# Linear Regression and Classification Revisited

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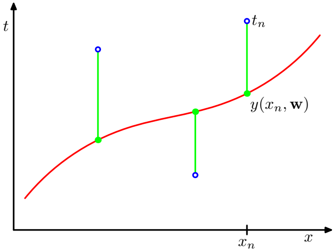
2. Regularized Linear Regression
3. Discriminant Functions for Classification
4. Fisher's Linear Discriminant

# Linear Regression



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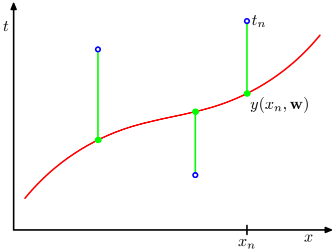


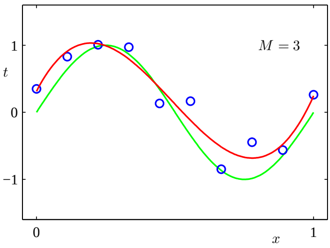

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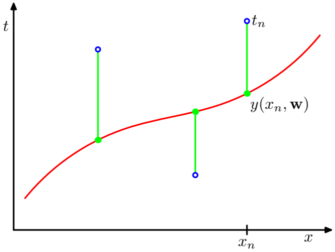


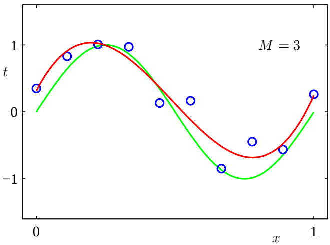


- $x$ is the input variable, $t$ is the output variable, w is the parameters vector of our model and the data points were generated from $\sin(2\pi x) + \varepsilon$.

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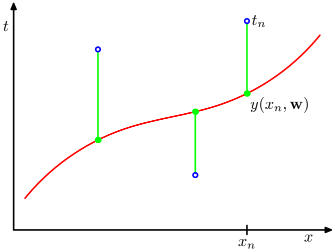


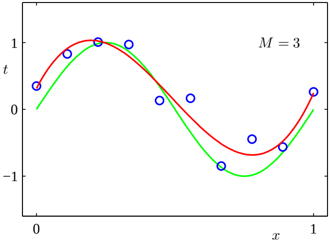


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- For our model $y(x, \mathrm{w}) = w_0 + w_1 x + \ldots + w_M x^M$, we need to search for the best $M$ and we need to learn the parameters w.

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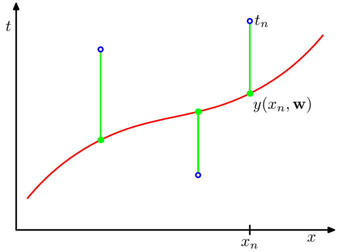


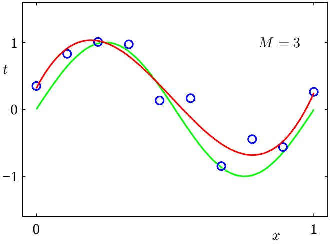


- $x$ is the input variable, $t$ is the output variable, w is the parameters vector of our model and the data points were generated from $\sin(2\pi x) + \varepsilon$.
- For our model $y(x, \mathrm{w}) = w_0 + w_1 x + \ldots + w_M x^M$, we need to search for the best $M$ and we need to learn the parameters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

# Estimating the Parameters w

## Stochastic Gradient Descent

Loop $\{$

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

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

$\}$

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**Normal Equations**

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

# Locally Weighted Linear Regression

The algorithm works as follows:

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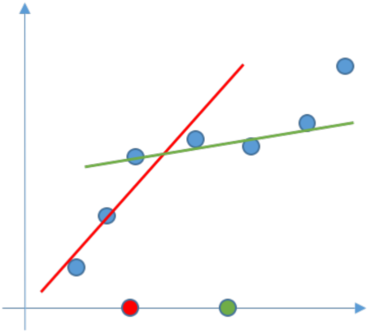
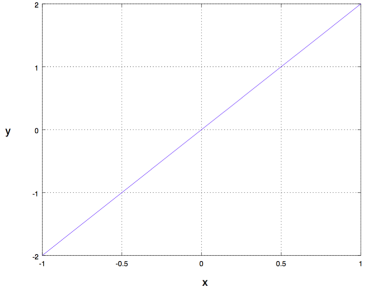


# Polynomial Functions

$y = 2x$



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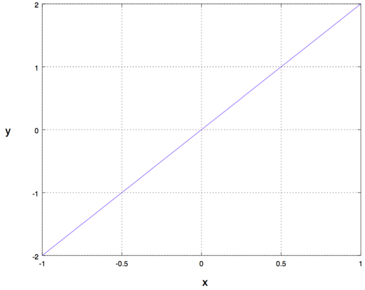
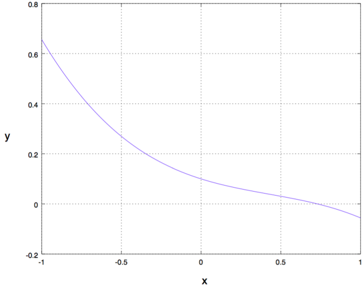



$y = 0.1 - 0.2x + 0.2x^2 - 0.156x^3$



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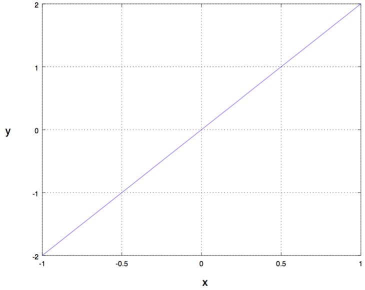


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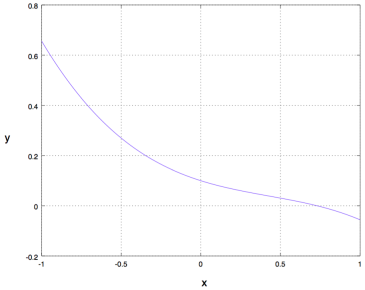
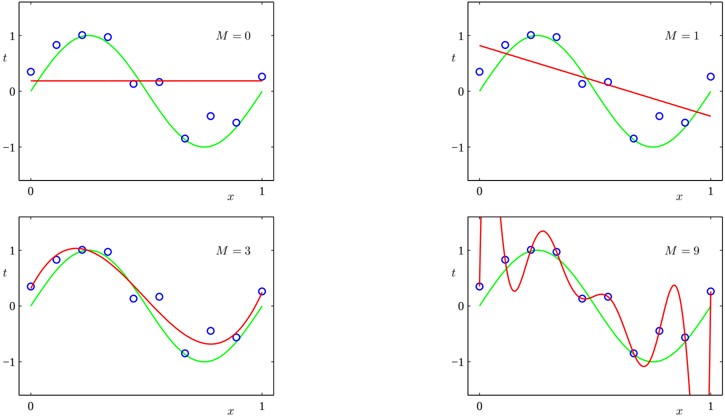



- For polynomial functions, we need to try systematically different $M'$s and evaluate the performance of our current model.

# 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 $E_{\mathrm{RMS}}$.

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

where

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

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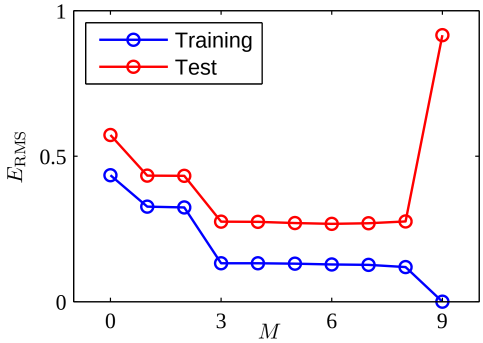
- This error can also be used to evaluate if our model's performance is improving after each iteration of the learning algorithm.

# Evaluation of Performance



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- The simplest linear model for regression is one that involves a linear combination of the input variables

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- 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

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

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  where $\phi_j(\mathrm{x})$ 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

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

where

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

and

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

# Basis Functions

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- 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

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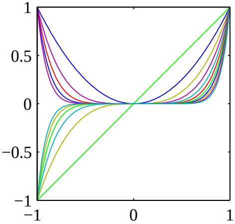
  where the $\mu_j$ govern the locations of the basis functions in input space, and the parameter $s$ governs their spatial scale.
- Sigmoidal basis functions:

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

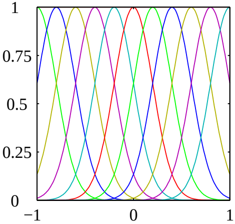
  where

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

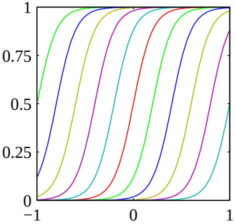
# Basis Functions




Polynomial

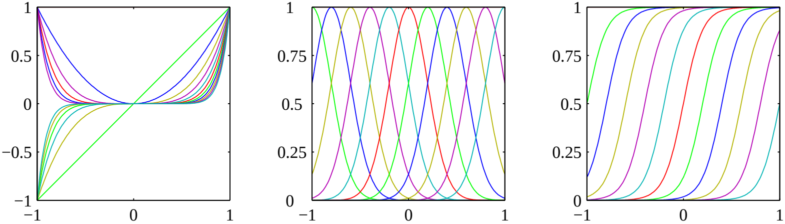



Gaussian




Sigmoidal

# Basis Functions




Polynomial Gaussian Sigmoidal

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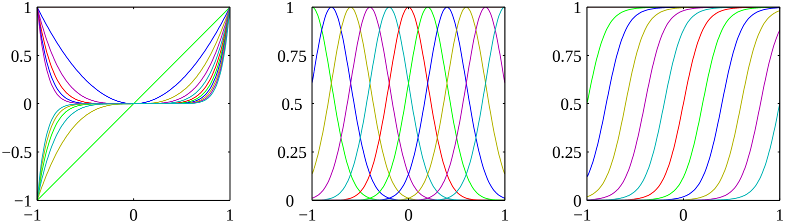
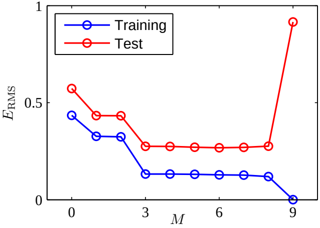



Polynomial Gaussian Sigmoidal

- 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



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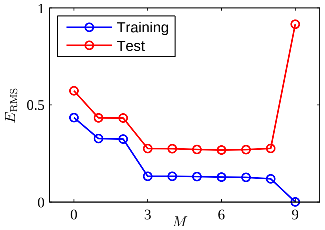
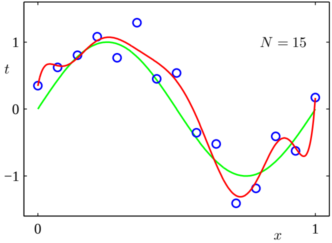



| | $M=0$ | $M=1$ | $M=3$ | $M=9$ |
|---|---|---|---|---|
| $w_0$ | 0.19 | 0.82 | 0.31 | 0.35 |
| $w_1$ | | -1.27 | 7.99 | 232.37 |
| $w_2$ | | | -25.43 | -5321.83 |
| $w_3$ | | | 17.37 | 48568.31 |
| $w_4$ | | | | -231639.30 |
| $w_5$ | | | | 640042.26 |
| $w_6$ | | | | -1061800.52 |
| $w_7$ | | | |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

# Importance of Dataset Size



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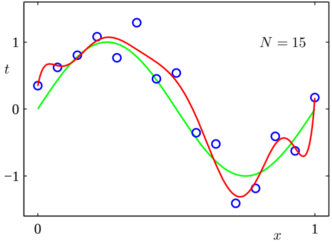


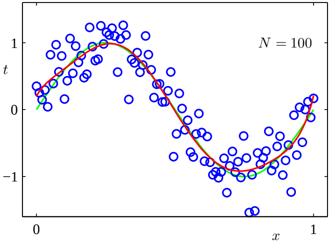

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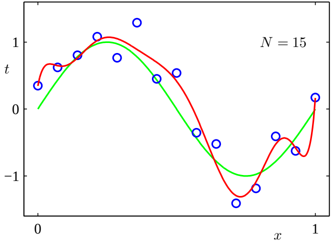


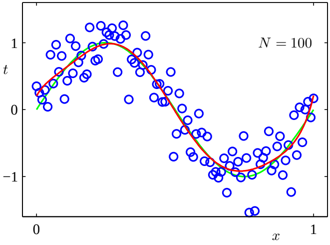


- Two solutions with $M = 9$. In the left using $N = 15$ training examples. In the right using $N = 100$ training examples.

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

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

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

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

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- We minimize

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

# Estimating the Parameters w with Regularization

Stochastic Gradient Descent

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Normal Equations

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

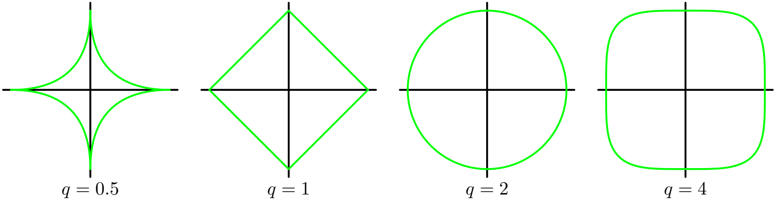
# Different Types of Regularizers

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

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

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

# Types of Regularizers and their Effects



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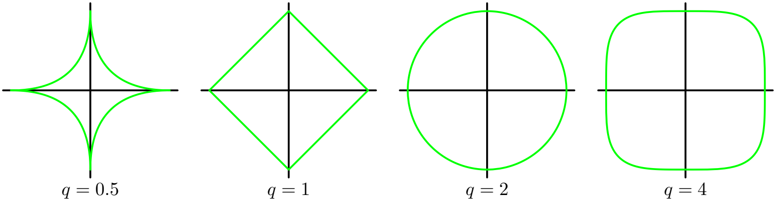


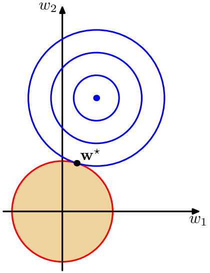

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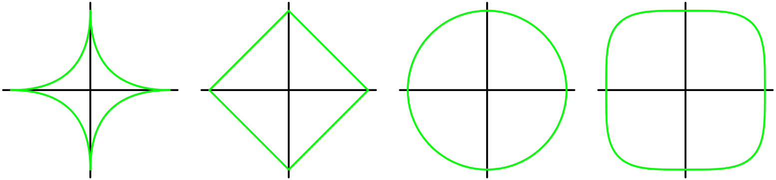
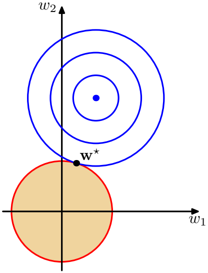
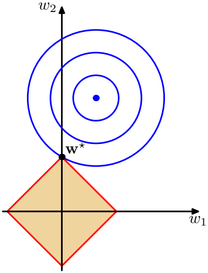


$q = 0.5$ $q = 1$ $q = 2$ $q = 4$



# Benefits of Regularization

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- 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 $\lambda$.

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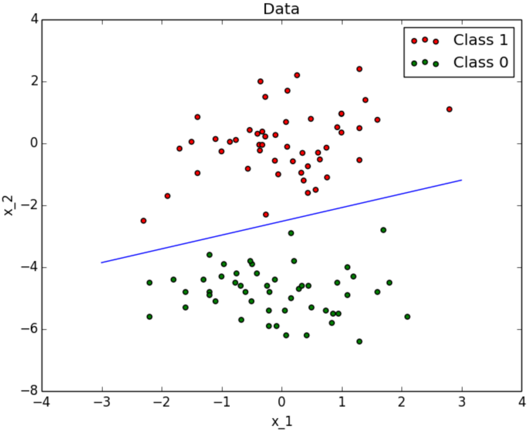
- Data sets whose classes can be separated exactly by linear decision surfaces are said to be linearly separable.

# Linear Classification




Two cloud of points linearly separable.

# Linear Classification

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

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- The simplest representation of a linear discriminant function is obtained by taking a linear function of the input vector so that

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

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

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- So w determines the orientation of the decision surface.

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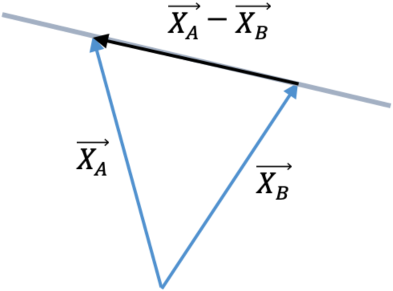

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- Similarly, if $\mathrm{x}$ is a point on the decision surface, then $y(x) = 0$, and so the normal distance from the origin to the decision surface is given by

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

# Discriminant Functions

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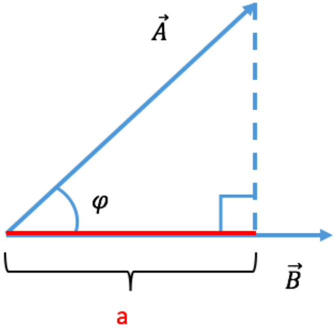

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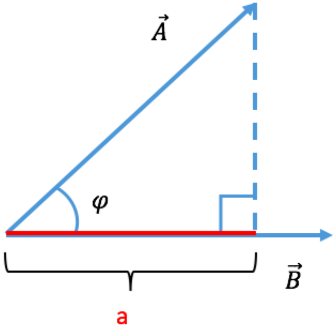


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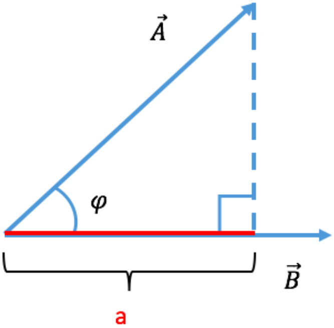


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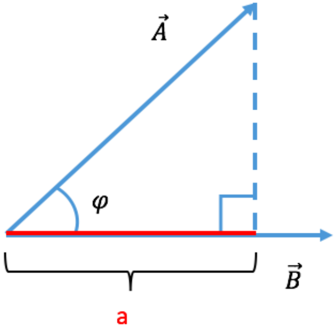


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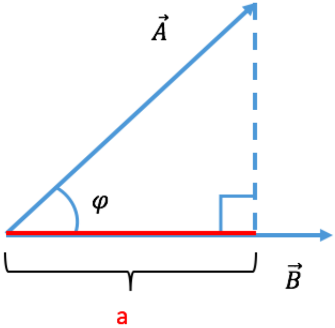


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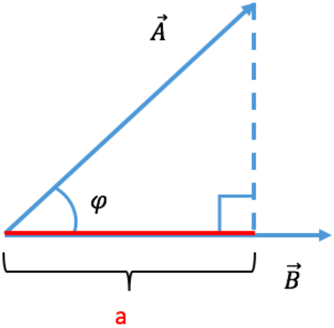


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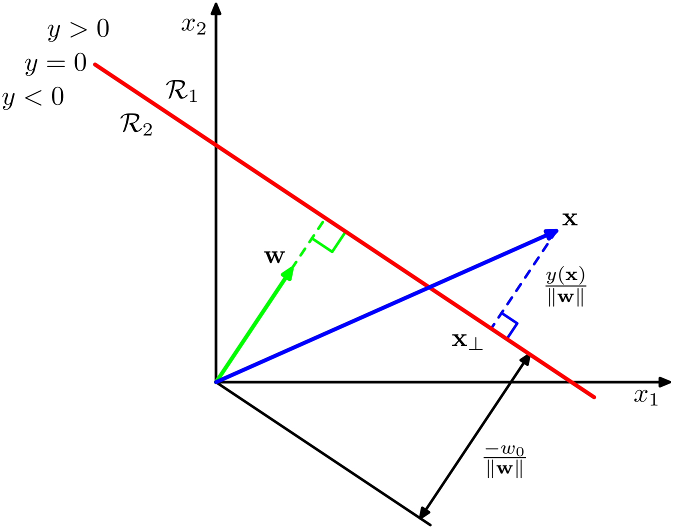

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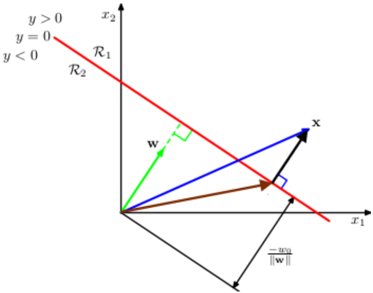

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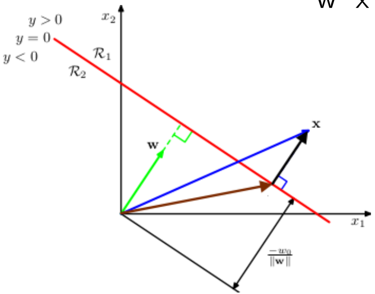


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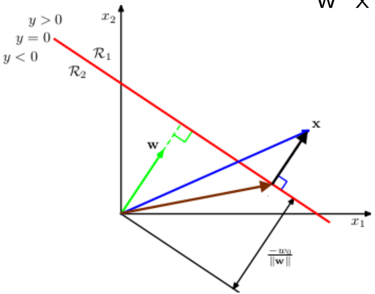


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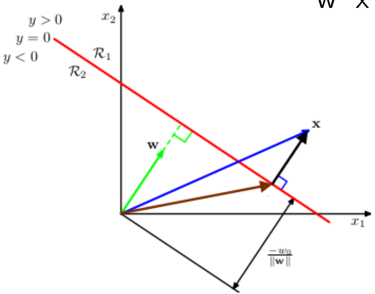


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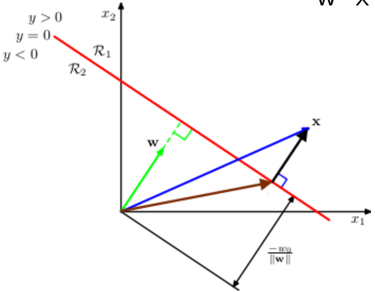


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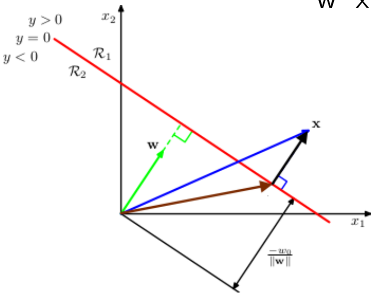


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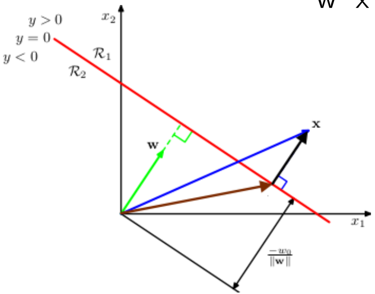


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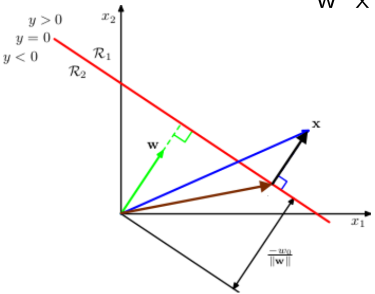


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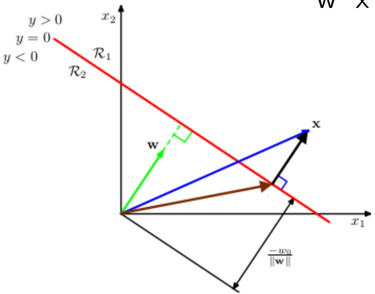


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Let $\mathrm{w} = (w_1, w_2, \ldots, w_n)$, then the following is true:
$\mathrm{w}^\top\mathrm{w} = w_1^2 + w_2^2 + \cdots + w_n^2 = \sqrt{w_1^2 + w_2^2 + \cdots + w_n^2}\sqrt{w_1^2 + w_2^2 + \cdots + w_n^2} = ||\mathrm{w}||\ ||\mathrm{w}||$

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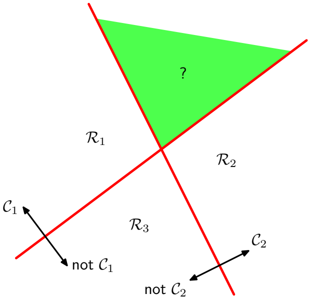
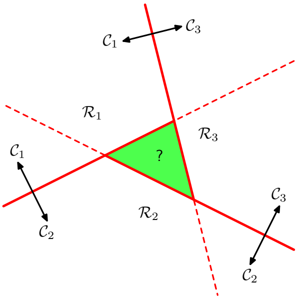
- One-versus-the-rest classifier: build a $K$-class discriminant by combining a number of two-class discriminant functions. However, this leads to some serious ambiguity difficulties.
- One-versus-one classifier: Introduce $K(K-1)/2$ binary discriminant functions, one for every possible pair of classes. 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

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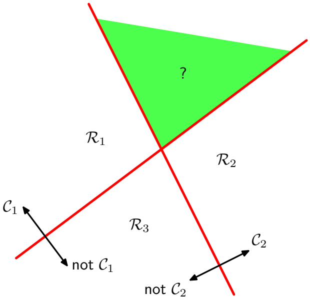


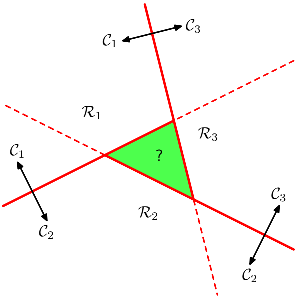


One-versus-the-rest

One-versus-one

- Both result in ambiguous regions of input space.

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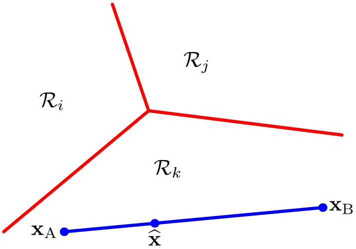
- Decision regions of such a discriminant are always singly connected and convex.

## Multiple Classes



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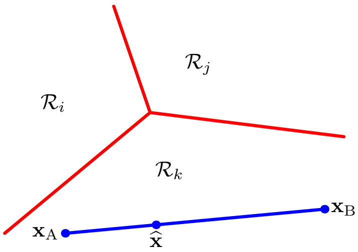


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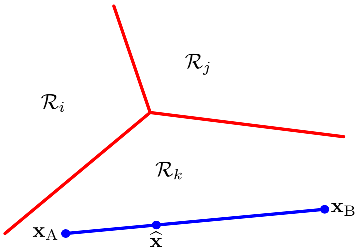
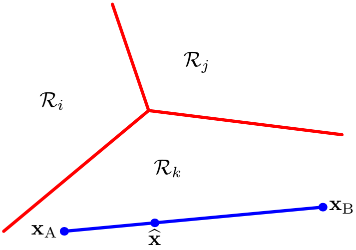



- Consider two points $x_A$ and $x_B$ both in decision region $R_k$.
- Any point $\hat{x}$ on line connecting $x_A$ and $x_B$ can be expressed as

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

where $0 \leq \lambda \leq 1$

# Multiple Classes

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

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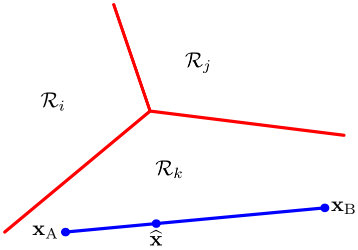


- Because both $x_A$ and $x_B$ lie inside $R_k$, it follows that

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for all $j \neq k$.

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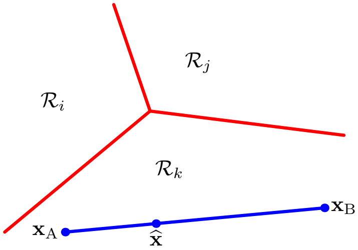


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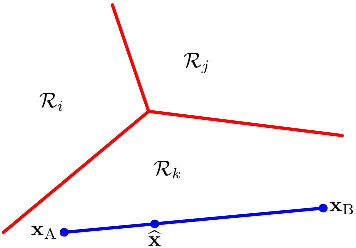


- Because both $x_A$ and $x_B$ lie inside $R_k$, it follows that

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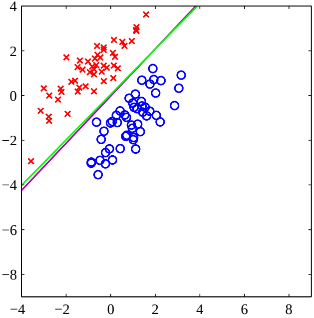
- Hence $y_k(\hat{x}) > y_j(\hat{x})$, and so $\hat{x}$ also lies inside $R_k$.
- Thus $R_k$ is singly connected and convex.

# Least Squares Vs Logistic Regression



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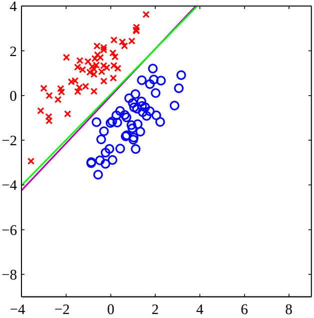


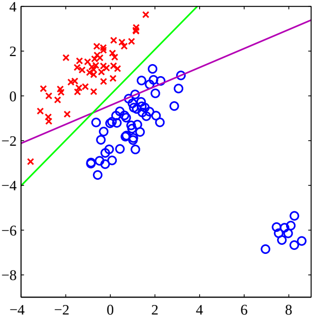

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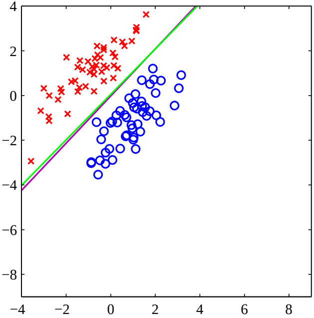


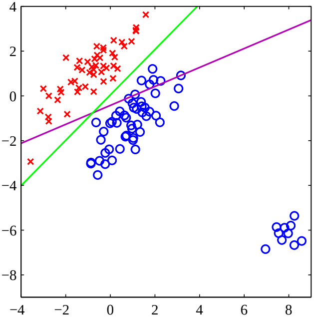


- Decision boundaries found by least squares (magenta curve) and also by the logistic regression model (green curve).

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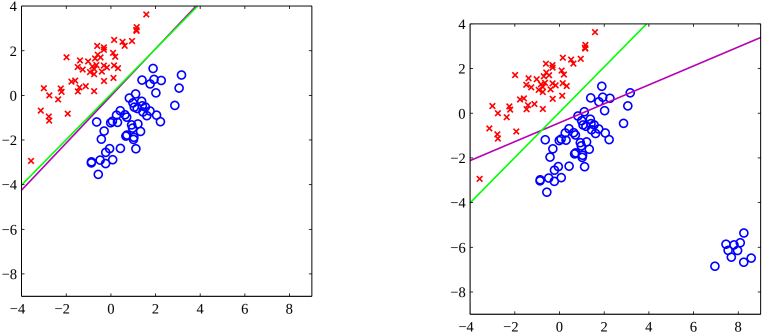


- Decision boundaries found by least squares (magenta curve) and also by the logistic regression model (green curve).
- The right-hand plot shows that least squares (Maximum Likelihood with Gaussian assumption) is highly sensitive to outliers, unlike logistic regression.

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- 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.

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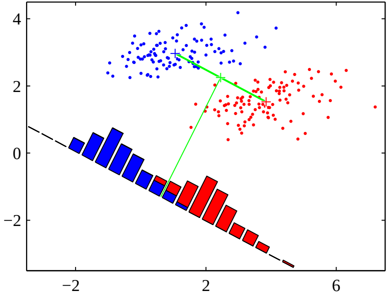

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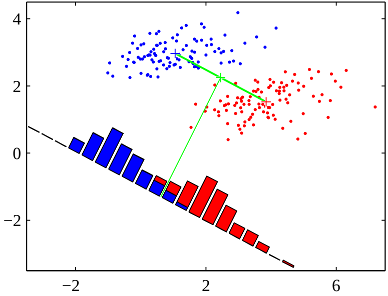


- However, by adjusting the components of the weight vector w, we can select a projection that maximizes the class separation.

# 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

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

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

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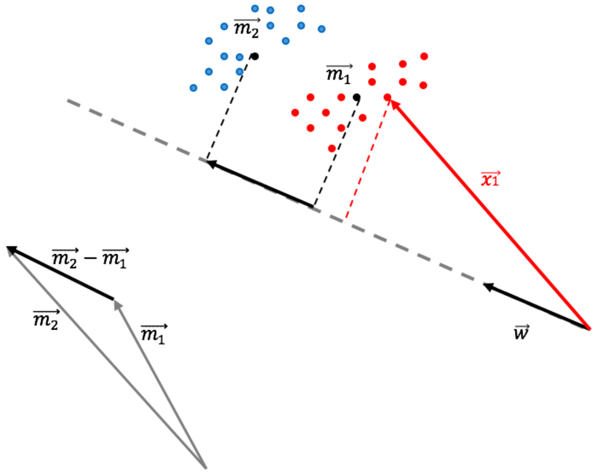

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- This suggests that we might choose $\mathrm{w}$ so as to maximize

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

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- However, this expression can be made arbitrarily large simply by increasing the magnitude of $\mathrm{w}$.
- To solve this problem we could constrain $\mathrm{w}$ to have unit length, so that $\sum_i w_i^2 = 1$.

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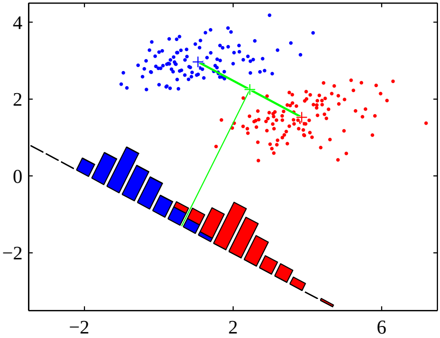

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- The projection then transforms the set of labelled data points in $\mathrm{x}$ into a labelled set in the one-dimensional space $y$.
- The within-class variance of the transformed data from class $C_k$ is therefore given by

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

where

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

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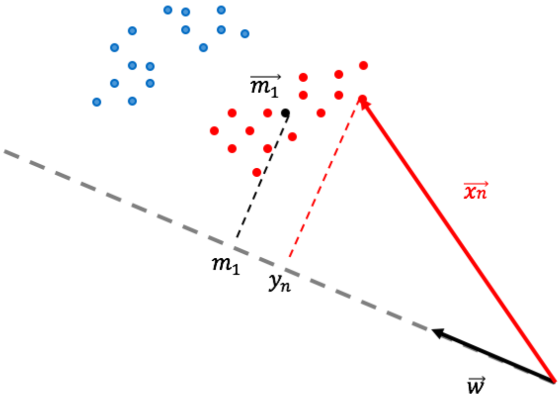

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- We can make the dependence on w explicit and rewrite the Fisher criterion in the form

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

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

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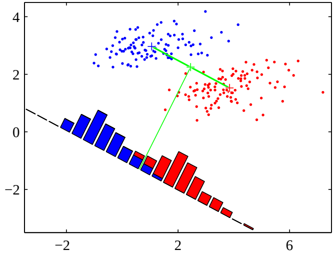

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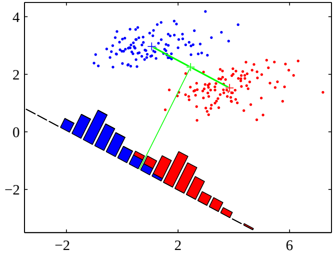


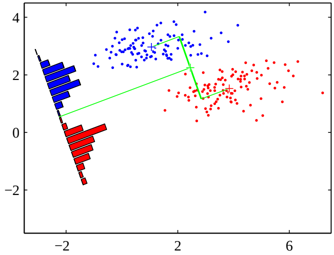

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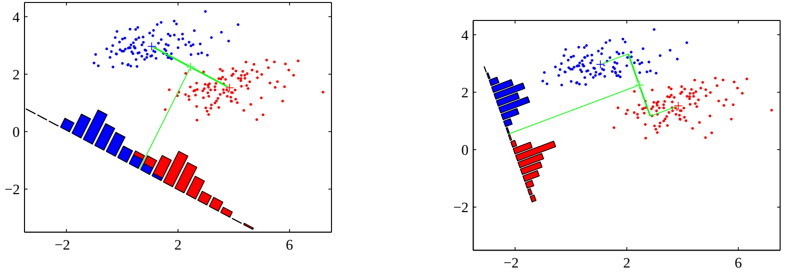


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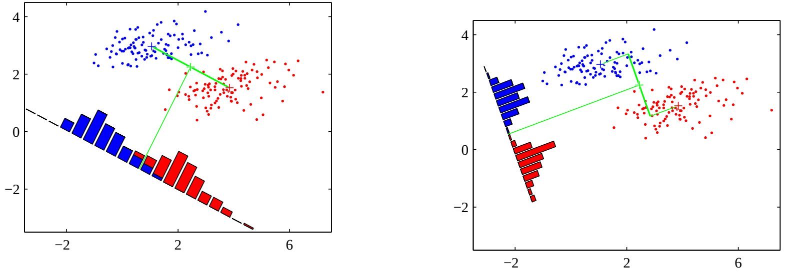


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- However, the projected data can subsequently be used to construct a discriminant, by choosing a threshold $y_0$ so that we classify a new point as belonging to $C_1$ if $y(\mathrm{x}) \geq y_0$ and classify it as belonging to $C_2$ otherwise.

# Reference


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

Thank you!

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