COMP472: Artificial Intelligence
Machine Learning
Evaluation

- Russell & Norvig: Sections 19.4

Today

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

我们怎么评价machine-learning model效率

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

Data Sets

还是supervised learning的领域（有f(x)）

- 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

指的就是test set

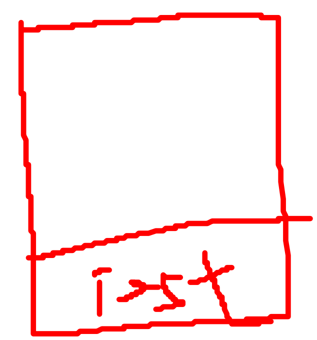
- Split data set into 3 sub-sets
  1. Actual **training** set (~80%)
  2. **Validation** set (~20%)
  3. **Test** set

~80%

~20%

training

no overlap



dataset被分为三部分，前两部分叫做training,，用来构建model,在构建完以后test set才会被投入使用将预测结果与实际结果进行比较

方法学

Standard Methodology

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

build the model

Loop:

conditional probability, prior probability...

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

validation set用来评估我们通过training set建立的model,
并且通过hyper parameters进行tweak,adjust微调

5. Measure performance with the test set

34无限重复，，直到你得到了一个好model， 开始5

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

Parameters:
basic values learned by the ML model. eg. ML学习的数据
- for NB: prior & conditional probabilities naive bayes:各种几率
- 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, smoothing曲线用的，1，0.5这种
- for DTs: pruning level
- for ANNs: nb of hidden layers, nb of nodes per layer...

Metrics 评判标准

- accuracy TEST SET里 我们模型准确预测的百分比
  - % of instances of the test set the algorithm correctly classifies
  - when all classes are equally important and represented

f(x),所有f(x)重要性相等

balanced,例如f(x)有80%class是狗，10%是猫，10%是老鼠，就不算represented/ballanced dataset.

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

如果没有满足equally important and balanced,我们要使用第二套标准

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

	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% !

accuracy其实挺好的，但生活中没用，我们更想检查出生病的人（sick is more important），所以unbalanced不能用第一种

Recall, Precision

比例

- Recall: What proportion of the instances in the class of interest (eg. sick) are labelled correctly? 所有实际sick的instance有几个被标出来了
- Precision: What proportion of instances labeled with the class of interest (eg. sick) are actually correct? 所有标出来的sick有几个是实际sick

		Correct class	
		instance should be in class *C*	instance should <u>not</u> be in class *C*
Model prediction	instance is put in class *C*	True Positive (TP)	False Positive (FP)
	instance is <u>not</u> 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

	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%	497/500 = 99.4%
Precision		1/1 = 100%	3/3 = 100%	4/6 = 66.7%
Recall		1/5 = 20%	3/5 = 60%	4/5 = 80%

标出来的sick有几个是真sick

实际5个sick，标出来了1个，3个，4个

Which system is better?

2肯定比一好
但是23不好说，看我们具体需求有的时候我们觉得查错不要紧，尽量查出来，选3
有的时候我们觉得舍弃掉一些哪怕正确的是可以接受的，而精度更重要，选2

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)~~ 500个。50个sick，你全标sick，但实际上你这模型很差

1. take harmonic mean 调和平均数
   - which penalizes extreme values 他让极端情况的评分下降

使..不利

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

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 <u>weighted</u> harmonic mean 如果recall与precision有时候有一个侧重点，我们就改变系数

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

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

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/a+1/b需要等于1

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

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

可以换成以下形式

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

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

可以改成这个形式，叫做F-measure

F-measure

- A weighted harmonic mean of precision and recall

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

F measure是一组measure，由β决定，例如F1 measure，F0.5measure...

- β represents the relative importance of recall to precision
  - when β = 1
    - F1 measure
    - precision & recall have same importance

β代表着recall相对重要性与precision相比，=1同样重要，大于1recall更重要
小于1precision更重要，

  - when β > 1
    - recall is given more weigth
    - e.g. F_2 measure, recall is considered 2x more important than precision

β等于2，说明recall两倍重要

  - when β < 1
    - precision is given more weigth
    - e.g. $F_{0.5}$ measure, precision is considered 2x more important than recall

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%	497/500 = 99.4%
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)	β等于1	2*100*20/ (100+20) = 33%	75%	72.9%

P, R and F for Multiclass Classification

上面的是偏重一项例如SICK的，如果我们偏重多个CLASS（鼠，猫，狗这种不同结果的F(X)），那么我们需要

- 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 把每个class的PRF算一遍
  - 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

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

FP.FN都是针对猫的

就是前面TP,FP,FN,TN一套，
红色圈的是猜了猫，实际也是猫，也就是好的TP
下划线就是猜了猫，实际上是狗或者实际上是鱼，那对于猫来说他是FP

X代表着FALSE NEGATIVE,我们猜没有猫（猜成别的了），实际上是猫，就是FN FALSE NEGATIVE

每一格代表的猜成X(行)，实际上是Y（列），横着的TOTAL代表一共猜了几次猫
竖着的TOTAL代表一共有几个猫

- 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%

precision就是猜了几次对了几个

- 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%

reccall就是有那么多你猜对了几个

Per-class F1-measure

	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)

- 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

有了PR求出F1

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:简单的就求平均
    - --> macro precision, macro recall, macro F1
  - take weighted average 实际上我们有6只猫，10只狗，9只鱼，每个人都有一个系数6/25，10/25，9/25
    - ie. weight the average based on the nb of samples from each class
    - --> weighted averaged precision, weighted averaged recall, weighted averaged F1

Confusion Matrix 也叫contingency table

- to do an error analysis and find out where the model went wrong ?
- aka contingency table 用来分析错误，找到Model哪儿出问题了
- eg. 6 classes, 100 test instances 就是第14页那个

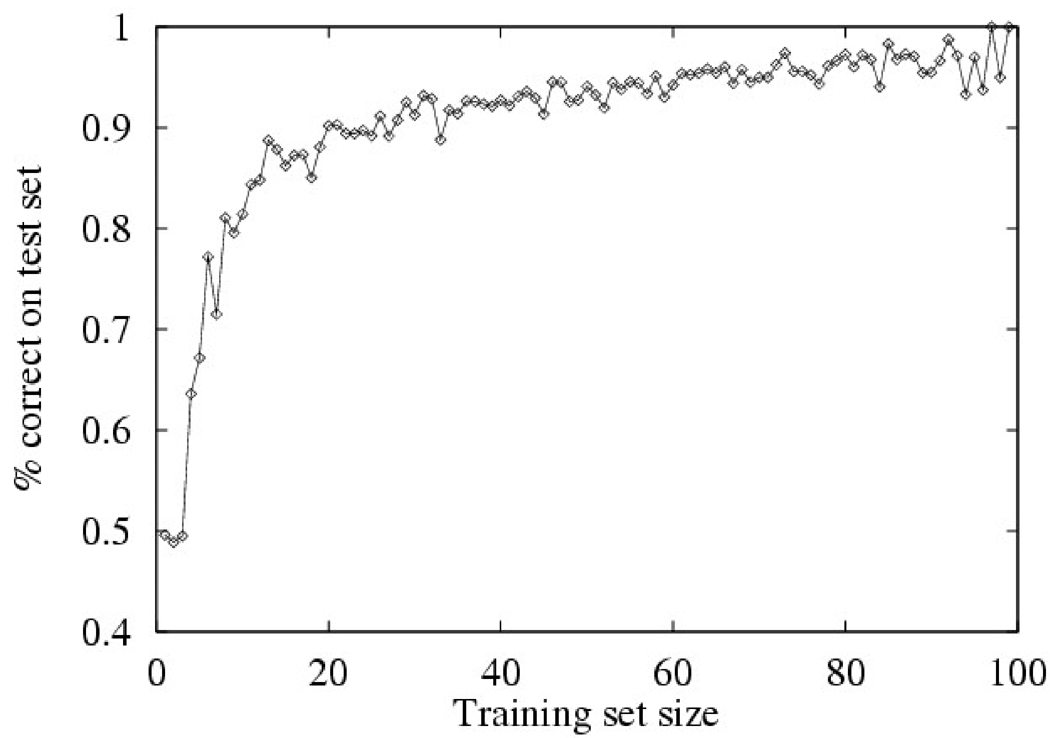
		Correct Class						
		C1	C2	C3	C4	C5	C6	Total
Predicted Class	C1	10✓	3×	0	0	3×	0	*16*
	C2	0	12✓	3×	4×	0	0	*19*
	C3	0	1×	9✓	2×	1×	2×	*15*
	C4	0	1×	3×	5✓	2×	0	*11*
	C5	0	0	3×	2×	10✓	3×	*18*
	C6	0	0	5×	0	5×	11✓	*21*
	Total	*10*	*17*	*23*	*13*	*21*	*16*	*100*

实际猜了16次C1

实际有10个C1

A Learning Curve

数据越多，the more you learn，但是到了后面加起来很微弱



理论上你可以得到一个完全精确地set，但实际上很难，因为生活中dataset很难完全正确，甚至你用同样的training set构建模型，再用同样的set作为test set，也很难达到1

- 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

Size	Color	Shape	Output
Big	Red	Circle	+
Big	Red	Circle	-

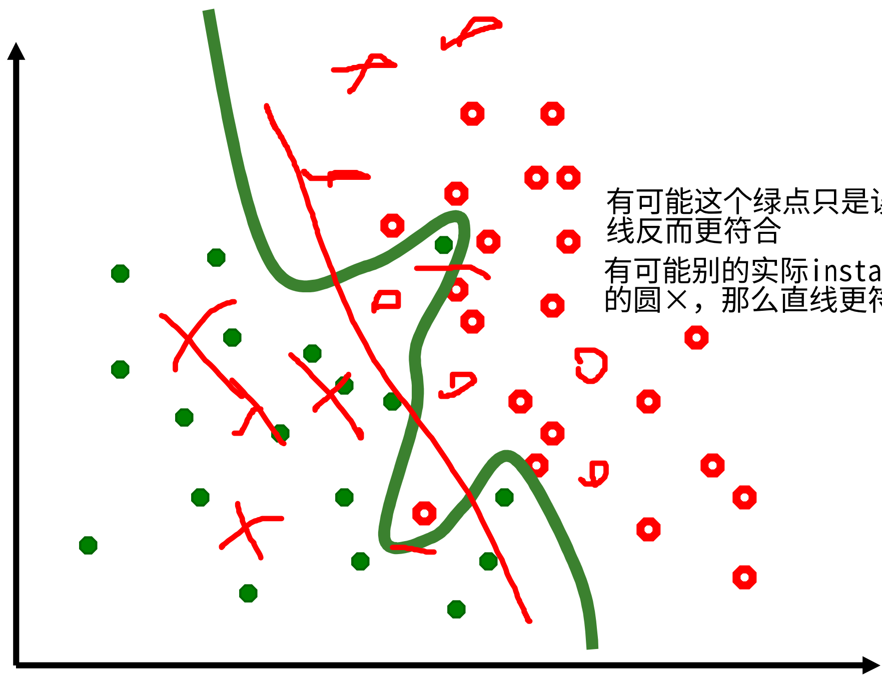
    - Some values of features are incorrect or missing (ex. errors in the data acquisition)
    - Some relevant attributes are not taken into account in the data set

可能第二个shape是circle，，也可能Output是+，或者是4TH feature没有被考虑到
这也是为什么即使你用你的training set作为test set，也可能做不到100%精确率

Overfitting

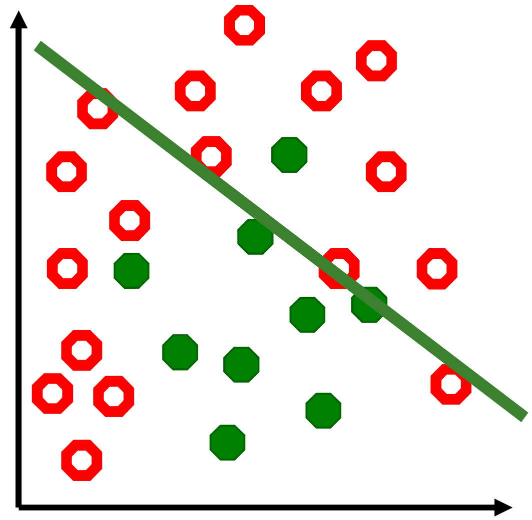
有很多实际上并不相关的feature，在这个training data里面因为巧合显得相关，我们如果面面俱到，会产生overfit，过于符合training data了

- 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 过于符合//吉他里的tune调音
- They do not *generalize* well to the new data 概括
- Extreme case: "rote learning" 死记硬背
- Training error is low training error少
- 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



过于简单，testing training两个都达不到

- Training error is high
- Testing error is high

Cross-validation

- K-fold cross-validation　　　　K就是折叠成几分
  - 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

exp1:	train									test
exp2:	train								test	train
exp3:	train							test	train	
…	…									

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