INFO411 Lecture - Classification II

Jeremiah Deng

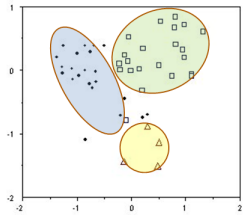
InfoSci, University of Otago

August 20, 2019

Overview

Bayesian Classifiers

- Use a *probabilistic* discriminant function $g_i(\mathbf{x})$
- Usually we can have
  - $g_i(\mathbf{x}) = P(\omega_i|\mathbf{x})$, or
  - $g_i(\mathbf{x}) = \ln p(\mathbf{x}|\omega_i) + \ln P(\omega_i)$.
- For $p(\mathbf{x}|\omega_i)$ of Gaussian (normal) density:
  $g_i(\mathbf{x}) = -\frac{1}{2}(\mathbf{x}-\mu_i)^T\Sigma_i^{-1}(\mathbf{x}-\mu_i) - \frac{1}{2}\ln|\Sigma_i| + \ln P(\omega_i)$
- Mixture of Gaussians: apply maximum-likelihood estimation of the Gaussian distribution for each class/each "mode"
- Conduct classification by assigning class labels according to the biggest discriminant function value



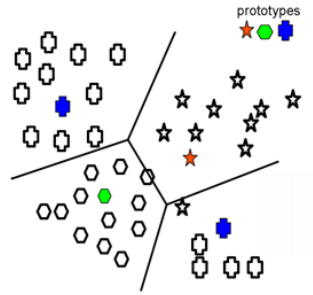
K-Nearest Neighbour (k-NN) Estimation

- Non-parametric: no need to estimate probability density ☺
- We have shown that k-NN classifier approximates the Bayes Classifier.
- Suppose we now place a cell of volume V around $\mathbf{x}$
- There are n labelled samples, of c classes
- The cell captures k samples, of which k_i belong to class i
- Then the estimate for the joint probability is
  $$p(\mathbf{x}, \omega_i) = \frac{k_i/n}{V}.$$
- And a reasonable estimate for *a posteriori* probability is
  $$P(\omega_i|\mathbf{x}) = \frac{p(\mathbf{x}|\omega_i)P(\omega_i)}{\sum_{j=1}^{c} p(\mathbf{x}, \omega_j)} = \frac{k_i}{k}$$
  i.e., k-NN is a an approximation to the Bayes Classifier.

Extending the clustering algorithms

- K-means, SOM etc. can all be augmented with a supervisory layer that tries to match to the class label of the training samples.
- For instance:
  - Linking prototypes with class labels;
  - Adopting supervised learning; or
  - Adding another layer and taking gradient descent on the weights.

Learning Vector Quantization (LVQ)



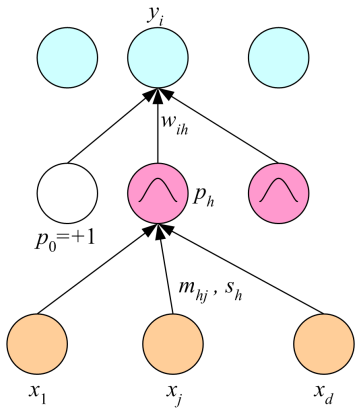
- Kohonen (1989)
- Similar to the idea of competitive learning and vector quantization
- However, since prototypes are labelled, we can make use of the supervisory learning

Algorithm

1. Initialize the prototype set $D^n = \{\mathbf{m}_1, \mathbf{m}_2, \cdots, \mathbf{m}_n\}$.
2. Given an input pattern $\mathbf{x}$, find the best matching prototype $\mathbf{m}_c$.
3. Update the winning prototype
   - $\Delta\mathbf{m}_c = \gamma(t)(\mathbf{x} - \mathbf{m}_c)$ if Class($\mathbf{x}$)==Class($\mathbf{m}_c$);
   - $\Delta\mathbf{m}_c = -\gamma(t)(\mathbf{x} - \mathbf{m}_c)$, otherwise.
4. Go back to Step 2 until convergence.

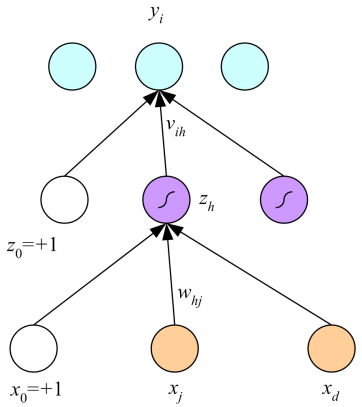
Radial Basis Functions

- Cluster data points around a few prototypes of Gaussian distribution
  $$p_h^t = \exp\left[-\frac{\|\mathbf{x}^t - \mathbf{m}_h\|^2}{2s_h^2}\right]$$
- Output is generated with a layer of "perceptron"
  $$y^t = \sum_{h=1}^{H} w_h p_h^t + w_0$$
- Use linear regression on the membership to clusters to predict the desired output r_i^t
  $$\Delta w_{ih} = \eta \sum_t (r_i^t - y_i^t) p_h^t$$

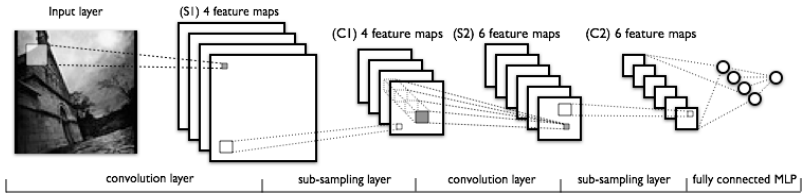


Multi-Layer Perceptron and Back Propagation

- Hidden layer employing "sigmoid" function to its weighted sum:
  $$z_h = \frac{1}{1 + \exp[-(\sum_{j=1}^{d} w_{hj} x_j + w_{h0})]}$$
- Output $y_i = \sum_{h=1}^{H} v_{ih} z_h + v_{i0}$
- Least-squares rule to update the 2nd layer weights: $\Delta v_h = \eta \sum_t (r^t - y^t) z_h^t$
- Back-Propagation rule for hidden layer:
  $$\begin{aligned}\Delta w_{hj} &= -\eta \frac{\delta E}{\delta w_{hj}} \\ &= -\eta \sum_t \frac{\delta E}{\delta y^t} \frac{\delta y^t}{\delta z_h^t} \frac{\delta z_h^t}{\delta w_{hj}} \\ &= \eta \sum_t (r^t - y^t) v_h z_h^t (1 - z_h^t) x_j^t\end{aligned}$$



A *Shallow* View on Deep Learning

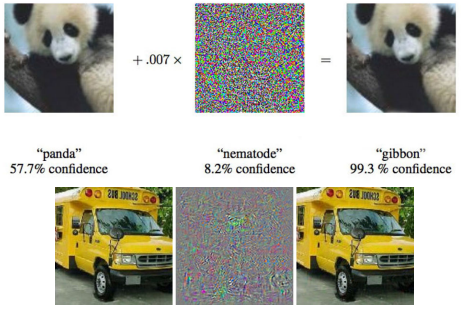


☹ Deep neural networks are very hard to train...

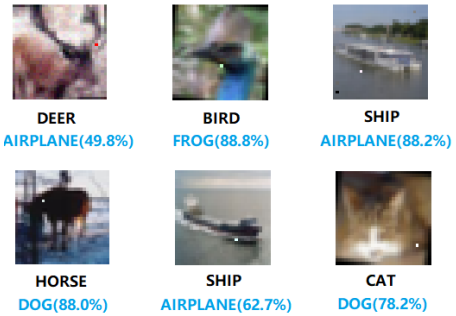
- Convolutional neural networks (CNN) are MLP-extensions inspired by biological vision.
- Dated back to Fukushima (1980), LeCun & Bengio (1998?) ...
- Multiple layers of nonlinear mechanisms: convolution, subsampling, sparsity
- Outcome: so far the best object recogniser

You see monkeys?

- Deep learning remains largely *unexplainable*.
- Also easily to be fooled, sometimes by perturbation of single pixels
- Nguyen et al. (2014), Szegedy et al. (2014), Goodfellow et al. (2015), Su et al. (2017), Athalye et al. (2018)



Or ostrich?



The Separation Hyperplane

Let's revisit the linear separation idea.

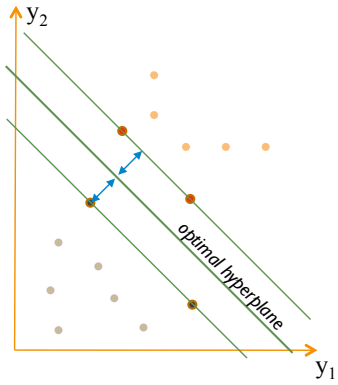
Consider a two-class problem, with sample $X = \{\mathbf{x}, r\}$, where $r = 1$ when $\mathbf{x} \in C_1$, and $r = -1$ if $\mathbf{x} \in C_2$.
We would like to find a hyperplane $g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0$ such that

$$g(\mathbf{x}) \geq +1, \text{for } r = +1$$
$$g(\mathbf{x}) \leq -1, \text{for } r = -1$$

Focusing on the margins

Note there exists a margin on either side of the hyperplane, of which we wish to maximize for better generalization. The above two lines are equivalent to $rg(\mathbf{x}) = r(\mathbf{w}^T\mathbf{x} + w_0) \geq 1$. To maximize the margin, we also need to add the constraint of minimizing $\|\mathbf{w}\|$. So our optimisation goal is

$$\min \frac{1}{2}\|\mathbf{w}\|^2 \text{ subject to } r(\mathbf{w}^T\mathbf{x} + w_0) \geq 1, \forall \mathbf{x}$$



Solving SVM

Using Lagrange multipliers α_t, the optimisation criterion becomes

$$L = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{t=1}^{N} \alpha_t [r_t(\mathbf{w}^T\mathbf{x}_t + w_0) - 1],$$

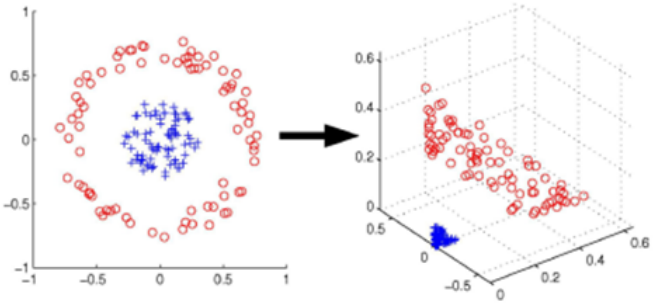
where $\mathbf{x}_t$ and r_t denote the t-th data point and its class label respectively.
By solving this quadratic optimization problem, it is found that most α_t are zero. Those $\mathbf{x}_t$ with $\alpha_t > 0$ satisfy

$$r_t(\mathbf{w}^T\mathbf{x}_t + w_0) = 1$$

lie on the margin. These are called 'support vectors'. One can easily worked out $w_0 = r_t - \mathbf{w}^T\mathbf{x}_t$ using these support vectors.

Challenge: Linear non-separability

- Not all classification problems can be solved using linear discriminant functions.
- Solutions:
  - Use multiple linear discriminant functions (divide-and-conquer)
  - Conduct nonlinear transformation using kernel methods, projecting data into higher dimensional kernel space with linear separability



SVM as a kernel machine

- First, use a nonlinear function to map the input data to a high-dimensional space.

$$z_k = \Phi(\mathbf{x}_k)$$

- Kernel function $\Phi(.)$ e.g. can be polynomials or Gaussians
- Defines a linear discriminant function in the augmented z space, where the problem becomes more linearly separable.
- Note because of the kernel trick $\Phi(\mathbf{x}_t)^T\Phi(\mathbf{x}_s) = K(\mathbf{x}_t, \mathbf{x}_s)$, we don't need to conduct dot product in the high-dimension space.

Kernel Trick: Example

Suppose we have 2-D data points $\mathbf{x}, \mathbf{y}$ and we project them to 3-D using $\Phi(.)$.

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}, \Phi(\mathbf{x}) = \begin{bmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{bmatrix}, \Phi(\mathbf{y}) = \begin{bmatrix} y_1^2 \\ \sqrt{2}y_1y_2 \\ y_2^2 \end{bmatrix}.$$

Now check out the dot product:

$$\begin{bmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{bmatrix} \cdot \begin{bmatrix} y_1^2 \\ \sqrt{2}y_1y_2 \\ y_2^2 \end{bmatrix} = \begin{matrix} x_1^2y_1^2 \\ + \ 2x_1x_2y_1y_2 \\ + \ x_2^2y_2^2 \end{matrix} = (x_1y_1 + x_2y_2)^2$$

i.e.

$$\langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle = \langle \mathbf{x}, \mathbf{y} \rangle^2$$

So $K(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle^2$: dot product can be done in 2-D instead of 3-D.
Not much savings? Think about the gains with 10-D, 100-D data ...

Popular kernel functions

- Polynomials of degree q: $K(\mathbf{x}_t, \mathbf{x}) = (\mathbf{x}^T\mathbf{x}_t + 1)^q$
- Radial-basis functions define a spherical kernel as in Parzen windows with a radius s:

$$K(\mathbf{x}_t, \mathbf{x}) = \exp[-\frac{\|\mathbf{x}_t - \mathbf{x}\|^2}{2s^2}]$$

  This can be extended to other definition of distance D between $\mathbf{x}$ and $\mathbf{x}_t$ (e.g., the geodesic distance used in Isomap):

$$K(\mathbf{x}_t, \mathbf{x}) = \exp[-\frac{\|D(\mathbf{x}_t, \mathbf{x})\|^2}{2s^2}]$$

- Sigmoidal functions: $K(\mathbf{x}_t, \mathbf{x}) = \tanh(2\mathbf{x}^T\mathbf{x}_t + 1)$
- ☺ Design your own?

Complications

- Often two classes are not perfectly linearly separable, and we have a soft margin instead:

$$r_t(\mathbf{w}^T\mathbf{x}_t + w_0) \geq 1 - \xi_t, \xi_t \geq 0$$

  and we penalise the ξ_t terms by modifying the optimisation function, with $C > 0$ controlling the extent of penalty:

$$\min \left[\frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{t=1}^{N}\xi_t\right]$$

- What about multi-class classification? Suppose k classes.
  - One-vs-one: build $k \times (k-1)/2$ pair-wise classifiers; the class with the highest vote wins;
  - One-vs-rest: build k binary classifiers; the one with the highest score wins. Faster, and almost as good.

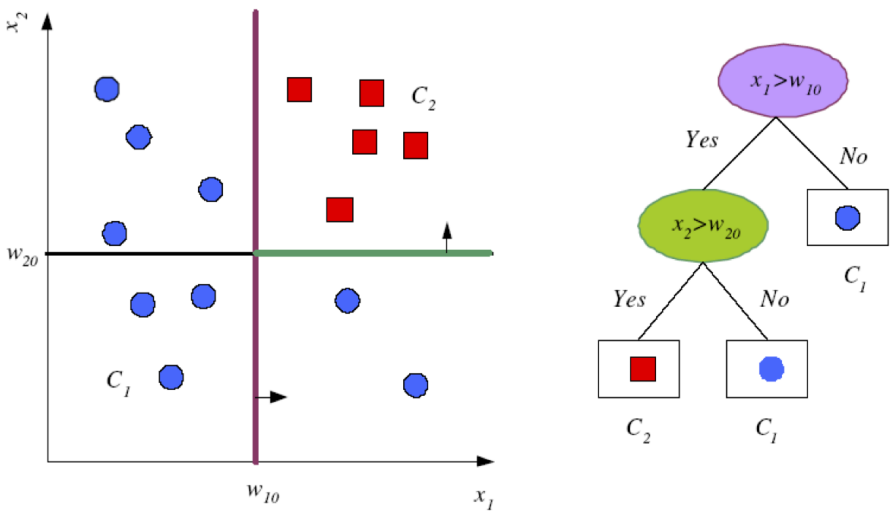
Non-metric data classification

- How can we handle non-numeric data?
- There are no distance measures, not even similarity definitions!

Decision Trees

- Similar to the idea of the "20-questions" game
- Useful for nonmetric data – all questions can be asked in a 'yes/no' or 'true/false' or 'which one' (from a finite set of values)
- The sequence of these questions (and answers) forms a decision tree, starting from the first question (root node), until it reaches the terminal or leaf nodes.
- Classification of a particular pattern begins at the root node and follows the appropriate link to a subsequent or descendent node.
- Famous algorithms: CART, C4.5 etc.
  - Can handle numeric data as well!

Tree Uses Nodes, and Leaves



Where to make the cut: minimize impurity

- Consider a node m
- Suppose it contains N_m training samples
- Of these, N_m^i instances belong to Class C_i
- Prob. for Class C_i is

$$p_m^i = \frac{N_m^i}{N_m}$$

- Measure the 'impurity' of node m using entropy:

$$H_m = -\sum_i p_m^i \log_2 p_m^i$$

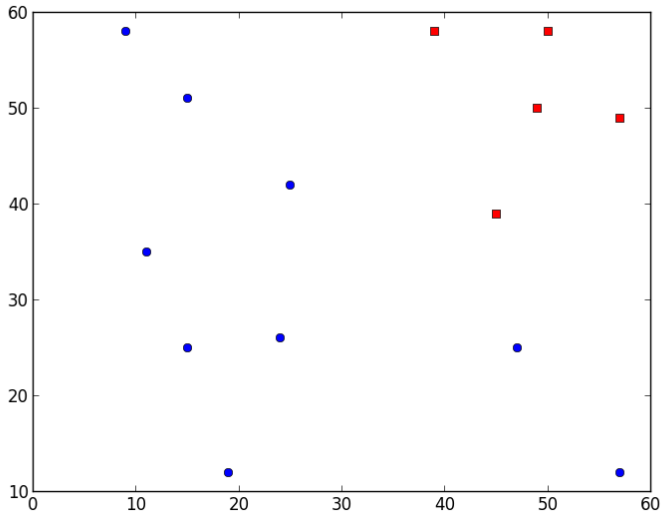
- For a 2-class problem
  - Entropy: $H = -p\log_2 p - (1-p)\log_2(1-p)$
  - Or, using the Gini index: $2p(1-p)$

A bit of DIY

```
### demo: finding where to make the 1st cut
data=np.array([[ 9.0, 58.0],
       [15, 51],
       [25, 42],
       [11, 35],
       [15, 25],
       [24, 26],
       [19, 12],
       [47, 25],
       [57, 12],
       [39, 58],
       [45, 39],
       [49, 50],
       [50, 58],
       [57, 49]])

cla=np.array([1, 1, 1, 1, 1, 1, 1, 1, 1, 2, 2, 2, 2, 2])

data=np.hstack((data,cla.reshape((-1,1))))
```

Try Out the Cuts

```
dim=0
d=np.unique(data[:,dim])
cuts=[]
for i in range(len(d)-1):
    cuts.append((d[i]+d[i+1])/2)    # cut amid two values

def impurity(a):
    labels=a[:,-1]
    p=(np.sum(labels==1)+0.)/len(a)
    if min(p,1-p)>1e-10:
        impu=-p*np.log2(p)-(1-p)*np.log2(1-p)
    else:
        impu=0.0
    return impu

print 'Imp_orig.', impurity(data)
for th in cuts:
    print 'Cut@',th,'Imp:',
    left=data[:,dim]<=th
    right=data[:,dim]>th
    p1=np.sum(data[left]==1)/(len(data)+0.)
    print impurity(data[left])*p1+impurity(data[right])*(1-p1)
```


Impurity from cuts

Original impurity: 0.940285958671

Outcome for Dimension #0

```
Cut@ 10.0 Impu 0.892576847243
Cut@ 13.0 Impu 0.839887505701
Cut@ 17.0 Impu 0.714285714286
Cut@ 21.5 Impu 0.637120324182
Cut@ 24.5 Impu 0.545390858814
Cut@ 32.0 Impu 0.431560284283
Cut@ 42.0 Impu 0.730930138627
Cut@ 46.0 Impu 0.867577550482
Cut@ 48.0 Impu 0.760220964704
Cut@ 49.5 Impu 0.876613035522
Cut@ 53.5 Impu 0.953311905174
```

Outcome for Dimension #1

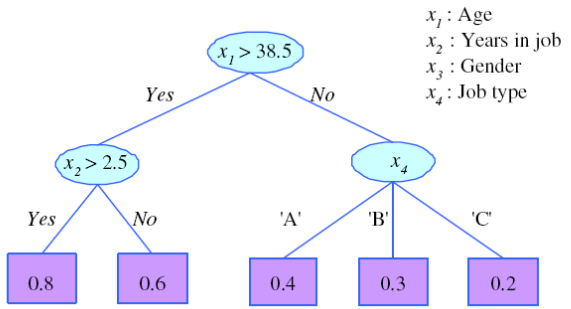
```
Cut@ 18.5 Impu 0.839887505701
Cut@ 25.5 Impu 0.714285714286
Cut@ 30.5 Impu 0.637120324182
Cut@ 37.0 Impu 0.545390858814
Cut@ 40.5 Impu 0.816561554269
Cut@ 45.5 Impu 0.730930138627
Cut@ 49.5 Impu 0.867577550482
Cut@ 50.5 Impu 0.940645449615
Cut@ 54.5 Impu 0.876613035522
```


Divide and Conquer

- Internal decision nodes
  - Univariate: Uses a single attribute, x_i
    - Numeric x_i : Binary split at w_m that reduces impurity the most
    - Discrete x_i : n-way split for n possible values
  - Multivariate: Uses all attributes, $\mathbf{x}$
- Leaves
  - Classification: Class labels, or proportions
  - Regression: Numeric; r average, or local fit
- Learning is greedy; find the best split recursively (Breiman et al., 1984; Quinlan, 1986, 1993)
- When to stop: use cross-validation, or thresholding on impurity reduction

Rule Extraction from Trees

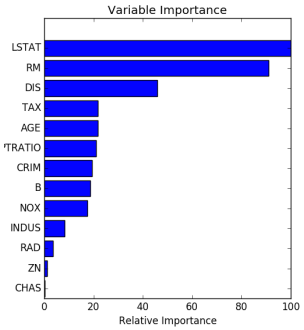
C4.5 rules (Quinlan 1993). Works also for regression.



R1: IF (age>38.5) AND (years-in-job>2.5) THEN y =0.8
R2: IF (age>38.5) AND (years-in-job≤2.5) THEN y =0.6
R3: IF (age≤38.5) AND (job-type='A') THEN y =0.4
R4: IF (age≤38.5) AND (job-type='B') THEN y =0.3
R5: IF (age≤38.5) AND (job-type='C') THEN y =0.2

Interpretation of trees

- Every time a split of a node is made on a variable results in reduction of the Gini impurity.
- Adding up the impurity reduction reveals the importance of variables.
- However, a single tree tends to be highly sensitive noises in data ☹
- In practice, random forests are preferred their better generalisation ability.
- Adding up the Gini decreases for each individual variable over all trees in the forest gives the importance measure.
- Variable important can also be found through permutation.



Recap

- Other classification methods: MLP, LVQ, RBF ...
  - Alpaydin Ch.11, “Multilayer Perceptrons”
  - Alpaydin Ch.12 “Local Models”
- SVM and kernel method (Alpaydin Ch.13)
- Decision Trees (Ch. 9)