

Bayesian Decision Theory

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- 1 Introduction
- 2 Minimum-Error-Rate Classification
 - Prior
 - Decision by Likelihood
 - Decision by Posterior
- 3 Minimum-Risk Classification
- 4 Gaussian (Normal) Density
- 5 Discriminant Functions
- 6 Discriminant Function for the Normal Density
 - Case $\Sigma_i = \sigma^2 \mathbf{I}$
 - Common covariance matrix
 - Different Σ for each class
- 7 Error Probabilities
- 8 Receiver Operating Characteristic (ROC)

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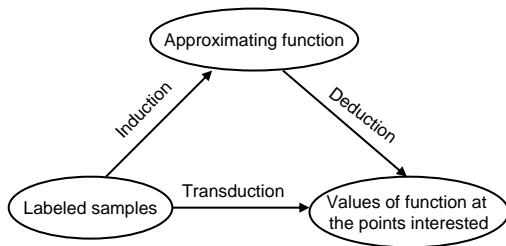
Learning Types

Imagine an organism or machine which experiences a series of sensory inputs: $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \dots$

- **Supervised learning:** The machine is also given desired outputs y_1, y_2, y_3, \dots , and its goal is to learn to produce the correct output given a new input
- **Unsupervised learning:** The goal of the machine is to build a model of \mathbf{x} that can be used for reasoning, decision making, predicting things, communicating etc.
- **Reinforcement learning:** The machine can also produce actions a_1, a_2, \dots which affect the state of the world, and receives rewards (or punishments) r_1, r_2, \dots . Its goal is to learn to act in a way that maximizes rewards in the long term

Inference Types

- **Inductive Learning** (specific-to-general): Learning is a problem of function estimation on the basis of empirical data
- **Transductive Learning** (specific-to-specific): To estimate the values of the function for a given finite number of samples of interest



General Decision Theory

Foundation of pattern recognition is **probability theory**

- Minimize the expected number of misclassifications by assigning each input \mathbf{x} to the class \mathcal{C}_k which maximizes the posterior

$$P(\mathcal{C}_k|\mathbf{x}).$$

General Decision Theory

Foundation of pattern recognition is **probability theory**

- Minimize the expected number of misclassifications by assigning each input \mathbf{x} to the class \mathcal{C}_k which maximizes the posterior

$$P(\mathcal{C}_k|\mathbf{x}).$$

- Two phases
 - 1 Inference: model the posterior probabilities
 - 2 Decision: choose the optimal output

Generative Vs. Discriminative Models

- **Generative approaches:** separately model the class-conditional densities and the priors

$$p(\mathbf{x}|\mathcal{C}_k), \quad P(\mathcal{C}_k)$$

then evaluate the posterior with the Bayes' Theorem

$$P(\mathcal{C}_k|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_k)P(\mathcal{C}_k)}{\sum_j p(\mathbf{x}|\mathcal{C}_j)P(\mathcal{C}_j)}$$

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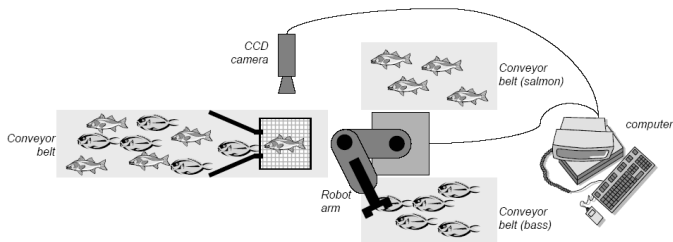
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- **Discriminative approaches:** directly model the posterior

$$P(\mathcal{C}_k|\mathbf{x})$$

Scenario

- Design of a classifier to separate two kinds of fish: sea bass and salmon
- What's the next emerging along the conveyor belt (prediction)?
- Does the sequence of types of fish appear to be random?



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Decision by Prior

- The type of fish, or **state of nature**, or class, ω , is a random variable
- As each fish emerges **nature** is in one or the other of the two possible states

$$\omega = \begin{cases} \omega_1 & \text{if fish is sea bass} \\ \omega_2 & \text{if fish is salmon} \end{cases}$$

- As the ω is unpredictable, it must be described probabilistically
- Assuming there is some *a priori* probability (**prior**), which reflects our knowledge of how likely each type of fish will appear before we actually see it.

Prior

- Assuming that the catch of salmon and sea bass is equiprobable (**uniform priors**),

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- Assuming that the catch of salmon and sea bass is equiprobable (**uniform priors**),
 - $P(\omega_1) = P(\omega_2)$
- Assume there are no other types of fish
 - $P(\omega_1) + P(\omega_2) = 1$ (exclusivity and exhaustivity)
- May use different values depending on the fishing area, time of the year, etc.

Decision with Prior

No more information available, if we are forced to make a decision

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$$\omega = \begin{cases} \omega_1 & \text{if } P(\omega_1) > P(\omega_2) \\ \omega_2 & \text{if } P(\omega_1) < P(\omega_2) \\ \omega_1/\omega_2 & \text{if } P(\omega_1) = P(\omega_2) \end{cases}$$

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Probability Density

- Let's try to improve the decision using the lightness measurement x
- different fish with different lightness values x_1, x_2, \dots

$\Rightarrow x$ is a random variable in probabilistic terms

- Assume x to be a continuous random variable whose distribution depends on the state of nature:

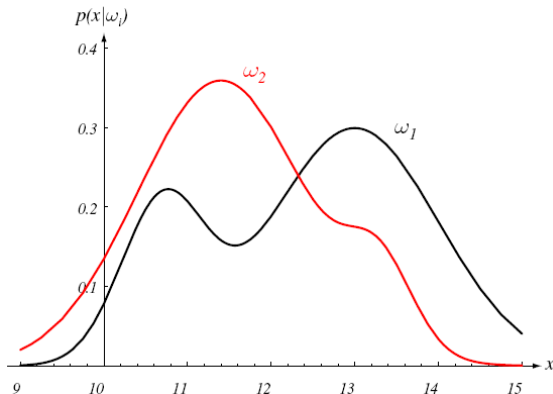
$$p(x|\omega)$$

which is class-conditional probability density of measuring a particular feature value x given the pattern is in category (class) ω

- likelihood: if all other things are equal, larger $p(x|\omega_i)$ is of more "likely" that the true category is ω_i

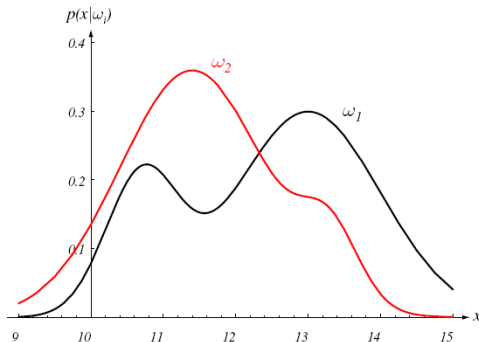
Probability Density

$p(x|\omega_1)$ and $p(x|\omega_2)$ describe the difference in lightness between **population** of sea bass and salmon



Decision by Likelihood

$$\omega = \begin{cases} \omega_1 & \text{if } p(x|\omega_1) > p(x|\omega_2) \\ \omega_2 & \text{if } p(x|\omega_1) < p(x|\omega_2) \\ \omega_1/\omega_2/\text{reject} & \text{if } p(x|\omega_1) = p(x|\omega_2) \end{cases}$$



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Decision-theoretic terminology

- state of nature: ω
- *a priori* probability (prior) $P(\omega)$
- class-conditional probability density function $p(x|\omega_i)$
the likelihood of ω_i wrt x
- *a posteriori* probability $P(\omega_i|x)$: the probability of the state of nature being ω_i given that feature value x has been measured

Posterior

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- Product of the likelihood and the prior probability
- Bayes formula:

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

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$$P(\omega_k|x) = \frac{p(x|\omega_k)P(\omega_k)}{\sum_{i=1}^2 p(x|\omega_i)P(\omega_i)}$$

Making Decision

- Suppose we know the likelihood and the prior probability
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$$\omega = \begin{cases} \omega_1 & \text{if } P(\omega_1|x) > P(\omega_2|x) \\ \omega_2 & \text{otherwise} \end{cases}$$

- We can rewrite the decision rule by

$$\omega = \begin{cases} \omega_1 & \text{if } \frac{p(x|\omega_1)}{p(x|\omega_2)} > \frac{P(\omega_2)}{P(\omega_1)} \\ \omega_2 & \text{otherwise} \end{cases}$$

Probability of the Error

What is the probability of error for this decision:

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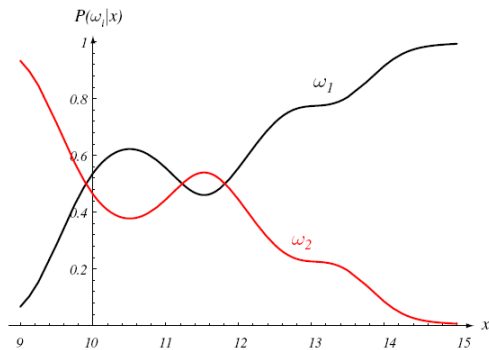
What is the average probability of error?

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

Bayes decision rule minimizes this error since

$$P(\text{error}|x) = \min[P(\omega_1|x), P(\omega_2|x)]$$

Bayes Decision Rule



MAP and MLE

Maximum a posteriori (MAP)

Decide ω_1 if $P(\omega_1|x) > P(\omega_2|x)$

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$$P(\omega_k|x) = \frac{p(x|\omega_k)P(\omega_k)}{p(x)} \quad \Downarrow \quad p(x) = \sum_{i=1}^2 p(x|\omega_i)P(\omega_i)$$

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Maximum Likelihood Estimation (MLE)

Decide ω_1 if $p(x|\omega_1)P(\omega_1) > p(x|\omega_2)P(\omega_2)$

$$\Downarrow \quad P(\omega_1) = P(\omega_2)$$

Decide ω_1 if $p(x|\omega_1) > p(x|\omega_2)$

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- more than one feature:
 - replacing the scalar x by the *feature vector* $\mathbf{x} \in \mathcal{R}^d$
- more than two states of nature
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- allowing actions other than just decision
 - allowing the possibility of rejection
- different risks for the decision
 - define how costly each action is

- Let \mathbf{x} be the d -dimensional random variable, called the **feature vector**

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- Let $\{\alpha_1, \dots, \alpha_a\}$ be the finite set of a possible **actions**
- Let $\lambda(\alpha_i|\omega_j)$ be the **loss** incurred for taking action α_i when the state of nature is ω_j

Bayesian Decision Theory

Posterior

- $P(\omega_i)$ is the prior probability when the state of nature is ω_i
- $p(x|\omega_i)$ is the class-conditional probability density function
- $P(\omega_i|x)$ is the posterior probability which can be computed by

$$P(\omega_k|x) = \frac{p(x|\omega_k)P(\omega_k)}{\sum_{i=1}^2 p(x|\omega_i)P(\omega_i)}$$

Conditional Risk

- Suppose we observe \mathbf{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

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

which is also called the **conditional risk**

Minimum Risk Classification

- The general **decision rule** $\alpha(\mathbf{x})$ tells us which action ($\alpha_i, i = 1, \dots, a$) to take for every possible observation
- 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 when $R(\alpha_i|\mathbf{x})$ is the minimum
- The resulting minimum overall risk is called the **Bayes risk** and is the best performance that can be achieved.

Binary-Class Case: Conditional risk

- α_1 : deciding ω_1
- α_2 : deciding ω_2
- $\lambda_{ij} = \lambda(\alpha_i|\omega_j)$:

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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 $i \neq j$

Conditional risk:

- $R(\alpha_1|\mathbf{x}) = \lambda_{11}P(\omega_1|\mathbf{x}) +$

Binary-Class Case: Conditional risk

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Conditional risk:

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

- α_1 : deciding ω_1
- α_2 : deciding ω_2
- $\lambda_{ij} = \lambda(\alpha_i|\omega_j)$

Minimum-risk decision rule:

$$\text{Decide } \begin{cases} \omega_1 & \text{if } R(\alpha_1|\mathbf{x}) < R(\alpha_2|\mathbf{x}) \\ \omega_2 & \text{otherwise} \end{cases}$$

This corresponds to

$$\begin{aligned} R(\alpha_1|\mathbf{x}) &< R(\alpha_2|\mathbf{x}) \\ \Rightarrow \lambda_{21} - \lambda_{11})P(\omega_1|\mathbf{x}) &> (\lambda_{12} - \lambda_{22})P(\omega_2|\mathbf{x}) \\ \Rightarrow \frac{p(\mathbf{x}|\omega_1)}{p(\mathbf{x}|\omega_2)} &= \frac{\lambda_{12} - \lambda_{22}}{\lambda_{21} - \lambda_{11}} \frac{P(\omega_2)}{P(\omega_1)} \end{aligned}$$

Likelihood Ratio

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

- the form of decision rule focuses on the \mathbf{x} -dependence of probability densities
- **likelihood ratio** exceeds a threshold value that is independent of the observation \mathbf{x}

Optimal decision property

If the likelihood ratio exceeds a threshold value independent of the input pattern \mathbf{x} , we can take optimal actions

Zero-One Loss

Recall: $\lambda_{ij} = \lambda(\alpha_i|\omega_j)$

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 $i \neq j$

- Define the **zero-one loss**

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

(all the errors are equally costly)

- Conditional risk becomes

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

Minimum Error Rate

$$R(\alpha_i|\mathbf{x}) = 1 - P(\omega_i|\mathbf{x})$$

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

Decide ω_i if $P(\omega_i|\mathbf{x}) > P(\omega_j|\mathbf{x}), \forall j \neq i$

- The resulting error is called the **Bayes error** and is the best performance that can be achieved

Example

Recall likelihood ratio

$$\frac{p(\mathbf{x}|\omega_1)}{p(\mathbf{x}|\omega_2)} = \frac{\lambda_{12} - \lambda_{22}}{\lambda_{21} - \lambda_{11}} \frac{P(\omega_2)}{P(\omega_1)} = \theta_\lambda \text{ then}$$

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- If Λ is the zero-one loss function,

$$\Lambda = \begin{pmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{pmatrix} =$$

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- If loss function penalizes misclassifying ω_2 as ω_1 more than the converse, say, 1.2 folds,

$$\Lambda =$$

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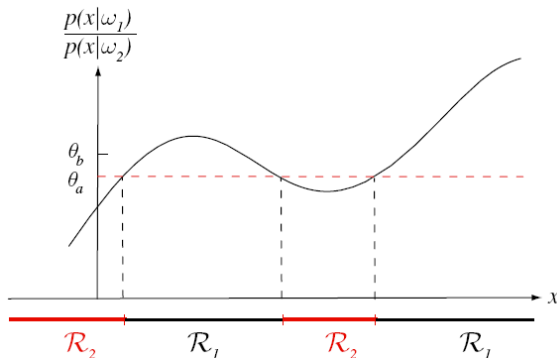
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$$\Lambda = \begin{pmatrix} 0 & 1.2 \\ 1 & 0 \end{pmatrix}, \quad \theta_\lambda = \frac{1.2P(\omega_2)}{P(\omega_1)} = \theta_b$$

Example

Table: A cost matrix.

	actual normal	actual cancer
predicted normal	$\lambda_{11} = 0$	$\lambda_{12} = 1.2$
predicted cancer	$\lambda_{21} = 1$	$\lambda_{22} = 0$



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Gaussian can be considered as a model where the feature vectors for a given class are continuous-valued, randomly corrupted versions of a single typical or prototype vector

Some properties of the Gaussian

- analytically tractable
- Completely specified by the 1st and 2nd moments
- A lot of processes are asymptotically Gaussian (Central Limit Theorem)
- Linear transformations of a Gaussian are also Gaussian
- Uncorrelatedness implies independence

Univariate Density

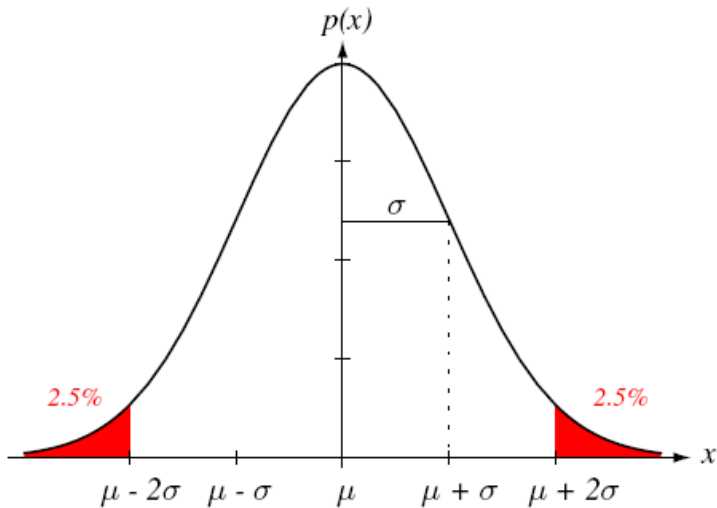
For $x \in \mathcal{R}$

$$\begin{aligned} p(x) &= \mathcal{N}(\mu, \sigma^2) \\ &= \frac{1}{\sqrt{2\pi}\sigma} \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] \end{aligned}$$

where

$$\begin{aligned} \mu &= E[x] = \int_{-\infty}^{\infty} xp(x)dx \\ \sigma^2 &= E[(x - \mu)^2] = \int_{-\infty}^{\infty} (x - \mu)^2 p(x)dx \end{aligned}$$

Univariate Density



Multivariate Density

For $\mathbf{x} \in \mathcal{R}^d$

$$\begin{aligned} p(\mathbf{x}) &= \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \\ &= \frac{1}{2\pi^{d/2}|\boldsymbol{\Sigma}|^{1/2}} \exp \left[-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}) \right] \end{aligned}$$

where

$$\begin{aligned} \boldsymbol{\mu} &= E[\mathbf{x}] = \int_{-\infty}^{\infty} \mathbf{x} p(\mathbf{x}) d\mathbf{x} \\ \boldsymbol{\Sigma} &= E[(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^\top] = \int_{-\infty}^{\infty} (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^\top p(\mathbf{x}) d\mathbf{x} \end{aligned}$$

statistically independent,

Multivariate Density

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statistically independent, $\sigma_{ij} = 0$

Linear Transformation

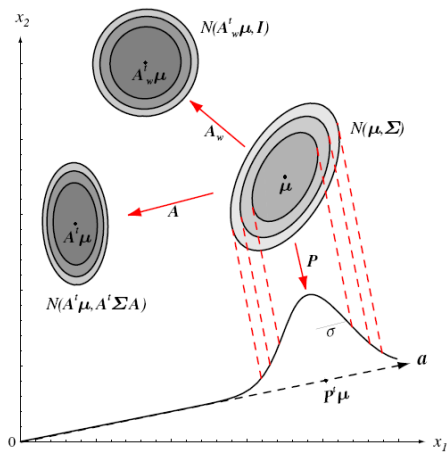
The linear transformation of a Gaussian is also Gaussian

- $p(\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$
- $\mathbf{z} = \mathbf{A}^\top \mathbf{x}, \mathbf{A} \in \mathcal{R}^{d \times k}$
- $p(\mathbf{z}) =$

Linear Transformation

The linear transformation of a Gaussian is also Gaussian

- $p(\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$
- $\mathbf{z} = \mathbf{A}^\top \mathbf{x}, \mathbf{A} \in \mathcal{R}^{d \times k}$
- $p(\mathbf{z}) = \mathcal{N}(\mathbf{A}^\top \boldsymbol{\mu}, \mathbf{A}^\top \boldsymbol{\Sigma} \mathbf{A})$



Projection onto a line

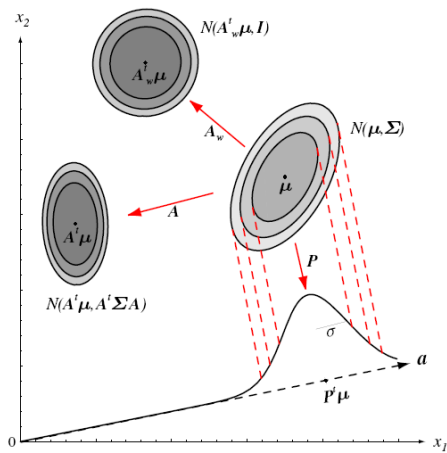
Remember $\mathbf{z} = \mathbf{P}^\top \mathbf{x}$, $\mathbf{P} \in \mathcal{R}^{d \times k}$

- if $k = 1$ and \mathbf{P} is a unit-length vector, \mathbf{a}
- then,

Projection onto a line

Remember $\mathbf{z} = \mathbf{P}^\top \mathbf{x}$, $\mathbf{P} \in \mathcal{R}^{d \times k}$

- if $k = 1$ and \mathbf{P} is a unit-length vector, \mathbf{a}
- then, $z = \mathbf{a}^\top \mathbf{x}$ is a scalar, representing a projection of \mathbf{x} onto a line in the direction \mathbf{a}



Whitening Transformation

Coordinate transformation

- arbitrarily Gaussian distribution \rightarrow a spherical one
- $p(\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \rightarrow p(\mathbf{z}) =$

Whitening Transformation

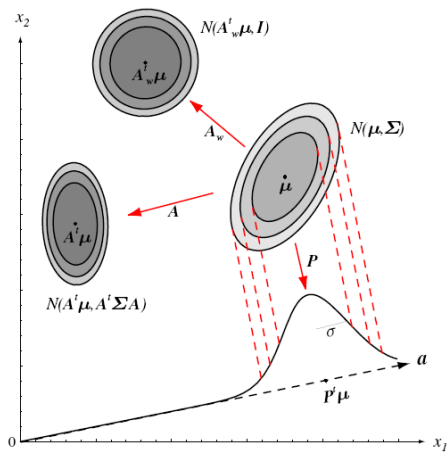
Coordinate transformation

- arbitrarily Gaussian distribution \rightarrow a spherical one
- $p(\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \rightarrow p(\mathbf{z}) = \mathcal{N}(\mathbf{A}_w^\top \boldsymbol{\mu}, \mathbf{I}_d)$
- finding \mathbf{A}_w

Whitening Transformation

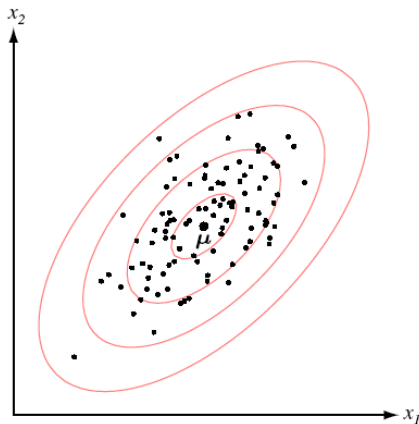
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- finding \mathbf{A}_w
 - $\mathbf{A}_w^\top \boldsymbol{\Sigma} \mathbf{A}_w = \mathbf{I}_d$
 - $\boldsymbol{\Sigma} = \mathbf{U} \boldsymbol{\Lambda} \mathbf{U}^\top$
 - $\mathbf{A}_w = \mathbf{U} \boldsymbol{\Lambda}^{-1/2}$



Cloud

- cluster
- position: mean
- shape: covariance matrix
- # parameters:
 $d + d(d - 1)/2$



Mahalanobis distance

- the shape of data points with equal density is a hyperellipsoid (locus of points of constant density)
- principle axes of hyperellipsoids:

Mahalanobis distance

- the shape of data points with equal density is a hyperellipsoid (locus of points of constant density)
- principle axes of hyperellipsoids: eigenvector of Σ
- distance for \mathbf{x} to μ : $r^2 = (\mathbf{x} - \mu)^\top \Sigma^{-1} (\mathbf{x} - \mu)$, called squared **Mahalanobis distance**
 - determining similarity of an unknown sample set to a known one
 - scale-invariant, i.e. not dependent on the scale of measurements
 - dissimilarity measure between two random vectors with covariance matrix Σ : $(\mathbf{x}_1 - \mathbf{x}_2)^\top \Sigma^{-1} (\mathbf{x}_1 - \mathbf{x}_2)$
 - $\Sigma = \mathbf{I}$, Euclidean distance
 - $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_d)$, **normalized Euclidean distance**

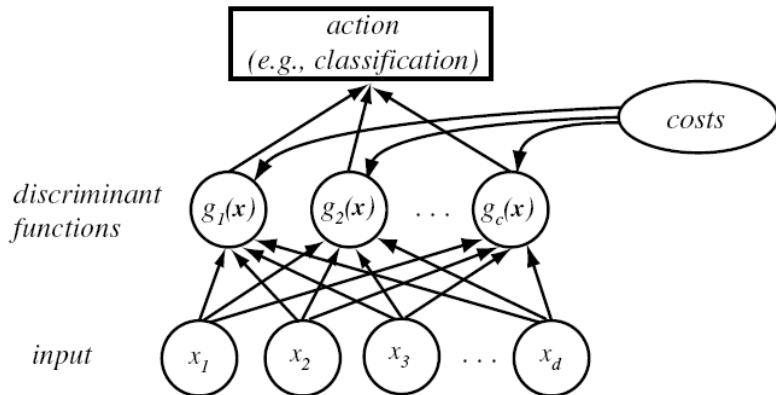
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- A useful way of representing classifiers is through discriminant functions $g_i(\mathbf{x})$, $i = 1, \dots, c$, where the classifier assigns a feature vector \mathbf{x} to class ω_i if

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

or

$$\mathbf{x} \in \omega_m \text{ if and only if } g_m(\mathbf{x}) = \arg \max_{i=1, \dots, c} \{g_i(\mathbf{x})\}$$



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- For the classifier that minimizes **error**

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

- These functions divide the feature space into c **decision regions**, $\mathcal{R}_1, \mathcal{R}_2, \dots, \mathcal{R}_c$, separated by **decision boundaries**
- the choice of discriminant function is not unique
 - multiplicative or additive operations without influencing the decision
 - with a monotonically increasing function $f(\cdot)$, replacing $g_i(\mathbf{x})$ by $f(g_i(\mathbf{x}))$, i.e.,

$$\begin{aligned} g_i(\mathbf{x}) &= p(\mathbf{x}|\omega_i)P(\omega_i) \Rightarrow \\ \ln g_i(\mathbf{x}) &= \ln p(\mathbf{x}|\omega_i) + \ln P(\omega_i) \end{aligned}$$

- This may lead to significant analytical and computational simplifications

Example for the Two-category case

- special case of multi-category case, dichotomizer
- discriminant function:

$$g(\mathbf{x}) \equiv g_1(\mathbf{x}) - g_2(\mathbf{x})$$
$$\omega = \begin{cases} \omega_1, & \text{if } g(x) > 0 \\ \omega_2, & \text{otherwise} \end{cases}$$

- for minimum-error-rate discriminant function,

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

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- Recall that the **minimum error-rate classification** can be achieved by the discriminant function

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

- For multivariate normal density, $p(\mathbf{x}|\omega_i) \sim \mathcal{N}(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$
- so we can have

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

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Linear Discriminant Function (1)

- features are statistically independent
- each feature has the same variance, σ^2
- Recall that the discriminant functions

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

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$$\begin{aligned} g_i(\mathbf{x}) &= -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_i)^\top \boldsymbol{\Sigma}_i^{-1}(\mathbf{x} - \boldsymbol{\mu}_i) - \frac{d}{2} \ln 2\pi - \frac{1}{2} \ln |\boldsymbol{\Sigma}_i| + \ln P(\omega_i) \\ &\Rightarrow -\frac{\|\mathbf{x} - \boldsymbol{\mu}_i\|^2}{2\sigma^2} + \ln P(\omega_i) \end{aligned}$$

where $\|\cdot\|$ denotes the Euclidean norm, i.e.,

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

Linear Discriminant Function (2)

- \mathbf{x} equal distance to mean, optimal decision by a priori
- otherwise, not necessary to compute distance

$$\begin{aligned} g_i(\mathbf{x}) &= -\frac{\|\mathbf{x} - \boldsymbol{\mu}_i\|^2}{2\sigma^2} + \ln P(\omega_i) \\ &= -\frac{1}{2\sigma^2} [\mathbf{x}^\top \mathbf{x} - 2\boldsymbol{\mu}_i^\top \mathbf{x} + \boldsymbol{\mu}_i^\top \boldsymbol{\mu}_i] + \ln P(\omega_i) \\ &\propto -\frac{1}{2\sigma^2} [-2\boldsymbol{\mu}_i^\top \mathbf{x} + \boldsymbol{\mu}_i^\top \boldsymbol{\mu}_i] + \ln P(\omega_i) \\ &= \mathbf{w}_i^\top \mathbf{x} + w_{i0} \end{aligned}$$

where $\mathbf{w}_i = \frac{\boldsymbol{\mu}_i}{\sigma^2}$ and $w_{i0} = -\frac{1}{2\sigma^2} \boldsymbol{\mu}_i^\top \boldsymbol{\mu}_i + \ln P(\omega_i)$

Linear Machine (1)

- A classifier that uses linear discriminant functions is called a **linear machine**
- decision surfaces $\mathcal{R}_i, \mathcal{R}_j$ are pieces of hyperplanes defined by

$$g_i(\mathbf{x}) \equiv g_j(\mathbf{x}) \Rightarrow \mathbf{w}^\top (\mathbf{x} - \mathbf{x}_0) = 0$$

$$\text{where } \begin{cases} \mathbf{w} = \mu_i - \mu_j \\ \mathbf{x}_0 = \frac{1}{2}(\mu_i + \mu_j) - \frac{\sigma^2}{\|\mu_i - \mu_j\|^2} \ln \frac{P(\omega_i)}{P(\omega_j)} (\mu_i - \mu_j) \end{cases}$$

Decision hyperplane

- separating \mathcal{R}_i and \mathcal{R}_j
- through the point \mathbf{x}_0
- orthogonal to $\mathbf{w} = \mu_i - \mu_j$ and so

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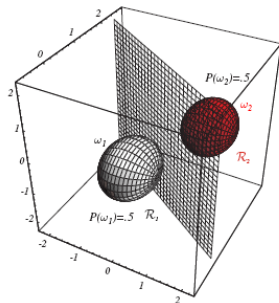
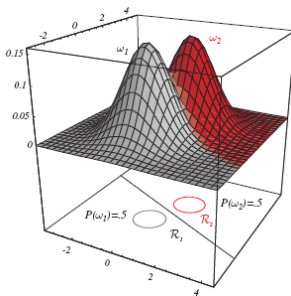
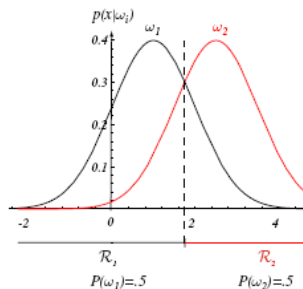
$$\text{where } \begin{cases} \mathbf{w} = \mu_i - \mu_j \\ \mathbf{x}_0 = \frac{1}{2}(\mu_i + \mu_j) - \frac{\sigma^2}{\|\mu_i - \mu_j\|^2} \ln \frac{P(\omega_i)}{P(\omega_j)} (\mu_i - \mu_j) \end{cases}$$

Decision hyperplane

- separating \mathcal{R}_i and \mathcal{R}_j
- through the point \mathbf{x}_0
- orthogonal to $\mathbf{w} = \mu_i - \mu_j$ and so orthogonal to the line linking the means

Equal Prior

$P(\omega_i) = P(\omega_j)$, the point \mathbf{x}_0 is halfway between the means, and the hyperplane is the perpendicular bisector of the line between the means



Equal Priors for multiple classes

If the priors are the same for all c classes, the $\ln P(\omega_i)$ term becomes unimportant constant

minimum-distance classifier

- measure the Euclidean distance $d_i = \|\mathbf{x} - \boldsymbol{\mu}_i\|$
- $\mathbf{x} \in \omega_m, d_m = \arg \min_{i=1, \dots, c} d_i$

If mean as ideal prototype or template, **template-matching**

Unequal Prior

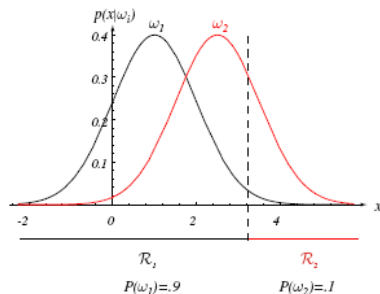
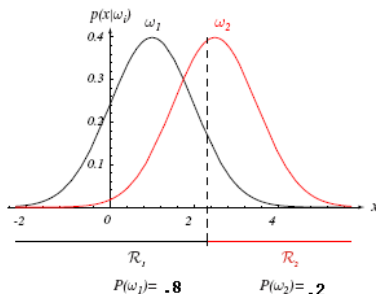
$$g_i(\mathbf{x}) \equiv g_j(\mathbf{x}) \Rightarrow \mathbf{w}^\top (\mathbf{x} - \mathbf{x}_0) = 0$$

$$\text{where } \begin{cases} \mathbf{w} = \boldsymbol{\mu}_i - \boldsymbol{\mu}_j \\ \mathbf{x}_0 = \frac{1}{2}(\boldsymbol{\mu}_i + \boldsymbol{\mu}_j) - \frac{\sigma^2}{\|\boldsymbol{\mu}_i - \boldsymbol{\mu}_j\|^2} \ln \frac{P(\omega_i)}{P(\omega_j)} (\boldsymbol{\mu}_i - \boldsymbol{\mu}_j) \end{cases}$$

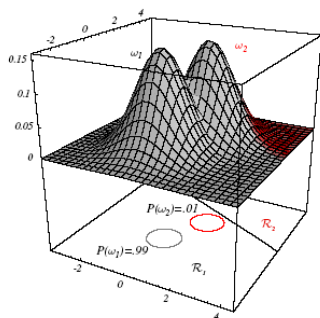
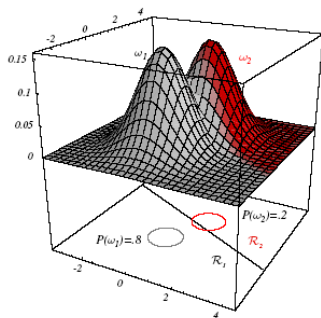
$$P(\omega_i) \neq P(\omega_j)$$

- the point \mathbf{x}_0 shifts away from the more likely mean
- if $\frac{\sigma^2}{\|\boldsymbol{\mu}_i - \boldsymbol{\mu}_j\|^2}$ is small, the position of the decision boundary is relatively insensitive to the exact values of the prior probability

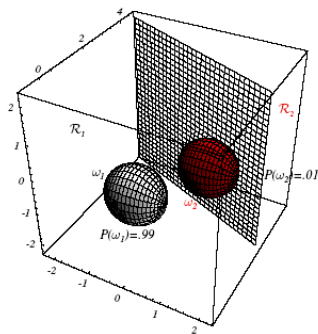
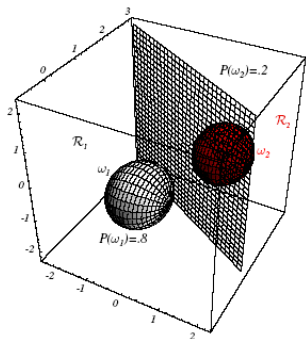
Unequal Prior (1-d)



Unequal Prior (2-d)



Unequal Prior (3-d)



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Linear discriminant

Common covariance matrix, i.e., $\Sigma_1 = \cdots = \Sigma_c = \Sigma$

Discriminant function is

$$\begin{aligned} g_i(\mathbf{x}) &= -\frac{1}{2}(\mathbf{x} - \mu_i)^\top \Sigma^{-1}(\mathbf{x} - \mu_i) + \ln P(\omega_i) \\ &= -\frac{1}{2}\mathbf{x}^\top \Sigma^{-1}\mathbf{x} + \mu_i^\top \Sigma^{-1}\mathbf{x} - \frac{1}{2}\mu_i^\top \Sigma^{-1}\mu_i + \ln P(\omega_i) \\ &\propto \mu_i^\top \Sigma^{-1}\mathbf{x} - \frac{1}{2}\mu_i^\top \Sigma^{-1}\mu_i + \ln P(\omega_i) \\ &= \mathbf{w}_i^\top \mathbf{x} + w_{i0} \end{aligned}$$

where $\mathbf{w}_i = \Sigma^{-1}\mu_i$ and $w_{i0} = -\frac{1}{2}\mu_i^\top \Sigma^{-1}\mu_i + \ln P(\omega_i)$

Decision boundary (1)

If \mathcal{R}_i and \mathcal{R}_j are continuous, we have

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

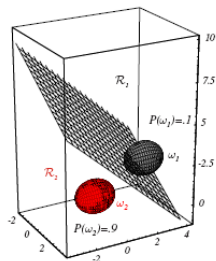
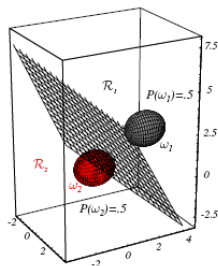
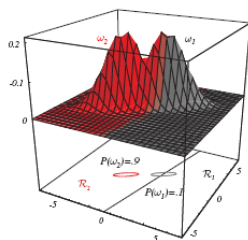
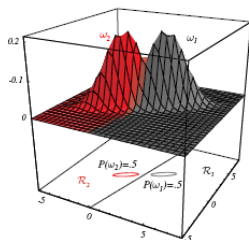
where

$$\mathbf{w} = \mathbf{\Sigma}^{-1}(\mu_i - \mu_j)$$

$$\mathbf{x}_0 = \frac{1}{2}(\mu_i + \mu_j) - \frac{\ln(P(\omega_i)/P(\omega_j))}{(\mu_i - \mu_j)^\top \mathbf{\Sigma}^{-1}(\mu_i - \mu_j)}(\mu_i - \mu_j)$$

the hyperplane passes through \mathbf{x}_0 but is necessarily not orthogonal to the line between the means

Decision boundary (2)



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Discriminant function

$$\begin{aligned} g_i(\mathbf{x}) &= -(\mathbf{x} - \boldsymbol{\mu}_i)^\top \boldsymbol{\Sigma}_i^{-1} (\mathbf{x} - \boldsymbol{\mu}_i) + \ln P(\omega_i) \\ &= -\frac{1}{2} \mathbf{x}^\top \boldsymbol{\Sigma}_i^{-1} \mathbf{x} + \boldsymbol{\mu}_i^\top \boldsymbol{\Sigma}_i^{-1} \mathbf{x} - \frac{1}{2} \boldsymbol{\mu}_i^\top \boldsymbol{\Sigma}_i^{-1} \boldsymbol{\mu}_i + \ln P(\omega_i) \\ &= \mathbf{x}^\top \mathbf{W}_i \mathbf{x} + \mathbf{w}_i^\top \mathbf{x} + w_{i0} \end{aligned}$$

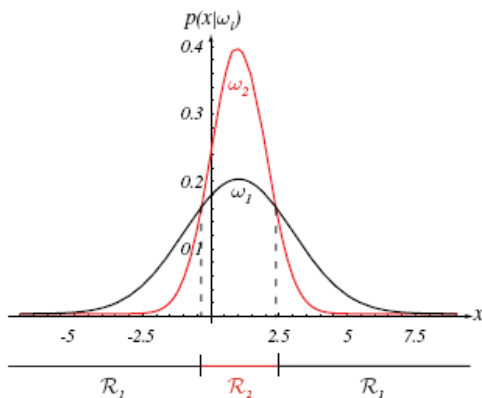
where

$$\begin{aligned} \mathbf{W}_i &= -\frac{1}{2} \boldsymbol{\Sigma}_i^{-1}, \quad \mathbf{w}_i = \boldsymbol{\Sigma}_i^{-1} \boldsymbol{\mu}_i \\ w_{i0} &= -\frac{1}{2} \boldsymbol{\mu}_i^\top \boldsymbol{\Sigma}_i^{-1} \boldsymbol{\mu}_i - \frac{1}{2} \ln |\boldsymbol{\Sigma}_i| + \ln P(\omega_i) \end{aligned}$$

g_i is **quadratic discriminant**

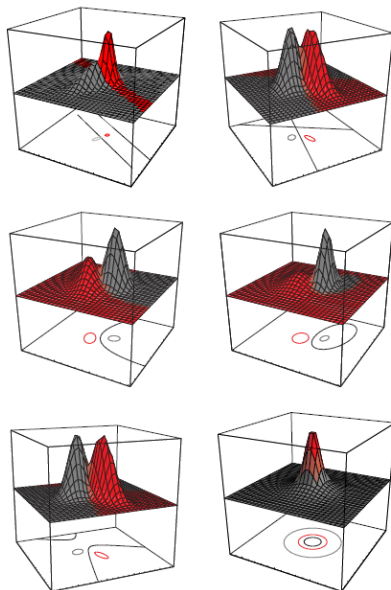
Decision boundary are hyperquadrics,

Decision boundary (1-d)

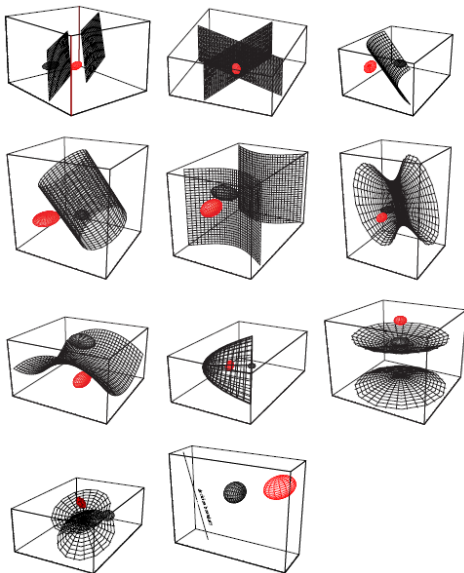


Equal prior

Decision boundary (2-d)



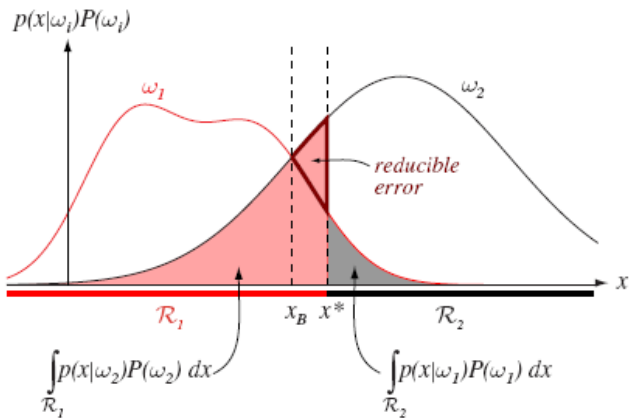
Decision boundary (3-d)



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- For binary classification

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



- For multcategory classification

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

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- 7 Error Probabilities
- 8 Receiver Operating Characteristic (ROC)

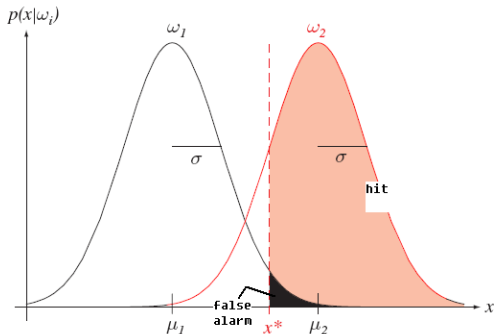
History

The ROC curve

- was first developed by electrical engineers and radar engineers during World War II for detecting enemy objects in battle fields, also known as the **signal detection theory**
 - ω_1 : object is not present (negative), e.g., detecting a weak pulse
 - ω_2 : object is present (positive)
- was soon introduced in psychology to account for perceptual detection of signals
- has been widely used in medicine, radiology, and other areas for many decades

An Example

- A detector to detect whether there is an external signal (pulse) denoted by a signal x
- x is a random variable due to the random noise within and outside the detector itself
 - ω_1 : when the signal is not present (negative), $p(x|\omega_1) = \mathcal{N}(\mu_1, \sigma^2)$
 - ω_2 : when the signal is present (positive), $p(x|\omega_2) = \mathcal{N}(\mu_2, \sigma^2)$



discriminability:

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

Confusion matrix

		Predicted		Total
		ω_1	ω_2	
State of	ω_1	correct rejection (true negative) $P(\mathbf{x} < \mathbf{x}^* \mathbf{x} \in \omega_1)$	false alarm (false positive) $P(\mathbf{x} > \mathbf{x}^* \mathbf{x} \in \omega_1)$	N
Nature	ω_2	miss (false negative) $P(\mathbf{x} < \mathbf{x}^* \mathbf{x} \in \omega_2)$	hit (true positive) $P(\mathbf{x} > \mathbf{x}^* \mathbf{x} \in \omega_2)$	P

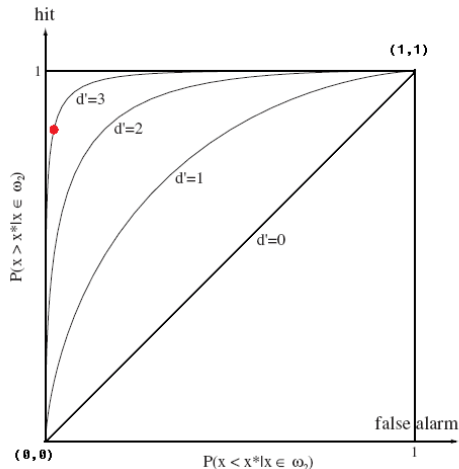
- **true positive rate, TPR** (hit rate, recall, sensitivity): $\frac{TP}{FN+TP}$, which determines a classifier or a diagnostic test performance on classifying positive instances correctly among all positive samples available during the test
- **false positive rate, FPR** (false alarm, 1 – sensitivity): $\frac{FP}{TN+FP}$, which defines how many incorrect positive results occur among all negative samples available during the test

ROC

- only TPR and FPR are needed to draw an ROC curve
- fixed density, i.e.,

ROC

- only TPR and FPR are needed to draw an ROC curve
- fixed density, i.e., d'
- changeable x^*

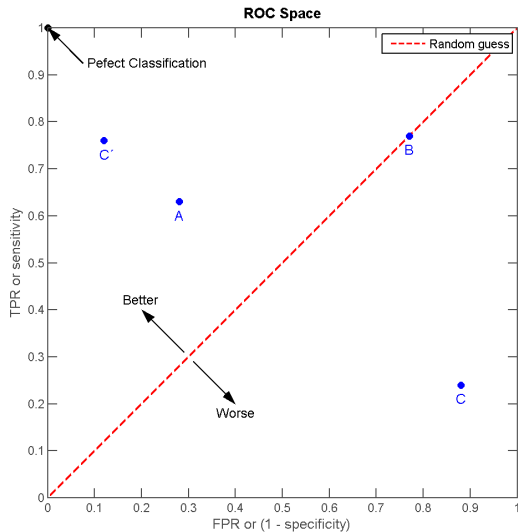


Example

- four prediction results from 100 positive and 100 negative instances
- C' is the mirror of C across the center point (0.5, 0.5)

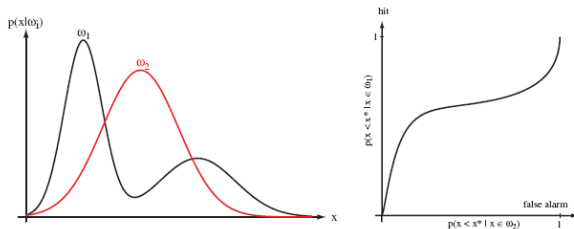
A				B				C				C'			
TP=63	FP=28	91		TP=77	FP=77	154		TP=24	FP=88	112		TP=76	FP=12	88	
FN=37	TN=72	109		FN=23	TN=23	46		FN=76	TN=12	88		FN=24	TN=88	112	
100	100	200		100	100	200		100	100	200		100	100	200	
TPR = 0.63				TPR = 0.77				TPR = 0.24				TPR = 0.76			
FPR = 0.28				FPR = 0.77				FPR = 0.88				FPR = 0.12			
ACC = 0.68				ACC = 0.50				ACC = 0.18				ACC = 0.82			

Example



Extension

to non-Gaussian assumption



- ROC analysis provides tools to select possibly optimal models