Introduction to Statistical Machine Learning

Cheng Soon Ong & Christian Walder

Machine Learning Research Group
Data61 | CSIRO
and
College of Engineering and Computer Science
The Australian National University

Canberra
February – June 2019

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

Part V

Linear Classification 1

Strategy in this course

- Estimate best predictor = training = learning
  Given data $(x_1, y_1), \ldots, (x_n, y_n)$, find a predictor $f_{\mathbf{w}}(\cdot)$.
  1. Identify the type of input x and output y data
  2. Propose a (linear) mathematical model for $f_{\mathbf{w}}$
  3. Design an objective function or likelihood
  4. Calculate the optimal parameter ($\mathbf{w}$)
  5. Model uncertainty using the Bayesian approach
  6. Implement and compute (the algorithm in python)
  7. Interpret and diagnose results

Classification

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

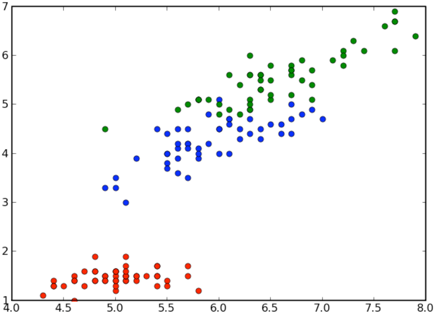


Figure: Length of the petal [in cm] for a given sepal [cm] for iris flowers (Iris Setosa, Iris Versicolor, Iris Virginica).

How to represent binary class labels?

- Class labels are no longer real values as in regression, but a discrete set.
- Two classes : $t \in \{0, 1\}$
  ($t = 1$ represents class $\mathcal{C}_1$ and $t = 0$ represents class $\mathcal{C}_2$)
- Can interpret the value of t as the probability of class $\mathcal{C}_1$, with only two values possible for the probability, 0 or 1.
- Note: Other conventions to map classes into integers possible, check the setup.

How to represent multi-class labels?

- If there are more than two classes ($K > 2$), we call it a multi-class setup.
- Often used: 1-of-K coding scheme in which $\mathbf{t}$ is a vector of length K which has all values 0 except for $t_j = 1$, where j comes from the membership in class C_j to encode.
- Example: Given 5 classes, $\{\mathcal{C}_1, \ldots, \mathcal{C}_5\}$. Membership in 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-classes into integers possible, check the setup.

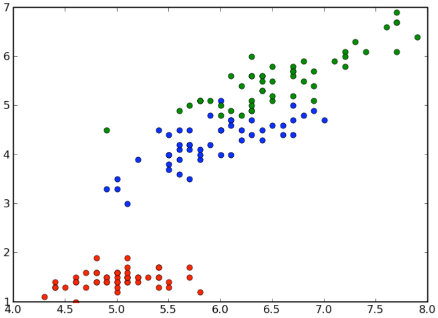
Ong & Walder & Webers
Data61 | CSIRO
The Australian National University

Linear Model

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

$$y(\mathbf{x}_n, \mathbf{w}) = \mathbf{w}^T \phi(\mathbf{x}_n)$$

- But generally $y(\mathbf{x}_n, \mathbf{w}) \in \mathbb{R}$.
  Example: Which class is $y(\mathbf{x}, \mathbf{w}) = 0.71623$?



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

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

- Activation function: $f(\cdot)$
- Link function : $f^{-1}(\cdot)$

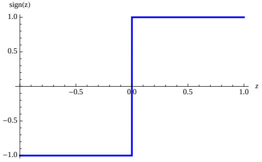


Figure: Example of an activation function $f(z) = \mathrm{sign}\,(z)$.

Three Models for Decision Problems

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

Two Classes

Definition

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

- Consider first two classes ($K = 2$).
- Construct a linear function of the inputs $\mathbf{x}$

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

  such that $\mathbf{x}$ being assigned to class $\mathcal{C}_1$ if $y(\mathbf{x}) \geq 0$, and to class $\mathcal{C}_2$ otherwise.
- weight vector $\mathbf{w}$
- bias w_0 (sometimes $-w_0$ called threshold)

Two Classes

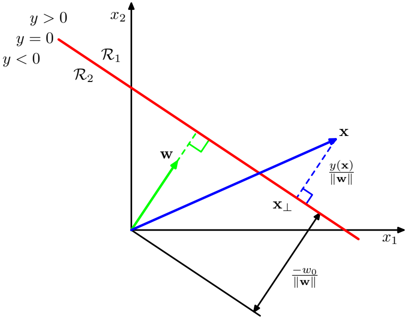
- Decision boundary $y(\mathbf{x}) = 0$ is a $(D-1)$-dimensional hyperplane in a D-dimensional input space (decision surface).
- $\mathbf{w}$ is orthogonal to any vector lying in the decision surface.
- Proof: Assume $\mathbf{x}_A$ and $\mathbf{x}_B$ are two points lying in the decision surface. Then,

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

Two Classes

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

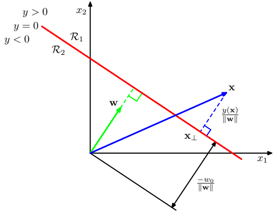
$$\frac{\mathbf{w}^T \mathbf{x}}{\|w\|} = -\frac{w_0}{\|w\|}$$



Two Classes

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

$$y(\mathbf{x}) = \mathbf{w}^T \overbrace{\left(\mathbf{x}_\perp + r\frac{\mathbf{w}}{\|w\|}\right)}^{\mathbf{x}} + w_0 = r\frac{\mathbf{w}^T\mathbf{w}}{\|w\|} + \overbrace{\mathbf{w}^T\mathbf{x}_\perp + w_0}^{0} = r\|w\|$$



Two Classes

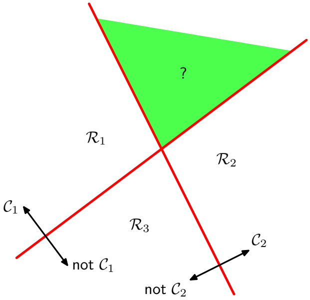
- More compact notation : Add an extra dimension to the input space and set the value to $x_0 = 1$.
- Also define $\widetilde{\mathbf{w}} = (w_0, \mathbf{w})$ and $\widetilde{\mathbf{x}} = (1, \mathbf{x})$

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

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

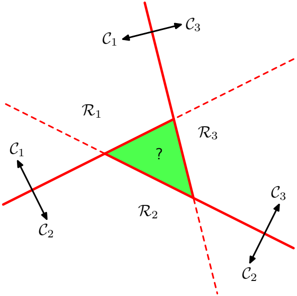
Multi-Class

- 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?



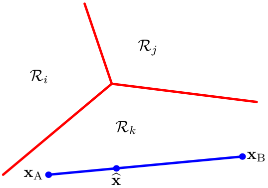
Ong & Walder & Webers
Data61 | CSIRO
The Australian National University

Multi-Class

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

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

- Assign input $\mathbf{x}$ to class $\mathcal{C}_k$ if $y_k(\mathbf{x}) > y_j(\mathbf{x})$ for all $j \neq k$.
- Decision boundary between class $\mathcal{C}_k$ and $\mathcal{C}_j$ given by $y_k(\mathbf{x}) = y_j(\mathbf{x})$



Least Squares for Classification

- Regression with a linear function of the model parameters and minimisation of sum-of-squares error function resulted in a closed-from solution for the parameter values.
- Is this also possible for classification?
- Given input data $\mathbf{x}$ belonging to one of K classes $\mathcal{C}_k$.
- Use 1-of-K binary coding scheme.
- Each class is described by its own linear model

$$y_k(\mathbf{x}) = \mathbf{w}_k^T \mathbf{x} + w_{k0} \qquad k = 1, \dots, K$$

Least Squares for Classification

- With the conventions

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

$$\widetilde{\mathbf{x}} = \begin{bmatrix} 1 \\ \mathbf{x} \end{bmatrix} \qquad \in \mathbb{R}^{D+1}$$

$$\widetilde{\mathbf{W}} = \begin{bmatrix} \widetilde{\mathbf{w}}_1 & \dots & \widetilde{\mathbf{w}}_K \end{bmatrix} \qquad \in \mathbb{R}^{(D+1)\times K}$$

- we get for the discriminant function (vector valued)

$$\mathbf{y}(\mathbf{x}) = \widetilde{\mathbf{W}}^T \widetilde{\mathbf{x}} \qquad \in \mathbb{R}^K.$$

- 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 $\{\mathbf{x}_n, \mathbf{t}\}$ where $n = 1, \dots, N$, and $\mathbf{t}$ is the class in the 1-of-K coding scheme.
- Define a matrix $\mathbf{T}$ where row n corresponds to $\mathbf{t}_n^T$.
- The sum-of-squares error can now be written as

$$E_D(\widetilde{\mathbf{W}}) = \frac{1}{2} \operatorname{tr}\left\{(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})^T (\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})\right\}$$

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

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

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

$$\mathbf{y}(\mathbf{x}) = \widetilde{\mathbf{W}}^T \widetilde{\mathbf{x}} = \mathbf{T}^T (\widetilde{\mathbf{X}}^\dagger)^T \widetilde{\mathbf{x}},$$

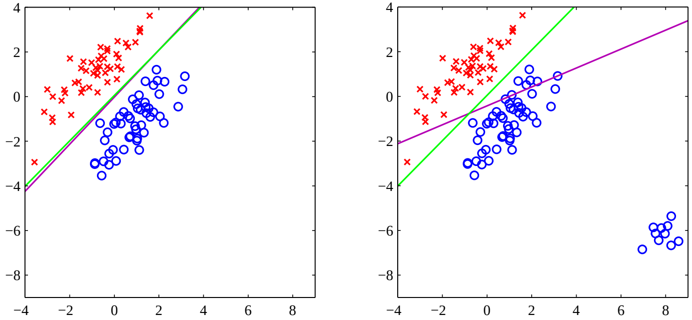
  where $\widetilde{\mathbf{X}}$ is given by the training data, and $\widetilde{\mathbf{x}}$ is the new input.
- Interesting property: If for every $\mathbf{t}_n$ the same linear constraint $\mathbf{a}^T \mathbf{t}_n + b = 0$ holds, then the prediction $\mathbf{y}(\mathbf{x})$ will also obey the same constraint

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

- 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 $(0, 1)$.

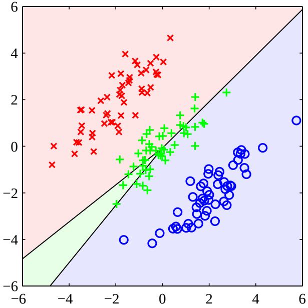
Deficiencies of the Least Squares Approach

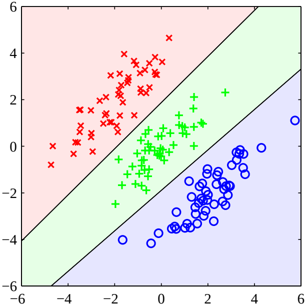
Magenta curve : Decision Boundary for the least squares approach (Green curve : Decision boundary for the logistic regression model described later)



Deficiencies of the Least Squares Approach

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





Fisher's Linear Discriminant

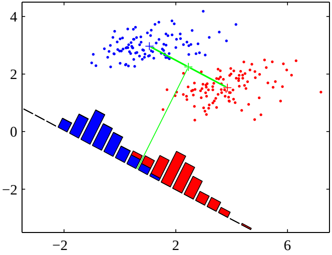
- View linear classification as dimensionality reduction.

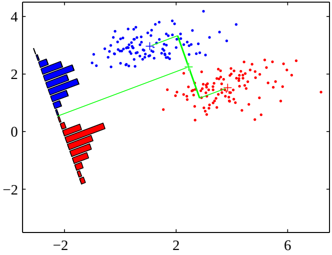
$$y(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$$

  If $y \geq -w_0$ then class $\mathcal{C}_1$, otherwise $\mathcal{C}_2$.
- But there are many projections from a D-dimensional input space onto one dimension.
- Projection always means loss of information.
- For classification we want to preserve the class separation 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

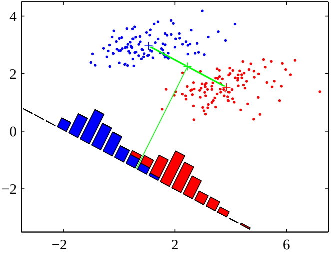
- Given N_1 input data of class $\mathcal{C}_1$, and N_2 input data of class $\mathcal{C}_2$, calculate the centres of the two classes

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

- Choose $\mathbf{w}$ so as to maximise the projection of the class means onto $\mathbf{w}$

$$m_1 - m_2 = \mathbf{w}^T (\mathbf{m}_1 - \mathbf{m}_2)$$

- Problem with non-uniform covariance



Fisher's Linear Discriminant

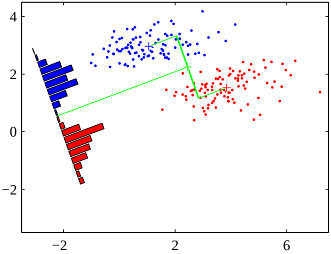
- Measure also the within-class variance for each class

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

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

- Maximise the Fisher criterion

$$J(\mathbf{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2}$$



Fisher's Linear Discriminant

- The Fisher criterion can be rewritten as

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

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

$$\mathbf{S}_B = (\mathbf{m}_2 - \mathbf{m}_1)(\mathbf{m}_2 - \mathbf{m}_1)^T$$

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

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

Fisher's Linear Discriminant

- The Fisher criterion

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

  has a maximum for Fisher's linear discriminant

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

- Fisher's linear discriminant is NOT a discriminant, but 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' $y_k = \mathbf{w}^T \mathbf{x}$ and write everything in vector form (no bias involved!)

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

- The within-class covariance is then the sum of the covariances for all K classes

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

where

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

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

Fisher's Discriminant For Multi-Class

- Between-class covariance

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

  where $\mathbf{m}$ is the total mean of the input data

$$\mathbf{m} = \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_n.$$

- One possible way to define a function of $\mathbf{W}$ which is large when the between-class covariance is large and the within-class covariance is small is given by

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

- 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)

The Perceptron Algorithm

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

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

$$y(\mathbf{x}) = f(\mathbf{w}^T \phi(\mathbf{x}))$$

with $\phi(\mathbf{x})$ containing some bias element $\phi_0(\mathbf{x}) = 1$.

- nonlinear activation function

$$f(a) = \begin{cases} +1, & a \geq 0 \\ -1, & a < 0 \end{cases}$$

- 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 therefore the gradient is zero almost everywhere.
- Better idea: Using the $(-1, +1)$ target coding scheme, we want all patterns to satisfy $\mathbf{w}^T \phi(\mathbf{x}_n) t_n > 0$.
- Perceptron Criterion : Add the errors for all patterns belonging to the set of misclassified patterns $\mathcal{M}$

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

Perceptron - Stochastic Gradient Descent

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

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

- One iteration at step τ
  1. Choose a training pair $(\mathbf{x}_n, t_n)$
  2. Update the weight vector $\mathbf{w}$ by

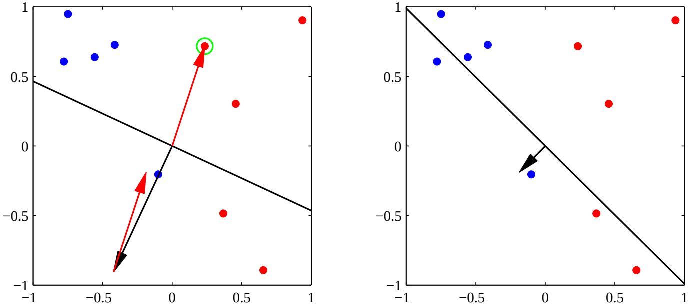
$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_P(\mathbf{w}) = \mathbf{w}^{(\tau)} + \eta \phi_n t_n$$

- As $y(\mathbf{x}, \mathbf{w})$ does not depend on the norm of $\mathbf{w}$, one can set $\eta = 1$

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

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

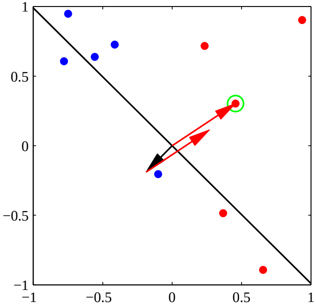
$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} + \phi_n t_n$$

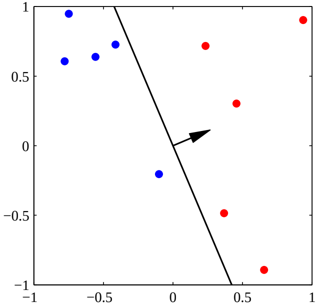


The Perceptron Algorithm - Update 2

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

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





The Perceptron Algorithm - Convergence

- Does the algorithm converge ?
- For a single update step

$$-\mathbf{w}^{(\tau+1)T}\boldsymbol{\phi}_n t_n = -\mathbf{w}^{(\tau)T}\boldsymbol{\phi}_n t_n - (\boldsymbol{\phi}_n t_n)^T\boldsymbol{\phi}_n t_n < -\mathbf{w}^{(\tau)T}\boldsymbol{\phi}_n t_n$$

  because $(\boldsymbol{\phi}_n t_n)^T\boldsymbol{\phi}_n t_n = \|\boldsymbol{\phi}_n t_n\| > 0$.
- BUT: contributions to the error from the other misclassified patterns might have increased.
- AND: some correctly classified patterns might now be 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.