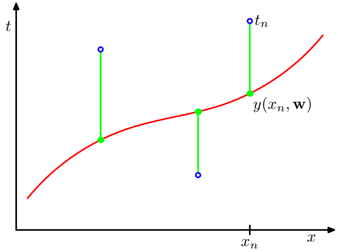
Linear Regression and Classification Revisited

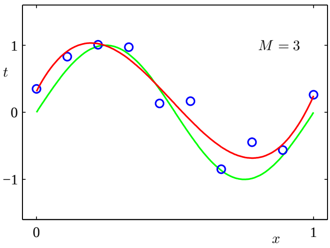
Dr. Víctor Uc Cetina

Universität Hamburg

Content

Linear Regression





- x is the input variable, t is the output variable, $\mathbf{w}$ is the parameters vector of our model and the data points were generated from $\sin(2\pi x) + \varepsilon$.
- For our model $y(x, \mathbf{w}) = w_0 + w_1 x + \ldots + w_M x^M$, we need to search for the best M and we need to learn the parameters $\mathbf{w}$.
- Such parameter vector $\mathbf{w}$ can be learned iteratively or directly.

Estimating the Parameters $\mathbf{w}$

Stochastic Gradient Descent

Loop {

for $i = 1$ to m {

$$w_j := w_j + \alpha\left[t^{(i)} - y(x^{(i)}, \mathbf{w})\right]x_j^{(i)} \qquad \text{(for every } j\text{)}.$$

}

}

Normal Equations

$\mathbf{w} = (\mathbf{X}^\top \mathbf{X})^{-1}\mathbf{X}^\top \mathbf{y}.$

Locally Weighted Linear Regression

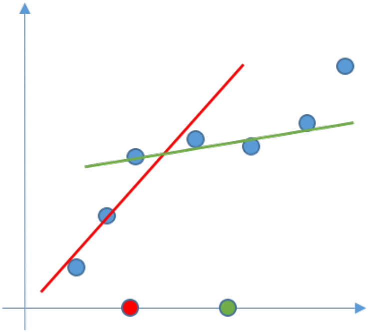
The algorithm works as follows:

1. Fit **w** to minimize $\sum_i \sigma^{(i)}(t^{(i)} - \mathbf{w}^\top x^{(i)})^2$.
2. Output $\mathbf{w}^\top x$.

Where $\sigma^{(i)}$'s are non-negative valued weights.

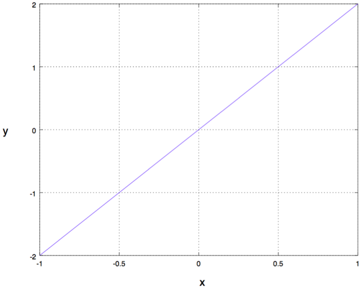
A good choice for the weights is:

$$\sigma^{(i)} = \exp\left(- \frac{(x^{(i)} - x)^2}{2\tau^2} \right)$$

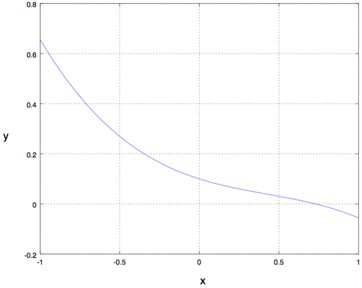


Polynomial Functions

$y = 2x$

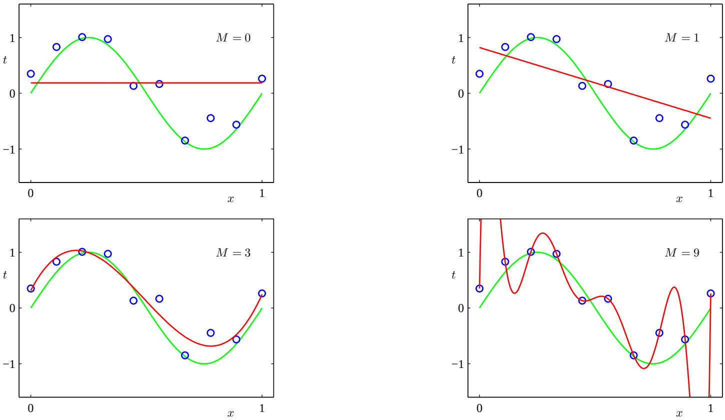


$y = 0.1 - 0.2x + 0.2x^2 - 0.156x^3$



- For polynomial functions, we need to try systematically different M's and evaluate the performance of our current model.

Polynomial Functions



- Polynomial functions with different orders M.

Evaluation of Performance

- For each choice of M we can evaluate the performance of the model using the root-mean-square error E_{RMS}.

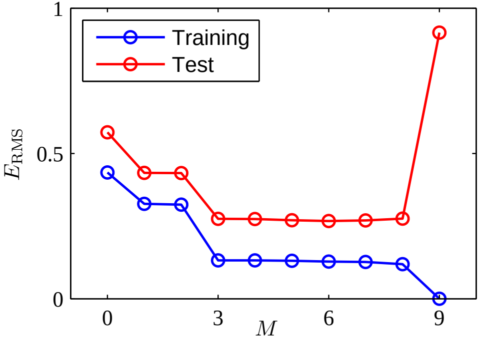
$$E_{\mathrm{RMS}} = \sqrt{2E(\mathbf{w})/N}$$

where

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2$$

- This error can also be used to evaluate if our model's performance is improving after each iteration of the learning algorithm.

Evaluation of Performance



Generalized Linear Regression

- The goal of regression is to predict the value of one or more continuous target variables t given the value of a D-dimensional vector $\mathbf{x}$ of input variables.
- The simplest linear model for regression is one that involves a linear combination of the input variables

$$y(\mathbf{x}, \mathbf{w}) = w_0 + w_1 x_1 + \ldots + w_D x_D$$

where

$$\mathbf{x} = (x_1, \ldots, x_D)^\top$$

- The key property of this model is that it is a linear function of the parameters $w_0, \ldots, w_D$. It is also, however, a linear function of the input variables x_i, and this imposes significant limitations on the model.

Generalized Linear Regression

- However, we can obtain a much more useful class of functions by taking linear combinations of a fixed set of nonlinear functions of the input variables, of the form

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x})$$

  where $\phi_j(\mathbf{x})$ are known as basis functions.
- Such models are linear functions of the parameters, which gives them simple analytical properties, and yet can be nonlinear with respect to the input variables.

Generalized Linear Regression

- It is often convenient to define an additional dummy basis function $\phi_0(x) = 1$ so that

$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^\top \phi(\mathbf{x})$$

where

$$w = (w_0, w_1, \ldots, w_{M-1})^\top$$

and

$$\phi = (\phi_0, \phi_1, \ldots, \phi_{M-1})^\top$$

Basis Functions

- Polynomial regression is a particular example of basis functions models in which there is a single input variable x, and the basis functions take the form of powers of x so that $\phi_j(x) = x^j$.
- One limitation of polynomial basis functions is that they are global functions of the input variable, so that changes in one region of input space affect all other regions.
- This can be resolved by dividing the input space into regions and fit a different polynomial in each region, leading to spline functions.

Basis Functions

- Other possible choices for the basis functions are Gaussian basis functions and sigmoidal basis functions
- Gaussian basis functions:

$$\phi_j(x) = \exp\left\{ -\frac{(x-\mu_j)^2}{2s^2} \right\}$$

where the μ_j govern the locations of the basis functions in input space, and the parameter s governs their spatial scale.

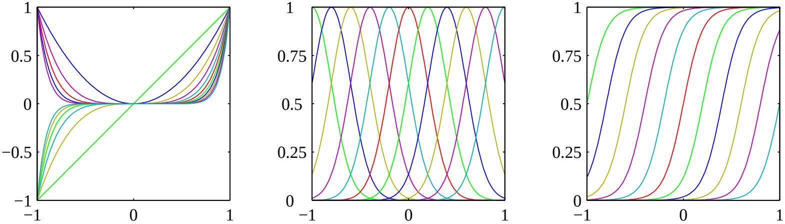
- Sigmoidal basis functions:

$$\phi_j(x) = \sigma\left(\frac{x-\mu_j}{s} \right)$$

where

$$\sigma(a) = \frac{1}{1+\exp(-a)}$$

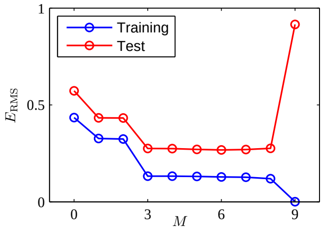
Basis Functions



Polynomial Gaussian Sigmoidal

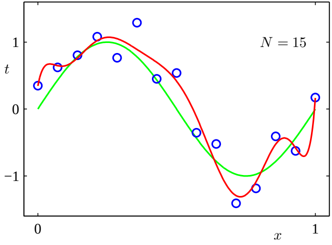
- Linear models have significant limitations as practical techniques for machine learning, particularly for problems involving input spaces of high dimensionality.
- However, they form the foundation of more sophisticated models such as neural networks and support vector machines.

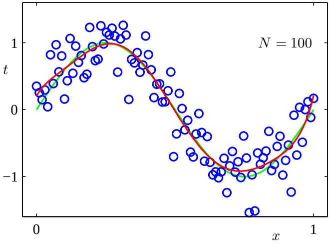
Parameters Going Wild



	$M = 0$	$M = 1$	$M = 3$	$M = 9$
w_0	0.19	0.82	0.31	0.35
w_1		-1.27	7.99	232.37
w_2			-25.43	-5321.83
w_3			17.37	48568.31
w_4				-231639.30
w_5				640042.26
w_6				-1061800.52
w_7				1042400.18
w_8				-557682.99
w_9				125201.43

Importance of Dataset Size





- Two solutions with $M = 9$. In the left using $N = 15$ training examples. In the right using $N = 100$ training examples.

Regularization Term

- We can add a regularization term to the error function in order to control over-fitting, so that the total error function to be minimized takes the form

$$E(\mathbf{w}) = E_D(\mathbf{w}) + \lambda E_W(\mathbf{w})$$

where λ is the regularization coefficient that controls the relative importance of the data-dependent error $E_D(\mathbf{w})$ and the regularization term $E_W(\mathbf{w})$.

$$E_D(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{t_n - \mathbf{w}^\top \phi(\mathbf{x}_n)\}^2$$

Regularization Term

- One of the simplest forms of regularizer is given by the sum-of-squares of the weight vector elements

$$E_W(\mathbf{w}) = \frac{1}{2}\mathbf{w}^\top\mathbf{w}$$

- Then, instead of minimizing

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^\top\phi(\mathbf{x}_n)\}^2.$$

- We minimize

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^\top\phi(\mathbf{x}_n)\}^2 + \frac{\lambda}{2}\mathbf{w}^\top\mathbf{w}.$$

Estimating the Parameters **w** with Regularization

Stochastic Gradient Descent

Loop $\{$

for $i = 1$ to m $\{$

$$w_j := w_j + \alpha\big[t^{(i)} - y(x^{(i)}, \mathbf{w})\big]x_j^{(i)} + \frac{\lambda}{m} w_j \qquad \text{(for every } j\text{).}$$

$\}$

$\}$

Normal Equations

$$\mathbf{w} = (\lambda \mathrm{I} + \mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

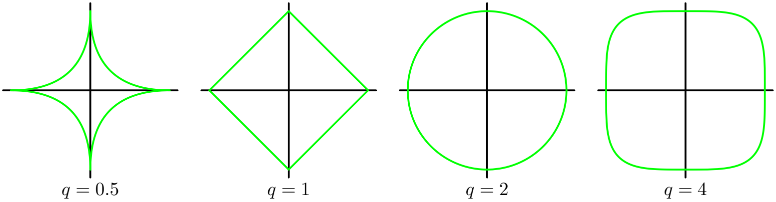
Different Types of Regularizers

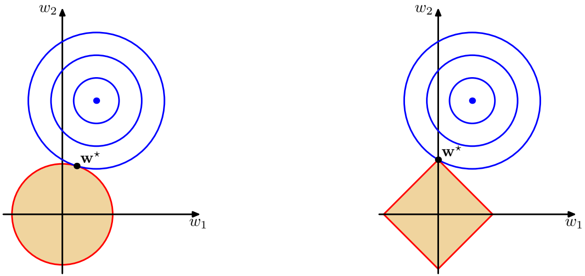
- Sometimes a more general regularizer is used, for which de regularized error takes the form

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^\top \phi(\mathbf{x}_n)\}^2 \; + \; \frac{\lambda}{2}\sum_{j=1}^{M}|w_j|^q.$$

where $q = 2$ corresponds to the quadratic regularizer.

Types of Regularizers and their Effects





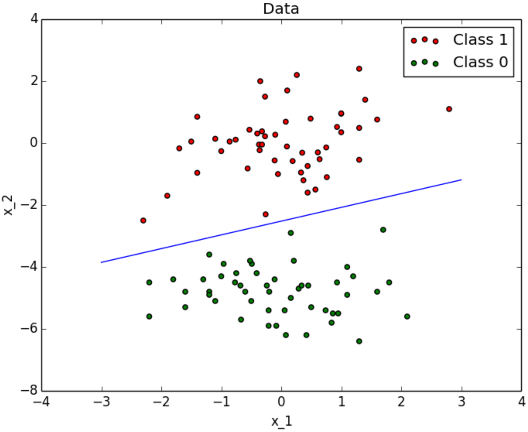
Benefits of Regularization

- Regularization allows complex models to be trained on data sets of limited size without severe over-fitting, essentially by limiting the effective model complexity.
- However, the problem of determining the optimal model complexity is then shifted from one of finding the appropriate number of basis functions to one of determining a suitable value of the regularization coefficient λ.

Linear Classification

- The goal in classification is to take an input vector $\mathbf{x}$ and to assign it to one of K discrete classes C_k where $k = 1, \ldots, K$.
- In the most common scenario, the classes are taken to be disjoint, so that each input is assigned to one and only one class.
- The input space is thereby divided into decision regions whose boundaries are called decision boundaries or decision surfaces.
- Data sets whose classes can be separated exactly by linear decision surfaces are said to be linearly separable.

Linear Classification



Two cloud of points linearly separable.

Linear Classification

- For classification problems, however, we wish to predict discrete class labels, or more generally posterior probabilities that lie in the range $(0, 1)$.
- To achieve this, we consider a generalization of this model in which we transform the linear function of $\mathbf{w}$ using a nonlinear function $f(\cdot)$ so that

$$y(\mathbf{x}) = f(\mathbf{w}^\top \mathbf{x} + w_o).$$

  where $f(\cdot)$ is known as the activation function.
- An input vector $\mathbf{x}$ is assigned to class C_1 if $y(\mathbf{x}) \geq 0$ and to class C_2 otherwise.

Discriminant Functions

- A discriminant is a function that takes an input vector $\mathbf{x}$ and assigns it to one of K classes, denoted C_k.
- The simplest representation of a linear discriminant function is obtained by taking a linear function of the input vector so that

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

where $\mathbf{w}$ is called a weight vector, and w_0 is a bias.

Discriminant Functions

- The corresponding decision boundary is therefore defined by the relation $y(x) = 0$, which corresponds to a (D-1)-dimensional hyperplane within the D-dimensional input space.
- Consider two points x_A and x_B both of which lie on the decision surface.
- Because $y(\mathbf{x}_A) = y(\mathbf{x}_B) = 0$, we have $\mathbf{w}^\top(\mathbf{x}_A - \mathbf{x}_B) = 0$ and hence the vector $\mathbf{w}$ is orthogonal to every vector lying within the decision surface.
- So $\mathbf{w}$ determines the orientation of the decision surface.

Discriminant Functions

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

$$y(\mathbf{x}_A) = y(\mathbf{x}_B) = 0$$

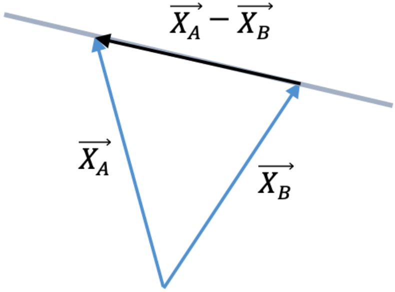
$$y(\mathbf{x}_A) = y(\mathbf{x}_B)$$

$$\mathbf{w}^\top \mathbf{x}_A + w_o = \mathbf{w}^\top \mathbf{x}_B + w_o$$

$$\mathbf{w}^\top \mathbf{x}_A = \mathbf{w}^\top \mathbf{x}_B$$

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

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



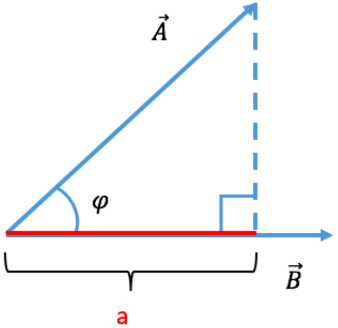
Discriminant Functions

- Similarly, if x is a point on the decision surface, then $y(x) = 0$, and so the normal distance from the origin to the decision surface is given by

$$\frac{\mathbf{w}^\top \mathbf{x}}{||\mathbf{w}||} = -\frac{w_o}{||\mathbf{w}||}$$

- We therefore see that the bias parameter w_0 determines the location of the decision surface.

Discriminant Functions



$$\cos\varphi = \frac{a}{||\vec{A}||}$$

$$a = ||\vec{A}||\cos\varphi \qquad (1)$$

$$\vec{A}\cdot\vec{B} = ||\vec{A}||\,||\vec{B}||\cos\varphi$$

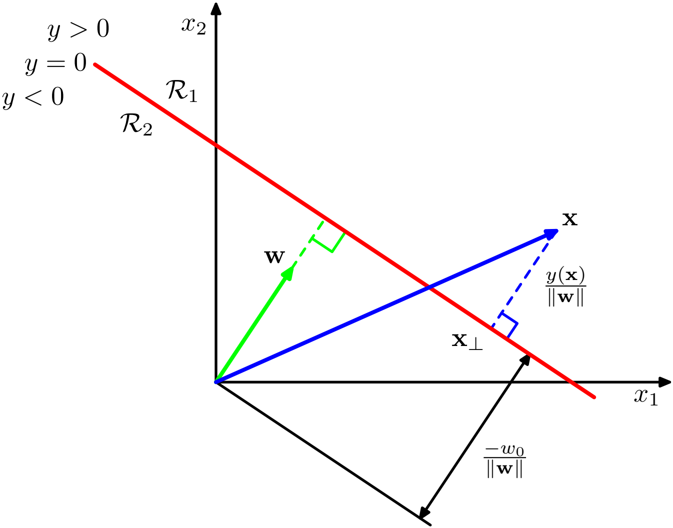
$$\cos\varphi = \frac{\vec{A}\cdot\vec{B}}{||\vec{A}||\,||\vec{B}||} \qquad (2)$$

Subst. (2) in (1)

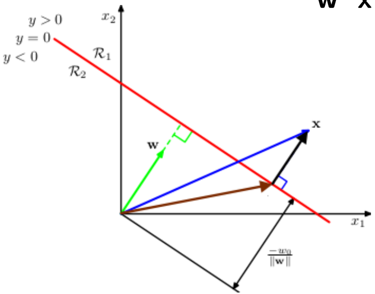
$$a = ||\vec{A}||\left(\frac{\vec{A}\cdot\vec{B}}{||\vec{A}||\,||\vec{B}||}\right)$$

$$= \frac{\vec{A}\cdot\vec{B}}{||\vec{B}||}$$

Discriminant Functions



Discriminant Functions



$$
\begin{aligned}
\mathbf{x} &= \mathbf{x}_\perp + r\frac{\mathbf{w}}{||\mathbf{w}||} \\
\mathbf{w}^\top \mathbf{x} + w_0 &= \mathbf{w}^\top\left(\mathbf{x}_\perp + r\frac{\mathbf{w}}{||\mathbf{w}||}\right) + w_0 \\
y(\mathbf{x}) &= \mathbf{w}^\top \mathbf{x}_\perp + r\frac{\mathbf{w}^\top \mathbf{w}}{||\mathbf{w}||} + w_0 \\
y(\mathbf{x}) &= \mathbf{w}^\top \mathbf{x}_\perp + w_0 + r\frac{\mathbf{w}^\top \mathbf{w}}{||\mathbf{w}||} \\
y(\mathbf{x}) &= r\frac{\mathbf{w}^\top \mathbf{w}}{||\mathbf{w}||} \\
y(\mathbf{x}) &= r\frac{||\mathbf{w}||\ ||\mathbf{w}||}{||\mathbf{w}||} \quad \text{(See explanation below)} \\
y(\mathbf{x}) &= r\ \ ||\mathbf{w}|| \\
r &= \frac{y(\mathbf{x})}{||\mathbf{w}||} \quad \text{(Dist. between } \mathbf{x} \text{ and decision boundary)}
\end{aligned}
$$

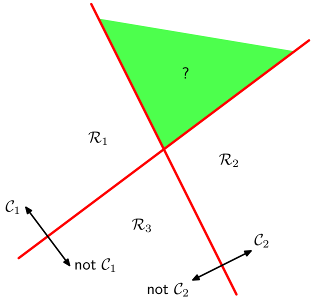
Let $\mathbf{w} = (w_1, w_2, \ldots, w_n)$, then the following is true:
$\mathbf{w}^\top \mathbf{w} = w_1^2 + w_2^2 + \cdots + w_n^2 = \sqrt{w_1^2 + w_2^2 + \cdots + w_n^2}\sqrt{w_1^2 + w_2^2 + \cdots + w_n^2} = ||\mathbf{w}||\ ||\mathbf{w}||$

Multiple Classes

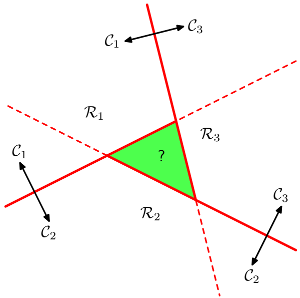
Consider the extension of linear discriminants to $K > 2$ classes. There are two approaches:

- One-versus-the-rest classifier: build a K-class discriminant by combining a number of two-class discriminant functions. However, this leads to some serious ambiguity difficulties.
- One-versus-one classifier: Introduce $K(K-1)/2$ binary discriminant functions, one for every possible pair of classes. Each point is then classified according to a majority vote amongst the discriminant functions. However, this too runs into the problem of ambiguous regions.

Multiple Classes



One-versus-the-rest



One-versus-one

- Both result in ambiguous regions of input space.

Multiple Classes

- Consider a single K class discriminant of the form

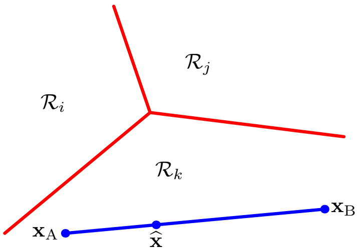
$$y_k(x) = w_k^\top x + w_{k0}.$$

- Then we can assign a point x to class C_k if

$$y_k(x) > y_j(x) \ \text{for all} \ j \neq k.$$

- Decision regions of such a discriminant are always singly connected and convex.

Multiple Classes



- Consider two points x_A and x_B both in decision region R_k.
- Any point $\hat{x}$ on line connecting x_A and x_B can be expressed as

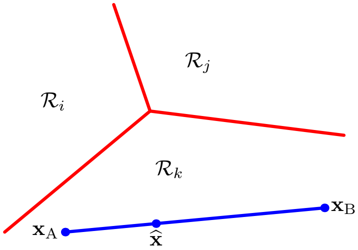
$$\hat{x} = \lambda x_A + (1 - \lambda) x_B$$

  where $0 \leq \lambda \leq 1$

- From linearity of discriminant functions, it follows that

$$y_k(\hat{x}) = \lambda y_k(x_A) + (1 - \lambda) y_k(x_B).$$

Multiple Classes



- Because both x_A and x_B lie inside R_k, it follows that

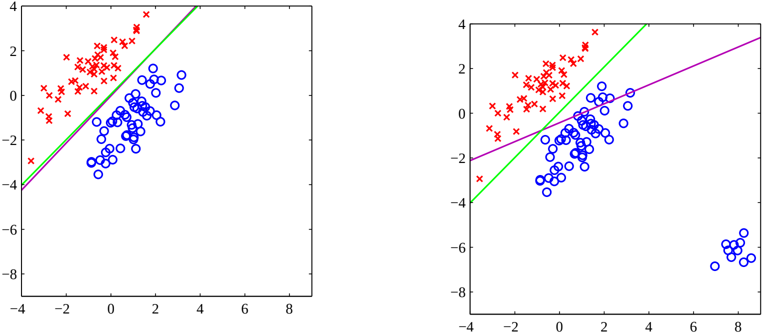
$$y_k(x_A) > y_j(x_A),$$

  and

$$y_k(x_B) > y_j(x_B),$$

  for all $j \neq k$.
- Hence $y_k(\hat{x}) > y_j(\hat{x})$, and so $\hat{x}$ also lies inside R_k.
- Thus R_k is singly connected and convex.

Least Squares Vs Logistic Regression



- Decision boundaries found by least squares (magenta curve) and also by the logistic regression model (green curve).
- The right-hand plot shows that least squares (Maximum Likelihood with Gaussian assumption) is highly sensitive to outliers, unlike logistic regression.

Fisher's Linear Discriminant

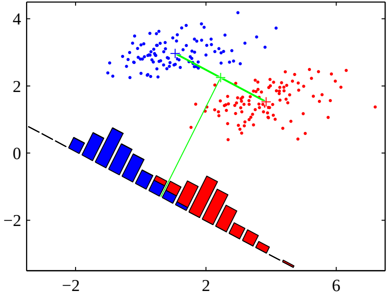
- One way to view a linear classification model is in terms of dimensionality reduction.
- Consider the case of two classes, and suppose we take D-dimensional input vector $\mathbf{x}$ and project it down to one dimension using

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

- If we place a threshold on y and classify $y \geq -w_o$ as class C_1, and otherwise class C_2, then we obtain a standard linear classifier.

Fisher's Linear Discriminant

- In general, the projection onto one dimension leads to a considerable loss of information, and classes that are well separated in the original D-dimensional space may become strongly overlapping in one dimension.



- However, by adjusting the components of the weight vector **w**, we can select a projection that maximizes the class separation.

Fisher's Linear Discriminant

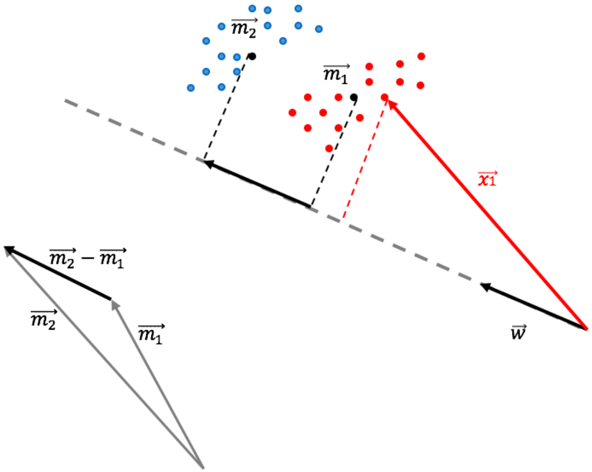
- Consider a two-class problem in which there are N_1 points of class C_1 and N_2 points of class C_2, so that the mean vectors of the two classes are given by

$$\mathbf{m}_1 = \frac{1}{N_1} \sum_{n \in C_1} \mathbf{x}_n,$$

$$\mathbf{m}_2 = \frac{1}{N_2} \sum_{n \in C_2} \mathbf{x}_n.$$

- The simplest measure of the separation of the classes, when projected onto $\mathbf{w}$, is the separation of the projected class means.

Fisher's Linear Discriminant



Fisher's Linear Discriminant

- This suggests that we might choose **w** so as to maximize

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

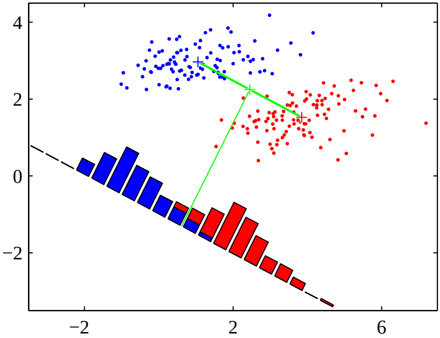
  where

$$m_k = \mathbf{w}^\top \mathbf{m}_k$$

  is the mean of the projected data from class C_k.
- However, this expression can be made arbitrarily large simply by increasing the magnitude of **w**.
- To solve this problem we could constrain **w** to have unit length, so that $\sum_i w_i^2 = 1$.

Fisher's Linear Discriminant

- Problem with this approach: two classes that are well separated in the original two-dimensional space may have considerable overlap when projected onto the line joining their means.
- This difficulty arises from strongly nondiagonal covariances of the class distributions.



Fisher's Linear Discriminant

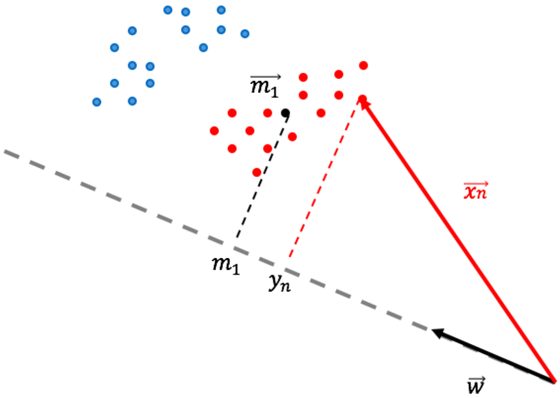
- The idea proposed by Fisher is to maximize a function that will give a large separation between the projected class means while also giving a small variance within each class, thereby minimizing the class overlap.
- The projection then transforms the set of labelled data points in $\mathbf{x}$ into a labelled set in the one-dimensional space y.
- The within-class variance of the transformed data from class C_k is therefore given by

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

where

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

Fisher's Linear Discriminant



Fisher's Linear Discriminant

- We can define the total within-class variance for the whole data set to be simply $s_1^2 + s_2^2$.
- The Fisher criterion is defined to be the ratio of the between-class variance to the within-class variance and is given by

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

- We can make the dependence on **w** explicit and rewrite the Fisher criterion in the form

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

Fisher's Linear Discriminant

- In

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

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

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

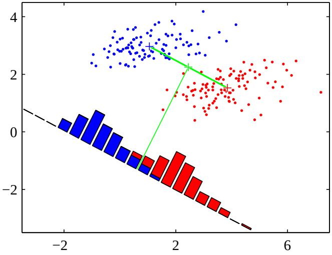
- and $\mathbf{S}_W$ is the within-class covariance matrix given by

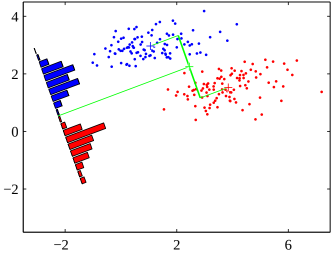
$$\mathbf{S}_W = \sum_{n \in C_1} (\mathbf{x}_n - \mathbf{m}_1)(\mathbf{x}_n - \mathbf{m}_1)^\top + \sum_{n \in C_2} (\mathbf{x}_n - \mathbf{m}_2)(\mathbf{x}_n - \mathbf{m}_2)^\top.$$

- Finally, by maximizing $J(\mathbf{w})$ we find that

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

Fisher's Linear Discriminant





- The result is known as Fisher's linear discriminant, although strictly it is not a discriminant but rather a specific choice of direction for projection of the data down to one dimension.
- However, the projected data can subsequently be used to construct a discriminant, by choosing a threshold y_0 so that we classify a new point as belonging to C_1 if $y(\mathbf{x}) \geq y_0$ and classify it as belonging to C_2 otherwise.

Reference

- Andrew Ng. **Machine Learning Course Notes**. 2003.
- Christopher Bishop. **Pattern Recognition and Machine Learning**. Springer. 2006.

Thank you!

Dr. Víctor Uc Cetina
cetina@informatik.uni-hamburg.de