# Linear discriminant functions

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Machine Learning

# Discriminative learning

## Discriminative vs generative

- Generative learning assumes knowledge of the distribution governing the data
- Discriminative learning focuses on directly modeling the discriminant function
- E.g. for classification, directly modeling decision boundaries (rather than inferring them from the modelled data distributions)

# Discriminative learning

## PROS

- When data are complex, modeling their distribution can be very difficult
- If data discrimination is the goal, data distribution modeling is not needed
- Focuses parameters (and thus use of available training examples) on the desired goal

## CONS

- The learned model is less flexible in its usage
- It does not allow to perform arbitrary inference tasks
- E.g. it is not possible to efficiently generate new data from a certain class

# Linear discriminant functions

## Description

$$f(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x} + w_0$$

- The discriminant function is a linear combination of example features
- $w_0$ is called *bias* or *threshold*
- it is the simplest possible discriminant function
- Depending on the complexity of the task and amount of data, it can be the best option available (at least it is the first to try)

# Linear binary classifier

## Description

$$f(\boldsymbol{x}) = \text{sign}(\boldsymbol{w}^T \boldsymbol{x} + w_0)$$

- It is obtained taking the sign of the linear function
- The decision boundary ($f(\mathbf{x}) = 0$) is a hyperplane ($H$)
- The weight vector $\boldsymbol{w}$ is orthogonal to the decision hyperplane:

$$\begin{aligned} &\forall \boldsymbol{x}, \boldsymbol{x}' : f(\boldsymbol{x}) = f(\boldsymbol{x}') = 0 \\ &\boldsymbol{w}^T \boldsymbol{x} + w_0 - \boldsymbol{w}^T \boldsymbol{x}' - w_0 = 0 \\ &\boldsymbol{w}^T (\boldsymbol{x} - \boldsymbol{x}') = 0 \end{aligned}$$

# Linear binary classifier

## Functional margin

- The value $f(\boldsymbol{x})$ of the function for a certain point $\boldsymbol{x}$ is called *functional margin*
- It can be seen as a confidence in the prediction

## Geometric margin

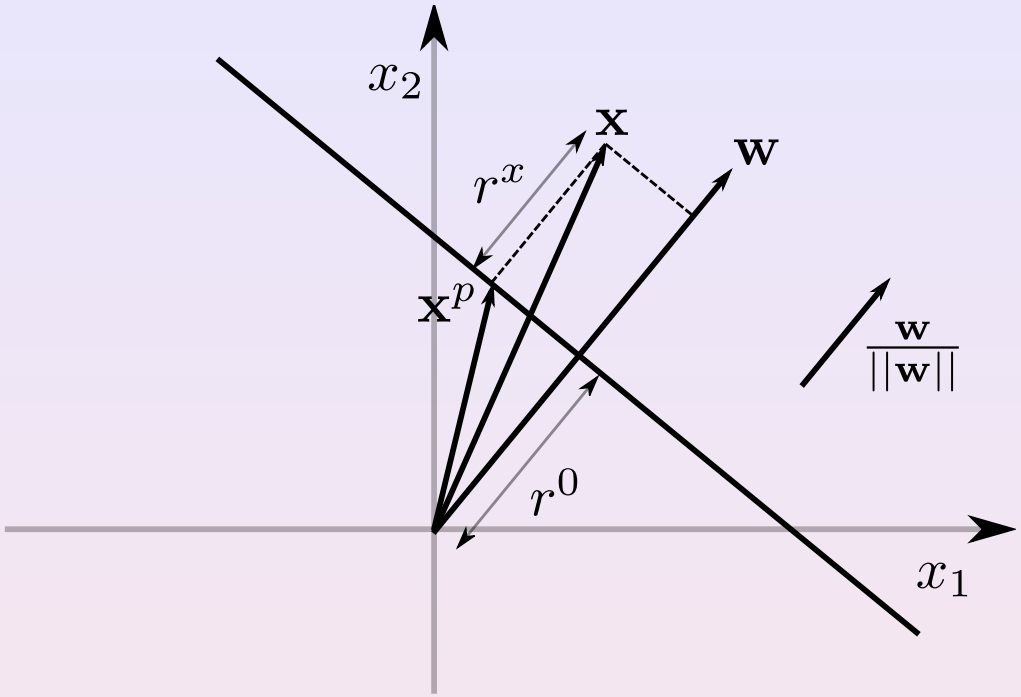
- The distance from $\boldsymbol{x}$ to the hyperplane is called *geometric margin*

$$r^x = \frac{f(\boldsymbol{x})}{||\boldsymbol{w}||}$$

- It is a normalize version of the functional margin
- The distance from the origin to the hyperplane is:

$$r^0 = \frac{f(\mathbf{0})}{||\boldsymbol{w}||} = \frac{w_0}{||\boldsymbol{w}||}$$

# Linear binary classifier




## Geometric margin (cont)

- A point can be expressed by its projection on $H$ plus its distance to $H$ times the unit vector in that direction:

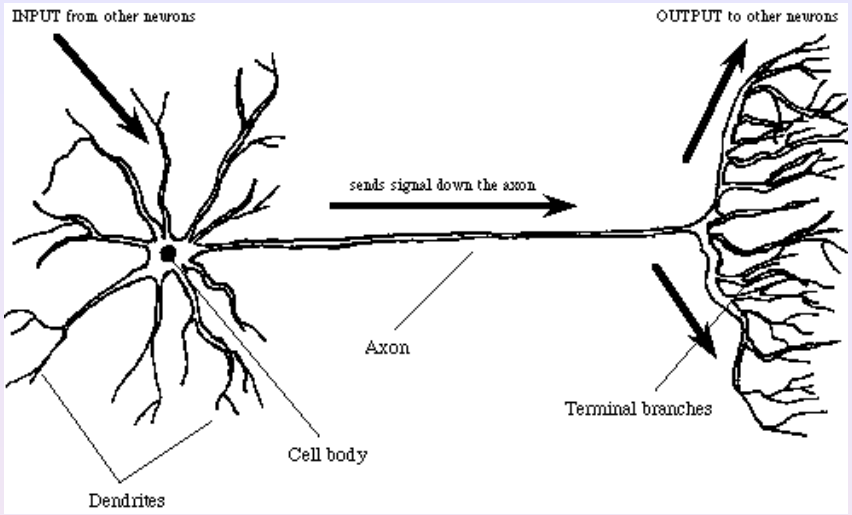
$$\boldsymbol{x} = \boldsymbol{x}^p + r^x \frac{\boldsymbol{w}}{||\boldsymbol{w}||}$$

## Geometric margin (cont)

- Then as $f(\boldsymbol{x}^p) = 0$:

$$
\begin{aligned}
f(\boldsymbol{x}) &= \boldsymbol{w}^T \boldsymbol{x} + w_0 \\
&= \boldsymbol{w}^T (\boldsymbol{x}^p + r^x \frac{\boldsymbol{w}}{||\boldsymbol{w}||}) + w_0 \\
&= \underbrace{\boldsymbol{w}^T \boldsymbol{x}^p + w_0}_{f(\boldsymbol{x}^p)} + r^x \boldsymbol{w}^T \frac{\boldsymbol{w}}{||\boldsymbol{w}||} \\
&= r^x ||\boldsymbol{w}|| \\
\frac{f(\boldsymbol{x})}{||\boldsymbol{w}||} &= r^x
\end{aligned}
$$

# Biological motivation

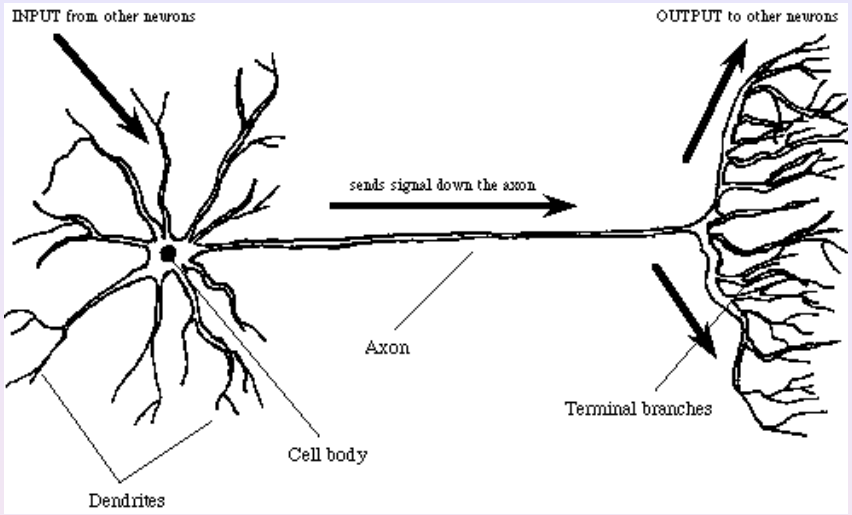



## Human Brain

- Composed of densely interconnected network of **neurons**
- A neuron is made of:

| | |
|---|---|
| soma | A central body containing the nucleus |
| dendrites | A set of filaments departing from the body |
| axon | a longer filament (up to 100 times body diameter) |
| synapses | connections between dendrites and axons from other neurons |

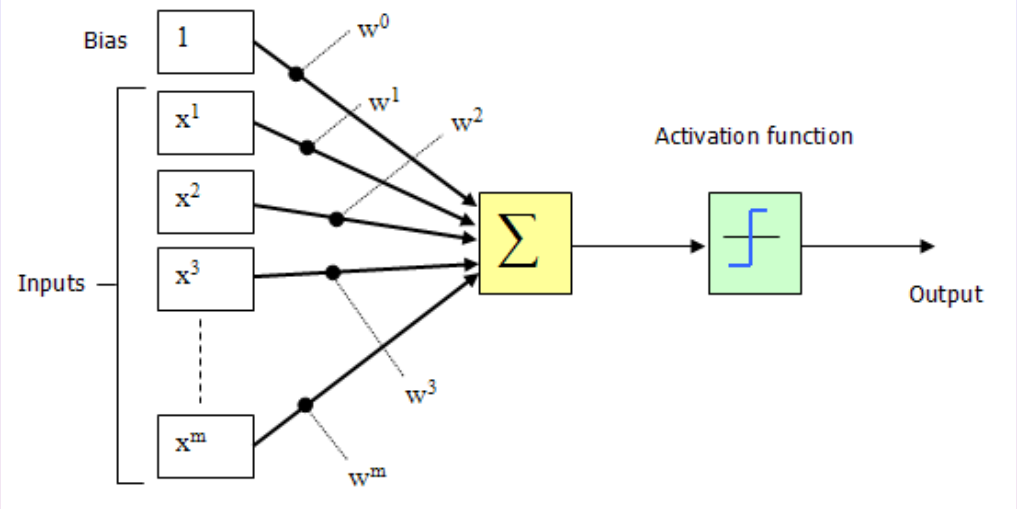
# Biological motivation




## Human Brain

- Electrochemical reactions allow signals to propagate along neurons via axons, synapses and dendrites
- Synapses can either *excite* on *inhibit* a neuron potentional
- Once a neuron potential exceeds a certain *threshold*, a signal is generated and transmitted along the axon

# Perceptron




## Single neuron architecture

$$f(x) = \text{sign}(\boldsymbol{w}^T \boldsymbol{x} + w_0)$$

- Linear combination of input features
- Threshold activation function

# Perceptron

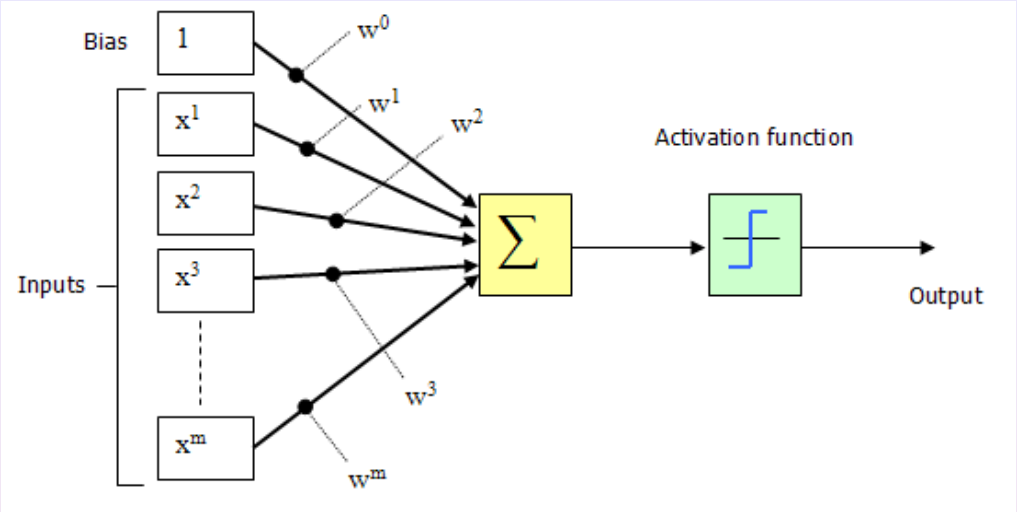
## Representational power

- *Linearly separable* sets of examples
- E.g. primitive boolean functions (AND,OR,NAND,NOT)
- $\Rightarrow$ any logic formula can be represented by a network of two levels of perceptrons (in disjunctive or conjunctive normal form).

## Problem

- *non-linearly separable* sets of examples cannot be separated
- Representing complex logic formulas can require a number of perceptrons *exponential* in the size of the input

# Perceptron




## Augmented feature/weight vectors

$$f(x) = \text{sign}(\hat{\boldsymbol{w}}^T \hat{\boldsymbol{x}})$$

- Where bias is incorporated in augmented vectors:

$$\hat{\boldsymbol{w}} = \begin{pmatrix} w_0 \\ \boldsymbol{w} \end{pmatrix} \qquad \hat{\boldsymbol{x}} = \begin{pmatrix} 1 \\ \boldsymbol{x} \end{pmatrix}$$

- Search for weight vector + bias is replaced by search for augmented weight vector (we skip the "^" in the following)

# Parameter learning

## Error minimization

- Need to find a function of the parameters to be optimized (like in maximum likelihood for probability distributions)
- Reasonable function is measure of error on training set $\mathcal{D}$ (i.e. the loss $\ell$):

$$E(\boldsymbol{w}; \mathcal{D}) = \sum_{(\boldsymbol{x}, y) \in \mathcal{D}} \ell(y, f(\boldsymbol{x}))$$

- Problem of overfitting training data (less severe for linear classifier, we will discuss it)

# Parameter learning

## Gradient descent

1. Initialize $\boldsymbol{w}$ (e.g. $\boldsymbol{w} = 0$)
2. Iterate until gradient is approx. zero:

$$\boldsymbol{w} = \boldsymbol{w} - \eta \nabla E(\boldsymbol{w}; \mathcal{D})$$

## Note

- $\eta$ is called *learning rate* and controls the amount of movement at each gradient step
- The algorithm is guaranteed to converge to a local optimum of $E(\boldsymbol{w}; \mathcal{D})$ (for small enough $\eta$)
- Too low $\eta$ implies slow convergence
- Techniques exist to adaptively modify $\eta$

# Parameter learning

## Problem

- The misclassification loss is piecewise constant
- Poor candidate for gradient descent

## Perceptron training rule

$$E(\boldsymbol{w}; \mathcal{D}) = \sum_{(\boldsymbol{x}, y) \in \mathcal{D}_E} -yf(\boldsymbol{x})$$

- $\mathcal{D}_E$ is the set of current training errors for which:

$$yf(\boldsymbol{x}) \leq 0$$

- The error is the sum of the functional margins of incorrectly classified examples

# Parameter learning

## Perceptron training rule

- The error gradient is:

$$\begin{aligned}\nabla E(\boldsymbol{w};\mathcal{D}) &= \nabla \sum_{(\boldsymbol{x},y)\in\mathcal{D}_E} -yf(\boldsymbol{x}) \\ &= \nabla \sum_{(\boldsymbol{x},y)\in\mathcal{D}_E} -y(\boldsymbol{w}^T\boldsymbol{x}) \\ &= \sum_{(\boldsymbol{x},y)\in\mathcal{D}_E} -y\boldsymbol{x}\end{aligned}$$

- the amount of update is:

$$-\eta\nabla E(\boldsymbol{w};\mathcal{D}) = \eta \sum_{(\boldsymbol{x},y)\in\mathcal{D}_E} y\boldsymbol{x}$$

# Perceptron learning

## Stochastic perceptron training rule

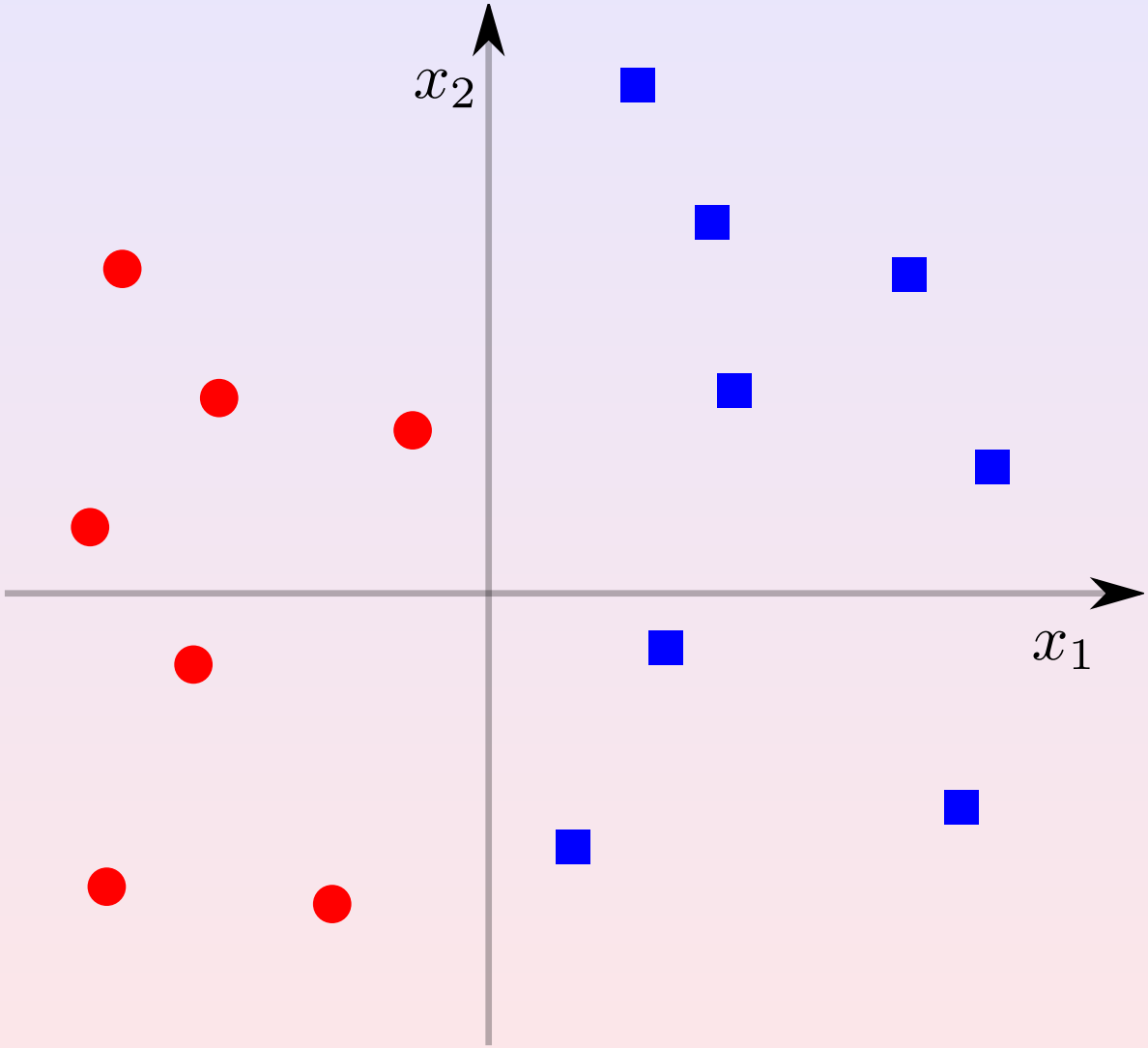
1. Initialize weights randomly
2. Iterate until all examples correctly classified:
   1. For each incorrectly classified training example $(\boldsymbol{x}, y)$ update weight vector:

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \eta y \mathbf{x}$$

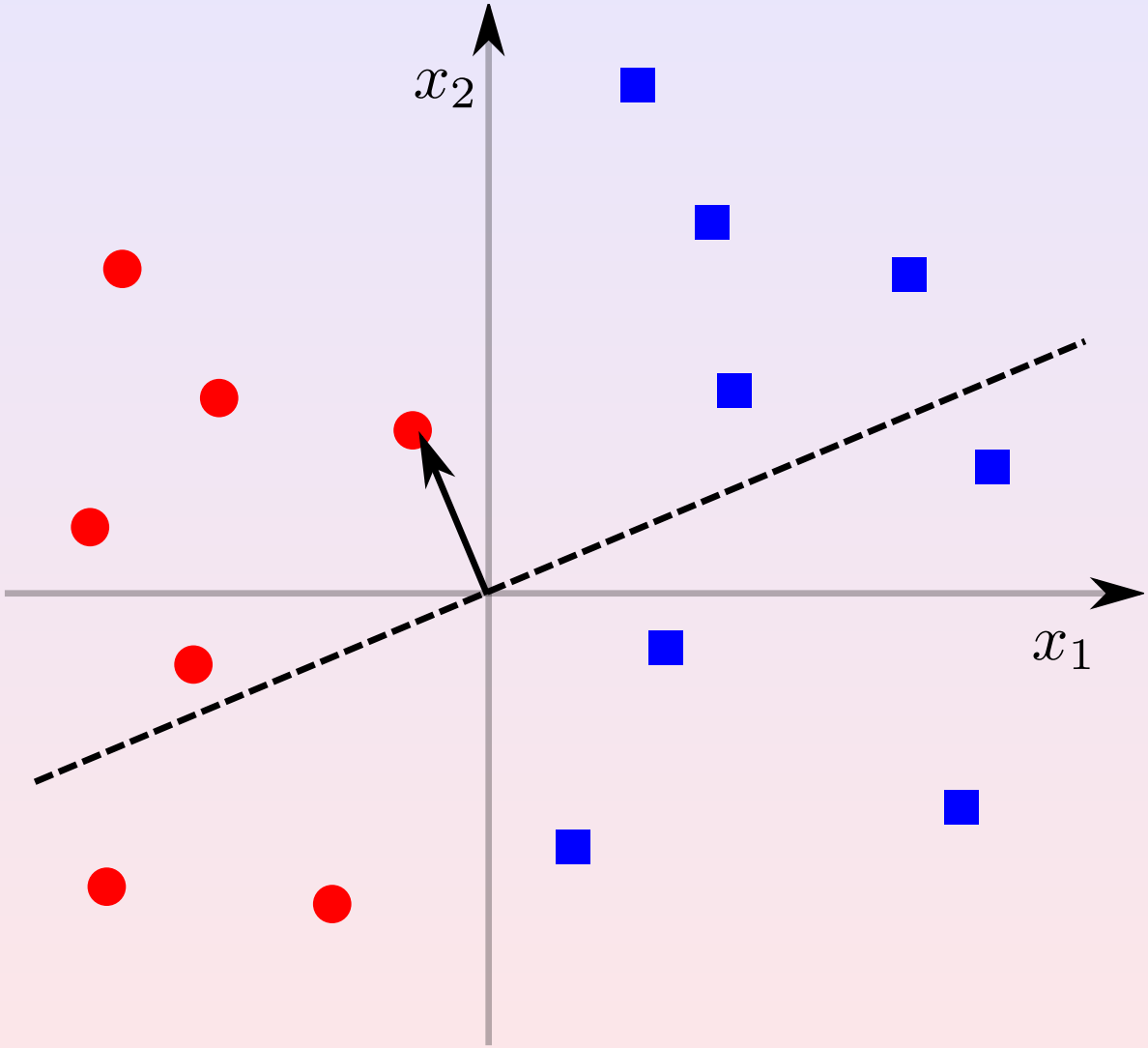
## Note on stochastic

- we make a gradient step for each training error (rather than on the sum of them in *batch* learning)
- Each gradient step is very fast
- Stochasticity can sometimes help to avoid local minima, being guided by various gradients for each training example (which won't have the same local minima in general)

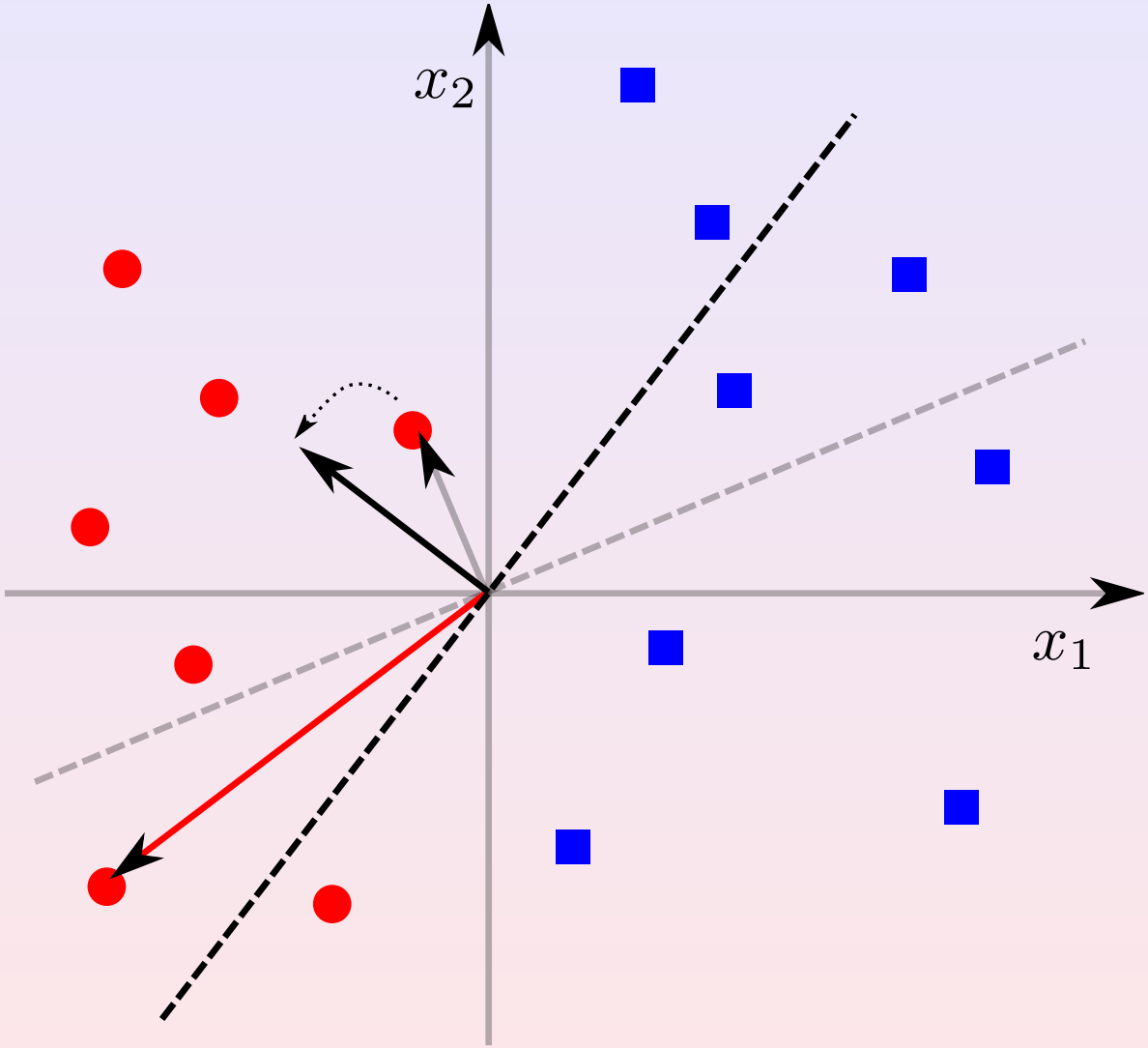
# Perceptron learning



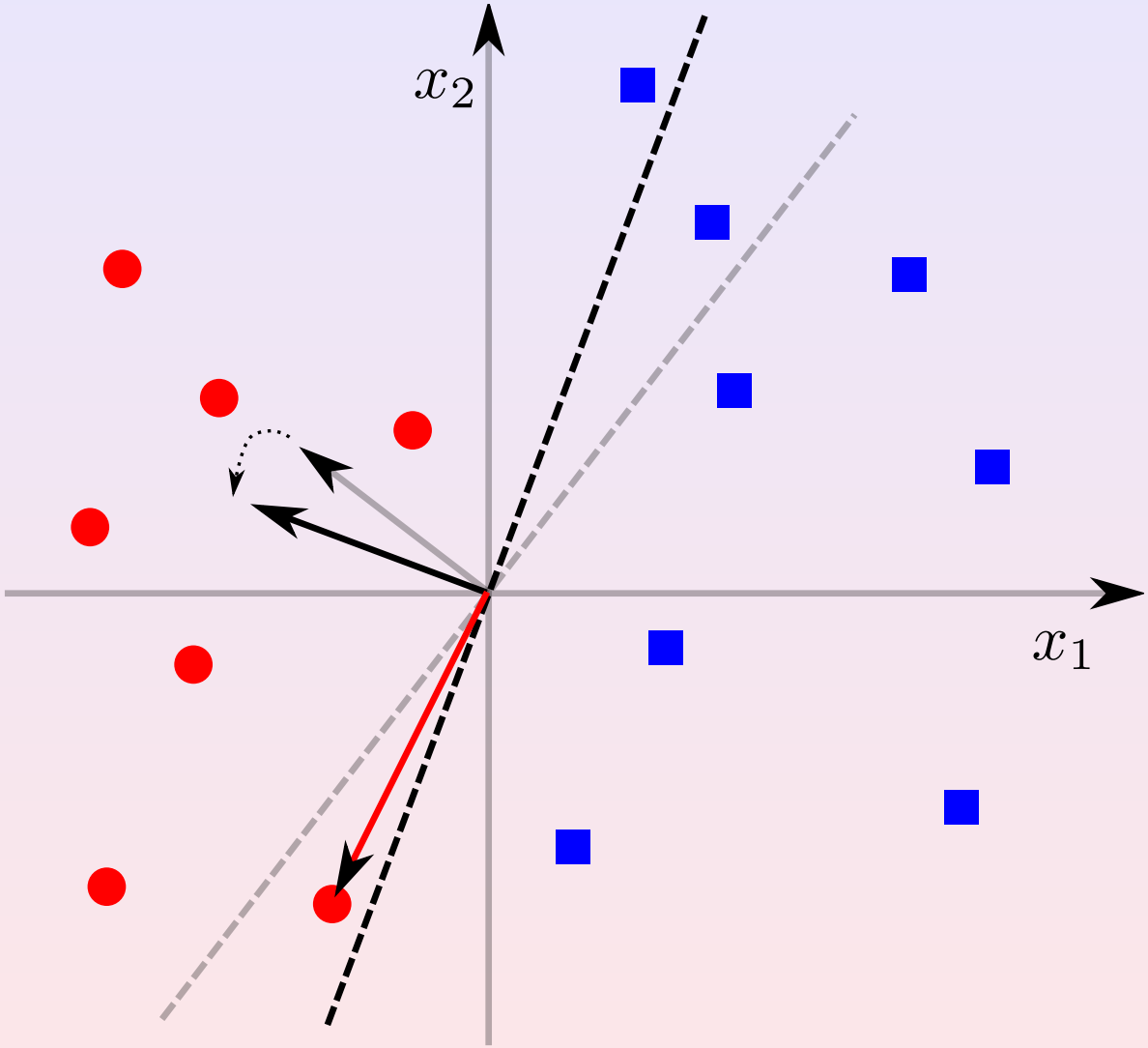
# Perceptron learning



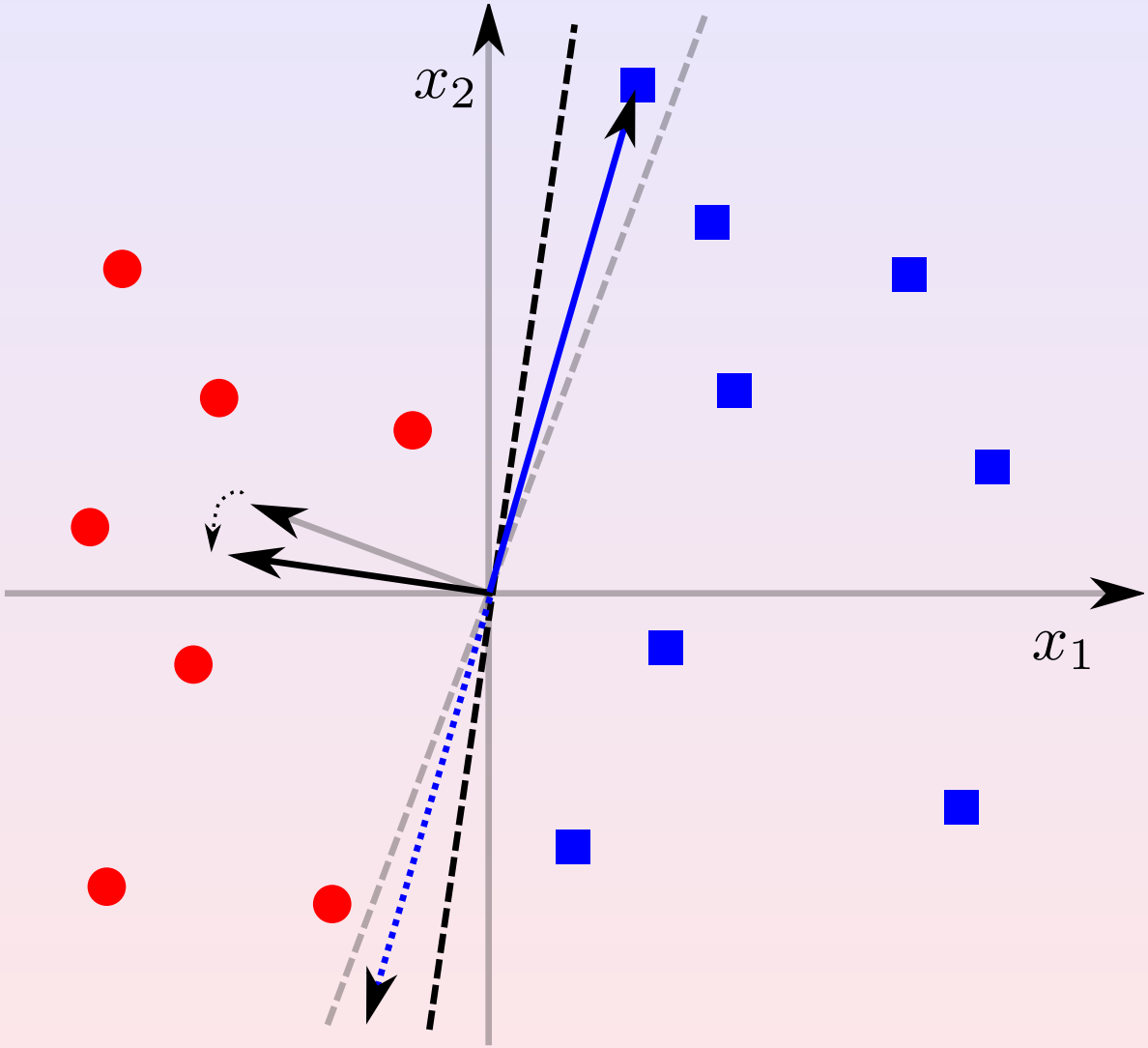
# Perceptron learning



# Perceptron learning



# Perceptron learning



# Perceptron regression

## Exact solution

- Let $X \in \mathbb{R}^n \times \mathbb{R}^d$ be the input training matrix (i.e. $X = [\boldsymbol{x}^1 \cdots \boldsymbol{x}^n]^T$ for $n = |\mathcal{D}|$ and $d = |\boldsymbol{x}|$)
- Let $\boldsymbol{y} \in \mathbb{R}^n$ be the output training matrix (i.e. $y_i$ is output for example $\mathbf{x}^i$)
- Regression learning could be stated as a set of linear equations):

$$X\boldsymbol{w} = \boldsymbol{y}$$

- Giving as solution:

$$\boldsymbol{w} = X^{-1}\boldsymbol{y}$$

# Perceptron regression

**Problem**

- Matrix $X$ is rectangular, usually more rows than columns
- System of equations is overdetermined (more equations than unknowns)
- No exact solution typically exists

# Perceptron regression

## Mean squared error (MSE)

- Resort to loss minimization
- Standard loss for regression is the mean squared error:

$$E(\boldsymbol{w}; \mathcal{D}) = \sum_{(\boldsymbol{x}, y) \in \mathcal{D}} (y - f(\boldsymbol{x}))^2 = (\boldsymbol{y} - X\boldsymbol{w})^T (\boldsymbol{y} - X\boldsymbol{w})$$

- Closed form solution exists
- Can always be solved by gradient descent (can be faster)
- Can also be used as a classification loss

# Perceptron regression

## Closed form solution

$$
\begin{aligned}
\nabla E(\boldsymbol{w}; \mathcal{D}) &= \nabla(\boldsymbol{y} - X\boldsymbol{w})^T(\boldsymbol{y} - X\boldsymbol{w}) \\
&= 2(\boldsymbol{y} - X\boldsymbol{w})^T(-X) = 0 \\
&= -2\boldsymbol{y}^T X + 2\boldsymbol{w}^T X^T X = 0 \\
\boldsymbol{w}^T X^T X &= \boldsymbol{y}^T X \\
X^T X\boldsymbol{w} &= X^T \boldsymbol{y} \\
\boldsymbol{w} &= (X^T X)^{-1} X^T \boldsymbol{y}
\end{aligned}
$$

# Perceptron regression

$$\boldsymbol{w} = (X^T X)^{-1} X^T \boldsymbol{y}$$

**Note**

- $(X^T X)^{-1} X^T$ is called *left-inverse*
- If $X$ is square and nonsingular, inverse and left-inverse coincide and the MSE solution corresponds to the exact one
- The left-inverse exists provided $(X^T X) \in \mathbb{R}^{d \times d}$ is full rank $\rightarrow$ features are linearly independent (if not, just remove the redundant ones!)

# Perceptron regression

## Gradient descent

$$
\begin{aligned}
\frac{\partial E}{\partial w_i} &= \frac{\partial}{\partial w_i}\frac{1}{2}\sum_{(\boldsymbol{x},y)\in\mathcal{D}}(y - f(\boldsymbol{x}))^2 \\
&= \frac{1}{2}\sum_{(\boldsymbol{x},y)\in\mathcal{D}}\frac{\partial}{\partial w_i}(y - f(\boldsymbol{x}))^2 \\
&= \frac{1}{2}\sum_{(\boldsymbol{x},y)\in\mathcal{D}} 2(y - f(\boldsymbol{x}))\frac{\partial}{\partial w_i}(y - \boldsymbol{w}^T\boldsymbol{x}) \\
&= \sum_{(\boldsymbol{x},y)\in\mathcal{D}}(y - f(\boldsymbol{x}))(-x_i)
\end{aligned}
$$

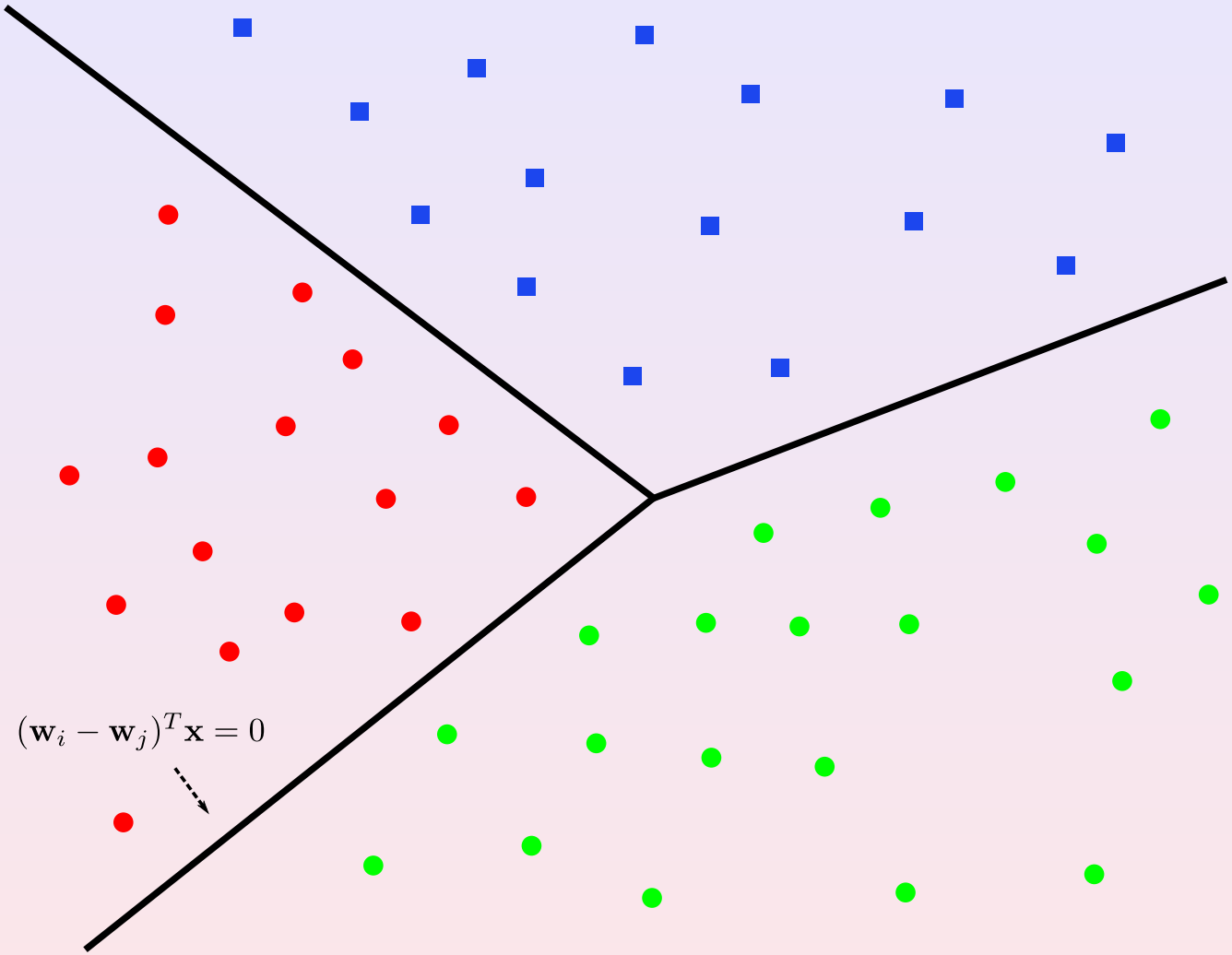
# Multiclass classification

## One-vs-all

- Learn one binary classifier for each class:
  - positive examples are examples of the class
  - negative examples are examples of all other classes
- Predict a new example in the class with maximum functional margin
- Decision boundaries for which $f_i(\boldsymbol{x}) = f_j(\boldsymbol{x})$ are pieces of hyperplanes:

$$\begin{aligned} \boldsymbol{w}_i^T \boldsymbol{x} &= \boldsymbol{w}_j^T \boldsymbol{x} \\ (\boldsymbol{w}_i - \boldsymbol{w}_j)^T \boldsymbol{x} &= 0 \end{aligned}$$

# Multiclass classification



# Multiclass classification

## all-pairs

- Learn one binary classifier for each pair of classes:
  - positive examples from one class
  - negative examples from the other
- Predict a new example in the class winning the largest number of pairwise classifications

# Generative linear classifiers

## Gaussian distributions

- linear decision boundaries are obtained when covariance is shared among classes ($\Sigma_i = \Sigma$)

## Naive Bayes classifier

$$f_i(\boldsymbol{x}) = P(\boldsymbol{x}|y_i)P(y_i) = \prod_{j=1}^{|\boldsymbol{x}|}\prod_{k=1}^{K}\theta_{ky_i}^{z_k(x[j])}\frac{|\mathcal{D}_i|}{|\mathcal{D}|}$$

$$= \prod_{k=1}^{K}\theta_{ky_i}^{N_k\boldsymbol{x}}\frac{|\mathcal{D}_i|}{|\mathcal{D}|}$$

- where $N_k\boldsymbol{x}$ is the number of times feature $k$ (e.g. a word) appears in $\boldsymbol{x}$

## Naive Bayes classifier (cont)

$$\log f_i(\boldsymbol{x}) = \underbrace{\sum_{k=1}^{K} N_k \boldsymbol{x} \log \theta_{k y_i}}_{\boldsymbol{w}^T \boldsymbol{x}'} + \underbrace{\log\left(\frac{|\mathcal{D}_i|}{|\mathcal{D}|}\right)}_{w_0}$$

- $\boldsymbol{x}' = [N_1 \boldsymbol{x} \cdots N_K \boldsymbol{x}]^T$
- $\boldsymbol{w} = [\log \theta_{1 y_i} \cdots \log \theta_{K y_i}]^T$
- Naive Bayes is a *log-linear* model (as Gaussian distributions with shared $\Sigma$)