Linear Threshold Units - II

Logisitic Regression and

Linear Discriminant Analysis

Logistic Regression

- Learn the conditional distribution P(y|**x**)
- Let p_y(x:w) be our estimate of P(y|x), where w is a vector of parameters (adjustable). Assume two classes y=0 and y=1

$$p(y=1\,|\,\mathbf{x};\mathbf{w}) = p_1(\mathbf{x}) = \frac{1}{1+e^{-\mathbf{w}\cdot\mathbf{x}}}$$

$$p(y=0\,|\,\mathbf{x};\mathbf{w}) = 1 - p_1(\mathbf{x})$$

- You will show in homework that, this is equivalent to

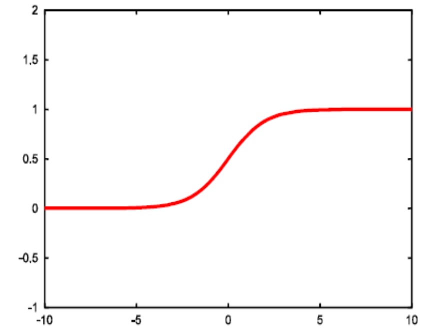
$$\log\frac{p(y=1\,|\,\mathbf{x};\mathbf{w})}{p(y=0\,|\,\mathbf{x};\mathbf{w})} = \mathbf{w}\cdot\mathbf{x}$$

i.e., the log odds of class 1 is a linear function of **x.**

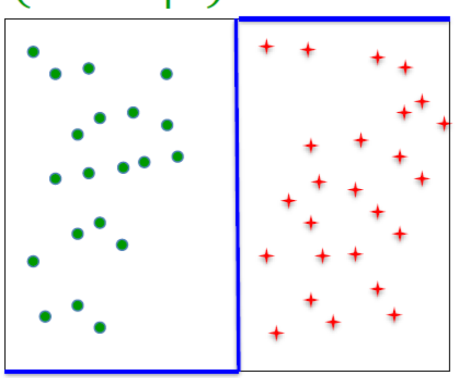
Why the exp function?

- Differentiable
- Easy to learn
- Handles noisy labels naturally

$$g(\mathbf{x},\mathbf{w}) = \frac{1}{1+\exp(-\mathbf{w}\cdot\mathbf{x})}$$

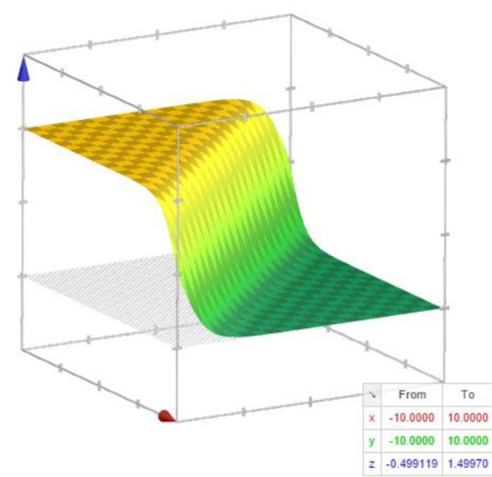


$p(Y = 1|x) = 0$



$p(Y = 1|x) = 1$

A linear function has a range from $[-\infty,\infty]$, the logistic function transforms the range to [0,1] to be a probability.



Not differentiable!

Deriving a Learning Algorithm

- Since we are fitting a conditional probability distribution, we no longer seek to minimize the loss on the training data. Instead, we are interested in finding the distribution *h* that is most likely given the training data
- Let S be the training sample. Our goal is to find h to maximize P(h|S)

$$\arg\max_h P(h \mid S) = \arg\max_h \frac{P(S \mid h)P(h)}{P(S)}$$ by Bayes' Rule

$$= \arg\max_h P(S \mid h)P(h)$$ because *P(S)* doesn't depend on *h*

$$= \arg\max_h P(S \mid h)$$ assuming *P(h)* is uniform

$$= \arg\max_h \log P(S \mid h)$$ Because log is montonic

The distribution of P(S|h) is called the <u>likelihood</u> function. The log likelihood is frequently used as the objective function for learning. It is often written as l(**w**).

The h that maximizes the likelihood on the training data is called the <u>maximum likelihood estimator (MLE)</u>

Computing the Likelihood

- In our framework, we assume that each training example is iid

- $$\begin{aligned} logP(S|\mathrm{h}) &= \log \prod_i P(\boldsymbol{x}_i, y_i|h) \\ &= \sum_i logP(\boldsymbol{x}_i, y_i|h) \end{aligned}$$

- This shows that the log likelihood of S is the sum of the log likelihoods of the individual training examples

Computing the Likelihood

- Recall that any joint distribution P(a,b) can be factored as P(a|b)P(b). Hence, we can write

$$\begin{aligned}\arg\max_h \log P(S \mid h) &= \arg\max_h \sum_i \log P(\mathbf{x}_i, y_i \mid h) \\ &= \arg\max_h \sum_i \log P(y_i \mid \mathbf{x}_i, h) P(\mathbf{x}_i \mid h)\end{aligned}$$

- In our case, P(**x**|h) = P(**x**), since it does not depend on h

$$\arg\max_h \log P(S \mid h) = \arg\max_h \sum_i \log P(y_i \mid \mathbf{x}_i, h)$$

Computing the Likelihood

- Consider an example ($\mathbf{x}_i$,y_i)
  - If y_i=0 the log likelihood is log [1 – $p_1(\mathbf{x};\mathbf{w})$]
  - If y_i=1 the log likelihood is log [$p_1(\mathbf{x};\mathbf{w})$]

- Note that these cases are mutually exclusive and hence can be combined

$$l(y_i;\mathbf{x}_i,\mathbf{w}) = \log P(y_i \mid \mathbf{x}_i,\mathbf{w}) = (1-y_i)\log[1-p_1(\mathbf{x}_i,\mathbf{w})] + y_i \log[p_1(\mathbf{x}_i,\mathbf{w})]$$

- The goal of our learning algorithm will be to find **w** to maximize

$$J(\mathbf{w}) = \sum_i l(y_i;\mathbf{x}_i,\mathbf{w})$$

Fitting Logistic Regression by Gradient Descent

On the board

Over all gradient is

$$\frac{\partial J(w)}{\partial w_j} = \sum_i (y_i - p_1(\mathbf{x}_i;\mathbf{w}))x_{ij}$$

Batch Gradient Ascent for Logistic Regression

Given: Training examples *($\mathbf{x}_i$, y_i), i = 1,…,N*

Let **w** = (0,0,…,0) be the initial weight vector

Repeat until convergence

Let g = (0,…,0) be the initial gradient vector

For i = 1 to N do

$$p_i = 1/(1+\exp[\mathbf{w}\cdot\mathbf{x}_i])$$

$$error = y_i - p_i$$

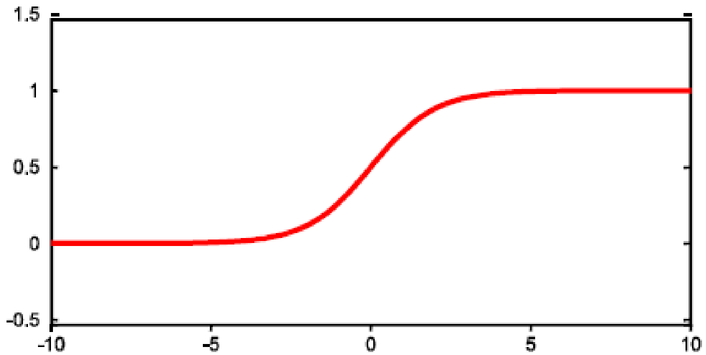
For j = 1 to n do

$$g_j = g_j + error \cdot x_{ij}$$

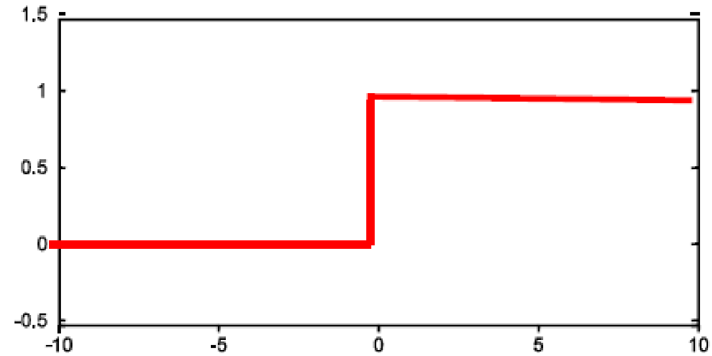
$$w := w + \eta g$$

Connection between Logistic Regression and Perceptron Algorithm

If we replace the logistic function with a step function:



$$h_{\mathbf{w}}(\mathbf{x}) = \frac{1}{1+e^{-\mathbf{w}\cdot\mathbf{x}}}$$



$$h_{\mathbf{w}}(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{w}\cdot\mathbf{x} > 0 \\ 0 & \text{otherwise} \end{cases}$$

Multi-Class Logistic Regression

- Choose class K to be the "reference class" and represent each of the other classes as a logistic function of the odds of class *k* versus class K:

$$\log \frac{P(y=1 \mid \mathbf{x})}{P(y=K \mid \mathbf{x})} = \mathbf{w}_1 \cdot \mathbf{x}$$
$$\log \frac{P(y=2 \mid \mathbf{x})}{P(y=K \mid \mathbf{x})} = \mathbf{w}_2 \cdot \mathbf{x}$$
$$\vdots$$
$$\log \frac{P(y=K-1 \mid \mathbf{x})}{P(y=K \mid \mathbf{x})} = \mathbf{w}_{K-1} \cdot \mathbf{x}$$

- Gradient ascent can be applied to simultaneously train all weight vectors $\mathbf{w}_k$

Multi-Class Logistic Regression

- Conditional probability for class k $\neq$ K can be computed as

$$P(y=k \mid \mathbf{x}) = \frac{\exp(\mathbf{w}_k \cdot \mathbf{x})}{1+\sum_{l=1}^{K-1} \exp(\mathbf{w}_l \cdot \mathbf{x})}$$

- For class K, the conditional probability is

$$P(y=K \mid \mathbf{x}) = \frac{1}{1+\sum_{l=1}^{K-1} \exp(\mathbf{w}_l \cdot \mathbf{x})}$$

Logistic Regression Implements a Linear Discriminant Function

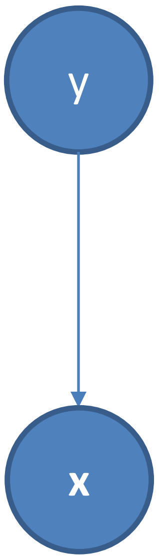
White board time!

Summary of Logistic Regression

- Learns conditional probability distribution P(y | $\mathbf{x}$)
- Local Search
  - begins with initial weight vector. Modifies it iteratively to maximize the log likelihood of the data
- Online or Batch
  - both online and batch variants of the algorithm exist

Linear Discriminant Analysis

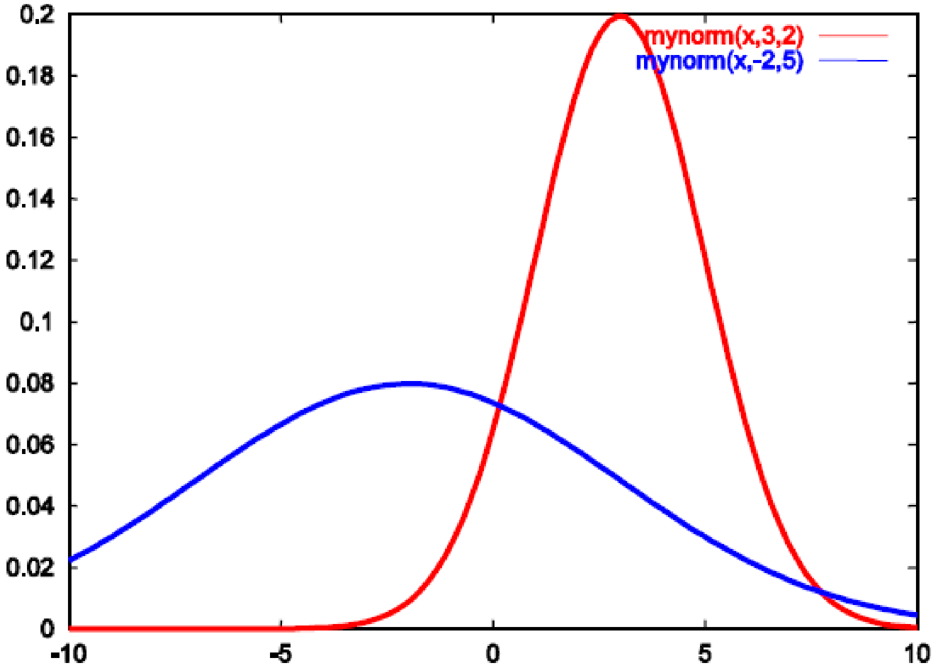
- Learn P(**x**,y). This is often called as generative approach, because we think of P(**x**,y) as a model of how the data has been generated.
  - For example, if we factor the joint distribution P(**x**,y) = P(y) P(**x**|y)
  - We can think of P(y) as generating a value for y according to the prior. Then we can think of P(**x**|y) as generating a value for **x** given the previously-generated value of y



LDA (2)

- P(y) is a discrete normal distribution
  - Ex: P(y=0) = 0.31 will generate 31% negative examples and 69% positive examples
- Recall that the univariate gaussian has the formula

$$p(x) = \frac{1}{\sqrt{2\pi\sigma}} \exp[\frac{-1}{2} \frac{(x-\mu)^2}{\sigma^2}]$$



Multivariate Gaussian

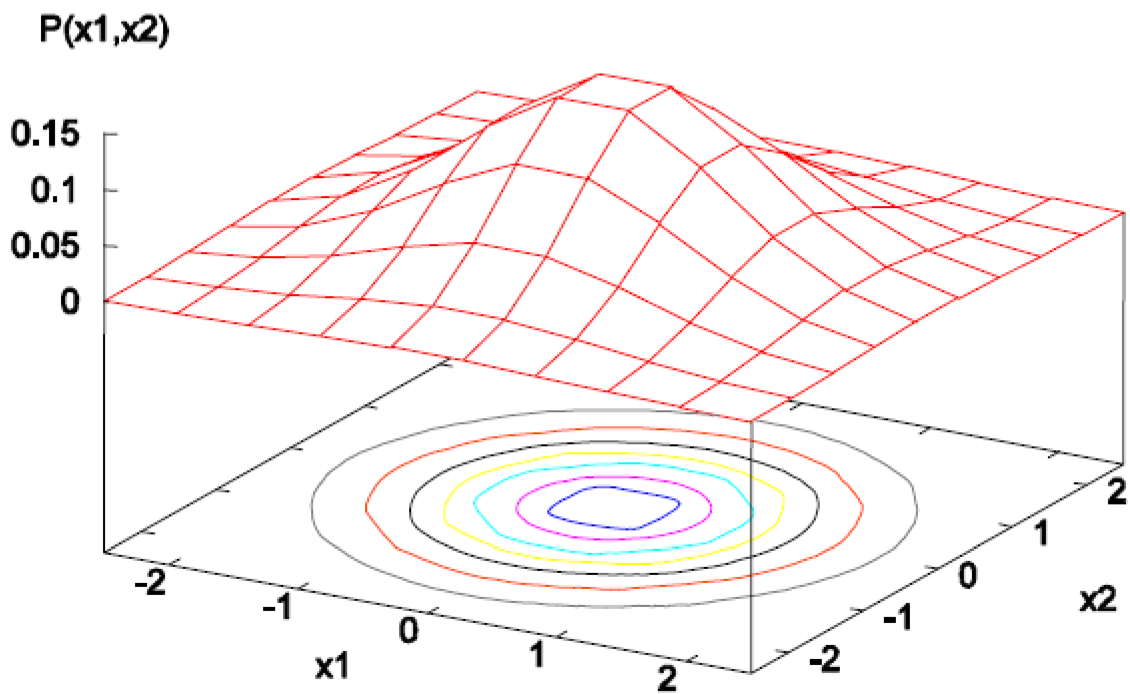
- A 2-dimensional Gaussian is defined by a mean vector $\mu = (\mu_1, \mu_2)$ and a covariance matrix

$$\Sigma = \begin{bmatrix} \sigma_{1,1}^2 & \sigma_{1,2}^2 \\ \sigma_{2,1}^2 & \sigma_{2,2}^2 \end{bmatrix}$$

where $\sigma_{i,j}^2 = E[(\mathbf{x}_i - \mu_i)((\mathbf{x}_j - \mu_j))]$ is the variance (if i=j) or the corvariance if (i≠j).

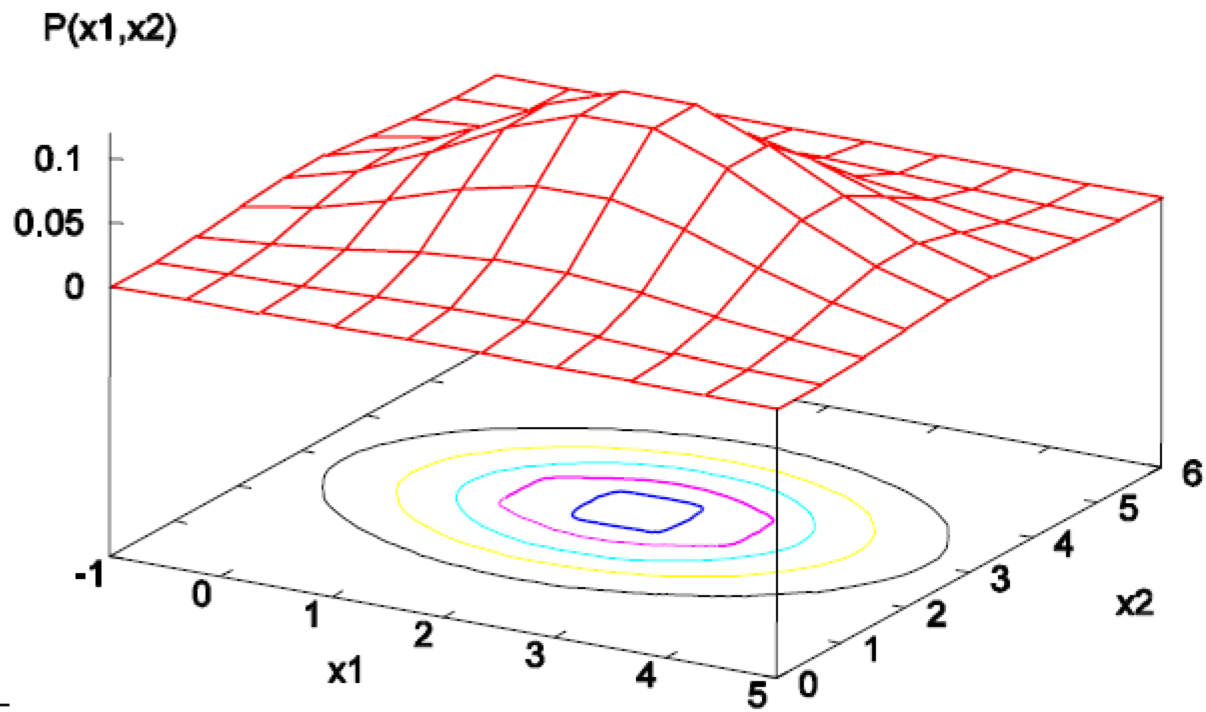
Multivariate Gaussian(2)

If Σ is the identity matrix, i.e., $\Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ and $\mu = (0,0)$ then we get the standard normal distribution



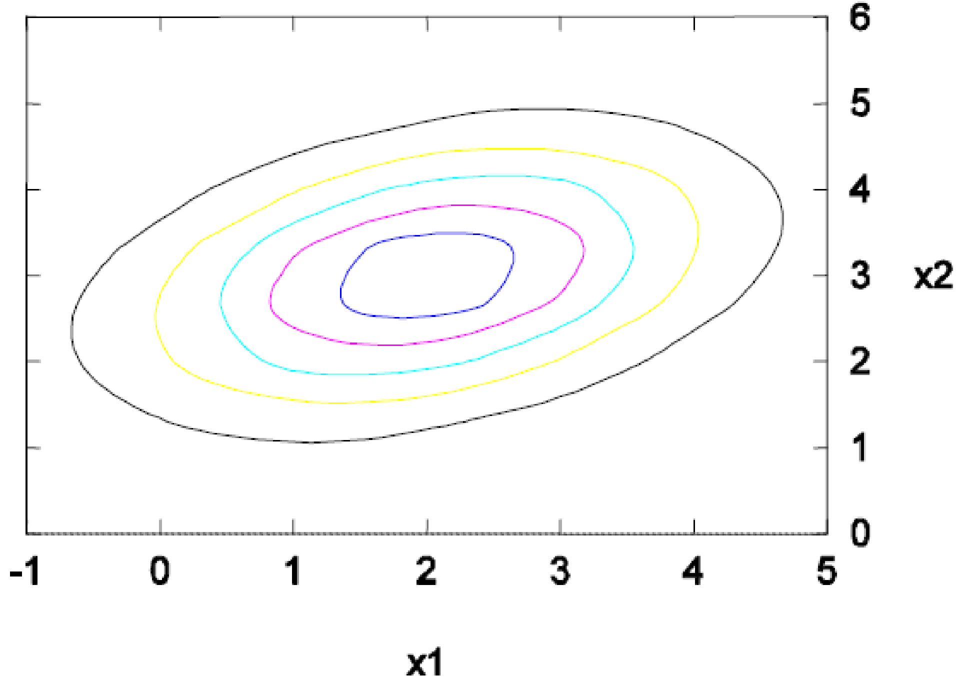
Multivariate Gaussian (3)

- If Σ is a diagonal matrix, for ex, $\Sigma = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}$ and $\mu = (2,3)$, the two variates x1 and x2 are independent random variables. In this case, we obtain



Multivariate Gaussian (4)

- If Σ is an arbitrary matrix, for ex, $\Sigma = \begin{bmatrix} 2 & 0.5 \\ 0.5 & 1 \end{bmatrix}$ and $\mu = (2,3)$, the two variates x1 and x2 are dependent variables. In this case, the lines are tilted to the coordinate axes.



Estimating a Multivariate Gaussian

- Given a set of N data points **{x1,…,xN}** we can compute the maximum likelihood estimate for the multivariate gaussian

$$\hat{\mu} = \frac{1}{N}\sum_i \mathbf{x}_i$$

$$\hat{\Sigma} = \frac{1}{N}\sum_i (\mathbf{x}_i - \hat{\mu})\cdot(\mathbf{x}_i - \hat{\mu})^T$$

- Note that the dot product in the second equation is an outer product. The outer product of two vectors is a matrix

- $x \cdot y^T = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \cdot [y_1 y_2 y_3] = \begin{bmatrix} x_1y_1 & x_1y_2 & x_1y_3 \\ x_2y_1 & x_2y_2 & x_2y_3 \\ x_3y_1 & x_3y_2 & x_3y_3 \end{bmatrix}$
- For comparison the usual dot product is written as $\boldsymbol{x^T} \cdot \boldsymbol{y}$

LDA Model

- LDA assumes that the joint distribution has the form

$$P(\mathbf{x}, y) = P(y)\frac{1}{2\pi^{n/2}\,|\sum|^{1/2}}\exp\left(\frac{1}{2}[(x-\mu_k)^T \sum^{-1}(x-\mu_k)]\right)$$

Where each μ_y is the mean of a multivariate Gaussian for examples belonging to class *y* and $\sum$ is a single covariance matrix <u>shared by all classes</u>.

Fitting the LDA Model

- It is easy to learn the LDA model in a single pass through the data
  - Let $\widehat{\pi_k}$ be our estimate of P(y=k)
  - Let N_k be the number of training examples belonging to class k

$$\hat{\pi}_k = \frac{N_k}{N}$$

$$\hat{\mu}_k = \frac{1}{N_k} \sum_{i; y_i = k} \mathbf{x}_i$$

$$\hat{\Sigma} = \frac{1}{N} \sum_i (\mathbf{x}_i - \hat{\mu}_{y_i}) \cdot (\mathbf{x}_i - \hat{\mu}_{y_i})^T$$

- Note that each $\mathbf{x_i}$ is subtracted from its corresponding $\widehat{\mu_{y_i}}$ prior to taking the outer product. This gives the “pooled” estimate of $\sum$
- It is easy to prove that LDA learns a LTU

Two Geometric Views of LDA
View 1: Mahalanobis Distance

- The term $D_M(x,\mathbf{u})^2 = (x-\mathbf{u})^T \sum^{-1}(x-\mathbf{u})$ is known as the (squared) Mahalanobis distance between **x** and **u**. We can think of the matrix $\sum^{-1}$ as a linear distortion of the coordinate system that converts the standard Euclidean distance to Mahalanobis distance
- Note that

$$\log P(\mathbf{x} \mid y=k) \propto \log \pi_k - \frac{1}{2}[(x-\mu_k)^T \sum^{-1}(x-\mu_k)]$$

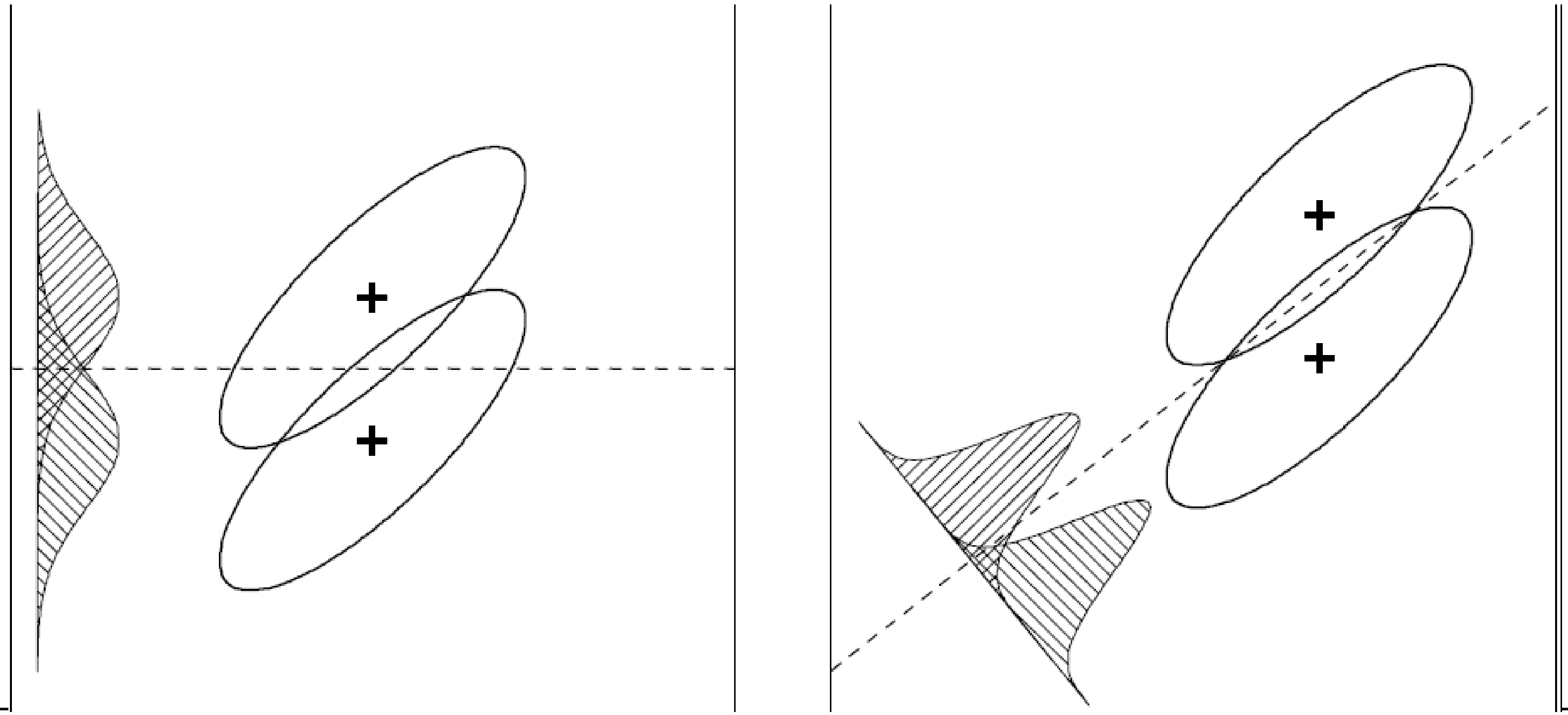
$$\log P(\mathbf{x} \mid y=k) \propto \log \pi_k - \frac{1}{2} D_M(x,\mu_k)^2$$

- Therefore, we can view LDA as computing $D_M(x,\mu_0)^2$ and $D_M(x,\mu_1)^2$

and then classifying **x** according to which mean is closest in Mahalanobis distance corrected by $\log \pi_k$

View 2: Most Informative Low-Dimensional Projection

- LDA can be also viewed as finding a hyperplane of dimension K-1 such that **x** and the $\{\mu_k\}$ are projected down into this hyperplane and then **x** is classified to the nearest μ_k using Euclidean distance inside this hyperplane



Summary of LDA

- Learns the joint probability distribution P(**x,**y)
- Direct Computation. The maximum likelihood estimate of P(**x**,y) can be computed from the data without search
- Eager. The classifier is constructed from training examples which can be discarded.
- Batch algorithm. Most implementations are batch algorithm. An online algorithm can be constructed if the matrix can be inverted incrementally.

Which should we use?

- Statistical Efficiency: If the generative model is correct, then LDA gives the highest accuracy, particularly if the data set is small. If the model is correct, LDA requires 30% less data than Logistic Regression in theory

- Computational Efficiency: Generative models are the easiest to learn. In our example, we do not need a gradient descent method to compute a LDA

- Robustness to changing loss functions: Both generative and conditional methods allow the loss function to be changed at runtime without re-learning. Perceptron requires re-training the classifier if the loss function changes.

Which should we use

- Robustness to model assumptions: The generative models generally have *strong* model assumptions. In turn they perform poorly when these are violated. For instance if $P(\mathbf{x}|y)$ is very non-Gaussian, then LDA will not work well. Logistic regression is more robust to model assumptions but perceptron is the most robust one.

- Robustness to missing values and noise: In many applications, some of the features may be missing or corrupted. Generative models typically provide better ways of handling this.