Lecture 2:

Classification I

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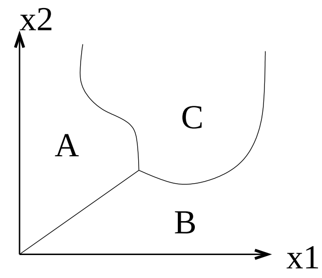
Voronoi Tessellation, Decision Surfaces

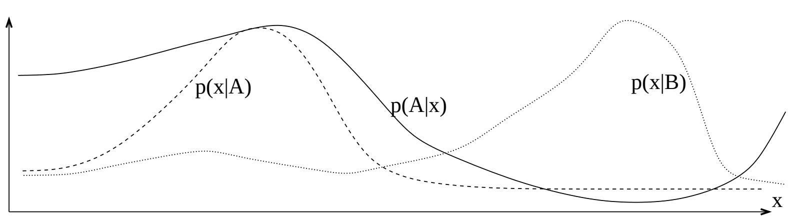
- For continuous inputs, we can view the problem as one of segmenting the input space into regions which belong to a single class, i.e. constant output.
- Such a segmentation is the "Voronoi tessellation" for our classifier.
- The boundaries between regions are the "decision surfaces".
- Training a classifier == defining decision surfaces.



Reminder: Classification

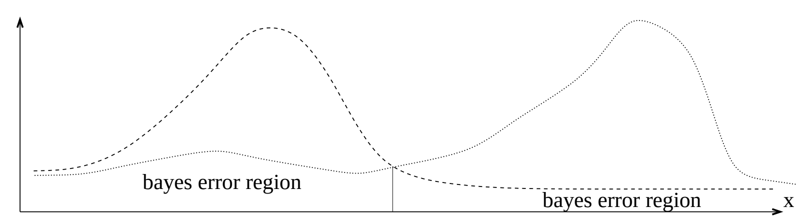
- Multiple inputs $\mathbf{x}$, mixed cts. and discrete.
- Single discrete output y.
- Goal: predict output on future unseen inputs.
- From a probabilistic point of view, we are using *Bayes rule*:

$$p(y|\mathbf{x}) = \frac{p(\mathbf{x}|y)p(y)}{p(\mathbf{x})} = \frac{p(\mathbf{x}|y)p(y)}{\sum_{y'} p(\mathbf{x}|y')p(y')}$$



Probabilistic Model, Bayes Error Rate

- Model original data as coming from joint pdf $p(\mathbf{x}, y)$.
  Classification == trying to learn conditional density $p(y|\mathbf{x})$.
- Even if we get the perfect model, our error rate may not be zero.
  Why? Classes may overlap.
- The best we could ever do if our cost function is number of errors is to guess $y^* = \mathrm{argmax}_y \; p(y|\mathbf{x})$.
  (The error rate of this procedure is known as the "Bayes error".)



K-Nearest-Neighbour

- Finally: a real algorithm!
- To classify a test point, chose the most common class amongst its K nearest neighbours in the training set.
- **Algorithm K-NN**

```
c-test ← KNN(K,x-train,c-train,x-test)   {
d(m,n) = distance between x-train(m) and x-test(n)
n(n,l) = index of l-th smallest entry of d(:,n) [*]
c(n,l) = c-train(n(n,l))
c-test(n) = most common value in c(n,1:K) [**]          }
```

- If ties at *, increase `K` for that `n` only.
- If ties at **, decrease `K` for that `n` only.
- confidence = (#votes for class) / K

Error Bounds for NN

- Amazing fact: asymptotically, err(1-NN) < 2 err(Bayes):

$$e_B \leq e_{1_{NN}} \leq 2e_B - \frac{M}{M-1}e_B^2$$

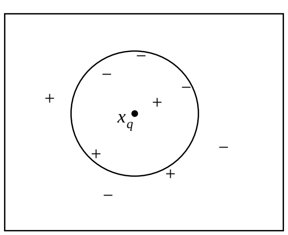
this is a tight upper bound, achieved in the "zero-information" case when the classes have identical densities.

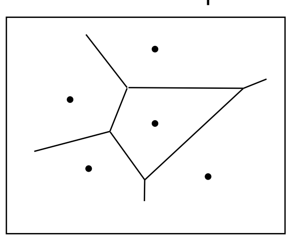
- For K-NN there are also bounds. e.g. for two classes and odd K:

$$e_B \leq e_{K_{NN}} \leq \sum_{i=0}^{(K-1)/2} \binom{k}{i} \left[e_B^{i+1}(1-e_B)^{k-i} + e_B^{k-i}(1-e_B)^{i+1} \right]$$

More on K-NN

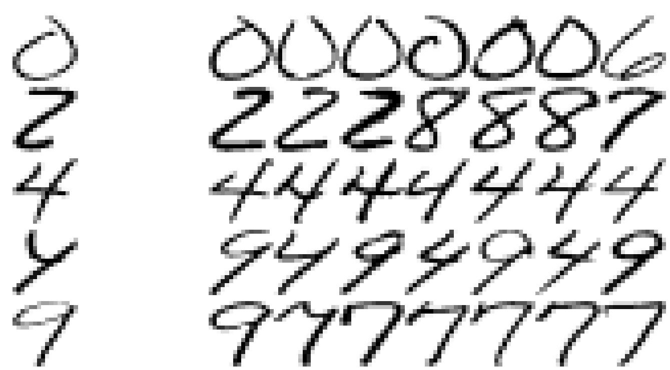
- Typical distance = squared Euclidean $d(m,n) = \sum_d (x_d^m - x_d^n)^2$
- Remember the K^{th} smallest distance so far, and stop the summation above when you exceed it.
- In high-d, save time by computing the distance of each training point from the min corner and using the "annulus bound".
- In low-d with lots of training points you can build "KD trees", "ball trees" or other data structures to speed up the query time.
- If Euclidean distance is used, decision surfaces are piecewise linear.





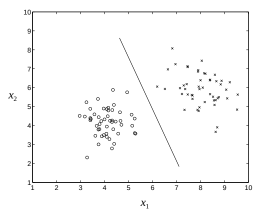
Example: USPS Digits

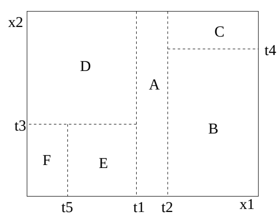
- Take 16x16 grayscale images (8bit) of handwritten digits.
- Use Euclidean distance in raw pixel space (dumb!) and 7-nn.
- Classification error: 4.85%.



Nonparametric (Instance-Based) Models

- Q: in K-NN, what are the parameters?
  A: the scalar K *and the entire training set*.
  A model which needs the entire training set at test time but (hopefully) has very few other parameters is known as *nonparametric*, *instance-based* or *case based*.
- What if we want a classifier that uses only a small number of parameters at test time? (e.g. for speed or memory reasons)
  Idea 1: single linear boundary, of arbitrary orientation
  Idea 2: many boundaries, but axis-parallel & tree structured





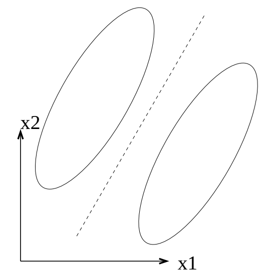
Fisher's Linear Discriminant

- Observation: If each class has a Gaussian distribution (with same covariances) then the Bayes decision boundary is linear:

$$\mathbf{w}^* = \Sigma^{-1}(\mu_0 - \mu_1)$$

$$w_0^* = \frac{1}{2}\mathbf{w}^\top(\mu_0 + \mu_1) - \mathbf{w}^\top(\mu_0 - \mu_1)\left[\frac{\log p_0 - \log p_1}{(\mu_0 - \mu_1)^\top\Sigma^{-1}(\mu_0 - \mu_1)}\right]$$

- Idea (Fisher'36):
  Assume each class is Gaussian even if they aren't!
  Fit μ_i and Σ as sample mean and sample covariance.



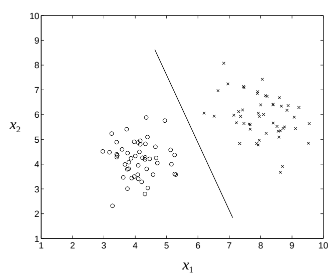
- This also maximizes the ratio of *cross-class scatter* to *within class scatter*: $(\bar{z}_0 - \bar{z}_1)^2/(\mathrm{var}(z_0) - \mathrm{var}(z_1))$

Linear Classification for Binary Output

- Goal: find the line (or hyperplane) which best separates two classes:

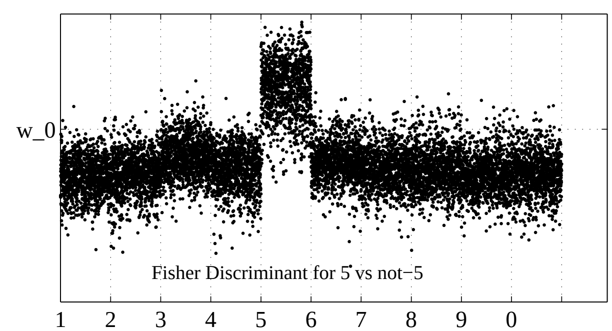
$$c(x) = \mathrm{sign}[\underbrace{\mathbf{x}^\top\mathbf{w}}_{weight} - \underbrace{w_0}_{threshold}]$$

- $\mathbf{w}$ is a vector perpendicular to decision boundary
- This is the opposite of non-parametric: only $d+1$ parameters!
- Typically we augment $\mathbf{x}$ with a constant term ± 1 ("bias unit") and then absorb w_0 into $\mathbf{w}$, so we don't have to treat it specially.



Digits again

Train to discriminant "5" from others.
Error = 3.59%

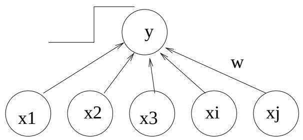


Linear Discriminants are Perceptrons

- The architecture we are using

  $$c(x) = \text{sign}[\mathbf{x}^\top \mathbf{w} - w_0]$$

  can be thought of as a circuit/network.



- It was studied extensively in the 1960s and is known as a *perceptron*.
- There is another way to train the weights, other than Fisher.

Algorithm perceptronTrain (Rosenblatt'56)

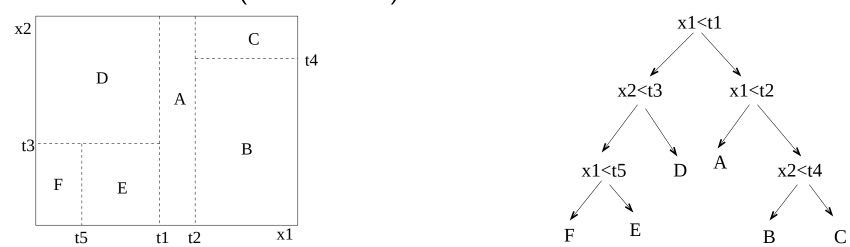
```
w ← perceptronTrain(x-train,c-train)   {
   w = ‘‘small’’ random values;
    do {   errors=0;
         for n=1:N {if(c-train(n) != sign[w’*xtrain(n)]) then {
         w = w + c - train(n)*xtrain(n);    errors++; } }
       } until(errors==0)
}
```

Perceptron Learning Rules

- Now: cycle through examples, when you make an error, add/subtract the example from the weight vector depending on its true class.
- Amazingly, for separable training sets, this always converges. (We absorb the threshold as a "bias" variable always equal to -1.)
- For non-separable datasets, you need to remember the sets of weights which you have seen so far, and combine them somehow.
- One way: keep the set that survived unchanged for the longest number of (random) pattern presentations. (Gallant's *pocket algorithm*.)
- Better way: Freund & Shapire's *voted perceptron* algorithm.
- Perceptron, voted-perceptron, weighted-majority, kernel perceptron, Winnow, and other algorithms have a frumpy reputation but they are actually extremely powerful and useful, especially using the kernel trick. Try these before more complex classifiers such as SVMs!

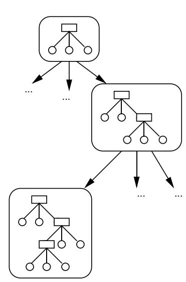
Tree Structured Axis-Aligned Classifiers

- What if we want more than two regions?
- We could consider a fixed number of arbitrary linear segments (*) but even cheaper is to use axis-aligned splits.
- If these form a hierarchical partition, then the classifier is called a *decision tree* or *classification tree*.
- Each internal node tests one attribute; leaves assign a class.
- Equivalent to a disjunction of conjunctions of constraints on attribute values (if-then rules).



Cost Function for Decision Trees

- Define a measure of "class impurity" in a set of examples.
- Goal: minimize expected sum of impurity at leaves.
- Two problems:
  1) We don't know true distribution $p(\mathbf{x}, y)$.
  2) Search: even if we knew $p(\mathbf{x}, y)$ finding optimal tree is NP.
- So we will take a suboptimal (greedy) approach.

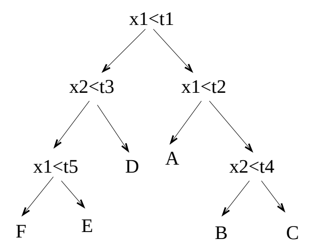


Learning (Inducing) Decision Trees

- Need to pick the order of split axes and values of split points. Many algorithms: CART, ID3, C4.5, C5.0.
- Almost all have the following structure:
  1. Put all examples into the root node.
  2. At each node: search all dimensions, on each one chose split which most reduces impurity; chose the best split.
  3. Sort the data cases into the daughter nodes based on the split.
  4. Recurse until a leaf condition:
     - number of examples at node is too small
     - all examples at node have same class
     - all examples at node have same inputs
  5. Prune tree down to some maximum number of leaves.

Binary Splits

- A better solution is to always constrain ourselves to binary splits.
- For ordered discrete or real valued nodes, split is natural.
  Also easy to compute (*).
- For a discrete attribute with M settings, looks like we need to consider $2^M - 1$ splits. But for two classes, there is a trick:
  1. Order the settings according to $p(c|x_i = m)$.
  2. Search exhaustively over q, grouping first q and last $M - q$.
  3. Optimal split is one of those.



Impurity Measures

- When considering splitting data D at a node on x_i, we measure:

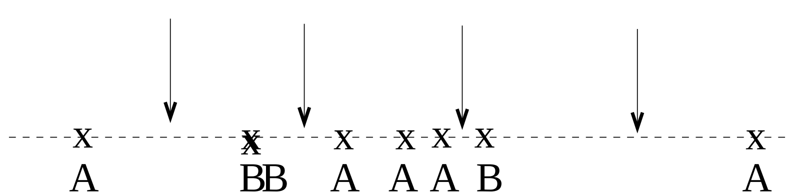
$$\mathrm{Gain}(D; x_i) = I(D) - \sum_{v \in split(x_i)} \frac{|D_{iv}|}{|D|} I(D_{iv})$$

- Common impurity measures:
  Entropy: $I(D) = -\sum_c p_c(D) \log p_c(D)$
  Misclass: $I(D) = 1 - p_{c^*}$
  Gini: $I(D) = \sum_c \sum_{c' \neq c} p_c(D) p_{c'}(D) = \ldots$
  (this is the avg. error if we stochastically classify with node prior)
- These often favour multi-way splits.
- One solution: normalize by "split information":

$$S(D) = -\sum_v \frac{|D_{iv}|}{|D|} \log \frac{|D_{iv}|}{|D|}$$

Real Valued Attributes

- For real valued attributes, what splits should we consider?
- Idea1: discretize the real value into M bins.
- Idea2: Search for a scalar value to split on.
  Sounds hard! Lots of real values. But there is a trick:
  Only need to consider splits at midpoints between observed values.
  In fact, only need to consider splits at midpoints between observed values with different classes.
- Complexity: $N \log N + 2N|C|$



Algorithm: DT

```
root of decision tree = SplitNode(train-data,nmin)

subtree ← SplitNode(D)  {
c = most common class in D
if (all class(D) same) or (all x(D) same) or (size(D) < nmin)
then return a leaf of class c
else for each xi measure Gain(D;xi)
return a node which splits on best xi and has daughters:
- SplitNode(Div) for all split vals v with nonempty Div
- leaf of class c for values with empty Div                    }

G ← Gain(D,i)  {
G = I(D)
for each value v in split(xi)
Div = cases in D with xi=v
G = G - I(Div)*size(Div)/size(D)                               }
```

Pruning Decision Trees

- Finding the "optimal" pruned tree.
  It can be shown that if you start with a tree T_0 and insist on using a rooted subtree of it, the following sequence of trees contains the optimum tree for all numbers of leaves:
  1. Let U(node) $=$ I(node)-I(subtree-rooted-at-node)
  2. Replace the non-leaf node with the smallest value of:
     U(node)/leaves-below-node
     with a leaf node having majority class.
- Still have problems:
  - cannot capture additive structure (OR)
  - cannot deal with linear combinations of variables

Overfitting in Trees

- Just as with most other models, decision trees can overfit. In fact they are quite powerful.
- eg: Expressive power of binary trees
  Q: If all input and outputs are binary, what class of Boolean functions can DTs represent?
  A: All Boolean functions.
- Hence we must *regularize* to control capacity.
- Typically we do this by limiting the number of leaf nodes.
  Formally, we define: $\Phi(T) = \sum_{leaves} I(l) + \alpha |leaves|$.
- Minimizing this for any α is equivalent to finding the tree of a fixed size with smallest impurity. (cf. Lagrange multipliers).
- Practically, we achieve this via pruning.

DT Variants

- ID3 (Quinlan)
  - split values are all possible values of x_i
  - I(D) is entropy - no pruning
- C4.5, C5.0 (Quinlan)
  - binary splits
  - I(D) is entropy - error-pruning
  - "rule simplification"
- CART (Breiman et. al)
  - binary splits
  - I(D) is Gini
  - minimum-leaf subtree pruning

Still to come...

- How do we chose K in K-NN?
- How do we chose T_{max} for decision trees?
- Can Fisher's Discriminant overfit?
- Logistic regression