THE UNIVERSITY *of* EDINBURGH
informatics

Applied Machine Learning (AML)

Logistic Regression

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Linear Classification

Generative Versus Discriminative Classifiers

- **Generative** classifiers (e.g. Naive Bayes) model how a class 'generated' the feature vector $p(\boldsymbol{x}|y)$
- Which we then used for classification

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- In contrast, **discriminative** classifiers do not waste effort modelling the generative process
- Instead, they model the posterior $p(y|\boldsymbol{x})$ *directly*

Generative Versus Discriminative Classifiers

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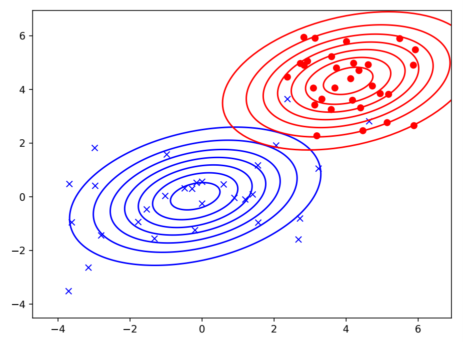
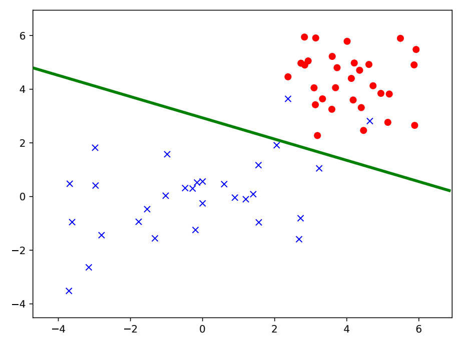
Generative Classifier



Discriminative Classifier



The Linear Classification Problem

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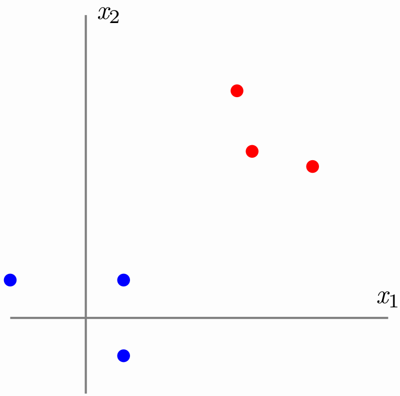

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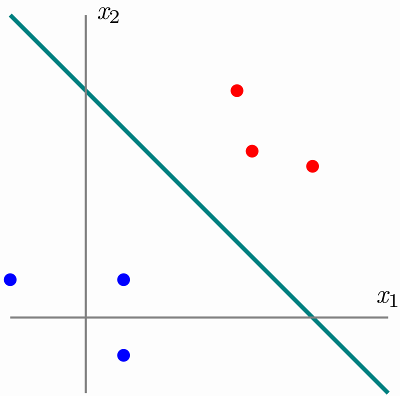

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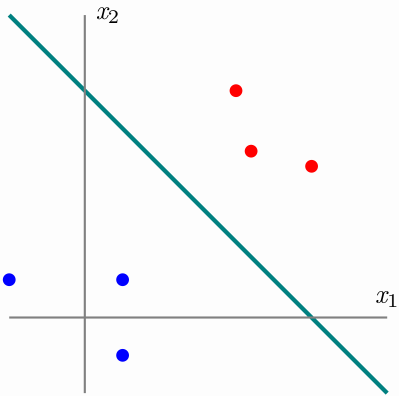
- The **decision boundary** is the boundary between these two regions, i.e. where the two classes are 'tied'



Linear Classifiers in Higher Dimensions

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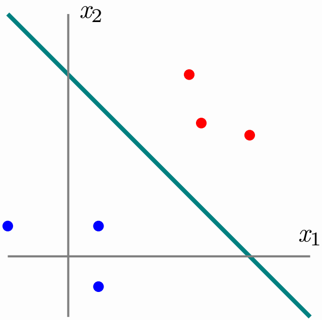

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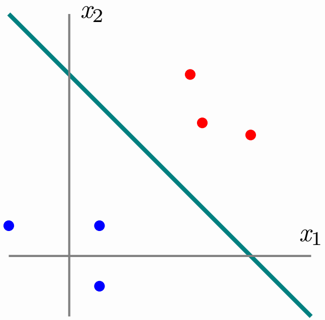

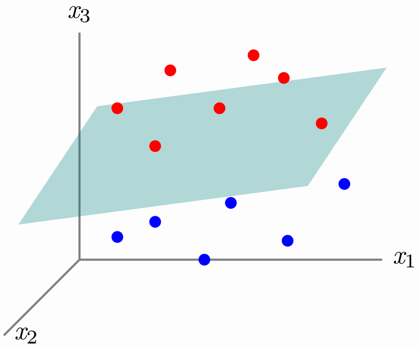

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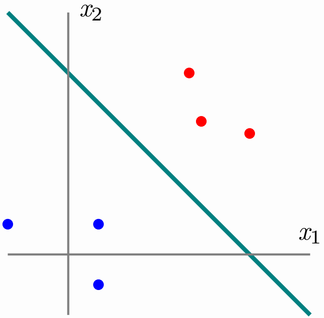
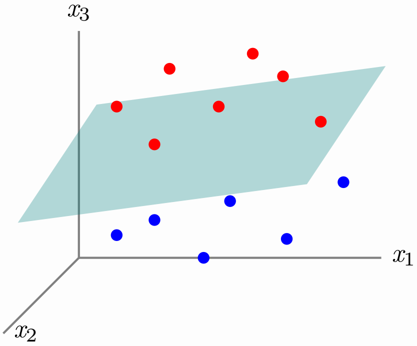
- In higher dimensions, it is a **hyperplane**





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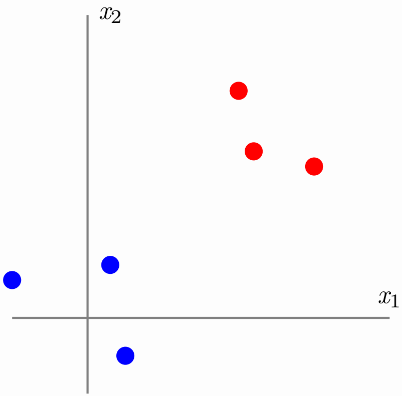
- To make a prediction we can threshold the output of the function

$$
\hat{y} = \begin{cases} 1 & \text{if } \boldsymbol{w}^\intercal \phi(\boldsymbol{x}) >= 0 \\ 0 & \text{if } \boldsymbol{w}^\intercal \phi(\boldsymbol{x}) < 0 \end{cases}
$$

Geometric Perspective



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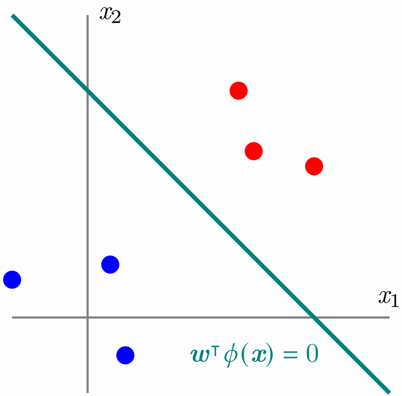

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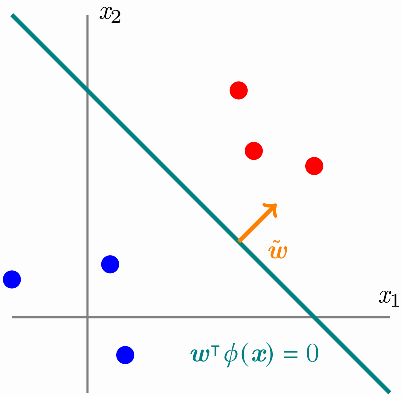

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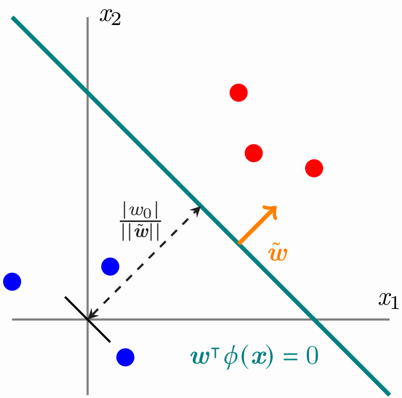

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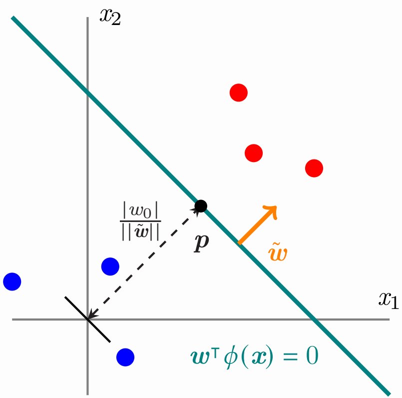
- If $\boldsymbol{p}$ is the point on the boundary closest to the origin, then the normal distance from the boundary to the origin is $\frac{|w_0|}{||\tilde{\boldsymbol{w}}||}$



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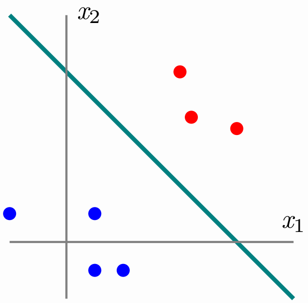

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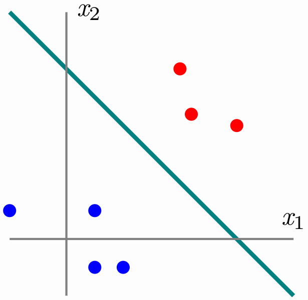

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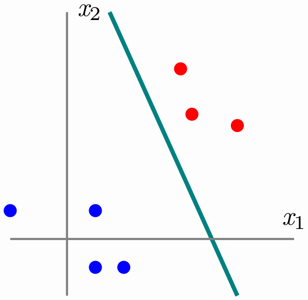

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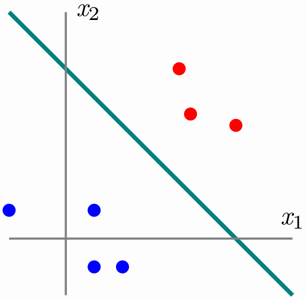

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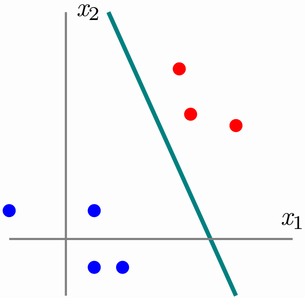

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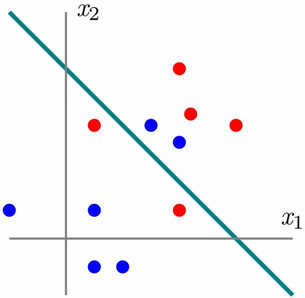

Linearly **non**-separable

Linear Separability

- If we can find a hyperplane to separate the data based on the classes, the problem is **linearly separable**

- Causes of non perfect separation
  - The linear model is too simple
  - Simple features that do not account for all variations
  - There is noise in the input features
  - There are errors in the class labels

Logistic Regression

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- One problem with our linear classifier, $f(\boldsymbol{x}; \boldsymbol{w}) = \boldsymbol{w}^\top \phi(\boldsymbol{x})$, is that the outputs are unbounded, i.e. $f(\boldsymbol{x}; \boldsymbol{w}) \in [-\infty, \infty]$

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- One solution is to 'squash' outputs of $f(\boldsymbol{x}; \boldsymbol{w})$ so that they remain in the range $[0, 1]$

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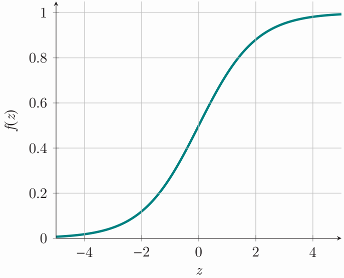
- As z goes from $-\infty$ to ∞, $\sigma(z)$ goes from 0 to 1,
- It has a ‘sigmoid’ shape, i.e. an ‘S’ like shape



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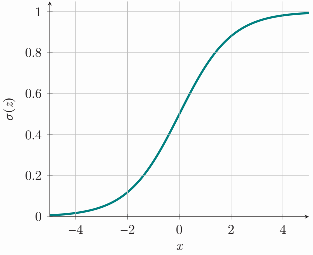

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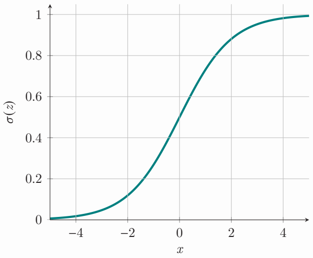

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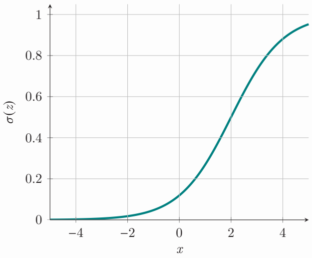

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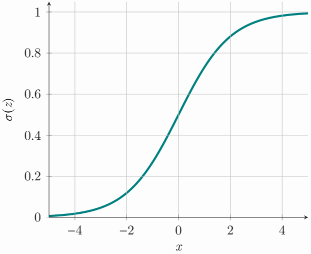

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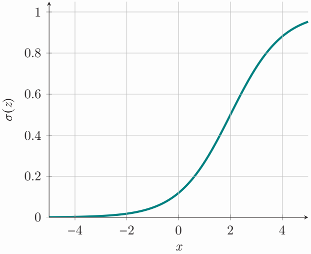

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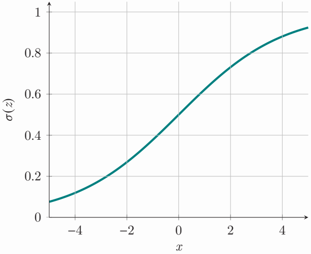

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- Despite the name, this is a model for **classification** not *regression*

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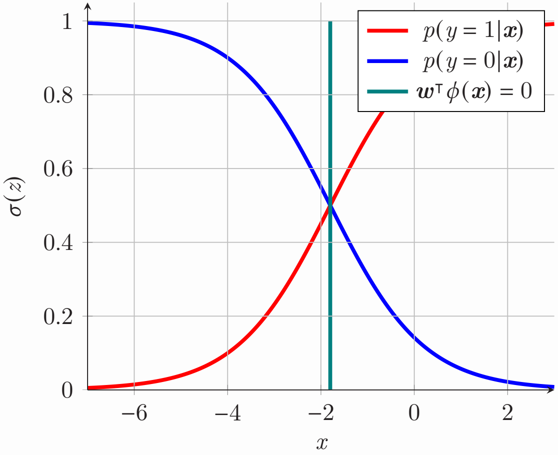

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- The magnitude of the weight vector $||\boldsymbol{w}||$ effects how certain the classifications are
- For small $||\boldsymbol{w}||$ most of the probabilities within the region of the decision boundary will be close to 0.5
- For large $||\boldsymbol{w}||$ probabilities in the same region will be close to 0 or 1

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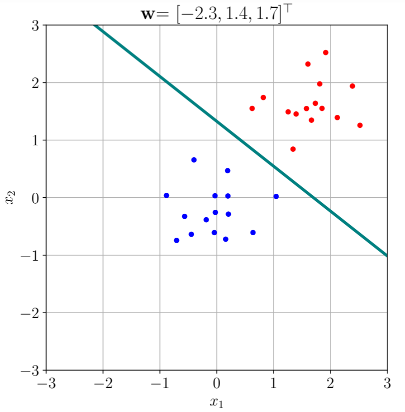

Input data

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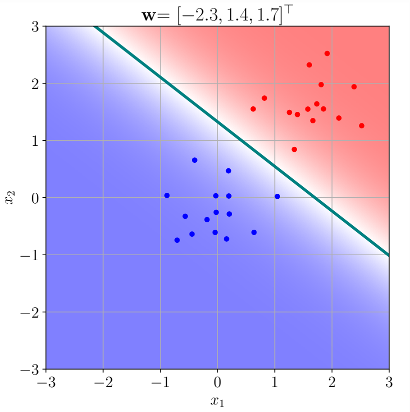
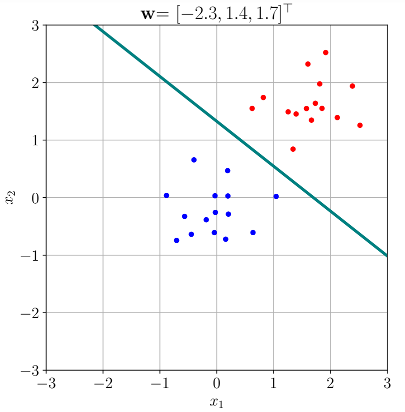


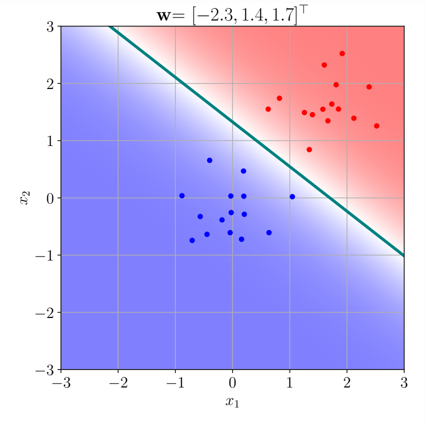
Standard model prediction



Input data

Impact of Weights on Classification

- On the right we set the bias to $w_0 = 0$



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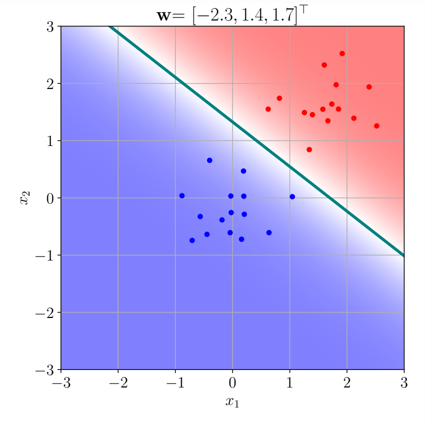

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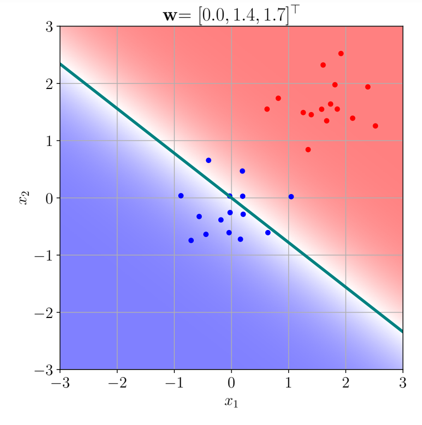

Zero bias

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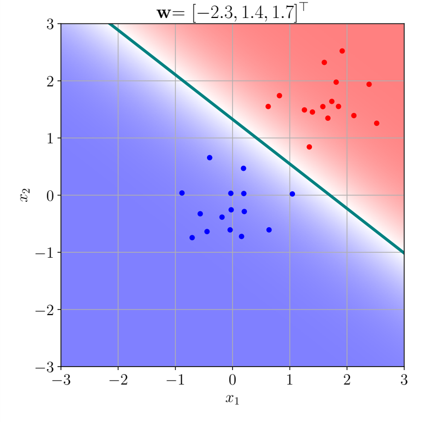

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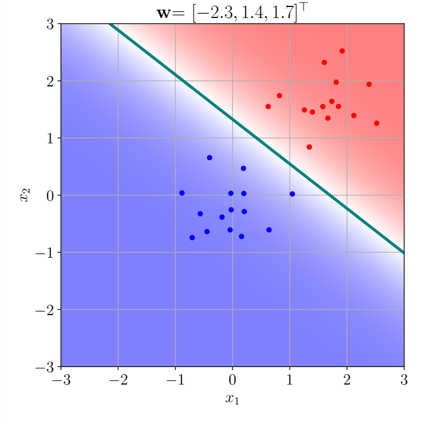

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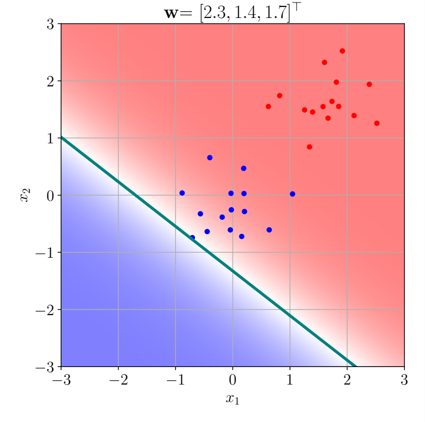

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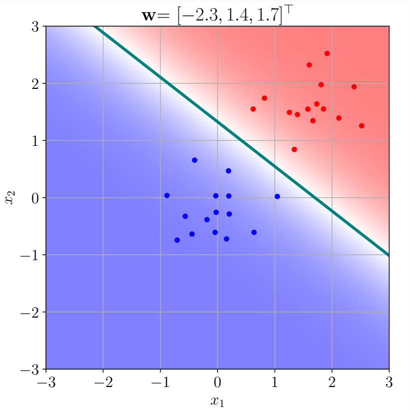

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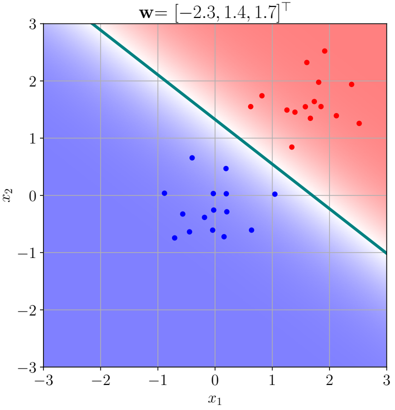

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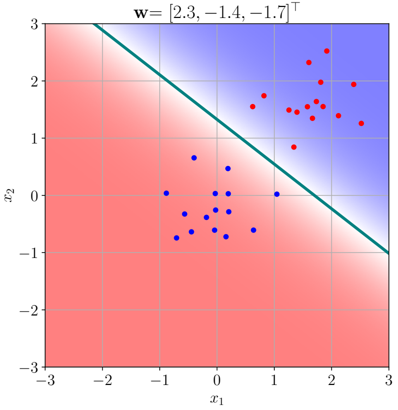

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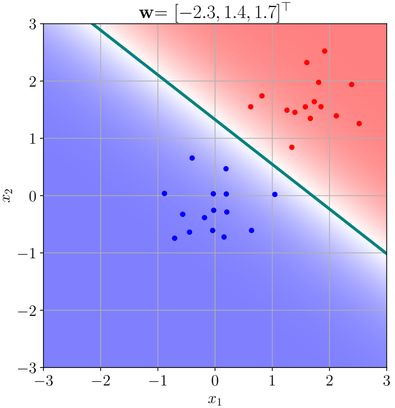

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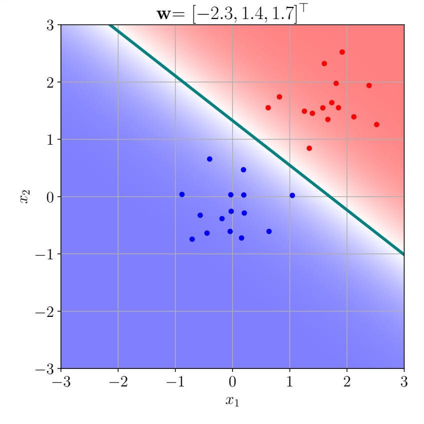

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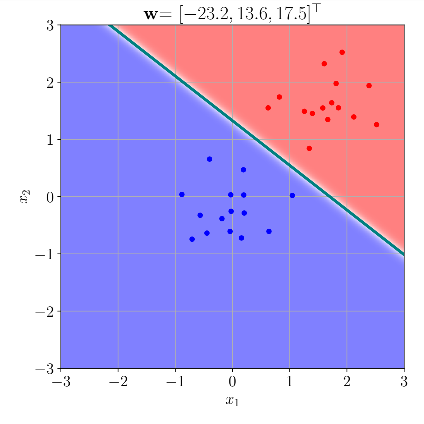

Scaled weights

Learning Logistic Regression

Maximum Likelihood Estimation

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- We will do this via *maximum likelihood estimation*

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- Main steps:
  - Write out the likelihood for the model
  - Find the derivatives of the negative log likelihood w.r.t the parameters
  - Adjust the parameters to minimise the negative log likelihood

Likelihood for Binary Classification

- We denote our dataset as $\mathcal{D} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), ...(\boldsymbol{x}_N, y_N)\}$, where $y \in \{0, 1\}$
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$$
\begin{aligned}
p(\mathcal{D}|\boldsymbol{w}) &= \prod_{n=1}^{N} p(y = y_n|\boldsymbol{x}_n; \boldsymbol{w}) \\
&= \prod_{n=1}^{N} p(y = 1|\boldsymbol{x}_n; \boldsymbol{w})^{y_n} (1 - p(y = 1|\boldsymbol{x}_n; \boldsymbol{w}))^{1-y_n}
\end{aligned}
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- Hence, the **negative log likelihood**, $\mathsf{NLL}(\boldsymbol{w}) = -\frac{1}{N}\log p(\mathcal{D}|\boldsymbol{w})$, is given by

$$\mathsf{NLL}(\boldsymbol{w}) = -\frac{1}{N}\sum_{n=1}^{N}\left[y_n \log\sigma(\boldsymbol{w}^\intercal\boldsymbol{x}_n) + (1-y_n)\log(1-\sigma(\boldsymbol{w}^\intercal\boldsymbol{x}_n))\right]$$

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- To minimise it, we solve for the gradient

$$\frac{\partial \mathsf{NLL}(\boldsymbol{w})}{\partial w_d} = \frac{1}{N}\sum_{n=1}^{N}(\sigma(\boldsymbol{w}^{\mathsf{T}}\boldsymbol{x}_n) - y_n)x_{nd}$$

Visualising the NLL Loss Surface

- NLL loss surface for binary logistic regression applied to the Iris dataset with one feature and one bias term

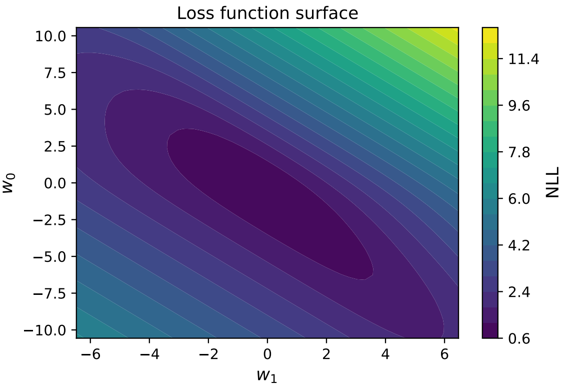

Figure adapted from Probabilistic Machine Learning: An Introduction, K. Murphy

Multiclass Classification

More Than Two Classes

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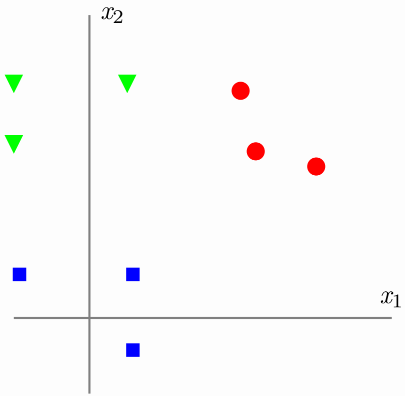

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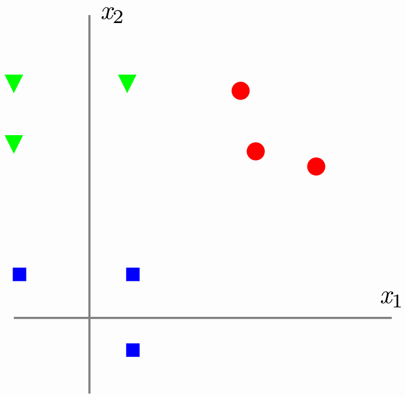

One-vs-Rest (OvR) Classification

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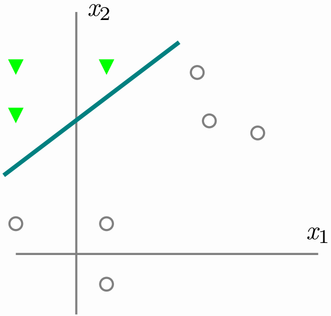

$y = 1$

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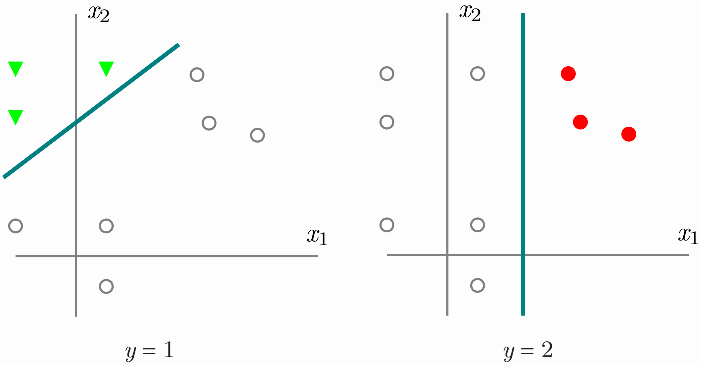

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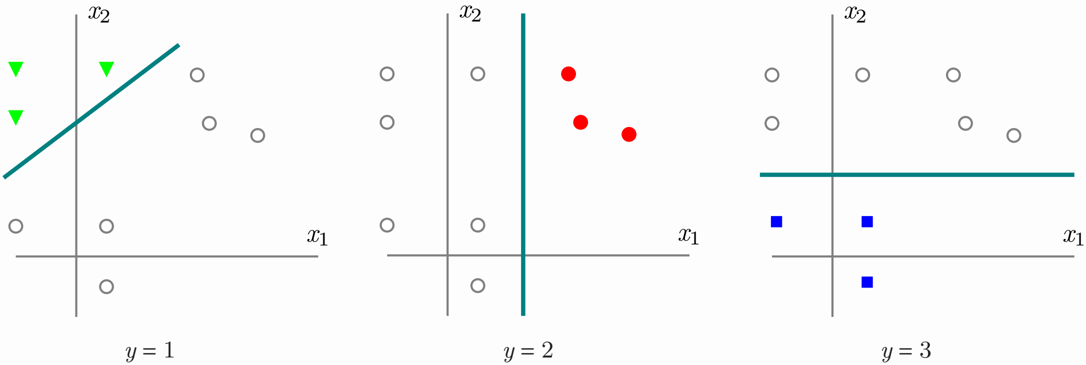

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- The OvR approach is a general one that can be applied to any binary classifier

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Properties of the Softmax Function

- The softmax function $\boldsymbol{s}()$ converts a vector of K real numbers, $\boldsymbol{z} \in \mathbb{R}^K$, into a probability distribution of K possible outcomes

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- The normalisation ensures that the sum of the components of the output vector is 1, i.e. $\sum_{i=1}^{K} \boldsymbol{s}(\boldsymbol{z})_i = 1$

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- For a D dimensional input space, there are $D + 1$ parameters (i.e. weights) that need to be learned in binary classification
- We showed that we can derive an expression for estimating the parameters for this model using maximum likelihood estimation
- It is a simple model, but can be very effective. Often it should be one of the first models to try