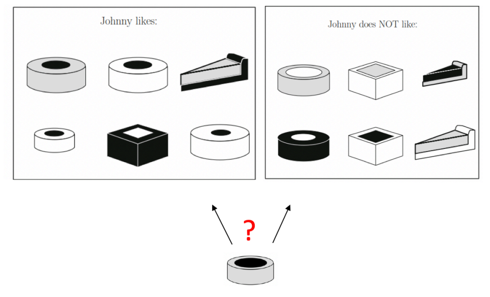
» Classification with Two Classes

- Will Johnny like or dislike the pie?
- Training data:



- Features: Shape (round, square, triangle), filling (white, gray, dark), crust (thick, thin, light, dark), size (big, small) etc
- To make prediction match features of pie against previous examples from training data

» Classification with Two Classes

* Examples:
  * *Movies reviews: positive or negative?*
  * Images: Does a picture contain human faces?
  * Finance: Is person applying for a loan likely to repay it?
  * Advertising: If display an ad on web page is the person likely to click on it?
  * Online transactions: fraudulent or not ?
  * Tumor: malignant or benign ?
* As before x="input" variable/features e.g. text of email, location, nationality
* Now y="output" variable/"target" variable only takes values -1 or 1 (with linear regression y was real valued). In classification y often referred to as the **label**[1].
* We want to build a **classifier** that predicts the label of a new object e.g whether a new email is spam or not.

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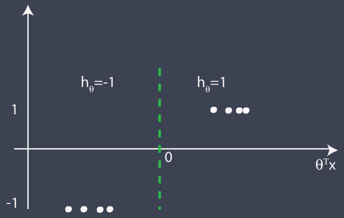
[1]Note could also use values 0 and 1 rather than -1 and 1, leave this as an exercise

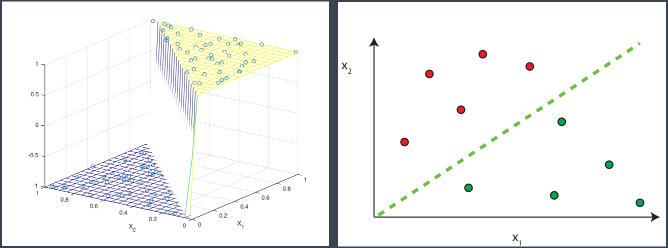
» Logistic Regression: Model



* As before $\theta^T x = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$ with $x_0 = 1$, $x_1, \ldots, x_n$ the input features and $\theta_0, \ldots, \theta_n$ the (unknown) parameters.
* Model: $sign(\theta^T x)$ i.e. predict output +1 when $\theta^T x > 0$ and output -1 when $\theta^T x < 0$. *Decision boundary* is $\theta^T x = 0$ (green line in plot above)
* $\theta^T x = 0$ defines a point in one dimension e.g. $1 + 0.5x_1 = 0 \rightarrow x_1 = -2$ ...
* ... a line in two dimensions e.g. $2 + x_1 + 2x_2 = 0 \Rightarrow x_2 = -x_1/2 - 1$ ...
* .. and a plane in higher dimensions

» Logistic Regression: Decision Boundary

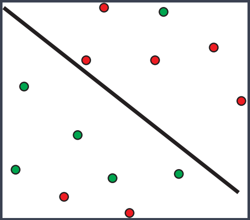
* Example: suppose x is vector $x = [1, x_1, x_2]^T$ e.g. x_1 might be tumour size and x_2 patient age.



* $\theta_0 = 0$, $\theta_1 = 0.5$, $\theta_2 = -0.5$.
* $sign(\theta^T x) = +1$ when $0.5x_1 - 0.5x_2 > 0$ i.e. when $x_1 > x_2$.
* When data can be separated in this way we say that it is *linearly separable*.
* Often the 3D plot on left is sketched in 2D as shown in right (easier to draw!)

» Logistic Regression: Decision Boundary

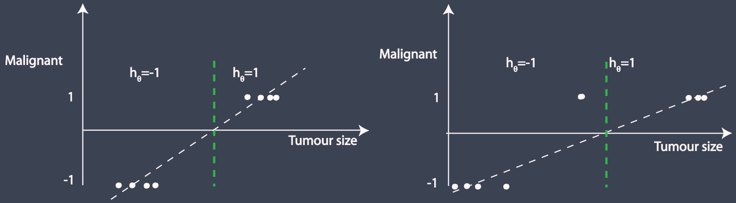
* Not all data is linearly separable e.g.



» Logistic Regression: Choice of Cost Function

* Training data: $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \cdots, (x^{(m)}, y^{(m)})\}$
* $x \in \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}, x_0 = 1, y \in \{-1, 1\}$
* Model: $h_\theta(x) = sign(\theta^T x)$
* How to choose parameters θ ?

» Logistic Regression: Choice of Cost Function



- Model: $sign(\theta^T x)$ i.e. predict output +1 when $\theta^T x > 0$ and output -1 when $\theta^T x < 0$
- Suppose we try square error $\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$.
  - Roughly speaking, minimising square error fits the same line to the data that we would fit by eye
  - Works ok on left-hand plot above: $sign(\theta^T x) = -1$ for points to the left of green line and $sign(\theta^T x) = +1$ for points to the right.
  - Not so good in right-hand plot - data points far to the right pull point where $\theta^T x$ crosses zero to the right, so causing misclassification

» Logistic Regression: Choice of Cost Function

* We might consider the **0-1 loss function**:

$$\frac{1}{m}\sum_{i=1}^{m}\mathbb{I}(h_\theta(x^{(i)}) \neq y^{(i)})$$

where indicator function $\mathbb{I}=1$ if $h_\theta(x^{(i)}) \neq y^{(i)}$ and $\mathbb{I}=0$ otherwise. But hard to work with.

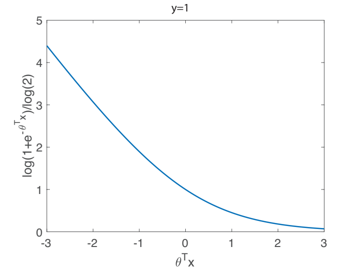
* For logistic regression we use:

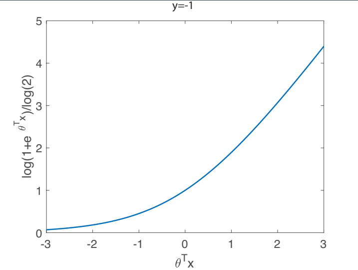
$$\frac{1}{m}\sum_{i=1}^{m}\log(1+e^{-y^{(i)}\theta^T x^{(i)}})/log(2)$$

noting that $y=-1$ or $y=+1$. Scaling by log(2) is optional, but makes the loss 1 when $y^{(i)}\theta^T x^{(i)}=0$.

» Logistic Regression: Choice of Cost Function

Loss function: $\log(1+e^{-y\theta^T x})/log(2)$





* So a small penalty when $\theta^T x \gg 0$ and $y = 1$, and when $\theta^T x \ll 0$ and $y = -1$.
* Minimising this thus gives preference to θ values that push $\theta^T x$ well away from the decision boundary $\theta^T x = 0$.

» Summary

* Model: $h_\theta(x) = sign(\theta^T x)$
* Parameters: θ
* Cost Function: $J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \log(1 + e^{-y^{(i)}\theta^T x^{(i)}})$
* Optimisation: Select θ that minimises $J(\theta)$

» Gradient Descent

As before, can find θ using gradient descent. For $J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \log(1 + e^{-y^{(i)}\theta^T x^{(i)}})$:

* $\frac{\partial}{\partial\theta_j}J(\theta) = \frac{1}{m}\sum_{i=1}^{m} -y^{(i)}x_j^{(i)}\frac{e^{-y^{(i)}\theta^T x^{(i)}}}{1+e^{-y^{(i)}\theta^T x^{(i)}}}$
* (Remember $\frac{d\log(x)}{dx} = \frac{1}{x}$, $\frac{d\exp(x)}{dx} = exp(x)$ and chain rule $\frac{df(z(x))}{dx} = \frac{df}{dz}\frac{dz}{dx}$)

So gradient descent algorithm is:

* Start with some θ
* Repeat:

  for j=0 to n $\{\delta_j := -\frac{\alpha}{m}\sum_{i=1}^{m} y^{(i)}x_j^{(i)}\frac{e^{-y^{(i)}\theta^T x^{(i)}}}{1+e^{-y^{(i)}\theta^T x^{(i)}}}\}$

  for j=0 to n $\{\theta_j := \theta_j + \delta_j\}$
* $J(\theta)$ is convex, has a single minimum. Iteration moves downhill until it reaches the minimum

» Python sklearn

Logistic regression:

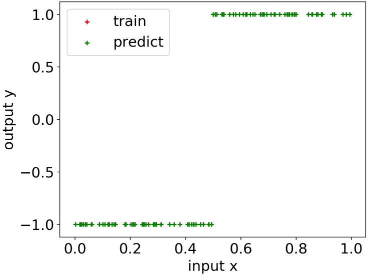
```
import numpy as np
Xtrain = np.random.uniform(0,1,100)
ytrain = np.sign(Xtrain-0.5)
Xtrain = Xtrain.reshape(-1, 1)
from sklearn.linear\_model import LogisticRegression
model = LogisticRegression(penalty='none',solver='lbfgs')
model.fit(Xtrain, ytrain)
print("intercept %f, slope %f"%(model.intercept_, model.coef_))
```

Typical output:
intercept -267.026565, slope 529.954559

* Prediction $\hat{y} = sign(-267.026565 + 529.954559x)$
* i.e. $y = +1$ when $-267.026565 + 529.954559x > 0$ and $y = -1$ when $-267.026565 + 529.954559x < 0$
* i.e. $y = +1$ when $x > 267.026565/529.954559 = 0.50392$ and $y = -1$ when $x < 267.026565/529.954559 = 0.5039$
* We generated data using $y = +1$ when $x > 0.5$ and $y = -1$ when $x < 0.5$. So model learned from training data is *roughly* correct, but not perfect. That's normal. *Why?*

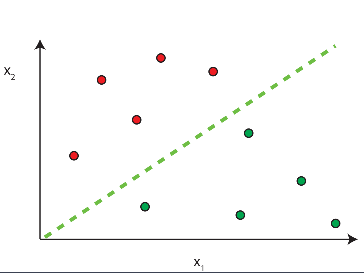
Plotting predictions

```
import matplotlib.pyplot as plt
plt.rc('font', size=18)
plt.rcParams['figure.constrained_layout.use'] = True
plt.scatter(Xtrain, ytrain, color='red', marker='+')
plt.scatter(Xtrain, ypred, color='green', marker='+')
plt.xlabel("input x"); plt.ylabel("output y")
plt.legend(["train","predict"])
plt.show()
```

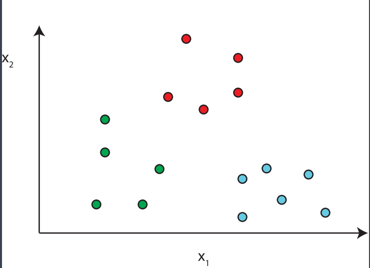


» Logistic Regression With Multiple Classes

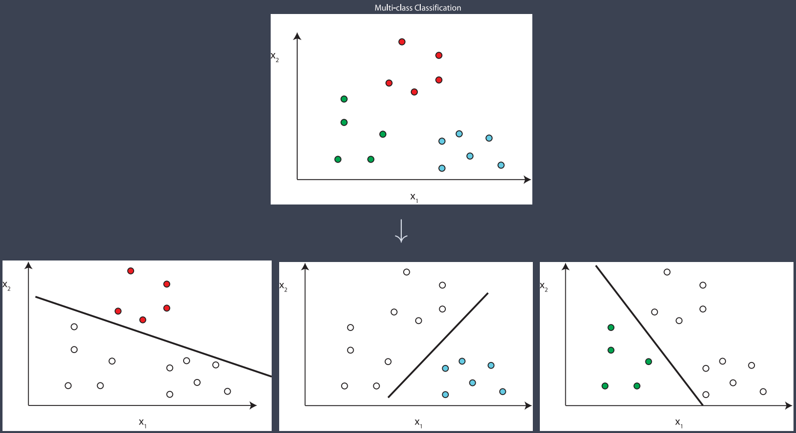
- Examples:
  - Email folder tagging: work, friends, family, hobby
  - Weather, sunny, cloudy, rain, snow
  - Given where I live in Dublin, predict which political party I'll vote for.
- Now y="output" variable/"target" variable takes values 0,1,2,.... E.g. $y = 0$ if sunny, $y = 1$ if cloudy, $y = 2$ if rain etc.



Multi-class Classification



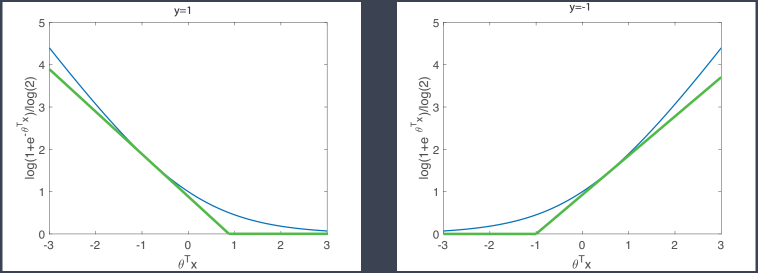
» Logistic Regression With Multiple Classes



* Train a classifier $sign(\theta^T x)$ for each class i to predict the probability that $y = i$. Training data: re-label data as $y = -1$ when $y \neq i$ and as $y == 1$ when $y = i$, so we're back to a binary classification task.

» SVM: Choice of Cost Function

In an SVM use the "hinge" loss function $\max(0, 1 - y\theta^T x)$:



Main differences from logistic loss function:

- hinge-loss is not differentiable ("non-smooth")
- hinge loss assigns zero penalty to all values of θ which ensure $\theta^T x \geq 1$ when $y = 1$, and $\theta^T x \leq -1$ when $y = -1$

» SVM: Choice of Cost Function

In an SVM use the "hinge" loss function $\text{max}(0, 1 - y\theta^T x)$:

* So long as $y\theta^T x > 0$ then by scaling up θ sufficiently, e.g. to 10θ or 100θ, then we can always force $y\theta^T x > 1$ i.e. $\text{max}(0, 1 - y\theta^T x) = 0$
* To get sensible behaviour we have to penalise large values of θ. We do this by adding penalty $\theta^T\theta = \sum_{j=1}^{n} \theta_j^2$
* Final SVM cost function is:

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \text{max}(0, 1 - y^{(i)}\theta^T x^{(i)}) + \theta^T\theta/C$$

where $C > 0$ is a weighting parameter that we have to choose (making C bigger makes penalty less important).

» SVM Summary

* Model: $h_\theta(x) = sign(\theta^T x)$
* Parameters: θ
* Cost Function: $J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \max(0, 1 - y^{(i)}\theta^T x^{(i)}) + \theta^T\theta/C$
* Optimisation: Select θ that minimise $J(\theta)$
* *Observe that only difference from Logistic Regression is in the choice of cost function.*
* SVM cost function:
  * Includes penalty $\theta^T\theta/C$. We can also add a penalty like this to Logistic Regression though $\rightarrow$ *regularisation*, we'll come back to this later
  * Terms in sum are zero for points where $y^{(i)}\theta^T x^{(i)} \geq 1 \rightarrow$ this is the important difference.
    * It means that training data points $(x^{(i)}, y^{(i)})$ with $y^{(i)}\theta^T x^{(i)} \geq 1$ don't contribute to the cost function
    * Only the training data points with $y^{(i)}\theta^T x^{(i)} < 1$ are relevant $\rightarrow$ *support vectors*. Can make computations more efficient.

» Gradient Descent for SVMs

Subgradient descent algorithm for SVMs is:

* Start with some θ
* Repeat:
  for j=0 to n
  $\{\delta_j := -\alpha(2\theta_j/C - \frac{1}{m}\sum_{i=1}^{m} y^{(i)} x_j^{(i)} \mathbb{1}(y^{(i)}\theta^T x^{(i)} \leq 1))$
  for j=0 to n $\{\theta_j := \theta_j + \delta_j\}$
  where $\mathbb{1}(y^{(i)}\theta^T x^{(i)} \leq 1) = 1$ when $y^{(i)}\theta^T x^{(i)} \leq 1$ and zero otherwise.

$J(\theta)$ is convex, has a single minimum. Iteration moves downhill until it reaches the minimum

» Python sklearn

Logistic regression:

```
from sklearn.svm import LinearSVC
model = LinearSVC(C=1.0).fit(Xtrain, ytrain)
print("intercept %f, slope %f"%(model.intercept_, model.coef_))
```

Typical output:
intercept -1.890453, slope 3.867570

* So prediction is $y = +1$ when $x > 1.890453/3.867570 = 0.4888$ and $y = -1$ when $x < 0.4888$
* cf Logistic Regression:intercept -267.026565, slope 529.954559 i.e. $y = +1$ when $x > 0.5039$ and $y = -1$ when $x < 0.5039$
* Recall penalty term encourages SVM to choose smaller θ. Changing to use $C = 1000$ gives intercept -19.830632, slope 40.271028 i.e. decision boundary $x = 19.830632/40.271028 = 0.4924$