Linear Regression and Classification Revisited

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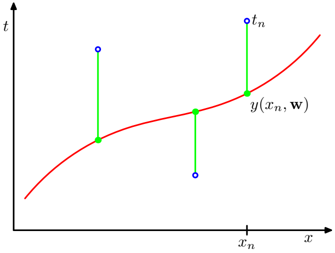
Content

Linear Regression



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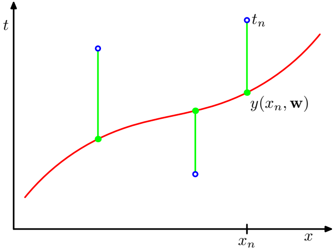

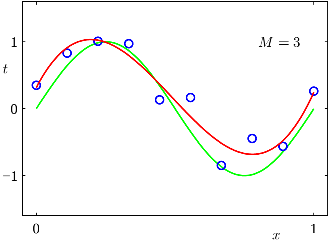

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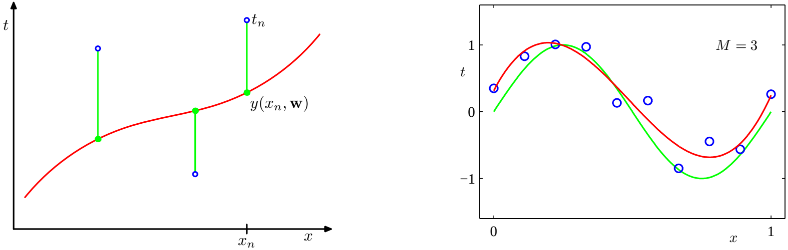

- x is the input variable, t is the output variable, $\mathbf{w}$ is the parameters vector of our model and the data points were generated from $\sin(2\pi x) + \varepsilon$.

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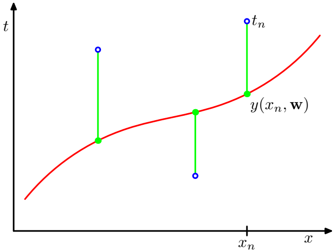

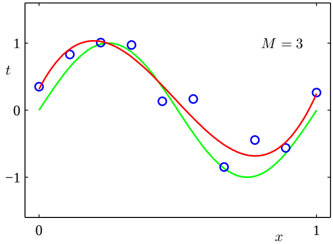

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- For our model $y(x, \mathbf{w}) = w_0 + w_1 x + \ldots + w_M x^M$, we need to search for the best M and we need to learn the parameters $\mathbf{w}$.

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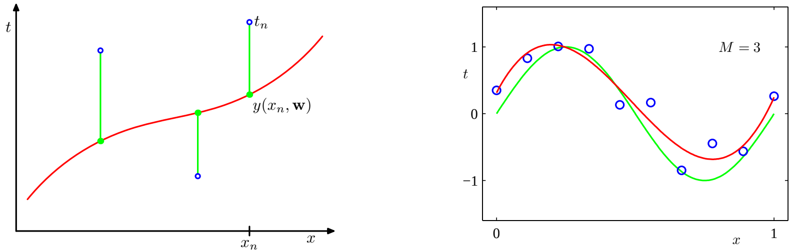

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- For our model $y(x, \mathbf{w}) = w_0 + w_1 x + \ldots + w_M x^M$, we need to search for the best M and we need to learn the parameters $\mathbf{w}$.
- Such parameter vector $\mathbf{w}$ can be learned iteratively or directly.

Estimating the Parameters $\mathbf{w}$

Stochastic Gradient Descent

Loop {

for $i = 1$ to m {

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

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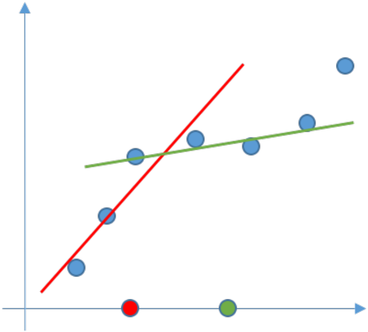
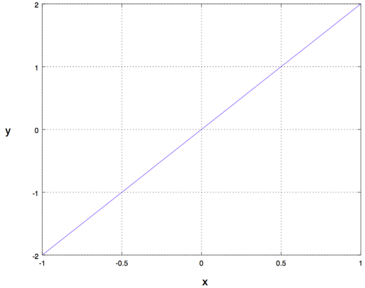


Polynomial Functions

$y = 2x$



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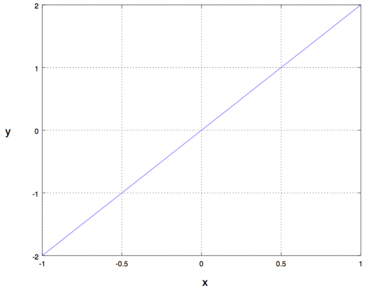
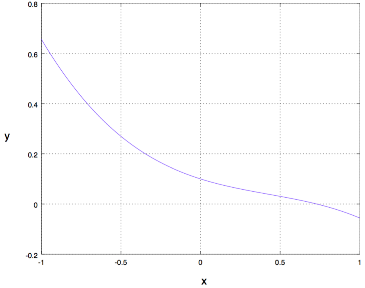


$y = 0.1 - 0.2x + 0.2x^2 - 0.156x^3$



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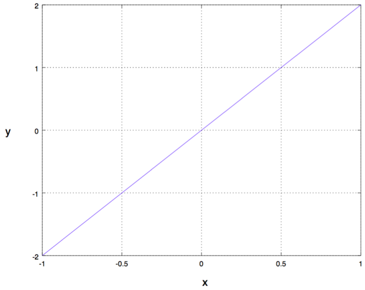

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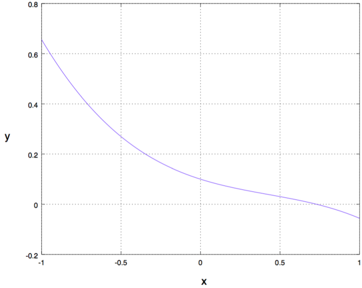
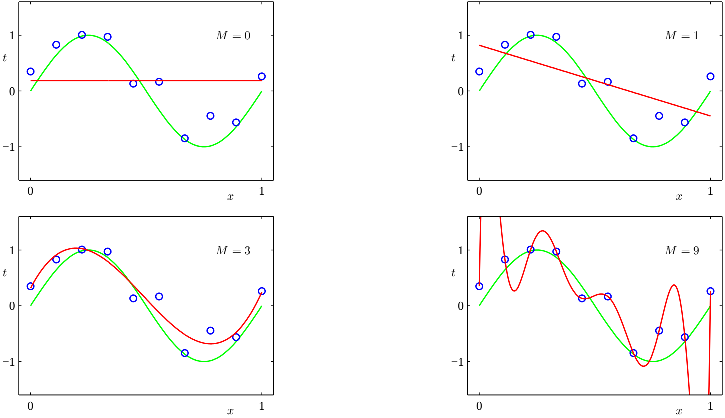


- For polynomial functions, we need to try systematically different M's and evaluate the performance of our current model.

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_{RMS}.

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

where

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

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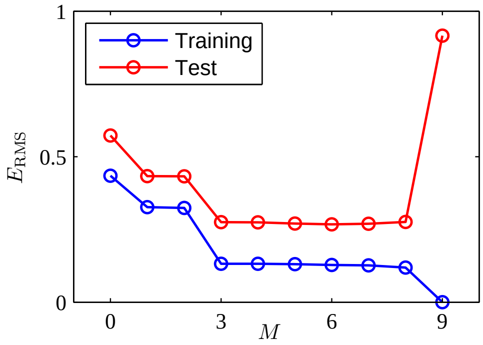
- This error can also be used to evaluate if our model's performance is improving after each iteration of the learning algorithm.

Evaluation of Performance



Generalized Linear Regression

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- 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

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

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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

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

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  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

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

Radial Basis Functions

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- 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.

Radial Basis Functions

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

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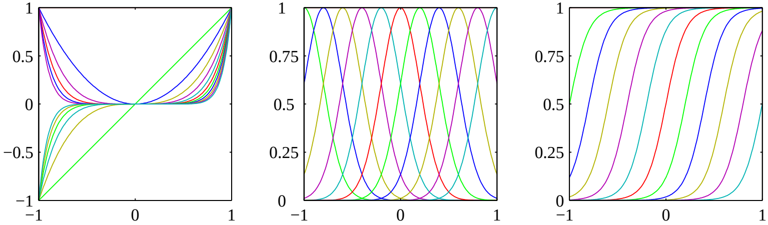
  where the μ_j govern the locations of the basis functions in input space, and the parameter s governs their spatial scale.
- Sigmoidal basis functions:

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

  where

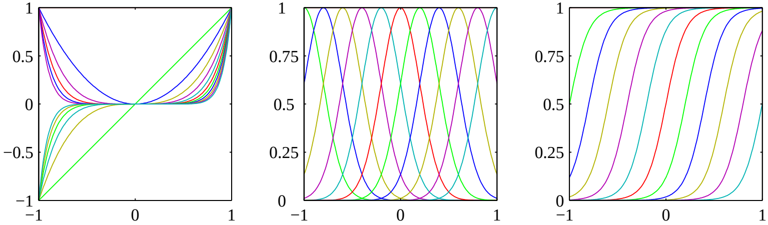
$$\sigma(a) = \frac{1}{1+\exp(-a)}$$

Radial Basis Functions



Polynomial Gaussian Sigmoidal

Radial Basis Functions



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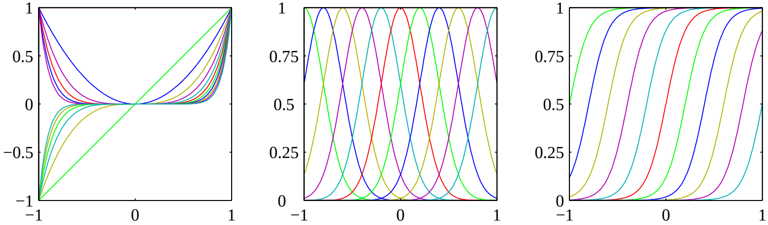
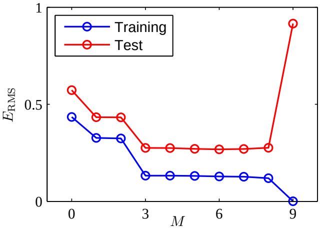


Polynomial Gaussian Sigmoidal

- 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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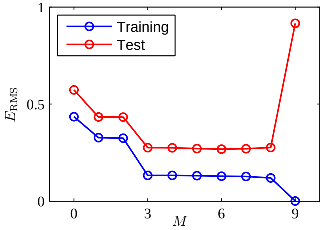
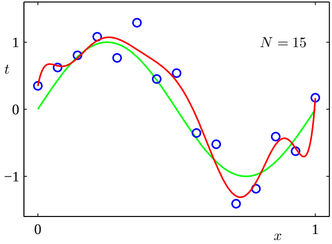


	$M = 0$	$M = 1$	$M = 6$	$M = 9$
w_0	0.19	0.82	0.31	0.35
w_1		-1.27	7.99	232.37
w_2			-25.43	-5321.83
w_3			17.37	48568.31
w_4				-231639.30
w_5				640042.26
w_6				-1061800.52
w_7				1042400.18
w_8				-557682.99
w_9				125201.43

Importance of Dataset Size



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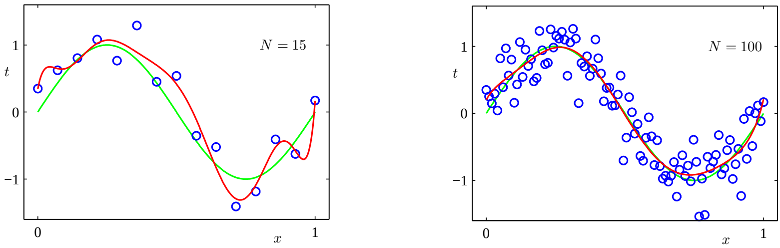

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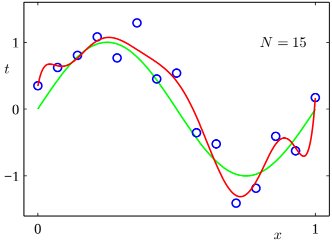

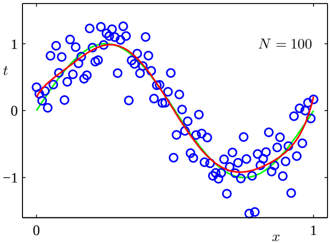

- Two solutions with $M = 9$. In the left using $N = 15$ training examples. In the right using $N = 100$ training examples.

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

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

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- 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 $E_W(\mathbf{w})$.

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

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- 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 $\mathbf{w}$ with Regularization

Stochastic Gradient Descent

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for $i = 1$ to m {

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Normal Equations

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

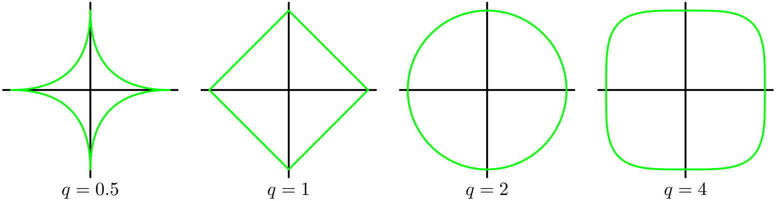
Different Types of Regularizers

- 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



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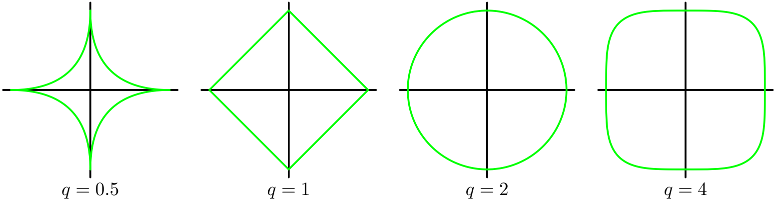

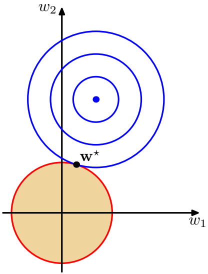

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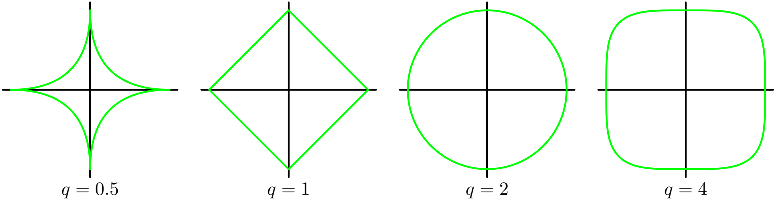

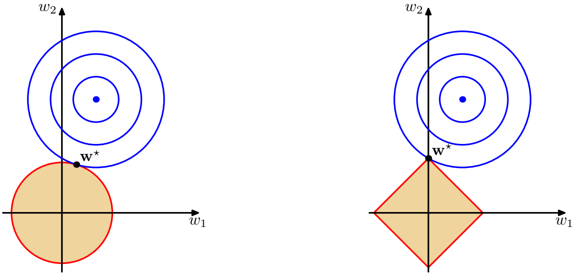

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- Regularization allows complex models to be trained on data sets of limited size without severe over-fitting, essentially by limiting the effective model complexity.
- However, the problem of determining the optimal model complexity is then shifted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

Linear Classification

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- In linear models for classification, the decision surfaces are linear functions of the input vector $\mathbf{x}$ and hence are defined by (D-1)-dimensional hyperplanes within the D-dimensional input space.
- Data sets whose classes can be separated exactly by linear decision surfaces are said to be linearly separable.

Linear Classification

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- 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

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

  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.

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- 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.

Discriminant Functions

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Discriminant Functions

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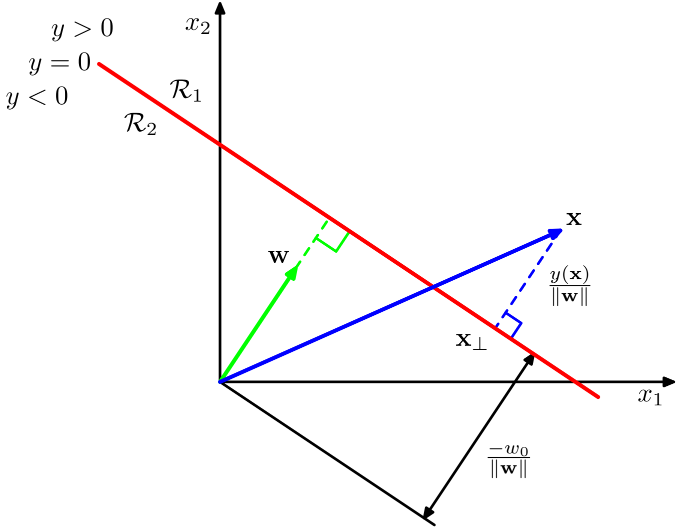
- We therefore see that the bias parameter w_0 determines the location of the decision surface.

Discriminant Functions



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Multiple Classes

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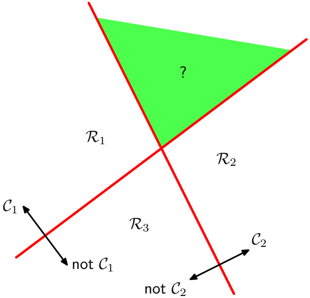
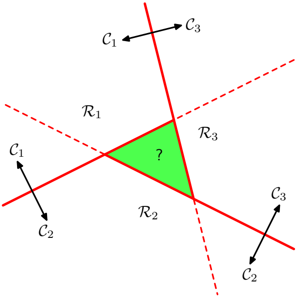
- One-versus-the-rest classifier: build a K-class discriminant by combining a number of two-class discriminant functions. However, this leads to some serious ambiguity difficulties.
- One-versus-one classifier: Introduce $K(K-1)/2$ binary discriminant functions, one for every possible pair of classes.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

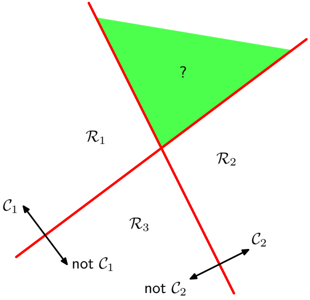


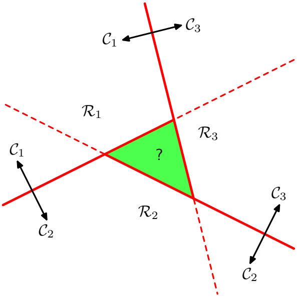
One-versus-the-rest



One-versus-one

Multiple Classes





One-versus-the-rest　　　　One-versus-one

- Both result in ambiguous regions of input space.

Multiple Classes

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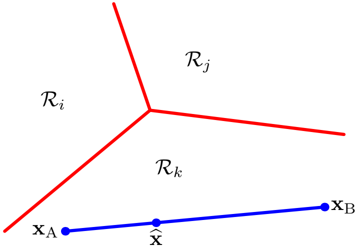
Multiple Classes



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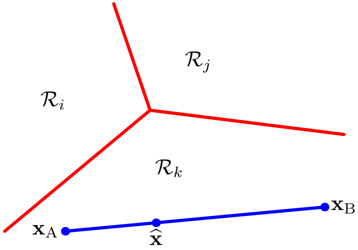

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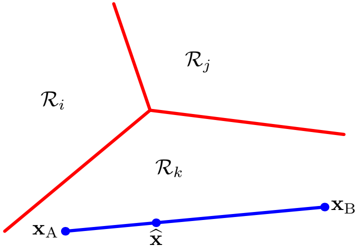

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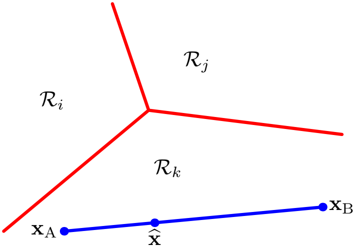

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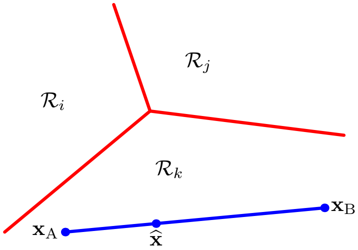
- From linearity of discriminant functions, it follows that

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

Multiple Classes



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

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

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for all $j \neq k$.

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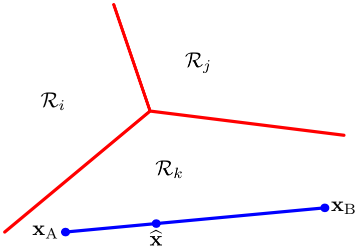

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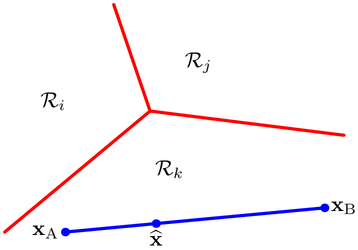

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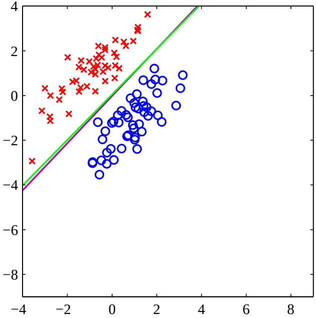
- Thus R_k is singly connected and convex.

Least Squares Vs Logistic Regression



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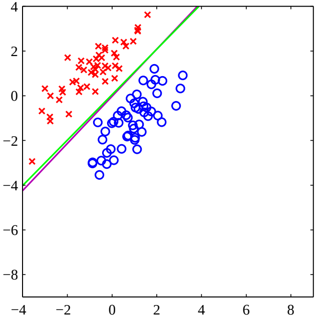

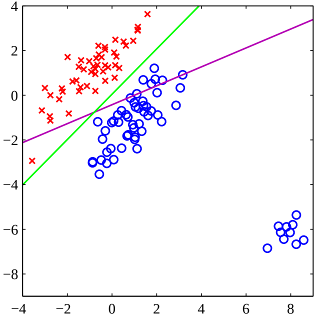

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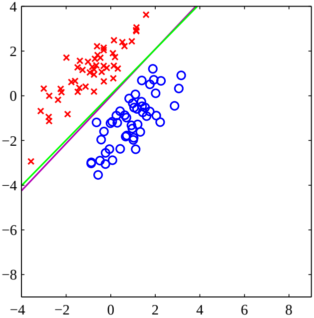
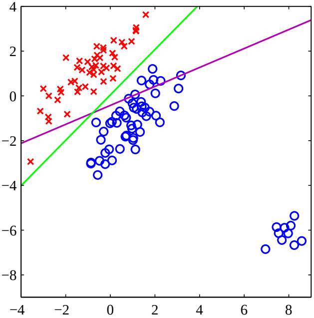
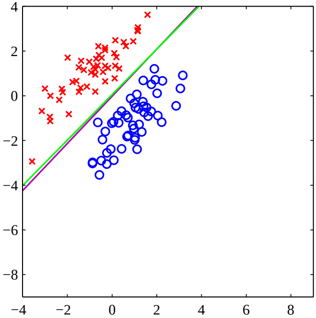
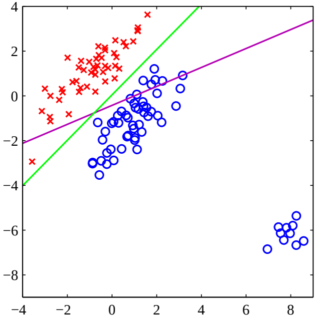




- Decision boundaries found by least squares (magenta curve) and also by the logistic regression model (green curve).

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

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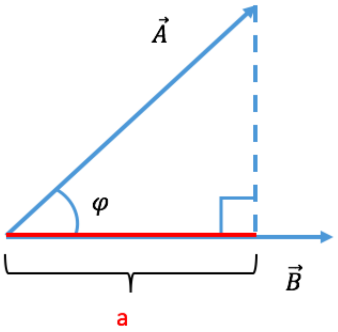
$$y = \mathbf{w}^\top \mathbf{x}.$$
- If we place a threshold on y and classify $y \geq -w_o$ as class C_1, and otherwise class C_2, then we obtain a standard linear classifier.

Fisher's Linear Discriminant

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



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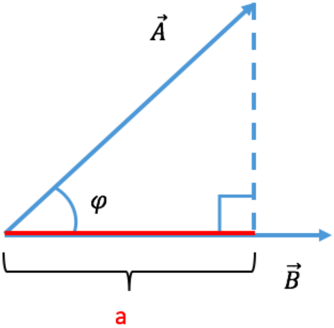

$$\begin{aligned} \cos\varphi &= \frac{a}{||\vec{A}||} \\ a &= ||\vec{A}||\cos\varphi \end{aligned} \tag{1}$$

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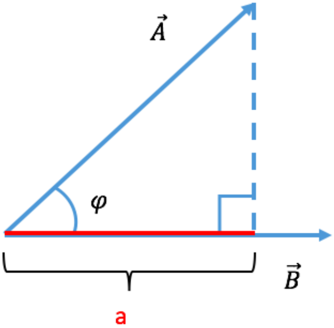

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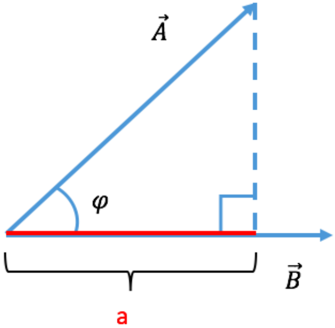

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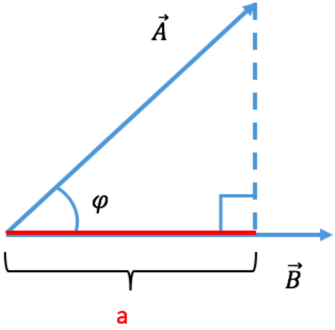
Fisher's Linear Discriminant



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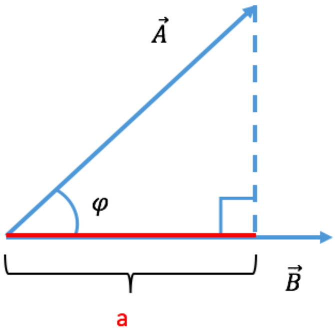

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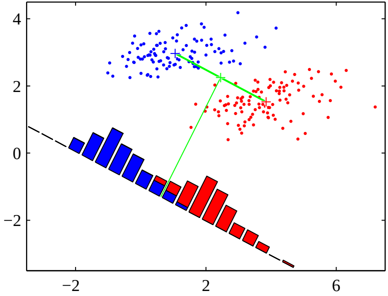

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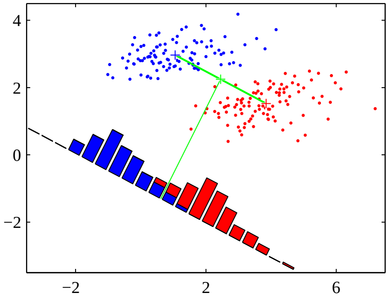

- However, by adjusting the components of the weight vector **w**, we can select a projection that maximizes the class separation.

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

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

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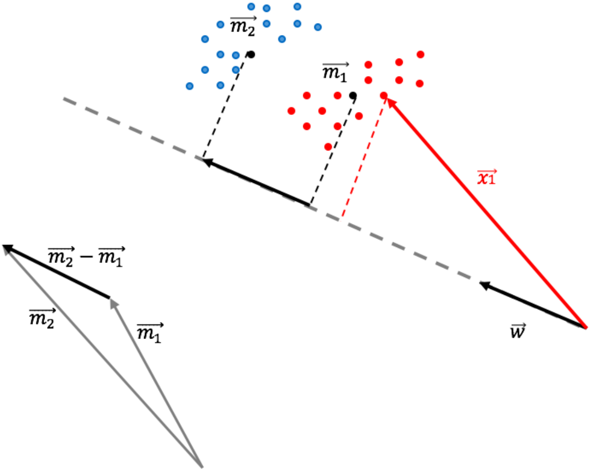
- The simplest measure of the separation of the classes, when projected onto $\mathbf{w}$, is the separation of the projected class means.

Fisher's Linear Discriminant



Fisher's Linear Discriminant

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

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

where

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- 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 $\sum_i w_i^2 = 1$.

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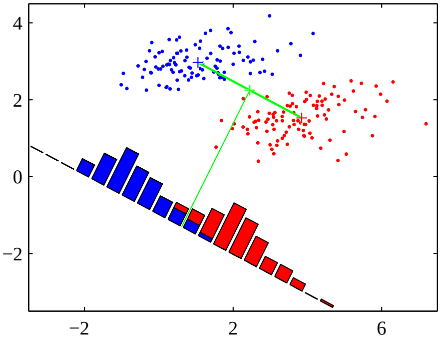

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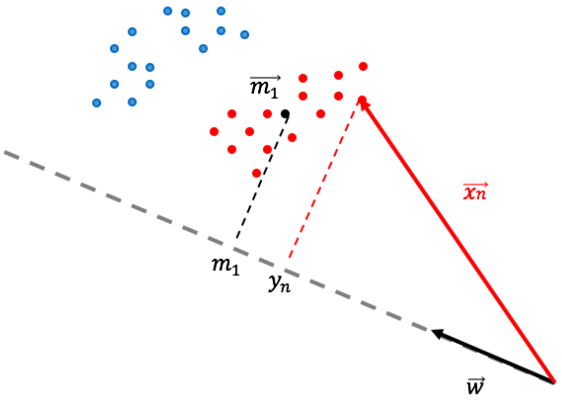
- The projection then transforms the set of labelled data points in $\mathbf{x}$ into a labelled set in the one-dimensional space y.
- The within-class variance of the transformed data from class C_k is therefore given by

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

where

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

Fisher's Linear Discriminant



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- We can make the dependence on $\mathbf{w}$ 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
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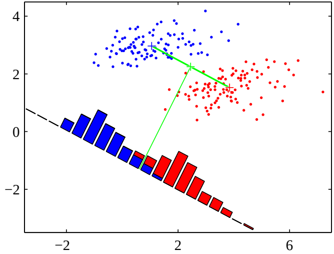
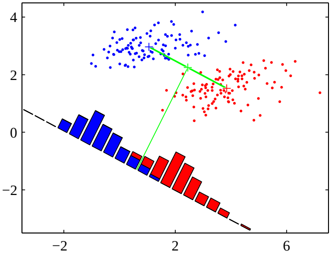
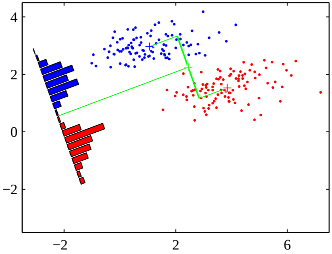
- Finally, by maximizing $J(\mathbf{w})$ we find that
$$\mathbf{w} \propto \mathbf{S}_W^{-1}(\mathbf{m}_2 - \mathbf{m}_1).$$

Fisher's Linear Discriminant

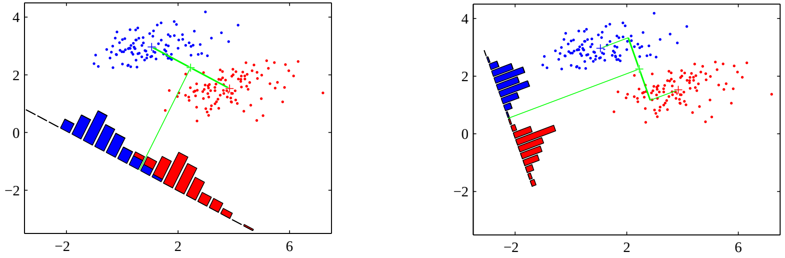


Fisher's Linear Discriminant



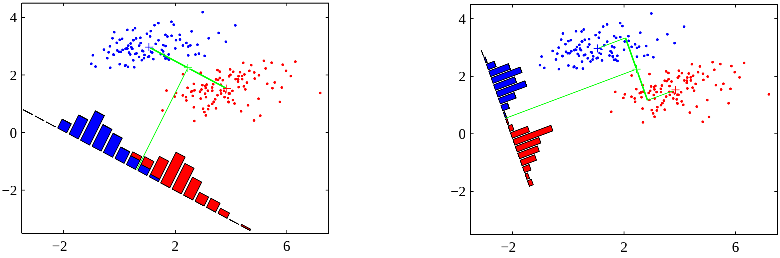


Fisher's Linear Discriminant



- 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.

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!