



Trinity College Dublin

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The University of Dublin

02 - Logistic Regression

(linear classifier, cross-entropy
gradient descent optimisation)

François Pitié

Assistant Professor in Media Signal Processing

Department of Electronic & Electrical Engineering, Trinity College Dublin

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Motivation

With **Linear Regression**, we looked at linear models, where the output of the problem was a **continuous variable** (eg. height, car price, temperature, ...).

分类器

Very often you need to design a **classifier** that can answer questions such as: what car type is it? is the person smiling? is a solar flare going to happen? In such problems the model depends on **categorical** variables.

分类

明确的

Logistic Regression (David Cox, 1958), considers the case of a **binary variable**, where the outcome is 0/1 or true/false.

There is a whole zoo of classifiers out there. Why are we covering logistic regression in particular?

Because logistic regression is the building block of 神经网络 Neural Nets.

Introductory Example

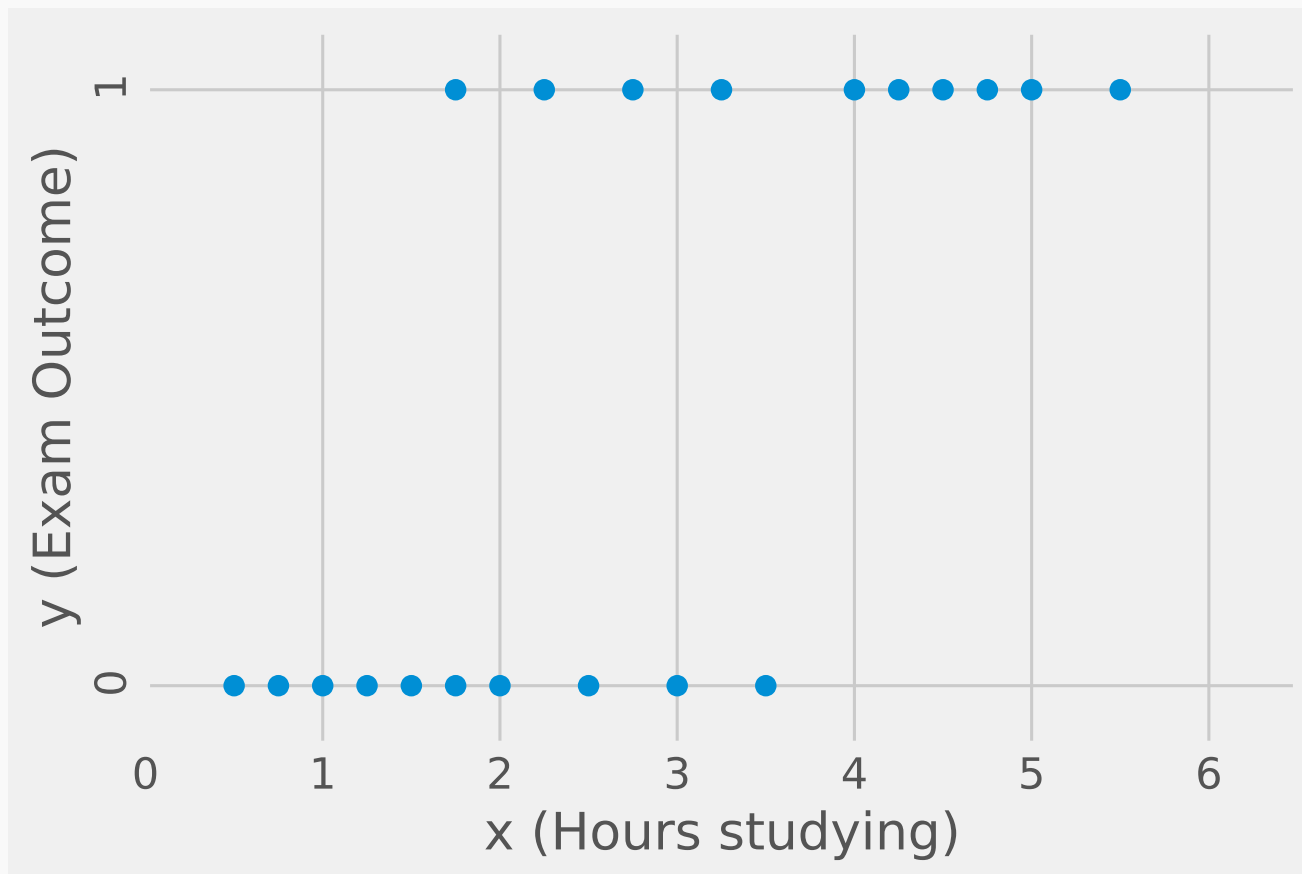
We'll start with an example from Wikipedia:

A group of 20 students spend between 0 and 6 hours studying for an exam. How does the number of hours spent studying affect the probability that the student will pass the exam?

Introductory Example

The collected data looks like so:

Studying Hours	:	0.75	1.00	2.75	3.50	...
result (1=pass,0=fail)	:	0	0	1	0	...



Regression?

Although the output y is binary, we could still attempt to fit a linear model via least squares:

线性模型

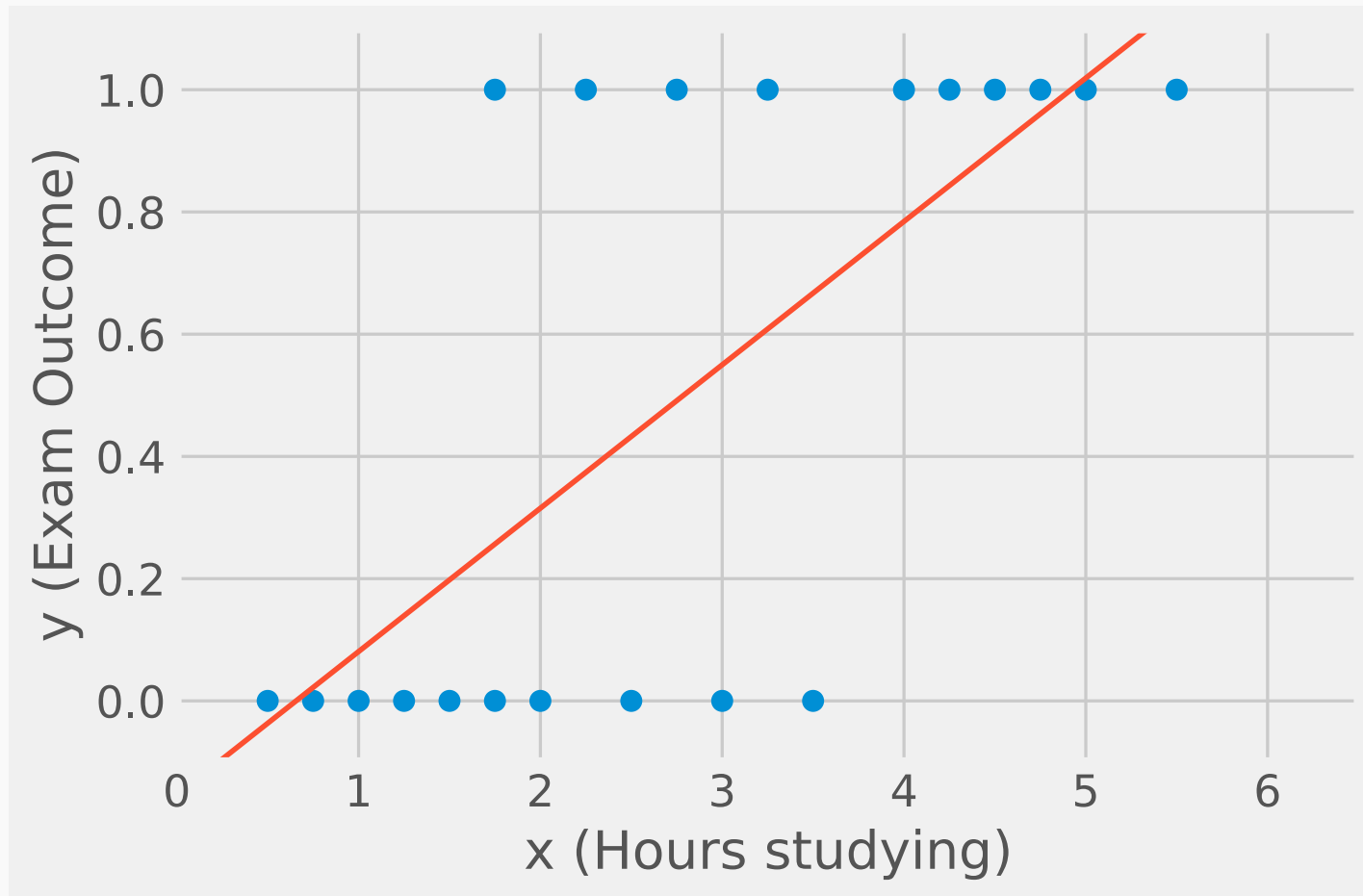
$$h_{\mathbf{w}}(\mathbf{x}) = \mathbf{x}^T \mathbf{w} = w_1 x_1 + \cdots + w_p x_p$$

where $h_{\mathbf{w}}(\mathbf{x})$ is the *prediction* given model parameters \mathbf{w} and input features \mathbf{x} .

Regression?

This is what the least squares estimate $h_w(\mathbf{x})$ looks like:

$$h_w(x) \approx 0.18 \times x + 0.08$$



Regression?

The model prediction $h_{\mathbf{w}}(\mathbf{x}) = \mathbf{x}^T \mathbf{w}$ is continuous, but we could apply a threshold to obtain the binary classifier as follows:

$$y = [\mathbf{x}^T \mathbf{w} > 0.5] = \begin{cases} 0 & \text{if } \mathbf{x}^T \mathbf{w} \leq 0.5 \\ 1 & \text{if } \mathbf{x}^T \mathbf{w} > 0.5 \end{cases}$$

and the output would be 0 or 1.

Numerically on our example we would have:

$$y = \begin{cases} 0 & \text{if } 0.18 \times x + 0.08 \leq 0.5 \\ 1 & \text{if } 0.18 \times x + 0.08 > 0.5 \end{cases}$$

Obviously, we have some issues with that approach...

Regression?

Example: a student studied 100 hours and is successful:

$$h_w(x) = 100 \times 0.18 + 0.08 = 18.08 > 0.5$$

But in terms of LS, the error $\varepsilon^2 = (1 - h_w(x))^2 = 17.1^2$ is large, when everything is in fact perfectly fine.

Regression?

The issue is that the our Least Squares loss is defined as:

$$E(\mathbf{w}) = \sum_i (\mathbf{w}^\top \mathbf{x}_i - y_i)^2$$

But we should include the threshold and have something like:

$$E(\mathbf{w}) = \sum_i (\underbrace{[\mathbf{w}^\top \mathbf{x}_i > 0.5]} - y_i)^2$$

So Least Squares doesn't really work...

Let's see what can be done.

General Linear Model

The general problem of **general linear models** can be presented as follows. We are trying to find a linear combination of the data $\mathbf{x}^T \mathbf{w}$, such that the sign of $\mathbf{x}^T \mathbf{w}$ tells us about the outcome y :


$$y = [\mathbf{x}^T \mathbf{w} + \epsilon > 0]$$

General Linear Model

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The quantity $\mathbf{x}^T \mathbf{w}$ is sometimes called the risk score. It is a scalar value that grades the certainty to belong to one class or the other:


$$\begin{aligned} \mathbf{x}^T \mathbf{w} &\gg 0 \Rightarrow y = 1 && \text{large} && \text{for sure} \\ \mathbf{x}^T \mathbf{w} &\ll 0 \Rightarrow y = 0 && \text{small} \\ \mathbf{x}^T \mathbf{w} &\approx 0 \Rightarrow \text{undecided} \end{aligned}$$

The risk score does a dimensional reduction: it combines multiple input features into a single number.

General Linear Model

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$$y = [\mathbf{x}^T \mathbf{w} + \epsilon > 0]$$

The error term is represented by the random variable ϵ . Multiple choices are possible for the distribution of ϵ .

逻辑分布

In **logistic regression**, the **error ϵ** is assumed to follow a **logistic distribution** and the **risk score $\mathbf{x}^T \mathbf{w}$** is also called the **logit**.

$\begin{cases} \mathbf{x}^T \mathbf{w} \geq 0 \Rightarrow y=1 \\ \mathbf{x}^T \mathbf{w} < 0 \Rightarrow y=0 \\ \mathbf{x}^T \mathbf{w} \approx 0 \Rightarrow \text{undecided} \end{cases}$

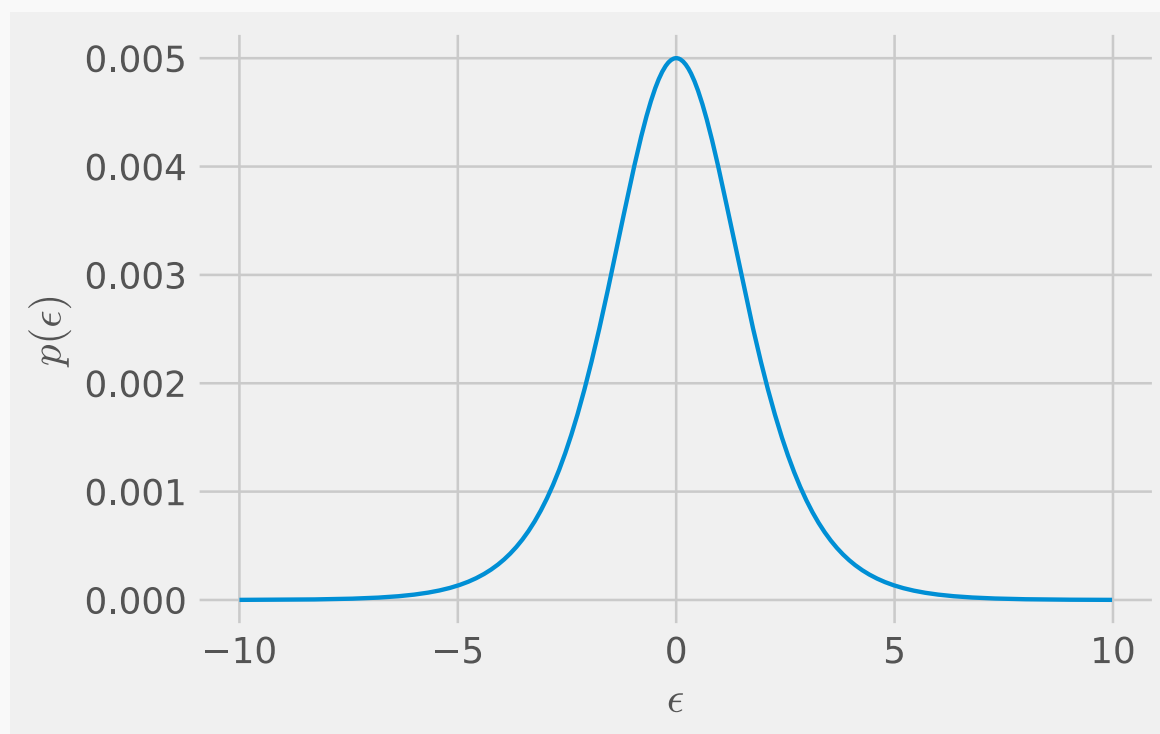


Figure: pdf of the logistic distribution

概率图规

正态分布

In **probit** regression, the error ϵ is assumed to follow a **normal distribution**, the risk score $\mathbf{x}^T \mathbf{w}$ is also called the **probit**.

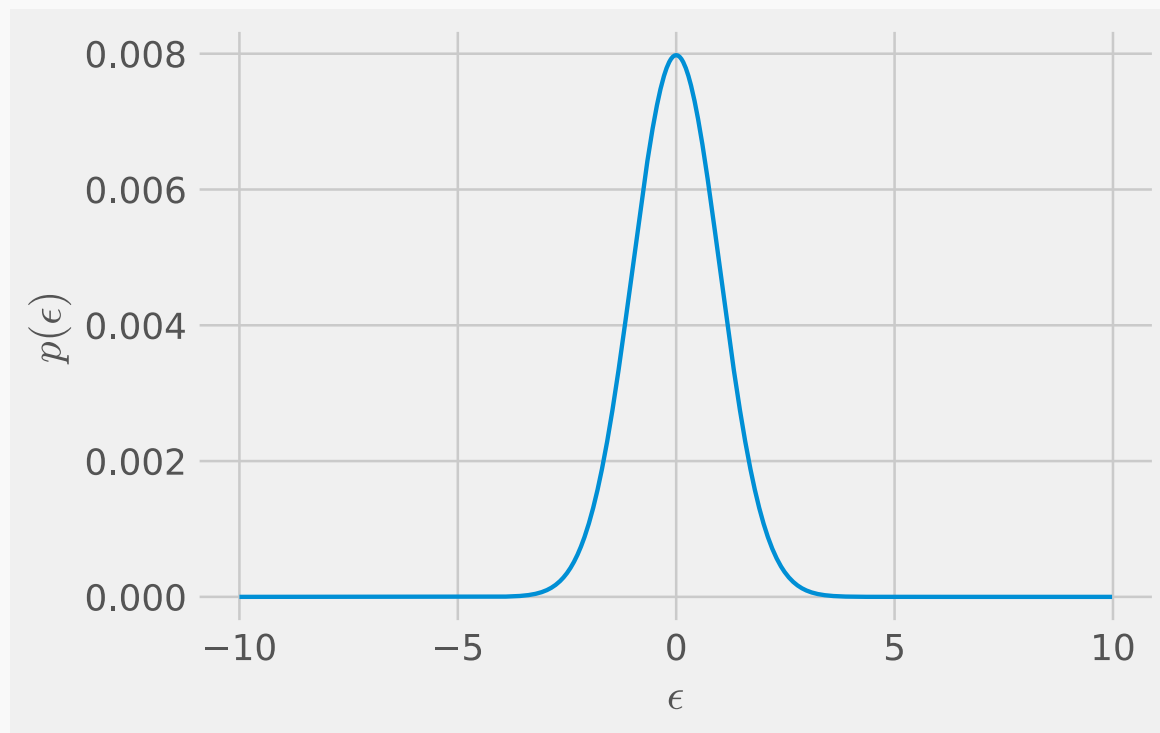


Figure: pdf of the normal distribution

For our purposes, there is not much difference between *logistic* and *logit* regression. The main difference is that logistic regression is numerically easier to solve.

From now on, we'll only look at the logistic model but note that similar derivations could be made for any other model.

Logistic Regression Model

Consider $p(y = 1|\mathbf{x}, \mathbf{w})$, the **likelihood** that the output is a success:

$$\begin{aligned} p(y = 1|\mathbf{x}, \mathbf{w}) &= p(\mathbf{x}^T \mathbf{w} + \epsilon > 0) \\ &= p(\epsilon > -\mathbf{x}^T \mathbf{w}) \end{aligned}$$

Handwritten notes: $y = \mathbf{x}^T \mathbf{w} + \epsilon$ (pink), and a pink wavy underline under the second equation.

since ϵ is symmetrically distributed around 0, it follows that

$$p(y = 1|\mathbf{x}, \mathbf{w}) = p(\epsilon < \mathbf{x}^T \mathbf{w})$$

Handwritten notes: "以 0 对称分布" (pink), and a pink wavy underline under the expression $\epsilon < \mathbf{x}^T \mathbf{w}$.

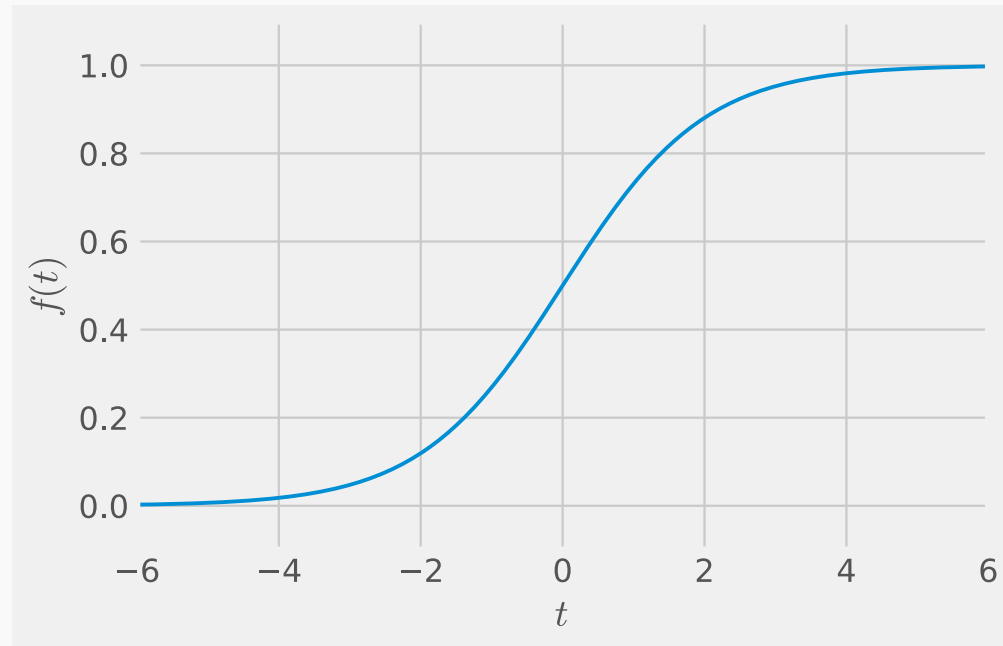
Because we have made some assumptions about the distribution of ϵ , we are able to derive a closed-form expression for the likelihood.

The Logistic Function

The function $f : t \mapsto f(t) = p(\epsilon < t)$ is the c.d.f. of the logistic distribution and is also called the **logistic function** or sigmoid:

Sigs

$$f(t) = \frac{1}{1 + e^{-t}}$$



Logistic Regression Model

Thus we have a simple model for the likelihood of success:

$$p(y = 1|\mathbf{x}, \mathbf{w}) = p(\epsilon < \mathbf{x}^\top \mathbf{w}) = f(\mathbf{x}^\top \mathbf{w}) = \frac{1}{1 + e^{-\mathbf{x}^\top \mathbf{w}}}$$

The likelihood of failure is simply given by:

$$p(y = 0|\mathbf{x}, \mathbf{w}) = 1 - p(y = 1|\mathbf{x}, \mathbf{w}) = \frac{1}{1 + e^{+\mathbf{x}^\top \mathbf{w}}}$$

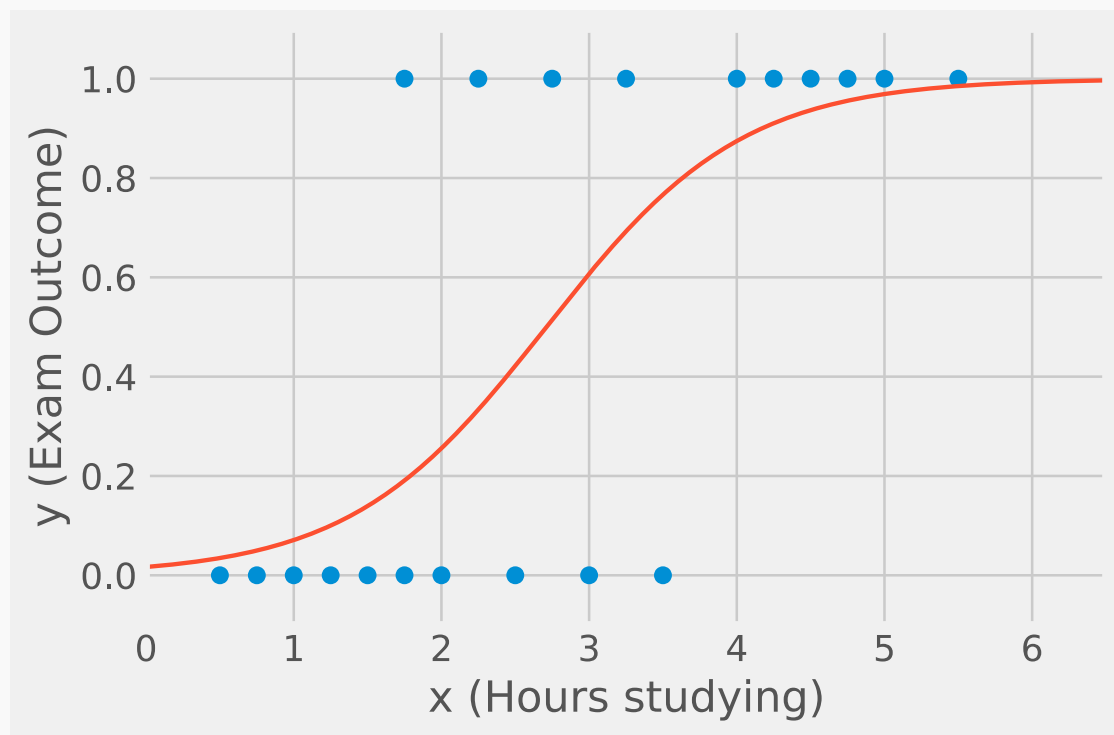
$$p(y=1|\mathbf{x}, \mathbf{w}) = p(\epsilon < \mathbf{x}^\top \mathbf{w})$$
$$h_{\mathbf{w}}(\mathbf{x}) = \mathbf{x}^\top \mathbf{w}$$

Exercise:

show that $p(y = 0|\mathbf{x}, \mathbf{w}) = h_{\mathbf{w}}(-\mathbf{x})$

Logistic Regression Model

Below is the plot of $p(y = 1|\mathbf{x}, \mathbf{w}) = 1/(1 + \exp(-(w_0 + w_1x)))$ for our problem (using optimal values of w_0 and w_1):



The results are easy to interpret: there is about 60% chance to pass the exam if you study for 3 hours.

Logistic Regression vs. Least Squares

In **linear regression**, the model prediction $h_{\mathbf{w}}(\mathbf{x})$ was a direct prediction of the outcome: 直接的预测值

$$h_{\mathbf{w}}(\mathbf{x}) = \hat{y}$$

In **logistic regression**, the model prediction $h_{\mathbf{w}}(\mathbf{x})$ is an estimate of the **likelihood** of the outcome: 一种可能性
computing which class

$$h_{\mathbf{w}}(\mathbf{x}) = p(y = 1 | \mathbf{x}, \mathbf{w})$$

Thus whereas in linear regression we try to answer the question:

What is the expected value of y given \mathbf{x} ?

In logistic regression (and any other general linear model), we try instead to answer the question:

What is the probability that $y = 1$ given \mathbf{x} ?

Maximum Likelihood

To estimate the weights \mathbf{w} , we will again use the concept of **Maximum Likelihood**.

Maximum Likelihood

As we've just seen, for a particular observation \mathbf{x}_i and model \mathbf{w} , the likelihood is given by:

$$p(y = y_i | \mathbf{x}_i, \mathbf{w}) = \begin{cases} p(y = 1 | \mathbf{x}_i, \mathbf{w}) = h_{\mathbf{w}}(\mathbf{x}_i) & \text{if } y_i = 1 \\ p(y = 0 | \mathbf{x}_i, \mathbf{w}) = 1 - h_{\mathbf{w}}(\mathbf{x}_i) & \text{if } y_i = 0 \end{cases}$$

As $y_i \in \{0, 1\}$, this can be written in a slightly more compact form:

$$\underline{p(y = y_i | \mathbf{x}_i, \mathbf{w}) = h_{\mathbf{w}}(\mathbf{x}_i)^{y_i} (1 - h_{\mathbf{w}}(\mathbf{x}_i))^{1-y_i}}$$

This works because $z^0 = 1$.

Assuming independent observations, the likelihood over all observations is:

$$p(\mathbf{y} | \mathbf{X}, \mathbf{w}) = \prod_{i=1}^n h_{\mathbf{w}}(\mathbf{x}_i)^{y_i} (1 - h_{\mathbf{w}}(\mathbf{x}_i))^{1-y_i}$$

Maximum Likelihood

We want to find \mathbf{w} that maximises the likelihood $p(\mathbf{y}|\mathbf{X})$. As always, it is equivalent but more convenient to minimise the negative log likelihood:

$$\begin{aligned} E(\mathbf{w}) &= -\ln(p(\mathbf{y}|\mathbf{X}, \mathbf{w})) \\ &= \sum_{i=1}^n -y_i \ln(h_{\mathbf{w}}(\mathbf{x}_i)) - (1 - y_i) \ln(1 - h_{\mathbf{w}}(\mathbf{x}_i)) \end{aligned}$$

This loss function we need to minimise is called the 交叉熵 cross-entropy.

Note that we can consider also the *average* cross-entropy:

$$E(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n -y_i \ln(h_{\mathbf{w}}(\mathbf{x}_i)) - (1 - y_i) \ln(1 - h_{\mathbf{w}}(\mathbf{x}_i))$$

We could have considered optimising the parameters \mathbf{w} using other loss functions. For instance we could have tried to minimise the least square error as we did in linear regression:

$$E_{LS}(\mathbf{w}) = \sum_{i=1}^n (h_{\mathbf{w}}(\mathbf{x}_i) - y_i)^2$$

The solution would not maximise the likelihood, as would the cross-entropy loss, but maybe that would still be a reasonable thing to do? The problem is that $h_{\mathbf{w}}$ is non-convex, which makes the minimisation of $E_{LS}(\mathbf{w})$ much harder than when using cross-entropy.

This is in fact a mistake that the Neural Net community did for a number of years before switching to the cross entropy loss function.

Optimisation: gradient descent

To minimise the error function, we need to resort to gradient descent, which is a general method for nonlinear optimisation and which will be at the core of neural networks optimisation.

We start at $\mathbf{w}^{(0)}$ and take steps along the steepest direction \mathbf{v} using a fixed size step as follows:

$$\mathbf{w}^{(n+1)} = \mathbf{w}^{(n)} + \eta \mathbf{v}^{(n)}$$

η 控制下降的速度

η is called the learning rate and controls the speed of the descent.

What is the steepest slope \mathbf{v} ?

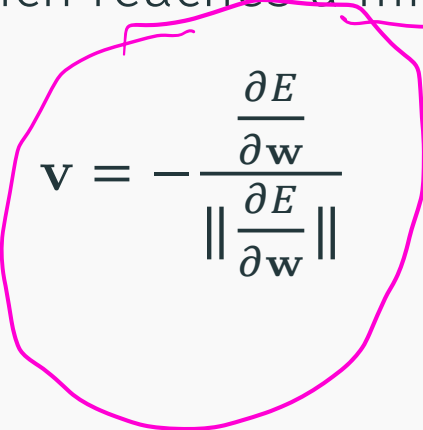
Optimisation: gradient descent

Without loss of generality we set \mathbf{v} to be a unit vector (ie. $\|\mathbf{v}\| = 1$).
Then, moving \mathbf{w} to $\mathbf{w} + \eta \mathbf{v}$ yields a new error as follows:

$$E(\mathbf{w} + \eta \mathbf{v}) = E(\mathbf{w}) + \eta \left(\frac{\partial E}{\partial \mathbf{w}} \right)^T \mathbf{v} + O(\eta^2)$$

高阶无穷小

which reaches a minimum when


$$\mathbf{v} = - \frac{\frac{\partial E}{\partial \mathbf{w}}}{\left\| \frac{\partial E}{\partial \mathbf{w}} \right\|}$$

Optimisation: gradient descent

now, it is hard to find a good value for the learning rate η and we usually adopt an adaptive step instead. Thus instead of using

$$\mathbf{w}^{(n+1)} = \mathbf{w}^{(n)} - \eta \frac{\frac{\partial E}{\partial \mathbf{w}}}{\left\| \frac{\partial E}{\partial \mathbf{w}} \right\|}$$

we usually use the following update step:

$$\mathbf{w}^{(n+1)} = \mathbf{w}^{(n)} - \eta \frac{\partial E}{\partial \mathbf{w}}$$

Optimisation: gradient descent

Recall that the cross-entropy loss function is:

$$E(\mathbf{w}) = \sum_{i=1}^n -y_i \ln(h_{\mathbf{w}}(\mathbf{x}_i)) - (1 - y_i) \ln(1 - h_{\mathbf{w}}(\mathbf{x}_i))$$

and that
$$h_{\mathbf{w}}(\mathbf{x}) = f(\mathbf{x}^{\top} \mathbf{w}) = \frac{1}{1 + e^{-\mathbf{x}^{\top} \mathbf{w}}}$$

Exercise:

Given that the derivative of the sigmoid f is $f'(t) = (1 - f(t))f(t)$, show that

$$\frac{\partial E}{\partial \mathbf{w}} = \sum_{i=1}^n (h_{\mathbf{w}}(\mathbf{x}_i) - y_i) \mathbf{x}_i$$

Optimisation: gradient descent

The overall gradient descent method looks like so:

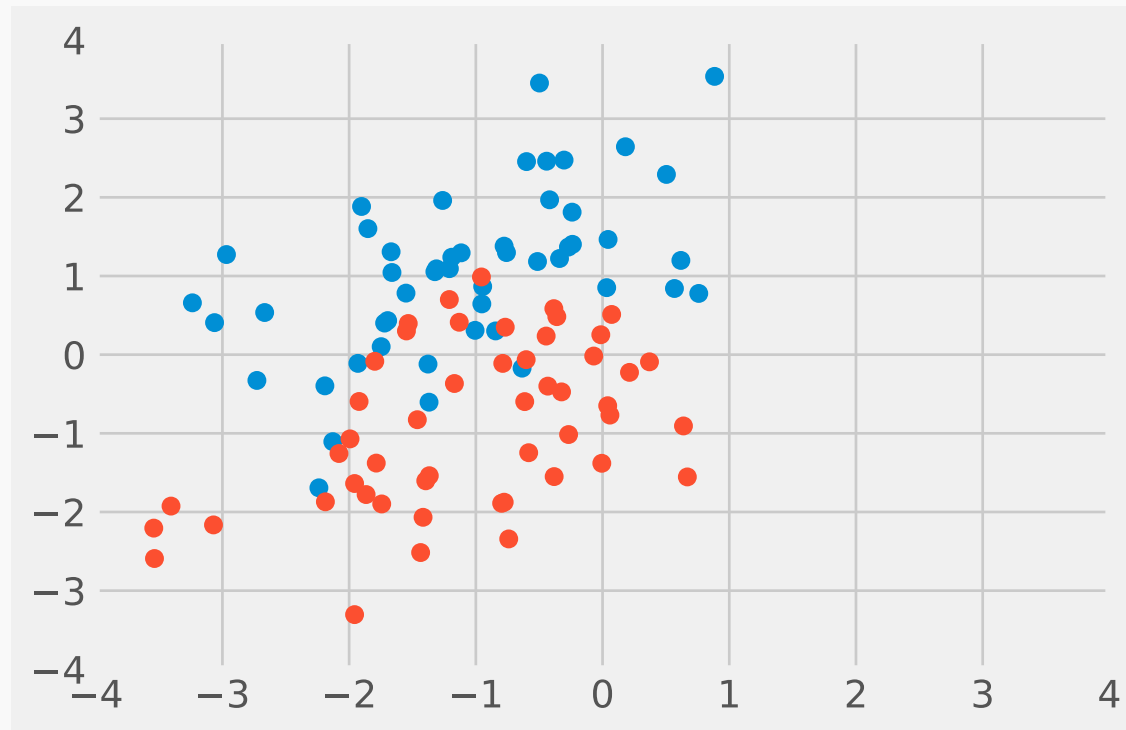
1. set an initial weight vector $\mathbf{w}^{(0)}$ and
2. **for** $t = 0, 1, 2, \dots$ **do until convergence**
3. compute the gradient

$$\frac{\partial E}{\partial \mathbf{w}} = \sum_{i=1}^n \left(\frac{1}{1 + e^{-\mathbf{x}_i^\top \mathbf{w}}} - y_i \right) \mathbf{x}_i$$

4. update the weights: $\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \frac{\partial E}{\partial \mathbf{w}}$

Example

Below is an example with 2 features.

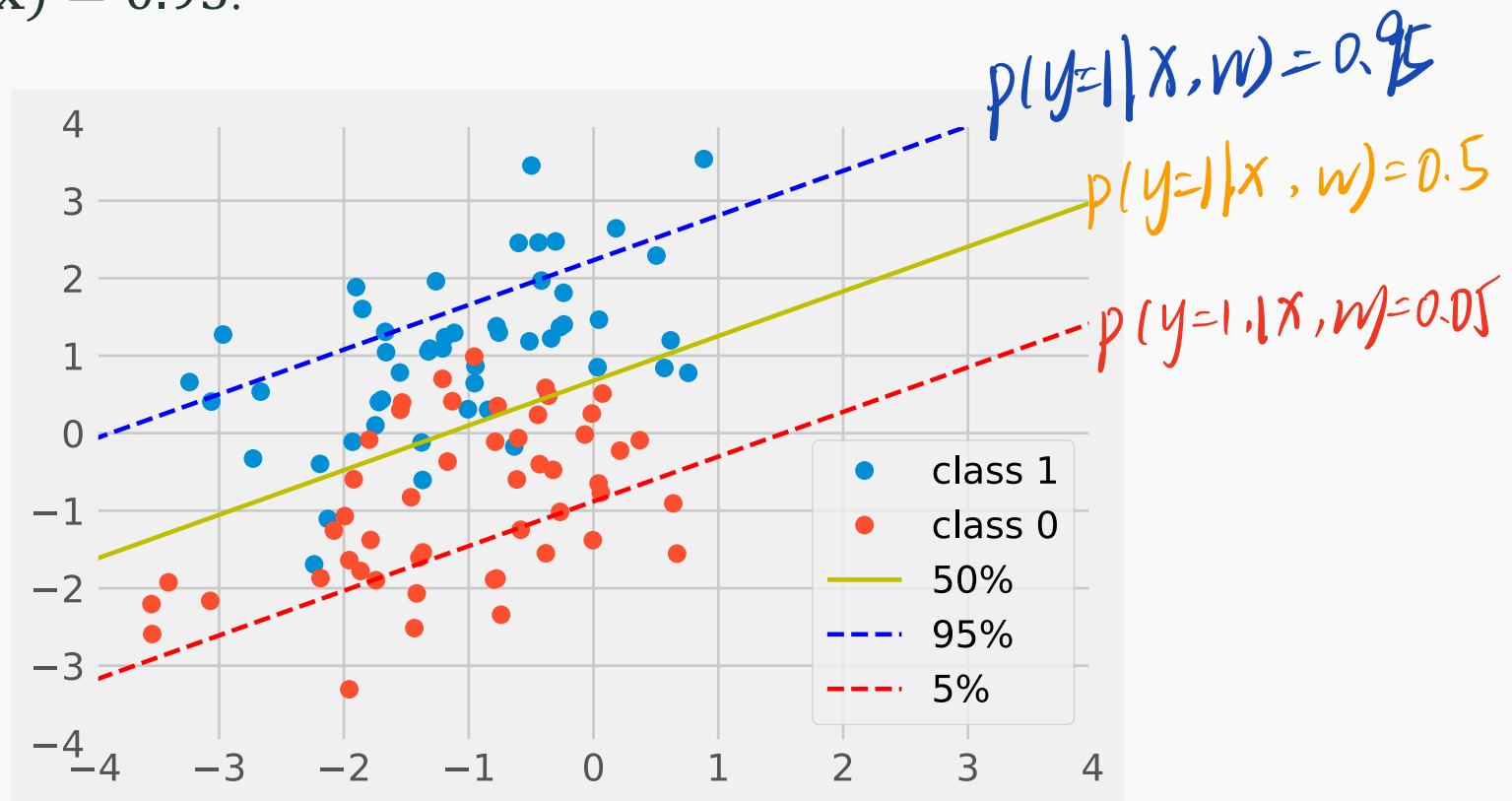


Example

The estimate for the probability of success is

$$h_{\mathbf{w}}(\mathbf{x}) = 1/(1 + e^{-(-1.28 - 1.09x_1 + 1.89x_2)})$$

Below are drawn the lines that correspond to $h_{\mathbf{w}}(\mathbf{x}) = 0.05$, $h_{\mathbf{w}}(\mathbf{x}) = 0.5$ and $h_{\mathbf{w}}(\mathbf{x}) = 0.95$.



Multiclass Classification

In many applications you have to deal with more than 2 classes.

In these cases, we need to use 多项式 multinomial logistic regression, which is an extension of logistic regression to more than 2 classes.

Multinomial Logistic Regression

多项式

In Multinomial Logistic Regression, each of the binary classifier is based on the following likelihood model:

$$p(y = C_k | \mathbf{x}, \mathbf{w}) = \text{softmax}(\mathbf{x}^\top \mathbf{w})_k = \frac{\exp(\mathbf{w}_k^\top \mathbf{x})}{\sum_{j=1}^K \exp(\mathbf{w}_j^\top \mathbf{x})}$$

C_k is the class k and $\text{softmax} : \mathbb{R}^K \rightarrow \mathbb{R}^K$ is the function defined as

$$\text{softmax}(\mathbf{t})_k = \frac{\exp(t_k)}{\sum_{j=1}^K \exp(t_j)}$$

In other words, softmax takes as an input the vector of logits for all classes and returns the vector of corresponding likelihoods.

Multinomial Logistic Regression

For instance, say we have 3 classes A, B, C, with

$$\mathbf{x} \rightarrow \begin{bmatrix} \mathbf{x}^\top \mathbf{w}_A = -1.2 \\ \mathbf{x}^\top \mathbf{w}_B = +3.1 \\ \mathbf{x}^\top \mathbf{w}_C = -0.9 \end{bmatrix} \xrightarrow{\text{softmax}} \begin{bmatrix} p(A|\mathbf{x}) = 0.0131 \\ p(B|\mathbf{x}) = 0.9691 \\ p(C|\mathbf{x}) = 0.0177 \end{bmatrix}$$

where $p(A|\mathbf{x}) = \exp(-1.2)/(\exp(-1.2)+\exp(3.1)+\exp(-0.9)) = 0.0131$

Multinomial Cross Entropy

To optimise for the parameters. We can take again the **maximum likelihood** approach.

Combining the likelihood for all possible classes gives us:

$$p(y|\mathbf{x}) = p(y = C_1|\mathbf{x})^{[y=C_1]} \times \dots \times p(y = C_K|\mathbf{x})^{[y=C_K]}$$

where $[y = C_1]$ is 1 if $y = C_1$ and 0 otherwise.

The total likelihood is:

$$p(y|\mathbf{X}) = \prod_{i=1}^n p(y_i = C_1|\mathbf{x}_i)^{[y=C_1]} \times \dots \times p(y_i = C_K|\mathbf{x}_i)^{[y=C_K]}$$

Multinomial Cross Entropy

Taking the negative log likelihood yields the cross entropy error function for the multiclass problem:

$$E(\mathbf{w}_1, \dots, \mathbf{w}_K) = -\ln(p(y|\mathbf{X})) = -\sum_{i=1}^n \sum_{k=1}^K [y_i = C_k] \ln(p(y_i = C_k | \mathbf{x}_i))$$

Similarly to logistic regression, we can use a gradient descent approach to find the K weight vectors $\mathbf{w}_1, \dots, \mathbf{w}_K$ that minimise this cross entropy expression.

Take Away

With **Logistic Regression**, we look at linear models, where the output of the problem is a **binary categorical** response.

Instead of directly predicting the actual outcome as in least squares, the model proposed in logistic regression makes a prediction about the **likelihood of belonging to a particular class**.

Finding the maximum likelihood parameters is equivalent to minimising the **cross entropy** loss function. The minimisation can be done using the **gradient descent** technique.

The extension of Logistic Regression to more than 2 classes is called the **Multinomial Logistic Regression**.