CS 559 Machine Learning

Linear Classification

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Plan for today

Generative vs Discriminative Classification

Linear Discriminant Analysis

The Perceptron Algorithm

Naive Bayes Classifier

Model Selection

Review of last lecture

- Linear regression: L2 loss, L1 loss; Ridge regression (L2 regularization), Lasso regression;
- Gradient descent algorithms: BGD, SGD, mini-batch GD;
- Features: non-monotonicity, saturation, interactions between features;
- Maximum Likelihood estimator;
- Model selection: under-fitting, over-fitting, bias-variance;
- The curse of dimensionality

Classification

Classification task: finding a function f that classifies examples into given set of categories $\{C_1, C_2, .., C_k\}$

$$\mathbf{x} \quad \rightarrow \quad \boxed{\text{function } f} \quad \rightarrow \quad y \in \{C_1, C_2, .., C_k\}$$

A classification example:

$\rightarrow \quad \boxed{\text{function } f} \quad \rightarrow$ "Cat"

Decision Theory for Classification

Decision theory, when combined with probability theory, allows us to make optimal decisions in situations involving uncertainty.

- Training data: input values X and target values $\mathbf{y}$
- Inference stage: use the training data to learn a model for $p(C_k|\mathbf{x})$
- Decision stage: use the given posterior probabilities to make optimal class assignments.

Generative Methods

- Solve the inference problem of estimating the class-conditional densities $p(\mathbf{x}|C_k)$ for each class C_k
- Infer the prior class probabilities $p(C_k)$
- Use Bayes' theorem to find the class posterior probabilities:

$$p(C_k|\mathbf{x}) = \frac{p(\mathbf{x}|C_k)p(C_k)}{p(\mathbf{x})}$$

  where

$$p(\mathbf{x}) = \sum_k p(\mathbf{x}|C_k)p(C_k)$$

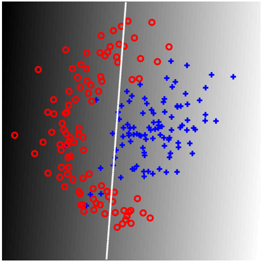
- Use decision theory to determine class membership for each new input $\mathbf{x}$

Discriminative Methods

- Solve directly the inference problem of estimating the class posterior probabilities $p(C_k|\mathbf{x})$
- Discriminative Functions: Find a function $f(x)$ which maps each input directly onto a class label. Probabilities play no role here.
- Use decision theory to determine class membership for each new input $\mathbf{x}$

Binary Classification

Task: Assign each data point to one of two classes.



Examples:

- Is there a face in this image?
- Will this neuron spike in response to this stimulus?
- Based on this brain-scan, does this patient have a given disease or not?
- Will this customer buy this product or not?
- Is this person likely to be a democrat/republican?

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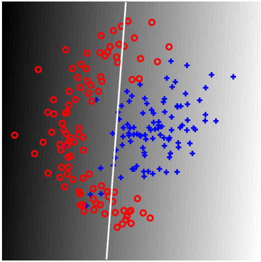

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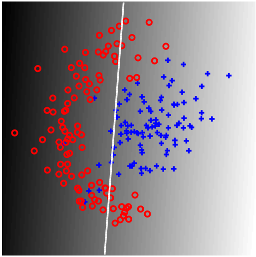
Notation: we have data $D = \{(x_1, y_1), \ldots, (x_N, y_N)\}$, with $y_n = 1$ if x_n belongs to class 1 and $y_n = -1$ if x_n belongs to class -1.

Linear Discriminant Functions



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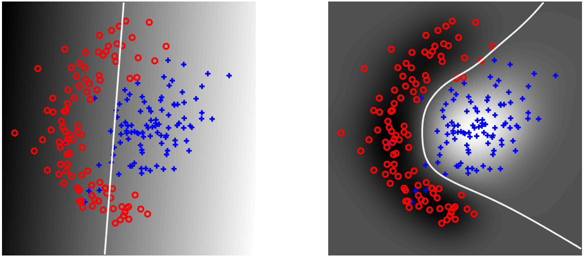

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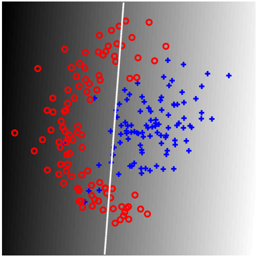 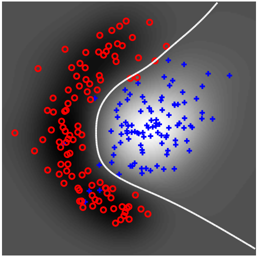

Of course, linear algorithms can be used together with nonlinear feature spaces or nonlinear basis functions in order to solve nonlinear classification problems!

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- $\mathbf{w}$ is the normal vector to the hyperplane, and points into the positive class or negative class.
- ω_o determines the location of the decision-surface
- $|f(\mathbf{x})|$ is proproptional to the perpendicular distance to the decision-surface (with factor 1 if $||\mathbf{w}|| = 1$).

Linear Discriminant Functions-Geometrical Properties

- Decision boundary:

$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + \omega_o = 0$$

- Let $\mathbf{x}_1, \mathbf{x}_2$ be two points which lie on the decision boundary

$$f(\mathbf{x}_1) = \mathbf{w}^\top \mathbf{x}_1 + \omega_o = 0, f(\mathbf{x}_2) = \mathbf{w}^\top \mathbf{x}_2 + \omega_o = 0$$
$$\Rightarrow \mathbf{w}^T(\mathbf{x}_1 - \mathbf{x}_2) = 0$$

- $\mathbf{w}$ represents the orthogonal direction to the decision boundary.

Linear Discriminant Functions-Geometrical Properties Cont.

- $\mathbf{w}^{*T} = \frac{\mathbf{w}^T}{||\mathbf{w}||}$
- $\mathbf{w}^{*T}(\mathbf{x} - \mathbf{x}_0)$ is the projection of $(\mathbf{x} - \mathbf{x}_0)$ onto the $\mathbf{w}^*$ direction
- Thus,

$$\frac{\mathbf{w}^T}{||\mathbf{w}||}(\mathbf{x} - \mathbf{x}_0) = \frac{1}{||\mathbf{w}||}(\mathbf{w}^T\mathbf{x} - \mathbf{w}^T\mathbf{x}_0)$$

$$= \frac{1}{||\mathbf{w}||}(\mathbf{w}^T\mathbf{x} + \omega_0) = \frac{f(\mathbf{x})}{||\mathbf{w}||}$$

when $\mathbf{x} = \mathbf{0}$, $\frac{f(\mathbf{x})}{||\mathbf{w}||} = \frac{\omega_0}{||\mathbf{w}||}$

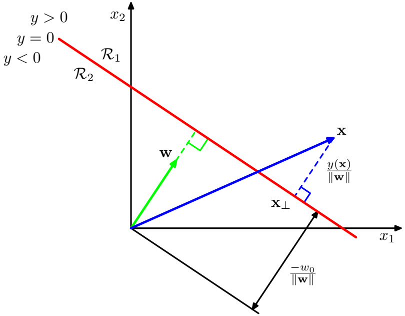
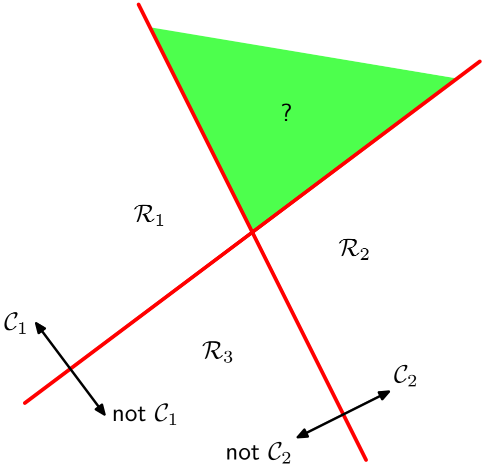


Figure: Signed orthogonal distance of the origin from the decision

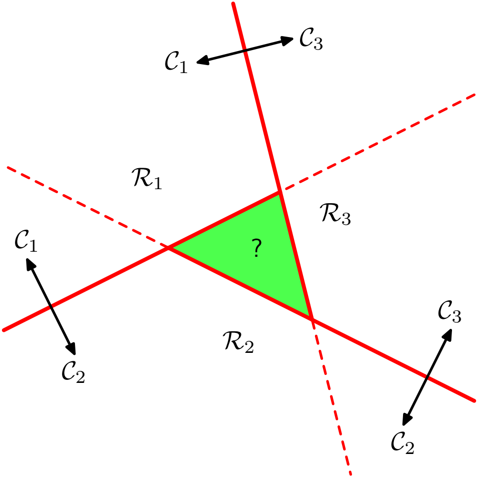
Linear Discriminant Functions: Multiple classes

one-versus-the-rest: K-1 classifiers each of which solves a two-class problem of separating points of C_k from points not in that class.



Linear Discriminant Functions: Multiple classes

<u>one-versus-one</u>: $\frac{K(K-1)}{2}$ binary discriminant functions, one for every possible pair of classes.

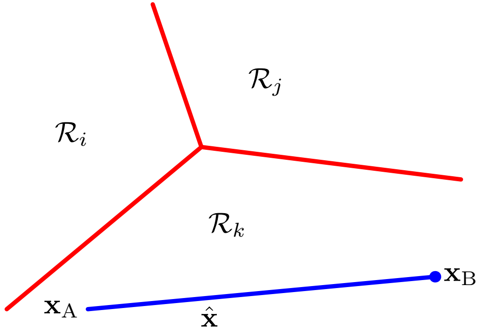


Linear Discriminant Functions: Multiple classes

- Solution: consider a single K-class discriminant comprising K linear functions of the form

$$f_k(\mathbf{x}) = \mathbf{w}_k^T \mathbf{x} + w_{k0}$$

- Assign a point $\mathbf{x}$ to class C_k if $f_k(\mathbf{x}) > f_j(\mathbf{x}) \forall j \neq k$
- The decision boundary between class C_k and class C_j is given by: $f_k(\mathbf{x}) = f_j(\mathbf{x}) \Rightarrow (\mathbf{w}_k - \mathbf{w}_j)^T \mathbf{x} + (w_{k0} - w_{j0}) = 0$



Multiple algorithms and methods

- Mis-classification rate $C(\mathbf{w}) = \frac{1}{N}\sum_n \delta\left[f(\mathbf{x}_n) = y_n\right]$ (i.e. average number of errors) difficult to optimize over $\mathbf{w}$, and might have multiple solutions.

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- Many algorithms can be derived by replacing C by another cost-function which can be optimized.
- Linear classification algorithms include Least-square classification, Fisher's linear Discriminant, Logistic regression, Support Vector Machines and Rosenblatts' perceptron.

Least square classification

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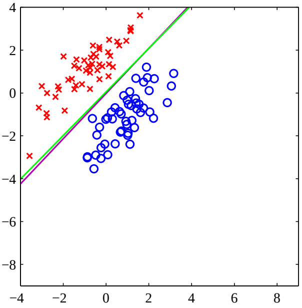

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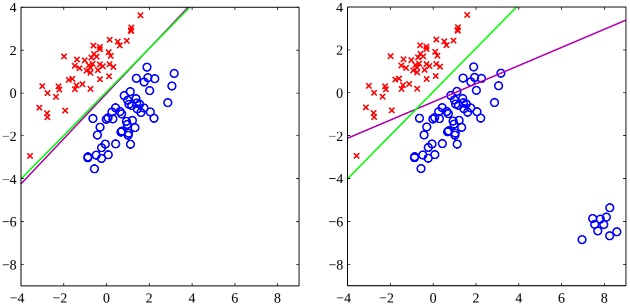

Bishop PRML Figure 4.4

Least square classification

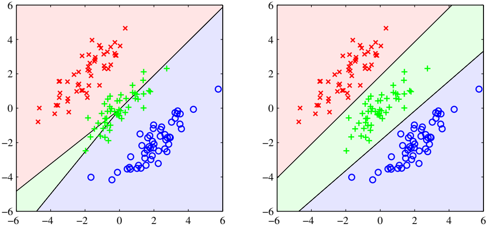

Figure: Left: using a least-squares discriminant; Right: using logistic regression

Bishop PRML Figure 4.5

Classification via projection

- A linear function: $f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + \omega_o$ assuming in 2D, projects each point $\mathbf{x} = [x_1, x_2]^T$ to a line parallel to $\mathbf{w}$:

point in $\mathcal{R}^d$	projected point in $\mathcal{R}$
$\mathbf{x}_1$	$z_1 = \mathbf{w}^T \mathbf{x}_1$
$\mathbf{x}_2$	$z_2 = \mathbf{w}^T \mathbf{x}_2$
$\cdots$	$\cdots$
$\mathbf{x}_n$	$z_n = \mathbf{w}^T \mathbf{x}_n$

- We can study how well the projected points $z_1, ..., z_n$ viewed as functions of $\mathbf{w}$ are separated across the classes.

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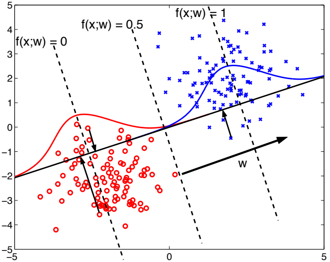

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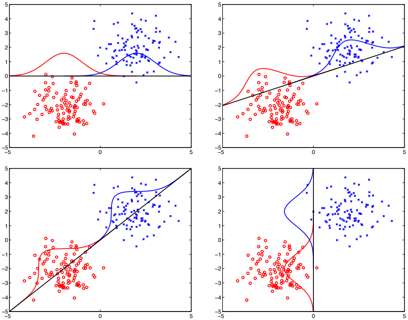
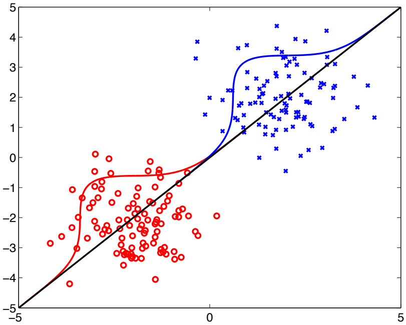
Classification via projection

- By varying **w** we get different levels of separation between the projected points



Optimizing the projection

- We would like to find $\mathbf{w}$ that somehow maximizes the separation of the projected points across classes.



- We can quantify the separation (overlap) in terms of means and variances of the resulting 1-dimensional class distributions

Fisher's linear discriminant

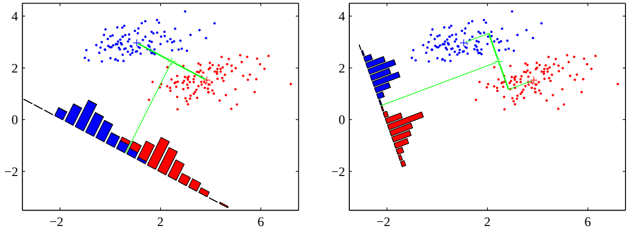
- One way to view a linear classification model is in terms of dimensionality reduction.
- Two class case: suppose we project $\mathbf{x}$ onto one dimension:

$$f = \mathbf{w}^T \mathbf{x}$$

- Set a threshold t:

$$\begin{array}{ll} \text{if } f \leq t & \text{assign } C_1 \text{ to } \mathbf{x} \\ \text{otherwise} & \text{assign } C_2 \text{ to } \mathbf{x} \end{array}$$

Fisher's linear discriminant



- Find an orientation along which the projected samples are well separated;
- This is exactly the goal of linear discriminant analysis (LDA);
- In other words: we are after the linear projection that best separates the data, i.e. best discriminates data of different classes.

Fisher's linear discriminant

- Two classes: $\{C_+, C_-\}$
- N_+ samples of class C_+
- N_- samples of class C_-
- Consider $\mathbf{w} \in \mathbb{R}^d$ with $||\mathbf{w}|| = 1$
- Then: $\mathbf{w}^T\mathbf{x}$ is the projection of $\mathbf{x}$ along the direction of $\mathbf{w}$.
- We want the projections $\mathbf{w}^T\mathbf{x}$ where $\mathbf{x} \in C_+$ separated from the projections $\mathbf{w}^T\mathbf{x}$ where $\mathbf{x} \in C_-$

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  - Sample mean for the projected points:

$$m_+ = \frac{1}{N_+} \sum_{\mathbf{x} \in C_+} \mathbf{w}^T \mathbf{x} = \mathbf{w}^T \mathbf{m}_+$$

$$\Rightarrow |m_+ - m_-| = \mathbf{w}^T (\mathbf{m}_+ - \mathbf{m}_-)$$

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- We wish to make the above difference as large as we can. In addition, ...

Fisher's linear discriminant

- To obtain good separation of the projected data, we really want the difference between the means to be large relative to some measure of the standard deviation of each class:

Fisher's linear discriminant

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  - Scatter of the projected samples of class C_+:

$$s_+^2 = \sum_{\mathbf{x} \in C_+} (\mathbf{w}^T \mathbf{x} - m_+)^2$$

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  - Total within-class scatter of the projected samples:

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  - Fisher linear discriminant analysis:

$$\text{arg max}_{\mathbf{w}} \frac{|m_+ - m_-|^2}{s_+^2 + s_-^2}$$

Fisher's linear discriminant

- $J(\mathbf{w}) = \frac{|m_+ - m_-|^2}{s_+^2 + s_-^2}$

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- $J(\mathbf{w}) = \frac{|m_+ - m_-|^2}{s_+^2 + s_-^2}$
- To obtain $J(\mathbf{w})$ as an explicit function of $\mathbf{w}$, we define the following matrices:

$$S_+ = \sum_{\mathbf{x} \in C_+} (\mathbf{x} - \mathbf{m}_+)(\mathbf{x} - \mathbf{m}_+)^T$$

Within-class scatter matrix:

$$S_w = S_+ + S_-$$

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Within-class scatter matrix:

$$S_w = S_+ + S_-$$

- Then:

$$\begin{aligned} s_+^2 &= \sum_{\mathbf{x} \in C_+} (\mathbf{w}^T \mathbf{x} - m_+)^2 = \sum_{\mathbf{x} \in C_+} (\mathbf{w}^T \mathbf{x} - \mathbf{w}^T \mathbf{m}_+)^2 \\ &= \sum_{\mathbf{x} \in C_+} \mathbf{w}^T (\mathbf{x} - \mathbf{m}_+)(\mathbf{x} - \mathbf{m}_+)^T \mathbf{w} = \mathbf{w}^T S_+ \mathbf{w} \end{aligned}$$

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\begin{aligned}
s_+^2 + s_-^2 &= \mathbf{w}^T S_+ \mathbf{w} + \mathbf{w}^T S_- \mathbf{w} \\
&= \mathbf{w}^T (S_+ + S_-) \mathbf{w} \\
&= \mathbf{w}^T S_w \mathbf{w}
\end{aligned}
$$

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- Similarly:

$$\begin{aligned} (m_+ - m_-)^2 &= (\mathbf{w}^T \mathbf{m}_+ - \mathbf{w}^T \mathbf{m}_-)^2 \\ &= \mathbf{w}^T (\mathbf{m}_+ - \mathbf{m}_-)(\mathbf{m}_+ - \mathbf{m}_-)^T \mathbf{w} \\ &= \mathbf{w}^T S_B \mathbf{w} \end{aligned}$$

where $S_B = (\mathbf{m}_+ - \mathbf{m}_-)(\mathbf{m}_+ - \mathbf{m}_-)^T$ (Between-class scatter matrix)

Fisher's linear discriminant

- We have obtained:

$$J(\mathbf{w}) = \frac{|m_+ - m_-|^2}{s_+^2 + s_-^2} = \frac{\mathbf{w}^T S_B \mathbf{w}}{\mathbf{w}^T S_W \mathbf{w}}$$

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- $J(\mathbf{w})$ is maximized when $(\mathbf{w}^T S_B \mathbf{w}) S_W \mathbf{w} = (\mathbf{w}^T S_W \mathbf{w}) S_B \mathbf{w}$

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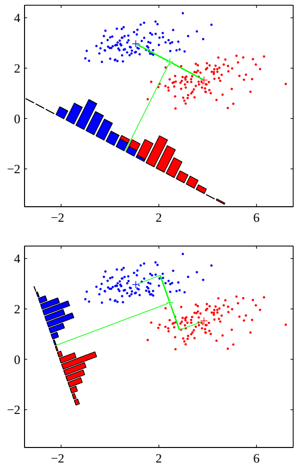
$$\mathbf{w} = S_W^{-1}(\mathbf{m}_+ - \mathbf{m}_-)$$

Fisher's linear discriminant-Summary



Bishop PRML Figure 4.6

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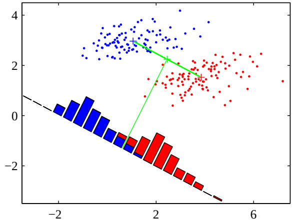

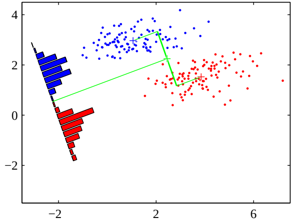

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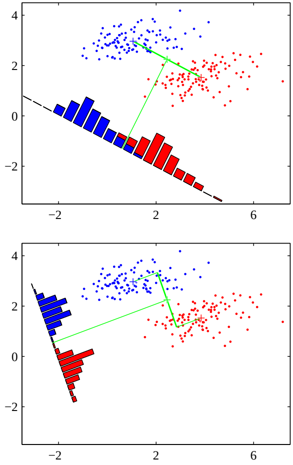

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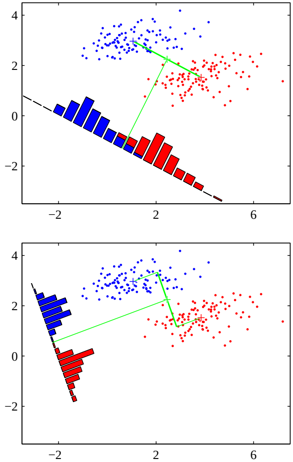

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- Fix: Maximize the ratio of between-class variance to within-class variance ('signal to noise'). Fisher criterion

$$J_{\mathbf{w}} = \frac{(m_{+} - m_{-})^2}{s_{+}^2 + s_{-}^2} \quad (1)$$

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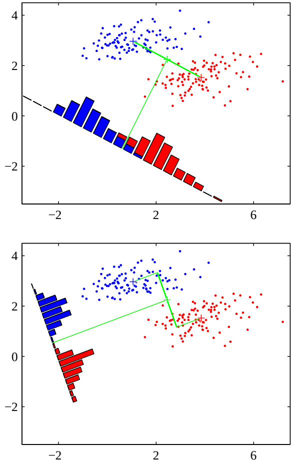

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Fisher's linear discriminant

- Gives the linear function with the maximum ratio of between-class scatter to within-class scatter.
- The problem, e.g. classification, has been reduced from a d-dimensional problem to a more manageable one-dimensional problem.
- Optimal for multivariate normal class conditional densities.

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- At most K-1 distinct solution eigenvalues
- The optimal projection matrix V to a subspace of dimension k is given by the eigenvectors corresponding to the largest k eigenvalues

Fisher's linear discriminant

- LDA is a linear technique for dimensionality reduction: it projects the data along directions that can be expressed as linear combination of the input features.
- The "appropriate" transformation depends on the data and on the task we want to perform on the data. Note that LDA uses class labels.
- Non-linear extensions of LDA exist (e.g., generalized LDA).

The Perceptron Algorithm (Frank Rosenblatt, 1957)

- First learning algorithm for neural networks.
- Originally introduced for character classification, where each character is represented as an image;
- Total input to output node:

$$\sum_j w_j x_j$$

- Output unit performs the function (activation function):

$$H(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0 \end{cases}$$

Perceptron: Learning Algorithm

- Goal: compute a mapping from inputs to the outputs.
- Example: two class character recognition problem.
  - Training set: set of images representing either the character 'a' or the character 'b' (supervised learning);
  - Learning task: learn the weights so that when a new unlabelled image comes in, the network can predict its label.
  - Setting: d input units (intensity level of a pixel), 1 output unit.

Perceptron: Learning Algorithm

The algorithm proceeds as follows:

- Initial random setting of weights;
- The input is a random sequence $\{\mathbf{x}_k\}$
- For each element of class C_1, if output $= 1$ (correct), do nothing; otherwise, update weights;
- For each element of class C_2, if output $= 0$ (correct), do nothing; otherwise, update weights;

Perceptron: Learning Algorithm

- More formally: $\mathbf{x} = (x_1, x_2, .., x_d)^T, \mathbf{w} = (w_1, w_2, .., w_d)^T$
- θ: Threshold of the output unit
- Unit output: $\mathbf{w}^T\mathbf{x} = w_1x_1 + w_2x_2 + ... + x_dx_d$
- Output class 1 if $\mathbf{w}^T\mathbf{x} - \theta \geq 0$
- To eliminate the explicit dependence on θ:
  Output class 1 if: $\mathbf{w}^T\mathbf{x} \geq 0$

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Perceptron: Learning Algorithm

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- Given $\mathbf{x}$ in input, if $\mathbf{x}$ is classified correctly, weights are unchanged, otherwise:

$$\mathbf{w} = \begin{cases} \mathbf{w} + \mathbf{x} & \text{if an element of class } C_1 \text{ was classified as in } C_2 \\ \mathbf{w} - \mathbf{x} & \text{if an element of class } C_2 \text{ was classified as in } C_1 \end{cases}$$

Perceptron: Learning Algorithm

- 1^{st} case: $\mathbf{x} \in C_1$ and was classified in C_2. The correct answer is 1, which corresponds to: $\mathbf{w}^T\mathbf{x} \geq 0$, we have $\mathbf{w}^T\mathbf{x} < 0$. We want to get closer to the correct answer: $\mathbf{w}^T\mathbf{x} < \mathbf{w}'^T\mathbf{x}$.

$$\mathbf{w}^T\mathbf{x} < \mathbf{w}'^T\mathbf{x}, \text{ iff } \mathbf{w}^T\mathbf{x} < (\mathbf{w}+\mathbf{x})^T\mathbf{x}$$

$$(\mathbf{w}+\mathbf{x})^T\mathbf{x} = \mathbf{w}^T\mathbf{x} + \mathbf{x}^T\mathbf{x} = \mathbf{w}^T\mathbf{x} + ||\mathbf{x}||^2$$

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- 2^{st} case: $\mathbf{x} \in C_2$ and was classified in C_1. The correct answer is 0, which corresponds to: $\mathbf{w}^T\mathbf{x} < 0$, we have $\mathbf{w}^T\mathbf{x} \geq 0$. We want to get closer to the correct answer: $\mathbf{w}^T\mathbf{x} > \mathbf{w}'^T\mathbf{x}$.

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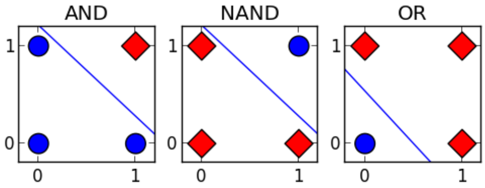
- Convergence theorem: regardless of the initial choice of weights, if the two classes are linearly separable, there exists $\mathbf{w}$ such that:

$$\begin{cases} \mathbf{w}^T\mathbf{x} \geq 0 & \text{if } \mathbf{x}_k \in C_1 \\ \mathbf{w}^T\mathbf{x} < 0 & \text{if } \mathbf{x}_k \in C_2 \end{cases}$$

then the learning rule will find such solution after a finite number of steps.

Representational Power of Perceptrons

- Marvin Minsky and Seymour Papert, "Perceptrons" 1969:
  The perceptron can solve only problems with linearly separable classes
- Examples of linearly separable Boolean functions:



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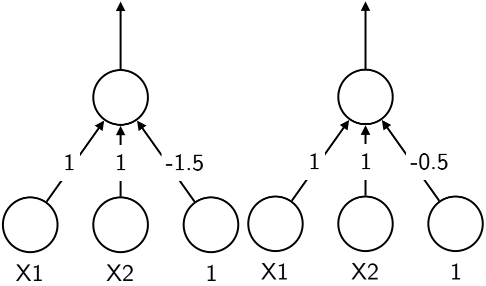
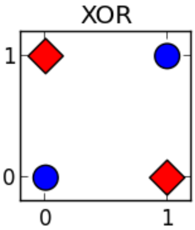


Figure: Left: AND; Right: OR

Representational Power of Perceptrons

- Examples of a non linearly separable Boolean function:



- The EX-OR function cannot be computed by a perceptron.

Naive Bayes: not (necessarily) a Bayesian method

- A and B are independent iff $p(A, B) = p(A)p(B)$
- A and B are conditionally independent given C iff $p(A, B|C) = p(A|C)p(B|C)$

Naive Bayes: Assumption

- Assume dimensions of **x** are conditionally independent given y.
- Example, bag of words:
  $p(\text{"Stevens"}, \text{"Institute"}, \text{"Technology"}|y) =$
  $p(\text{"Stevens"}|y)p(\text{"Institute"}|y)p(\text{"Technology"}|y)$
- Optimizaing:

$$
\begin{aligned}
f(x) &= \arg\max_y p(y|x) \\
&= \arg\max_y p(x|y)p(y)/p(x) \\
&= \arg\max_y p(x|y)p(y) \\
&= \arg\max_y p(y)\prod_j p(x_j|y)
\end{aligned}
$$

Naive Bayes: Solution

- $p(y) :\leftarrow \frac{\#\text{ examples where } Y{=}y}{(\#\text{ examples})}$
- $p(X_j = x_j | y) \leftarrow \frac{\#\text{ ex where } Y{=}y \text{ and } X_j{=}x_j}{(\#\text{ ex where } Y{=}y)}$
- Learning by counting!

Gaussian naive Bayes: Continuous data

- $p(y) :\leftarrow \frac{\#\text{ examples where } Y{=}y}{(\#\text{ examples})}$
- $p(X_j = v|y) \leftarrow \frac{1}{\sqrt{2\pi\sigma_k^2}} exp\{-\frac{(v-\mu_k)^2}{2\sigma_k^2}\}$
- μ_k and σ_k are determined from the training data set.
- Learning by counting!

Gaussian naive Bayes: example (from Wikipedia)

Training data set:

Sex	height	weight	foot size
male	6	180	12
male	5.92	1990	11
male	5.58	170	12
male	5.92	165	10
female	5	100	6
female	5.5	150	8
female	5.42	140	7
female	5.75	150	9

Mean and variance

Sex	mean-height	var-height	mean-weight	var-weight	mean-footsize	var-footsize
male	5.855	$3.5 * 10^{-2}$	176.25	$1.2292 * 10^{2}$	11.25	$9.1667 * 10^{-1}$
female	5.4175	$9.7225 * 10^{-2}$	132.5	$5.5833 * 10^{2}$	7.5	1.6667

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Testing:

Sex	height	weight	foot size
?	6	130	8

$$p(m|x) \approx p(\mathrm{m})p(\mathrm{height}|m)p(\mathrm{weight}|m)p(\mathrm{footsize}|m) = 6.1984 * 10^{-9}$$

$$p(f|x) \approx p(\mathrm{f})p(\mathrm{height}|f)p(\mathrm{weight}|f)p(\mathrm{footsize}|f) = 5.3778 * 10^{-4}$$

What is Model Selection?

Given a set of models $\mathcal{M} = \{M_1, M_2, ..., M_R\}$, choose the model that is expected to do the best on the test data. $\mathcal{M}$ may consist of:

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- Different learning models (e.g. SVM, kNN, DT, etc)

Note: usually considered in supervised learning but unsupervised learning faces this issue too.

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  - wastes training data

Held-out Data

- Set aside a fraction (10-20%) of the training data.
- This part becomes our held-out data (validation/development)
- **Remember**: Held-out data is NOT the test data
- Train each model using the remaining training data
- Evaluate error on the held-out data
- Choose the model with the smallest held-out error
- Problems:
  - wastes training data
  - if there was an unfortunate split (can be alleviated by repeated random subsampling)

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K-fold Cross-Validation on N training examples

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- can be expensive for large N. Typically used when N is small

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- Repeat K times, each with a different randomly chosen validation set
- Choose the model with the smallest average validation error
- Usually α is chose as 0.1, K as 10

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- This can break down if we overfit and $e_{\text{training}} = 0$

Bradley Efron & Robert Tibshirani. *Improvements on Cross-Validation: The 632+ Bootstrap Method*

Information Criteria based methods

- Akaike Information Criteria (AIC)

$$\mathrm{AIC} = 2k - 2\log(\mathcal{L})$$

- Bayesian Information Criteria (BIC)

$$\mathrm{BIC} = k\log(N) - 2\log(\mathcal{L})$$

- k: # of model parameters
- n: # of data examples
- $\mathcal{L}$: maximum value of the model likelihood
- Applicable for probabilistic models
- AIC/BIC penalize model complexity

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Selecting a useful subset from all the features. Why?

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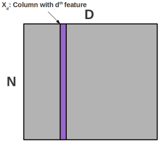
  - More on feature extraction when we cover **Dimensionality Reduction**

Feature Selection Methods

- Methods agnostic to the learning algorithm
  - Preprocessing based methods
    - E.g., remove a binary feature if its ON in very few or most examples
  - Filter Feature Selection methods
    - Use some ranking criteria to rank features
    - Select the top ranking features
- Wrapper Methods (keep the learning algorithm in the loop)
  - Requires repeated runs of the learning algorithm with different set of features
  - Can be computationally expensive

Filter Feature Selection

- Uses heuristics but is much faster than wrapper methods



- **Correlation Criteria**: Rank features in order of their correlation with the labels

$$R(X_d, \mathbf{y}) = \frac{cov(X_d, \mathbf{y})}{\sqrt{var(X_d)var(\mathbf{y})}}$$

- **Mutual Information Criteria**:

$$MI(X_d, \mathbf{y}) = \sum_{X_d \in \{0,1\}} \sum_{y \in \{-1,+1\}} P(X_d, \mathbf{y}) \log \frac{P(X_d, \mathbf{y})}{P(X_d)P(y)}$$

  - high mutual information means high relevance of that feature
  - Note: these probabilities can be easily estimated form the data

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- Inclusion/Removal criteria uses cross-validation

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