



June, 2014

AA ML Course – Theoretical Session 4

Courtesy of Amitai & Tom



Agenda



1. Introduction

- 2. Bayesian decisions
- 3. Naïve Bayes
- 4. Evaluation measures
- 5. K-Nearest Neighbors
- 6. Decision Trees
- 7. Support Vector Machines



Introduction

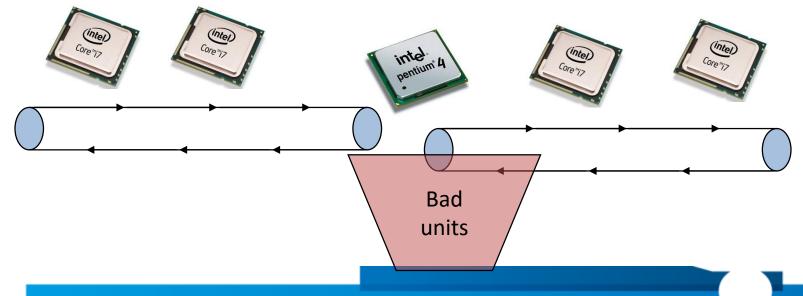


- Today we discuss prediction, mainly classification
- Classification/prediction as an optimal decision problem
- Some specific models to help us
- Different ways to evaluate ourselves





- For each unit, we want to use multiple features (physical tests) to decide whether to discard it, or send it to market
 - Or more generally: Classify it to class **C** (i3/i5/i7/etc.)
- Inherent uncertainty probabilistic decision
- Different decisions have different costs
- Formalize our problem to help us reach 'optimal' choices



Additional Examples....



 Determine whether an email is Spam or legitimate (e.g. based on its words, sender domain)

 Determine if a Parkinson's patients disease is On/ Off, based on motion sensors data

 Determine whether a lawn mower/washing machine/refrigerator needs maintenance based on physical sensors (IOT)





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Bayesian view in a (very small) nutshell



- We see evidence X, such as the CPU tests results
- We have **Prior** probabilities for having a bad CPU, e.g.: P(C=good) = 0.99; P(C=bad) = 1-0.99 = 0.01
- We obtain the Likelihood: Probability of evidence, given each class, e.g.: P(X | C= good) = 0.17
- We compute **Posterior** probabilities: Probability of class, <u>after</u> seeing the evidence, e.g. P(C=good | X)

Bayes rule:

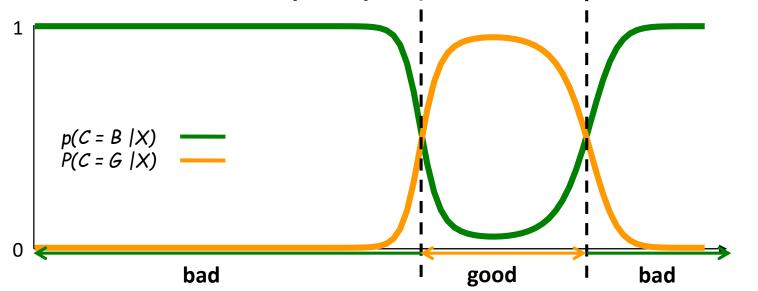
posterior
$$P(C \mid X) = \frac{P(C) p(X \mid C)}{p(X)}, \text{ where } p(x) = \sum_{C} P(C) p(x \mid C)$$
evidence



Classification as decision



- Our classification choice is a decision rule, where our decided 'action' is one of {Good,Bad}
- Our action usually depends on the evidence:







What is the Optimal Decision?



- We want optimal decisions but optimal by what criteria?
- Need to define our costs or **loss function**, L(C, a): What loss we incur for prediction a when the class is C
- **0-1 loss** (misclassification loss):

Predicted/Actual	Bad	Good
Bad	0	1
Good	1	0

Other/better appropriate losses for our CPU problem?



Optimal Decisions – Bayes decision rule



- By optimal, we mean the action that minimizes the expected loss
- In the Bayesian approach to decision theory, the optimal action having observed x is defined as the action a that minimizes the expected loss given the data

$$\sum_{C} L(C,a) p(C|x)$$

- A decision policy that minimizes the above quantity for each X, is called a Bayes decision rule
- Explanation: When *C=good* and we classify it as *a=bad*, we may lose a lot (depending on our loss function). But, the probability of getting C = good given the features x could be very low... so the expected loss doesn't give much weight to this particular error



Bayes decision rule – 0-1 Loss

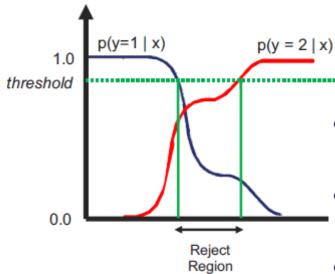


- Let's see this for 0-1 loss
- If we decide predicted = 1 ("good"): Loss(real = 0, pred = 1) P(real = 0|x) + Loss(real = 1, pred = 1) P(real = 1|x)= P(real = 0 and pred = 1|x)
- If we decide predicted = 0 ("bad"): Loss(real = 0, pred = 0) P(real = 0|x) + Loss(real = 1, pred = 0) P(real = 1|x)= P(real = 1 and pred = 0|x)
- So our total expected loss for predicting 'pred' is $P(real \neq pred | x)$
- To **minimize** the above, we simply choose *prediction* that **maximizes** P(real = pred | x). This is the **MAP classification rule** (Maximum A-Posterior)
- The misclassification loss is minimized by selecting the class having the largest posterior probability (probability given the features X)



Reject option + other Loss Functions





• 0-1 Loss: gives 0 loss when arguments agree, 1 otherwise

$$\mathcal{L}_{0-1}(x,y) = I[x \neq y]$$

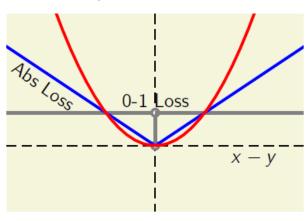
• **Absolute Loss**: gives the absolute difference in x & y

$$\mathcal{L}_{abs}\left(x,y\right) = \left|x - y\right|$$

• **Squared Loss**: gives the squared difference in x & y

$$\mathcal{L}_{sq}(x,y) = (x-y)^2$$

For some regions in input space, where the class posteriors are too low, we may prefer to say "don't know"



Bayesian decision theory: Summary



 Formulating as Bayesian decision problem tells us how to make optimal decisions, in terms of minimal risk

 But, where do we get all the 'components' to make the decision? Prior probabilities, conditional probabilities, etc...

 We need to construct models to learn these components from data, and combine prior domain knowledge if available



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Naïve Bayes Classification



A simple approach for computing the required components for the Bayes rule, specifically the Likelihood

A good and robust algorithm, recommended as one of the first 'house models' to try





Bayesian Classification: Binary Domain

Recall our situation:

- Two classes: **Bad**, **Good** (e.g., CPUs)
- Assume each instance has N attributes (test results)
 - $-X_n$ is a binary variable with value 0.1

Example:

	X_1	X_2	 X _N	C
	0	1	1	G
	1	0	1	В
	1	1	0	G
	•••	•••	•••	•••
_	0	0	0	G



Binary Domain - Priors



How do we estimate P(C)?

- Simple Binomial estimation
 - Count # of instances with C = B, and with C = G

X_1	X_2	 X_N	C
0	1	1	G
1	0	1	В
1	1	0	G
•••	•••	•••	
0	0	0	G





How do we estimate $P(X_1,...,X_N/C)$?

Two sub-problems in this case:

Compute
$$P(X_1,...,X_N|C=G)$$

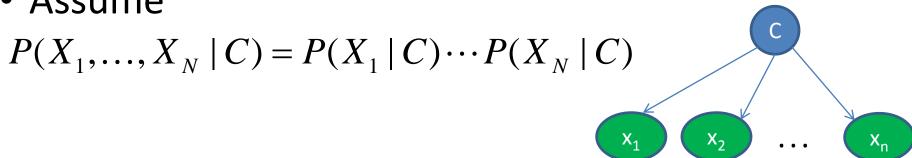
Compute
$$P(X_1,...,X_N|C=B)$$

X_1	X_2	 X_N	C
0	1	1	G
1	0	1	В
1	1	0	G
		•••	•••
0	0	0	G
0		O	

Naïve Bayes Likelihood



Assume



This is an independence assumption:

Each attribute X_i is independent of the other attributes once we know the value of C

 In our example: Test results are independent once we know whether the CPU is Good or Bad





Naïve Bayes: Boolean Domain

We only need to compute for each i:

$$P(X_i = 1 \mid C = G)$$

$$P(X_i = 1 \mid C = B)$$

How do we estimate $P(X_1 = 1 | G)$?

• Simple binomial estimation:

Count #1 and #0 values of X_1 in instances where C=G (Similar for non-boolean discrete features)

X_1	X_2	 X _N	C
0	1	1	G
1	0	1	В
1	1	0	G
•••		•••	•••
0	0	0	G

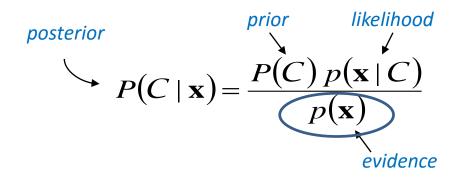






Interpretation of Naïve Bayes

Now we can almost compute this:



Note that computing the denominator is not required, since it does not depend on *C*

We choose the class with maximum posterior probablity



What About Continuous Features?



If the features are continuous, the likelihoods
 P(X_i|C) may be computed in several ways

- Binning to obtain discrete variables, and then estimating by count of the bin in the training set
- Assuming normal distribution:

Computing mean μ and standard deviation σ of X_i for each class in the training set, and assuming $X_i \sim N(\mu, \sigma)$



When Is Naïve Bayes helpful?



 High input-space dimension, making it difficult to estimate probability density in that space

Input contains both continuous and discrete variables



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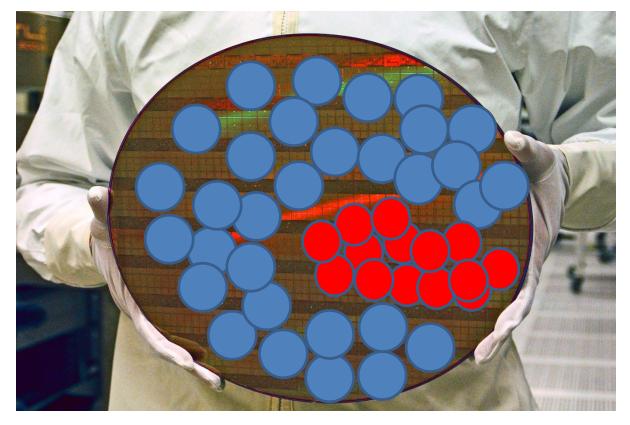
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kNN – tell me who your neighbors are...



- Back to our CPU problem
- A wafer, good units, bad units

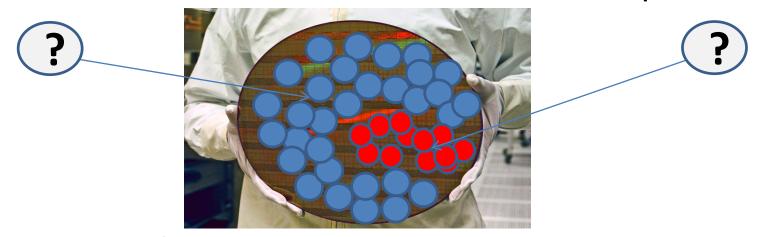




kNN – tell me who your neighbors are...



- Basic idea: Use local structure of data itself
- Store all data, and when new unit comes, find K nearest units, and classify by majority
- Known as "lazy" or "instance-based" learning
- 1-NN: Give new unit the label of closest data point



- Probabilistic / Bayesian decision formulation?
- 'Nearest' by what measure?





kNN as probability estimation



- kNN estimates the conditional probability p(y|x)
- Count of data points in class y in the neighborhood of x

$$p(y|x) = \frac{|\{(x_i, y_i) : y_i = y, x_i \in N(x)\}|}{|N(x)|}$$

Where N(x) are the (indices of) points in the neighborhood of x

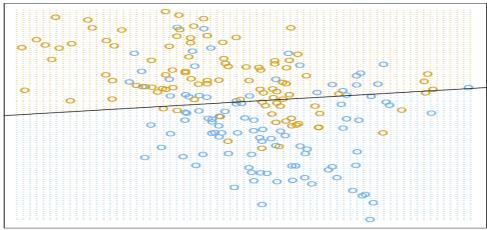
- A form of density estimation
- We can then use Bayes decision rule MAP classification
- Recall that to minimize **0-1 Loss**, we choose c that maximizes $P(y=c \mid x)$ i.e. majority class in neighborhood



Decision Boundaries



 Recall: Classification as decision problem. Classifier partitions the feature space into volumes called decision regions.



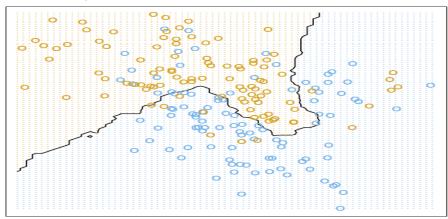
 The decision regions are separated by surfaces called the decision boundaries. These separating surfaces represent points where there are ties (in terms of loss) between categories.



kNN – non-linear decision boundaries



No assumptions are made about the shape of the decision boundary



 We can expect this approach to dominate linear classifier when the real (Bayes) decision boundary is highly non-linear.



From K=1 and beyond



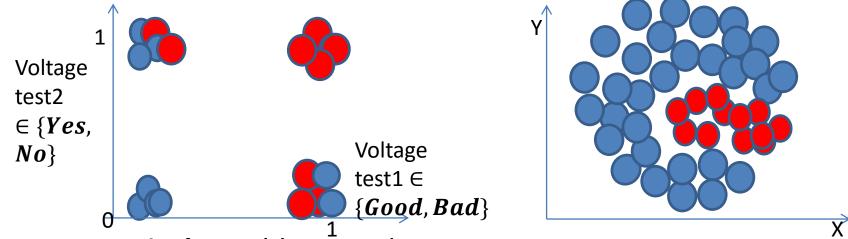
- 1NN induces a rough boundary (previous slide)
- The larger the K, the smoother the decision boundary;
 small K could lead to overfitting
- Bias-variance tradeoff: Smaller K ->
 larger variance (instability of prediction);
 Larger K->larger bias (inaccuracy of prediction)
- If we take just a "small neighborhood" it's likely to be homogenous (low bias) but we are basing ourselves on a small number of points (high variance)
- For large enough dataset $(n \to \infty)$, and large enough K, approaches optimal Bayes classifier (Bayes error)



'Nearest' according to what distance?



- Most common distance metric is Euclidean
- In our wafer example, with location as an input, this has the intuitive explanation of "geographic" proximity, but:



- For categorical variables, need an appropriate metric
- Weights: Give decaying importance to neighbors as they get further away
- In general, many different options and practicalities: choose according to problem and accuracy (using validation)



kNN's curse (of dimensionality)



- Main problem: kNN does not work well with high dimensional inputs; in high dimensions, "everything is distant"
- How do we find "near" people by their various "features"? Location, job, religion, education, height...
- Method is no longer very local, despite the name "nearest neighbor"
- The trouble with looking at "neighbors" that are so far away is that they may not be good predictors about the behavior of the input-output function at a given point

Home and Away

קרוב רחוק...



kNN summary + a note about interpretability



- Local method for complicated decision boundaries
- Fast training: Just store the data (but iterating and validating over different metrics and K-neighbors could change the picture...)
- But no assumption about decision boundary comes with a big cost: Needs a lot of data, sensitive to smoothing choice and mostly severely sensitive to dimensionality: Rapidly increasing sparsity of 'neighborhood' in highdimensions
- Interpretability/insight: kNN does not directly tell us which predictors are important: Harder to gain understanding... Decision Trees to the rescue?

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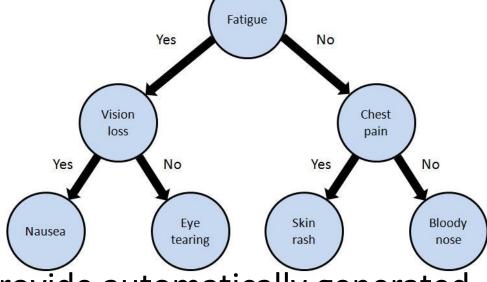
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Motivating example: Medical diagnosis



- Build a Healthcare diagnosis system for doctors
- Goal: Predict (diagnose) illness with sequence of questions
- Each question leads to another question based on previous answer



 We aim to provide automatically generated, accurate and interpretable (transparent) sequence of such questions

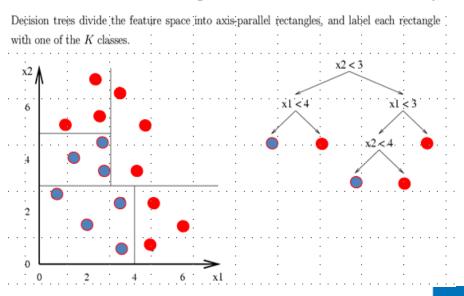


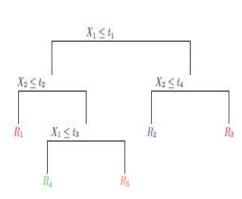


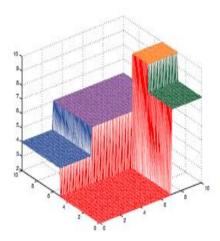
Decision Trees: Prediction by partition



- Binary partitions of the input space, and defining a local model in each resulting decision regions (boxes) of input space, represented by leaf nodes
- In trees used for classification, boxes hold class labels for predictions we associate each region with majority class
- We can easily also use trees for continuous target we simply use the average in each box for prediction







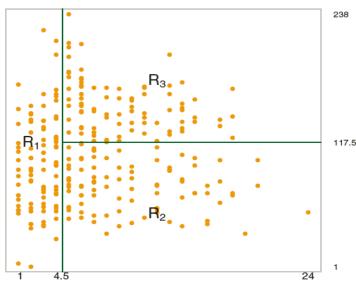


Decision Trees – big picture



For example, predict tablet sales with clear insight into model (screen size, weight, battery life)

Big picture: Two main steps:



- 1. We divide the feature space into J distinct and nonoverlapping regions $R_1, R_2, ... R_I$
- 2. For every observation falling in region R_i , predict (majority/average) for training observations in R_i



How to partition?



- Divide predictor space into high-dimensional boxes
- Find boxes $(R_1, R_2, ... R_J)$ that minimize Loss Function a key component for building the tree, determining its type and inner workings we will see examples
- Computationally infeasible to consider
 every possible partition of the feature space
- Heuristic solution: Recursive binary splitting
- Top-down: Begin at the top of the tree (all points in same region), successively split the predictor space
- 2. Greedy: At each step, best feature for split is found locally for the immediate split, rather than looking ahead and picking a split that may lead to a better tree in some future step further down



Recursive partitioning



- Basic method (example with continuous target tablet sales)
- Loss function: $\sum_{Boxes} \sum_{i \in Box} (y_i average(y_{box}))^2$ (Sum of Squared Errors)
- e.g. sum in one box: $(3.1 3)^2 + (2.9 3)^2$
- 1. Initialization: First select feature X_j and split (s) that leads to greatest reduction in SSE:

$$R_1(j,s) = \{X | X_j < s\} \text{ and } R_2(j,s) = \{X | X_j \ge s\}$$

That minimize

$$\sum_{i: x_i \in R_1(j,s)} (y_i - \hat{y}_{R_1})^2 + \sum_{i: x_i \in R_2(j,s)} (y_i - \hat{y}_{R_2})^2$$

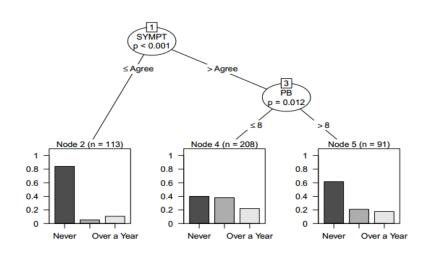
- 2. Recursion: Split one of the two previously identified regions in same way
- 3. Continue until a stopping criterion is reached



Classification – node purity



- Criteria for splitting (loss function) changes, basic idea same!
- Define node purity as a measure of how homogenous the node is
- We classify by which class k maximizes \hat{p}_{mk} , the proportion of class k observations in box m the majority class
- Just like SSE, purity will be used for our loss function







Purity measures



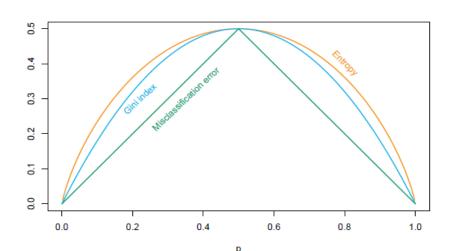
Unlike in continuous problem, there are several "natural

candidates" to choose from

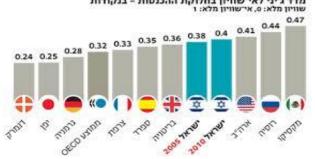
Misclassification error:
$$\frac{1}{N_m} \sum_{i \in R_m} I(y_i \neq k(m)) = 1 - \hat{p}_{mk(m)}.$$

Gini index:
$$\sum_{k \neq k'} \hat{p}_{mk} \hat{p}_{mk'} = \sum_{k=1}^{K} \hat{p}_{mk} (1 - \hat{p}_{mk}).$$

Cross-entropy or deviance: $-\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$.



- In words:
- Misclassification: Fraction of points in box for which we were wrong
- Entropy, Gini : Behave similarly, measure of general uncertainty in art ג'יני לאי שוויון בחלוקת ההכנסות בנקודות box
- Gini, entropy are more sensitive criteria than misclassification for splitting
 - often better to use them



Gain measures

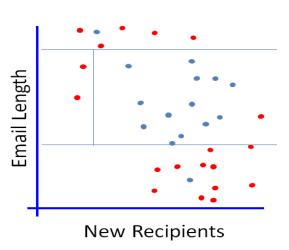


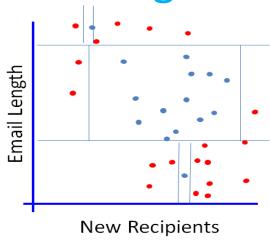
- Rather than decreasing Loss in splitting criteria, we can increase Gain
- Information Gain: By how much will we reduce the entropy after splitting a node using attribute X? We want this as large as we can
- H(Y) H(Y|X). Recognize this?
- Maximizing infoGain is equivalent to minimizing entropy
- Categorical features: Number of partitions grows exponentially in number of values; the more choices we have, the more likely we can overfit – infoGain weakness
- GainRatio: In practice, correct for the entropy of the attribute itself by reducing its weight in infoGain



How much partitioning?







- Too much splitting likely to overfit data tree might be too complex; Fewer splits -> Simpler decision boundaries
- Should we grow only while decrease in loss is large enough?
- No too short-sighted. Small decreases early in splitting process could lead to big decreases further down in tree



Pruning

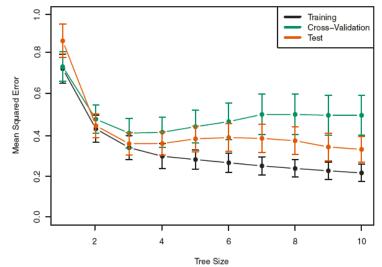


 Better solution: Grow a large tree until each node contains a small number of instances

• Then use pruning to remove nodes (splits) that do not

provide additional information

 One natural way is to penalize size of tree (rpart package in R)



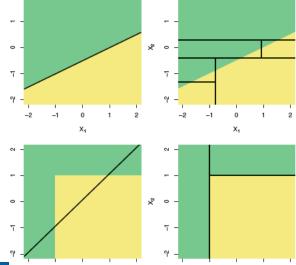
 Also use prediction accuracy – prune by node contribution to misclassification rate



DT issues: White box, but at what cost?



- Very transparent (with related advantage of Feature Selection)
- But aside from previous issues we saw, 2 major problems
- Instability: Small changes in data can cause very different splits; the effect of an error in the top split is propagated down to all of the splits below it (in next session, you will see how Random Forests fix this)
- Lack of smoothness: Boundary
 or true function could be smooth,
 but we search for partitions.
 Real-world examples?



Decision Trees summary



- Explanation for end-use by far strongest point
- Suitable for segmented (disjoint) decision boundaries
- Fast learning, easy handling of discrete features
- Instable, prone to overfitting
- Difficulty with smoother structures
- Generally not a state-of-the-art method, but a subroutine in some that are
- Can we trade-in for the interpretability, and get a model that can both predict very well and capture complex structures?

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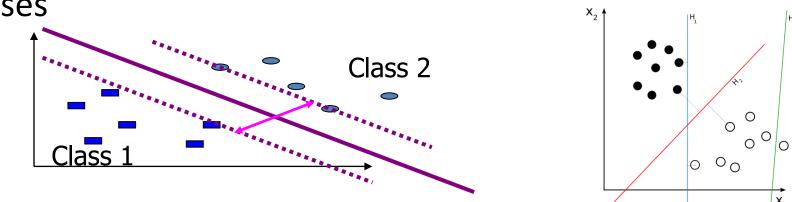


Support Vector Machines – the basics



- First thing, some key building blocks for SVM
- What is a hyperplane? A high-dimensional plane

Separating hyperplane – a hyperplane that separates the classes



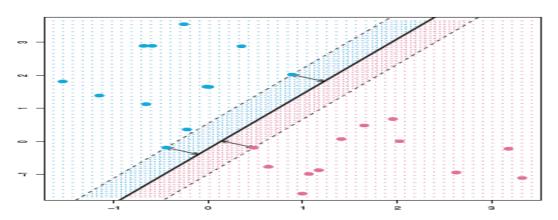
- Margin defined by points nearest to hyperplane
- The maximal margin hyperplane is the separating hyperplane for which the margin is largest
- Why? Greater generalization ability, more stability





Support Vectors – what do they 'support'?



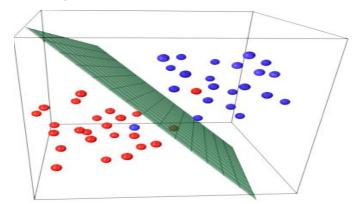


- Our data points are just vectors in p-dimensional space (feature1...featurep)
- Support vectors: if these data points were moved slightly, hyperplane would move as well; others "don't matter"
- Our decision (prediction) rule potentially based on only a small subset of the observations; stable to the behavior of observations that are far away from the hyperplane – less sensitive to outliers

Can we really have total separation?



- Real-world: Some points will be on wrong side of the hyperplane
- **Soft margin:** Allow some observations to be on the **incorrect side**



Why not just always find a perfectly separating hyperplane (if at all possible)? This is called a hard margin - usually leads to instability

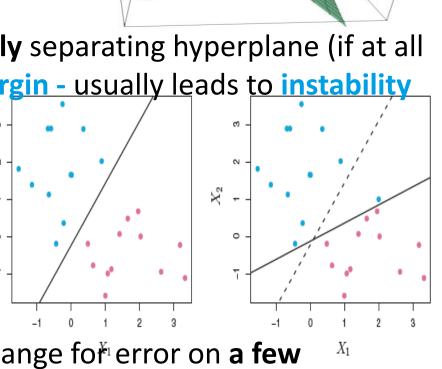
(hence poor generalization)

Example: add just 1 new point. Margin changes drastically,

and is now very narrow

With soft margin, get better

classification for most points in exchange for error on a few



Formulization as optimization problem



$$\min_{\mathbf{w}, w_0, \boldsymbol{\xi}} \frac{1}{2} ||\mathbf{w}||^2 + C \sum_{i=1}^{N} \xi_i$$

$$\text{s.t.} \quad \xi_i \geq 0, \quad y_i(\mathbf{x}_i^T \mathbf{w} + w_0) \geq 1 - \xi_i$$

$$\text{Class 1} \quad \mathbf{w}^T \mathbf{x} + b = 0$$

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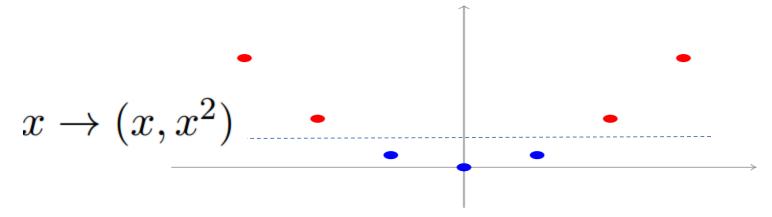
- In words: Maximize margin $(\frac{2}{||w||^2})$ while allowing some deviations (ξ_i), and penalize their sum with **C**
- C determines the number and severity of the violations, controls bias-variance tradeoff/overfitting: large C -> narrow margins rarely violated; small C -> margin is wider, fitting less hard

Kernels - for nonlinear boundaries



Data are not linearly separable





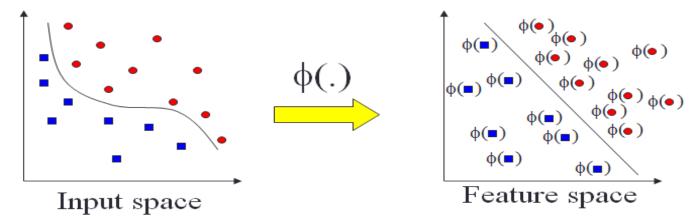
- Problem: Feature space grows exponentially
- Better solution: Kernels to avoid carrying out transformations explicitly (avoid computing and storing massive number of extracted features)



Kernel Trick



 With a few mathematical tricks, kernels allow us to fit linear SVM classifier in higher-dimensional space, without actually computing all these features



- Turns out that SVM easily allows us to do this mapping
- Polynomial kernel: Map feature space to polynomials (and their products i.e. interactions), for example $(x_1, x_2) \longmapsto (x_1^2, \sqrt{2}x_1x_2, x_2^2)$

RBF kernel – one important kernel



- Radial Basis Function Kernel
- Often first kernel to try (when no prior knowledge)

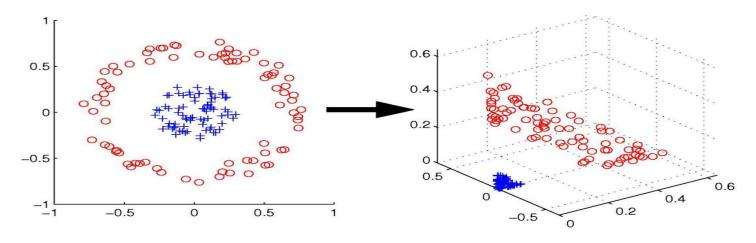


Figure 1: Transforming the data can make it linearly separable

 For a new observation we predict on, points that are far from it play essentially no role (kernel gives exponential decay in distance) – captures local ("circular") structure



SVM summary



- Classifier with strong performance, "general-purpose"
- Natural, efficient use of high-dimensional feature space
- Flexible use of kernel types capture many structures
- But no "analytic" way of finding right one
- Sparse solution that depends on support vectors only
- This is also a computational problem need to keep carrying SVs (for kernel SVMs)
- Especially when using kernels, not immediately clear how to interpret/extract insights



Evaluation: Algorithm Preference

intel

- Criteria (Application-dependent):
 - Accuracy
 - Misclassification error, or risk (loss functions)
 - Training time/space complexity
 - Testing time/space complexity
 - Interpretability (Model Complexity, for instance number of hidden units)
 - Easy tuning
 - Easy programmability
 - Easy embedding



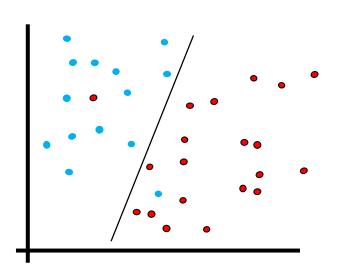
"Fast is fine, but accuracy is everything."

Xenophon
(Greek historian, 430 – 354 BC)

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Evaluating What's Been Learned The Test Set Method

- Randomly select a portion of the data to be used for training (the training set)
- Train the model on the training set
- Once the model is trained, run the model on the remaining instances (the test set) to see how it performs



Confusion Matrix

Predicted

Blue Red
Blue 13 1
Red 1 19



Confusion Matrix – Terms



		Predicted	
		0	1
Actual	0	True Negative (TN)	False Positive (FP) B
	1	False Negative (FN)	True Positive (TP)

If we have more than two classes, we can compute this matrix for each class vs. the others, and then average all matrices

Evaluation Considerations



- Higher accuracy does not necessarily imply better performance on target task
- Classes are often very imbalanced
 - Buying customers are much rarer than non buying customers
 - What if 99:1 split? Always say "no" -- 99% default accuracy
- Errors have different costs
 - Cost of eating poisonous mushroom is greater than cost of going hungry
 - Goals need to be defined by business understanding



Confusion Matrix – Error Measures



$$\bigcirc \text{Error rate} = \frac{FN + FP}{TN + FP + FN + TP} = \frac{C + B}{n}$$

		Predicted	
		0	1
Actual	0	True Negative (TN) A	False Positive (FP) B
Act	1	False Negative (FN) C	True Positive (TP)

$$\bigcirc Accuracy = \frac{TN+TP}{TN+FP+FN+TP} = \frac{A+D}{n}$$

○ Recall =
$$\frac{TP}{FN+TP} = \frac{D}{C+D}$$
 (= Sensitivity = Hit rate)

○ Specificity =
$$\frac{TN}{TN+FP} = \frac{A}{A+B}$$
 (= 1- False Positive rate)

$$\bigcirc \text{ Precision} = \frac{TP}{FP + TP} = \frac{D}{B + D}$$



Confusion Matrix – Error Measures



○ Specificity =
$$\frac{TN}{TN+FP} = \frac{A}{A+B}$$

○ False positive rate =
$$\frac{FP}{TN+FP} = \frac{B}{A+B}$$

		Predicted	
		0	1
Actual	0	True Negative (TN) A	False Positive (FP) B
	1	False Negative (FN)	True Positive (TP)

○ Recall =
$$\frac{TP}{FN+TP} = \frac{D}{C+D}$$
 (= True positive rate)

- When there are few positives, or when every positive should be detected, then high recall is crucial.
- When there are many positives and we just need some of them, we settle for lower recall and require high specificity. For example: Find 1000 programmers according to their LinkedIn profiles.

Confusion Matrix – Error Measures



F-Measure =
$$2 * \frac{Precision*Recall}{Precision+Recall}$$

		Predicted	
		0	1
Actual	0	True Negative (TN) A	False Positive (FP) B
	1	False Negative (FN)	True Positive (TP) D

F-measure is the harmonic average of precision and recall.

Provides a unified measure for both of them.

Worst value is 0, best value is 1, when both precision and recall are 1.

Commonly used in document retrieval/classification.



ROC Curve



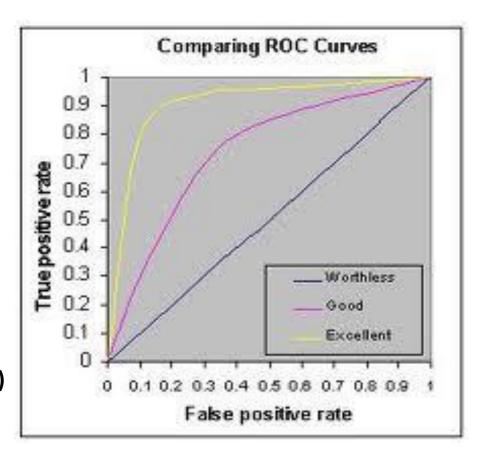
A way to assess and visualize the tradeoffs between classifiers and choose between them

False positive rate =
$$\frac{FP}{TN+FP}$$

(e.g. fraction of bad CPUs considered good)

True positive rate =
$$\frac{TP}{FN+TP}$$

(e.g. fraction of good CPUs considered good)

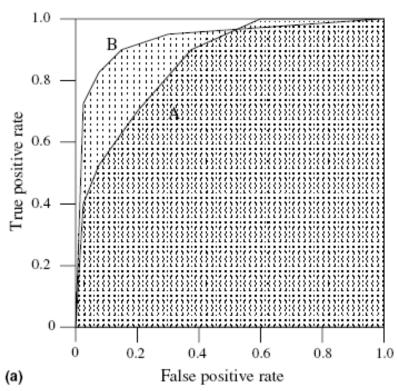


Area under ROC curve (AUC)



Comparing two ROC curves:

- The graph represents the areas under two ROC curves, A and B.
 Classifier B has greater area and therefore better average performance
- Note: Since the AUC is a portion of the area of the unit square, its value will always be between 0 and 1.
- AUC is equivalent to the probability that the classifier will rank a positive instance higher than a negative instance





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ROC and AUC - Summary

 ROC curve provides a popular visualization for the tradeoff between false positive rate (cost) and true positive rate (benefit) of a classifier

• AUC reduces the ROC curve to one number, reflecting the classifier's quality (probability that true will rank higher than false).

 It is better to review the full ROC curve, as a single number does not reflect it in full. For example, high false positives are incorporated in AUC but less interesting.

