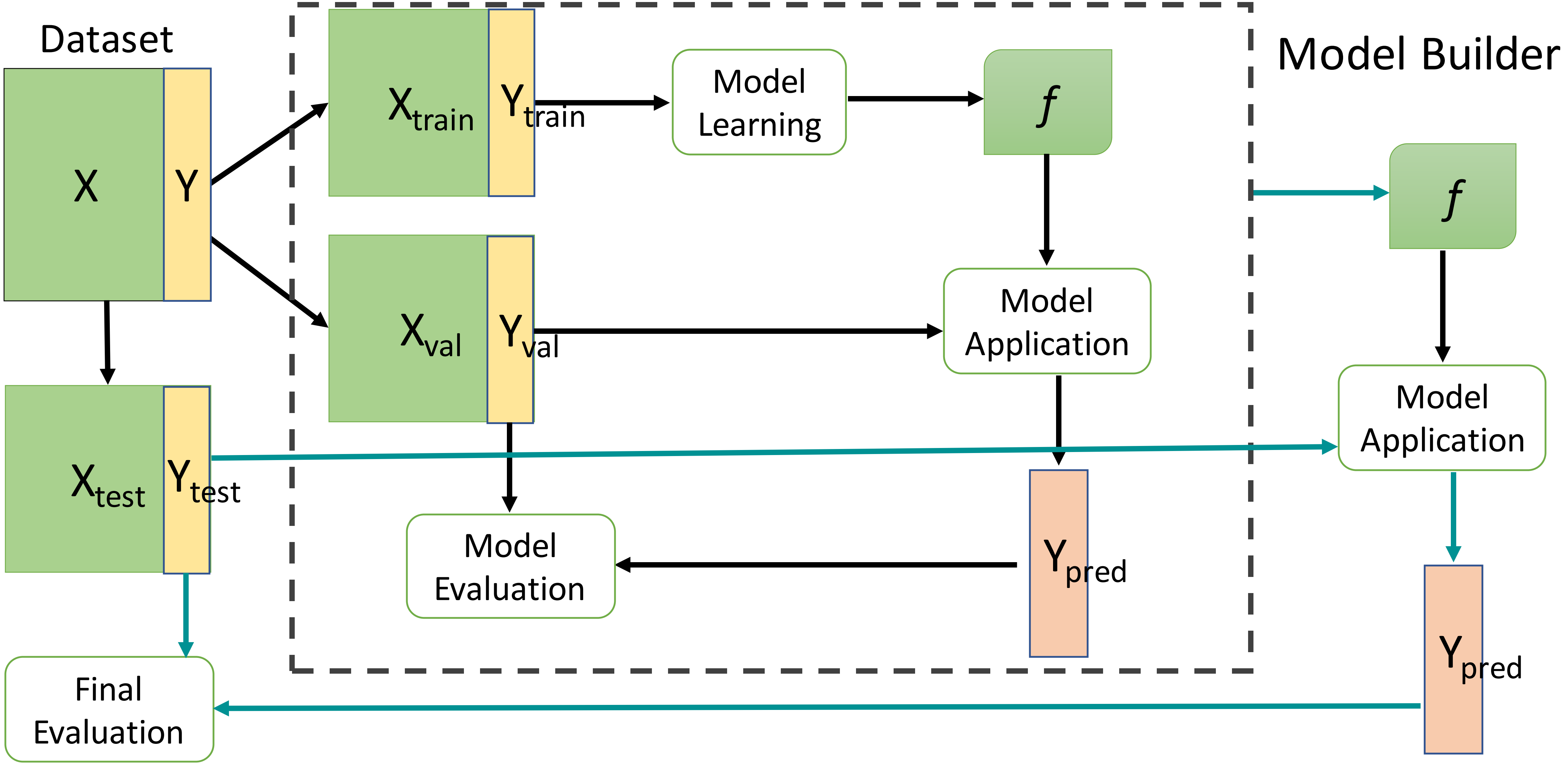


- Avoids overlapping test sets
  - **First step:** data is split into k subsets of equal size
  - **Second step:** each subset in turn is used for testing and the remainder for training
- This is called **k-fold cross-validation**
- Often the subsets are stratified before cross-validation is performed
- The **error estimates** are **averaged** to yield an overall error estimate
- **Even better:** repeated stratified cross-validation E.g. ten-fold cross-validation is repeated ten times and results are averaged (reduces the variance)

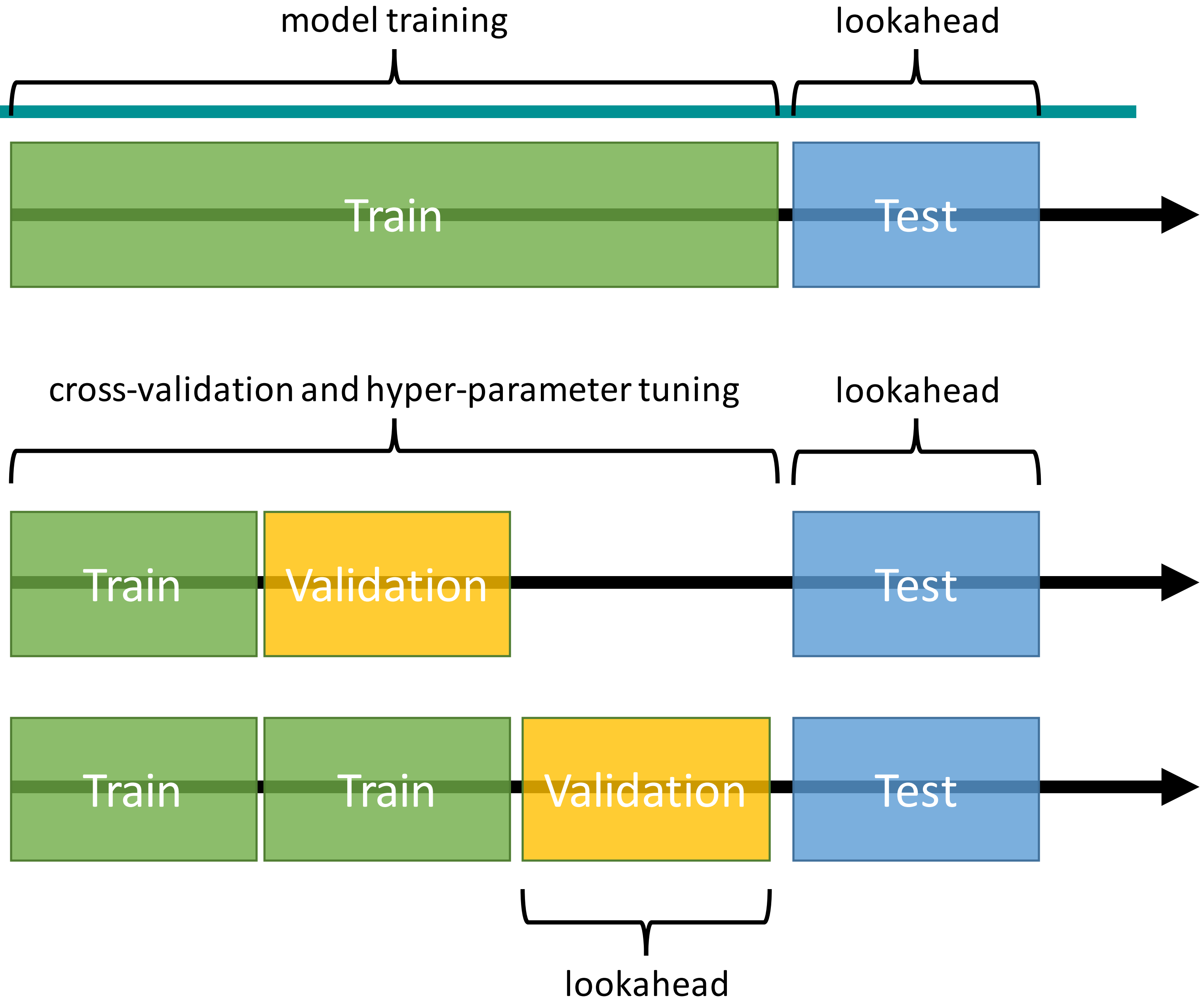
Data Partitioning



Evaluation: Training, Validation, Tests



Cross Validation with Time



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ROC (Receiver Operating Characteristic)

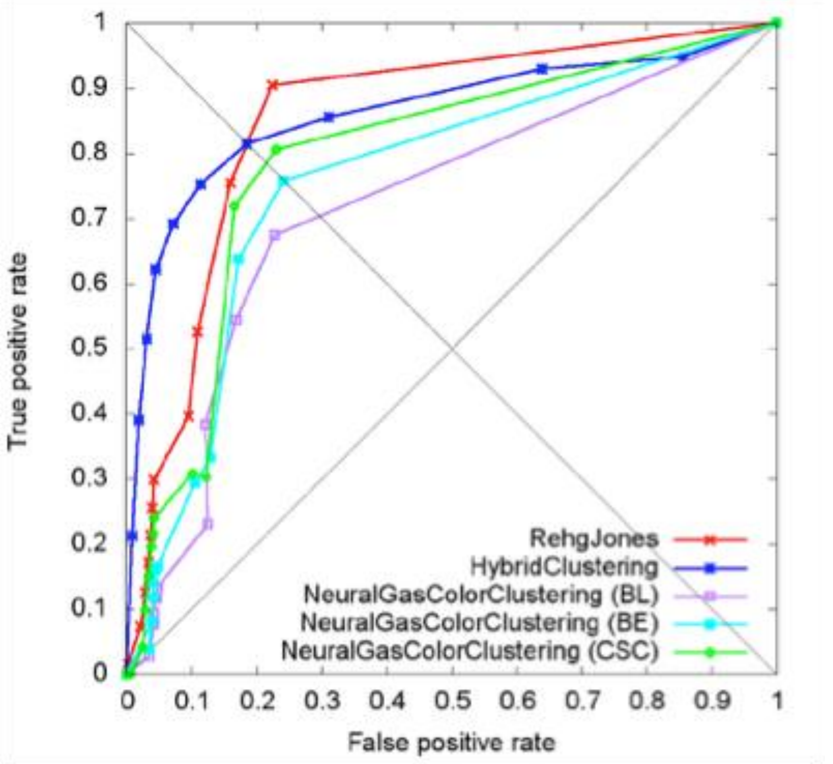
- Developed in 1950s for signal detection theory to analyze noisy signals
  - Characterize the trade-off between positive hits and false alarms

- ROC curve plots TP (on the y-axis) against FP (on the x-axis)

- **Performance of each classifier represented as a point on the ROC curve**
  - changing the threshold of algorithm, sample distribution or cost matrix changes the location of the point

Receiver Operating Characteristic Curve

- It illustrates the ability of a binary classifier as its discrimination threshold THR is varied.
- The ***ROC*** curve is created by plotting the true positive rate (TPR) against the false positive rate (FPR) at various THR.
- The TPR = TP / (TP + FN) is also known as ***sensitivity***, ***recall*** or probability of detection.
- The FPR = FP / (TN + FP) is also known as probability of ***false alarm*** and can be calculated as (1 − specificity).



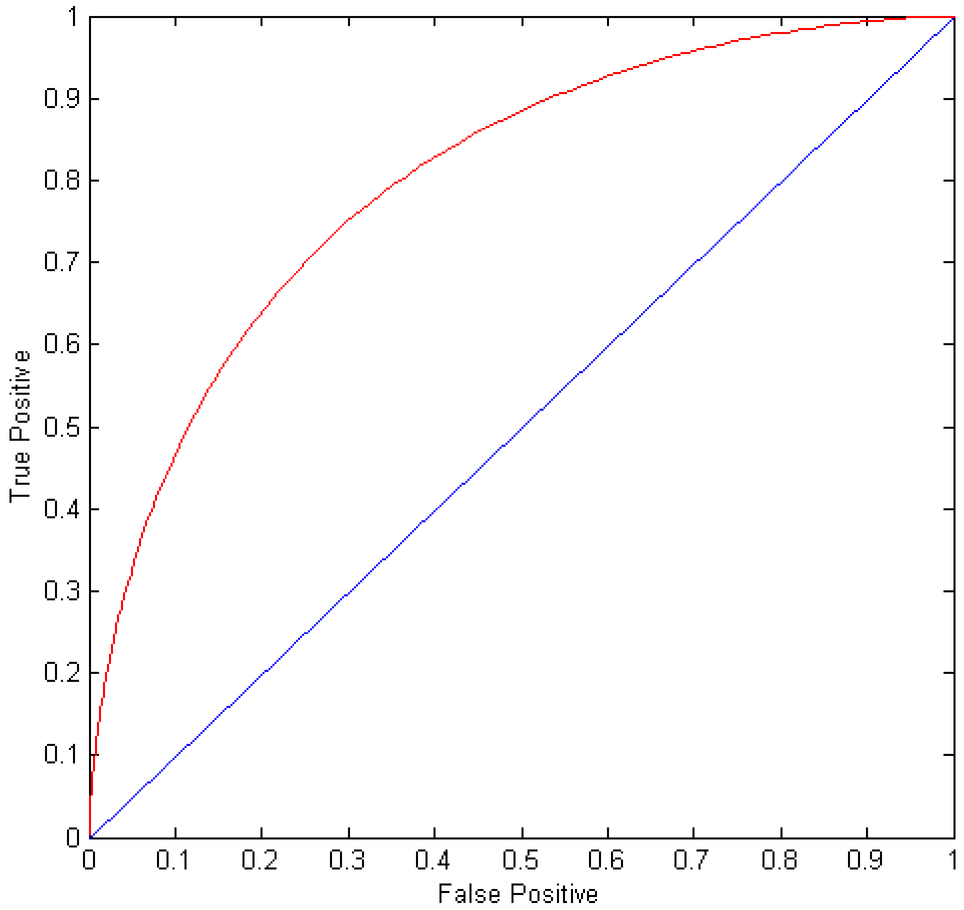
https://towardsdatascience.com/understanding-auc-roc-curve-68b2303cc9c5

ROC Curve

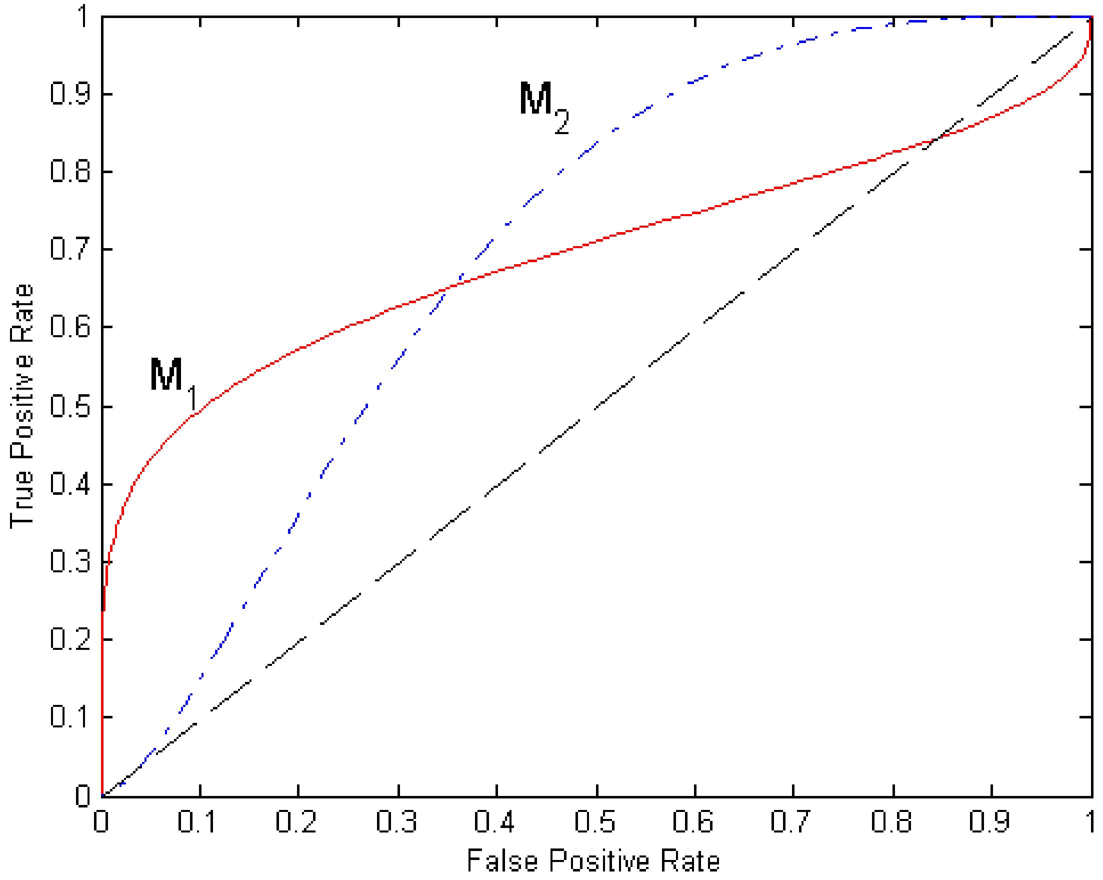
(TP,FP):

- (0,0): declare everything
  to be negative class
- (1,1): declare everything
  to be positive class
- (0,1): ideal

- Diagonal line:
  - Random guessing
  - Below diagonal line:
    - prediction is opposite of the true class



Using ROC for Model Comparison



- No model consistently outperform the other
  - M_1 is better for small FPR
  - M_2 is better for large FPR
- Area Under the ROC curve
  - Ideal: Area = 1
  - Random: Area = 0.5

How to Construct the ROC curve

Instance	P(+|A)	True Class
1	0.95	+
2	0.93	+
3	0.87	-
4	0.85	-
5	0.85	-
6	0.85	+
7	0.76	-
8	0.53	+
9	0.43	-
10	0.25	+

- Use classifier that produces posterior probability for each test instance P(+|A)
- Sort the instances according to P(+|A) in decreasing order
- Apply threshold at each unique value of P(+|A)
- Count the number of TP, FP, TN, FN at each threshold
- TP rate, TPR = TP/(TP+FN)
- FP rate, FPR = FP/(FP + TN)

TPR = TP / (TP + FN)
FPR = FP / (TN + FP)

How to Construct the ROC curve

Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP											
FP											
TN											
FN											
TPR											
FPR											

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How to Construct the ROC curve

TPR = TP / (TP + FN)

FPR = FP / (TN + FP)

Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5										
FP	5										
TN	0										
FN	0										
TPR	1										
FPR	1										

Inst.	P(+|A)	True Class
1	0.95	+
2	0.93	+
3	0.87	-
4	0.85	-
5	0.85	-
6	0.85	+
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8	0.53	+
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How to Construct the ROC curve

TPR = TP / (TP + FN)
FPR = FP / (TN + FP)

Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4									
FP	5	5									
TN	0	0									
FN	0	1									
TPR	1	0.8									
FPR	1	1									

Inst.	P(+|A)	True Class
1	0.95	+
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How to Construct the ROC curve

TPR = TP / (TP + FN)
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Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4	4								
FP	5	5	4								
TN	0	0	1								
FN	0	1	1								
TPR	1	0.8	0.8								
FPR	1	1	0.8								

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TPR = TP / (TP + FN)
FPR = FP / (TN + FP)

How to Construct the ROC curve

Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4	4	3							
FP	5	5	4	4							
TN	0	0	1	1							
FN	0	1	1	2							
→ TPR	1	0.8	0.8	0.6							
→ FPR	1	1	0.8	0.8							

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How to Construct the ROC curve

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Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4	4	3	3						
FP	5	5	4	4	3						
TN	0	0	1	1	2						
FN	0	1	1	2	2						
TPR	1	0.8	0.8	0.6	0.6						
FPR	1	1	0.8	0.8	0.6						

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TPR = TP / (TP + FN)
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Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4	4	3	3	3	3				
FP	5	5	4	4	3	2	1				
TN	0	0	1	1	2	3	4				
FN	0	1	1	2	2	2	2				
TPR	1	0.8	0.8	0.6	0.6	0.6	0.6				
FPR	1	1	0.8	0.8	0.6	0.4	0.2				

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Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4	4	3	3	3	3	2			
FP	5	5	4	4	3	2	1	1			
TN	0	0	1	1	2	3	4	4			
FN	0	1	1	2	2	2	2	3			
TPR	1	0.8	0.8	0.6	0.6	0.6	0.6	0.4			
FPR	1	1	0.8	0.8	0.6	0.4	0.2	0.2			

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FP	5	5	4	4	3	2	1	1	0		
TN	0	0	1	1	2	3	4	4	5		
FN	0	1	1	2	2	2	2	3	3		
TPR	1	0.8	0.8	0.6	0.6	0.6	0.6	0.4	0.4		
FPR	1	1	0.8	0.8	0.6	0.4	0.2	0.2	0		

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How to Construct the ROC curve

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TP	5	4	4	3	3	3	3	2	2	1	
FP	5	5	4	4	3	2	1	1	0	0	
TN	0	0	1	1	2	3	4	4	5	5	
FN	0	1	1	2	2	2	2	3	3	4	
→ TPR	1	0.8	0.8	0.6	0.6	0.6	0.6	0.4	0.4	0.2	
→ FPR	1	1	0.8	0.8	0.6	0.4	0.2	0.2	0	0	

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How to Construct the ROC curve

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FP	5	5	4	4	3	2	1	1	0	0	0
TN	0	0	1	1	2	3	4	4	5	5	5
FN	0	1	1	2	2	2	2	3	3	4	5
TPR	1	0.8	0.8	0.6	0.6	0.6	0.6	0.4	0.4	0.2	0
FPR	1	1	0.8	0.8	0.6	0.4	0.2	0.2	0	0	0

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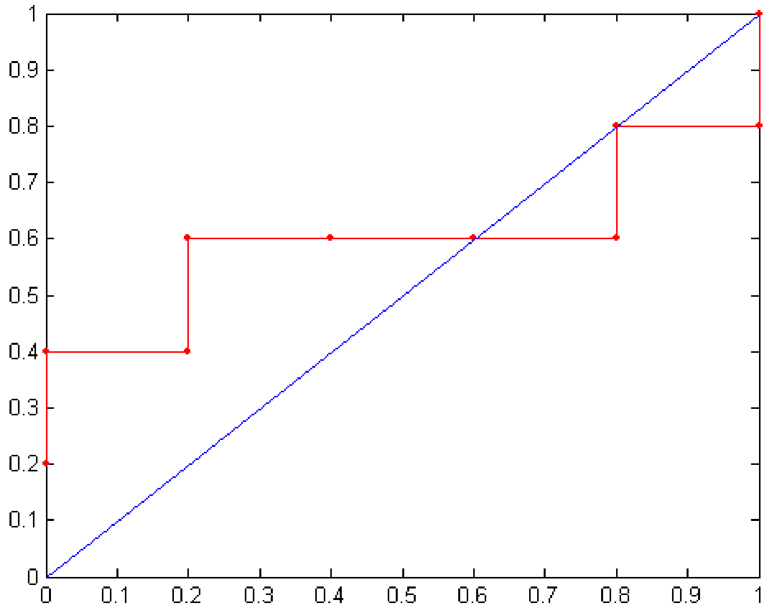
FN	0	1	1	2	2	2	2	3	3	4	5
TPR	1	0.8	0.8	0.6	0.6	0.6	0.6	0.4	0.4	0.2	0
FPR	1	1	0.8	0.8	0.6	0.4	0.2	0.2	0	0	0

TPR = TP / (TP + FN)

FPR = FP / (TN + FP)

ROC Curve:



Inst.	P(+|A)	True Class
1	0.95	+
2	0.93	+
3	0.87	-
4	0.85	-
5	0.85	-
6	0.85	+
7	0.76	-
8	0.53	+
9	0.43	-
10	0.25	+

Lift Chart

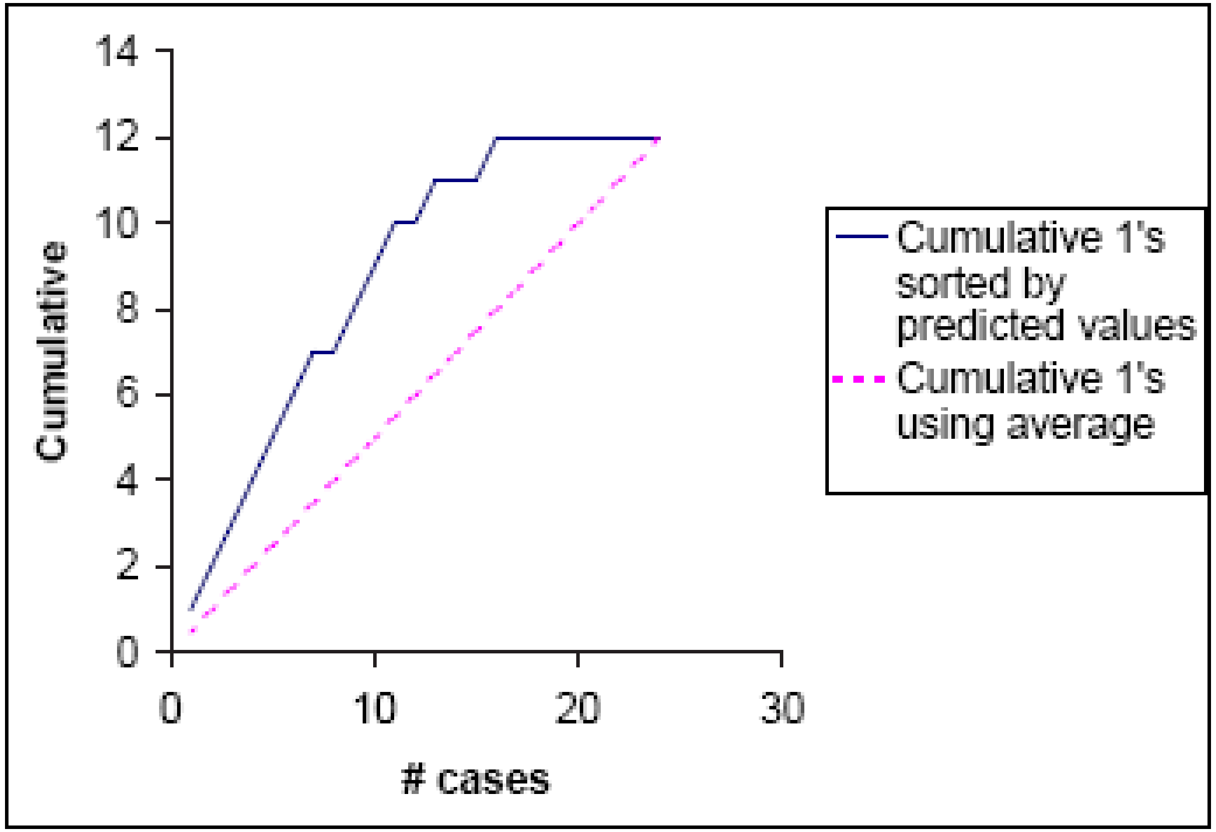
http://www2.cs.uregina.ca/~dbd/cs831/notes/lift_chart/lift_chart.html
http://mlwiki.org/index.php/Cumulative_Gain_Chart

- The lift curve is a popular technique in direct marketing.
- The input is a dataset that has been “scored’’ by appending to each case the estimated probability that it will belong to a given class.
- The cumulative ***lift chart*** (also called ***gains chart***) is constructed with the cumulative number of cases (descending order of probability) on the x-axis and the cumulative number of true positives on the y-axis.
- The dashed line is a reference line. For any given number of cases (the x-axis value), it represents the expected number of positives we would predict if we did not have a model but simply selected cases at random. It provides a benchmark against which we can see performance of the model.

Notice: “Lift chart” is a rather general term, often used to identify also other kinds of plots. Don’t get confused!

Lift Chart – Example

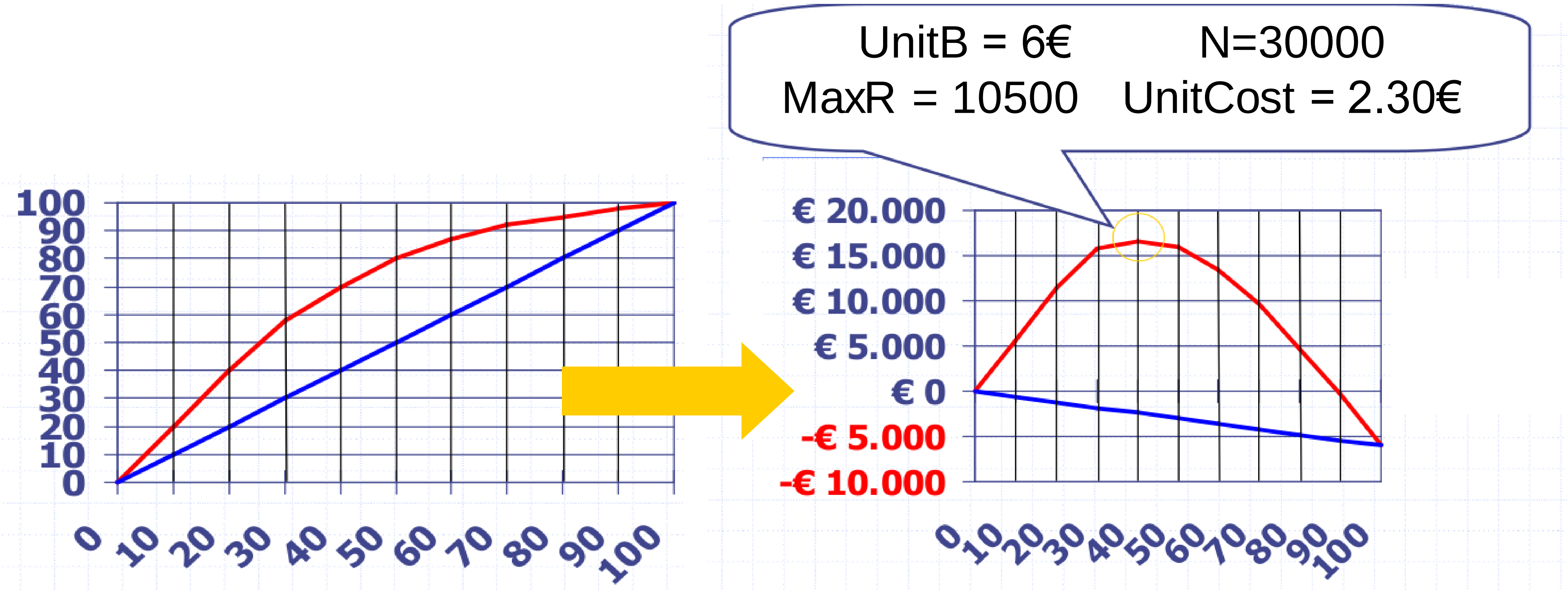
Serial no.	Predicted prob of 1	Actual Class	Cumulative Actual class
1	0.995976726	1	1
2	0.987533139	1	2
3	0.984456382	1	3
4	0.980439587	1	4
5	0.948110638	1	5
6	0.889297203	1	6
7	0.847631864	1	7
8	0.762806287	0	7
9	0.706991915	1	8
10	0.680754087	1	9
11	0.656343749	1	10
12	0.622419543	0	10
13	0.505506928	1	11
14	0.47134045	0	11
15	0.337117362	0	11
16	0.21796781	1	12
17	0.199240432	0	12
18	0.149482655	0	12
19	0.047962588	0	12
20	0.038341401	0	12
21	0.024850999	0	12
22	0.021806029	0	12
23	0.016129906	0	12
24	0.003559986	0	12



Lift Chart – Application Example

- From Lift chart we can easily derive an "economical value" plot, e.g. in target marketing.
- Given our predictive model, how many customers should we target to maximize income?
- Profit = UnitB*MaxR*Lift(X) - UnitCost*N*X/100
- UnitB = unit benefit, UnitCost = unit postal cost
- N = total customers
- MaxR = expected potential respondents in all population (N)
- Lift(X) = lift chart value for X, in [0,..,1]

Lift Chart – Application Example



References

- Chapter 3. Classification: Basic Concepts and Techniques.