Machine learning

Bayesian Decision Theory

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Bayesian Decision Theory

- **Bayesian Decision Theory** is a fundamental statistical approach that quantifies the tradeoffs between various decisions using **probabilities** and **costs** that accompany such decisions.
- **First**, we will assume that all probabilities are known.
- **Then**, we will study the cases where the probabilistic structure is not completely known.

Fish Sorting Example Revisited

- **State of nature** is a random variable.
  - Define ω as the **type** of fish we observe (state of nature, class) where

    $\omega = \omega_1$ for sea bass,

    $\omega = \omega_2$ for salmon.
- $P(\omega_1)$ is the a **priori probability** that the next fish is a sea bass.
- $P(\omega_2)$ is the a priori probability that the next fish is a salmon.

Prior Probabilities

- Prior probabilities **reflect our knowledge** of how likely each type of fish will appear **before we actually see it**.
- How can we choose $P(\omega_1)$ and $P(\omega_2)$?
  - Set $\mathbf{P(\omega_1) = P(\omega_2)}$ if they are **equiprobable** (uniform priors).
  - May use different values **depending** on the fishing area, time of the year, etc.
- Assume there are no other types of fish
  - $P(\omega_1) + P(\omega_2) = 1$
- (**exclusivity** and **exhaustivity**).

Approaches for building a classifier.

- In classification, the goal is to find a mapping from inputs X to outputs ω given a labeled set of input-output pairs (training set)
  - Binary classification (two classes labels)
  - Multi-class classification.
- Approaches for building a classier.
  - **Generative approach**: This approach creates a joint model of feature vectors and classes ($p(x,\omega)$) and then drive $p(\omega_j|k)$
  - **Discriminative approach**: This approach creates a model of the form of $p(\omega_j|k)$ directly.

Making a Decision

- How can we make a decision with only the prior information? (**Decision Rule**)

$$\text{Decide} \quad \begin{cases} w_1 & \text{if } P(w_1) > P(w_2) \\ w_2 & \text{otherwise} \end{cases}$$

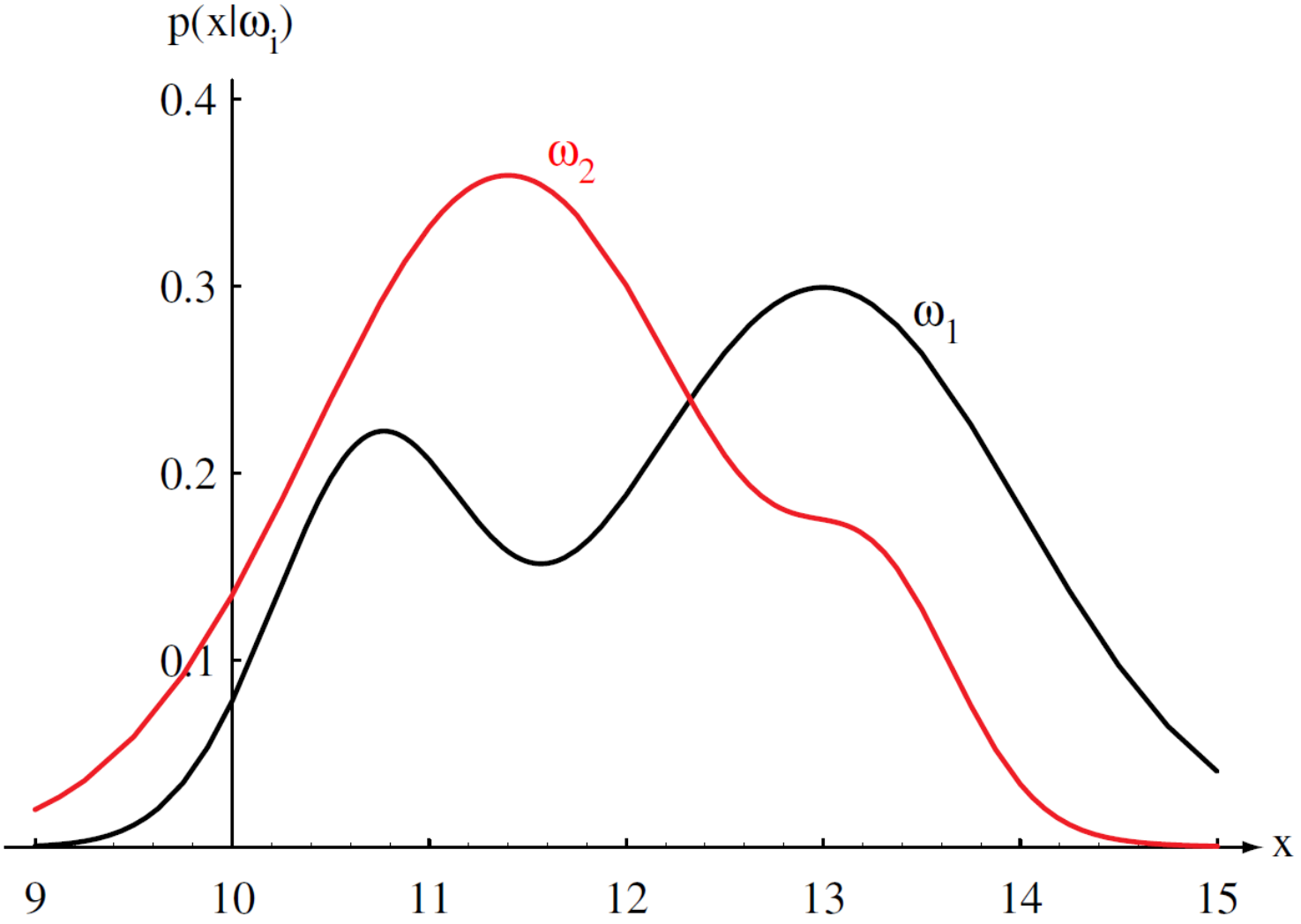
- What is the **probability of error** for this decision?

$$P(error) = \min\{P(w_1), P(w_2)\}$$

Class-Conditional Probabilities

- Let's try to **improve** the decision using the lightness measurement x. (importing **data** to decision model)
  - Let x be a **continuous random** variable.
- Define $p(x|\omega_j)$ as the **class-conditional probability** density (probability of x given that the **state of nature** is ω_j for $j = 1, 2$).
- $p(x|\omega_1)$ and $p(x|\omega_2)$ describe the **difference** in lightness between populations of sea bass and salmon.

Hypothetical class-conditional probability density functions for two classes.



Posterior Probabilities

- Suppose **we know** $P(\omega_j)$ and $p(x|\omega_j)$ for j = 1, 2, and measure the lightness of a fish as the value x.
- Define $P(\omega_j|x)$ as the a **posteriori probability** (probability of the state of nature being ω_j **given** the measurement of feature value x).
- We can use the **Bayes formula** to **convert** the prior probability to the posterior probability

$$P(\omega_j|x) = \frac{p(x|\omega_j)P(\omega_j)}{p(x)},$$

- Where $p(x) = \sum_{j=1}^{2} p(x|\omega_j)P(\omega_j).$

Bayes' formula

- Bayes' formula can be expressed informally in English by saying that

$$posterior = \frac{likelihood \times prior}{evidence}.$$

- $p(x|\omega_j)$ is called the **likelihood** and $p(x)$ is called the **evidence**.

Making a Decision

- How can we make a decision **after observing the value of** x?

$$\text{Decide } \omega_1 \text{ if } P(\omega_1|x) > P(\omega_2|x); \text{otherwise decide } \omega_2,$$

- Rewriting the rule gives

$$\text{Decide} \begin{cases} w_1 & \text{if } \frac{p(x|w_1)}{p(x|w_2)} > \frac{P(w_2)}{P(w_1)} \\ w_2 & \text{otherwise} \end{cases}$$

- Note that, at every x, $P(\omega_1|x) + P(\omega_2|x) = 1$.

Evidence

- The *evidence*, $p(x)$ is **unimportant** as far as **making a decision is concerned**
- It is basically just a **scale factor** that states how frequently we will actually measure a pattern with feature value x;
- By **eliminating** this scale factor, we obtain the following completely equivalent decision rule:

$$\text{Decide } \omega_1 \text{ if } p(x|\omega_1)P(\omega_1) > p(x|\omega_2)P(\omega_2); \quad \text{otherwise decide } \omega_2.$$

Where do Probabilities come from?

- There are two competitive answers:

  Relative frequency (**objective**) approach.
  - Probabilities can only come **from experiments**.

  Bayesian (**subjective**) approach.
  - Probabilities may reflect **degree of belief** and can be based on opinion.

Probability of Error (misclassification)

- What is the **probability of error** for this decision?

$$P(error|x) = \begin{cases} P(\omega_1|x) & \text{if we decide } \omega_2 \\ P(\omega_2|x) & \text{if we decide } \omega_1. \end{cases}$$

- What is the **average probability** of error?

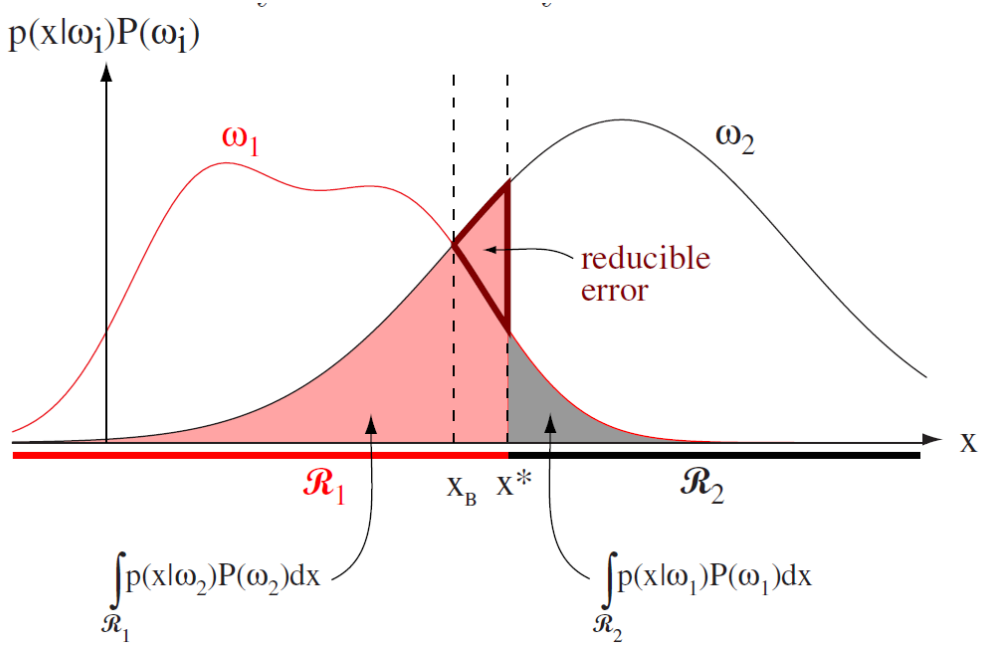
$$P(error) = \int_{-\infty}^{\infty} P(error, x)\, dx = \int_{-\infty}^{\infty} P(error|x)p(x)\, dx$$

- Bayes decision rule **minimizes this error** because

$$P(error|x) = \min\,[P(\omega_1|x), P(\omega_2|x)].$$

Bayesian classifier

The Bayesian classifier is optimal with respect to minimizing the classification probability



Decision region:

Let $R_1(R_2)$ be the region in the feature space in which we decide in favor of ω_1 (ω_2).

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

$$= \int_{\mathcal{R}_1} P(x|\omega_2)P(\omega_2)dx + \int_{\mathcal{R}_2} P(x|\omega_1)P(\omega_1)dx$$

Proof of optimality

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

$$= \int_{\mathcal{R}_1} P(x|\omega_2)P(\omega_2)dx + \int_{\mathcal{R}_2} P(x|\omega_1)P(\omega_1)dx$$

$$= \int_{\mathcal{R}_1} P(\omega_2|x)p(x)dx + \int_{\mathcal{R}_2} P(\omega_1|x)p(x))dx$$

Since $R_1 \cup R_2$ covers all the feature space ,we have

$$P(\omega_1) = \int_{\mathcal{R}_1} P(\omega_1|x)p(x)dx + \int_{\mathcal{R}_2} P(\omega_1|x)p(x)\,dx$$

The probability of error equals to

$$P(error) = \int_{\mathcal{R}_1} P(\omega_2|x)p(x)dx + \int_{\mathcal{R}_2} P(\omega_1|x)p(x))dx + \int_{\mathcal{R}_1} P(\omega_1|x)p(x)dx - \int_{\mathcal{R}_1} P(\omega_1|x)p(x)dx$$

$$P(error) = P(\omega_1) - \int_{\mathcal{R}_1} [P(\omega_1|x) - P(\omega_2|x)]p(x)dx$$

Proof of optimality

- The probability of error equals to

$$P(error) = P(\omega_1) - \int_{\mathcal{R}_1} [P(\omega_1|x) - P(\omega_2|x)]p(x)dx$$

- The probability of error is minimized if R_1 is the region of the space in which

$$[P(\omega_1|x) - P(\omega_2|x)] > 0 \rightarrow x \in \omega_1$$

- Then R_2 becomes the region where the reverse is true, i.e. is the region of the space in which

$$[P(\omega_1|x) - P(\omega_2|x)] < 0 \rightarrow x \in \omega_2$$

x can belong to R1 or R2 (not both of them)

Bayesian Decision Theory

- How can we generalize to more **than one feature**?
  - replace the scalar x by the **feature vector x**
- More than **two states of nature**?
  - just a difference in **notation**
- Allowing **actions** other than just **decisions**?
  - allow the **possibility of rejection**
- Different **risks** in the decision?
  - define how **costly** each action is

Bayesian Decision Theory (more than two classes)

- $p(\mathbf{x}|\omega_j)$ is the class-conditional probability density function.
- $P(\omega_j)$ is the prior probability that nature is in state ω_j
- The posterior probability can be computed as

$$P(\omega_j|\mathbf{x}) = \frac{p(\mathbf{x}|\omega_j)P(\omega_j)}{p(\mathbf{x})},$$

- Where

$$p(\mathbf{x}) = \sum_{j=1}^{c} p(\mathbf{x}|\omega_j)P(\omega_j).$$

A More General Theory

- Employ a more general **error function** (i.e., expected "**risk**") by associating a "**cost**" (based on a "**loss**" function) with different errors
- Let $\{\omega_1, \ldots, \omega_c\}$ be the finite set of c states of nature (**classes**, **categories**).
- Let $\{\alpha_1, \alpha_2, \ldots, \alpha_a\}$ be the finite set of a **possible actions.**
- Let $\boldsymbol{\lambda(\alpha_i|\omega_j)}$ be the **loss** incurred for taking action α_i when the state of nature is ω_j.
- Let **x** be the d-component vector-valued random variable called the **feature vector** .

Conditional Risk

- Suppose we observe **x** and take **action** α_i.
  - If the **true state** of nature is ω_j , we incur the **loss** $\lambda(\alpha_i|\omega_j)$.
- The **expected loss** with taking action α_i is

$$R(\alpha_i|\mathbf{x}) = \sum_{j=1}^{c} \lambda(\alpha_i|\omega_j) P(\omega_j|\mathbf{x}).$$

- which is also called the **conditional risk**

Minimum-Risk Classification

- The general **decision rule** $\alpha(\mathbf{x})$ tells us which action to take for observation **x**.
- We want to find the **decision rule** that minimizes the **overall risk**

$$R = \int R(\alpha(\mathbf{x})|\mathbf{x})p(\mathbf{x})\ d\mathbf{x},$$

- Bayes decision rule **minimizes the overall risk** by selecting the action α_i for **which $R(\alpha_i|\mathbf{x})$ is minimum**.

$$R(\alpha_i|\mathbf{x}) = \sum_{j=1}^{c} \lambda(\alpha_i|\omega_j)P(\omega_j|\mathbf{x})$$

  - $R(\alpha_i|\mathbf{x})$ is the **conditional risk associated** with action $\boldsymbol{\alpha_i}$
- The resulting minimum overall risk is called the **Bayes risk** and is the best performance that can be achieved.

Two-Category Classification

- Define
  - α_1: deciding ω_1,
  - α_2: deciding ω_2,
  - $\lambda_{ij} = \lambda(\alpha_i|\omega_j)$
- **Conditional risks** can be written as:

$$R(\alpha_1|\mathbf{x}) = \lambda_{11}P(\omega_1|\mathbf{x}) + \lambda_{12}P(\omega_2|\mathbf{x})$$
$$R(\alpha_2|\mathbf{x}) = \lambda_{21}P(\omega_1|\mathbf{x}) + \lambda_{22}P(\omega_2|\mathbf{x}).$$

- The fundamental rule is to decide ω_1 if $R(\alpha_1|\mathbf{x}) < R(\alpha_2|\mathbf{x})$

Two-Category Classification

- The **minimum-risk decision** rule becomes

$$\text{Decide} \begin{cases} w_1 & \text{if } (\lambda_{21} - \lambda_{11})P(w_1|\mathbf{x}) > (\lambda_{12} - \lambda_{22})P(w_2|\mathbf{x}) \\ w_2 & \text{otherwise} \end{cases}$$

- This corresponds to deciding ω_1 if

$$(\lambda_{21} - \lambda_{11})p(\mathbf{x}|\omega_1)P(\omega_1) > (\lambda_{12} - \lambda_{22})p(\mathbf{x}|\omega_2)P(\omega_2)$$

$$\frac{p(\mathbf{x}|\omega_1)}{p(\mathbf{x}|\omega_2)} > \frac{\lambda_{12} - \lambda_{22}}{\lambda_{21} - \lambda_{11}} \frac{P(\omega_2)}{P(\omega_1)}.$$

- Comparing **the likelihood ratio** to a threshold that is **independent** of the observation **x**

Minimum-Error-Rate Classification

- In classification problems, actions are decisions on classes (α_i is deciding ω_i).
  - If action α_i is taken and the true state of nature is ω_j, then the **decision is correct** if $i = j$ and in **error** if $i \neq j$.
- If errors are to be avoided, it is natural to seek a **decision rule** that **minimizes the probability of error**, i.e., the ***error rate***

zero-one loss function

- Define the zero-one loss function

$$\lambda(\alpha_i|\omega_j) = \begin{cases} 0 & i = j \\ 1 & i \neq j \end{cases} \qquad i, j = 1, ..., c.$$

(all errors are **equally** costly).

- **Conditional risk** becomes

$$\begin{aligned} R(\alpha_i|\mathbf{x}) &= \sum_{j=1}^{c} \lambda(\alpha_i|\omega_j) P(\omega_j|\mathbf{x}) \\ &= \sum_{j \neq i} P(\omega_j|\mathbf{x}) \\ &= 1 - P(\omega_i|\mathbf{x}) \end{aligned}$$

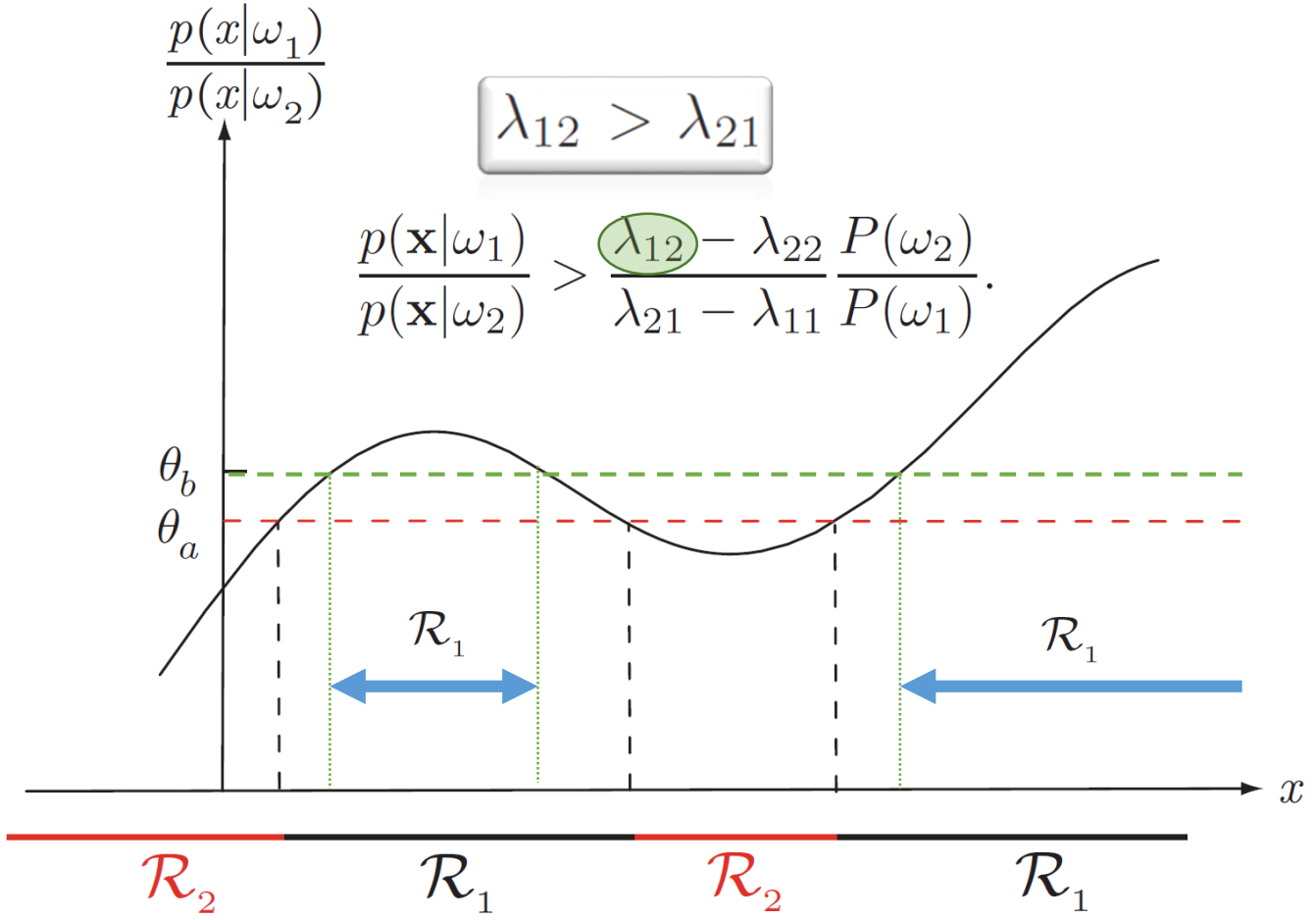
Minimum-Error-Rate Classification

- **Minimizing** the risk requires **maximizing** $P(\omega_i|\mathbf{x})$ and results in the **minimum-error decision** rule

$$\text{Decide } \omega_i \text{ if } P(\omega_i|\mathbf{x}) > P(\omega_j|\mathbf{x}) \qquad \text{for all } j \neq i.$$

- Decide base on **posterior**
- The resulting error is called the **Bayes error** and is the best performance that can be achieved.

Minimum-Error-Rate Classification



The likelihood ratio $p(\mathbf{x}|w_1)/p(\mathbf{x}|w_2)$. The threshold θ_a is computed using the priors $P(w_1) = 2/3$ and $P(w_2) = 1/3$, and a zero-one loss function. If we penalize mistakes in classifying w_2 patterns as w_1 more than the converse, we should increase the threshold to θ_b.

Neyman-Pearson Criterion

- In some problems, we may wish to minimize the overall risk **subject to a constraint**
- For example, we might wish to minimize the total risk subject to the constraint

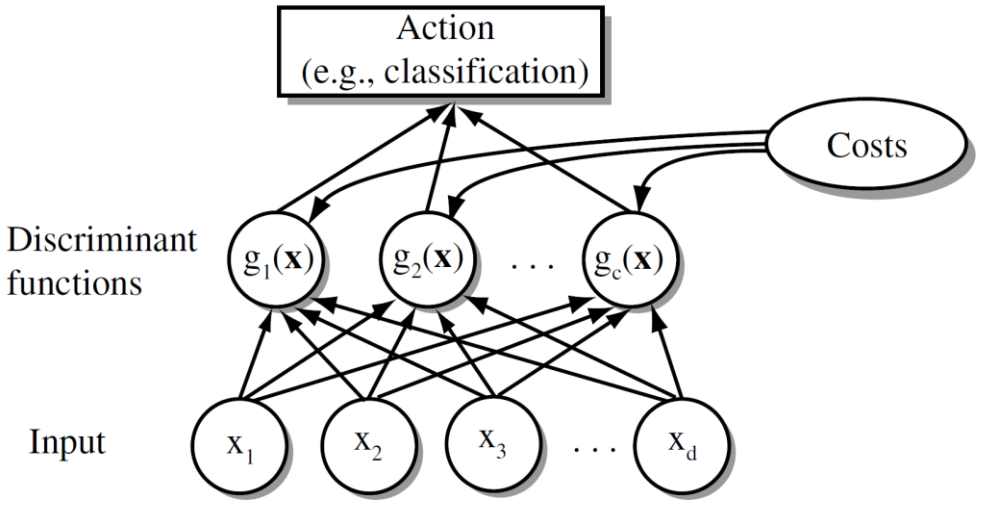
$$\int R(\alpha_i|\mathbf{x})\ d\mathbf{x} < constant \text{ for some particular } i.$$

- For instance, in our fish example, there might be some **government regulation** that we **must not misclassify more than 1% of salmon as sea bass**

Discriminant Functions

- A useful way of **representing classifiers** is through discriminant functions $g_i(\mathbf{x})$, i = 1, . . . , c, where the classifier **assigns** a feature vector **x** to class ω_i **if**

$$g_i(\mathbf{x}) > g_j(\mathbf{x}) \qquad \text{for all } j \neq i.$$



Discriminant Functions

- For the classifier that minimizes **conditional risk**

$$g_i(\mathbf{x}) = -R(\alpha_i|\mathbf{x})$$

- For the classifier that minimizes error

$$g_i(\mathbf{x}) = P(\omega_i|\mathbf{x})$$

Discriminant Functions

- These functions **divide the feature space into** c **decision regions** $(\mathcal{R}_1, \ldots, \mathcal{R}_c)$, separated by **decision boundaries**.
- Note that the results do not change even if we replace every $g_i(\mathbf{x})$ by $f(g_i(\mathbf{x}))$ where $f(\cdot)$ is a **monotonically increasing** function (e.g., logarithm).
- This may lead to significant analytical and computational **simplifications**.

e. g. for minimum-error-rate classification

- Any of the following choices gives identical classification results

$$g_i(\mathbf{x}) = P(\omega_i|\mathbf{x}) = \frac{p(\mathbf{x}|\omega_i)P(\omega_i)}{\sum_{j=1}^{c} p(\mathbf{x}|\omega_j)P(\omega_j)}$$

$$g_i(\mathbf{x}) = p(\mathbf{x}|\omega_i)P(\omega_i)$$

$$g_i(\mathbf{x}) = \ln\, p(\mathbf{x}|\omega_i) + \ln\, P(\omega_i),$$

The Two-Category Case; *dichotomizer*

- It is more common to define a **single discriminant** function

$$g(\mathbf{x}) \equiv g_1(\mathbf{x}) - g_2(\mathbf{x}),$$

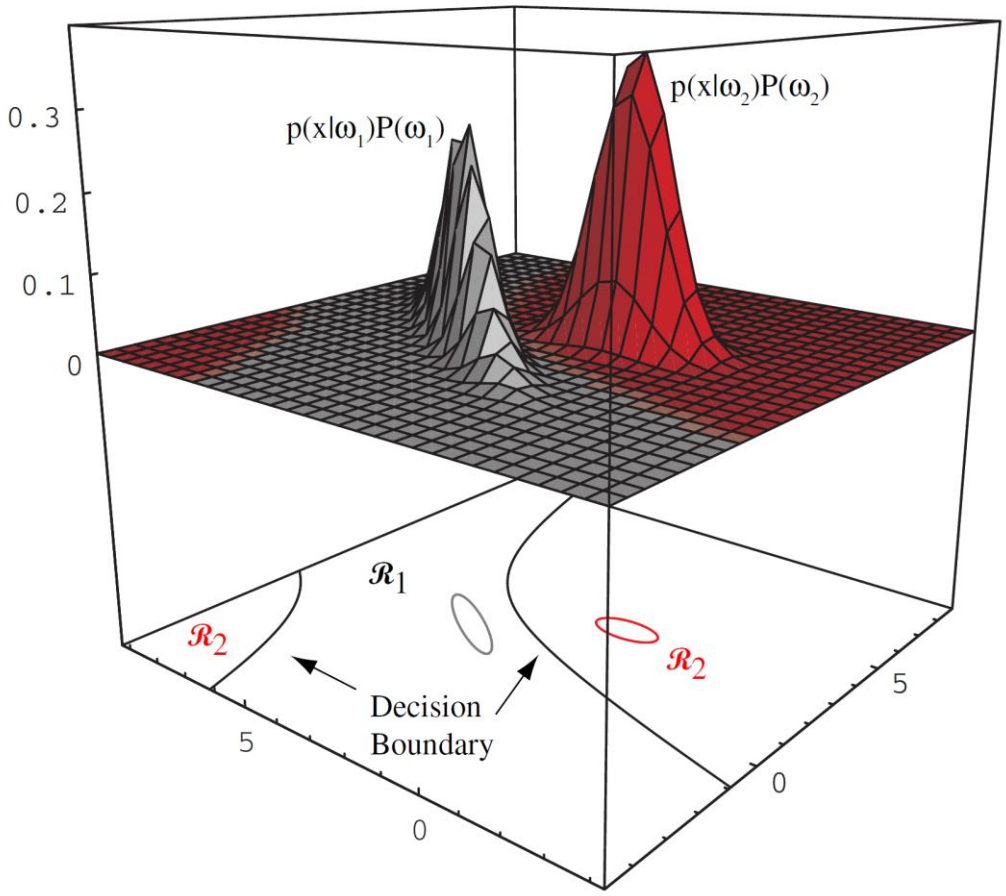
$$\text{Decide } \omega_1 \text{ if } g(\mathbf{x}) > 0; \text{ otherwise decide } \omega_2$$

- the minimum-error-rate discriminant function can be written:

$$g(\mathbf{x}) = P(\omega_1|\mathbf{x}) - P(\omega_2|\mathbf{x})$$

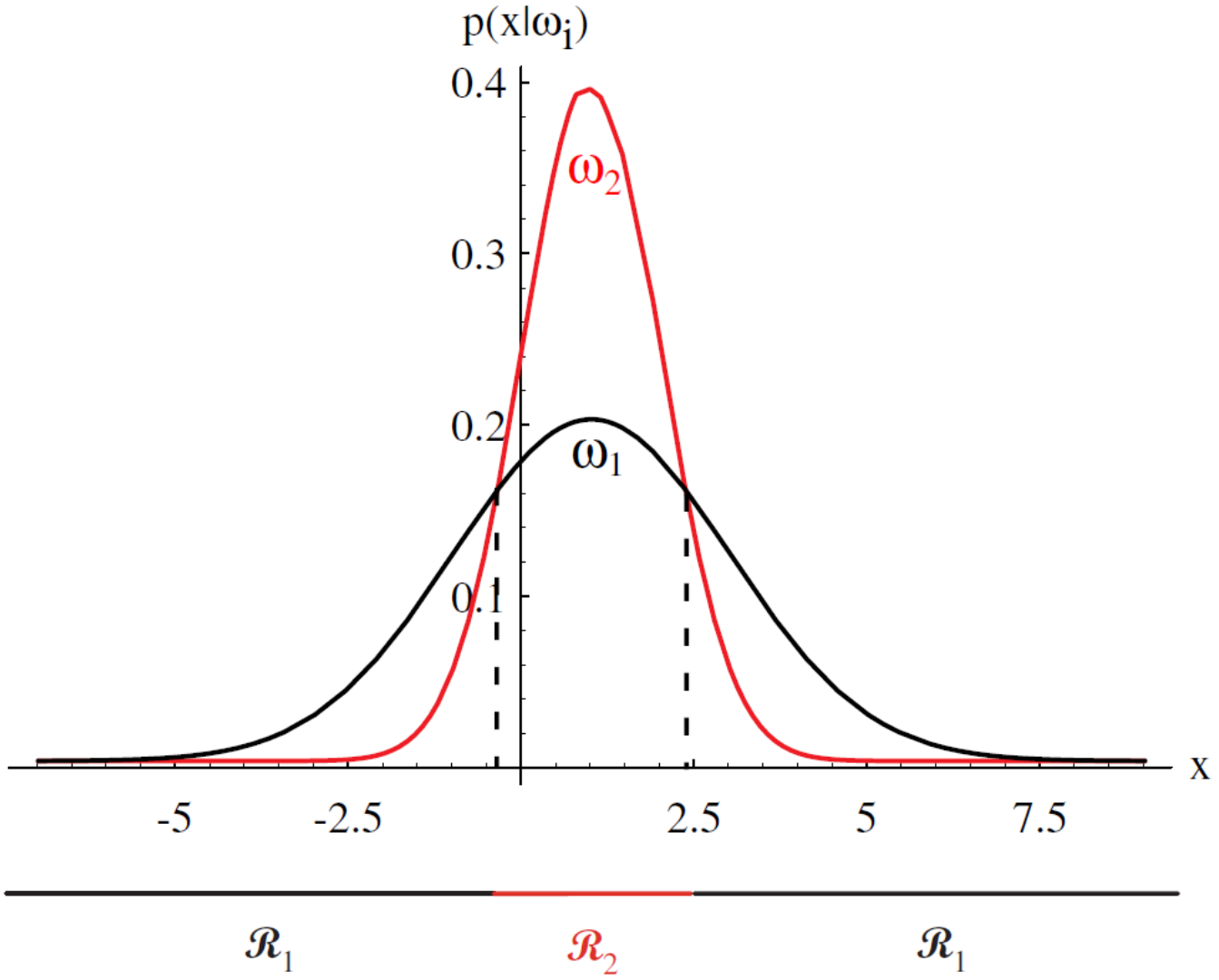
$$g(\mathbf{x}) = \ln\frac{p(\mathbf{x}|\omega_1)}{p(\mathbf{x}|\omega_2)} + \ln\frac{P(\omega_1)}{P(\omega_2)}.$$

Two-dimensional two-category classifier



the probability densities are Gaussian (with $1/e$ ellipses shown), the **decision boundary consists of two hyperbolas**, and thus the decision region $\boldsymbol{R_2}$ **is not simply connected**.

Non-simply connected decision regions



The Gaussian Density

- Gaussian can be considered as a model where the feature vectors for a given class are **continuous-valued**.
- Some properties of the Gaussian:
  - Analytically tractable.
  - Completely specified by the **1st and 2nd moments**.
  - Has the **maximum entropy** of all distributions with a given mean and variance.
  - Many processes are **asymptotically** Gaussian (Central Limit Theorem).
  - **Linear transformations** of a Gaussian are also Gaussian.
  - **Uncorrelatedness** implies **independence**.

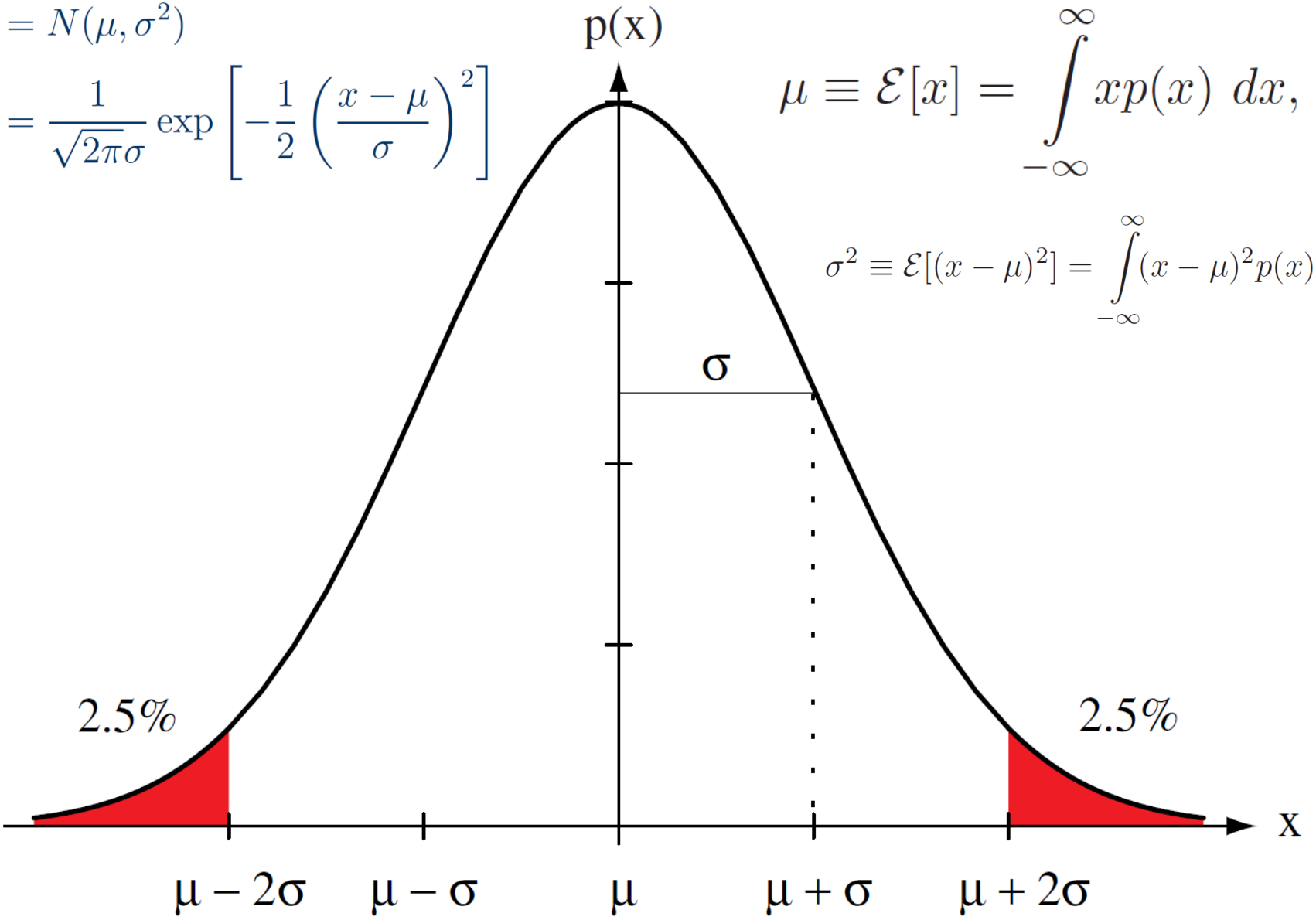
Univariate Gaussian

$$p(x) = N(\mu, \sigma^2)$$

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

$$\mu \equiv \mathcal{E}[x] = \int_{-\infty}^{\infty} xp(x)\ dx,$$

$$\sigma^2 \equiv \mathcal{E}[(x-\mu)^2] = \int_{-\infty}^{\infty} (x-\mu)^2 p(x)\ dx.$$



entropy

- The entropy is a non-negative quantity that describes the **fundamental uncertainty** in the values of points selected randomly from a distribution

$$H(p(x)) = -\int p(x)\,\ln\,p(x)\,dx,$$

- It measured in ***nats*** **(The natural unit of information)**.
- If a $\log_2$ at is used instead, the unit is the ***bit***.

Multivariate Gaussian

- General multivariate normal density in *d* dimensions

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

- Where

$$\boldsymbol{\mu} \equiv \mathcal{E}[\mathbf{x}] = \int \mathbf{x} p(\mathbf{x})\, d\mathbf{x}$$

$$\boldsymbol{\Sigma} \equiv \mathcal{E}[(\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^t] = \int (\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^t p(\mathbf{x})\, d\mathbf{x},$$

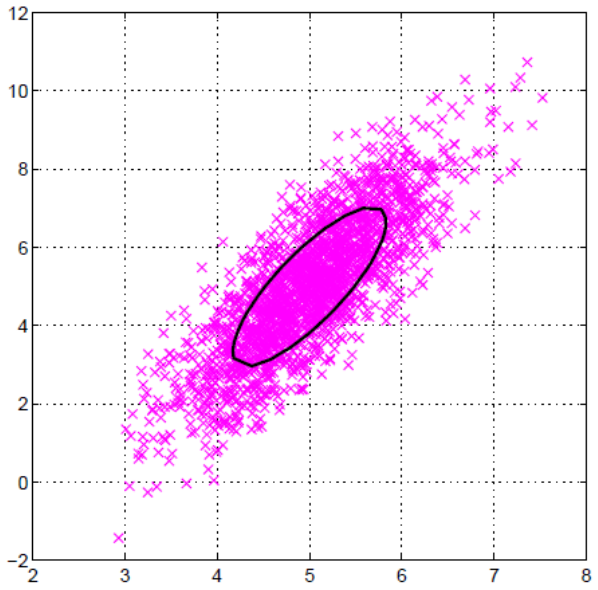
$$\mu_i = \mathcal{E}[x_i] \qquad \sigma_{ij} = \mathcal{E}[(x_i-\mu_i)(x_j-\mu_j)].$$

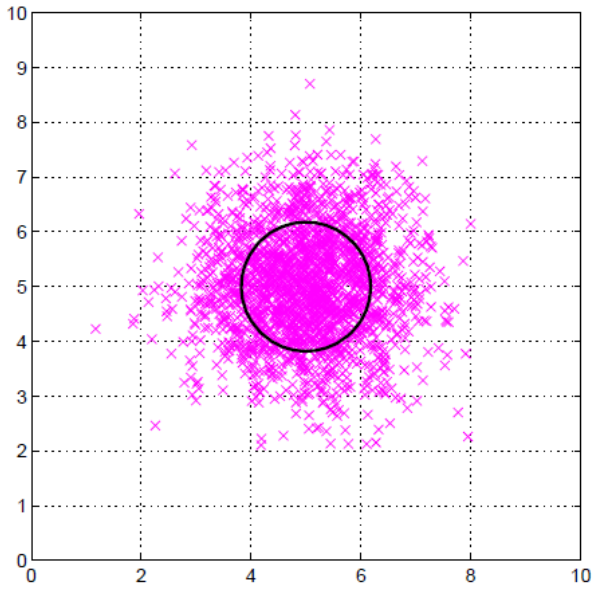
- $\boldsymbol{\Sigma}$ is **positive definite**, so that the determinant of $\boldsymbol{\Sigma}$ is strictly **positive**

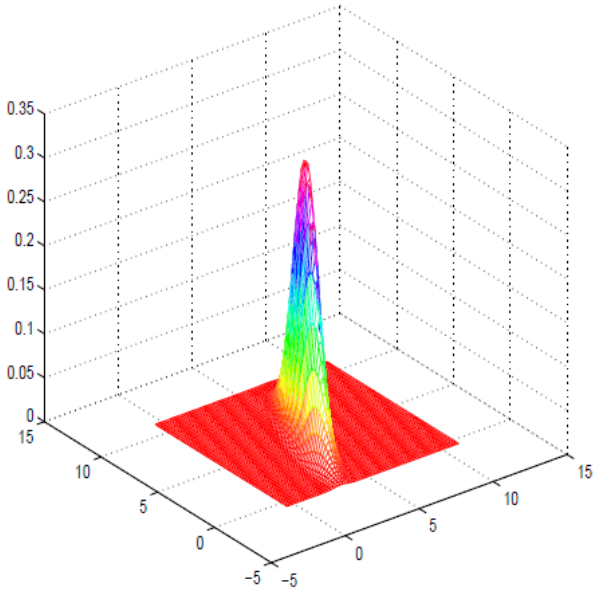
Example

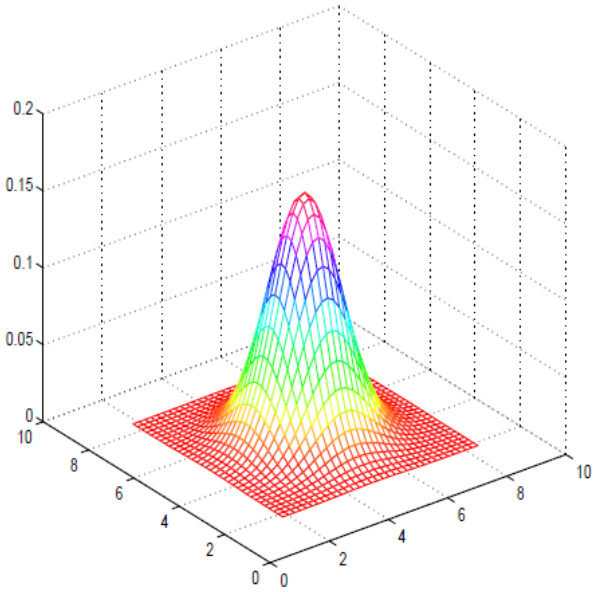
$$\Sigma = \begin{pmatrix} 3 & 1 \\ 1 & 0.5 \end{pmatrix}$$

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



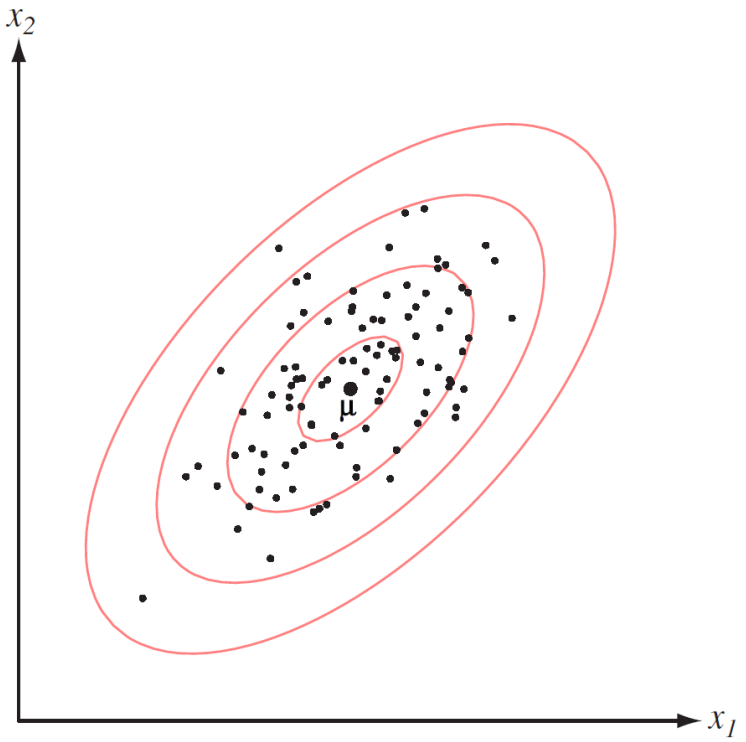






Samples drawn from a two-dimensional Gaussian lie in a cloud centered on the mean μ.

- The loci of **points of constant density** are the **ellipses** for which $(x - \mu)^T \Sigma^{-1} (x - \mu)$ is constant, where the **eigenvectors** of Σ determine the **direction** and the corresponding **eigenvalues** determine the **length** of the principal axes.
- The quantity $r^2 = (x-\mu)^T \Sigma^{-1} (x-\mu)$ is called the squared **Mahalanobis** distance from x to μ.



Linear Transformations

Recall that, given $\mathbf{x} \in \mathbb{R}^d$, $\mathbf{A} \in \mathbb{R}^{d \times k}$, $\mathbf{y} = \mathbf{A}^T\mathbf{x} \in \mathbb{R}^k$, if $x \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, then $y \sim N(\mathbf{A}^T\boldsymbol{\mu}, \mathbf{A}^T\boldsymbol{\Sigma}\mathbf{A})$.

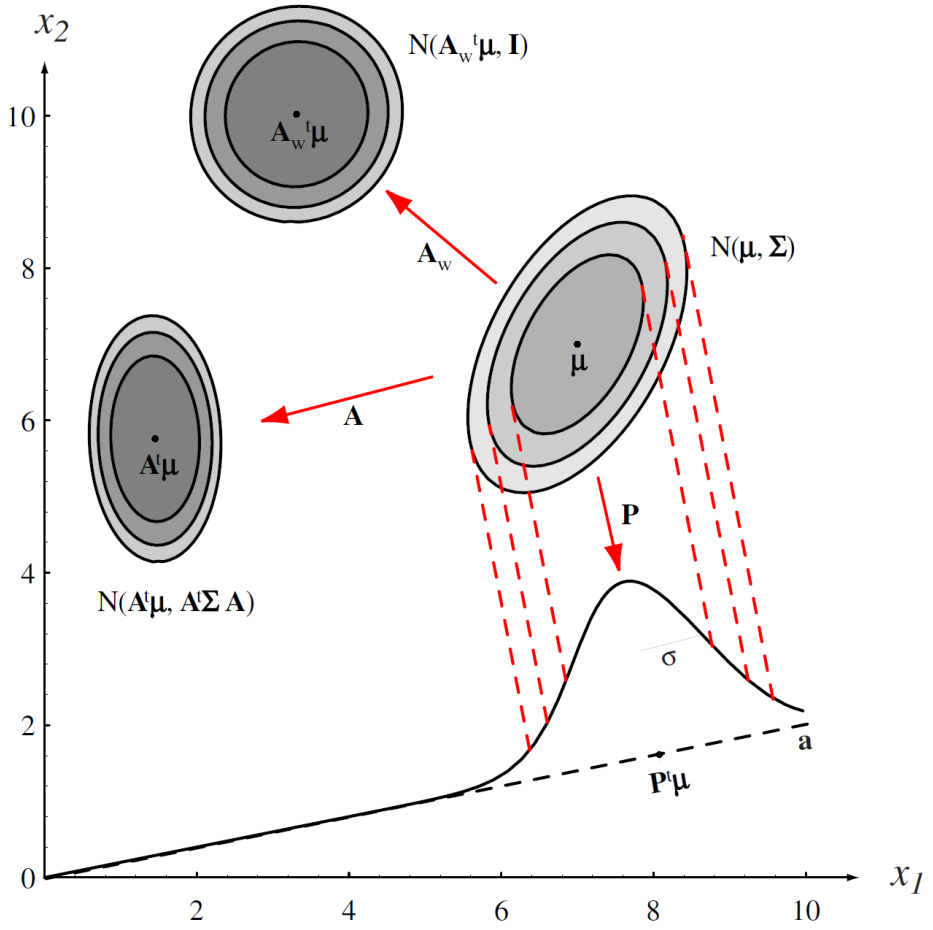
- As a special case, the whitening transform:

$$\mathbf{A_w} = \boldsymbol{\Phi}\boldsymbol{\Lambda}^{-1/2}$$

- Where
  - $\boldsymbol{\Phi}$ is the matrix whose **columns** are the **orthonormal eigenvectors** of $\boldsymbol{\Sigma}$
  - $\boldsymbol{\Lambda}$ is the **diagonal** matrix of the corresponding eigenvalues,
- Gives a **covariance matrix** equal to the identity matrix $\mathbf{I}$.

Linear Transformations

- **A** is a *d*-by-*k* *m*atrix and **y**=**A**^{t}**x** is a *k*-component vector,
- If $k = 1$ and **A** is a unit-length vector **a**, $y = \mathbf{a}^t\mathbf{x}$ is a scalar that represents the **projection of x onto a line** in the **direction** of **a**;
- In general then, **knowledge of the covariance matrix** allows us to calculate the dispersion of the data in ***any direction***, or in any **subspace**.



Discriminant Functions for the Gaussian Density

- Discriminant functions for **minimum-error-rate** classification can be written as

$$g_i(\mathbf{x}) = \ln\, p(\mathbf{x}|\omega_i) + \ln\, P(\omega_i).$$

- For $p(\mathbf{x}|\omega_i) \sim N(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$

$$g_i(\mathbf{x}) = -\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_i)^t \boldsymbol{\Sigma}_i^{-1}(\mathbf{x}-\boldsymbol{\mu}_i) - \frac{d}{2}\ln 2\pi - \frac{1}{2}\ln|\boldsymbol{\Sigma}_i| + \ln\, P(\omega_i).$$

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

- Features are **statistically independent**, and each feature has the **same variance**, σ^2
- Samples fall in equal-size **hyperspherical clusters**
- $|\boldsymbol{\Sigma}_i| = \sigma^{2d}$ and $\boldsymbol{\Sigma}_i^{-1} = (1/\sigma^2)\mathbf{I}$
- $|\boldsymbol{\Sigma}_i|$ and the $(d/2)$ ln 2π term are **independent of *i***

$$g_i(\mathbf{x}) = -\frac{\|\mathbf{x} - \boldsymbol{\mu}_i\|^2}{2\sigma^2} + \ln P(\omega_i),$$

$$g_i(\mathbf{x}) = -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_i)^t \boldsymbol{\Sigma}_i^{-1}(\mathbf{x} - \boldsymbol{\mu}_i) - \frac{d}{2}\ln 2\pi - \frac{1}{2}\ln |\boldsymbol{\Sigma}_i| + \ln P(\omega_i).$$

where $\|\cdot\|$ is the *Euclidean norm*, that is,

$$\|\mathbf{x} - \boldsymbol{\mu}_i\|^2 = (\mathbf{x} - \boldsymbol{\mu}_i)^t(\mathbf{x} - \boldsymbol{\mu}_i).$$

linear discriminant functions

- Expansion of the quadratic form $(\mathbf{x}-\boldsymbol{\mu})^{\mathsf{T}}(\mathbf{x}-\boldsymbol{\mu})$ yields

$$g_i(\mathbf{x}) = -\frac{1}{2\sigma^2}[\mathbf{x}^t\mathbf{x} - 2\boldsymbol{\mu}_i^t\mathbf{x} + \boldsymbol{\mu}_i^t\boldsymbol{\mu}_i] + \ln P(\omega_i),$$

- It seems quadratic, but term $\mathbf{x}^t\mathbf{x}$ is the same for all *i*, making it an **ignorable additive constant**

- Thus, we obtain the **linear discriminant functions**

$$g_i(\mathbf{x}) = \mathbf{w}_i^t\mathbf{x} + w_{i0},$$

- **Where**

$$\mathbf{w}_i = \frac{1}{\sigma^2}\boldsymbol{\mu}_i$$

$$w_{i0} = \frac{-1}{2\sigma^2}\boldsymbol{\mu}_i^t\boldsymbol{\mu}_i + \ln P(\omega_i).$$

We call w_{i0} the *threshold* or *bias* in the i^{th} category

Decision Boundaries

- Decision boundaries are the hyperplanes $g_i(x)=g_j(x)$, and can be written as

$$\mathbf{w}^t(\mathbf{x}-\mathbf{x}_0)=0,$$

- Where

$$\mathbf{w}=\boldsymbol{\mu}_i-\boldsymbol{\mu}_j$$

$$\mathbf{x}_0=\frac{1}{2}(\boldsymbol{\mu}_i+\boldsymbol{\mu}_j)-\frac{\sigma^2}{\|\boldsymbol{\mu}_i-\boldsymbol{\mu}_j\|^2}\ln\frac{P(\omega_i)}{P(\omega_j)}(\boldsymbol{\mu}_i-\boldsymbol{\mu}_j).$$

- Hyperplane separating R_i and R_j passes through the **point $\mathbf{x_0}$** and is **orthogonal** to the **vector w**.

Minimum-distance classifier

- Special case when $P(\omega_i)$ are the same for c classes the $\ln P(\omega_i)$ term becomes unimportant additive **constant** that can be ignored and it is **minimum-distance classifier**

$$g_i(\mathbf{x}) = -\frac{\|\mathbf{x}-\mu_i\|^2}{2\sigma^2} + \ln P(\omega_i) \longrightarrow g_i(\mathbf{x}) = -\|\mathbf{x}-\boldsymbol{\mu}_i\|^2$$

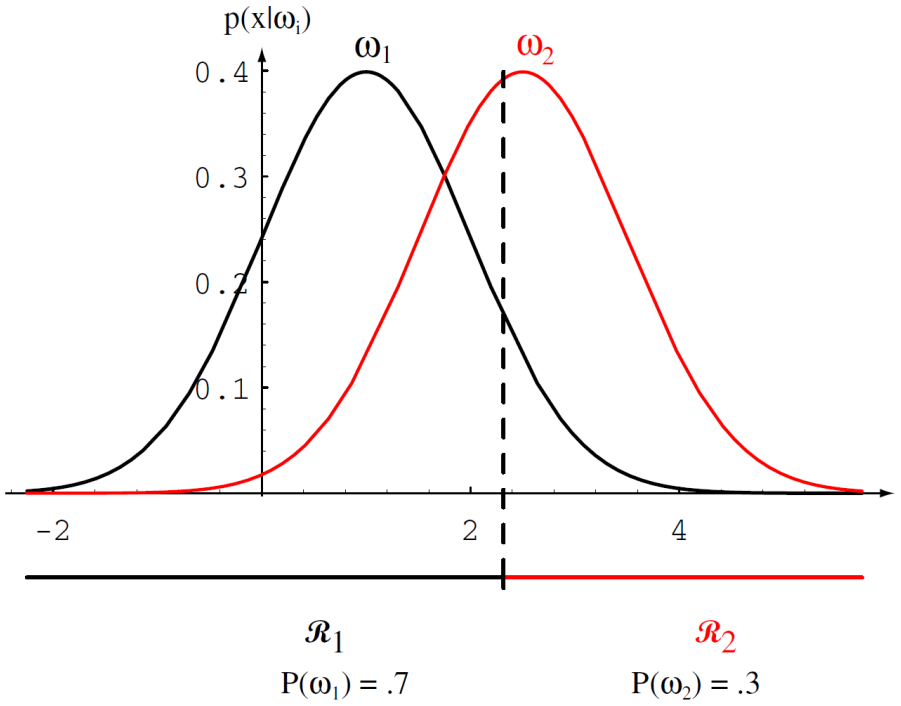
- The minimum-distance classifier that uses the decision rule

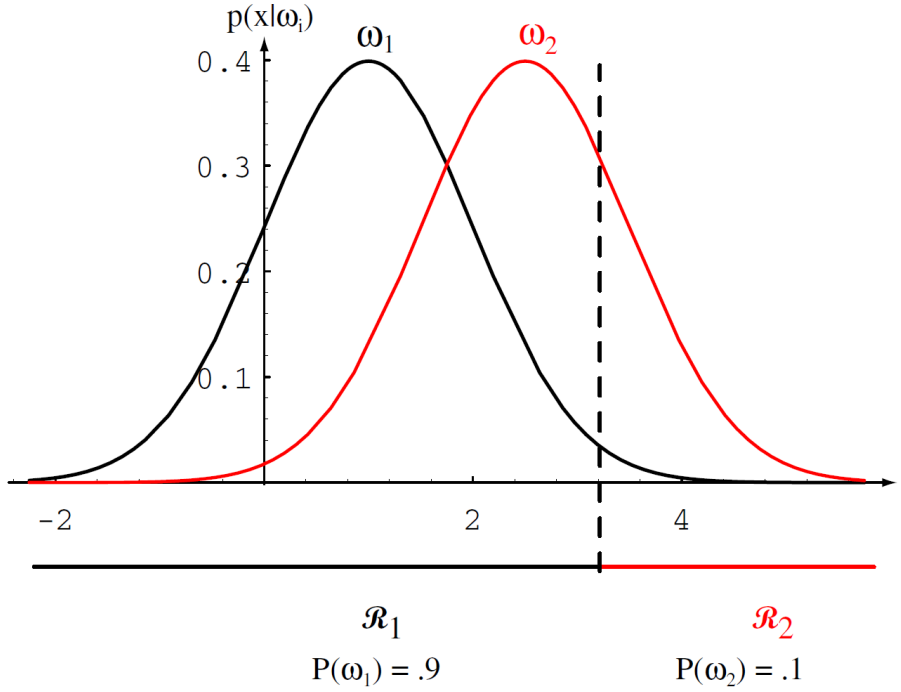
assign $\mathbf{x}$ to w_{i^*} where $i^* = \arg\min_{i=1,\ldots,c} \|\mathbf{x}-\boldsymbol{\mu}_i\|$.

Shift of decision boundary by changing priors

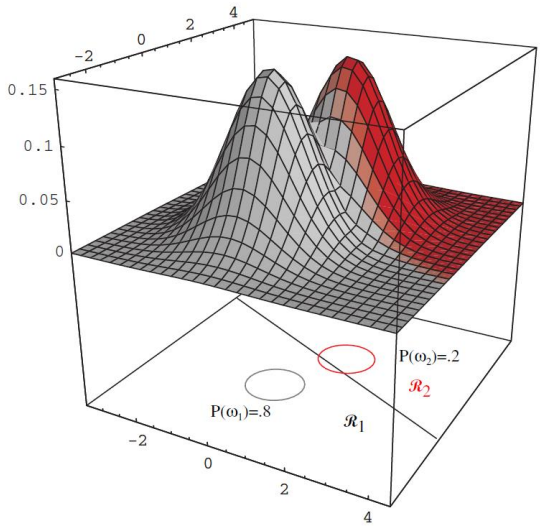
- If $P(\omega_i) \neq P(\omega_j)$, then $\mathbf{x_0}$ **shifts away** from the **most likely category.**
- If σ is **very small**, the position of the boundary is **insensitive** to $P(\omega_i)$ and $P(\omega_j)$

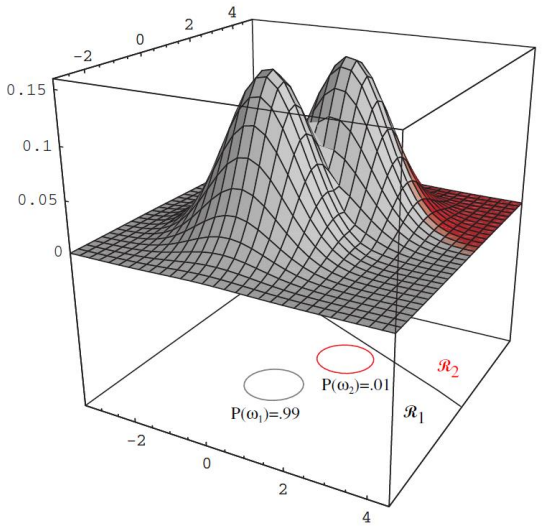
$$w_{i0} = \frac{-1}{2\sigma^2}\boldsymbol{\mu}_i^t\boldsymbol{\mu}_i + \ln P(\omega_i).$$

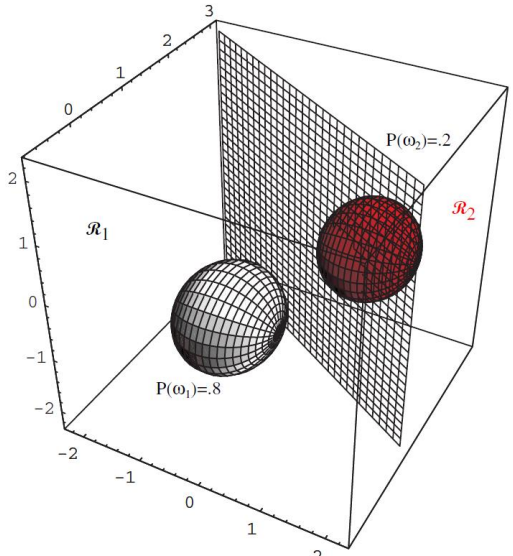


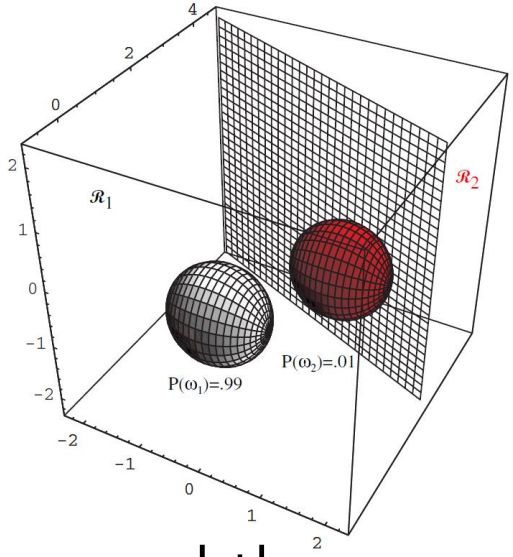


$$\Sigma_i = \sigma^2 \mathbf{I}$$









The distributions are **spherical in d dimensions**, and the boundary is a **generalized hyperplane of d–1 dimensions**, **perpendicular** to the **line separating the means**.
The decision boundary **shifts** as the priors are changed.

Case 2: $\Sigma_i = \Sigma$

- When the **covariance** matrices **for all of the classes** are **identical** but otherwise arbitrary
- Samples fall in **hyperellipsoidal** clusters of **equal size and shape**
- $|\mathbf{\Sigma}_i|$ and the $(d/2)$ ln 2π term are **independent of *i***

$$g_i(\mathbf{x}) = -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_i)^t \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}_i) + \ln P(\omega_i).$$

- To classify a feature vector **x**, measure the squared **Mahalanobis distance from x** to each of the *c* mean vectors, and assign **x** to the category of the **nearest mean**

Discriminant functions

- In the expansion of **quadratic** form $(\mathbf{x} - \boldsymbol{\mu}_i)^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}_i)$, the **quadratic** term $\mathbf{x}^t \boldsymbol{\Sigma}^{-1} \mathbf{x}$ is **independent of *i*; so**

$$g_i(\mathbf{x}) = \mathbf{w}_i^t \mathbf{x} + w_{i0},$$

- Where

$$\mathbf{w}_i = \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_i$$

$$w_{i0} = -\frac{1}{2} \boldsymbol{\mu}_i^t \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_i + \ln P(\omega_i).$$

Decision boundaries

- Since the discriminants are **linear**, the resulting decision boundaries are again **hyperplanes**

$$\mathbf{w}^t(\mathbf{x}-\mathbf{x}_0)=0,$$

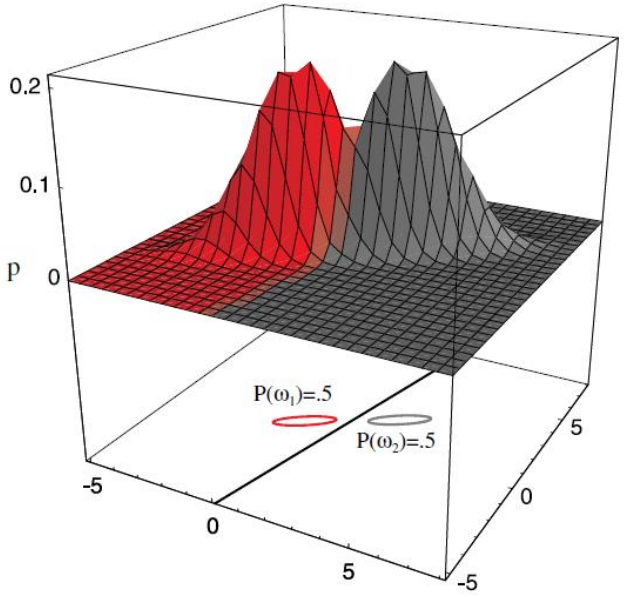
- Where

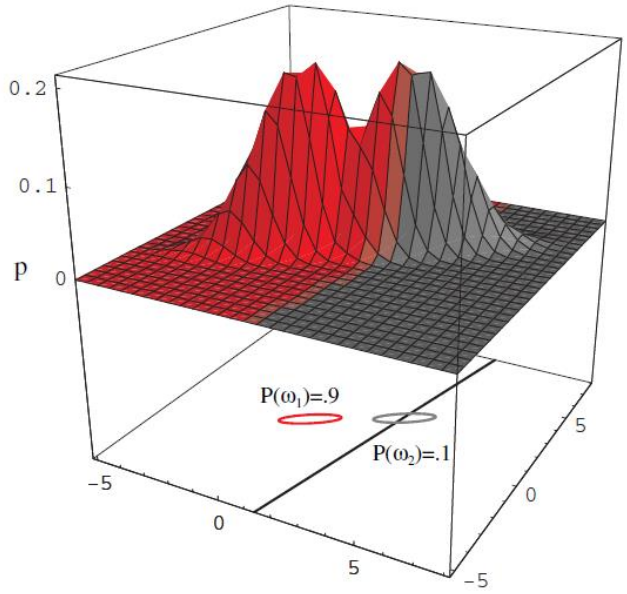
$$\mathbf{w}=\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_i-\boldsymbol{\mu}_j)$$

$$\mathbf{x}_0=\frac{1}{2}(\boldsymbol{\mu}_i+\boldsymbol{\mu}_j)-\frac{\ln\left[P(\omega_i)/P(\omega_j)\right]}{(\boldsymbol{\mu}_i-\boldsymbol{\mu}_j)^t\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_i-\boldsymbol{\mu}_j)}(\boldsymbol{\mu}_i-\boldsymbol{\mu}_j).$$

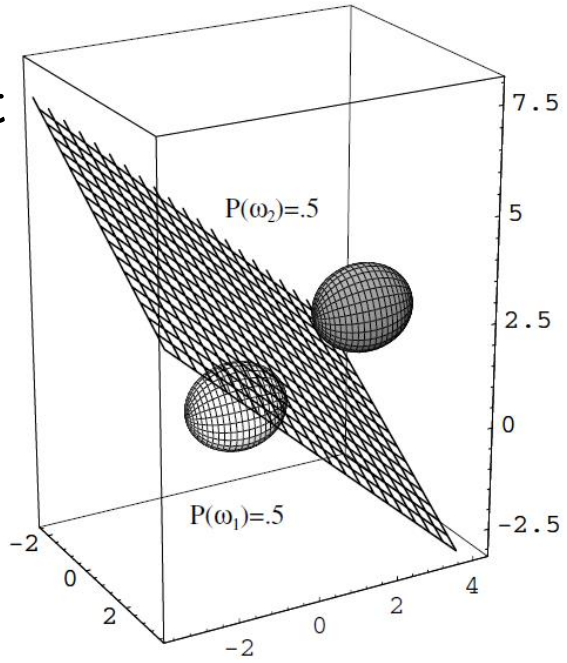
- Hyperplane passes through $\mathbf{x_0}$ but is **not necessarily orthogonal** to the line between the means. Since $\mathbf{w}=\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_i-\boldsymbol{\mu}_j)$ is generally not in the direction of $\boldsymbol{\mu}_i-\boldsymbol{\mu}_j$

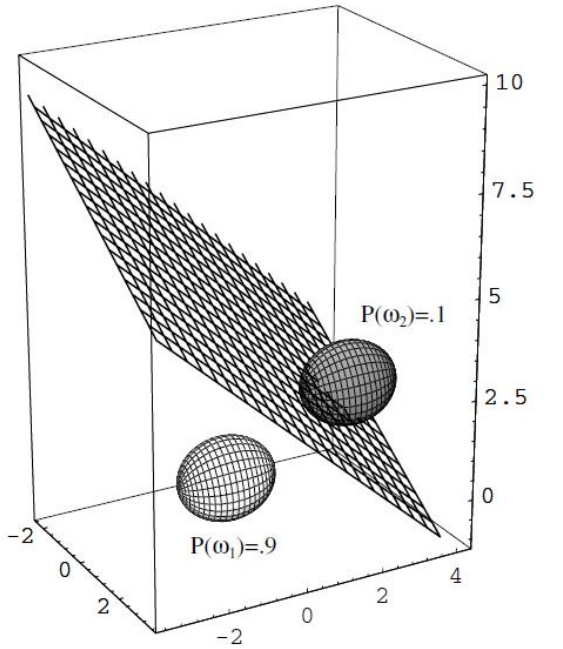
Probability densities with equal but **asymmetric Gaussian distributions**.





The decision hyperplanes **are not necessarily perpendicular** to the line connecting the means.





Case 3: Σ_i = arbitrary

$$g_i(\mathbf{x}) = -\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_i)^t\boldsymbol{\Sigma}_i^{-1}(\mathbf{x}-\boldsymbol{\mu}_i) - \frac{d}{2}\ln 2\pi - \frac{1}{2}\ln|\boldsymbol{\Sigma}_i| + \ln P(\omega_i).$$

- Only **$(d/2)\ln 2\pi$** term will dropped
- Discriminant functions are:

$$g_i(\mathbf{x}) = \mathbf{x}^t\mathbf{W}_i\mathbf{x} + \mathbf{w}_i^t\mathbf{x} + w_{i0},$$

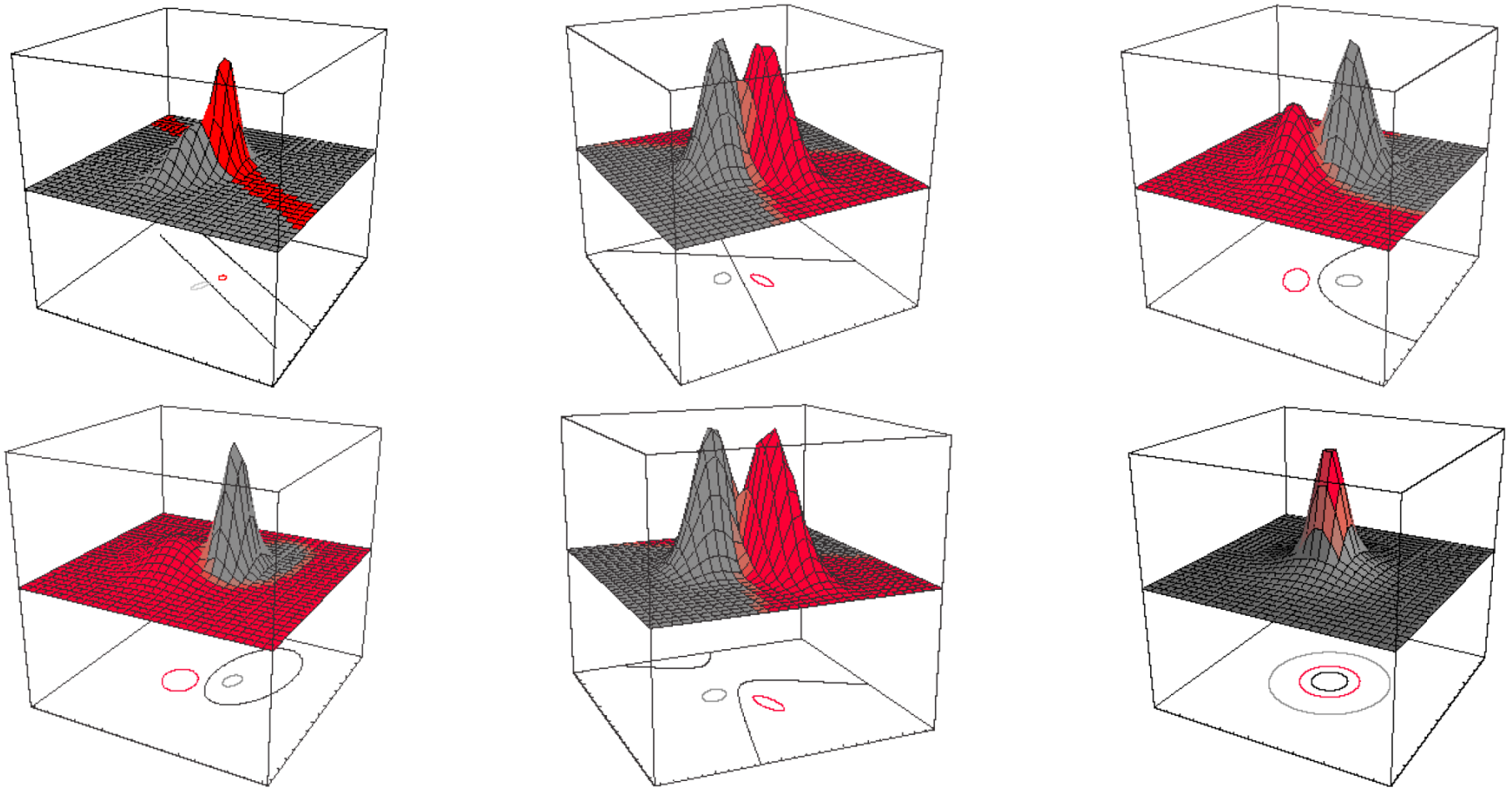
- Where

$$\mathbf{W}_i = -\frac{1}{2}\boldsymbol{\Sigma}_i^{-1},$$

$$\mathbf{w}_i = \boldsymbol{\Sigma}_i^{-1}\boldsymbol{\mu}_i$$

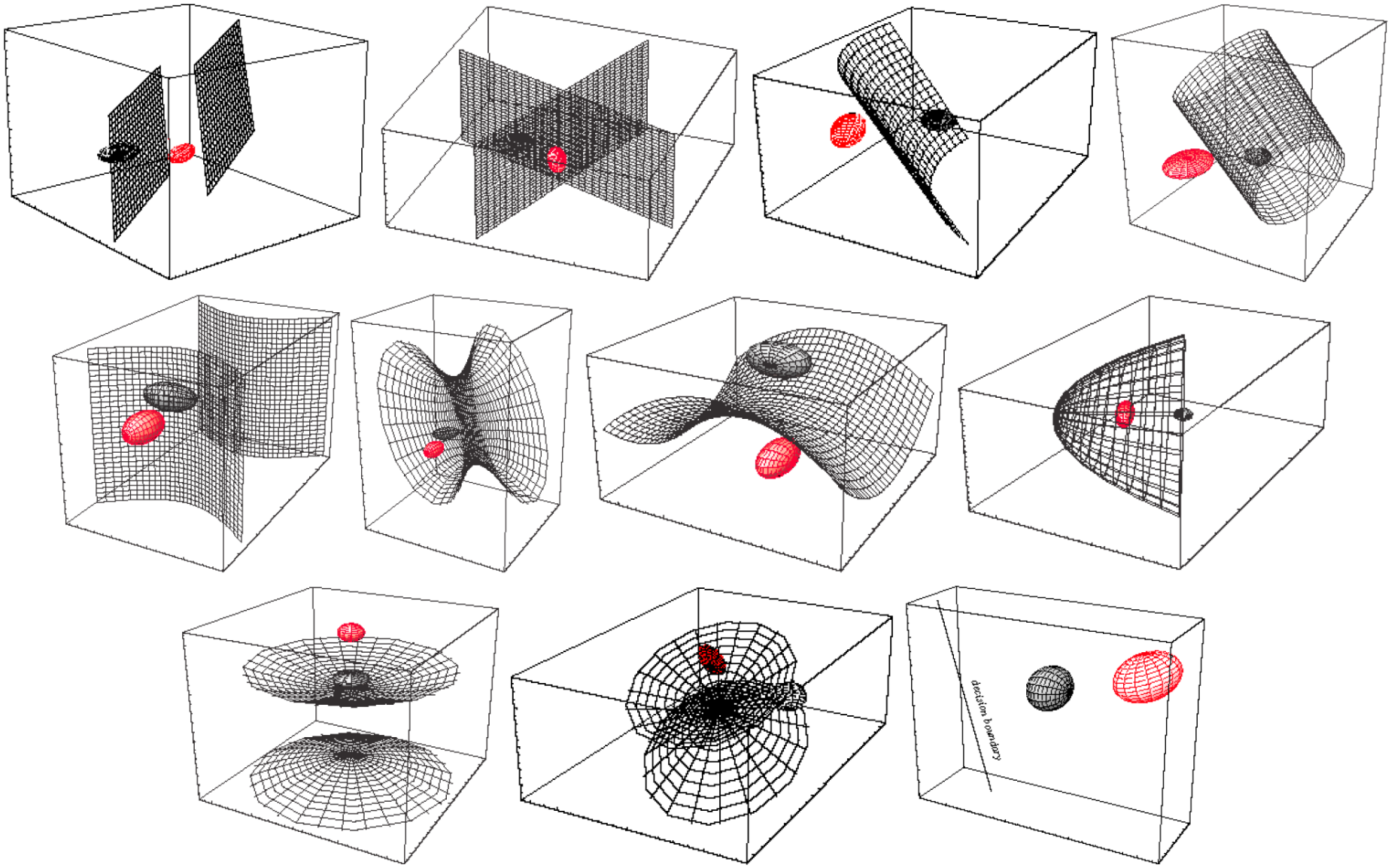
$$w_{i0} = -\frac{1}{2}\boldsymbol{\mu}_i^t\boldsymbol{\Sigma}_i^{-1}\boldsymbol{\mu}_i - \frac{1}{2}\ln|\boldsymbol{\Sigma}_i| + \ln P(\omega_i).$$

- Decision boundaries are **hyperquadrics**



Arbitrary Gaussian distributions lead to Bayes decision boundaries that are **general hyperquadrics**.

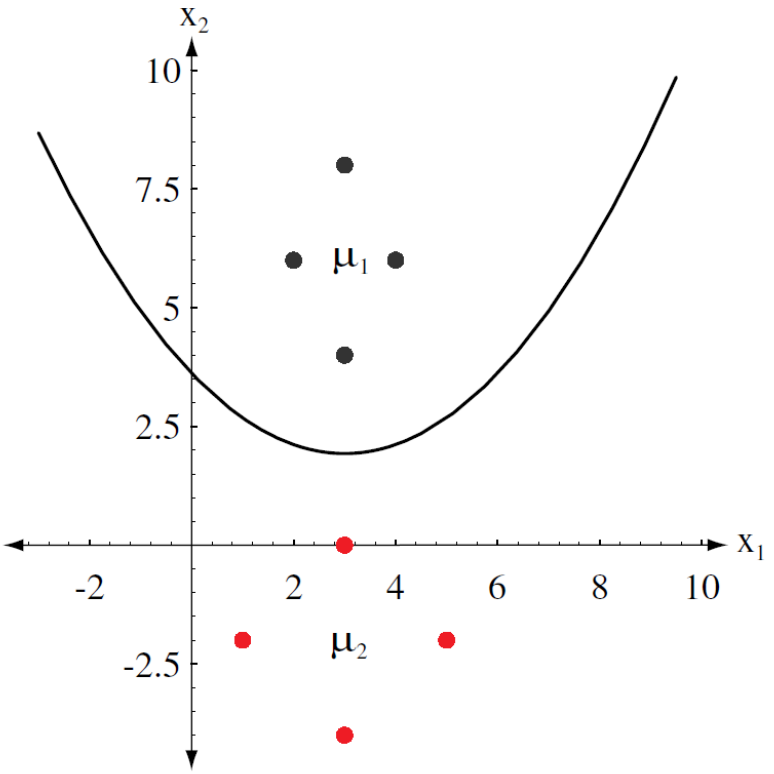
Case 3: Σ_i = arbitrary



Decision regions for two-dimensional Gaussian data

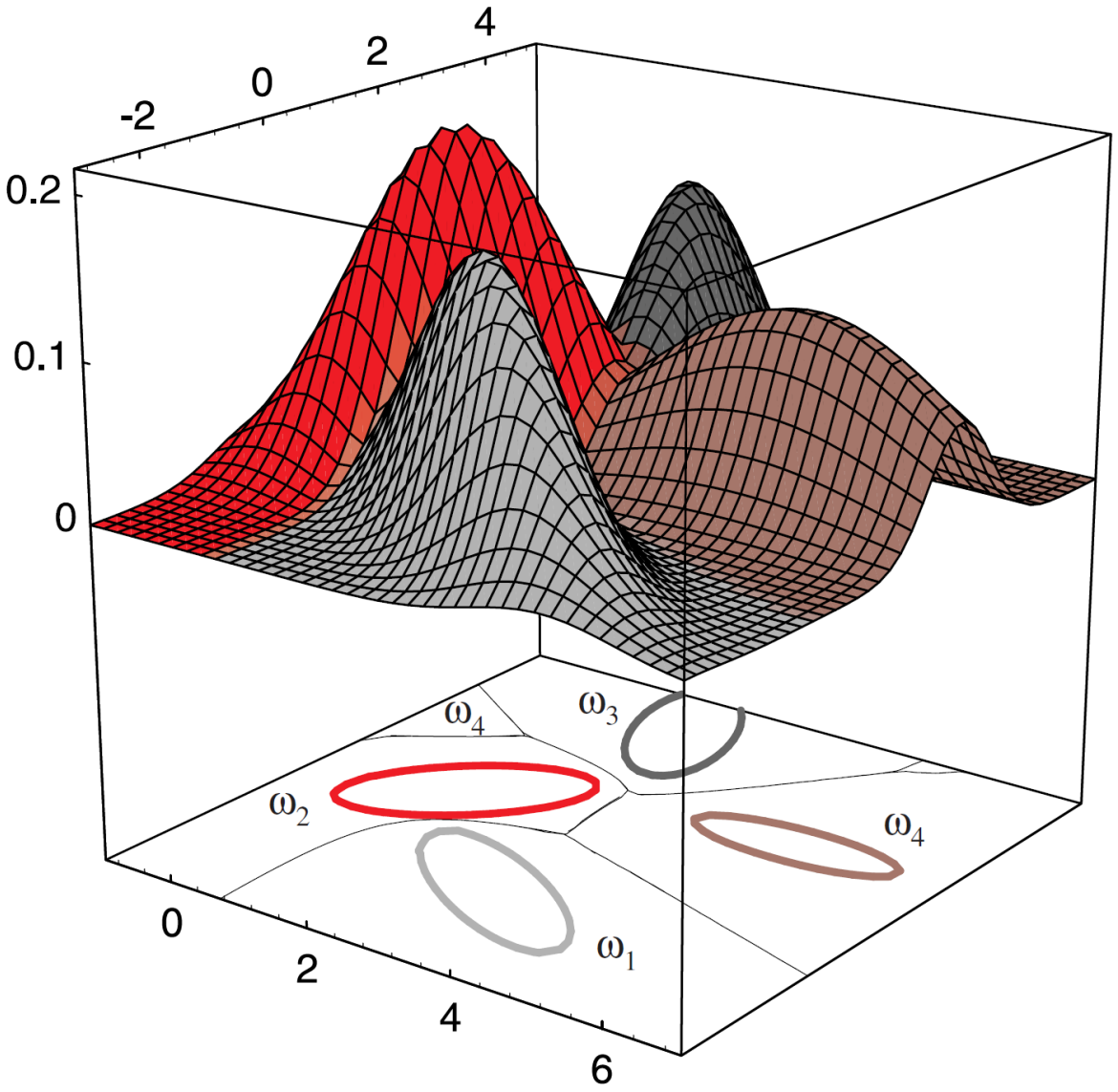
$$\boldsymbol{\mu}_1 = \begin{bmatrix} 3 \\ 6 \end{bmatrix}; \quad \boldsymbol{\Sigma}_1 = \begin{pmatrix} 1/2 & 0 \\ 0 & 2 \end{pmatrix} \text{ and } \boldsymbol{\mu}_2 = \begin{bmatrix} 3 \\ -2 \end{bmatrix}; \quad \boldsymbol{\Sigma}_2 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}.$$

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



decision boundary:

$$x_2 = 3.514 - 1.125x_1 + 0.1875x_1^2.$$



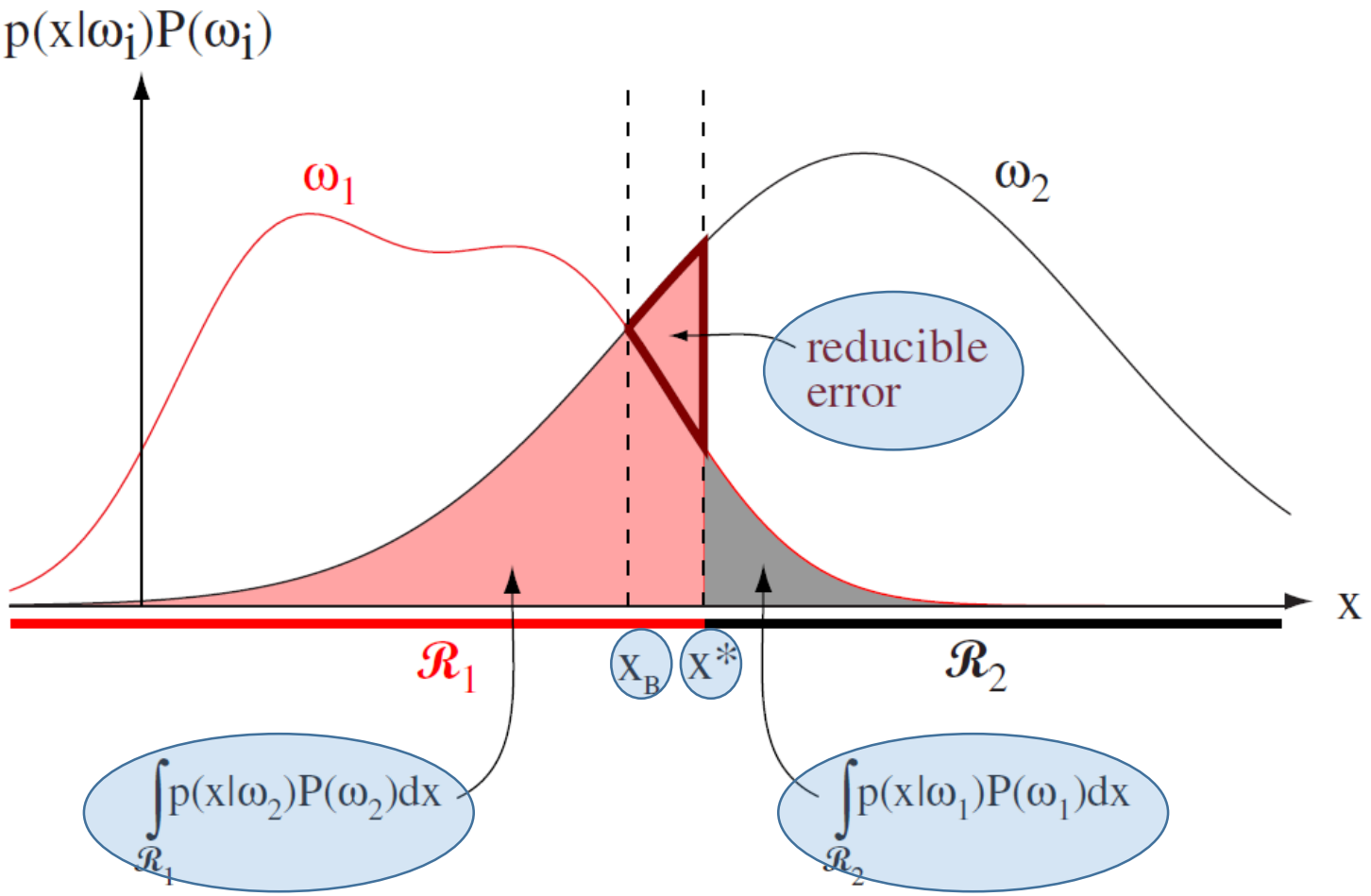
The **decision regions** for four normal distributions. Even with such a **low number of categories**, the shapes of the boundary regions can be rather complex.

Error Probabilities and Integrals

- For the two-category case

$$
\begin{aligned}
P(error) &= P(\mathbf{x} \in \mathcal{R}_2, \omega_1) + P(\mathbf{x} \in \mathcal{R}_1, \omega_2) \\
&= P(\mathbf{x} \in \mathcal{R}_2 | \omega_1) P(\omega_1) + P(\mathbf{x} \in \mathcal{R}_1 | \omega_2) P(\omega_2) \\
&= \int_{\mathcal{R}_2} p(\mathbf{x}|\omega_1) P(\omega_1) \, d\mathbf{x} + \int_{\mathcal{R}_1} p(\mathbf{x}|\omega_2) P(\omega_2) \, d\mathbf{x}.
\end{aligned}
$$

Optimal classifier



Components of the probability of error for equal priors and the **non-optimal decision point x*.**

The optimal point **x^B minimizes** the total shaded area and gives the Bayes error rate.

Error Probabilities and Integrals

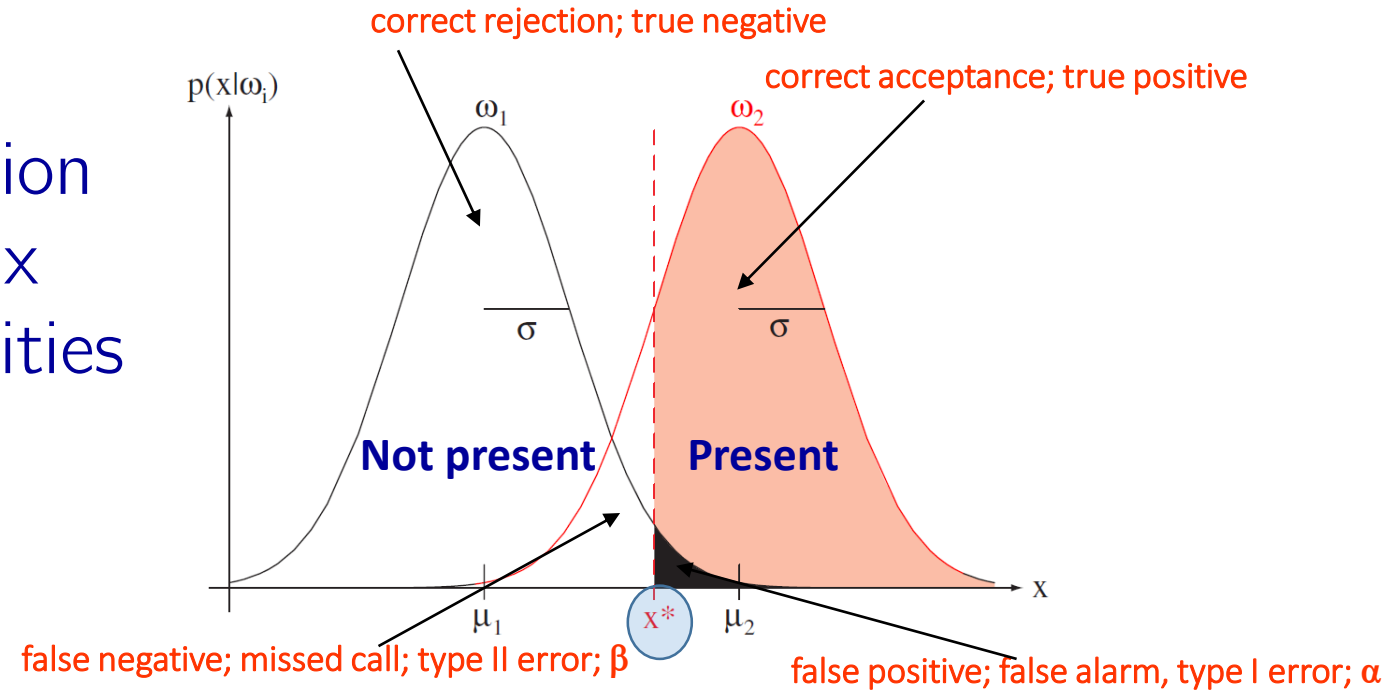
- For the **multicategory** case

$$
\begin{aligned}
P(error) &= 1 - P(correct) \\
&= 1 - \sum_{i=1}^{c} P(\mathbf{x} \in \mathcal{R}_i, w_i) \\
&= 1 - \sum_{i=1}^{c} P(\mathbf{x} \in \mathcal{R}_i | w_i) P(w_i) \\
&= 1 - \sum_{i=1}^{c} \int_{\mathcal{R}_i} p(\mathbf{x}|w_i)\, P(w_i)\, d\mathbf{x}.
\end{aligned}
$$

Signal Detection Theory

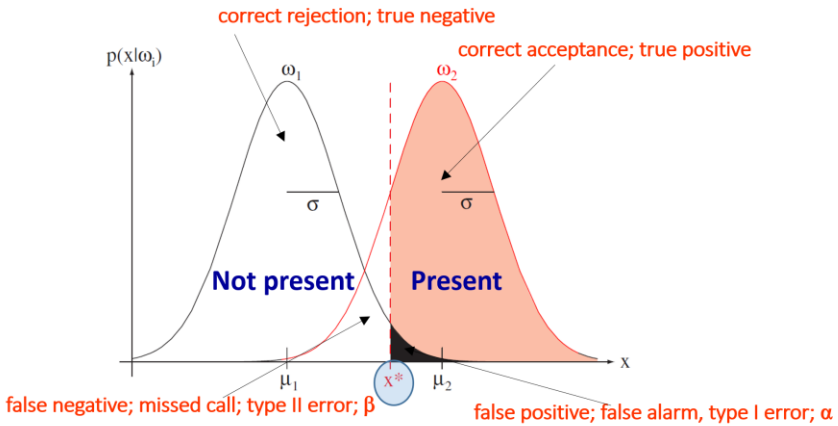
- There is an **internal signal** (such as a voltage) x, whose value has mean μ_2 when the external signal (pulse) is **present**, and mean μ_1 when it is **not present**.
- Because of noise the actual value is a **random variable**

Confusion matrix probabilities



- The detector (classifier) employs a **threshold** value x^* for determining whether the external pulse is present,

2 classes confusion matrix



Predicted Class

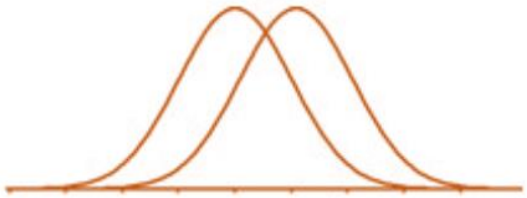
Actual Class	Positive	Negative	
ω_2 Positive	True Positive (TP)	False Negative (FN) Type II Error	**Sensitivity** $\frac{TP}{(TP+FN)}$
Negative ω_1	False Positive (FP) Type I Error	True Negative (TN)	**Specificity** $\frac{TN}{(TN+FP)}$
	Precision $\frac{TP}{(TP+FP)}$	**Negative Predictive Value** $\frac{TN}{(TN+FN)}$	**Accuracy** $\frac{TP+TN}{(TP+TN+FP+FN)}$

Discriminability

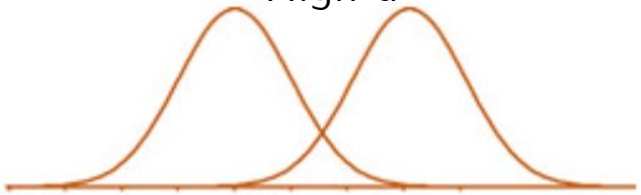
- A measure for discriminating whether the pulse is present or not
- Independent of the **choice of x*** and the **decision strategy**
- Describes the **inherent** and unchangeable properties due to noise and the strength of ability the external signal

$$d' = \frac{|\mu_2 - \mu_1|}{\sigma}.$$

Low d'

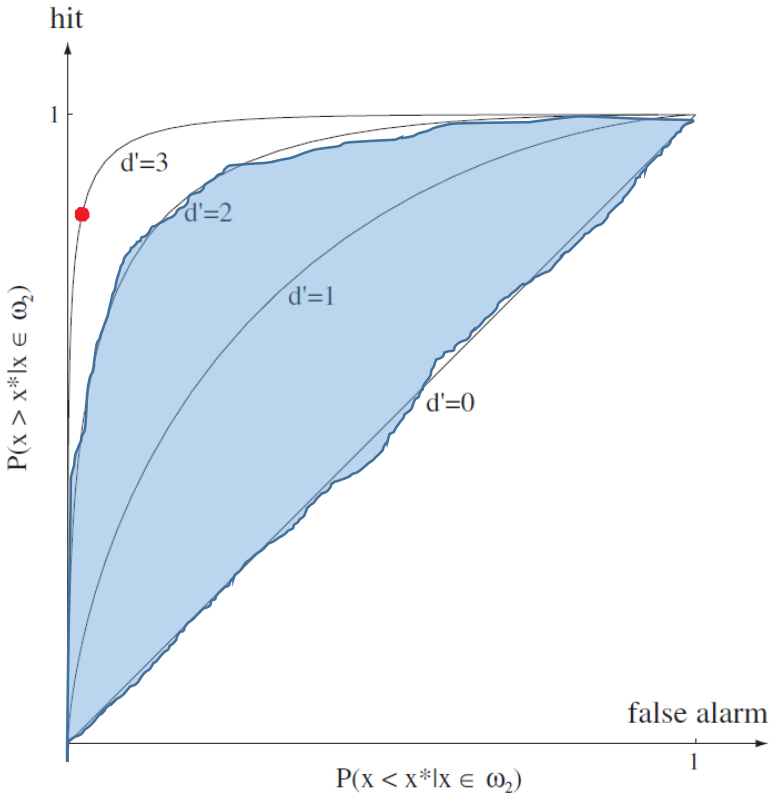


High d'



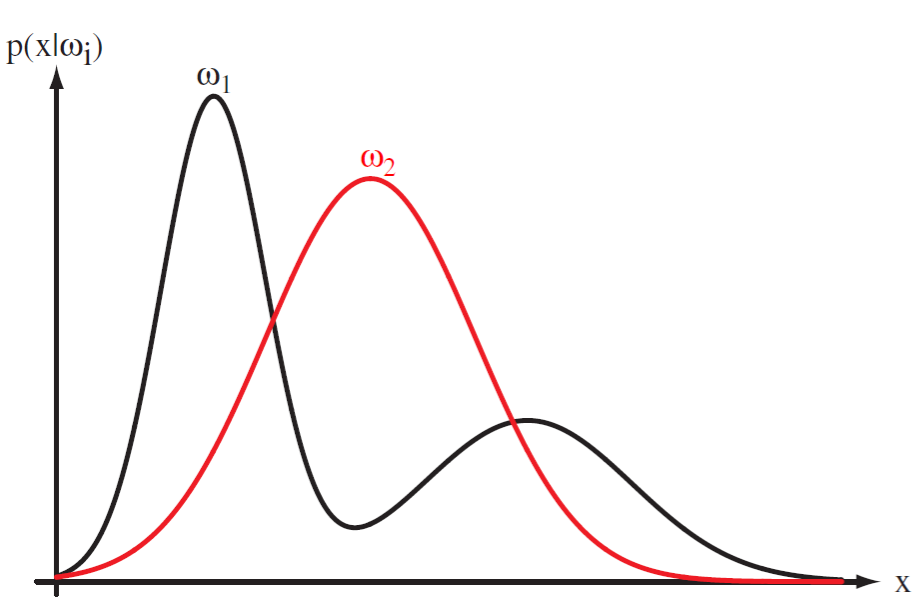
Operating Characteristics

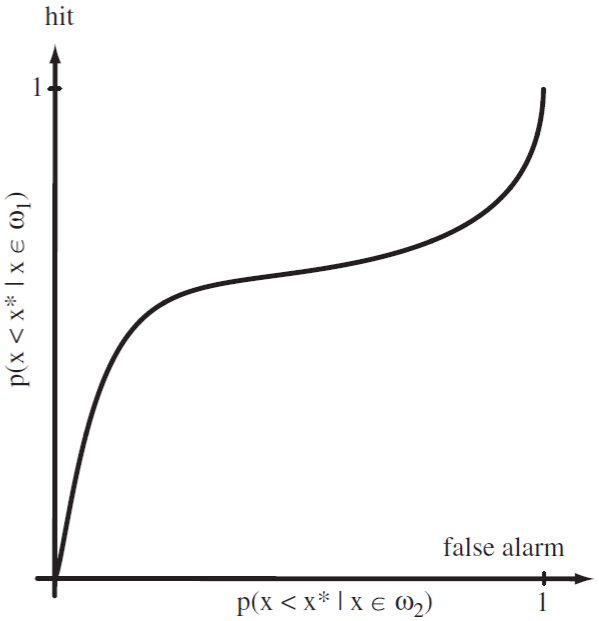
- We **do not know** μ_1, μ_2, σ nor x*, but **we know** the state of nature and the **decision of the system**. **We want to find d'**
- **Hit** an **false alarm** can be computed by large number of trials. (assume x* **is fixed)**
- If the **densities are fixed** but the **threshold *x∗* is changed**, then our **hit** and **false alarm** rates will also change.
- Thus we see that **for a given discriminability** *d*, our point will move along a smooth curve — a *receiver operating characteristic* or **ROC curve**



The area under a receiver operating characteristic (ROC) curve, abbreviated as AUC, is a single scalar value that measures the overall performance of a binary classifier Non-parametric measure

Example: general operating characteristic curve





operating characteristic curves are generally **not symmetric,**