# Classification

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# Overview

1. Classification (2.5 hours)
2. Clustering (1.5 hours)
3. Practical sessions (1 hour)

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- Understand what is a classification problem and when it can be applied.
- Being able to reason about new models and derive learning algorithms.
- **Being able to learn more by yourself!**

# Outline


1. What is classification?
2. Decision theory
3. Generative classifiers
4. Discriminative classifiers
5. Summary
6. Exercises

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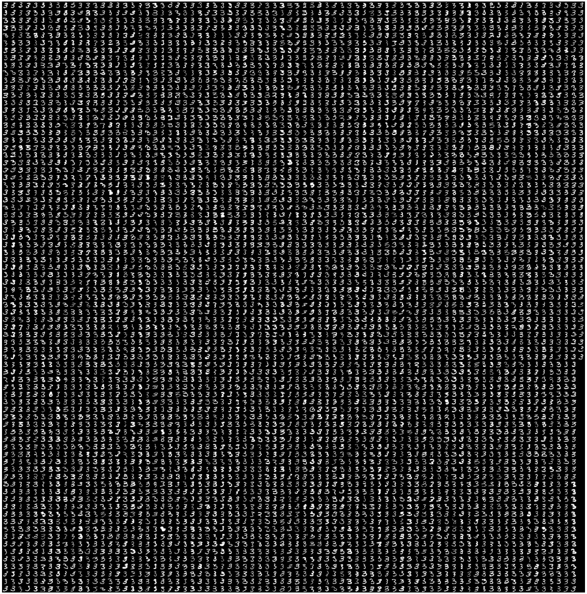
# A first example: digit classification



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Can we learn $f : \boldsymbol{x} \mapsto f(\boldsymbol{x}) = t$?

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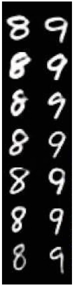

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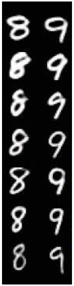

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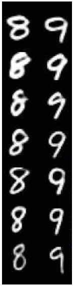


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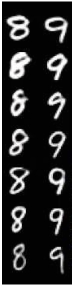

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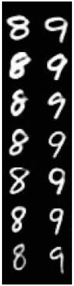

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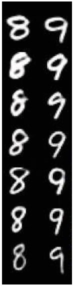

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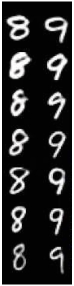

We would like to distinguish digit 8 from digit 9:

$$f(\boldsymbol{x}) = \mathrm{sign}(y(\boldsymbol{x})) = \begin{cases} +1 & \text{if } y(\boldsymbol{x}) > 0, \\ -1 & \text{if } y(\boldsymbol{x}) < 0. \end{cases}$$

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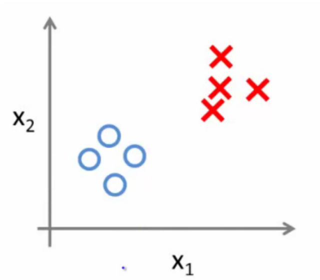
# Linear discriminant function (aka linear classifier)




We assume the instances can be separated by a linear subspace (or hyperplane):

$$y(\boldsymbol{x}) = \boldsymbol{w}^\top \boldsymbol{x} + b, \quad f_{\mathrm{LIN}}(\boldsymbol{x}) = \mathrm{sign}(y(\boldsymbol{x})),$$

where $\boldsymbol{w} \in \mathbb{R}^d \setminus \{\mathbf{0}\}$, $b \in \mathbb{R}$.

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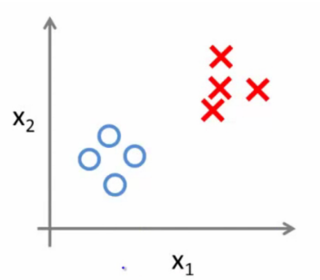


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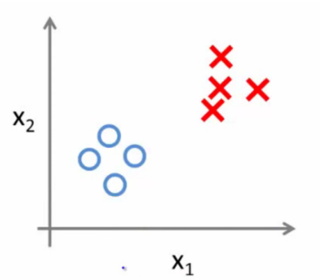


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- The decision boundary is the set $\{\boldsymbol{x} : y(\boldsymbol{x}) = 0\}$.
- Learning is to find $\boldsymbol{w}$ and $b$ such that $\forall i : f_{\mathrm{LIN}}(\boldsymbol{x}_i) \approx t_i$.

# Relation to nearest neighbour classification?

$$
\begin{aligned}
& \|\boldsymbol{x}_* - \boldsymbol{w}_{+1}\| < \|\boldsymbol{x}_* - \boldsymbol{w}_{-1}\| \quad \Leftrightarrow \quad \|\boldsymbol{x}_* - \boldsymbol{w}_{+1}\|^2 < \|\boldsymbol{x}_* - \boldsymbol{w}_{-1}\|^2 \\
\Leftrightarrow \; & \|\boldsymbol{x}_*\|^2 - 2\boldsymbol{w}_{+1}^T \boldsymbol{x}_* + \|\boldsymbol{w}_{+1}\|^2 < \|\boldsymbol{x}_*\|^2 - 2\boldsymbol{w}_{-1}^T \boldsymbol{x}_* + \|\boldsymbol{w}_{-1}\|^2 \\
\Leftrightarrow \; & \boldsymbol{w}_{+1}^T \boldsymbol{x}_* - \|\boldsymbol{w}_{+1}\|^2/2 > \boldsymbol{w}_{-1}^T \boldsymbol{x}_* - \|\boldsymbol{w}_{-1}\|^2/2 \\
\Leftrightarrow \; & (\boldsymbol{w}_{+1} - \boldsymbol{w}_{-1})^T \boldsymbol{x}_* + \frac{1}{2}\left(\|\boldsymbol{w}_{-1}\|^2 - \|\boldsymbol{w}_{+1}\|^2\right) > 0.
\end{aligned}
$$

# How can we picture a linear discriminant function?

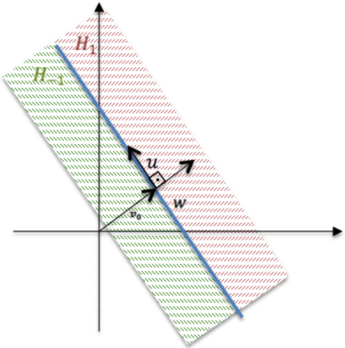


Figure 2.6: Separating hyperplane in $\mathbb{R}^2$. The decision boundary (blue) is defined by the normal vector $\boldsymbol{w}$ and an offset $b \in \mathbb{R}$. $\boldsymbol{v}_0$ is a point on the hyperplane, obtained by orthogonal projection of the origin. The plane separates $\mathbb{R}^2$ into two halfspaces $\mathcal{H}_{+1}$ $(\boldsymbol{w}^T\boldsymbol{x} + b > 0)$ and $\mathcal{H}_{-1}$ $(\boldsymbol{w}^T\boldsymbol{x} + b < 0)$, the decision regions of the corresponding linear discriminant.

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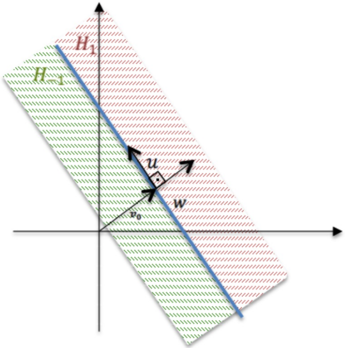


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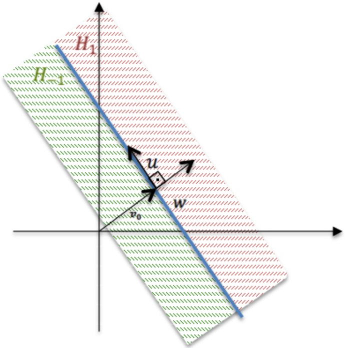


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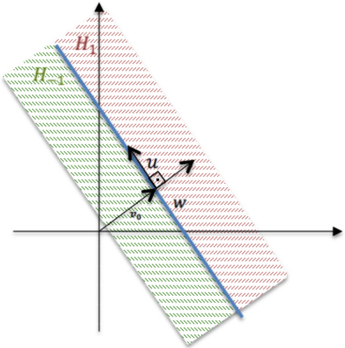


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- We restrict weight vectors to be unit norm: $\{\boldsymbol{w} : \|\boldsymbol{w}\| = 1\}$.

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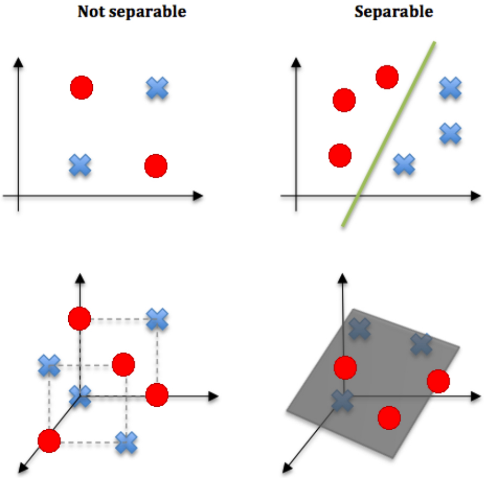

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Example: linear classifier with quadratic features

$$\phi(\boldsymbol{x}) = \begin{bmatrix} x_1 \\ \vdots \\ x_d \\ x_1 x_1 \\ \vdots \\ x_1 x_d \\ x_2 x_2 \\ \vdots \\ x_2 x_d \\ \vdots \\ x_d x_d \end{bmatrix} \in \mathbb{R}^{d(d+3)/2}. \qquad y(x) = \boldsymbol{w}^\top \phi(\boldsymbol{x}) + b = \sum_j w_j x_j + \sum_j \sum_{k \leqslant j} w_{jk} x_j x_k + b$$

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- If the data is not linearly separable, then the perceptron will not converge :-(

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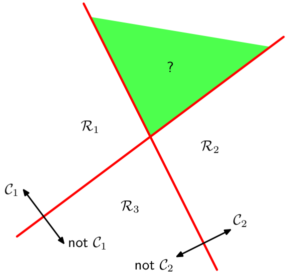

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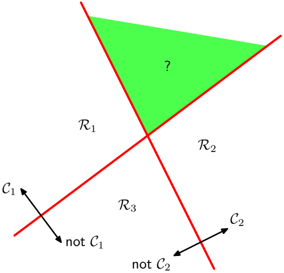


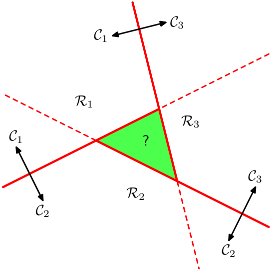

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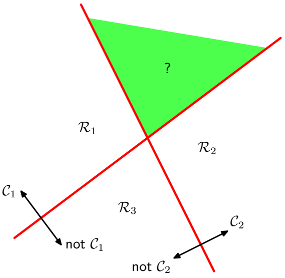


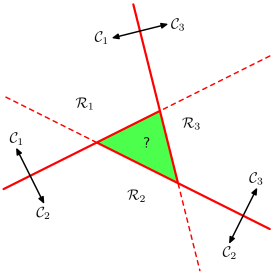


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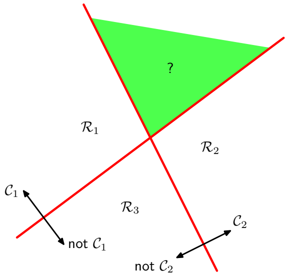


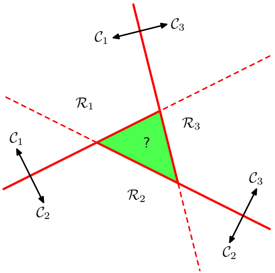


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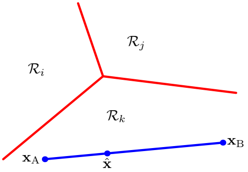


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# Outline


1. What is classification?
2. Decision theory
3. Generative classifiers
4. Discriminative classifiers
5. Summary
6. Exercises

# Bayes' rule

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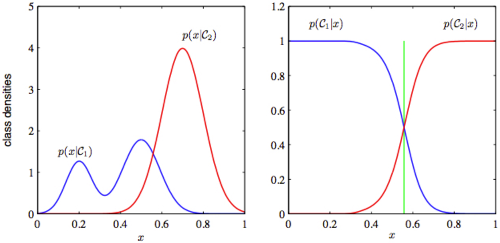
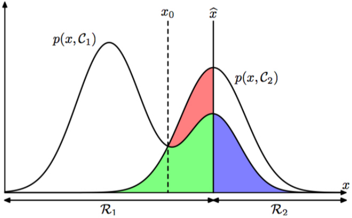



$$P(C_1) = P(t = -1),$$
$$P(C_1|x) = P(t = -1|x),$$
$$p(x, C_1) = p(x, t = -1).$$

# Minimising the classification error

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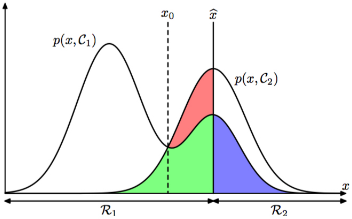


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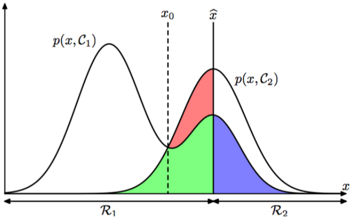


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$$P(\mathrm{error}) = P(x \in \mathcal{R}_1, C_2) + P(x \in \mathcal{R}_2, C_1),$$

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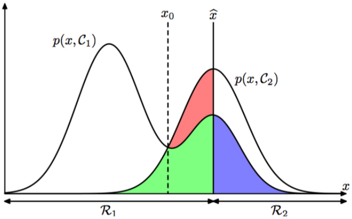


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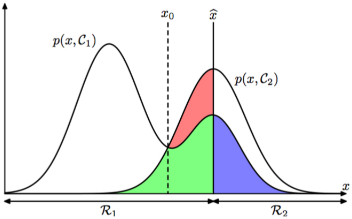


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- Bayes error at $x = x_0$: blue+green area.

# Example of a Bayes optimal classifier

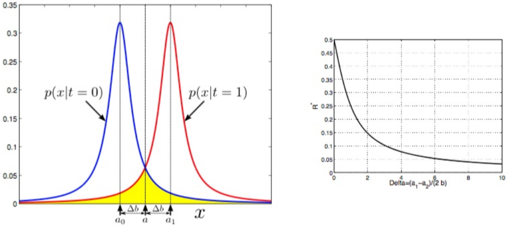
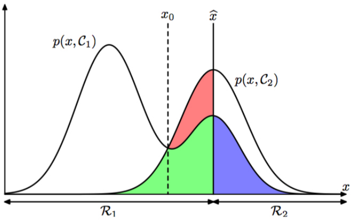



Figure 5.5: Bayes-optimal classifier and Bayes error for two class-conditional Cauchy distributions, centered at $a_0$ and $a_1$. The optimal rule thresholds at the midpoint $a = (a_0 + a_1)/2$. Since the class prior is $P(t = 0) = P(t = 1) = 1/2$, the Bayes error $R^*$ is twice the yellow area. Right plot show $R^*$ as function of separation parameter $\Delta$. The slow decay of $R^*$ is due to the very heavy tails of the Cauchy distributions.

# Precision and recall




| | $t = 1$ | $t = -1$ |
|---|---|---|
| $x > x_0$ | $TP$ | $FP$ |
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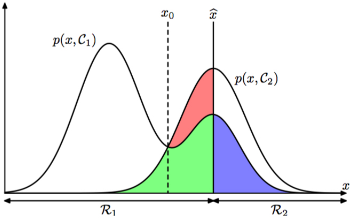


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- The precision is the proportion of positives in the instances classified as being positive:

$$P(x) = \frac{TP(x)}{TP(x) + FP(x)},$$

where $TP$ are the true positives and $FP$ the false positives.

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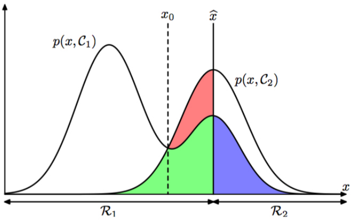


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where $FN$ are the false negatives.

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In a hospital, a tissue sample is taken from a patient, giving rise to an input vector $\boldsymbol{x}$. A classifier $f(\boldsymbol{x})$ is to predict whether the patient has cancer ($t = 1$) or not ($t = -1$). Is the cost of predicting that the patient has cancer while he/she has not the same, as predicting that the patient has not contracted cancer while he/she has the disease?

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Let us define a loss function, which assigns a unique loss to every decision we could take:

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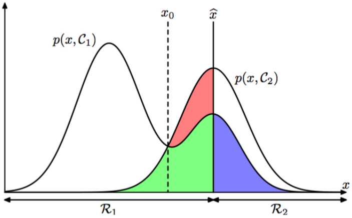
The expected loss is given by

$$\mathbb{E}(L) = \sum_k \sum_l \int_{x \in \mathcal{R}_l} L_{kl}\, p(x, C_k) dx.$$

# How can we make a trade-off?

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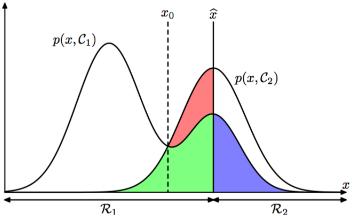


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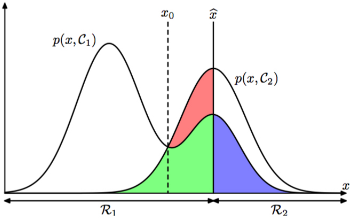


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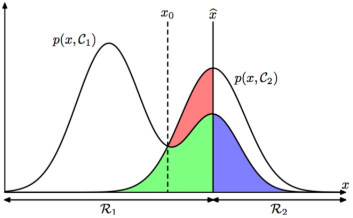


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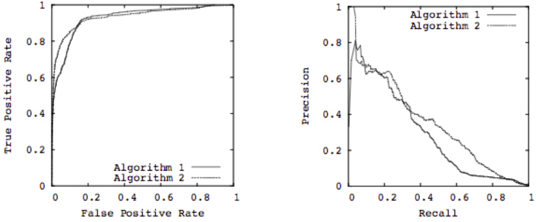


(a) Comparison in ROC space

(b) Comparison in PR space

- AUC enables us to compare classifiers irrespective of the decision threshold.

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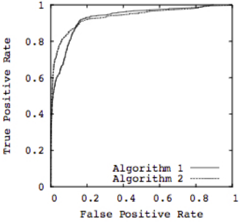


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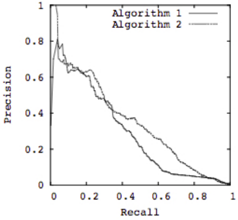


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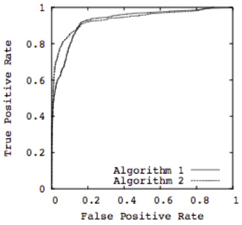


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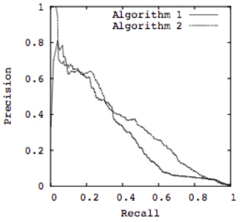


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- Precision-recall:
  - Non-monotonic
  - One to one mapping with ROC

# How do we measure the performance in multi-class classification?

- Confusion matrix:

| | $t=1$ | $t=2$ | $t=3$ |
|---|---|---|---|
| $f(\boldsymbol{x})=1$ | $c_{11}$ | $c_{12}$ | $c_{13}$ |
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- What are the expressions of precision and recall?

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# Generative classifiers

Consider the data set $\mathcal{D} = \{(\boldsymbol{x}_i, t_i) | i = 1, \ldots, n\}$. We are interested in the **posterior class probability**:

$$P(t = k|\boldsymbol{x}) = \frac{\overbrace{p(\boldsymbol{x}|t = k)}^{\text{class}-\text{conditional density}} \overbrace{P(t = k)}^{\text{class prior}}}{p(\boldsymbol{x})}, \qquad k = \{1, \ldots, m\}.$$

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$$\arg\max_{\boldsymbol{\theta}} \; \ln \prod_i p(t_i|\boldsymbol{\theta}) \quad \text{(maximum likelihood estimation)}$$

where $p(t_i|\boldsymbol{\theta}) = \mathrm{Categorical}\left(\pi_1 \mathrm{Gaussian}\left(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1\right), \dots, \pi_m \mathrm{Gaussian}\left(\boldsymbol{\mu}_m, \boldsymbol{\Sigma}_m\right)\right)$.

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- Discrete features: $p(\boldsymbol{x}|t = k) = \mathrm{Multinomial}\left(\boldsymbol{\mu}_k\right)$.

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# Definitions

Multivariate Gaussian probability density:

$$\boldsymbol{x} \sim \mathrm{Gaussian}\left(\boldsymbol{\mu}, \boldsymbol{\Sigma}\right) = \frac{1}{(2\pi)^{D/2}|\boldsymbol{\Sigma}|^{1/2}} e^{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})}.$$

Multinomial probability distribution:

$$\boldsymbol{x} \sim \mathrm{Multinomial}\left(\boldsymbol{\mu}\right) = \frac{(\sum_j x_j)!}{\prod_j x_j!} \prod_{j=1}^{d} \mu_j^{x_j}.$$

Categorical probability distribution:

$$t \sim \mathrm{Categorical}\left(\boldsymbol{p}\right) = \prod_{k=1}^{m} p_k^{\delta_k(t)},$$

where $\delta_z(\cdot)$ is the kronecker delta centred at $z$.

# Binary classification

$$P(t=1|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|t=1)P(t=1)}{\sum_k p(\boldsymbol{x}|t=k)P(t=k)}$$

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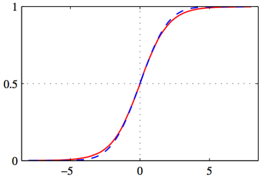


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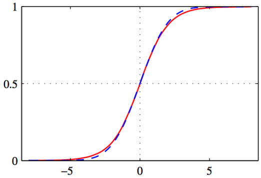


Sigmoid: $\sigma(z) = \frac{1}{1+\exp(-z)}$.

Let $\alpha \in [0,1]$. The classifier is defined as follows:

$$f(\boldsymbol{x}) = \begin{cases} +1 & \text{if } P(t=1|\boldsymbol{x}) > \alpha, \\ -1 & \text{if } P(t=1|\boldsymbol{x}) < \alpha. \end{cases}$$

# Binary classification with continuous features

- The classifier is defined by the following priors and class-conditionals:

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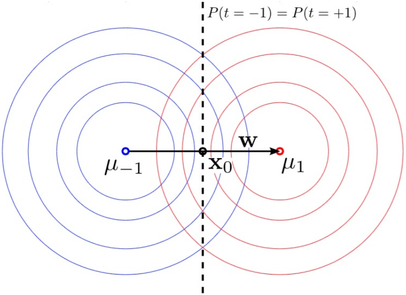

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where $p(\boldsymbol{\theta}) = \mathrm{Dirichlet}\,(\alpha \mathbf{1})$:

- Parameter $\alpha$ can be interpreted as a pseudo-count. $(\star)$
- Adding a prior is equivalent to regularisation.

# Naive Bayes classifier

- Generative classifier making the simplifying assumption that features are independent given the class:

$$P(t = k|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|t = k)P(t = k)}{p(\boldsymbol{x})} \approx \frac{\prod_{j=1}^{d} p(x_j|t = k)P(t = k)}{p(\boldsymbol{x})}.$$

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Tue Aug 1, 2006 3:20am ET

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- $\boldsymbol{x}_i$ represents document $i$; it contains the word counts.

# Maximum likelihood (ML) estimation: summary

The likelihood is the joint probability of observing i.i.d. data:

$$\ell(\boldsymbol{\theta}; \boldsymbol{t}) = \ln p(\boldsymbol{t}; \boldsymbol{\theta}) = \ln \prod_{i=1}^{n} p(t_i; \boldsymbol{\theta}).$$

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The goal is to find the parameters that maximise the log-likelihood function:

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \ell(\boldsymbol{\theta}; \boldsymbol{t}).$$

- ML leads to a point estimate of $\boldsymbol{\theta}$ and is asymptotically consistent.
- The likelihood is unbounded, so ML estimator can overfit!

# Maximum a posteriori (MAP) estimation: summary

Penalise unreasonable values ($\sim$ regularisation) by imposing a prior distribution on the parameters:

$$p(\boldsymbol{\theta}|\boldsymbol{X}) \propto p(\boldsymbol{X}|\boldsymbol{\theta})p(\boldsymbol{\theta}).$$

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- MAP leads to a point estimate of $\boldsymbol{\theta}$ and asymptotically agrees with ML estimate.
- MAP is not invariant under reparametrisation!

# Outline


1. What is classification?
2. Decision theory
3. Generative classifiers
4. Discriminative classifiers
5. Summary
6. Exercises

# Generative versus discriminative classification

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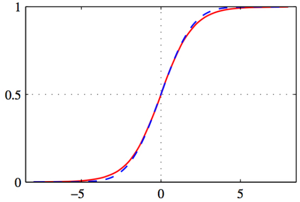
- Discriminative classifier:

$$P(t=k|\boldsymbol{x}) = \sigma(y(\boldsymbol{x};\boldsymbol{\theta}))$$

  - Does not rely on class-conditionals
  - Less parameters to learn (or optimise)
  - Easy to change the feature map $\phi(\boldsymbol{x})$

# (Binary) logistic regression




- Linear discriminant: $y(\boldsymbol{x}) = \boldsymbol{w}^\top \phi(\boldsymbol{x}) + b$ .

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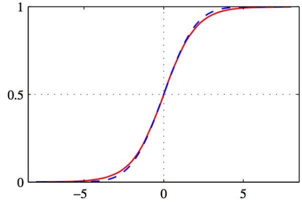


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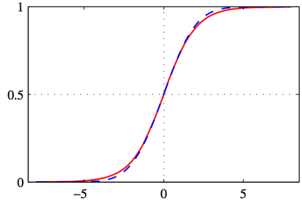


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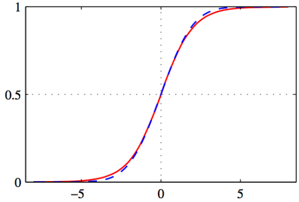


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- Alternative formulation: $P(t|\boldsymbol{x}) = \sigma\left(ty(\boldsymbol{x})\right)$ . $(\star)$

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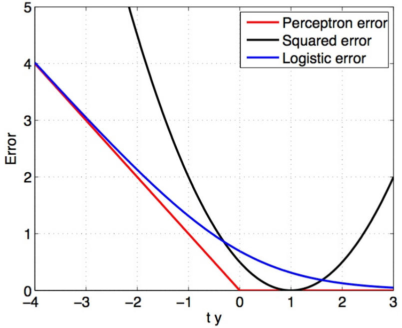
# Classification losses



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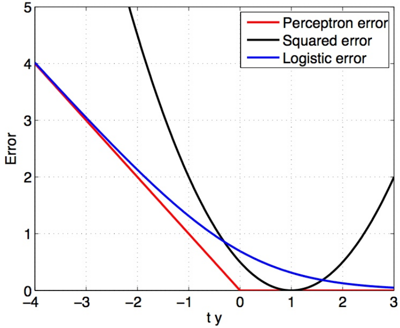


- Perceptron loss:

$$E(\mathbf{x}_i) = \begin{cases} 0 & \text{if } t_i y(\mathbf{x}_i) > 0, \\ t_i y(\mathbf{x}_i) & \text{if } t_i y(\mathbf{x}_i) < 0. \end{cases}$$

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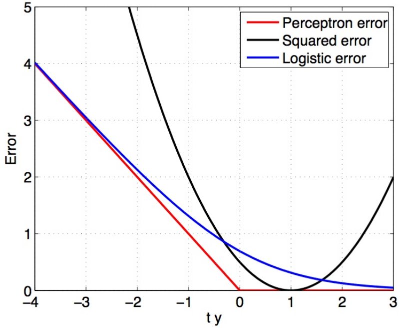


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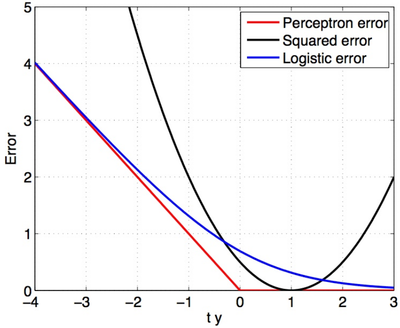


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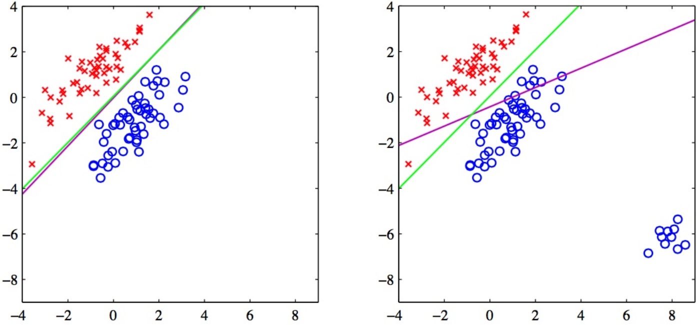
$$E(\boldsymbol{x}_i) = \ln\left(1 + e^{-t_i y(\boldsymbol{x}_i)}\right).$$

- Squared error:

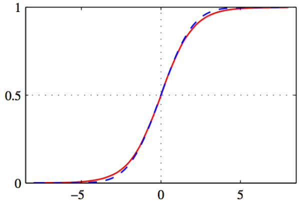
$$E(x_i) = \frac{1}{2}\left(t_i y(\boldsymbol{x_i}) - 1\right)^2.$$

# Is the squared error suitable for classification?




(Green: perceptron. Magenta: squared error.)

# Other link functions?




- Probit regression:

$$\Phi(y(\boldsymbol{x})) = \int_{-\inf}^{y(\boldsymbol{x})} \text{Gaussian}\,(0,1)\, dz, \quad y(\boldsymbol{x}) = \boldsymbol{w}^\top \boldsymbol{x} + b.$$

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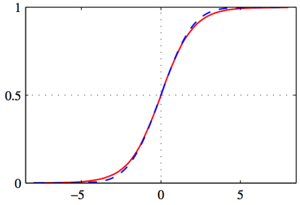


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- Latent variable view:

$$t|z \sim I(tz > 0), \qquad z \sim \text{Gaussian}\,(\boldsymbol{y}(\boldsymbol{x}), 1)\,.$$

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- Conditional likelihood:

$$t|\boldsymbol{x} \sim \mathrm{Categorical}(\boldsymbol{\mu}),$$

where $\mu_k = P(t = k|x)$.

# Outline


1. What is classification?
2. Decision theory
3. Generative classifiers
4. Discriminative classifiers
5. Summary
6. Exercises

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# Exercise 1

Can you propose a Naive Bayes classifier with continuous features? Derive the maximum likelihood estimates of the parameters.

# Exercise 2

Derive the update equations of a generative classifier with discrete binary features.

# Exercise 3

What is the form of the decision boundary for a binary classifier with Gaussian features with different covariance matrices?

# Exercise 3$^\star$

What are the expressions of the precision and the recall in the multi-class case?

# References


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