Aalto University
School of Electrical Engineering

CS-C3240 – Machine Learning D

Classification

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Learning goals

- Logistic Regresion
  - Logistic Loss
- Support Vector Machines
  - Hinge loss
  - Maximum margin principle
- The perceptron algorithm
- Multiclass and multilabel problems

Outline

Recap: linear regression

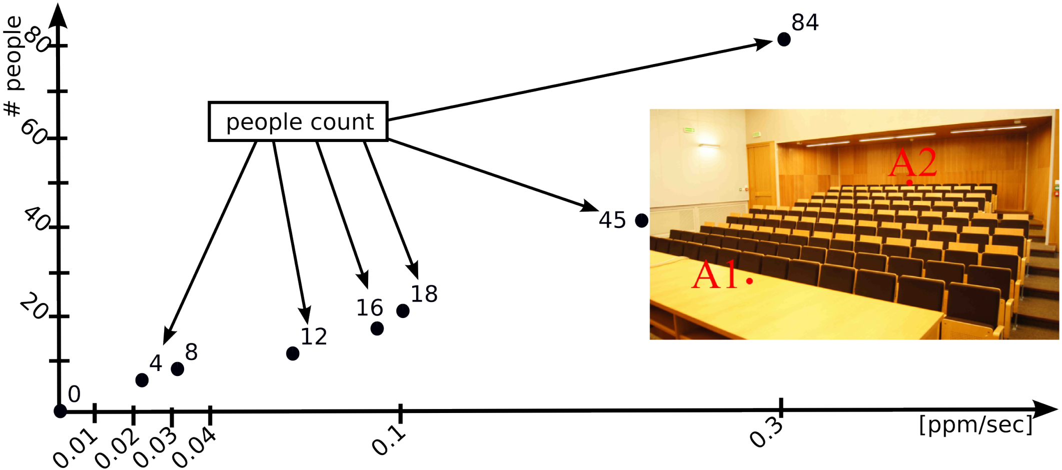
Logistic regression

The Perceptron algorithm

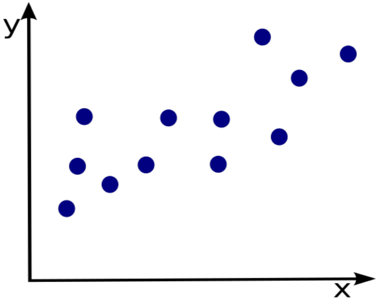
Support Vector Machines

Multiclass classification

Recap: linear regression



Recap: linear regression



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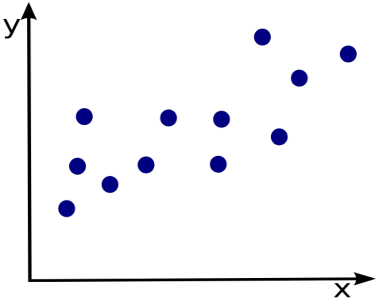
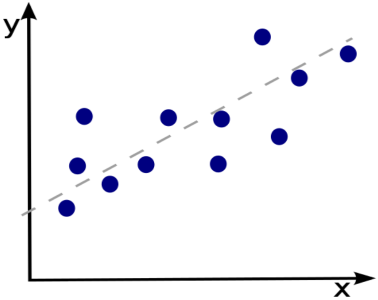


What do we try to find with linear regression?

Recap: linear regression



Hypothesis: $h(x) = w_0 + w_1 x$

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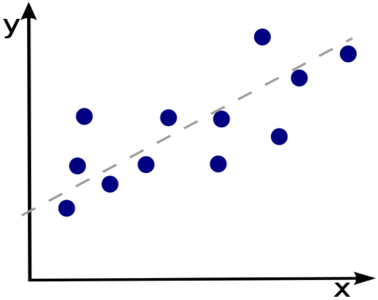

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- How do we find proper parameters w_0 and w_1 ?

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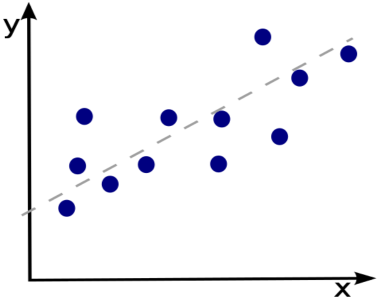

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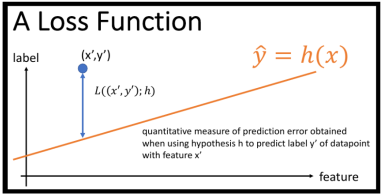

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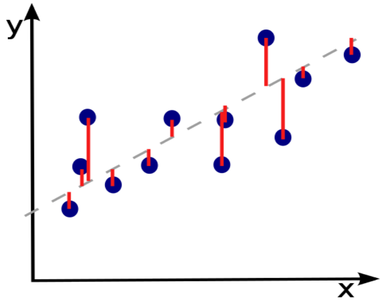

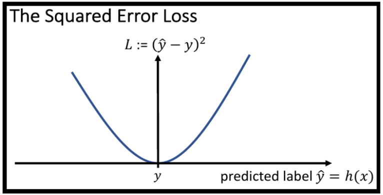

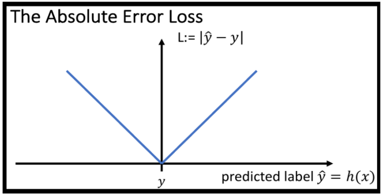

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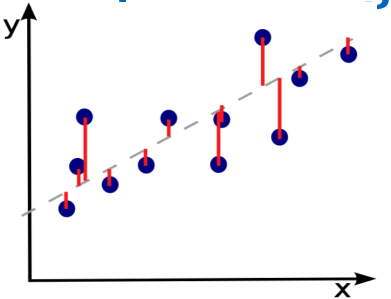

Loss function: estimates quality of current solution;

sometimes called *error function* or *cost function*.

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$$\text{minimize } L[(\mathcal{X},\mathcal{Y}),h(\cdot)] = \frac{1}{2n}\sum_{i=1}^{n}(h(x_i)-y_i)^2$$

$$\text{weight update (step } t \rightarrow t+1\text{): } w_1^{t+1} = w_1^{t} - \delta \cdot \frac{\partial L[(\mathcal{X},\mathcal{Y}),h(\cdot)]}{\partial w_1}$$

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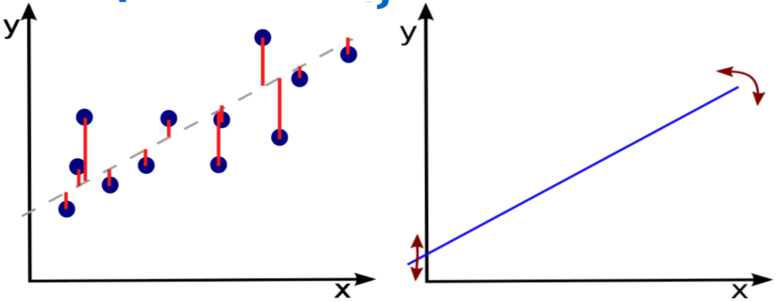

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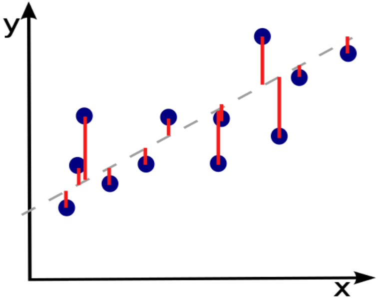

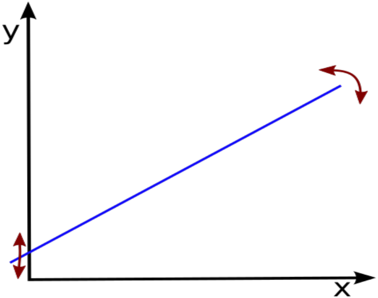

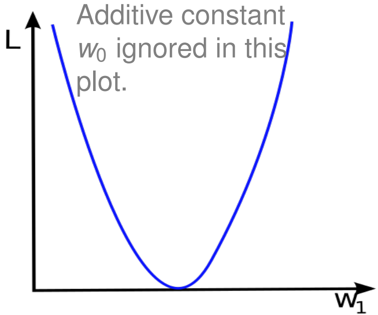

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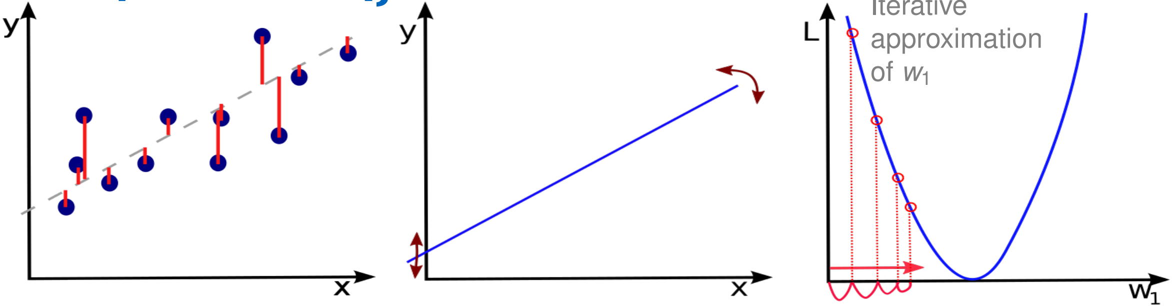

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Logistic regression

The Perceptron algorithm

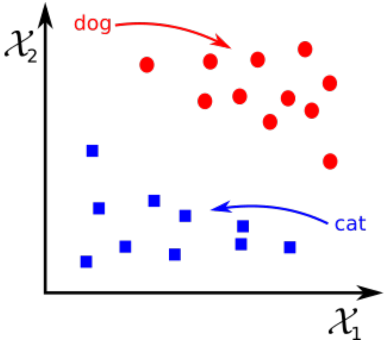
Support Vector Machines

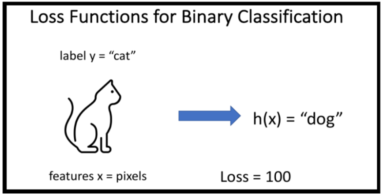
Multiclass classification

Logistic regression

Nominal classes

Classes might be nominal in real-world problems





Logistic regression

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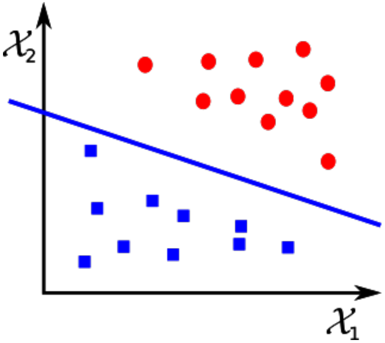

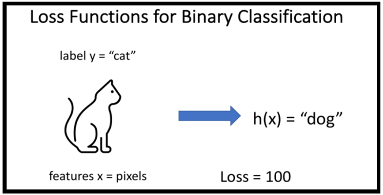

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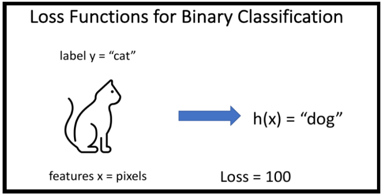
Weather	Sunny, rainy
Medical	positive diagnosis, negative diagnosis
Localisation	indoor, outdoor



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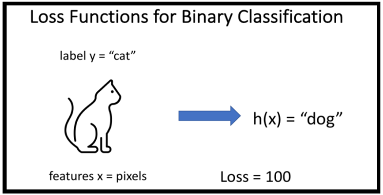

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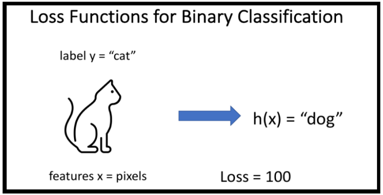

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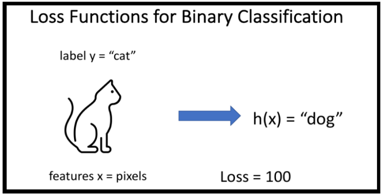
Logistic regression: $0 \leq h(x) \leq 1$



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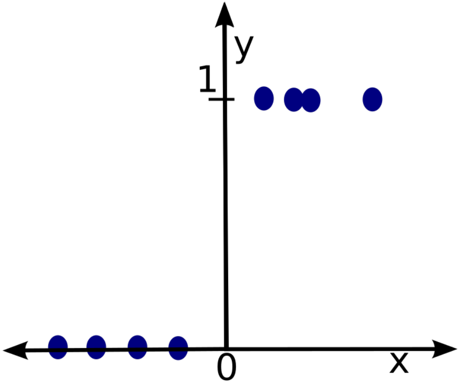

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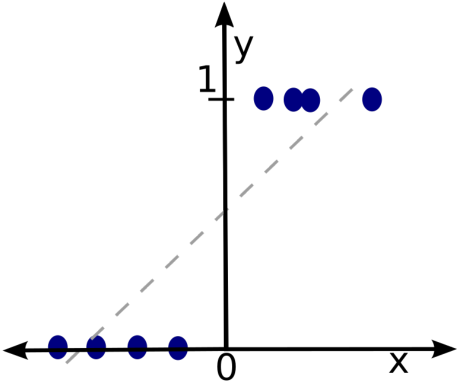
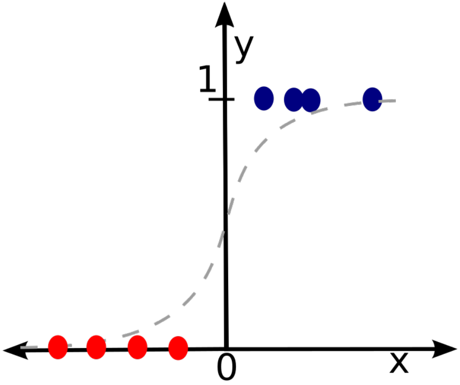


Logistic regression

Loss function



Logistic regression

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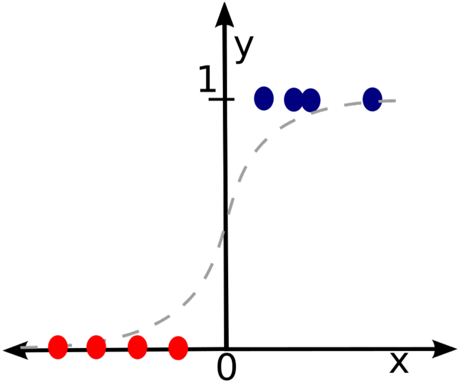
Linear regression

$$h(x) = \vec{w}^T x$$

Logistic regression

$$h(x) = \frac{1}{1+e^{-\vec{w}^T x}}$$



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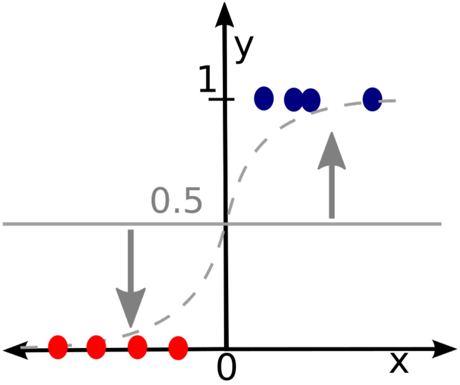

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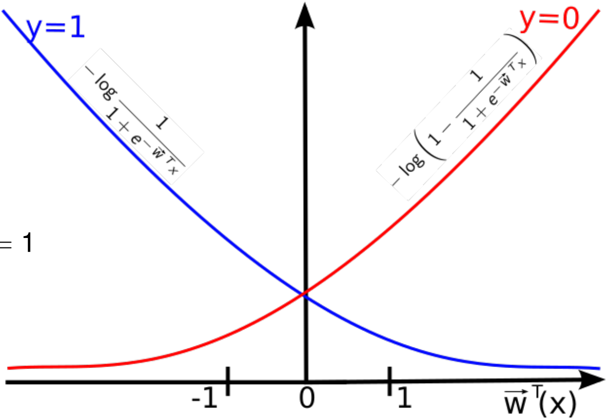
$$L[(\mathcal{X}, \mathcal{Y}), h(\cdot)] = \begin{cases} -\log(h(x)) & \text{if } y = 1 \\ -\log(1 - h(x)) & \text{else} \end{cases}$$



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Binary classification ($\overrightarrow{y} \in \{-1, 1\}^n$) with $\overrightarrow{x_i} \in \mathcal{X}$, $i \in \{1, \ldots, n\}$.

The perceptron algorithm

Binary classification ($\overrightarrow{y} \in \{-1, 1\}^n$) with $\overrightarrow{x_i} \in \mathcal{X}$, $i \in \{1, \ldots, n\}$.

We define a nonlinear hypothesis function as:

$$h(\overrightarrow{w}^T \overrightarrow{x}) = \begin{cases} +1, & \overrightarrow{w}^T \overrightarrow{x} \geq 0 \\ -1, & \overrightarrow{w}^T \overrightarrow{x} < 0. \end{cases}$$

The perceptron algorithm

Let $\mathcal{D}^t \subseteq \mathcal{X}$ describe the set of all misclassified x_i at step t and the loss function

$$L[\overrightarrow{x_i}, \overrightarrow{y}, \overrightarrow{w}, h(\cdot)] = \begin{cases} -\overrightarrow{w}^T \overrightarrow{x_i} y_i & ; \overrightarrow{x_i} \in \mathcal{D} \\ 0 & ; \text{else} \end{cases}$$

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$L[\overrightarrow{x_i}, \overrightarrow{y}, \overrightarrow{w}, h(\cdot)]$ is piecewise linear:

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Apply stochastic gradient descent to this loss function:

$$\overrightarrow{w}^{t+1} = \overrightarrow{w}^t - \begin{cases} \delta \frac{\partial L[\overrightarrow{x_i}, \overrightarrow{y}, \overrightarrow{w}, h(\cdot)]}{\partial \overrightarrow{w}} & ; x_i \in \mathcal{D} \\ 0 & ; \text{else} \end{cases}$$

$$= \overrightarrow{w}^t + \begin{cases} \delta \overrightarrow{x_i} y_i & ; x_i \in \mathcal{D} \\ 0 & ; \text{else} \end{cases}$$

The perceptron algorithm

Interpretation of the learning function

$$\overrightarrow{w}^{t+1} = \overrightarrow{w}^{t} + \begin{cases} \delta \overrightarrow{x_i} y_i & x_i \in \mathcal{D} \\ 0 & \text{else} \end{cases}$$

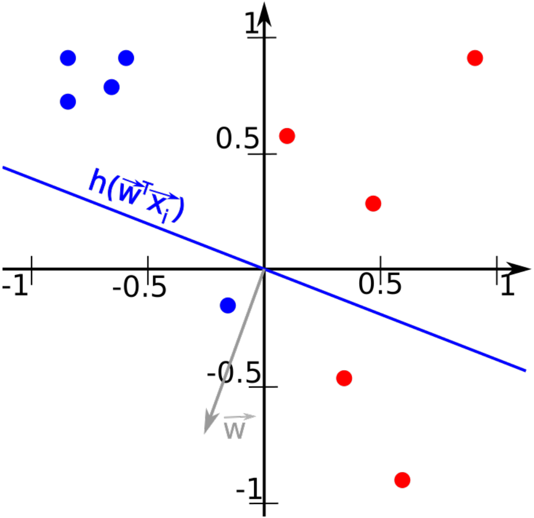
for each x_i:

correct classification: weight vector remains unchanged

incorrect classification:

$$\begin{aligned} y_i = 1 &: \quad \text{add vector } \overrightarrow{x_i} \\ y_i = -1 &: \quad \text{subtract vector } \overrightarrow{x_i} \end{aligned}$$

The perceptron algorithm



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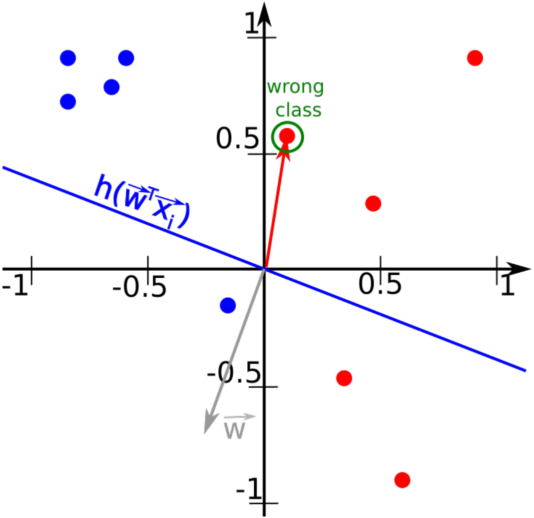

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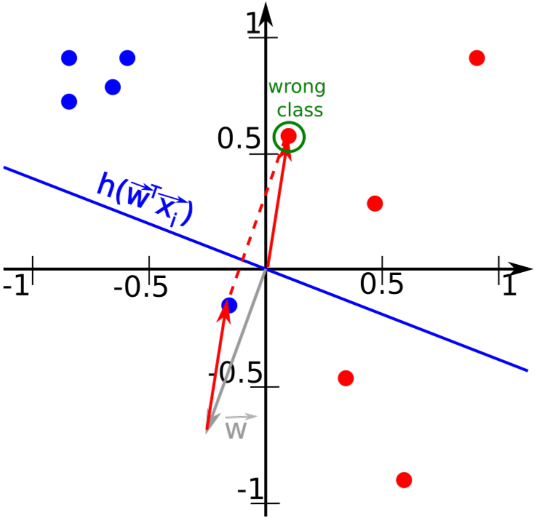

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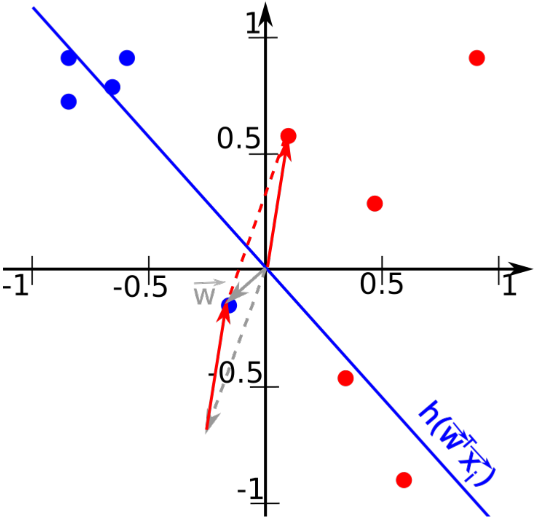

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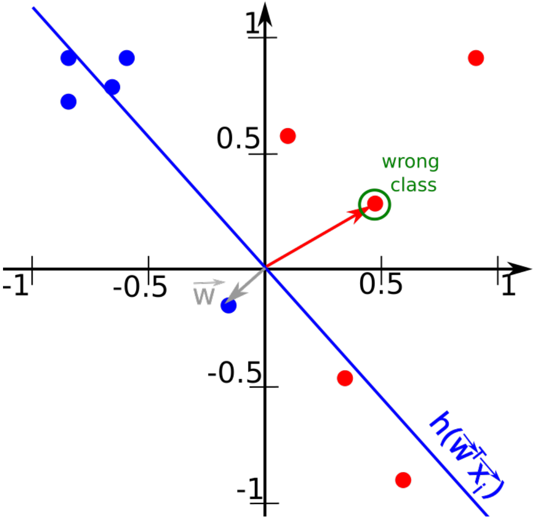

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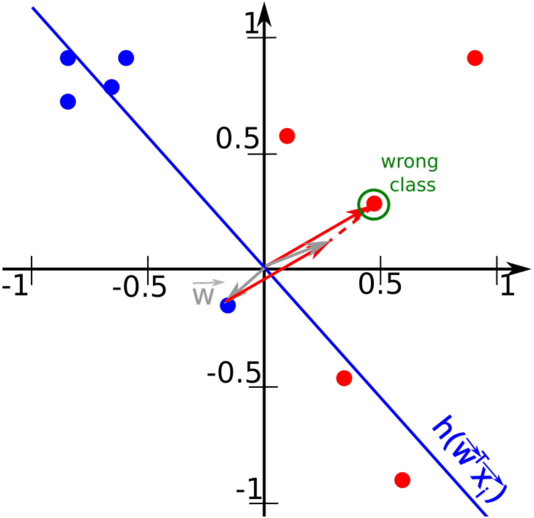

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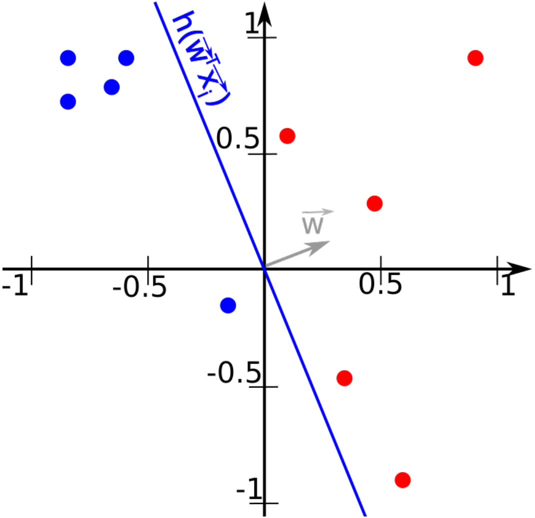

The perceptron algorithm

Perceptron convergence theorem

IFF the training data is linearly separable, then the perceptron learning algorithm will always find an exact solution in finite number of steps.

- → Number of steps required might be large
- → Until convergence, not possible to distinguish separable problem from non-separable
- → For non-separable data sets the algorithm will never converge

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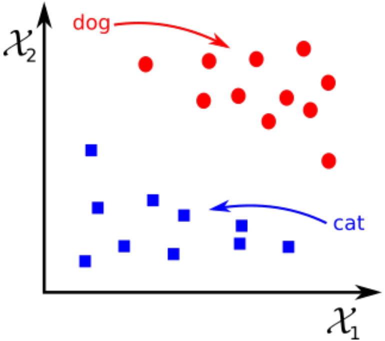
Support vector machines (SVM)

Large margin classifier



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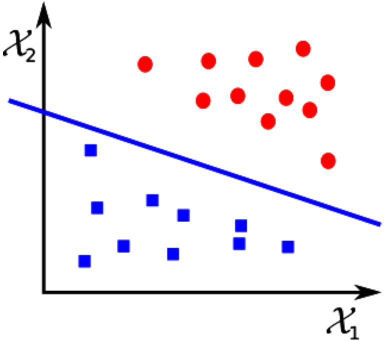
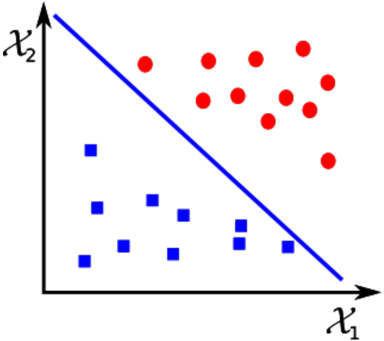


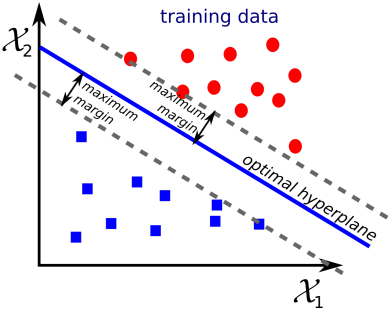


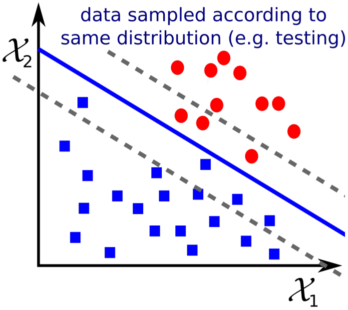
Support vector machines (SVM)

Large margin classifier

The goal for support vector machines is to find a linear and separating hyperplane with the largest margin to the outer points in all sets

If needed, map all points into a higher dimensional space until such a plane exists

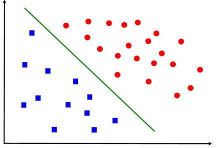




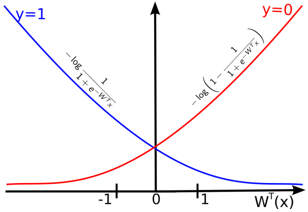
Support vector machines (SVM)

Contribution of a single sample to the overall loss:

Logistic regression



$$L[(\mathcal{X},\mathcal{Y}),h(\cdot)] = -y\cdot\log\left(1-\frac{1}{1+e^{-\vec{w}^T x}}\right)-(1-y)\cdot\log\frac{1}{1+e^{-\vec{w}^T x}}$$



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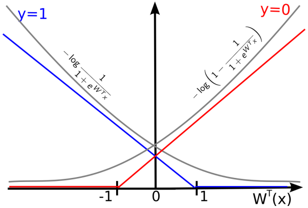

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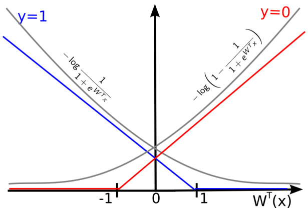
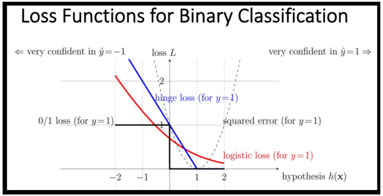
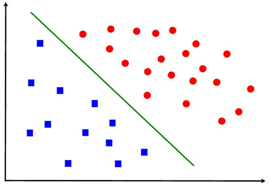




Support vector machines (SVM)

Cost function



Logistic regression

$$\min_{W} \quad \frac{1}{m}\left[\sum_{i=1}^{m} y_i \left(-\log\left(1-\frac{1}{1+e^{-\vec{w}^T x_i}}\right)\right)+(1-y_i)\left(-\log\frac{1}{1+e^{-\vec{w}^T x_i}}\right)\right]+\frac{\lambda}{2m}\sum_{j=1}^{n} w_j^2$$

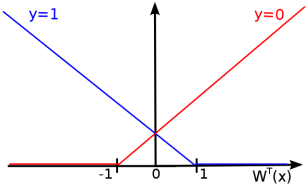
SVM

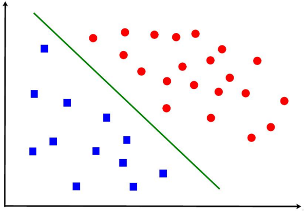
$$\min_{W} \quad \frac{1}{\lambda'}\sum_{i=1}^{m}\left[y_i \mathrm{cost}_{y=1}(\vec{w}^T x_i)+(1-y_i)\mathrm{cost}_{y=0}(\vec{w}^T x_i)\right]+\frac{1}{2}\sum_{j=1}^{n} w_j^2$$

λ has a similar effect on the overall term as $\frac{1}{\lambda'}$

Support vector machines (SVM)

SVM hypothesis

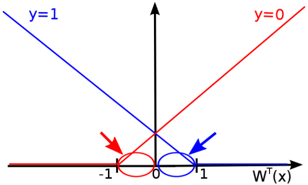


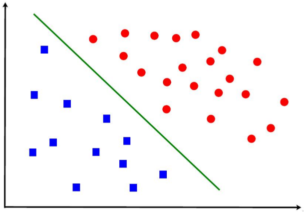


$$\min_{W} \frac{1}{\lambda'} \sum_{i=1}^{m} \left[y_i \text{cost}_{y=1}(\vec{w}^T x_i) + (1 - y_i)\text{cost}_{y=0}(\vec{w}^T x_i) \right] + \frac{1}{2} \sum_{j=1}^{n} w_j^2$$

Support vector machines (SVM)

SVM hypothesis



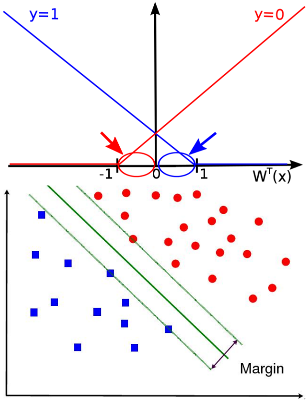


$$\vec{w}^T x \begin{cases} \geq 0 \\ < 0 \end{cases} \text{ sufficient}$$

$$\min_W \frac{1}{\lambda'} \sum_{i=1}^{m} \left[y_i \text{cost}_{y=1}(\vec{w}^T x_i) + (1 - y_i) \text{cost}_{y=0}(\vec{w}^T x_i) \right] + \frac{1}{2} \sum_{j=1}^{n} w_j^2$$

Support vector machines (SVM)

SVM hypothesis



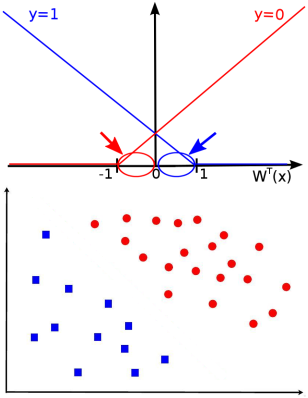
$$\vec{w}^T x \begin{cases} \geq 0 \\ < 0 \end{cases} \text{sufficient}$$

$$\vec{w}^T x \begin{cases} \geq \ 1 \\ \leq -1 \end{cases} \Rightarrow \text{confidence}$$

$$\min_W \frac{1}{\lambda'} \sum_{i=1}^{m} \left[y_i \text{cost}_{y=1}(\vec{w}^T x_i) + (1 - y_i) \text{cost}_{y=0}(\vec{w}^T x_i) \right] + \frac{1}{2} \sum_{j=1}^{n} w_j^2$$

Support vector machines (SVM)

SVM hypothesis



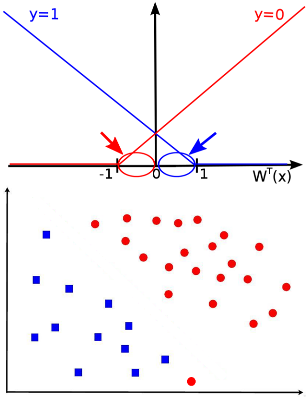
$$\overrightarrow{w}^T x \begin{cases} \geq & 1 \\ \leq & -1 \end{cases} \Rightarrow \text{confidence}$$

Outliers: Elastic decision boundary

$$\min_W \frac{1}{\lambda'} \sum_{i=1}^{m} \left[y_i \text{cost}_{y=1}(\overrightarrow{w}^T x_i) + (1 - y_i)\text{cost}_{y=0}(\overrightarrow{w}^T x_i) \right] + \frac{1}{2} \sum_{j=1}^{n} w_j^2$$

Support vector machines (SVM)

SVM hypothesis



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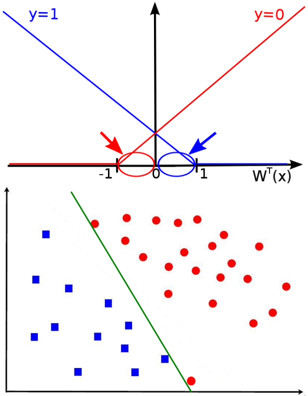
Support vector machines (SVM)

SVM hypothesis



$$\vec{w}^T x \begin{cases} \geq & 1 \\ \leq & -1 \end{cases} \Rightarrow \text{confidence}$$

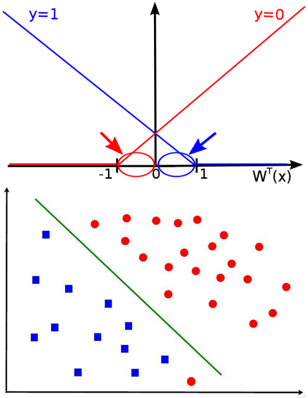
Outliers: Elastic decision boundary

small λ' stricter boundary at the cost of smaller margin

$$\min_W \frac{1}{\lambda'} \sum_{i=1}^{m} \left[y_i \text{cost}_{y=1}(\vec{w}^T x_i) + (1 - y_i)\text{cost}_{y=0}(\vec{w}^T x_i) \right] + \frac{1}{2} \sum_{j=1}^{n} w_j^2$$

Support vector machines (SVM)

SVM hypothesis



$$\vec{w}^T x \begin{cases} \geq & 1 \\ \leq & -1 \end{cases} \Rightarrow \text{confidence}$$

Outliers: Elastic decision boundary

large λ' tolerates outliers

$$\min_W \frac{1}{\lambda'} \sum_{i=1}^{m} \left[y_i \text{cost}_{y=1}(\vec{w}^T x_i) + (1 - y_i)\text{cost}_{y=0}(\vec{w}^T x_i) \right] + \frac{1}{2} \sum_{j=1}^{n} w_j^2$$

Support vector machines (SVM)

Large margin classifier

$$\min_{W} \frac{1}{\lambda'} \sum_{i=1}^{m} \left[y_i \text{cost}_{y=1}(\overrightarrow{w}^T x_i) + (1 - y_i)\text{cost}_{y=0}(\overrightarrow{w}^T x_i) \right] + \frac{1}{2} \sum_{j=1}^{n} w_j^2$$

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Large margin classifier

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Rewrite the SVM optimisation problem as

$$\begin{aligned} \min_{W} \quad & \tfrac{1}{2} \textstyle\sum_{j=1}^{n} w_j^2 \\ s.t. \quad & \overrightarrow{w}^T x_i \geq 1 \quad \text{if } y_i = 1 \\ & \overrightarrow{w}^T x_i \leq -1 \quad \text{if } y_i = 0 \end{aligned}$$

Support vector machines (SVM)

Large margin classifier

$$\min_{w} \quad \frac{1}{2}\sum_{j=1}^{n} w_j^2$$

$$s.t. \qquad \vec{w}^T x_i \geq 1 \ \text{ if } y_i = 1$$

$$\vec{w}^T x_i \leq -1 \text{ if } y_i = 0$$

Support vector machines (SVM)

Large margin classifier

$$\min_{w} \quad \frac{1}{2}\sum_{j=1}^{n} w_j^2 = \frac{1}{2}\left(\sqrt{w_1^2 + \cdots + w_n^2}\right)^2$$

$$s.t. \quad \overrightarrow{w}^T x_i \geq 1 \ \text{ if } y_i = 1$$

$$\overrightarrow{w}^T x_i \leq -1 \text{ if } y_i = 0$$

Support vector machines (SVM)

Large margin classifier

$$\min_{w} \quad \frac{1}{2}\sum_{j=1}^{n} w_j^2 = \frac{1}{2}\left(\sqrt{w_1^2 + \cdots + w_n^2}\right)^2 \quad = \frac{1}{2}||\vec{w}||^2$$

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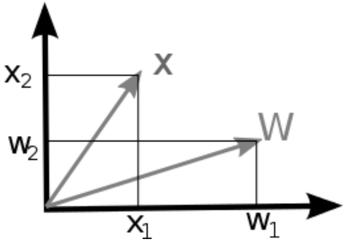

$$\overrightarrow{w}^T x = w_1 x_1 + w_2 x_2$$

Support vector machines (SVM)

Large margin classifier

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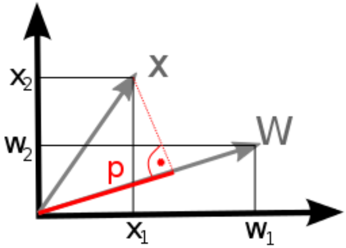

$$\vec{w}^{\,T}x = w_1x_1 + w_2x_2 = ||\vec{w}|| \cdot p$$

Support vector machines (SVM)

Large margin classifier

$$\min_{w} \quad \frac{1}{2}\sum_{j=1}^{n} w_j^2 = \frac{1}{2}\left(\sqrt{w_1^2+\cdots+w_n^2}\right)^2 \quad = \frac{1}{2}||\vec{w}||^2$$

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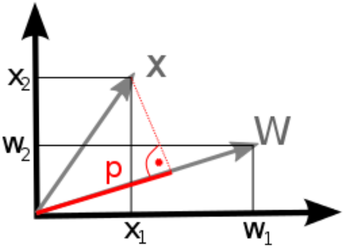

$$\vec{w}^T x = w_1 x_1 + w_2 x_2 = ||\vec{w}|| \cdot p$$

Support vector machines (SVM)

Large margin classifier

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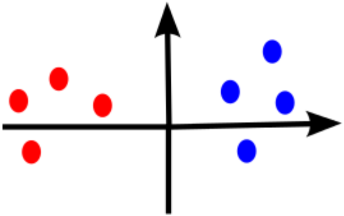

Which decision boundaray is found?

Support vector machines (SVM)

Large margin classifier

$$\min_{W} \quad \tfrac{1}{2}\sum_{j=1}^{n} w_j^2 = \tfrac{1}{2}\left(\sqrt{w_1^2+\cdots+w_n^2}\right)^2 \quad = \frac{1}{2}||\vec{w}||^2$$

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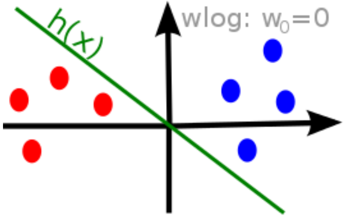

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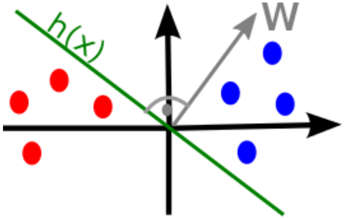

Which decision boundaray is found?

$$h(x) = w_1 x_1 + w_2 x_2$$

$\rightarrow$ W orthogonal to all x with $h(x) = 0$

Support vector machines (SVM)

Large margin classifier

$$\min_{W} \quad \frac{1}{2}\sum_{j=1}^{n} w_j^2 = \frac{1}{2}\left(\sqrt{w_1^2+\cdots+w_n^2}\right)^2 \quad = \frac{1}{2}||\vec{w}||^2$$

$$s.t. \quad \vec{w}^T x_i \geq 1 \text{ if } y_i = 1 \quad \rightarrow ||\vec{w}|| \cdot p_i \geq 1$$

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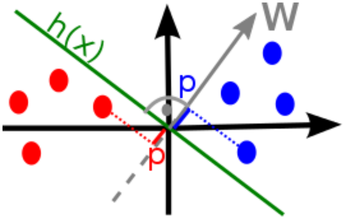

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Support vector machines (SVM)

Large margin classifier

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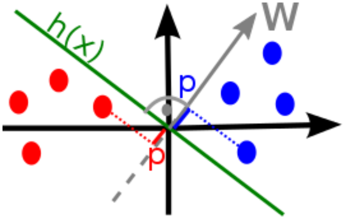

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$$h(x) = w_1 x_1 + w_2 x_2$$

$\rightarrow$ W orthogonal to all x with $h(x) = 0$

$\Rightarrow$ $\min \frac{1}{2}||\vec{w}||^2$ and $||\vec{w}|| \cdot p_i \geq 1$ necessitate larger p_i

Support vector machines (SVM)

Large margin classifier

$$\min_{W} \quad \tfrac{1}{2}\sum_{j=1}^{n} w_j^2 = \tfrac{1}{2}\left(\sqrt{w_1^2+\cdots+w_n^2}\right)^2 \qquad = \frac{1}{2}||\vec{w}||^2$$

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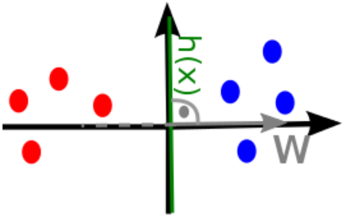

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Support vector machines (SVM)

Large margin classifier

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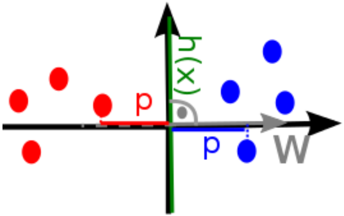

Which decision boundaray is found?

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Outline

Recap: linear regression

Logistic regression

The Perceptron algorithm

Support Vector Machines

Multiclass classification

Multiclass classification

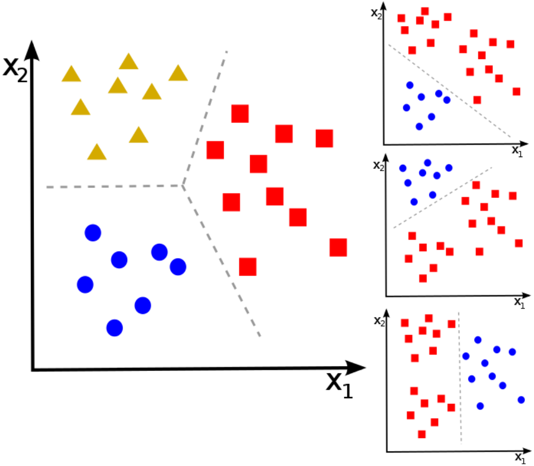
Multi-class: One-versus all:

Train classifiers for each class to obtain probability that x belongs to class i:

$$h_i(x) = P(y = i | \vec{x}, \vec{W})$$

then, choose

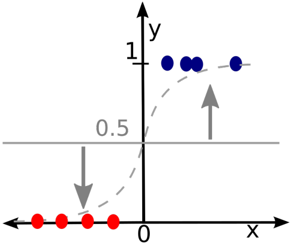
$$max_i\,(h_i(x))$$

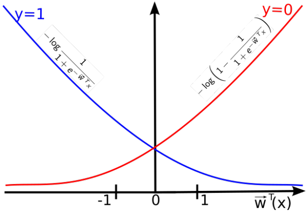


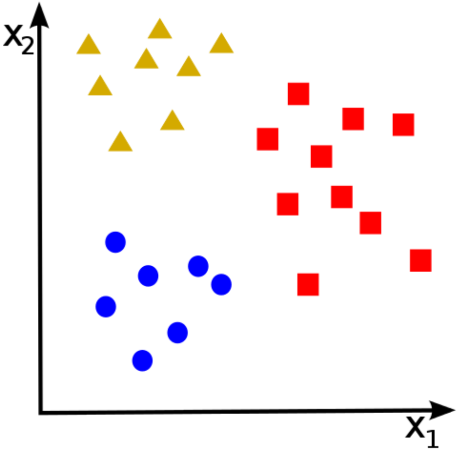
Multiclass classification

Multiple classes

Can we use logistic regression for problems with more than two classes?





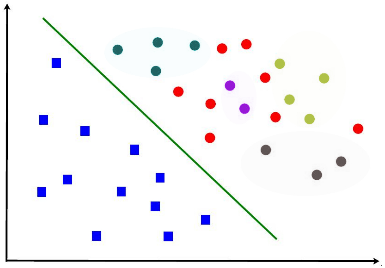


Application to several classes iteratively: One-versus-all

belongs to class 1 or not?

belongs to class 2 or not?

...



Questions?

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Si Zuo
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Literature

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- R.O. Duda, P.E. Hart, D.G. Stork: Pattern Classification, Wiley, 2001.