COMP472: Artificial Intelligence
Machine Learning
Evaluation

video #5

- Russell & Norvig: Sections 19.4

Today

1. Introduction to ML
2. Naïve Bayes Classification Model #1
   a. Application to Spam Filtering
3. Decision Trees Model #2
4. Evaluation 

5. Unsupervised Learning
6. Neural Networks
   a. Perceptrons
   b. Multi Layered Neural Networks

Data Sets

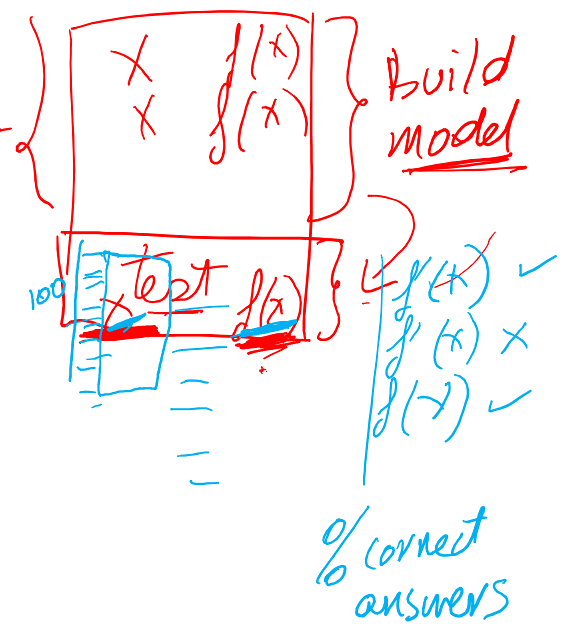
supervised learning

- How do you know if what you learned is correct?
- You run your classifier on a data set of unseen examples (that you did not use for training) for which you know the correct classification

- Split data set into 3 sub-sets
  1. Actual **training** set (~80%)
  2. **Validation** set (~20%)
  3. **Test** set

$\left.\begin{array}{l}\text{Actual training set (~80\%)}\\ \text{Validation set (~20\%)}\end{array}\right\}$ ~80%

Test set } ~20%



Standard Methodology

1. Collect a large set of examples (all with correct classifications)
2. Divide collection into training, validation and test set

Loop:

3. Apply learning algorithm to the training set to learn the parameters
4. Measure performance with the validation set, and adjust hyper-parameters* to improve performance

5. Measure performance with the test set

- DO NOT LOOK AT THE TEST SET until step 5.

Parameters: basic values learned by the ML model. eg.

- for NB: prior & conditional probabilities likelihood
- for DTs: features to split
- for ANNs: weights

Hyper-parameters: parameters used to set up the ML model. eg.

- for NB: value of delta for smoothing, ex. add-1 0.5 0.3
- for DTs: pruning level
- for ANNs: nb of hidden layers, nb of nodes per layer…

Metrics

- 1 Accuracy
  - % of instances of the test set the algorithm correctly classified
  - when all classes are equally important and represented

f(x)

balanced dataset

- 2 Recall, Precision & F-measure
  - when one class is more important and the others

80% dolph
10% dog
10% cat

not balanced

no-fracture 99%

fracture 1%

Accuracy

- % of instances of the test set the algorithm correctly classifies
- when all classes are equally important and represented
- problem:
  - when one class (eg. sick) is more important and the others
  - eg. when data set is unbalanced

correct classification

prediction

5 mistakes

	Target	system 1
X1	sick	ok ×
X2	sick	ok ×
X3	sick	ok ×
X4	sick	ok ×
X5	sick	ok ×
X6	ok	ok ✓
X7	ok	ok ✓
…	…	…
…	…	…
X500	ok	ok ✓
Accuracy		495/500 = 99% !

Recall, Precision

- Recall: What proportion of the instances in the class of interest (eg. sick) are labelled correctly?
- Precision: What proportion of instances labeled with the class of interest (eg. sick) are actually correct?

		Correct class	
		instance should be in class C	instance should not be in class C
Model prediction	instance is put in class C	True Positive (TP)	False Positive (FP)
	instance is not put in class C	False Negative (FN)	True Negative (TN)

$$\text{Precision} = \frac{TP}{TP+FP}$$

TP: nb of instances that are in class C and that the model identified as class C

TP+FP: nb of instances that the model labelled as class C

$$\text{Recall} = \frac{TP}{TP+FN}$$

TP: nb of instances that are in class C and that the model identified as class C

TP+FN: All instances that are in class C

Example

correct classification

class of interest = sick

	Target	system 1	system 2	system 3
X1	sick	sick ✓	sick ✓	ok ×
X2	sick	ok ×	ok ×	sick ✓
X3	sick	ok ×	sick ✓	sick ✓
X4	sick	ok ×	sick ✓	sick ✓
X5	sick	ok ×	ok ×	sick ✓
X6	ok	ok ✓	ok ✓	sick ×
X7	ok	ok ✓	ok ✓	sick ×
..	ok	ok ✓	ok ✓	ok ✓
..	ok	ok ✓	ok ✓	ok ✓
X500	ok	ok ✓	ok ✓	ok ✓
Accuracy		496/500 = 99%	498/500 = 99.6%	498/500 = 99.6%
Precision		1/1 = 100%	3/3 = 100%	4/6 = 66.7%
Recall		1/5 = 20%	3/5 = 60%	4/5 = 80%

Which system is better?

A Single Measure

- cannot take mean of P&R
  - if R = 50% P = 50% M = 50%
  - if R = 100% P = 10% M = 55% (not fair)

1. take harmonic mean
   - which penalizes extreme values

$$HM = \frac{2}{\frac{1}{R} + \frac{1}{P}}$$

HM is high only when both P&R are high

if R = 50% and P = 50% HM = 50%

if R = 100% and P = 10% HM = 18.2%

2. if P and R should not have the same importance in the problem domain, take weighted harmonic mean

$$WHM = \frac{1}{\frac{1}{2}\frac{1}{R} + \frac{1}{2}\frac{1}{P}}$$ // if weight R = weight P = $\frac{1}{2}$

$\frac{1}{2} + \frac{1}{2} = 1$

$$WHM = \frac{1}{\frac{1}{a}\frac{1}{R} + \frac{1}{b}\frac{1}{P}}$$ // if weight R = $\frac{1}{a}$ weight P = $\frac{1}{b}$ and $\boxed{\frac{1}{a} + \frac{1}{b} = 1}$

Weighted Harmonic Mean of P&R

$$WHM = \frac{1}{\frac{1}{a}\frac{1}{R} + \frac{1}{b}\frac{1}{P}}$$ // if weight R = $\frac{1}{a}$ weight P = $\frac{1}{b}$ and $\frac{1}{a} + \frac{1}{b} = 1$

1. let $w_R = \frac{\delta}{\delta+1}$ $w_P = \frac{1}{\delta+1}$ // so that $w_R + w_P = \frac{\delta+1}{\delta+1} = 1$

$$WHM = \frac{1}{\left(\frac{\delta}{\delta+1}\right)\frac{1}{R} + \left(\frac{1}{\delta+1}\right)\frac{1}{P}} = \frac{\delta+1}{\delta\frac{1}{R} + 1\frac{1}{P}} = \frac{(\delta+1)PR}{\delta P + 1R}$$

2. let $\delta = \beta^2$

$$WHM = \boxed{\frac{(\beta^2+1)PR}{\beta^2 P + 1R}}$$ // called the F-measure

F-measure

- A weighted harmonic mean of precision and recall

$$F_{\beta} = \frac{(\beta^2 + 1)PR}{(\beta^2 P + R)}$$

- β represents the relative importance of recall to precision
  - when β = 1
    - F1 measure
    - precision & recall have same importance
  - when β > 1
    - recall is given more weigth
    - e.g. F_2 measure, recall is considered 2x more important than precision
  - when β < 1
    - precision is given more weigth
    - e.g. $F_{0.5}$ measure, precision is considered 2x more important than recall

$\beta = 2$

$\beta = 0.5$

Example

	Target	system 1	system 2	system 3
X1	sick	sick ✓	sick ✓	ok ×
X2	sick	ok ×	ok ×	sick ✓
X3	sick	ok ×	sick ✓	sick ✓
X4	sick	ok ×	sick ✓	sick ✓
X5	sick	ok ×	ok ×	sick ✓
X6	ok	ok ✓	ok ✓	sick ×
X7	ok	ok ✓	ok ✓	sick ×
..	ok	ok ✓	ok ✓	ok ✓
..	ok	ok ✓	ok ✓	ok ✓
X500	ok	ok ✓	ok ✓	ok ✓
Accuracy		496/500 = 99%	498/500 = 99.6%	498/500 = 99.6%
Precision		1/1 = 100%	3/3 = 100%	4/6 = 66.7%
Recall		1/5 = 20%	3/5 = 60%	4/5 = 80%
F1-measure 2PR/(P+R)		2*100*20/ (100+20) = 33%	75%	72.9%

$\beta = 1$ $F_1 = \frac{2PR}{P+R}$

P, R and F for Multiclass Classification

- previous P, R and F are ok when 1 particular class interests us (eg. sick)
- What if several classes interest us?
- then
  - compute *per-class* P, R, F
  - and to have a single measure for all classes: combine per-class F-measures via
    - macro F-measure, or
    - weighted-average F-measure

Per-class Precision & Per-class Recall

gold

model prediction

		Correct Class			
		Cat	Dog	Fish	Total
Predicted Class	Cat	4	6	3	Σ 13
	Dog	1	2	0	3
	Fish	1	2	6	9
	Total	6	10	9	25

images

- precision of class Cat: 4/(4+6+3) = 30.8%
- precision of class Dog: 2/(1+2+0) = 66.7%
- precision of class Fish: 6/(1+2+6) = 66.7%

- recall of class Cat: 4/(4+1+1) = 66.7%
- recall of class Dog: 2/(2+6+2) = 20%
- recall of class Fish: 6/(3+0+6) = 66.7%

Per-class F1-measure

Model #1

Model #2

F1

	Precision	Recall	F1
Cat	30.8%	66.7%	42.1%
Dog	66.7%	20.0%	30.8%
Fish	66.7%	66.7%	66.7%

F1 = 2PR/(P+R)

$F_{b=1}$

- F1 of class Cat: (2 x .308 x .667) / (.308 + .667) = 0.421
- F1 of class Dog: (2 x .667 x .200) / (.667 + .200) = 0.308
- F1 of class Fish: (2 x .667 x .667) / (.667 + .667) = 0.667

Macro and Weighted-Average Measures

macro precision,
macro recall,
macro F1

	Precision	Recall	F1
Cat	30.8%	66.7%	42.1%
Dog	66.7%	20.0%	30.8%
Fish	66.7%	66.7%	66.7%
average	(30.8+66.7+66.7) / 3 = 54.7%	(66.7 + 20.0 + 66.7) / 3 = 51.1%	(42.1+30.8+66.7) = 46.5%
weighted-average	(6x30.8 // 6 cat + 10x66.7 // 10 dog + 9x66.7) // 9 fish / (6+10+9) // 25 samples = 58.1%	(6x66.7 + 10x20.0 + 6x66.7) / 25 = 48.0%	(6x42.1 + 10x30.8 + 6x66.7) / 25 = 46.4%

weighted-averaged precision,
weighted-averaged recall,
weighted-averaged F1

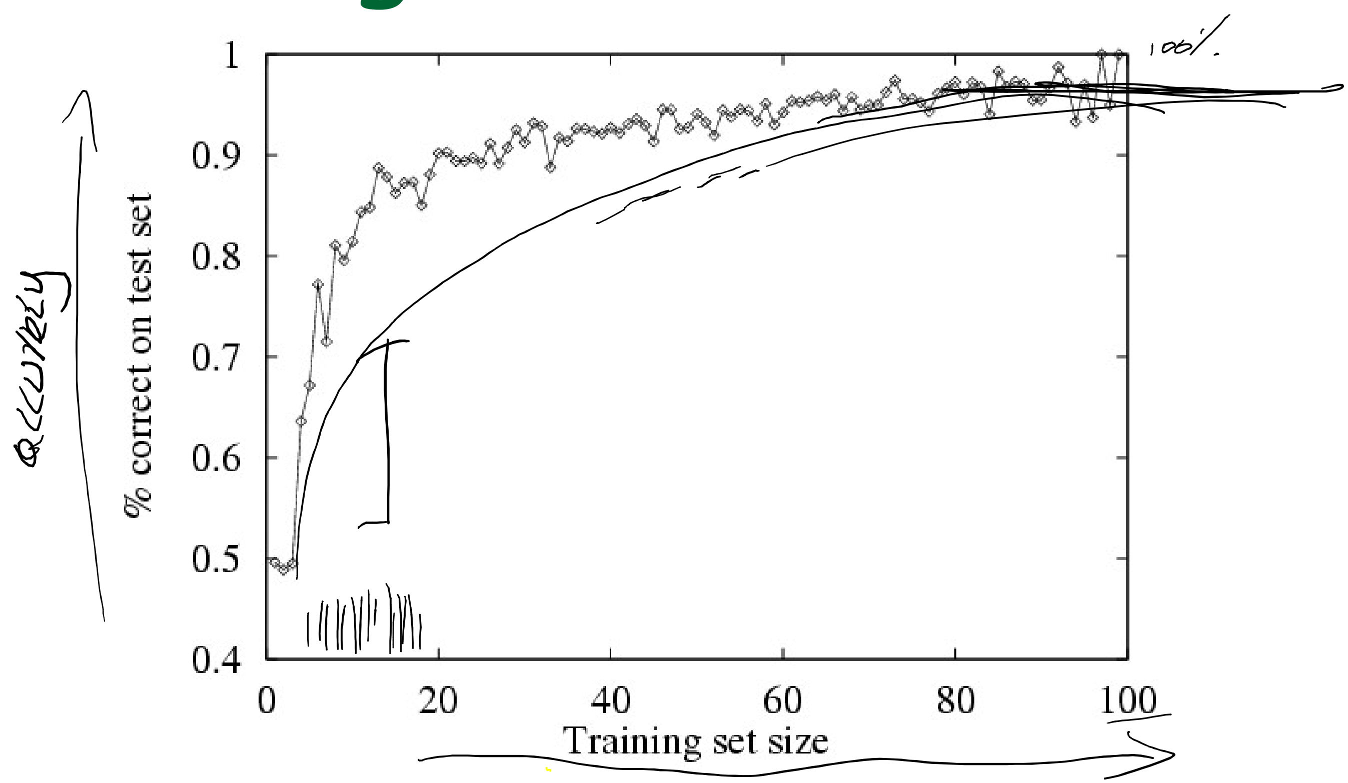
- To combine measures into a single one, we can:
  - take simple average
    - --> macro precision, macro recall, macro F1
  - take weighted average
    - ie. weight the average based on the nb of samples from each class
    - --> weighted averaged precision, weighted averaged recall, weighted averaged F1

Confusion Matrix

- to do an error analysis and find out where the model went wrong ?
- aka contingency table
- eg. 6 classes, 100 test instances

		Correct Class						
		C1	C2	C3	C4	C5	C6	Total
Predicted Class	C1	10✓	3×	0	0	3×	0	16
	C2	0	12✓	3×	4×	0	0	19
	C3	0	1×	9✓	2×	1×	2×	15
	C4	0	1×	3×	5✓	2×	0	11
	C5	0	0	3×	2×	10✓	3×	18
	C6	0	0	5×	0	5×	11✓	21
	Total	10	17	23	13	21	16	100

A Learning Curve



- Size of training set
  - the more, the better
  - but after a while, not much improvement…

source: Mitchell (1997)

Some Words on Training

- In all types of learning… watch out for:
  - Noisy input
  - Overfitting/underfitting the training data

Noisy Input

- In all types of learning… watch out for:
  - Noisy Input:
    - Two examples have the same feature-value pairs, but different outputs

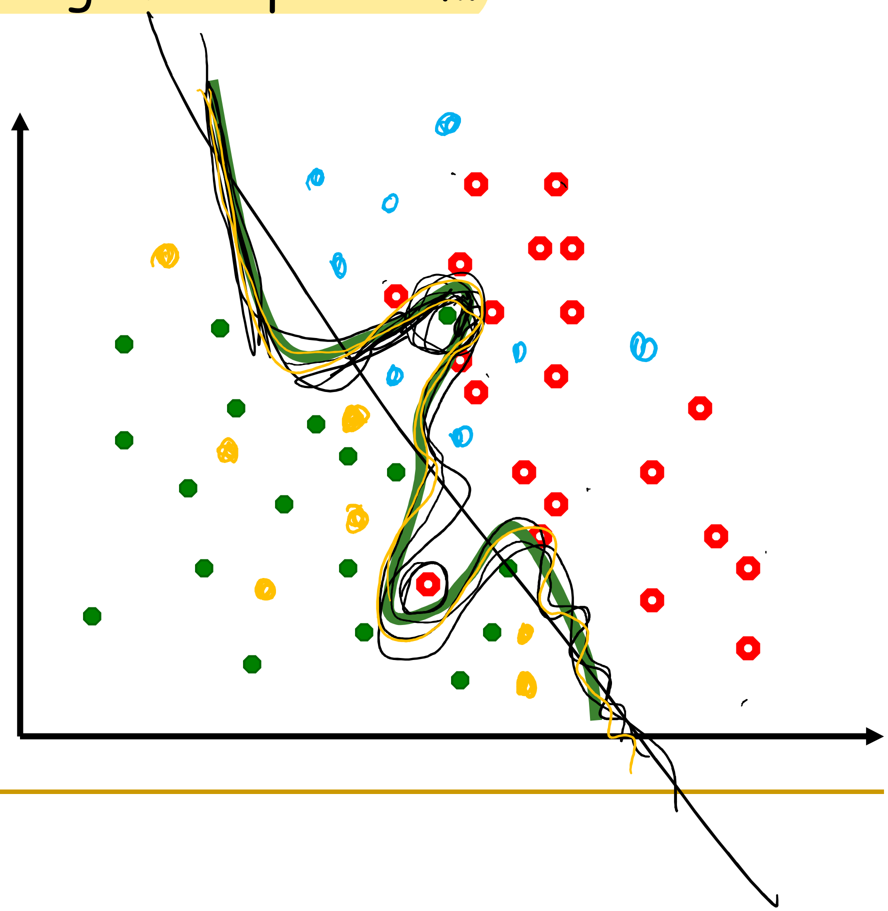
4th feature

Size	Color	NF	Shape	Output
Big	Red	a	Circle	+
Big	Red	b	Circle square	+

    - Some values of features are incorrect or missing (ex. errors in the data acquisition)
    - Some relevant attributes are not taken into account in the data set

Overfitting

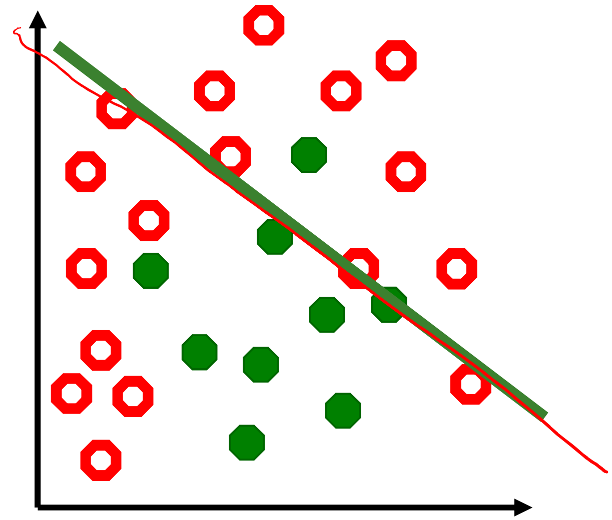
- If a large number of irrelevant features are there, we may find meaningless regularities in the data that are particular to the training data but irrelevant to the general problem.
- Complicated boundaries *overfit* the data
- they are too tuned to the particular training data at hand
- They do not *generalize* well to the new data
- Extreme case: "rote learning"



- Training error is low
- Testing error is high

Underfitting

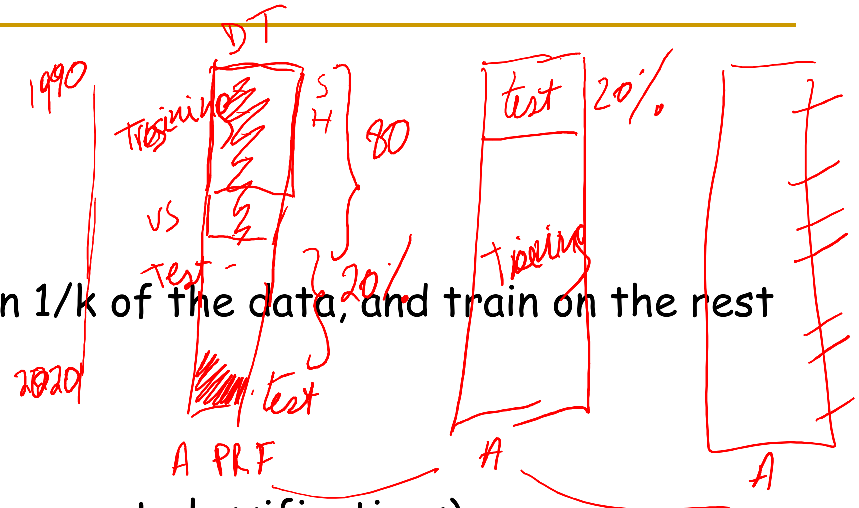
- We can also underfit data, i.e. find a decision boundary that is too simple
- Model is not expressive enough (not enough features, or not enough capacity)
- eg. There is no way to fit a linear decision boundary so that the training examples are well separated



- Training error is high
- Testing error is high

Cross-validation

- K-fold cross-validation
  - run k experiments, each time you test on 1/k of the data, and train on the rest
  - than you average the results



- ex: 10-fold cross validation
  1. Collect a large set of examples (all with correct classifications)
  2. Divide collection into two disjoint sets: training (90%) and test (10% = 1/k)
  3. Apply learning algorithm to training set
  4. Measure performance with the test set
  5. Repeat steps 2-4, with the 10 different portions
  6. Average the results of the 10 experiments

entire DS

1990 … 2020

exp1:	train									test 1/k
exp2:	train								test 1/k	train
exp3:	train							test	train	
…	…									

exp 10

F-measure = 80
F-measure 8/60
F - 83 99
F - 82 50
F

stable unstable

average

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2. Naïve Bayes Classification
   a. Application to Spam Filtering
3. Decision Trees
4. Evaluation
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6. Neural Networks
   a. Perceptrons
   b. Multi Layered Neural Networks

Up Next

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4. (Evaluation
5. Unsupervised Learning)
6. Neural Networks
   a. Perceptrons
   b. Multi Layered Neural Networks