Statistical Machine Learning

Christian Walder

College of Engineering and Computer Science
The Australian National University

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(Many figures from C. M. Bishop, "Pattern Recognition and Machine Learning")

Outlines

Part V

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Strategy in this course

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- Estimate best predictor = training = learning

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1.
2.
3.
4. Calculate the optimal parameter ($\mathbf{w}$)
5. Model uncertainty using the Bayesian appro
6. Implement and compute (the algorithm in py
7. Interpret and diagnose results

Classification

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- Goal : Given input data $\mathbf{x}$, assign it to one of K discrete classes $\mathcal{C}_k$ where $k = 1, \ldots, K$.
- Divide the input space into different regions.
- Eq

Length of petal [in cm] vs sepal [cm] for three types of flowers (Iris Setosa, Iris Versicolor, Iris Virginica).

How to represent binary class labels?

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- Class labels are no longer real values as in regression, but a dis
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with only two values possible for the probability
- Note: Other conventions to map classes into int
possible, check the setup.

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How to represent multi-class labels?

- If there are more than two classes ($K > 2$), we call it a multi-class setup.
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  class $\mathcal{C}_2$ will be encoded as the target vector

$$\mathbf{t} = (0, 1, 0, 0, 0)^T$$

- Note: Other conventions to map multi-classe
  possible, check the setup.

Linear Model

- Idea: Use again a Linear Model as in regression: $y(\mathbf{x}, \mathbf{w})$ is a linear function of the parameters $\mathbf{w}$

$$y(\mathbf{x}, \mathbf{w}) = \mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x})$$

- But
  Exa

Generalised Linear Model

- Apply a mapping $f : \mathbb{R} \to \mathbb{Z}$ to the linear model to get the discrete class labels.
- Generalised Linear Model

$$y(\mathbf{x}_n, \mathbf{w}) = f(\mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x}_n))$$

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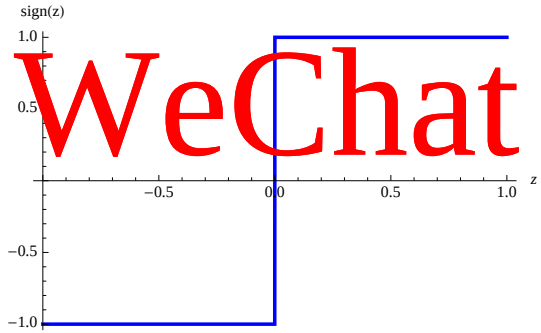

Figure: Example of an activation function $f(z) = \text{sign}(z)$.

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Three Models for Decision Problems

- Find a discriminant function $f(\mathbf{x})$ which maps each input directly onto a class label.
- Discriminative Models
  1.
  2.
- Generative Models
  1. Solve the inference problem of determining th class-conditional probabilities $p(\mathbf{x}|\mathcal{C}_k)$
  2. *Also infer the prior class probabilities*
  3. *Use Bayes' theorem to find the posterior* $p(\mathcal{C}_k|\mathbf{x})$
  4. *Alternatively model the joint distribution* $p(\mathbf{x}, \mathcal{C}_k)$ directly.
  5. Use decision theory to assign each new $\mathbf{x}$ to one of the classes.

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Definition

A discriminant is a function that maps from an input vector $\mathbf{x}$ to one of K classes, denoted by $\mathcal{C}_k$.

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$$y(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + w_0$$

such that $\mathbf{x}$ being assigned to class $\mathcal{C}_1$ class $\mathcal{C}_2$ otherwise.

- weight vector $\mathbf{w}$
- bias w_0 (sometimes $-w_0$ called threshold)

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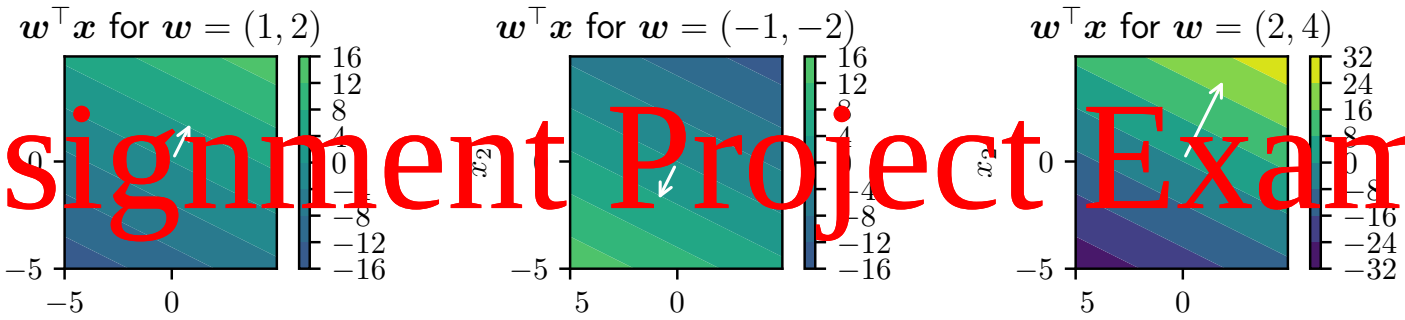
Linear Functions



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- The $+ \quad_0 =$
- Projecting $\mathbf{x}$ on that hyper-plane means find $\arg\min_{\mathbf{x}_\perp} \|\mathbf{x} - \mathbf{x}_\perp\|$ subject to the constrain $\mathbf{w}^\top \mathbf{x}_\perp + w_0 = 0$. Geometrically: move in the d $\quad -$
- Rate of change of function value in that direction is $\frac{\mathrm{d}}{\mathrm{d}a}\left(a\frac{\mathbf{w}}{\|\mathbf{w}\|}\right)^\top \mathbf{w} = a\|\mathbf{w}\|$.
- The length $\left\|a\frac{\mathbf{w}}{\|\mathbf{w}\|}\right\| = \frac{a}{\|\mathbf{w}\|}\|\mathbf{w}\| = a$.
- For a fixed change in $\mathbf{w}^\top\left(a\frac{\mathbf{w}}{\|\mathbf{w}\|}\right)$, $a \propto \frac{1}{\|\mathbf{w}\|}$.

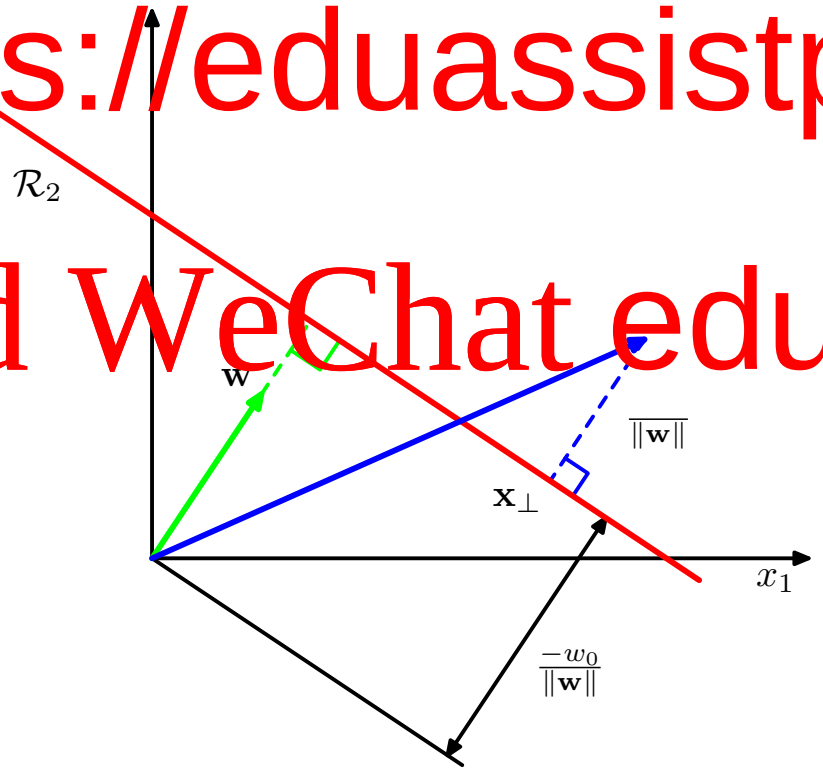
Two Classes

- Decision boundary $y(\mathbf{x}) = 0$ is a $(D-1)$-dimensional hyp
surf
- $\mathbf{w}$ is
- Pro
decision surface. Then,

$$0 = y(\mathbf{x}_A) - y(\mathbf{x}_B) = \mathbf{w}^\top(\mathbf{x}_A - \mathbf{x}_B)$$

- $y(\mathbf{x})$ gives a **signed** measure of the perpendicular distance r **from** the decision surface **to** $\mathbf{x}$, that is $r = y(\mathbf{x})/\|w\|$.

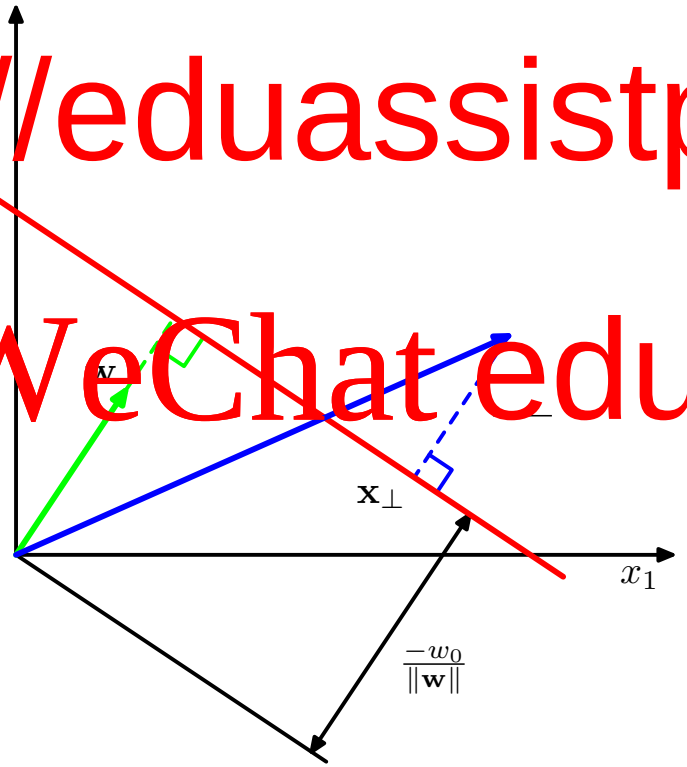
$$y(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + r\frac{\mathbf{w}}{\|\mathbf{w}\|} + w_0 = r\frac{\mathbf{w}^\top \mathbf{w}}{\|\mathbf{w}\|} + \mathbf{w}^\top \mathbf{x} + w_0 = r\,\|w\| + 0$$



Two Classes

- The normal distance from the origin to the decision surface is therefore

$$-\frac{y(\mathbf{0})}{\|w\|} = -\frac{w_0}{\|w\|}$$



Two Classes

- More compact notation : Add an extra dimension to the inp
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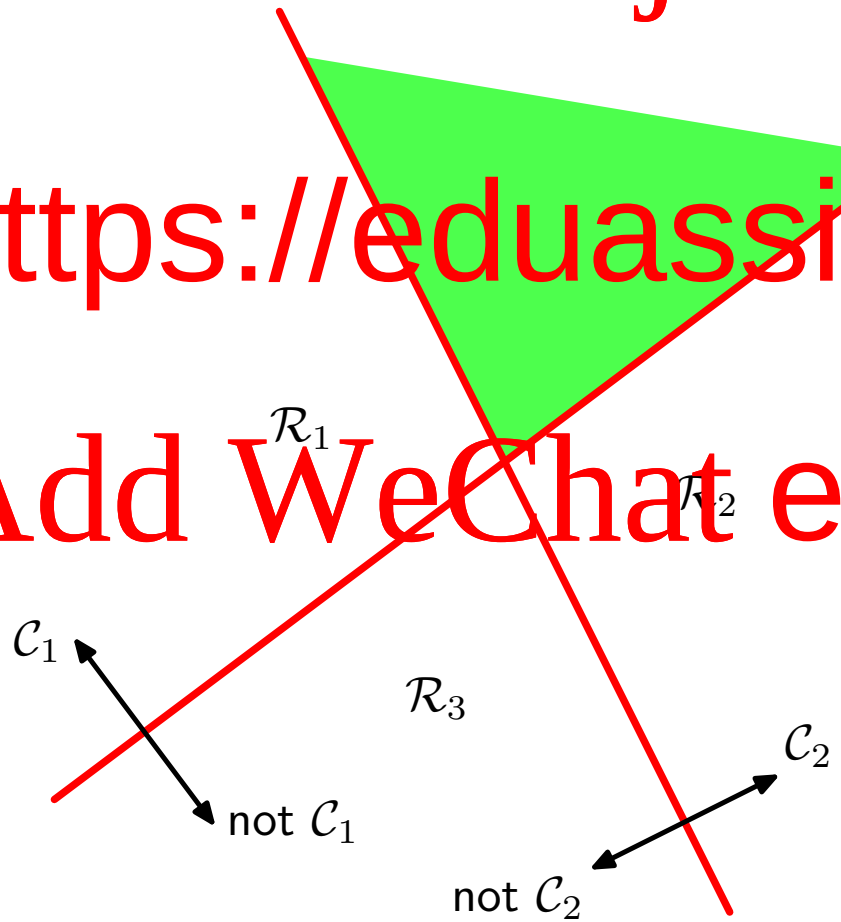
(if it helps, you may think of $\widetilde{\mathbf{w}}^\top$ as a func

- Decision surface is now a D-dimension $D+1$-dimensional expanded input space.

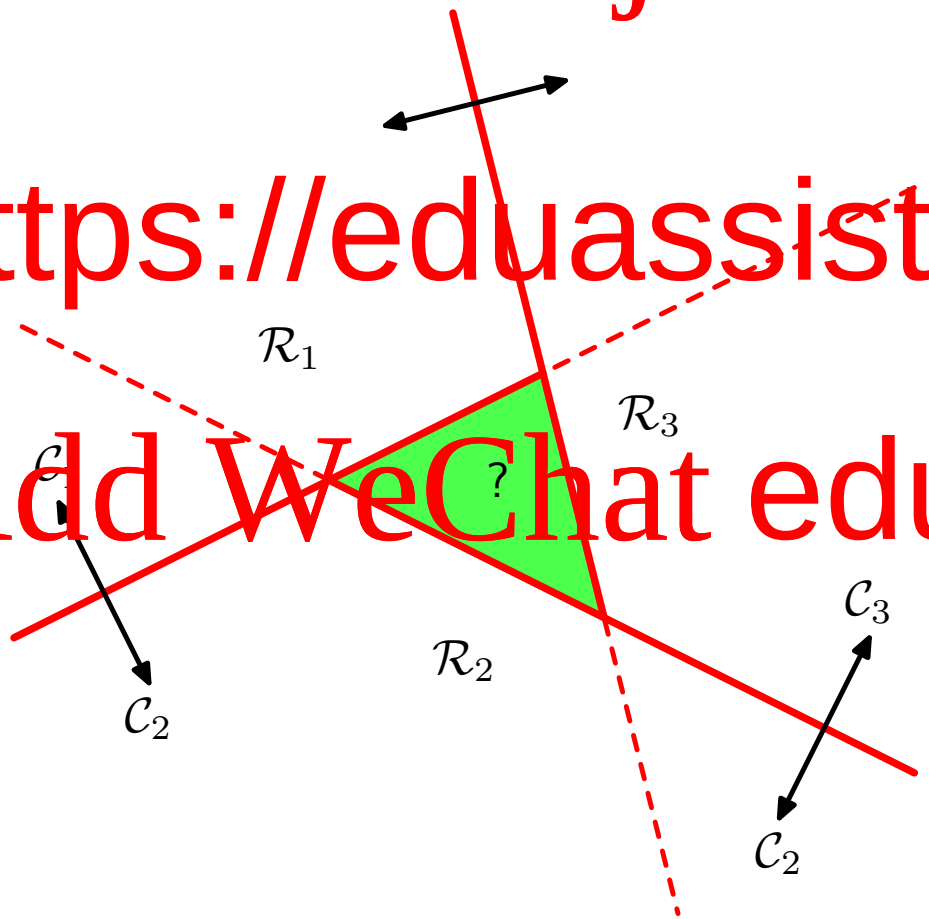
Multi-Class

- Number of classes $K > 2$
- Can we combine a number of two-class discriminant functions using $K - 1$ one-versus-the-rest classifiers?



Multi-Class

- Number of classes $K > 2$
- Can we combine a number of two-class discriminant functions using $K(K-1)/2$ one versus one classifiers?



- Number of classes $K > 2$
- Solution: Use K linear functions

$$y_k(\mathbf{x}) = \mathbf{w}_k^\top \mathbf{x} + w_{k0}$$

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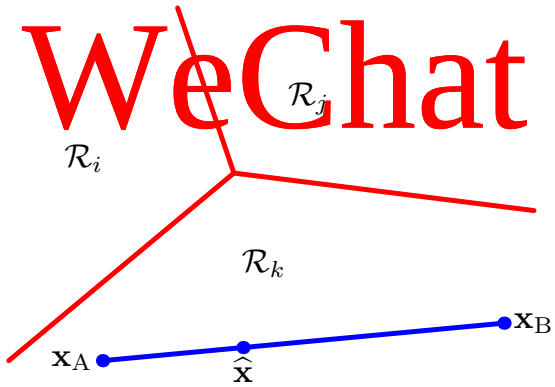
$y_k(\mathbf{x}$ j



Least Squares for Classification

- Regression with a linear function of the model parameters and minimisation of sum-of-squares error function resulted in a cl
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- Use 1-of-K binary coding scheme.
- Each class is described by its own linear model

$$y_k(\mathbf{x}) = \mathbf{w}_k^\top \mathbf{x} + w_{k0} \qquad k =$$

- With the conventions

$$\widetilde{\mathbf{w}}_k = \begin{bmatrix} w_{k0} \\ \mathbf{w}_k \end{bmatrix} \in \mathbb{R}^{D+1}$$

- we get for the (vector valued) discriminant func

$$\mathbf{y}(\mathbf{x}) = \widetilde{\mathbf{W}}^\top \widetilde{\mathbf{x}}$$

(if it helps, you may think of $\widetilde{\mathbf{W}}^\top$ as a **vector-valued** function).

- For a new input $\mathbf{x}$, the class is then defined by the index of the largest value in the row vector $\mathbf{y}(\mathbf{x})$

Determine $\widetilde{\mathbf{W}}$

- Given a training set $\{\mathbf{x}_n, \mathbf{t}_n\}$ where $n = 1, \ldots, N$, and $\mathbf{t}_n$ is the class in the 1-of-K coding scheme.
- Define a matrix $\mathbf{T}$ where row n corresponds to $\mathbf{t}_n^\top$.
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(ch

$$E_D(\widetilde{\ }) = \frac{}{2}\,\mathrm{tr}\ \ (\widetilde{\ }\ \widetilde{\ } - \ \ )\ (\qquad\qquad)$$

- The minimum of $E_D(\widetilde{\mathbf{W}})$ will be reached for

$$\widetilde{\mathbf{W}} = (\widetilde{\mathbf{X}}^\top \widetilde{\mathbf{X}})^{-1} \widetilde{\mathbf{X}}^\top \mathbf{T} = \widetilde{\mathbf{X}}^\dagger \mathbf{T}$$

where $\widetilde{\mathbf{X}}^\dagger$ is the pseudo-inverse of $\widetilde{\mathbf{X}}$.

Discriminant Function for Multi-Class

- The discriminant function $\mathbf{y}(\mathbf{x})$ is therefore

$$\mathbf{y}(\mathbf{x}) = \mathbf{W}^\top \mathbf{x} = \mathbf{T}^\top (\mathbf{X}^\top)^\top \mathbf{x}$$

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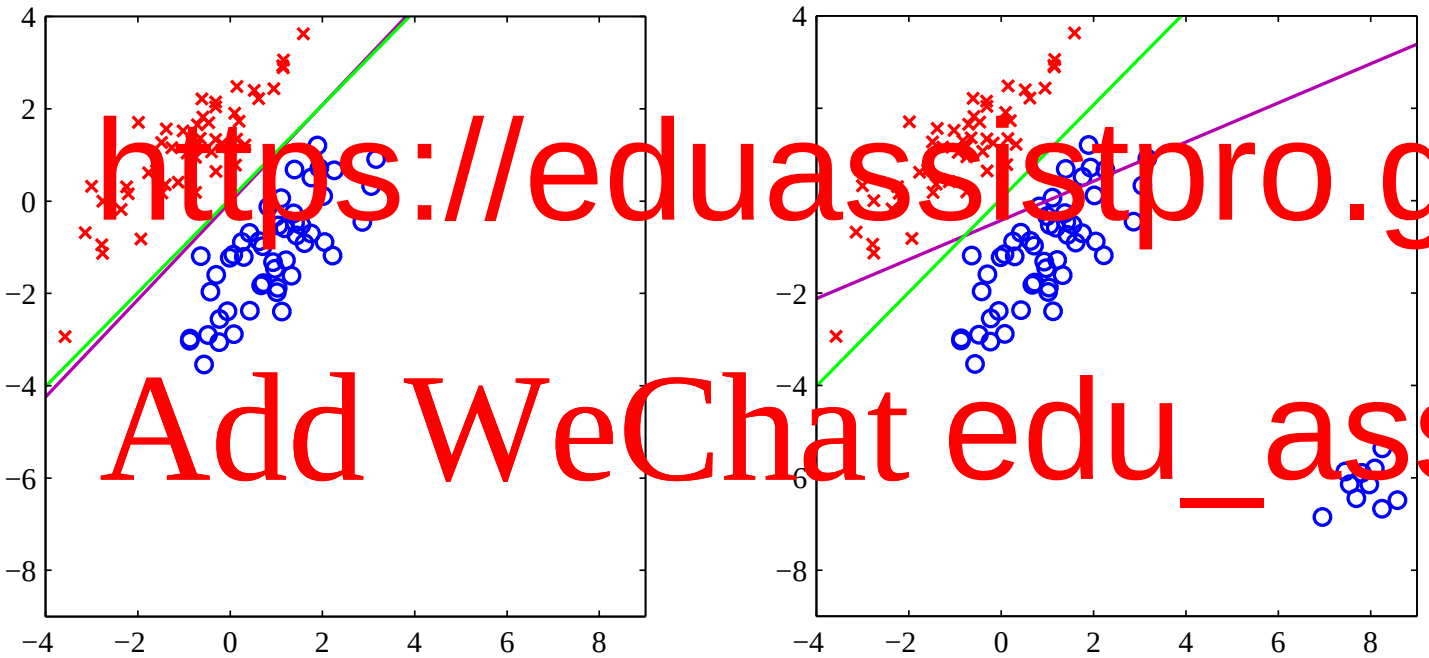
also obey the same constraint

$$\mathbf{a}^\top \mathbf{y}(\mathbf{x}) + b = \mathbf{0}.$$

- For the 1-of-K coding scheme, the sum of all components in $\mathbf{t}_n$ is one, and therefore all components of $\mathbf{y}(\mathbf{x})$ will sum to one. BUT: the components are not probabilities, as they are not constraint to the interval $(0, 1)$.

Deficiencies of the Least Squares Approach

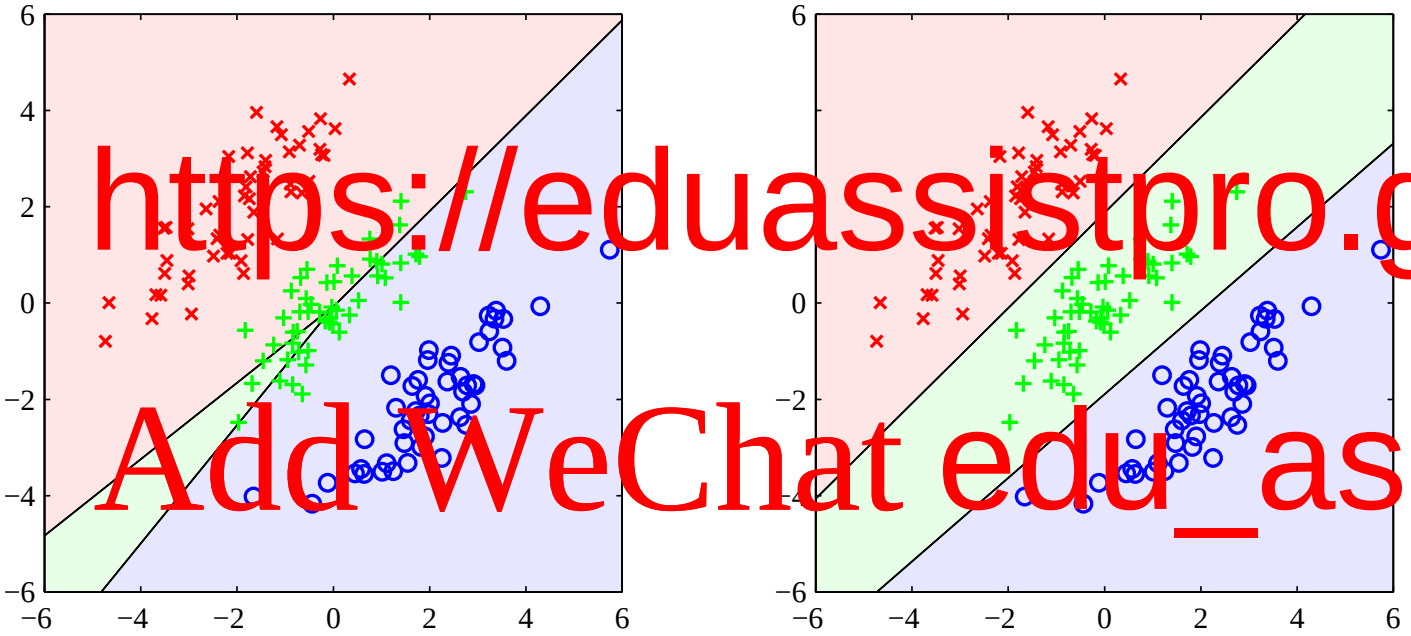
Magenta curve :
Decision Boundary for the least squares approach
Green curve :
Decision boundary for the logistic regression (described later)



(Imagine heat-maps of the quadratic penalty function, similarly to those of the linear functions earlier in the slides.)

Deficiencies of the Least Squares Approach

Left plot : Decision Boundary for least squares
Right plot : Boundaries for logistic regression (described later)



Fisher's Linear Discriminant

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- View linear classification as dimensionality reduction.

$$y(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}$$

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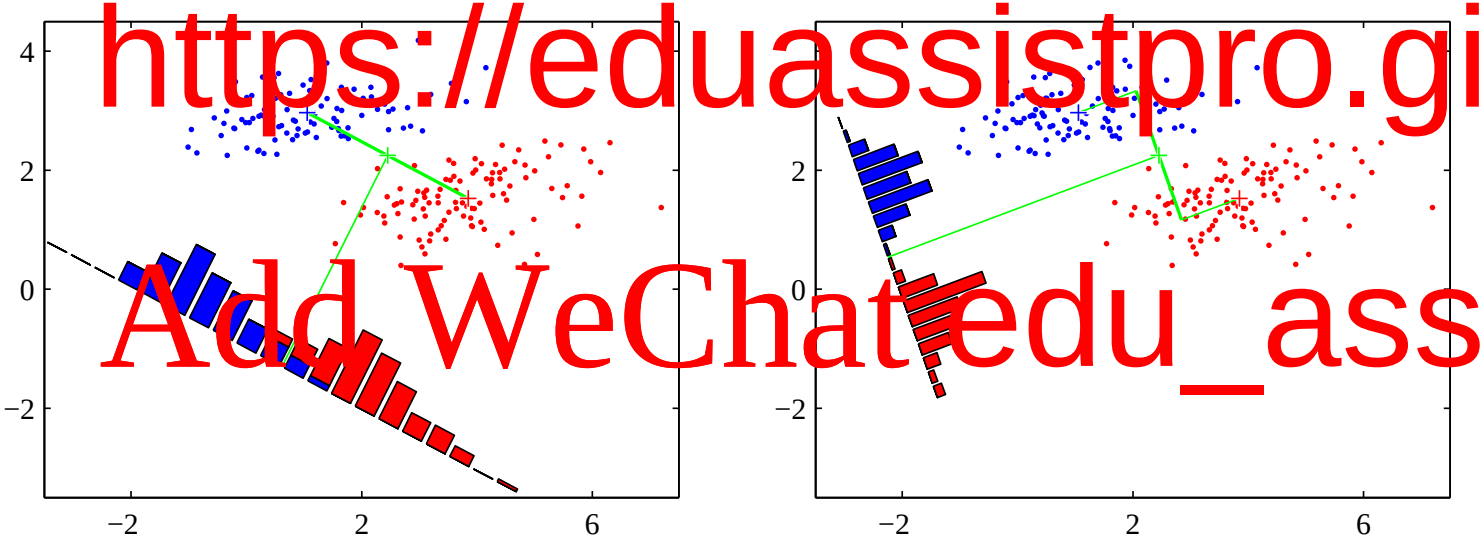
- Projection always means loss of information.
- For classification we want to preserve the class in one dimension.
- Can we find a projection which maximally preserves the class separation ?

Fisher's Linear Discriminant

Samples from two classes in a two-dimensional input space and their histogram when projected to two different one-dimensional spaces.



Fisher's Linear Discriminant - First Try

- Given N_1 input data of class $\mathcal{C}_1$, and N_2 input data of class $\mathcal{C}_2$, calculate the centres of the two classes

$$\mathbf{m}_1 = \frac{1}{N_1} \sum_{n \in \mathcal{C}_1} \mathbf{x}_n, \qquad \mathbf{m}_2 = \frac{1}{N_2} \sum_{n \in \mathcal{C}_2} \mathbf{x}_n$$

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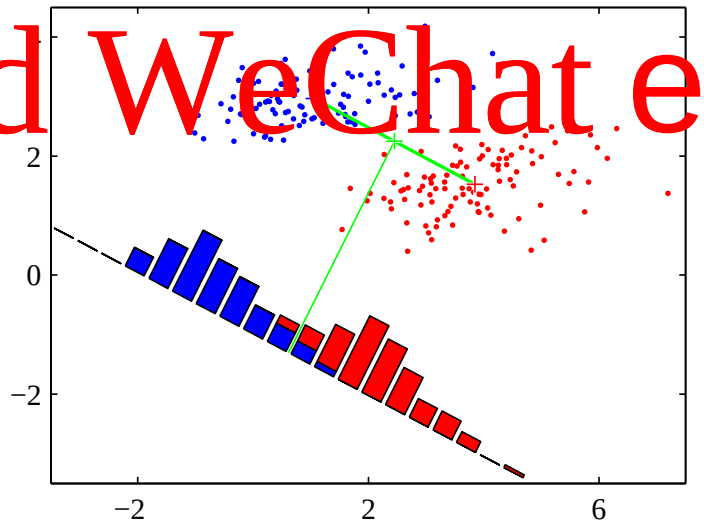
proj

- Problem with non-uniform covariance



Fisher's Linear Discriminant

- Measure also the within-class variance for each class

$$s_k^2 = \sum_{n \in \mathcal{C}_k} (y_n - m_k)^2$$

where $y_n = \mathbf{w}^\top \mathbf{x}_n$.

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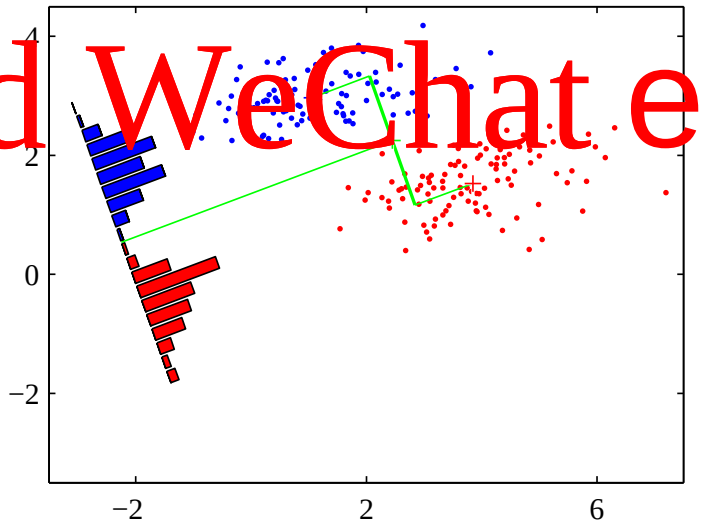

Primer: Bilinear form with a Covariance Matrix

Let

$$\begin{aligned}\boldsymbol{\mu} &= \mathbb{E}[\mathbf{x}] \\ \Sigma &= \mathrm{cov}[\mathbf{x}] \\ &= \mathbb{E}[(\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^\top].\end{aligned}$$

Then

$$\begin{aligned}&= \mathbb{E}\left[(\mathbf{w}^\top\mathbf{x} - \mathbf{w}^\top\mathbb{E}[\mathbf{x}])^2\right] \\ &= \mathbb{E}\left[(\mathbf{w}^\top\mathbf{x} - \mathbf{w}^\top\boldsymbol{\mu})^2\right] \\ &= \mathbb{E}\left[(\mathbf{w}^\top\mathbf{x} - \mathbf{w}^\top\boldsymbol{\mu})(\mathbf{w}^\top\mathbf{x} - \mathbf{w}^\top\boldsymbol{\mu})^\top\right] \\ &= \mathbb{E}\left[(\mathbf{w}^\top\mathbf{x} - \mathbf{w}^\top\boldsymbol{\mu})(\mathbf{x}^\top\mathbf{w} - \boldsymbol{\mu}^\top\mathbf{w})\right] \\ &= \mathbb{E}\left[\mathbf{w}^\top(\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^\top\mathbf{w}\right] \\ &= \mathbf{w}^\top\mathbb{E}\left[(\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^\top\right]\mathbf{w} \\ &= \mathbf{w}^\top\Sigma\mathbf{w}.\end{aligned}$$

Fisher's Linear Discriminant

- The Fisher criterion can be rewritten as

$$J(\mathbf{w}) = \frac{\mathbf{w}^\top \mathbf{S}_B \mathbf{w}}{\mathbf{w}^\top \mathbf{S}_W \mathbf{w}}$$

- $\mathbf{S}_B$ is the between-class covariance

so b

the variance of the projection of the means

- $\mathbf{S}_W$ is the within-class covariance

$$\mathbf{S}_W = \sum_{n \in \mathcal{C}_1} (\mathbf{x}_n - \mathbf{m}_1)(\mathbf{x}_n - \mathbf{m}_1)^T + \sum_{n \in \mathcal{C}_2} ($$

so so by the previous slide and $\mathbf{w}^\top (A + B)\mathbf{w} = \mathbf{w}^\top A\mathbf{w} + \mathbf{w}^\top B\mathbf{w}$, the denominator of $J(\mathbf{w})$ is:
(the variance of the projection of the points in class $\mathcal{C}_1$) +
(the variance of the projection of the points in class $\mathcal{C}_2$)

Fisher's Linear Discriminant

- The Fisher criterion

$$\frac{\mathbf{w}^\top \mathbf{S}_B \mathbf{w}}{}$$

has

$$\mathbf{w} \propto \mathbf{S}_W^{-1}(\mathbf{m}_2 - \mathbf{m}_1)$$

- Fisher's linear discriminant is NOT a discriminant but it can be used to construct one by choosing a threshold y_0 in the projection space.

Fisher's Discriminant For Multi-Class

- Assume that the dimensionality of the input space D is greater than the number of classes K.
- Use $D' > 1$ linear 'features' $y_k = \mathbf{w}^\top \mathbf{x}$ and write everything in vector form (with no bias term)

$$\mathbf{y} = \mathbf{W}^\top \mathbf{x}.$$

- The cov

$$\mathbf{S}_W = \sum_{k=1}^{K} \mathbf{S}_k$$

where

$$\mathbf{S}_k = \sum_{n \in \mathcal{C}_k} (\mathbf{x}_n - \mathbf{m}_k)(\mathbf{x}_n - \mathbf{m}_k)^\top$$

$$\mathbf{m}_k = \frac{1}{N_k} \sum_{n \in \mathcal{C}_k} \mathbf{x}_n$$

Fisher's Discriminant For Multi-Class

- Between-class covariance

$$\mathbf{S}_B = \sum_{k=1}^{K} N_k (\mathbf{m_k} - \mathbf{m})(\mathbf{m_k} - \mathbf{m})^T$$

wh

$$n=1$$

- One possible way to define a function of when the between-class covariance is large a within-class covariance is small is given by

$$J(\mathbf{W}) = \mathrm{tr}\left\{(\mathbf{W}^\top \mathbf{S}_W \mathbf{W})^{-1}(\mathbf{W}^\top \mathbf{S}_B \mathbf{W})\right\}$$

- The maximum of $J(\mathbf{W})$ is determined by the D' eigenvectors of $\mathbf{S}_W^{-1}\mathbf{S}_B$ with the largest eigenvalues.

The Perceptron Algorithm

- Frank Rosenblatt (1928 - 1969)
- "Principles of neurodynamics: Perceptrons and the theory of brain mechanisms" (Spartan Books, 1962)

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The Perceptron Algorithm

- Perceptron ("MARK 1") was the first computer which could learn new skills by trial and error

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The Perceptron Algorithm

- Two class model
- Create feature vector $\phi(\mathbf{x})$ by a fixed nonlinear transformation of the input $\mathbf{x}$.
- Generalised linear model

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$$f(a) = \begin{cases} +1, & a \geqslant \\ -1, & a < \end{cases}$$

- Target coding for perceptron

$$t = \begin{cases} +1, & \text{if } \mathcal{C}_1 \\ -1, & \text{if } \mathcal{C}_2 \end{cases}$$

The Perceptron Algorithm - Error Function

- Idea : Minimise total number of misclassified patterns.
- Problem : As a function of $\mathbf{w}$, this is piecewise constant and t
- Bet wa
- Perceptron Criterion : Add the errors for all patterns belonging to the set of misclassified patterns

$$E_P(\mathbf{w}) = -\sum_{n \in \mathcal{M}} \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}$$

Perceptron - Stochastic Gradient Descent

- Perceptron Criterion (with notation $\phi_n = \phi(\mathbf{x}_n)$)

$$E_P(\mathbf{w}) = -\sum_{n \in \mathcal{M}} \mathbf{w}^\top \phi_n t_n$$
$$\equiv E_P^{(n)}(\mathbf{w})$$

- On
  1.
  2. Update the weight vector $\mathbf{w}$ by

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E$$

where

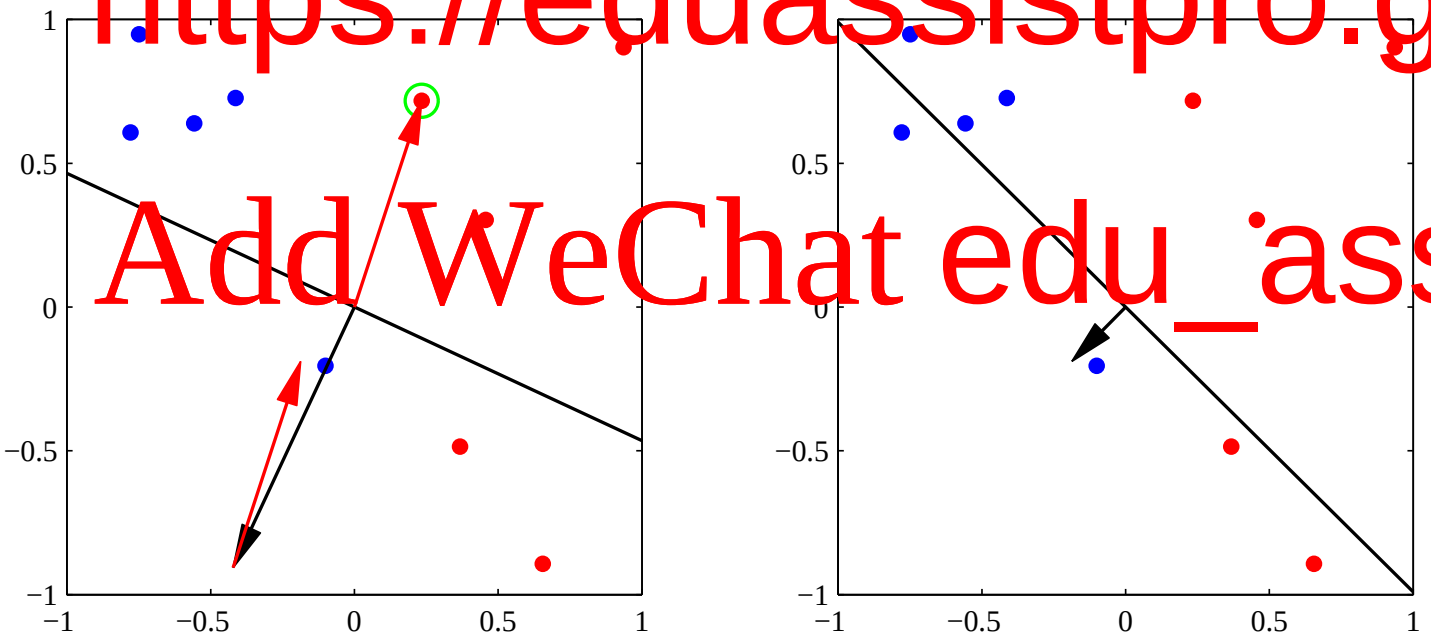
$$\nabla E_P^{(n)}(\mathbf{w}) = \begin{cases} -\phi_n t_n & \text{if } \left(\mathbf{w}^{(\tau)\top} \phi(\mathbf{x}_n) \cdot t_n\right) \leq 0 \\ 0 & \text{otherwise.} \end{cases}$$

- As $y(\mathbf{x}, \mathbf{w})$ is invariant to the norm of $\mathbf{w}$, we may set $\eta = 1$.

The Perceptron Algorithm - Update 1

Update of the perceptron weights from a misclassified pattern (green)

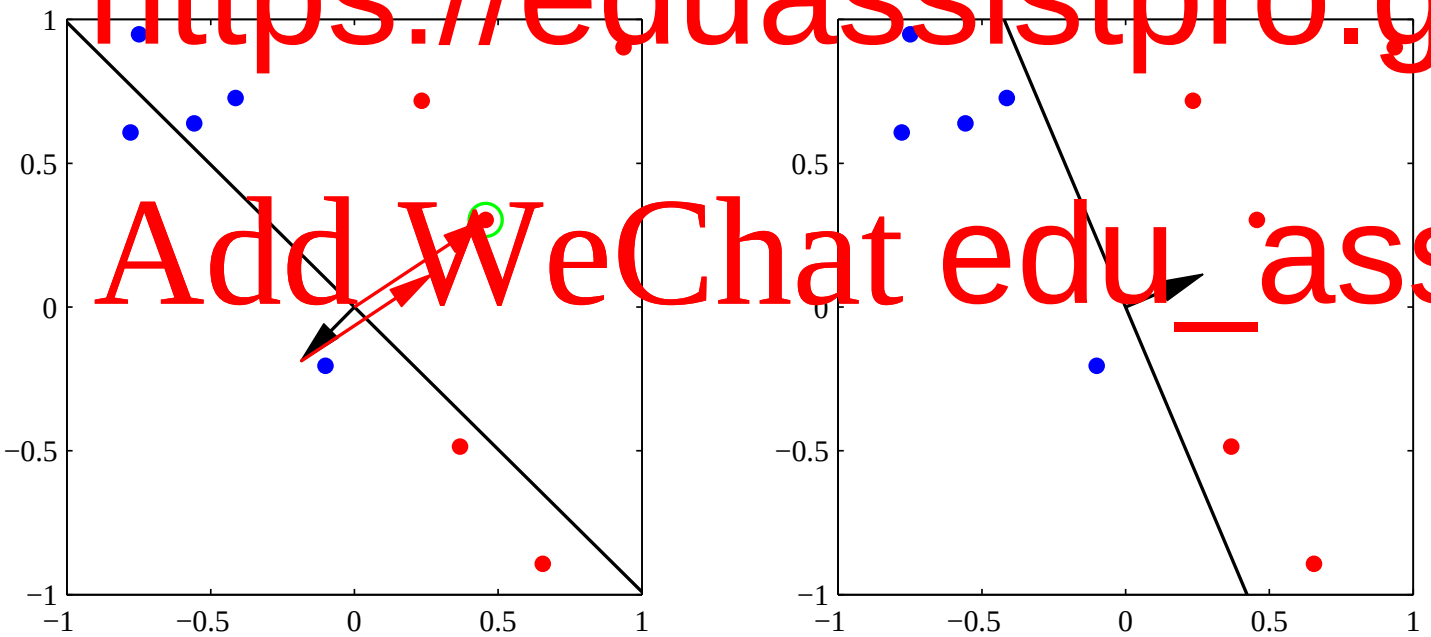
$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} + \boldsymbol{\varphi}_n t_n$$



The Perceptron Algorithm - Update 2

Update of the perceptron weights from a misclassified pattern (green)

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} + \varphi_n t_n$$



The Perceptron Algorithm - Convergence

- Does the algorithm converge ?
- For a single update step, letting $\eta = 1$, and considering the error from a single point,

$$\mathbf{w}^{(\tau+1)T} = \mathbf{w}^{(\tau)T} - \nabla E_n(\mathbf{w}^{(\tau)T})$$

  bec
  gra
  function.

- BUT: contributions to the error from the other mi
  patterns might have increased.

- AND: some correctly classified patterns migh
  misclassified.
- Perceptron Convergence Theorem : If the training set is linearly separable, the perceptron algorithm is guaranteed to find a solution in a finite number of steps.