# CO395 - Introduction to Machine Learning (70050)

## Week 2 (Introduction to ML)

## Week 3 (Instance-based Learning + Decision Trees)

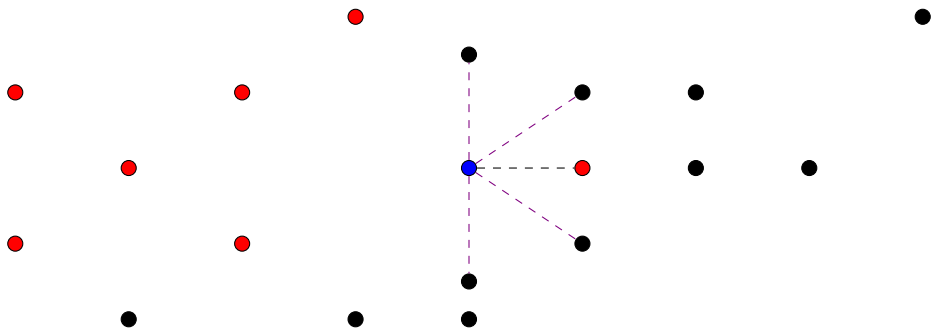
The **k Nearest Neighbours (k-NN)** classifier is classified as a **lazy learner**. A lazy learner stores all the training examples in the data set, and postpone any processing until a request is made (such as a prediction). On the other hand, **decision trees** are classified as a **eager learner**. An eager learner will attempt to construct a general target decision function, which is prepared prior to a query being made.

### Classification with Instance-based Learning

The concept behind instance-based learning is that we will use samples in a training data set in order to make inference on a query.

The **Nearest Neighbour** classifier is a specific example, where it classifies a test instance to the label of the nearest training instance, where nearest is subject to some distance metric. This is a **non-parametric model**, which means it naturally emerges from the training set. Note in the example below, an issue with this is that it can be sensitive to noise, as it would classify the blue point to be red, as it is the closest instance in the training set, even though it's more likely to be black - it is very sensitive to noise, and can **overfit** to the training data.

On the other hand, if we consider the **k Nearest Neighbours**, highlighted by the lines in violet, we get the class to be black, as we have 4 against 1. Usually, we need $k$ to be odd, to ensure a winner for the decision task.



Increasing $k$ will give the classifier have a smoother decision boundary (higher bias), and less sensitive to training data (lower variance). Choosing $k$ is dependant on the dataset, normally with a validation dataset.

The distance metric can be defined in many different ways, including the $\ell_1$, $\ell_2$ and $\ell_\infty$-norms as seen in **CO233**. Other metrics exist such as the **Mahalanobis distance** for non-isotropic spaces, typically used for Gaussian distributions, or the **Hamming distance** for binary strings.

Another variation is the **Distance Weighted k-NN**. For example, we may not want to trust neighbours which are further away, such as in the example below.

The idea is that we add weights to each neighbour (depending on distance), typically a higher weight for closer neighbours. We then assign the class based on which class has the largest sum. This metric, $w^{(i)}$, is any measure favouring the votes of nearby neighbours, such as;

- inverse of distance

$$w^{(i)} = \frac{1}{d(x^{(i)}, x^{(q)})}$$

- Gaussian distribution

$$w^{(i)} = \frac{1}{\sqrt{2\pi}} e^{-\frac{d\left(x^{(i)}, x^{(q)}\right)^2}{2}}$$

The value of $k$ is less important in the weighted case, as distant examples won't greatly affect classification. If $k = N$, where $N$ is the size of the training set, it is a global method, otherwise it is a local method (only considering the samples close by). This method is also more robust to noisy training data, however it can be slow for large datasets.

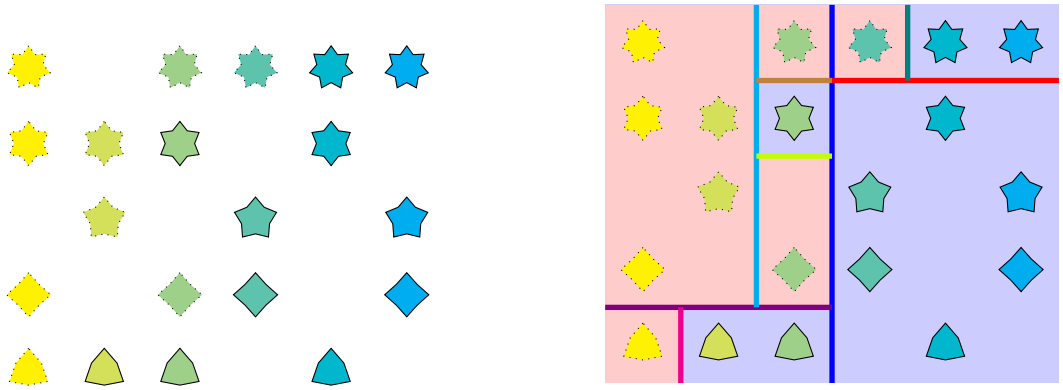
As this method relies on distance metrics, it may not work well if using all features in high dimensional spaces. If these features are irrelevant, instances in the same class may be far from each other. One solution to this is to weight features differently.

k-NN can also be used for regression, either by computing the mean value across $k$ nearest neighbours (which leads to a very rough curve), or by using locally weighted regression, which computes the weighted mean value across $k$ nearest neighbours, leading to a smoother curve.

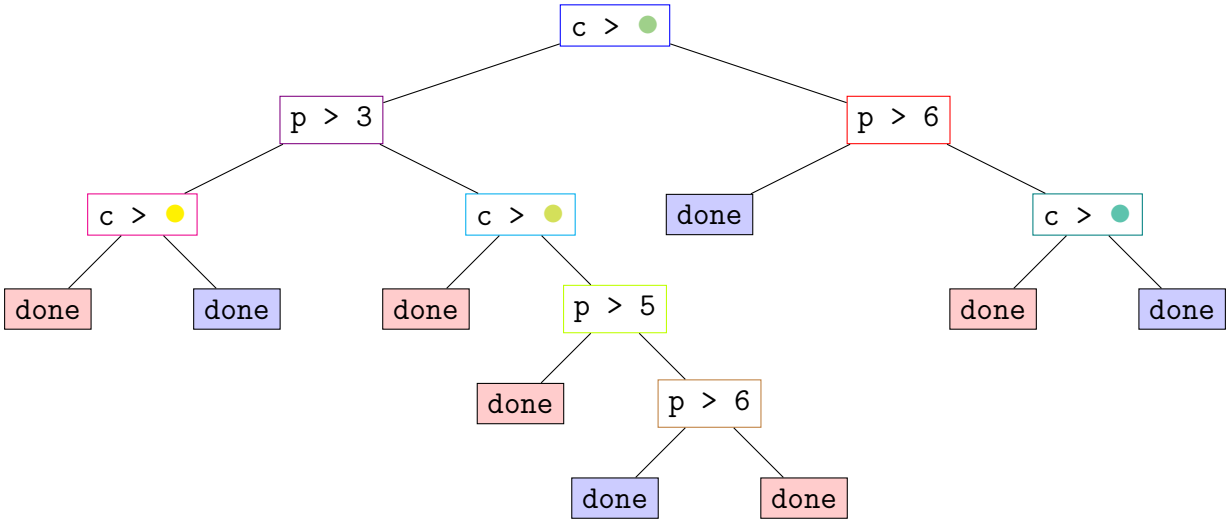
### Classification with Decision Trees

Decisions trees are the principal of focusing on a subset or single feature of each sample and then make a decision whether it's true or false (for each feature), and repeat this process to finer decisions until we manage to classify the sample that we want to check.

In decision trees, we learn a succession of linear decision boundaries that we can use to eventually correctly classify samples.



In the example above, we repeatedly choose divisions that result in the fewest number of errors, until we are able to classify everything. This results in the following decision tree, when we are using the attributes of colour and number of points. For brevity, the left branch is the `false` branch, `p` means points, and `c` means colour.




Decision trees are a method of approximating discrete classification functions, by representing them as a tree (a set of if-then rules). The general algorithm (ID3) for constructing a decision tree is as follows;

1. search for the optimal splitting rule on training data
2. split data according to rule
3. repeat 1 and 2 on each subset until each subset is pure (only containing a single class)

### How to select the 'optimal' split rule

Intuitively, we want to partition the datasets such that they are more pure than the original set. To do this, we have several metrics;

- **Information gain** ID3, C4.5

  quantifies the reduction of **entropy**

- **Gini impurity** CART

  if we randomly select a point in the feature space and randomly classify it according to the class label distribution, what is our probability of getting it incorrect?

- **Variance reduction** CART

  mostly used for regression trees, with a continuous target variable

To do this, we need to understand information entropy. Entropy is a measure of uncertainty of a random variable. It can also be seen as the average amount of information needed to define a random state / variable. If something has low entropy, it's predictable, and vice versa for high entropy.

Imagine we have two boxes, with something stored in one of the two, with an equal probability in each. To be fully certain, we need a single bit of information, if it's in the left box, the bit is `0`, otherwise (if it's in the right box), it's `1`. Similarly, if we have four boxes, with a uniform distribution, we would need 4 bits to encode the 4 states. In general;

$$
\begin{aligned}
2^B &= K \text{ states} \\
B &= \log_2(K) \\
I(x) &= \log_2(K) && \text{amount of information to determine the state of a random variable} \\
P(x) &= \frac{1}{K} && \Rightarrow \\
K &= \frac{1}{K} && \Rightarrow \\
I(x) &= -\log_2(P(x))
\end{aligned}
$$

As such, we can say;

$$I(x = \text{box}_1) = I(x = \text{box}_2) = I(x = \text{box}_3) = I(x = \text{box}_4) = -\log_2(P(x)) = 2 \text{ bits}$$

However, assume a non-uniform distribution, with the probabilities being 97%, 1%, 1%, and 1% respectively. If we were told it was in box 1, we do not get a lot of new information (low entropy); however if we were told it was in one of the other three, we high entropy (represents very important information).

$$\begin{aligned} I(x = \text{box}_1) &= -\log_2(0.97) \\ &\approx 0.0439 \text{ bits} \\ I(x = \text{box}_2) &= -\log_2(0.1) \\ &\approx 6.6439 \text{ bits} \end{aligned}$$

Entropy is defined as the average amount of information;

$$H(X) = -\sum_{k}^{K} P(x_k) \log_2(P(x_k))$$

In our example, we therefore have;

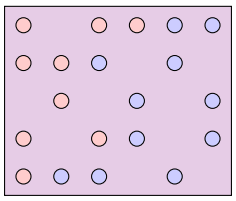
$$H(X) = -(0.97 \cdot \log_2(0.97) + 0.01 \cdot \log_2(0.01) + 0.01 \cdot \log_2(0.01) + 0.01 \cdot \log_2(0.01)) \approx 0.2419 \text{ bits}$$

We therefore need, on average, less information to know where the key is (compared to the uniform distribution).

For continuous entropy, we can use the probability density function $f(x)$ - this is imperfect (it can have negative values), but is still often used in Deep Learning.;

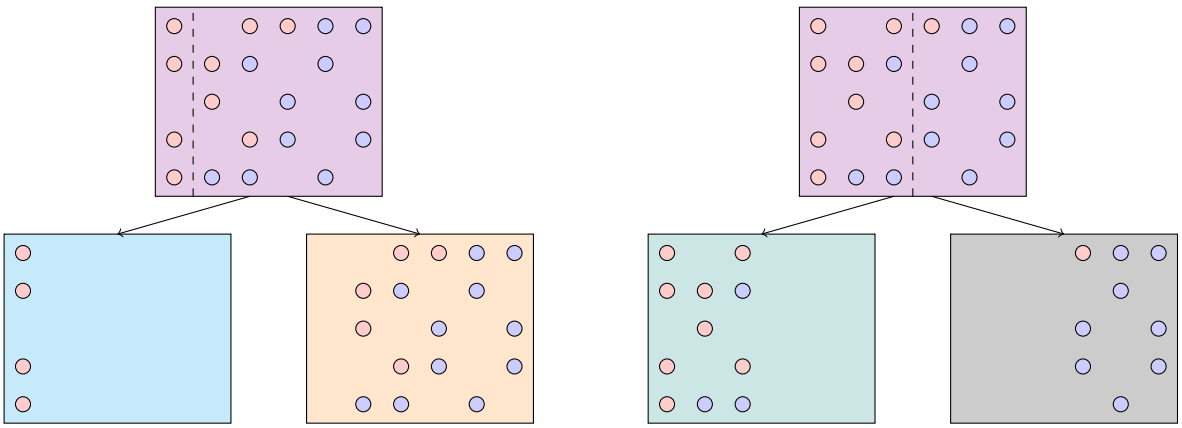
$$H(X) = -\int_{x} f(x) \log_2(f(x)) \, \mathrm{d}x$$

Consider the following example;



$$\begin{aligned} P(\bullet) &= \frac{11}{20} \\ P(\bullet) &= \frac{9}{20} \\ H(\blacksquare) &= -\left(\frac{11}{20} \cdot \log_2\left(\frac{11}{20}\right) + \frac{9}{20} \cdot \log_2\left(\frac{9}{20}\right)\right) \\ &\approx 0.9928 \end{aligned}$$

An entropy value close to 1 would indicate a maximum amount of information needed.



$$
\begin{aligned}
H(\blacksquare) &= 0 \\
H(\blacksquare) &\approx 0.896 \\
H(\{\blacksquare, \blacksquare\}) &\approx \frac{4}{20} \cdot 0 + \frac{16}{20} \cdot 0.896 \\
&\approx 0.7168 \\
H(\blacksquare) - H(\{\blacksquare, \blacksquare\}) &\approx 0.276 \qquad \text{information gain}
\end{aligned}
$$

$$
\begin{aligned}
H(\blacksquare) &\approx 0.8454 \\
H(\blacksquare) &\approx 0.5033 \\
H(\{\blacksquare, \blacksquare\}) &\approx \frac{11}{20} \cdot 0.8454 + \frac{9}{20} \cdot 0.5033 \\
&\approx 0.6915 \\
H(\blacksquare) - H(\{\blacksquare, \blacksquare\}) &\approx 0.3013 \qquad \text{information gain}
\end{aligned}
$$

As the second split has the larger information gain, that is the one we will end up selecting (and generally we want to split to maximise information gain). A formulation of this is as follows;

$$
IG(\text{dataset}, \text{subsets}) = H(\text{dataset}) - \sum_{S \in \text{subsets}} \frac{\mid S \mid}{\mid \text{dataset} \mid} H(S)
$$

$$
\mid \text{dataset} \mid = \sum_{S \in \text{subsets}} \mid S \mid
$$

We can have the following types of input;

- **ordered values**
  - attribute and split point
  - for each attribute, sort the values and consider split points between two examples with different classes
- **categorical / symbolic values**
  - search for the most informative feature and create as many branches as there are values for this feature

### Worked example for construction decision tree

Skipped, as this is basically done for the coursework.

### Summary and other considerations with decision tree

Note that in general, if we have real-valued attributes, we will end up with a binary tree, with an attribute and threshold at each node. On the other hand, if we have categorical values, we can end up with a **multiway tree**.

Decision trees will **overfit**, like with many machine learning algorithms. This means the algorithm will take into account every sample in the dataset, to the point where it picks up the noise in the dataset. On the other hand, we have an underfitted algorithm, which has low variance and high bias (in contrast).

In decision trees, to deal with overfitting, we can employ the following strategies;

- **early stopping**

  basically stop the algorithm when a condition is met, rather than when the subset is pure (such as maximum depth of tree, or a minimum number of examples in the subset)

- **pruning** will be covered more next week

  1. identify internal nodes connected to only leaf nodes
  2. turn each into a leaf node (with the majority class label)
  3. if the validation accuracy of the pruned tree is greater, we keep it, and then repeat the process until no other pruning can improve the accuracy

To test this, we can reserve part of the dataset for training, and another part for validation. This is called **cross-validation**.

Another approach is to use a random forest. This involves training multiple decision trees, each with a subset of the training dataset, with a random subset of the features, and therefore each focuses on one subset of the features. We then take the majority vote by each of the decision trees as the final outcome.

Decision trees can also be used for regression (**regression trees**). Instead of class labels, each leaf node predicts a real-valued number.

## Week 4 (Machine Learning Evaluation)

### Evaluation Set-up

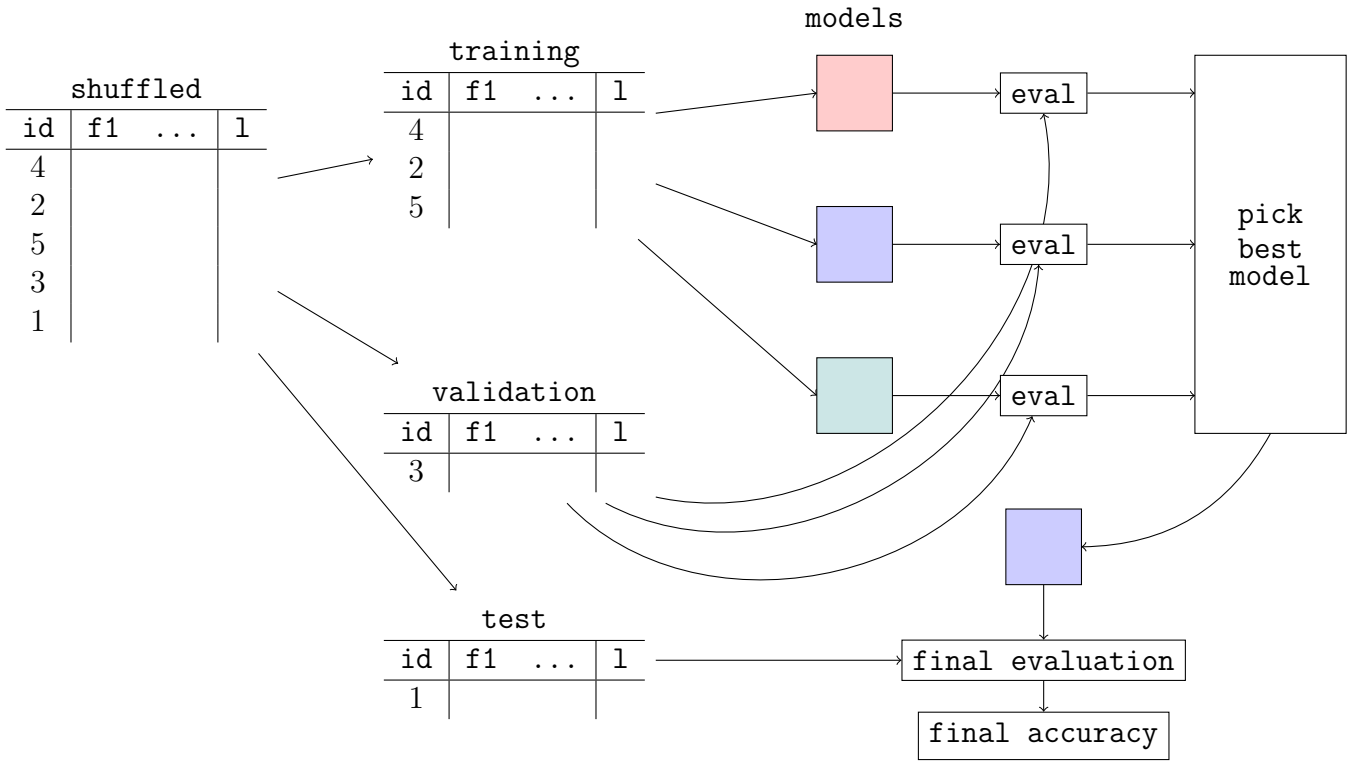
The goal is to create models and algorithms that can generalise to unseen data. We have good accuracy for the training set, since we trained the model for that, however we care more about the accuracy of unknown data.

To ensure meaningful evaluation, we need to split the training dataset from the test dataset (the test dataset should **never** be used to train, as it needs to simulate unknown data). This is done by first shuffling the dataset, and then splitting it into training and test datasets. The training dataset is used to train the model, and the test dataset is then fed into the trained model for final evaluation.

**Hyperparameters** are model parameters chosen before the training, such as the $k$ value for $k$-NN algorithm. Our overall objective is to find the values that lead to best performance for unknown data. An incorrect approach for hyperparameter tuning is to try different values on the training dataset, and then select the ones that lead to the best accuracy on the test dataset. This is incorrect because we now use the test dataset as part of the training process, and therefore we cannot say that it is unknown.

As such, the correct approach is to split the dataset into 3; training, validation, and test. The splits for this are between somewhere between $60:20:20$ and $80:10:10$. Different hyperparameter values are attempted on the **training** set, and then the result with the best accuracy on the **validation** set is chosen. The final evaluation is still done on the **test** dataset.

We want to keep the classifier that leads to the maximum performance on the validation test. We can extend this even further by adding the validation dataset to the training dataset and training it on the model with the best parameters to give it more data. Once again, the final evaluation is still done with the test dataset.




### Cross-validation

The idea of cross-validation is that the dataset can be divided into $k$ (usually 10) equal splits. $k-1$ of these folds can be used for training and validation, and the remaining split can be used for testing. This is done $k$ times, each time testing on a different portion of the data, in which we test on all of the data (but notice we never train and test on the same data at the same time). The performance on all $k$ held-out test sets can be averaged;

$$\text{global error estimate } = \frac{1}{N}\sum_{i=1}^{N} e_i$$

Note that this is used to evaluate an algorithm, not a particular model.

This method needs to be slightly modified when doing parameter tuning, in which we have the following options;

option 1: At each iteration, we use 1 fold for testing, 1 for validation, and the remaining $k-2$ folds for training. However, this will give us a different set of optimal parameters in each fold.

option 2: Another approach is to do cross-validation within cross-validation. As before, we still separate 1 fold for testing, however we run another internal cross-validation over the remaining $k-1$ folds to obtain the optimal hyperparameters. Once we obtain the best hyperparameters, we can then test it against the fold reserved for testing to obtain the final evaluation. This isn't always practical, as it requires a lot of computation for complex models.

When we go into production (not as common in academia), we may use all the remaining reserved test data for training as well (once we have the optimal parameters). However, this comes with the downside that we are no longer able to estimate the performance of the final trained model.

### Performance Metrics

Once we have a model, we want to have a quantifiable way to judge the quality of a model against another. Consider the following results from the test dataset;

| id | label | prediction |
|---|---|---|
| 1 | + | + |
| 2 | + | + |
| 3 | + | - |
| 4 | + | + |
| 5 | - | - |
| 6 | - | + |
| 7 | - | - |
| 8 | - | + |

| | class 1 (predicted) | class 2 (predicted) |
|---|---|---|
| class 1 (actual) | true positive (3) | false negative (1) |
| class 2 (actual) | false positive (2) | true negative (2) |

This confusion matrix highlights the risk of each prediction - sometimes it can be more important to have fewer false negatives than fewer false positives (such as diagnosing a disease) It also allows for easy identification of confusion between classes (when one class is commonly mislabelled as another). Many other measures can be computed from the confusion matrix. In our example, we have two classes (positive and negative). The common measures are as follows;

- **accuracy** $\frac{TP+TN}{TP+TN+FP+FN}$

  This is simply the number of correctly classified examples divided by the total number of examples. The classification error is $1 -$ accuracy.

- **precision** $\frac{TP}{TP+FP}$

  This is the number of correctly classified positive examples divided by the total number of predicted positive examples. We can also think about it as;

  $$P(\texttt{positive} \mid \texttt{example classified as positive})$$

  A high precision implies that an example labelled as positive is actually positive (few false positives).

- **recall** $\frac{TP}{TP+FN}$

  This can be considered as the inverse of precision. It is the number of correctly classified positive examples divided by the number of actual positive examples. It can be thought of as

  $$P(\texttt{correctly classified as positive} \mid \texttt{actually positive})$$

  A high recall implies that the class is correctly recognised (therefore a small number of false negatives).

- **F-measure / F-score** $F_1 = \frac{2 \cdot \texttt{precision} \cdot \texttt{recall}}{\texttt{precision} + \texttt{recall}}$

  Sometimes it is useful to measure the performance of the classifier with a single number. More generally it can be written as (with more emphasis on precision for higher $\beta$);

  $$F_\beta = (1 + \beta^2) \cdot \frac{\texttt{precision} \cdot \texttt{recall}}{(\beta^2 \cdot \texttt{precision}) + \texttt{recall}}$$

For something to be high recall and low precision, most of the positive examples are correctly recognised, but with many false positives. On the other hand if something has low recall and high precision, we miss a lot of positive examples, but the ones that we predict as positive are more likely to be actually positive.

The macro-averaged recall is the mean of the recalls for all the classes. The same can be done for precision and F-measure. In the multi-class case, precision, recall, and F-measure are computed for each class separately (we define one class each time as being the positive class). Note that macro-averaging is done on the class level, and is the average of the metrics for each class. On the other hand, micro-averaging does it on the item level (adding the TP, FP, TN, FN values for each class before calculating the metrics). Note that micro-averaged P, R and F1 will be equal to accuracy.

Another measure is regression tasks, where a lower mean squared error (MSE) is better (where $Y_i$ is a sample from the dataset and $\hat{Y}_i$ is the prediction from the model);

$$\frac{1}{N}\sum_{i=1}^{N}(Y_i - \hat{Y}_i)^2$$

However, we don't only care about accuracy, our models should be;

- **accurate** — makes correct predictions
- **fast** — fast to train and query
- **scalable** — works with large datasets
- **simple** — understandable and robust
- **interpretable** — can explain predictions

### Imbalanced Datasets

In a balanced dataset, we have an equal number of positive and negative data points. However, this will not always be the case, and we may have an unbalanced dataset where classes are not equally represented. The accuracy goes down, as it tends to follow the majority class. Additionally, the precision may also go down for the minority class. Consider the following case;

| | class 1 (predicted) | class 2 (predicted) |
|---|---|---|
| class 1 (actual) | 700 | 300 |
| class 2 (actual) | 100 | 0 |

From this, we obtain the following metrics where the accuracy may be high, but class 2 is completely misclassified;

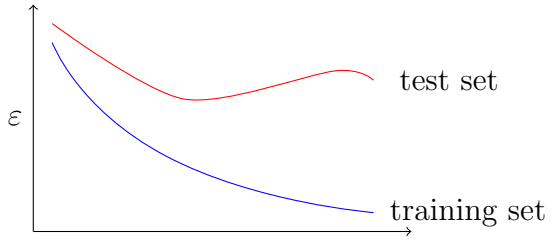
$$\begin{aligned} R(c1) &= 0.7 \\ P(c1) &= 0.875 \\ F_1(c1) &\approx 0.778 \\ R(c2) &= 0 \\ P(c2) &= 0 \\ F_1(c2) &= \texttt{N/A} \\ A &\approx 0.636 \end{aligned}$$

In conclusion, we need to look at different metrics, as well as the confusion matrix as a single metric may be misleading by itself.

We can normalise the confusion matrix by dividing each member of a row by the sum of that row (such that each row adds to one). We can also downsample the majority class, by picking less examples to get the two classes equal, or upsample the minority class by duplicating data. Neither will reflect how the model will generalise.

### Overfitting

An overfitted model has good performance on training data, but poor generalisation to other data. On the other hand, underfitting has poor performance on the training data, as well as poor generalisation.



In the example above, it starts off with an underfitted model, and then ends up overfitted. The point where it's correct is just as the error of the test set begins to increase again.

Overfitting can occur under these scenarios (and how we could avoid it);

- model used is too complex (learns too many fine details)

  use the validation set to decide the complexity
- examples in the training set are not representative of all possible situations

  obtain more data
- learning is performed for too long (such as neural networks)

  stopping the training earlier (using the validation set to decide when)

**Confidence Intervals**

The amount of data used in our test set also affects our confidence of the performance evaluation. A 90% accuracy score on a test set with 10 samples is still less trustworthy than an 84% accuracy score on a test set with 10,000 samples.

We define the true error of the model $h$ as the probability that it will misclassify a randomly drawn example $x$ from distribution $D$;

$$error_D(h) \equiv P[f(x) \neq h(x)]$$

The **sample error** of the model $h$ based on a data sample $S$ is as follows;

$$\begin{aligned} n &= \text{number of samples} \\ \delta(f(x), h(x)) &= \begin{cases} 1 & f(x) \neq h(x) \\ 0 & f(x) = h(x) \end{cases} \\ error_S(h) &\equiv \frac{1}{n} \sum_{x \in S} \delta(f(x), h(x)) \end{aligned}$$

We can say an $N\%$ confidence interval for some parameter $q$ is an interval with probability $N$ to contain the true value of $q$. Given a sample $S$, with more than 30 examples;

$$error_S(h) \pm Z_N \underbrace{\sqrt{\frac{error_S(h) \cdot (1 - error_S(h))}{n}}}_{\text{est. standard deviation of sample error}}$$

Due to the $n$ in the estimation of the standard deviation, if we have a very large $n$, we can obtain a very tight confidence interval. An example of this applied is as follows;

Emotion recognition results for 3 samples, using 156 training and 50 testing samples.

| | attributes | number of classes | classifier | correctly classified |
|---|---|---|---|---|
| face | 67 * 8 | C4.5 | 78% | |
| body | 140 | 6 | BayesNet | 90% |

We want to classify the 95% confidence interval for this error ($Z_N = 1.96$)

$$\begin{aligned} error_S(h) &= 0.22 \\ n &= 50 \\ Z_N &= 1.96 \\ \text{interval} &= \left[0.22 - 1.96\sqrt{\frac{0.22 \cdot (1 - 0.22)}{50}}, 0.22 + 1.96\sqrt{\frac{0.22 \cdot (1 - 0.22)}{50}}\right] \\ &= [0.11, 0.33] \end{aligned}$$

### Significance Testing

Statistical tests can tell us if the means of two sets are significantly different;

- **randomisation test**

  Randomly switch some predictions between two models and measure if the performance difference that we get is greater than or equal to the original difference.

- **two-sample T-test**

  This is used to estimate if two metrics from different populations are actually different. This has lower computational requirements and is easier to calculate.

- **paired T-test**

  Examining significance over multiple matched results, such as classification error over the same folds in cross-validation.

The **null hypothesis** (see **CO245**) is the hypothesis that the two algorithms / models perform the same and the differences are only due to sampling error. These tests return a **p-value**, which is the probability of obtaining the differences we see, assuming the null hypothesis is correct. A small p-value implies that we can be more confident that one system is actually different.

We consider a performance difference to be **statistically significant** of $p < 0.05$. However, $p > 0.05$ does not mean the algorithms are similar, just that we cannot observe a statistical difference.

There's a fairly long bit on **P-hacking**, but not sure why. A way to protect against P-hacking is to use an adaptive p-value;

1. rank p-values from $M$ experiments;

$$p_1 \leq p_2 \leq p_3 \leq \cdots \leq p_M$$

2. calculate the **Benjamini-Hochberg** critical value for each experiment;

$$z_i = 0.05\frac{i}{M}$$

3. significant results are the ones where the p-value is smaller than the critical value

## Week 5 (Artificial Neural Networks I)

### The Rise of Neural Networks

**Artificial neural networks** are a class of machine learning algorithms, similar to **kNN** or **decision trees**. They consist of connected neurons, normally optimised with **gradient descent**. On the other hand **deep learning** refers to the use of neural network models with multiple hidden layers (hence deep) - they are usually trained on larger datasets for longer periods of time.

Using neural network models, there was a large improvement in speech recognition. *AlphaGo* allows for board analysis to beat human players (an exhaustive search isn't feasible compared to chess). Another example is realistic text generation, as well as video editing (see *DeepFakes*) - automating what would take hours to do manually. The aforementioned example of video editing works by sharing an encoder, and feeding it to a decoder which specialises in generating a single face. To change a face, the encoded output from the first person is put into the decoder of the second. Another application is combining different information mediums (such as images and text) - for example generating descriptive outputs for a given image.

The theory for neural networks had already existed (perceptrons in 1958, backpropagation in 1964, convolutional neural networks and LSTMs in the 1990s). However, today there is more data for training, as well as improved methods for storing and managing data. Similarly, neural networks benefit from faster hardware for computation (especially GPUs, since the matrix computation can be easily parallelised on GPUs). Finally, better software (such as automatic differentiation libraries) reduces the amount of work required (compared to manual calculation).

### Linear Regression

We can think of linear regression as a very simplified method of a neural network model. This is a form of **supervised learning**, where we assume we have a dataset of input and output pairs;

- **dataset** $\{\langle x^{(1)}, y^1\rangle, \langle x^{(N)}, y^N\rangle, \ldots, \langle x^{(N)}, y^N\rangle\}$
- **input features** $X = \{x^{(1)}, x^{(2)}, \ldots, x^{(N)}\}$
- **known (desired) outputs** $Y = \{y^{(1)}, y^{(2)}, \ldots, y^{(N)}\}$

Our aim is to learn the mapping $f : X \to Y$, such that $\forall i \in [1, N]\ f(x^{(i)}) = y^{(i)}$. In linear regression, $f$ is a linear function.

It's important to note the difference between continuous and discrete problems;

- **classification** desired labels are discrete
  - obtaining digit labels from handwriting
  - obtaining sentiment from text
- **regression** desired labels are continuous
  - obtaining price of a house depending on some features
  - determining stock price from data on a company

An example of simple linear regression, with one input variable can be modelled as $y = ax + b$. $a$ denotes the slope, which controls the angle, $b$ denotes the intercept / bias (which controls the height) - with respect to a graph with the standard axes.

Consider a dataset which contains GDP per capita ($x$) and enrolment rate ($y$). To find the best values for $a$ and $b$ in $\hat{y} = ax + b$, we must first determine what we mean by best.

### Loss Function

A loss / cost function determines how well we are doing on our dataset, where a smaller value of $E$ means our predictions are close to our real values. Consider the **sum-of-squares** loss function;

$$\begin{aligned} E &= \frac{1}{2}\sum_{i=1}^{N}\left(\hat{y}^{(i)} - y^{(i)}\right)^2 \\ &= \frac{1}{2}\sum_{i=1}^{N}\left(ax^{(i)} + b - y^{(i)}\right)^2 \end{aligned}$$

Note that the division by two is optional, however it allows for easier differentiation since it cancels with the two that will come from the square. By using a squared function, we are allowing for small errors that are close to the actual value, but we want to penalise the model for large errors.

### Updating Parameters with Derivatives

Working out the partial derivative of the previously mentioned loss function with respect to each of the parameters, we get the following;

$$\begin{aligned} E &= \frac{1}{2}\sum_{i=1}^{N}\left(ax^{(i)} + b - y^{(i)}\right)^2 \\ \frac{\partial E}{\partial a} &= \frac{\partial}{\partial a}\frac{1}{2}\sum_{i=1}^{N}\left(ax^{(i)} + b - y^{(i)}\right)^2 \end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{2}\sum_{i=1}^{N}\frac{\partial}{\partial a}\left(ax^{(i)}+b-y^{(i)}\right)^2 \\
&= \sum_{i=1}^{N}\left(ax^{(i)}+b-y^{(i)}\right)x^{(i)} \\
&= \sum_{i=1}^{N}\left(\hat{y}^{(i)}-y^{(i)}\right)x^{(i)} \\
\frac{\partial E}{\partial b} &= \frac{\partial}{\partial b}\frac{1}{2}\sum_{i=1}^{N}\left(ax^{(i)}+b-y^{(i)}\right)^2 \\
&= \frac{1}{2}\sum_{i=1}^{N}\frac{\partial}{\partial b}\left(ax^{(i)}+b-y^{(i)}\right)^2 \\
&= \sum_{i=1}^{N}\left(ax^{(i)}+b-y^{(i)}\right) \\
&= \sum_{i=1}^{N}\left(\hat{y}^{(i)}-y^{(i)}\right)
\end{aligned}
$$

**Gradient Descent**

**Gradient descent** is the process of repeated updating our parameters by taking small steps (of learning rate / step size $\alpha$) in the negative direction of the partial derivative (worked out above). Note that we use := to denote a reassignment (not equality) in our **update rules**.

$$
\begin{aligned}
a &:= a - \alpha\frac{\partial E}{\partial a} \\
&:= a - \alpha\sum_{i=1}^{N}\left(\hat{y}^{(i)}-y^{(i)}\right)x^{(i)} \\
b &:= b - \alpha\frac{\partial E}{\partial b} \\
&:= b - \alpha\sum_{i=1}^{N}\left(\hat{y}^{(i)}-y^{(i)}\right)
\end{aligned}
$$

This can be implemented manually as follows;

```
X = data["GDP"].values
Y = data["Enrolment Rate"].values

a = 0.0
b = 0.0
learning_rate = 1e-11

for epoch in range(5): # an epoch is a single iteration
    update_a = 0.0
    update_b = 0.0
    error = 0.0
    for i in range(len(Y)):
        y_pred = a * X[i] + b
        update_a += (y_predicted - Y[i]) * X[i]
        update_b += (y_predicted - Y[i])
        error += np.square(y_predicted - Y[i])
```

```
    # Update rule for gradient descent
    a = a - learning_rate * update_a
    b = b - learning_rate * update_b

    # the lines above can be shortened to the following
    y_predicted = a * X + b
    a = a - learning_rate * ((y_predicted - Y) * X).sum()
    b = b - learning_rate * (y_predicted - Y).sum()
    rmse = np.sqrt(np.square(y_predicted - Y).mean())
```

It can often be more convenient to work with vector notation. The gradient is a vector of all the partial derivatives. For a function $f : \mathbb{R}^K \to \mathbb{R}$ (where there are $K$ parameters) the gradient is;

$$\nabla_\theta f(\theta) = \begin{bmatrix} \frac{\partial f(\theta)}{\partial \theta_1} \\ \frac{\partial f(\theta)}{\partial \theta_2} \\ \vdots \\ \frac{\partial f(\theta)}{\partial \theta_K} \end{bmatrix}$$

Using this, there is an **analytical solution** for solving a single variable linear regression;

$$\boldsymbol{X} = \begin{bmatrix} x^{(1)} & 1.0 \\ x^{(2)} & 1.0 \\ \vdots & \vdots \\ x^{(N)} & 1.0 \end{bmatrix}$$

$$\boldsymbol{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(N)} \end{bmatrix}$$

$$\boldsymbol{\theta} = \begin{bmatrix} a \\ b \end{bmatrix}$$

$$\begin{aligned} \nabla_\theta E(\boldsymbol{\theta}) &= \boldsymbol{X}^\top(\boldsymbol{X}\boldsymbol{\theta} - y) \\ &= 0 \qquad \Rightarrow \\ \boldsymbol{\theta}^* &= (\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top \boldsymbol{y} \end{aligned}$$

While this requires no iteration to directly find the optimal parameter values, it's not great for large problems as the matrix inversion has cubic complexity. The analytical solution, presented here with *Scikit-Learn*, has another benefit over gradient descent;

```
from sklearn.linear_model import LinearRegression

model = LinearRegression(fit_intercept=True)
X = data["GDP"].values.reshape(-1, 1)
Y = data["Enrolment Rate"]
model.fit(X, Y)

mse = np.square(Y - model.predict(X)).mean()
```

The analytical method manages to find the **global minimum**, whereas gradient descent finds a **local minimum**.

### Multiple Linear Regression

The previous example only took into account a single feature, which likely is insufficient for most complex problems. **multiple linear regression** considers many input features as follows, where each

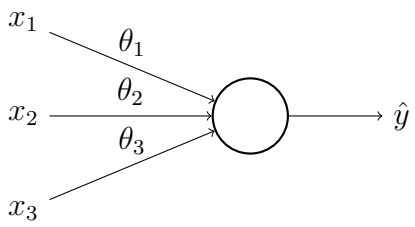
input feature has its own parameter as well as an extra parameter which acts as a bias;

$$y^{(i)} = \sum_{j=1}^{K} \theta_j x_j^{(i)} + \theta_{K+1}$$

Note that compared to before, when this is graphed on a two dimensional plane, it will be discontinuous, as it will exist in higher dimensions.

### Artificial Neuron

In the example below, we have the **features** $x_i$ and a corresponding weight (**parameter**) $\theta_i$.




The output value of the neuron above is as follows, where $g$ is the **activation function** (this is what makes it a neuron instead of just linear regression) and $b$ is the **bias**;

$$\hat{y} = g(\underbrace{\theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + b}_{\text{linear regression}})$$

Note that the bias is often implicit, since we can simply add an extra input feature that has a value of 1. Note that it's also possible to represent the weights as a vector $\boldsymbol{W}$, which simplifies the equation to be the following;

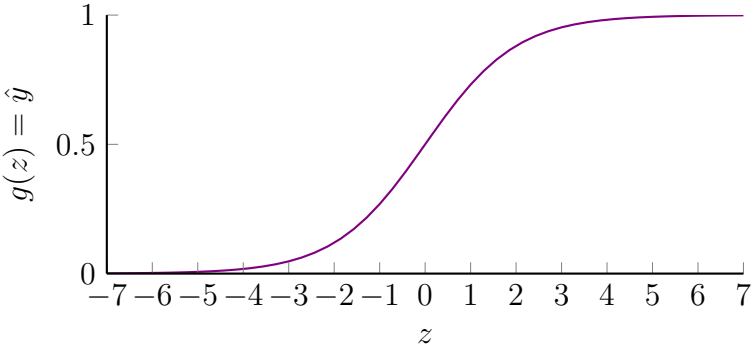
$$\hat{y} = g(\boldsymbol{W}^\top \boldsymbol{x})$$

Note that the part inside the activation function, concerning $W$ and $x$, can be written in any way (depending on the representation), as long as the dimensions line up to give a single scalar result.

### Logistic Activation Function

The **logistic function** is also known as the **sigmoid function**;

$$g(z) = \frac{1}{1 + e^{-z}}$$
$$z \in \mathbb{R}$$
$$\hat{y} \in [0, 1]$$




In logistic regression (which actually isn't regression), we can pass the output of linear regression through a logistic function, allowing us to get either 0 or 1 (binary classification). The model is optimised using gradient descent.

### Perceptron

This is another algorithm for supervised binary classification (similarly has the two classes 0 and 1). It uses a threshold function as the activation function;

$$h(x) = f(\boldsymbol{W}^\top \boldsymbol{x}) = \begin{cases} 1 & \text{if } \boldsymbol{W}^\top \boldsymbol{x} > 0 \\ 0 & \text{otherwise} \end{cases}$$

The learning rule is as follows;

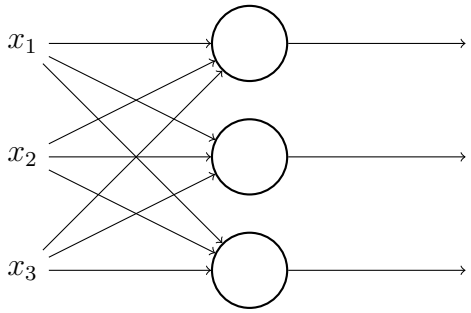
$$\theta_i \leftarrow \theta_i + \alpha(y - h(x))x_i$$

The reasoning is as follows; if the desired output ($y$) is equal to our prediction ($h(x)$), then the right hand side of the summation becomes 0, thus the parameter is unchanged - we don't fix it if it isn't broken. On the other hand, if the true value is 1 and the prediction is 0, we want to make $\boldsymbol{W}^\top \boldsymbol{x}$ bigger since the desired output is bigger than our prediction (therefore our prediction is too small to be set to 1 by the activation function). Since $y - h(x) = 1$ in this case, we increase $\theta_i$ if $x_i$ is positive, and decrease it if it is negative. The reasoning holds the other way around, when the true value is 0 but we predict 1.

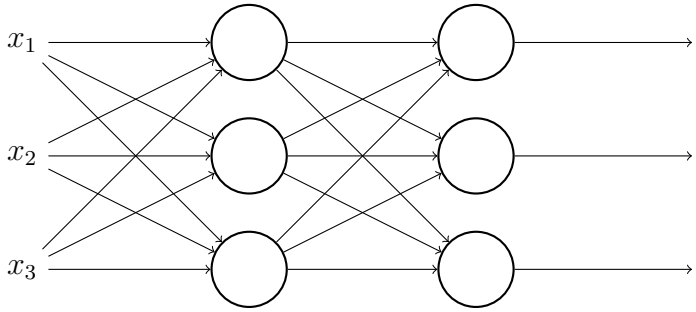
Any linearly separable function can be learnt with a perceptron, such as logical `OR` or `AND`, however something like `XOR` cannot be learnt. The activation function is also very sharp (and also not differentiable) so it's not used in most complex neural networks.

### Connecting Neurons

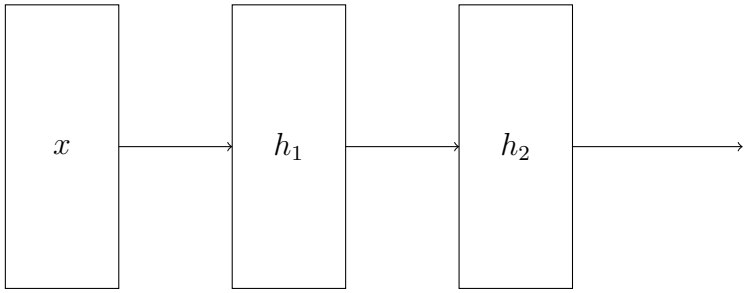
We can connect multiple neurons in parallel and consider each one as a **feature detector**;



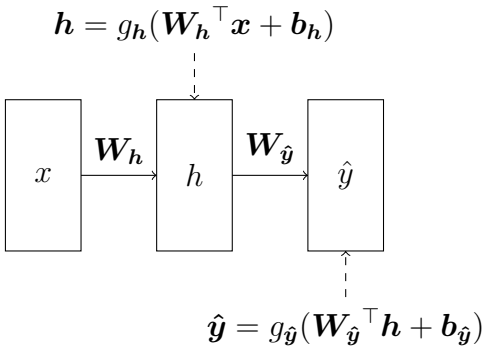

Similarly, we can connect neurons in sequence to learn from higher-order features (this is a multilayer perceptron, which isn't actually a perceptron);




A multilayer perceptron with a sufficient number of neurons can theoretically model an arbitrary function over an input. However, drawing this can be tedious (and isn't even feasible for large networks), we can represent each layer as a block, and each fully connected matrix of weights as an arrow (the diagram below represents the diagram above);




We typically refer to the first layer as the **input layer**, the final layer as the **output layer**, and everything in between the two as **hidden layers**. Consider a network with an input layer $x$, an output layer $\hat{y}$, and a hidden layer $h$;




When something doesn't work, it's often a good idea to verify the dimensions match up (possibly missing a transpose);

$$\begin{aligned}
\boldsymbol{x} &\in \mathbb{R}^{K\times 1} \\
\boldsymbol{h} &\in \mathbb{R}^{H\times 1} \\
\boldsymbol{W_h} &\in \mathbb{R}^{K\times H} \\
\boldsymbol{b_h} &\in \mathbb{R}^{H\times 1} \\
\hat{\boldsymbol{y}} &\in \mathbb{R}^{C\times 1} \\
\boldsymbol{W_{\hat{y}}} &\in \mathbb{R}^{H\times C} \\
\boldsymbol{b_{\hat{y}}} &\in \mathbb{R}^{C\times 1}
\end{aligned}$$

### Learning Representations and Features

It's also important to note the difference between traditional pattern recognition and end-to-end training. For example with image recognition, traditional pattern recognition would require someone to manually craft a feature extractor, which then goes into a trainable classifier to give an output. This is in contrast to end-to-end training, where useful features are learnt from the data and trained with the classifier. This is useful as the feature extractor (typically at the lower levels of the network) can change to help the higher levels of the network make better decisions.

For example (at a very abstract level), a face detector would be structured as follows - note how the lower levels generally learn individual features, and the higher levels learn features of the features from lower levels);

- initially works on individual pixels
- detects edges
- detects components of a face
- detects full faces

### Activation Functions

If we are able to use a linear model to capture all the features of our data, then we should do so (use the simplest model we can). However, more likely than not, our data will not be linearly separable, and therefore complex patterns cannot be captured with linear models. For multilayer networks, activation functions become more important.

- **linear activation** equivalent to having no activation function

$$f(x) = x$$

We cannot only use linear activation as multi-layer linear networks are equivalent to a single layer;

$$\begin{aligned} \boldsymbol{U} &= \boldsymbol{W_1 W_2} \\ \hat{\boldsymbol{y}} &= \boldsymbol{W_1}(\boldsymbol{W_2 x}) \\ &= \boldsymbol{U x} \end{aligned}$$

becomes a single layer

- **sigmoid activation** smoothly compresses the output into $[0, 1]$

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

- **tanh activation** similar shape to sigmoid, but range in $[-1, 1]$

$$f(x) = \tanh(x) = \frac{e^{x} - e^{-x}}{e^{x} + e^{-x}}$$

- **ReLU activation** rectified linear unit (linear in positive part)

$$f(x) = \text{ReLU}(x) = \begin{cases} 0 & \text{if } x \leq 0 \\ x & \text{otherwise} \end{cases} = \max(0, x)$$

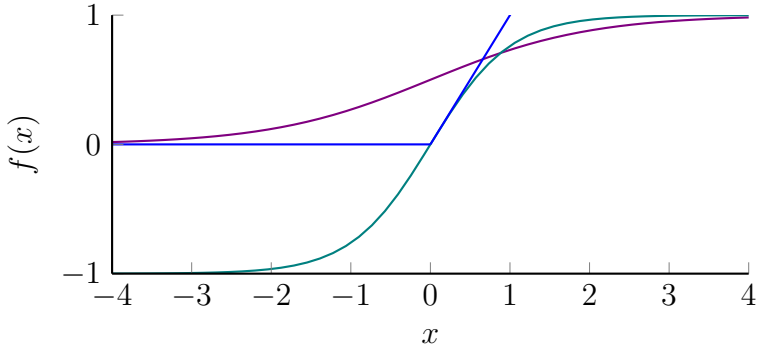
- **softmax activation**

scales inputs into a probability distribution (largest will be large, rest small), all output values sum to 1

$$\text{softmax}(z_i) = \frac{e^{z_i}}{\sum_k e^{z_k}}$$

This acts as a differentiable version of the max function, as it pushes the highest values close to 1 and the lower (remaining) values to 0. It identifies the value with the highest confidence and assigns more probability to it - very useful for image classification.

We can see the functions graphically as follows;



Note that most activation functions are applied **element-wise**, where each element is passed through the function independently (with the exception of softmax).

ReLU is used commonly for very deep networks, however tanh and sigmoid also work well and can be argued to be more robust. Those functions are more robust as ReLU is unbounded (if something is broken in the network, ReLU will give a large value which leads to more problems in the higher levels of the network). Therefore, the activation functions used are also a hyperparameter. The activation of the output layer should depend on the task (since it determines what the model can actually output);

- classifying into two classes — sigmoid or tanh
- predicting an unbounded score — linear
- predicting a probability distribution — softmax

### Feedforward Network in PyTorch

```
import torch
import torch.nn as nn

class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.layer_h = nn.Linear(10, 5) # input->hidden (input of size 10)
        self.layer_y = nn.Linear(5, 1) # hidden->output (hidden layer of size 5,
            gives 1 output)

    def forward(self, x):
        h = torch.tanh(self.layer_h(x)) # hidden layer with tanh activation
        y = torch.sigmoid(self.layer_y(h)) # output with sigmoid activation

net = Net()
input = torch.FloatTensor([x for x in range(10)]) # sample input
output = net(input) # execution
```

## Week 6 (Artificial Neural Networks II)

## Week 7 (Unsupervised Learning)

## Week 8 (Genetic Algorithms)