Discriminant functions and decision boundaries for normal distributions

Univariate normal density (normal = Gaussian)

$$p(x) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left(-\frac{1}{2} \frac{(x-\mu)^2}{\sigma^2} \right)$$

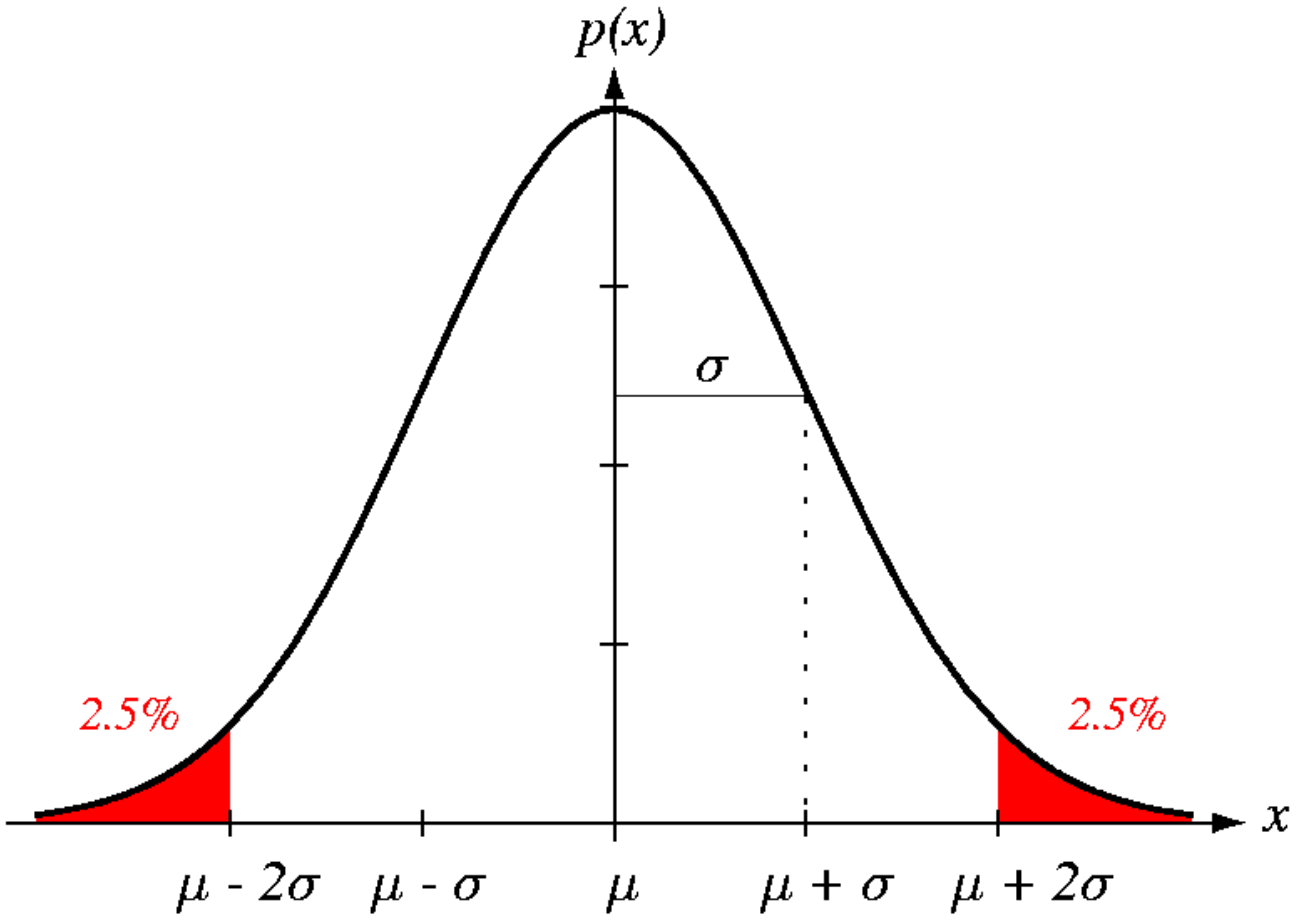
Mean:

$$\varepsilon[x] = \int_{-\infty}^{\infty} x\; p(x)\, dx = \mu$$

Variance:

$$\varepsilon[(x-\mu)^2] = \int_{-\infty}^{\infty} (x-\mu)^2\, p(x)\, dx = \sigma^2$$

Univariate normal density



In 95% of the cases x is in the range $|x - \mu| \leq 2\sigma$

from Duda, Hart, Stork (2001) Pattern classification

Multivariate normal density

$$p(\mathrm{x}) = \frac{1}{(2\pi)^{d/2} |\sum|^{1/2}} \exp\left[-\frac{1}{2}(\mathrm{x}-\mu)^t \sum^{-1} (\mathrm{x}-\mu)\right]$$

- $\mathrm{x} \in \mathrm{R}^{\mathrm{d}}$ is a d dimensional vector
- μ is the mean (a d-dimensional vector itself)
- Σ is the covariance matrix ($|\Sigma|$ its determinant and Σ^{-1} its inverse)

Common notation:

$$p(\mathrm{x}) \sim N(\mu, \Sigma)$$

Covariance matrix

$$\varepsilon[(x_i-\mu_i)(x_j-\mu_j)] = \int (x_i-\mu_i)(x_j-\mu_j)\,p(x)\,dx = \sigma_{i,j}$$

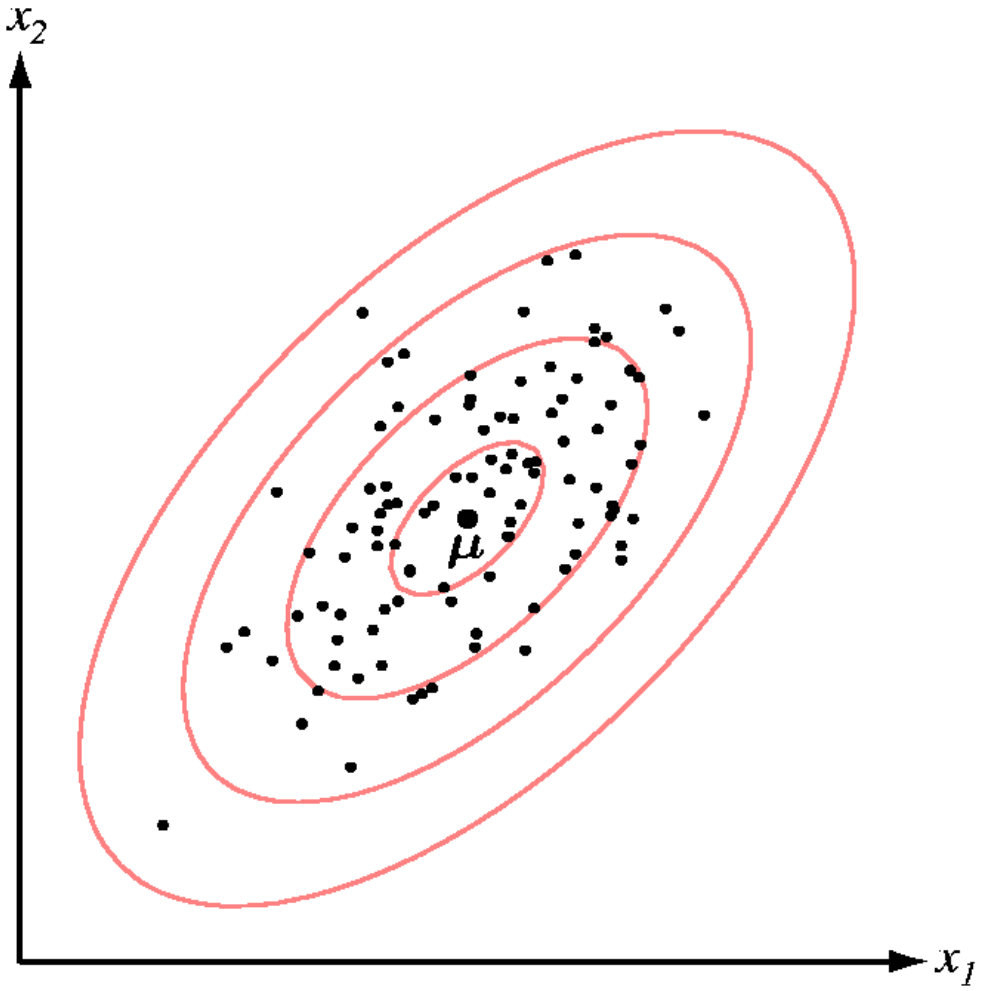
Covariance matrix

$$\Sigma = \begin{bmatrix} \sigma_{11} & \sigma_{21} & \cdots & \sigma_{1d} \\ \sigma_{21} & \sigma_{22} & \cdots & \sigma_{2d} \\ \cdots & \cdots & & \\ \sigma_{d1} & \sigma_{d2} & \cdots & \sigma_{dd} \end{bmatrix} = \begin{bmatrix} \sigma_1^2 & \sigma_{21} & \cdots & \sigma_{1d} \\ \sigma_{21} & \sigma_2^2 & \cdots & \sigma_{2d} \\ \cdots & \cdots & & \\ \sigma_{d1} & \sigma_{d2} & \cdots & \sigma_d^2 \end{bmatrix}$$

Σ is always symmetric and positive semi-definite ($|\Sigma| \geq 0$)

For statistically independent events x_i and x_j, $\sigma_{ij} = 0$.

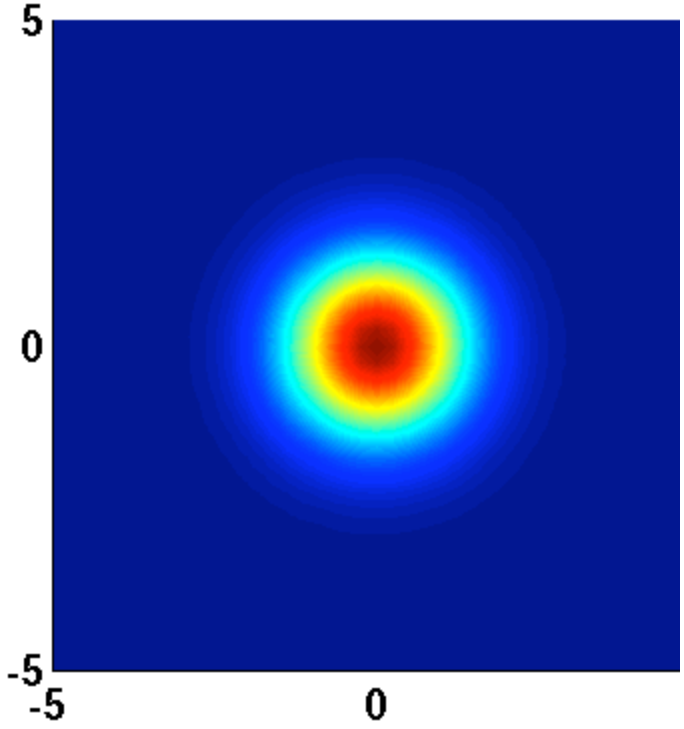
Thus it becomes a diagonal matrix.

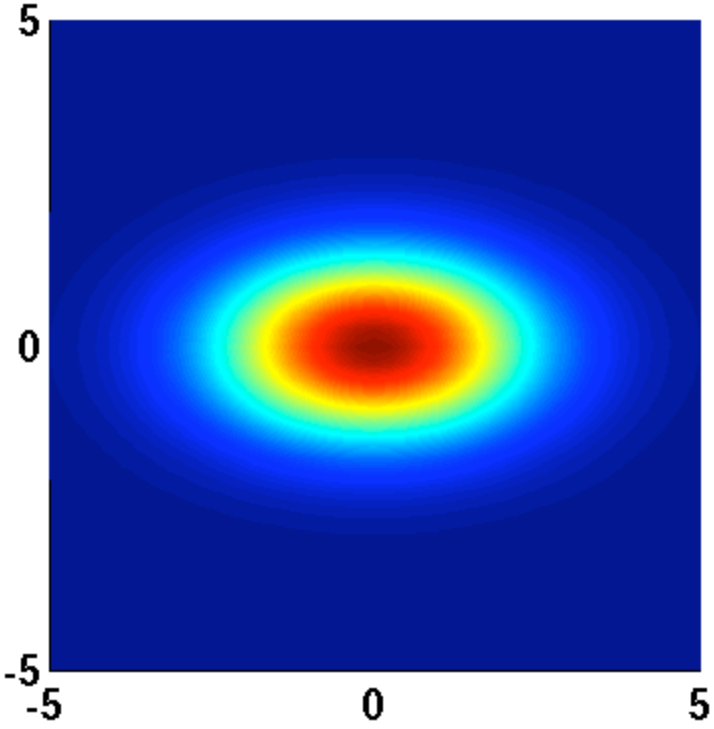


A hyperellipsoidal cluster formed by points drawn from a population which has normal distribution

from Duda, Hart, Stork (2001) Pattern classification

Multivariate Gaussians



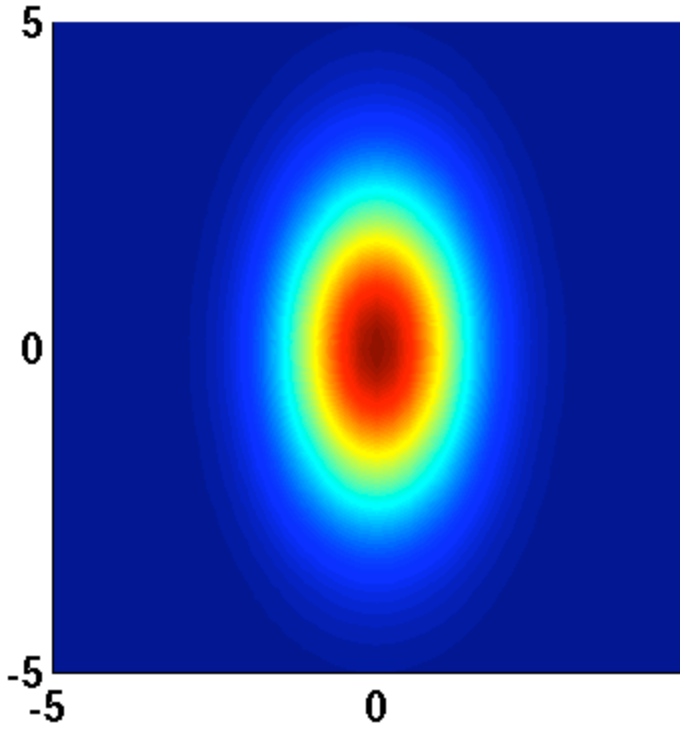


$$\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

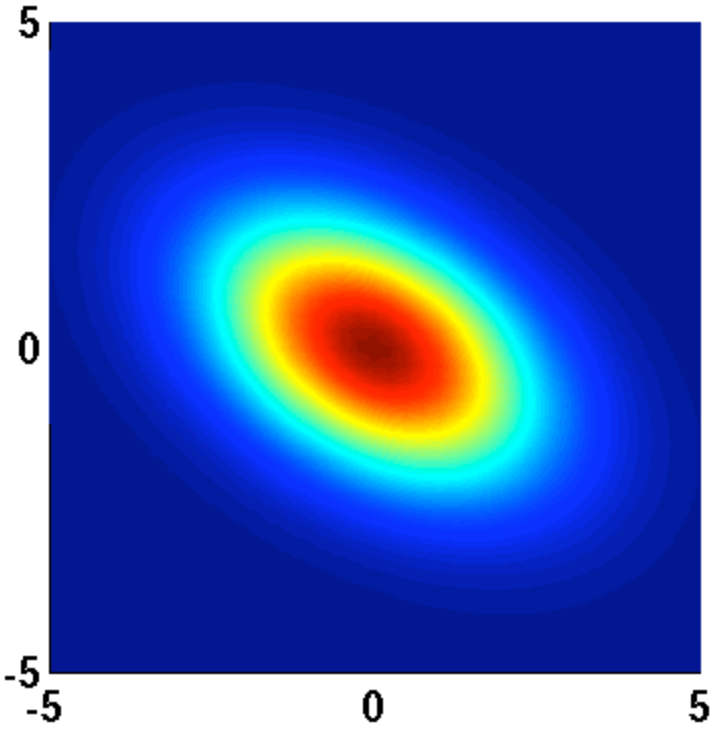
The principal axes of the hyperellipsoids are given by the eigenvectors of Σ. The eigenvalues determine the length of these axes.

$$\Sigma = \begin{pmatrix} 3 & 0 \\ 0 & 1 \end{pmatrix}$$

Multivariate Gaussians



$$\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix}$$



$$\Sigma = \begin{pmatrix} 3 & -1 \\ -1 & 1 \end{pmatrix}$$

Mahalanobis distance

The squared Mahalanobis distance from a point x to a class $N(\mu, \Sigma)$

$$r^2 = (\mathrm{x} - \mu)^t \Sigma^{-1} (\mathrm{x} - \mu)$$

The contours of constant density are hyperellipsoids of constant Mahalanobis distance.

Linear combinations

Linear combinations of normally distributed random variables (independent or not) are normally distributed, i.e.

$$p(\mathrm{x}) \sim N(\mu, \Sigma)$$
$$\mathrm{y} = \mathrm{A}^{\mathrm{t}}\mathrm{x} \qquad \Rightarrow \qquad p(\mathrm{y}) \sim N(\mathrm{A}^{\mathrm{t}}\mu, \mathrm{A}^{\mathrm{t}}\Sigma\mathrm{A})$$

where

- A is a d x k matrix
- y is a k dimensional vector

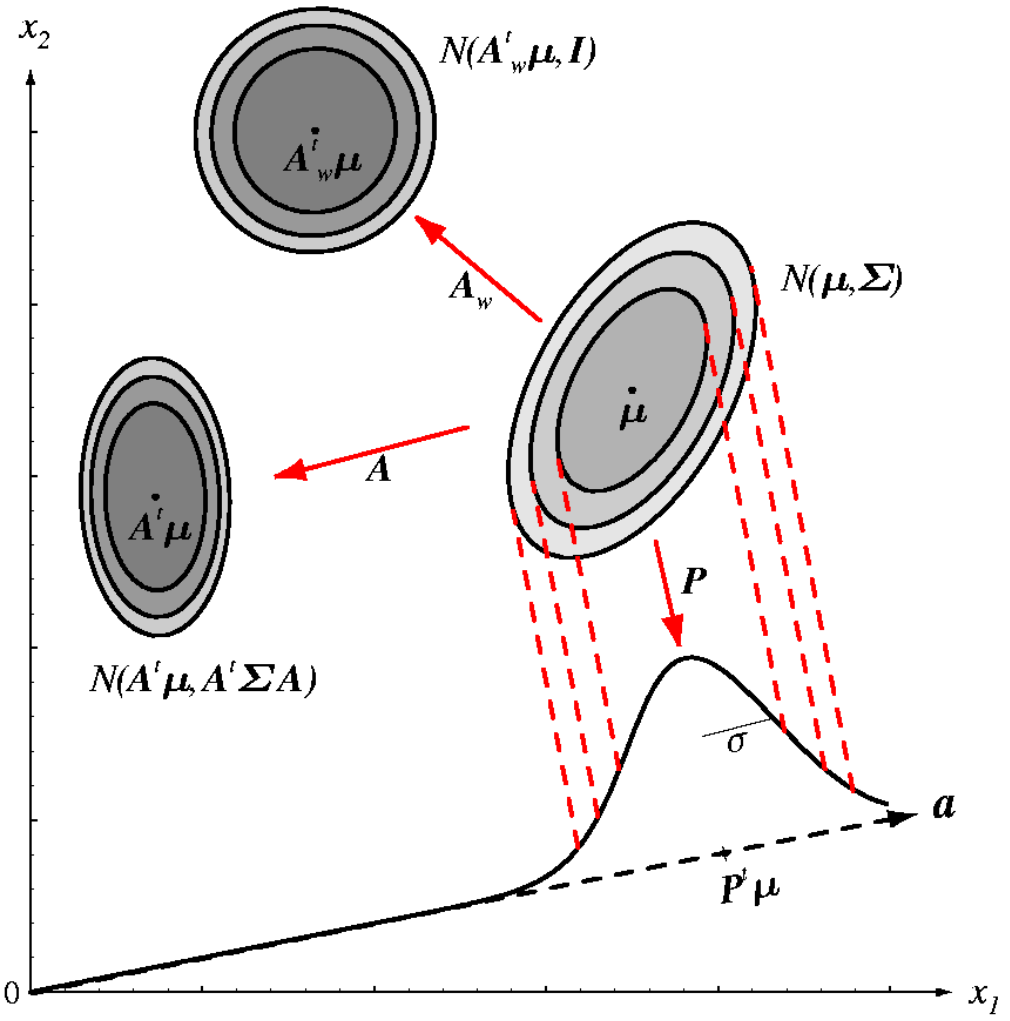
If $\mathrm{k} = 1$, then $\mathrm{A} = [\mathrm{a}]$, and $y = \mathrm{a}^{\mathrm{t}}\mathrm{x}$ is a scalar and represents the projection of x onto a.

Linear combinations

Whitening transform Aw

General transform A

Projection P



from Duda, Hart, Stork (2001) Pattern classification

Discriminant functions for normal densities

Minimum error rate classification can be achieved using the following discriminant functions:

$$g_i(\mathrm{x}) = \ln p(\mathrm{x} \mid \omega_i) + \ln P(\omega_i)$$

Bayesian Decision Theory

If the densities $p(\mathrm{x} \mid \omega_i)$ are multivariate normal densities

$p(\mathrm{x} \mid \omega_\mathrm{i}) \sim N(\mu_i, \Sigma_i)$, then from:

$$p(\mathrm{x} \mid \omega_\mathrm{i}) = \frac{1}{(2\pi)^{d/2} \mid \Sigma_i \mid^{1/2}} \exp\left[-\frac{1}{2} (\mathrm{x} - \mu_i)^t \Sigma_i^{-1} (\mathrm{x} - \mu_i) \right]$$

it follows:

$$g_i(\mathrm{x}) = -\frac{1}{2} (\mathrm{x} - \mu_i)^t \Sigma_i^{-1} (\mathrm{x} - \mu_i) - \frac{d}{2} \ln 2\pi - \frac{1}{2} \ln \mid \Sigma_i \mid + \ln P(\omega_i)$$

Statistically independent features of equal variance

Case 1: $\Sigma_i = \sigma^2 I$

Features are statistically independent and each feature has the same variance σ^2. The determinant of the covariance matrix and the inverse are $|\Sigma_i| = \sigma^{2d}$, respectively,

$$\Sigma_i^{-1} = (1/\sigma^2) I$$

The form of the discriminant functions simplifies to:

$$g_i(\mathrm{x}) = -\frac{\| \mathrm{x} - \mu_i \|^2}{2\sigma^2} + \ln P(\omega_i)$$

where $\| \mathrm{x} - \mu_i \|^2 = (\mathrm{x} - \mu_i)^t (\mathrm{x} - \mu_i)$ is the Euclidian norm.

Equivalently:

$$g_i(\mathrm{x}) = -\frac{\| \mathrm{x} - \mu_i \|^2}{2\sigma^2} + \ln P(\omega_i)$$

$$\Leftrightarrow \qquad g_i(\mathrm{x}) = -\frac{1}{2\sigma^2}(\mathrm{x} - \mu_i)^t (x - \mu_i) + \ln P(\omega_i)$$

$$\Leftrightarrow \qquad g_i(\mathrm{x}) = -\frac{1}{2\sigma^2}[\mathrm{x}^{\mathrm{t}}\mathrm{x} - 2\mu_i^{\mathrm{t}}\mathrm{x} + \mu_i^t \mu_i] + \ln P(\omega_i)$$

The discriminant function:

$$g_i(\mathrm{x}) = -\frac{1}{2\sigma^2}[\mathrm{x}^{\mathrm{t}}\mathrm{x} - 2\mu_i^{\mathrm{t}}\mathrm{x} + \mu_i^t\mu_i] + \ln P(\omega_i)$$

can be rewritten as a *linear discriminant*:

$$g_i(\mathrm{x}) = \mathrm{w}_{\mathrm{i}}^{\mathrm{t}}\mathrm{x} + w_{i0}$$

$$\mathrm{w}_{\mathrm{i}} = \frac{1}{\sigma^2}\mu_i$$

$$w_{i0} = -\frac{1}{2\sigma^2}\mu_i^{\,t}\mu_i + \ln P(\omega_i) \qquad \cancel{\left(-\mathrm{x}^{\mathrm{t}}\mathrm{x}/(2\sigma^2)\right)}$$

The term w_{i0} is called the *bias* for the *i*-th category.

Linear machine

A classifier that uses linear discriminant functions is called a linear machine.

If the priors are equal, the optimum decision rule can be stated as:

Classify a feature vector in the class with the closest mean.

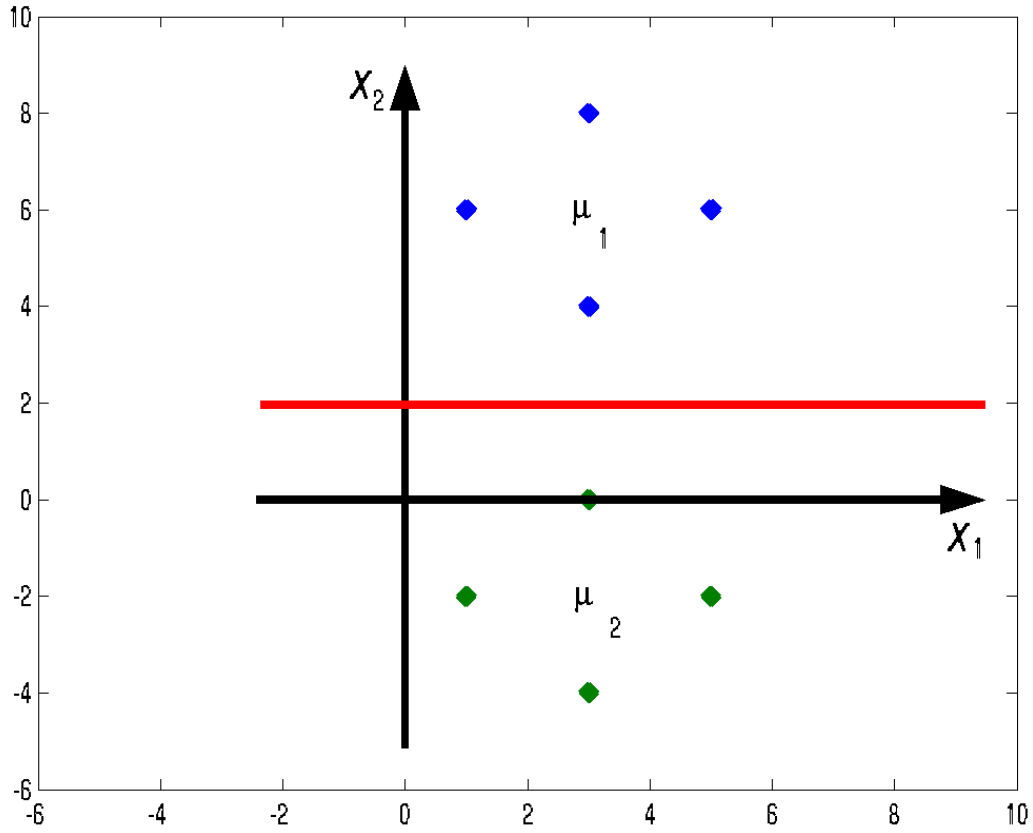
This classifier is known as a minimum-distance classifier.

Example

$$\mu_1 = \begin{bmatrix} 3 \\ 6 \end{bmatrix} \qquad \mu_2 = \begin{bmatrix} 3 \\ -2 \end{bmatrix}$$

$$\sigma_1 = \sigma_2 = \sqrt{2}$$

$$P(\omega_1) = P(\omega_2) = 0.5$$



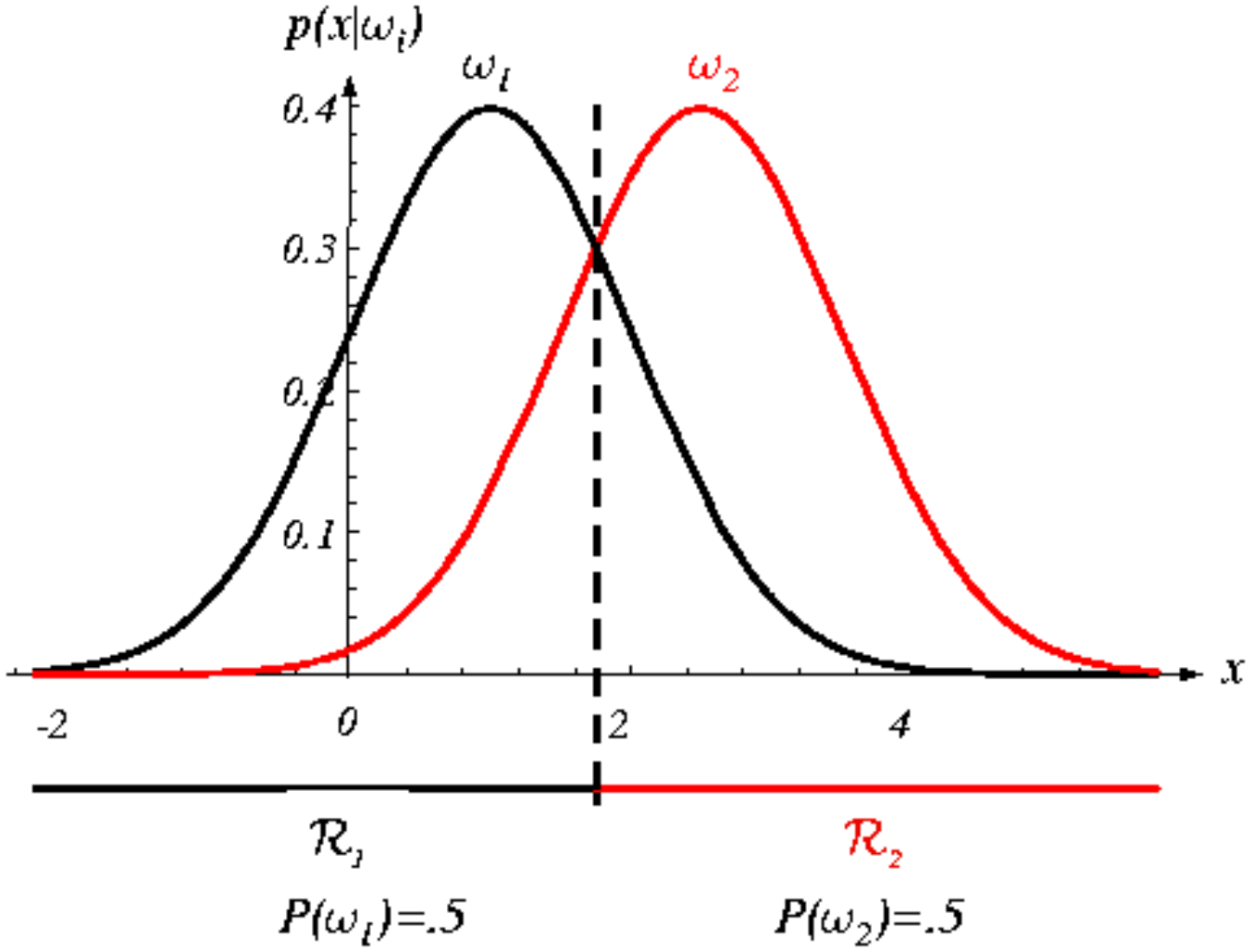
$$g_1(\mathrm{x}) = g_2(\mathrm{x}) \Rightarrow$$

$$(\mathrm{x} - \mu_1)^t(\mathrm{x} - \mu_1) = (\mathrm{x} - \mu_2)^t(\mathrm{x} - \mu_2) \Rightarrow$$

$$\begin{bmatrix} x_1 - 3 & x_2 - 6 \end{bmatrix} \begin{bmatrix} x_1 - 3 \\ x_2 - 6 \end{bmatrix} = \begin{bmatrix} x_1 - 3 & x_2 + 2 \end{bmatrix} \begin{bmatrix} x_1 - 3 \\ x_2 + 2 \end{bmatrix} \Rightarrow \quad x_2 = 2$$

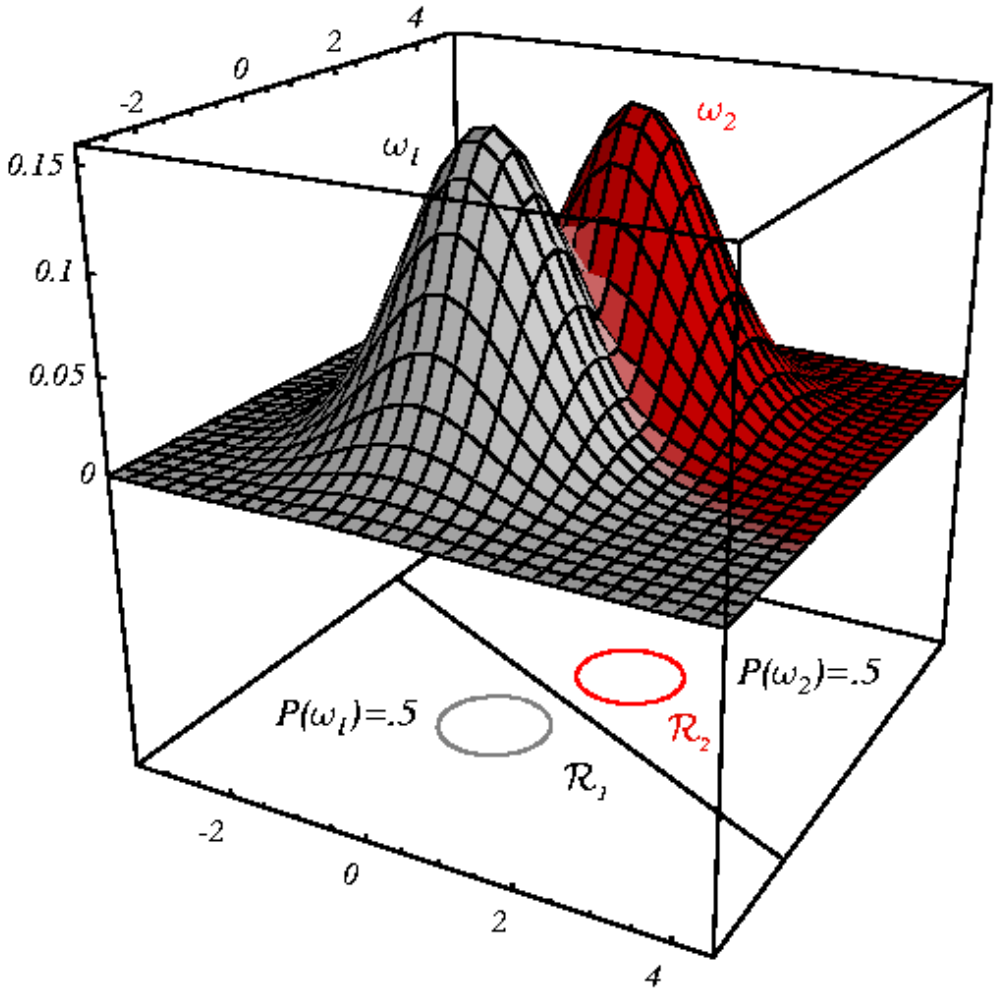
from Duda, Hart, Stork (2001) Pattern classification

One-dimensional case



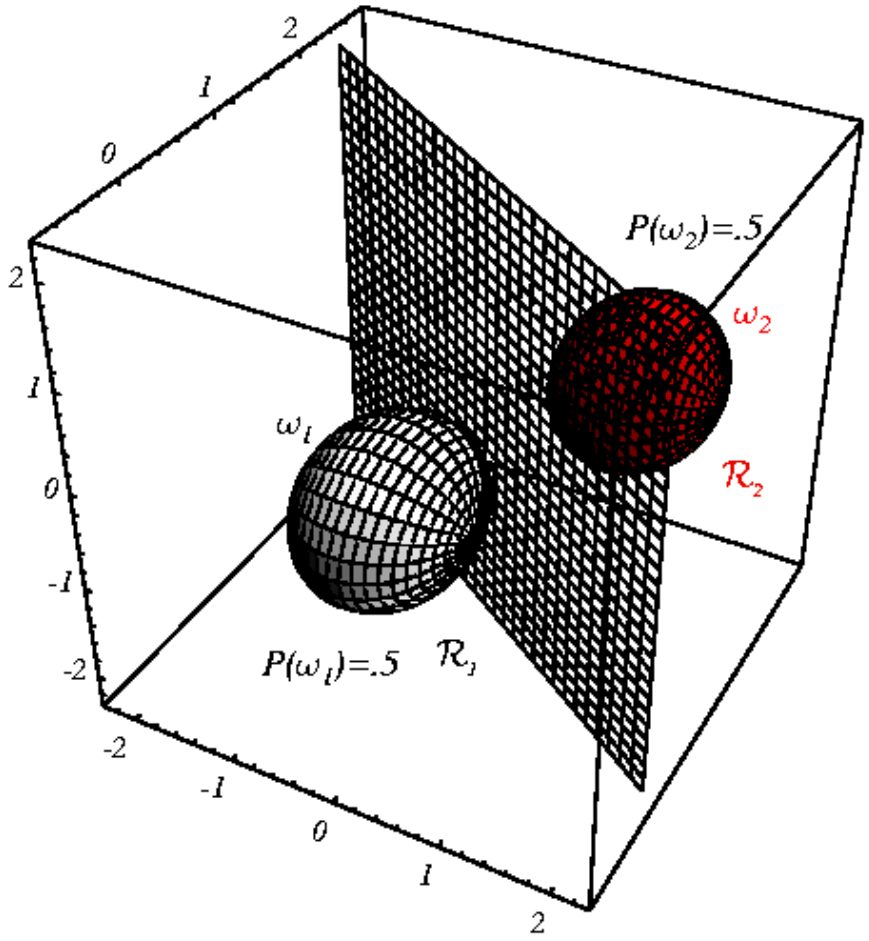
from Duda, Hart, Stork (2001) Pattern classification

Two-dimensional case



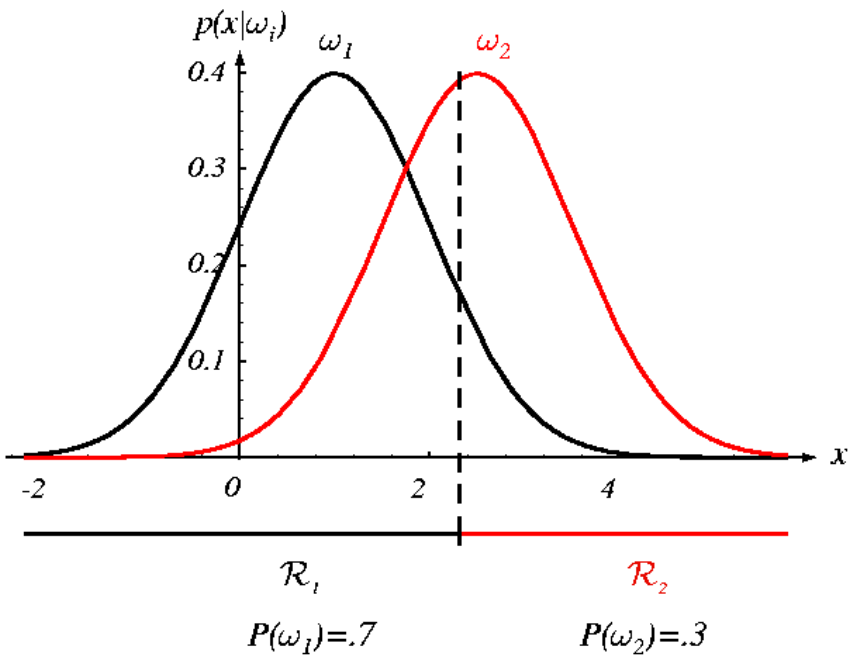
from Duda, Hart, Stork (2001) Pattern classification

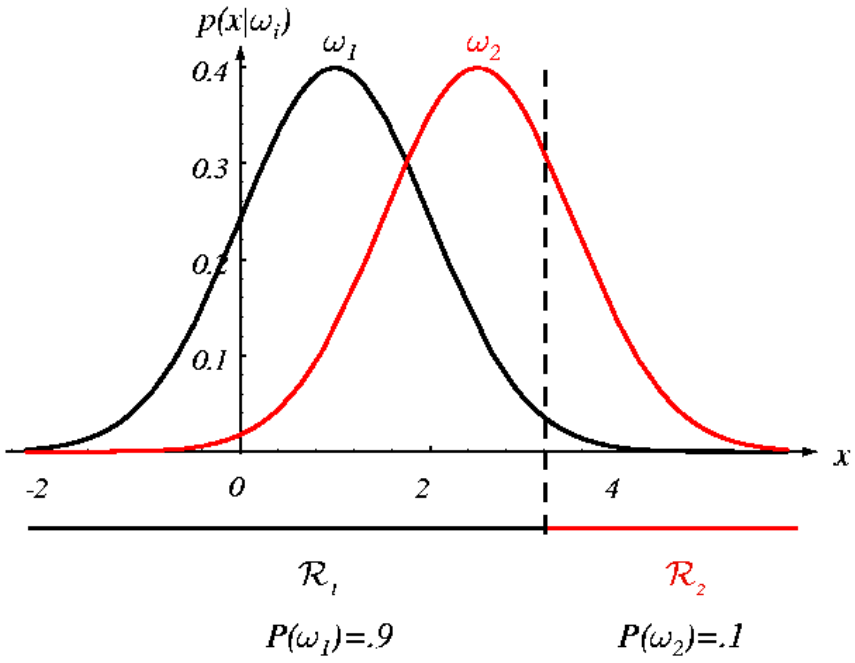
Three-dimensional case



from Duda, Hart, Stork (2001) Pattern classification

Unequal priors

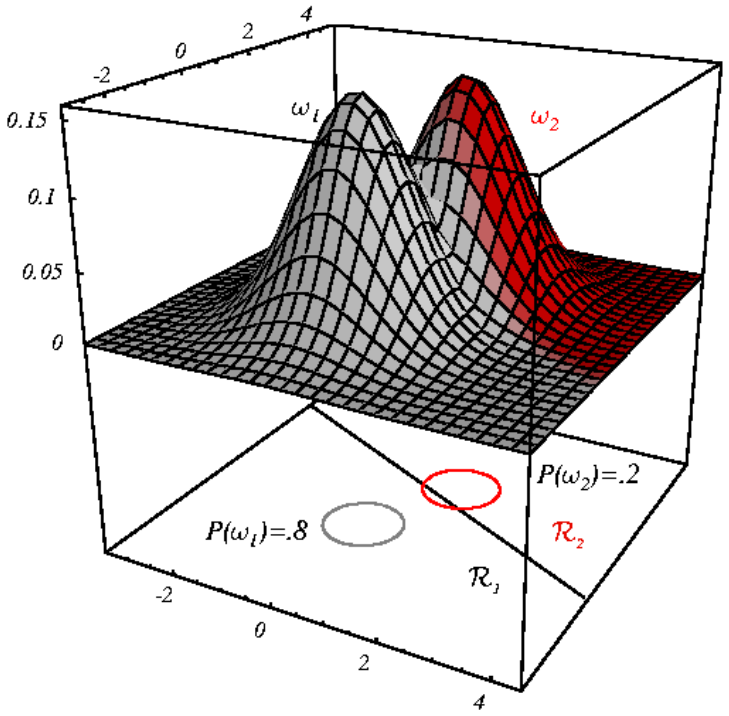


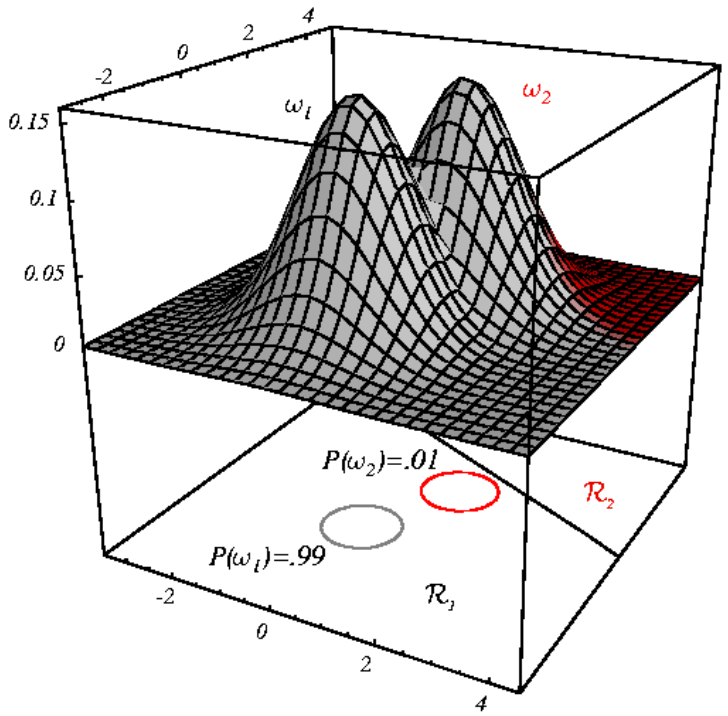


When $P(\omega_i) \neq P(\omega_j)$, the decision boundary is shifted

from Duda, Hart, Stork (2001) Pattern classification

Unequal priors

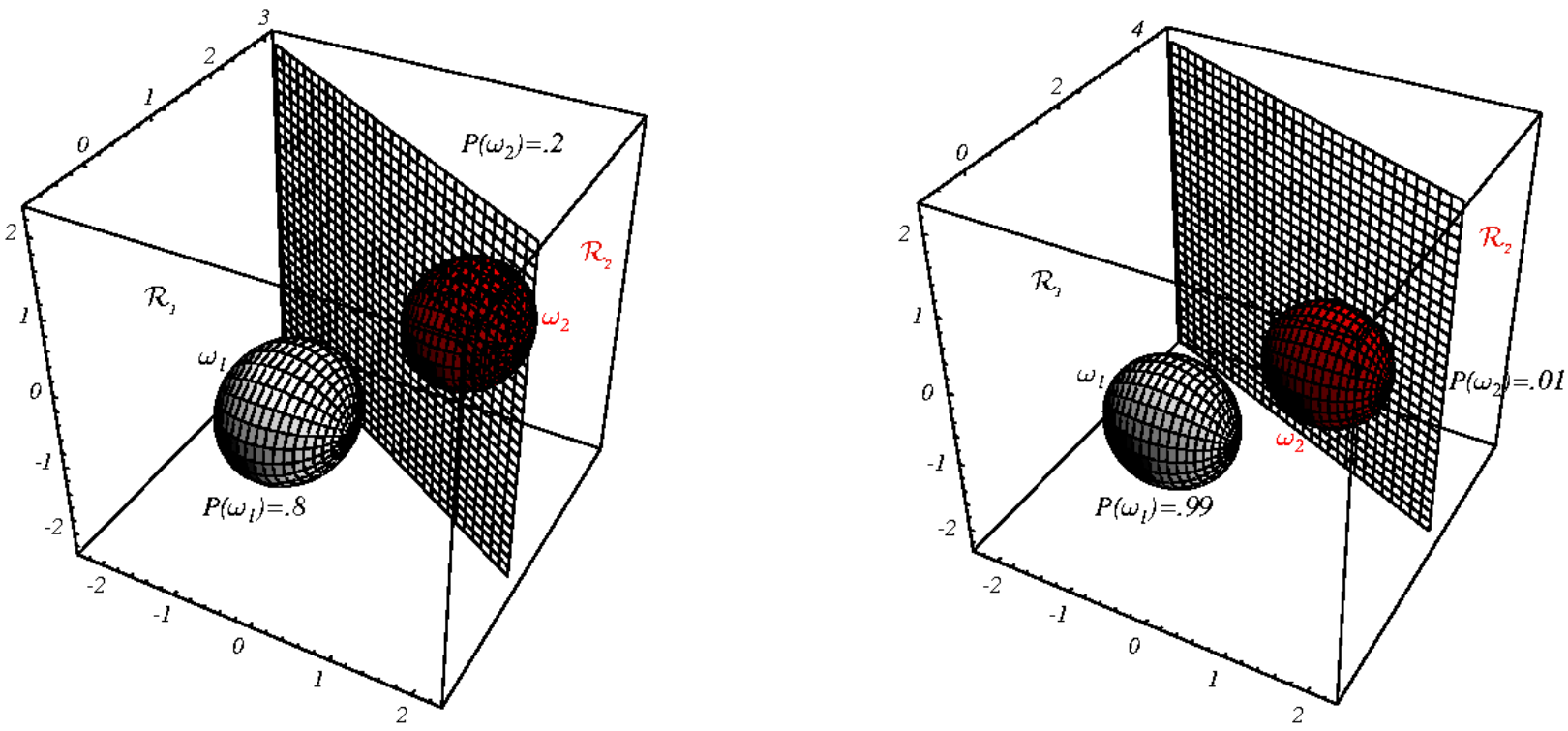




When $P(\omega_i) \neq P(\omega_j)$, the decision boundary is shifted (but still orthogonal to the segment connecting the means).

from Duda, Hart, Stork (2001) Pattern classification

Unequal priors



from Duda, Hart, Stork (2001) Pattern classification

Arbitrary covariance matrices

Example: $\Sigma_1 = \begin{pmatrix} 1/2 & 0 \\ 0 & 2 \end{pmatrix}$ $\Sigma_2 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$ $\mu_1 = \begin{bmatrix} 3 \\ 6 \end{bmatrix}$ $\mu_2 = \begin{bmatrix} 3 \\ -2 \end{bmatrix}$

$\Rightarrow$ $\Sigma_1^{-1} = \begin{pmatrix} 2 & 0 \\ 0 & 1/2 \end{pmatrix}$ $\Sigma_1^{-1} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$ $|\Sigma_1| = 1$ $|\Sigma_2| = 4$

Let $P(\omega_1) = P(\omega_2) = 0.5 \Rightarrow \ln P(\omega_1) = \ln P(\omega_2) = -\ln 2$

$$g_i(\mathrm{x}) = -\frac{1}{2}(\mathrm{x}-\mu_i)^t \Sigma_i^{-1}(\mathrm{x}-\mu_i) - \frac{1}{2}\ln|\Sigma_i| + \ln P(\omega_i)$$

$$g_1(\mathrm{x}) = -\frac{1}{2}[x_1-3, x_2-6]\begin{pmatrix} 2 & 0 \\ 0 & 1/2 \end{pmatrix}\begin{bmatrix} x_1-3 \\ x_2-6 \end{bmatrix} - \ln 2$$

$$g_2(\mathrm{x}) = -\frac{1}{2}[x_1-3, x_2+2]\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}\begin{bmatrix} x_1-3 \\ x_2+2 \end{bmatrix} - \frac{1}{2}\ln 4 - \ln 2$$

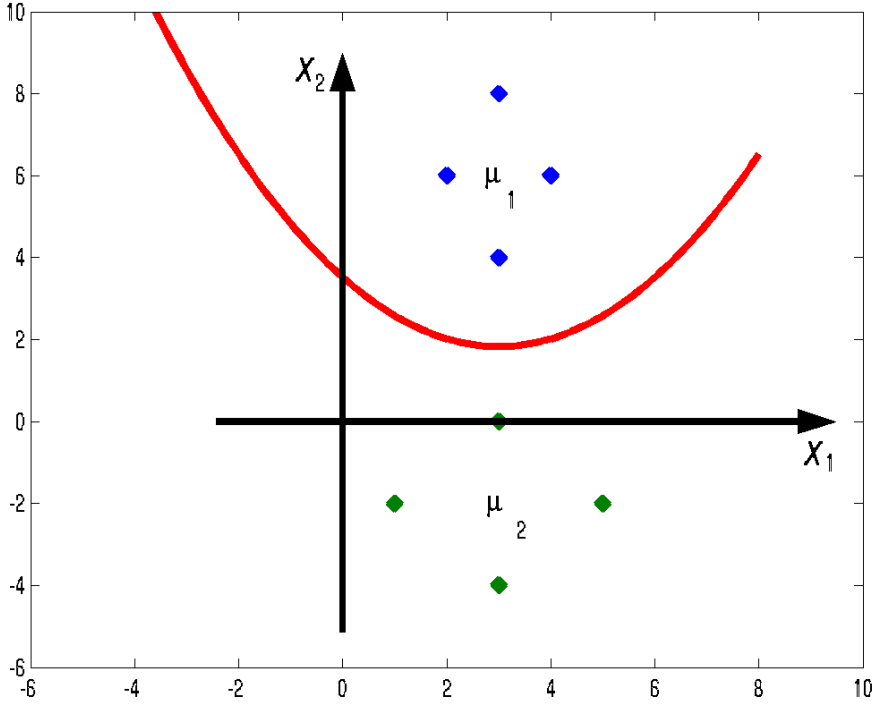
$$g_1(\mathrm{x}) = -(x_1-3)^2 - \frac{1}{4}(x_2-6)^2 - \ln 2$$

$$g_2(\mathrm{x}) = -\frac{1}{4}(x_1-3)^2 - \frac{1}{4}(x_2+2)^2 - \frac{1}{2}\ln 4 - \ln 2$$

Decision boundary is determined by $g_1(x) = g_2(x) \Rightarrow$

$$-(x_1-3)^2 - \frac{1}{4}(x_2-6)^2 - \ln 2 = -\frac{1}{4}(x_1-3)^2 - \frac{1}{4}(x_2+2)^2 - \frac{1}{2}\ln 4 - \ln 2$$

$$-(x_1-3)^2 - \frac{1}{4}(x_2-6)^2 = -\frac{1}{4}(x_1-3)^2 - \frac{1}{4}(x_2+2)^2 - \frac{1}{2}\ln 4$$

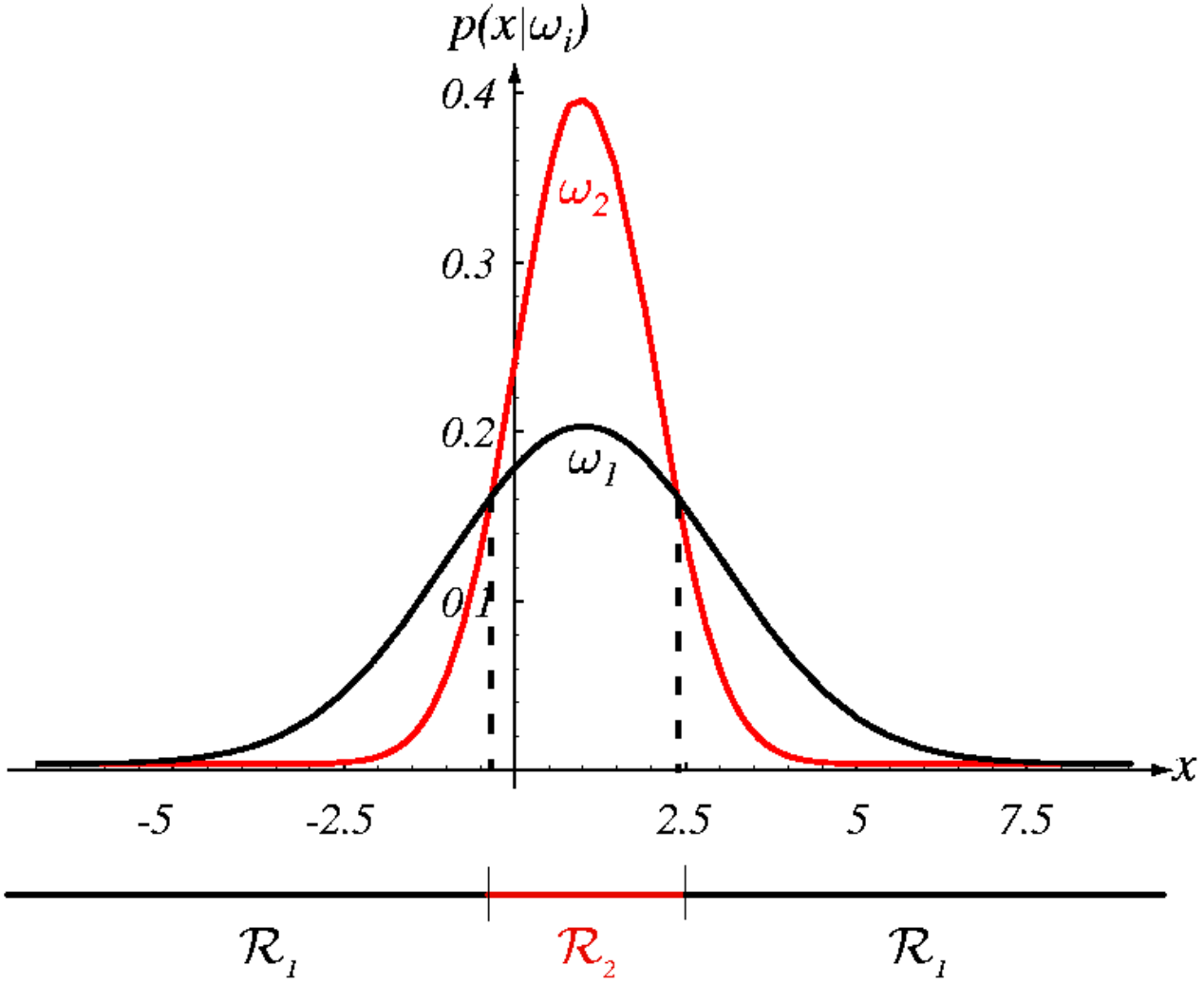


$\Rightarrow$

$$x_2 = 3.514 - 1.125\, x_1 + 0.1875\, x_1^2$$

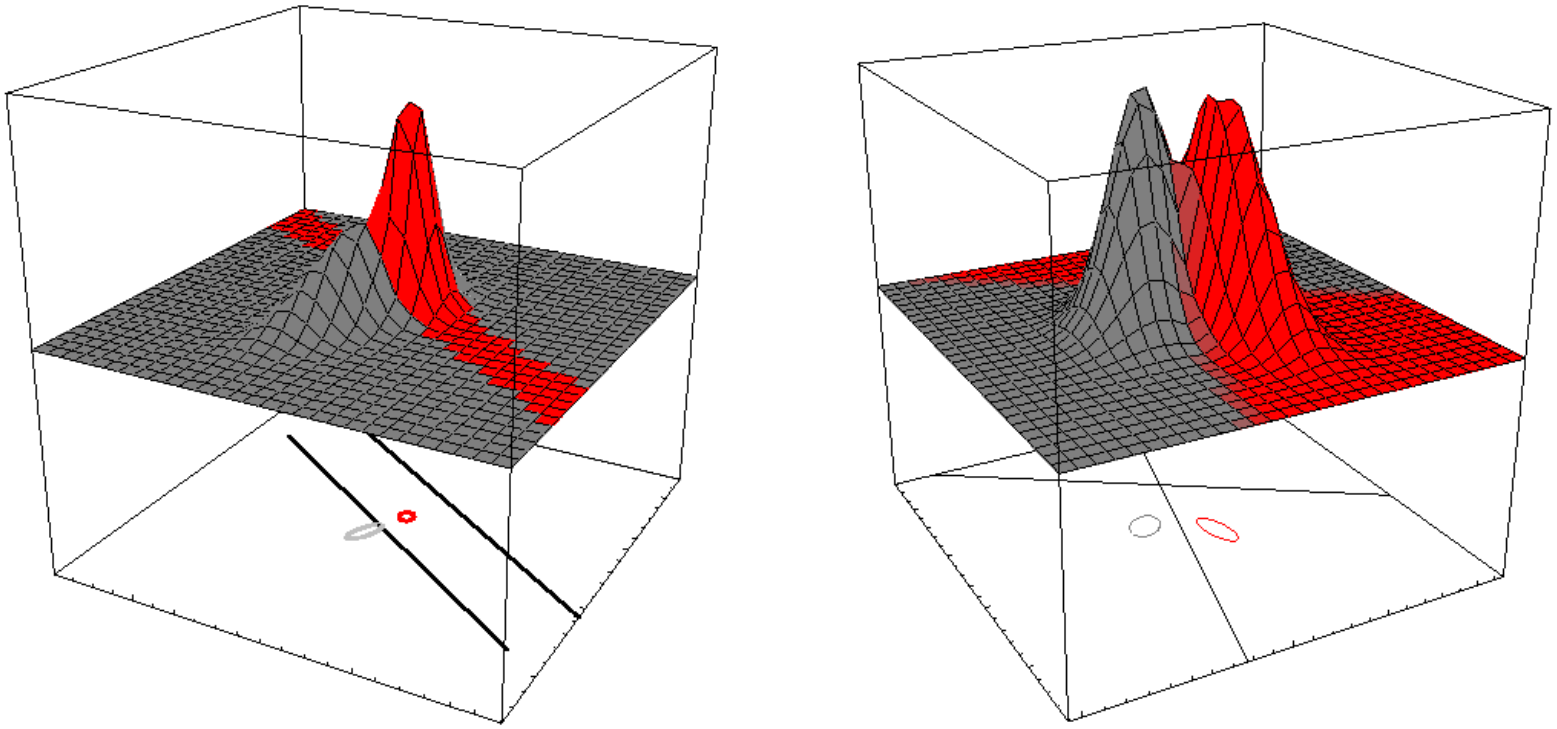
from Duda, Hart, Stork (2001) Pattern classification

One dimension



from Duda, Hart, Stork (2001) Pattern classification

Two dimensions



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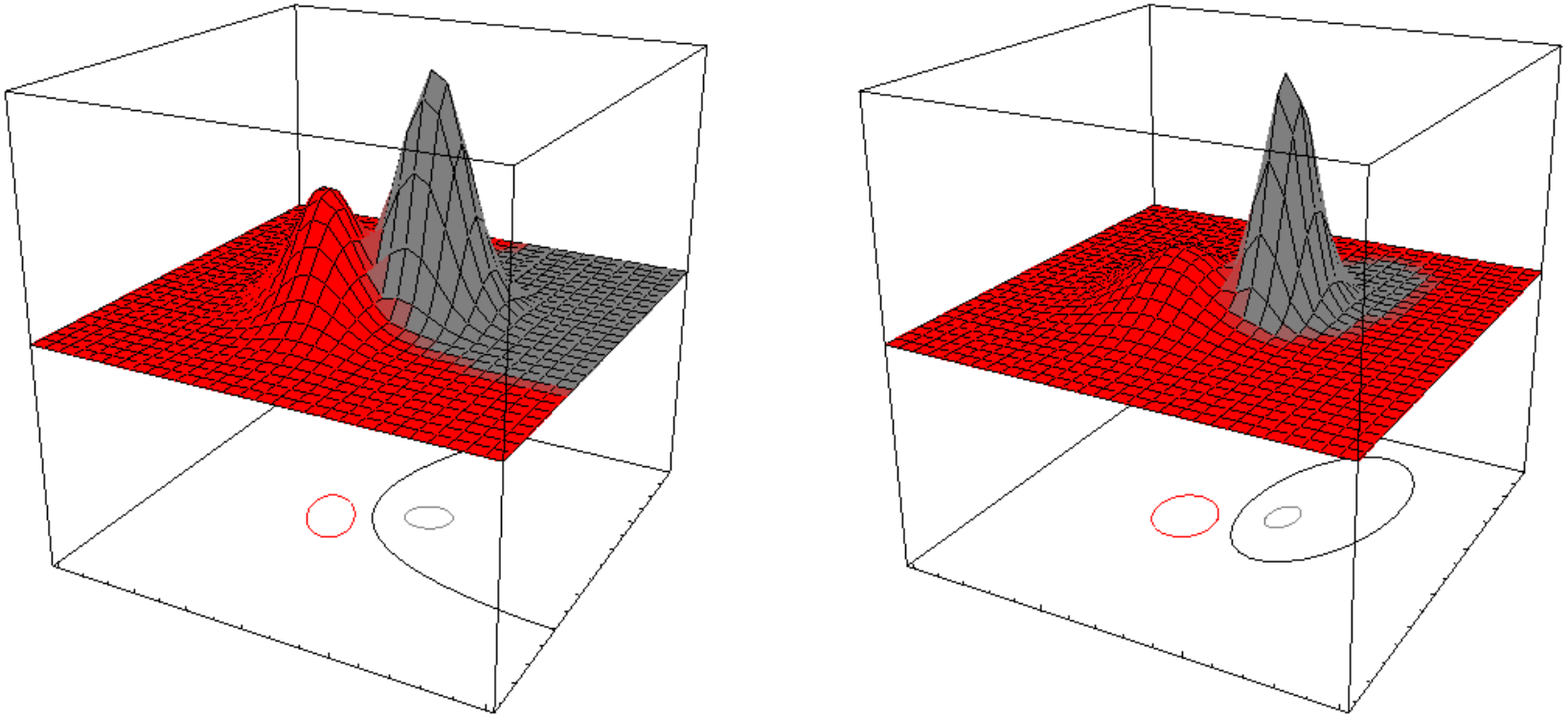
Two dimensions



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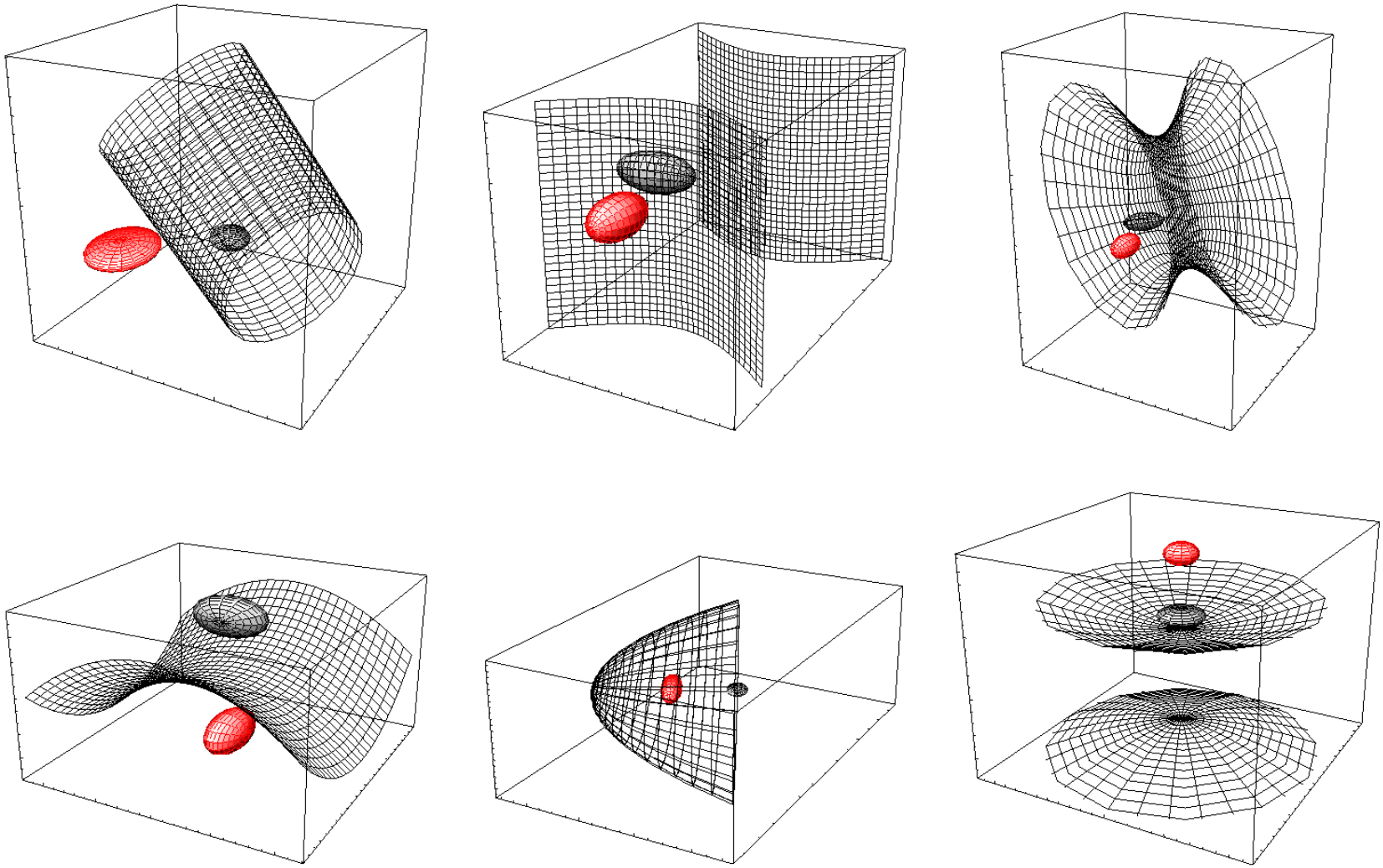
Three dimensions



from Duda, Hart, Stork (2001) Pattern classification

Conclusion

For multidimensional normal distributions, the discriminant functions can be computed analytically.

Classification Error

After we design a classifier, we need also to characterize it by means of the total classification error that it will make.
Total error concerns not just the classification of one point in the feature space, but all such points.
When the class conditional probability density functions are available in analytical form, the total error can be evaluated as follows.

Classification Error

Example: Two-class problem

Suppose that a dichotomizer has divided the space into two regions $\mathcal{R}_1$ and $\mathcal{R}_2$ The probability of error is:

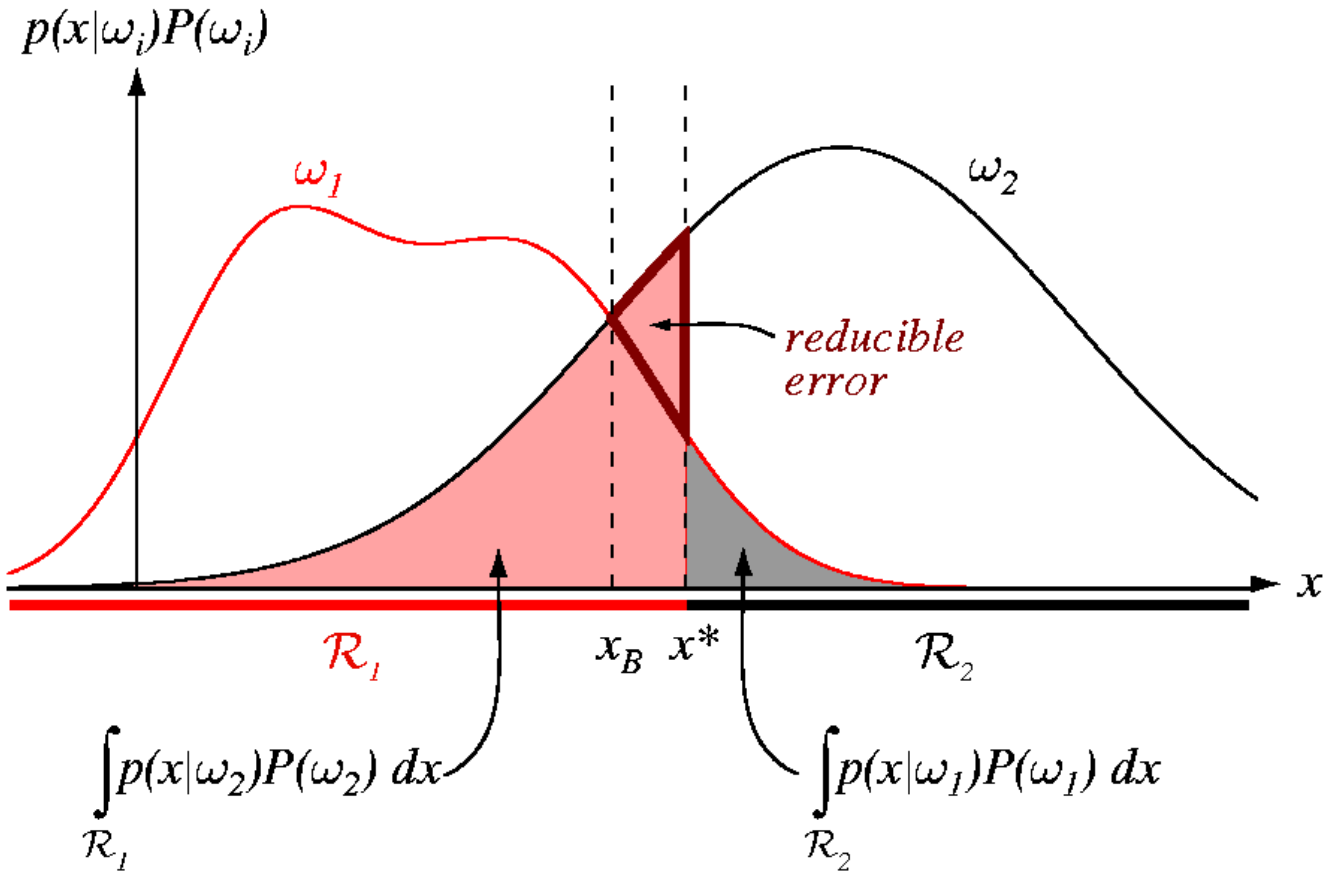
$$P(error) = P(\mathrm{x} \in \mathcal{R}_2, \omega_1) + P(\mathrm{x} \in \mathcal{R}_1, \omega_2)$$

$$= P(\mathrm{x} \in \mathcal{R}_2 \mid \omega_1) P(\omega_1) + P(\mathrm{x} \in \mathcal{R}_1 \mid \omega_2) P(\omega_2)$$

$$= \int_{\mathcal{R}_2} p(\mathrm{x} \mid \omega_1) P(\omega_1) d\mathrm{x} + \int_{\mathcal{R}_1} p(\mathrm{x} \mid \omega_2) P(\omega_2) d\mathrm{x}$$

When the class conditional pdf's are available, the above integrals can be evaluated analytically or numerically.

Classification Error – 1D case



The total error is the sum of the grey and pink areas. Bayes optimal decision boundary gives the lowest probability of total error.

from Duda, Hart, Stork (2001) Pattern classification

Classification Error

In the multi-category case, it is simpler to compute the probability of being correct

$$P(correct) = \sum_{1=1}^{c} P(\mathrm{x} \in \mathcal{R}_i, \omega_i)$$

$$= \sum_{1=1}^{c} P(\mathrm{x} \in \mathcal{R}_i \mid \omega_i) P(\omega_i)$$

$$= \sum_{1=1}^{c} \int_{\mathcal{R}_i} p(\mathrm{x} \mid \omega_i)\, P(\omega_i)\, d\mathrm{x}$$

Summary of concepts

- Discriminant functions. Classifier
- Transformations of discriminant functions
- Dichotomizer
- Discriminant functions and decision boundaries for normal distributions
- Univariate/Multivariate normal density
- Covariance matrix. Mahalanobis distance
- Linear combinations of normally distributed random variables. Whitening transform
- Discriminant functions for normal densities
- Statistically independent features of equal variance, linear discriminant functions, linear machine, minimum-distance classifier
- Arbitrary covariance matrices, quadratic forms
- Total classification error and its evaluation.