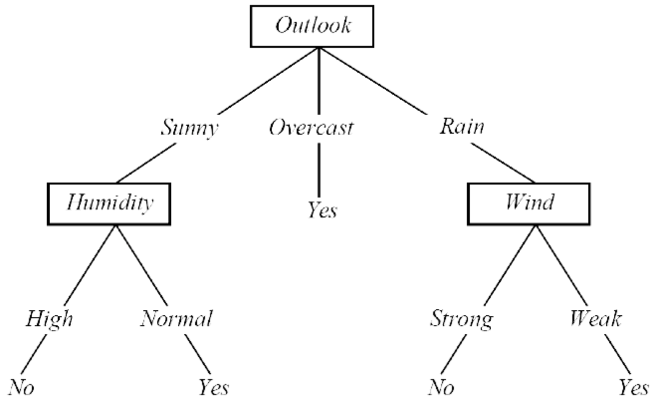
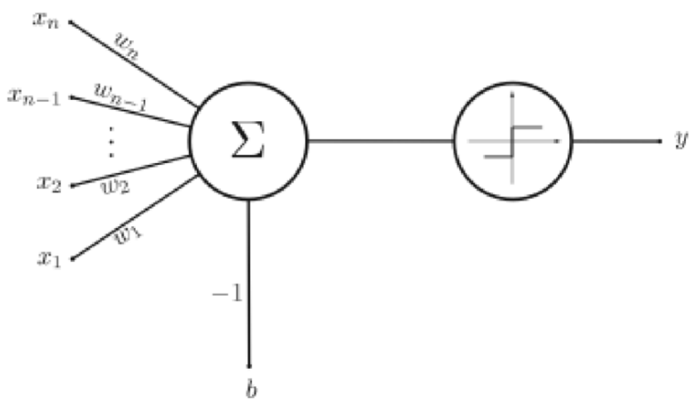
Learning

We have seen machine learning with different representations:

(1) Decision trees -- symbolic representation of various decision rules -- “disjunction of conjunctions”

(2) Perceptron -- learning of weights that represent alinear decision surface classifying a set of objects into two groups



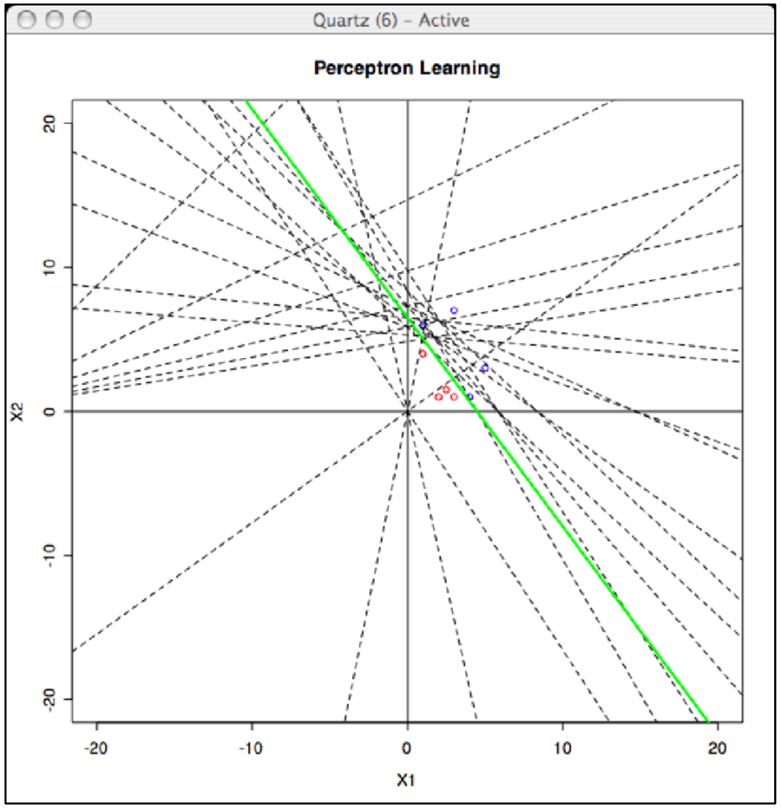


Different representations give rise to different <u>hypothesis</u> or <u>model spaces</u>.

Machine <u>learning algorithms search</u> these model spaces for the <u>best fitting model</u>.

Perceptron Learning Revisited

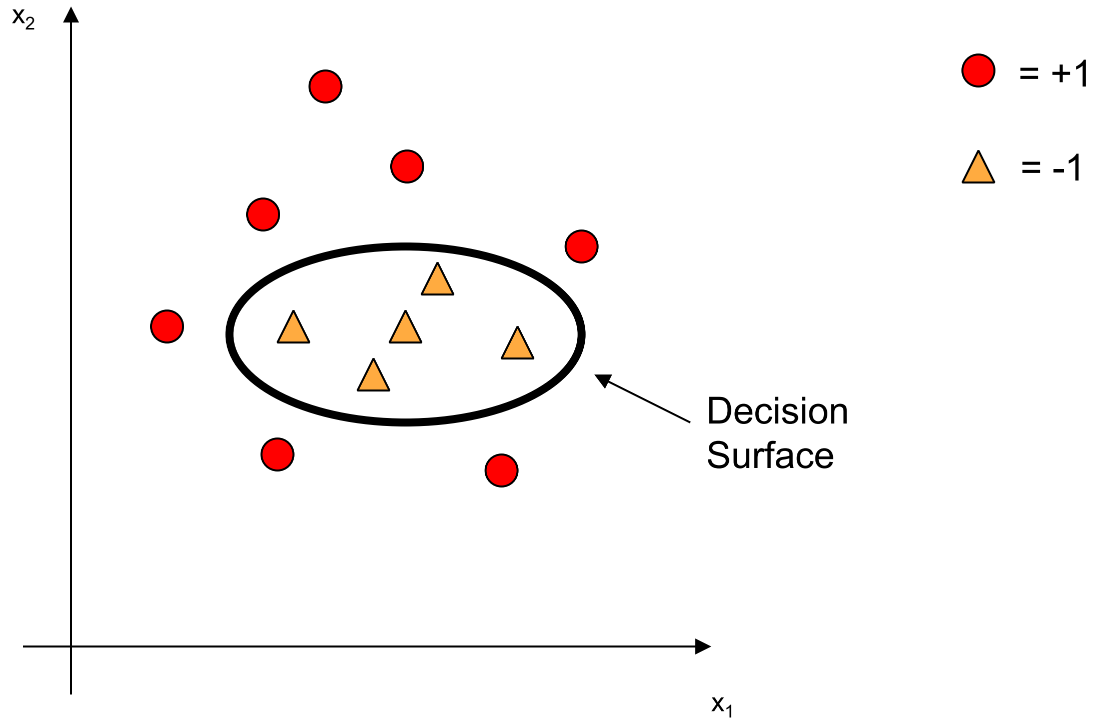
```
Initialize $\overline{w}$ and $b$ to random values.
repeat
    for each $(\overline{x}_i, y_i) \in D$ do
        if $\hat{f}(\overline{x}_i) \neq y_i$ then
            Update $\overline{w}$ and $b$ incrementally.
        end if
    end for
until $D$ is perfectly classified.
return $\overline{w}$ and $b$
```



Constructs a line (hyperplane) as a classifier.

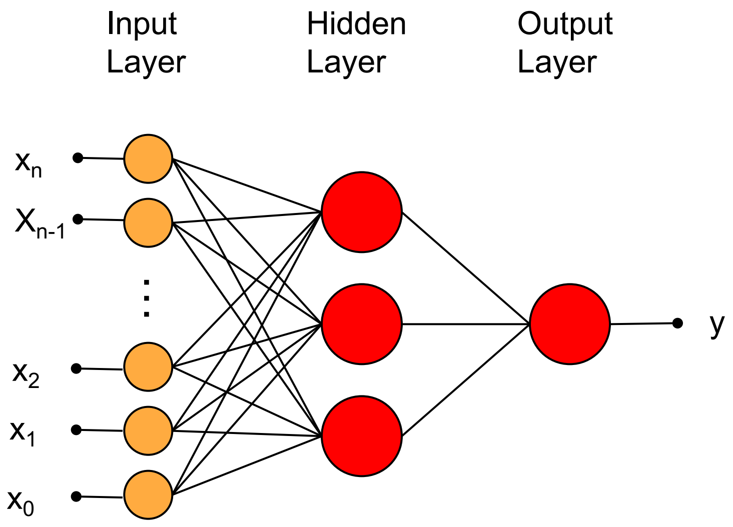
R Demo

What About Non-Linearity?



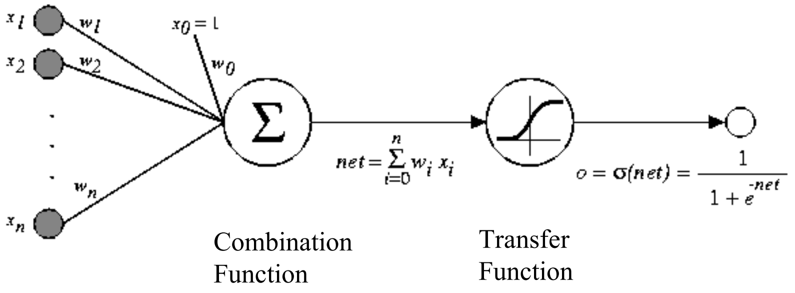
Can we learn this decision surface? …Yes! Multi-Layer Perceptronsl.

Multi-Layer Perceptrons



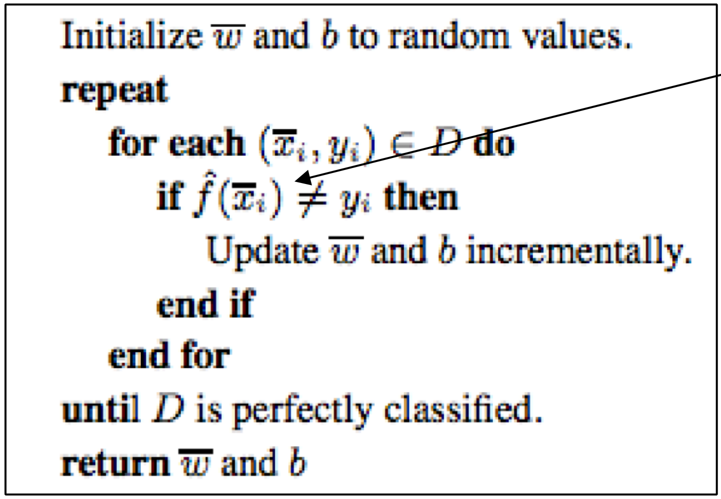
● ≡ Linear Unit

● ≡



How do we train?

Perceptron was easy:



```
Initialize $\overline{w}$ and $b$ to random values.
repeat
    for each $(\overline{x}_i, y_i) \in D$ do
        if $\hat{f}(\overline{x}_i) \neq y_i$ then
            Update $\overline{w}$ and $b$ incrementally.
        end if
    end for
until $D$ is perfectly classified.
return $\overline{w}$ and $b$
```

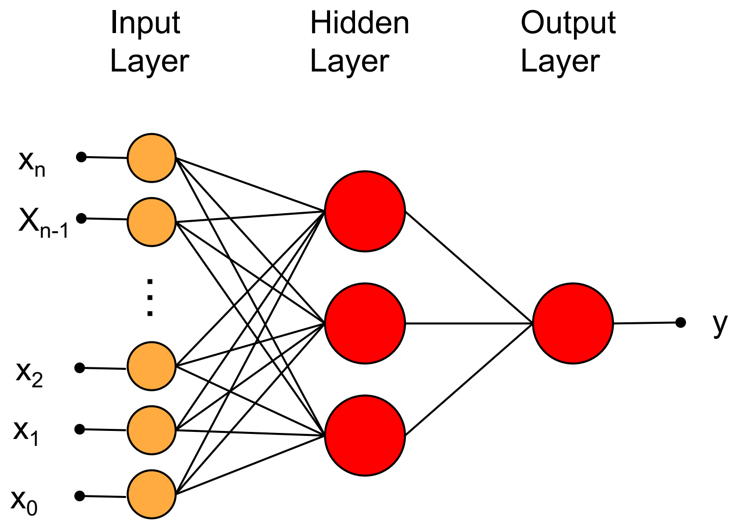
error

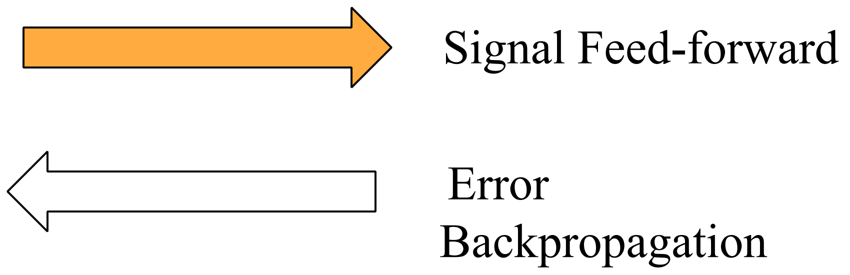
Every time we found an error of the predicted value $f(x_i)$ compared to the label in the training set y_i, we update w and b.

Artificial Neural Networks

Feed-forward with Backpropagation

We have to be a bit smarter in the case of ANNs: compute the error (feed forward) and then use the error to update all the weights by propagating the error back.



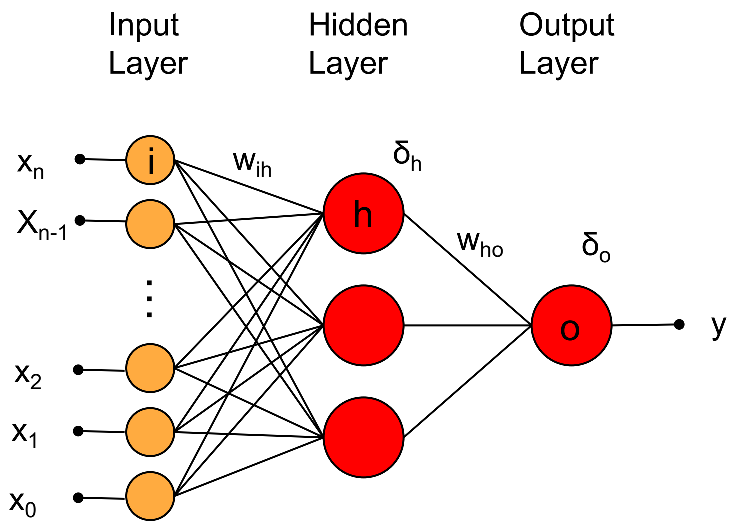


Backpropagation

$\Delta = (t - y)^2$

$$\delta_o = y(1-y)\Delta$$
$$w_{ho} \leftarrow w_{ho} + \alpha_o \delta_o$$

$$\delta_h = y(1-y) w_{ho} \delta_o$$
$$w_{ih} \leftarrow w_{ih} + \alpha_h \delta_h$$



This only works because

$$\delta_o = y(1-y)\Delta = \frac{\partial \Delta}{\partial \vec{w} \bullet \vec{x}} = \frac{\partial (t-y)^2}{\partial \vec{w} \bullet \vec{x}}$$

and the output y is differentiable because the transfer function is differentiable. Also note, everything is based on the *rate of change* of the error…we are searching in the direction where the rate of change will minimize the output error.

Backpropagation Algorithm

Note: this algorithm is for a NN with a single output node o and a single hidden layer. It can easily be generalized.

```
Initialize the weights in the network (often randomly)
  Do
        For each example e in the training set
             // forward pass
             y = compute neural net output
             t = label for e from training data
             Calculate error $\Delta = (t - y)^2$ at the output units
              // backward pass
             Compute error $\delta_o$ for weights from a hidden node h to the output node o using $\Delta$
             Compute error $\delta_h$ for weights from an input node i to hidden node h using $\delta_o$
             Update the weights in the network
  Until all examples classified correctly or stopping criterion satisfied
  Return the network
```

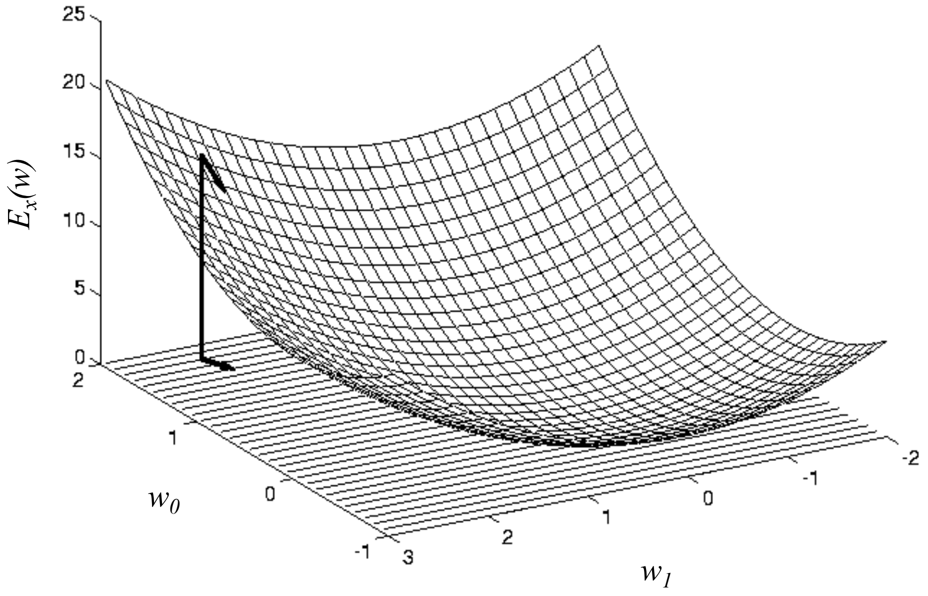
Source: http://en.wikipedia.org/wiki/Backpropagation

Neural Network Learning

- Define the network error as

$$\Delta_x = (t - y)^2$$

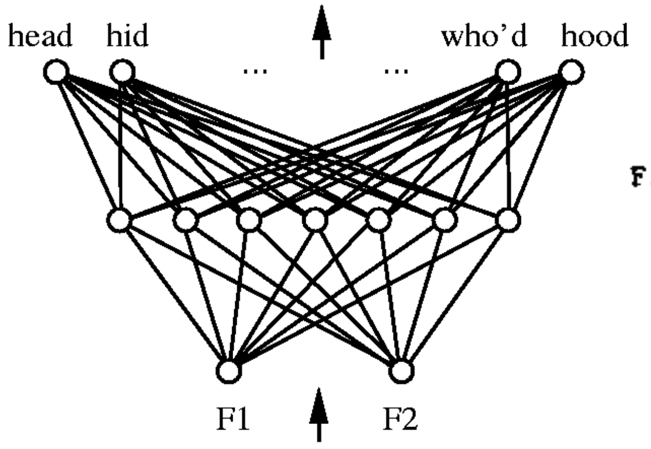
for some $x \in X$, where *i* is an index over the output units.
- Let $\Delta_x(w)$ be the error E_x as a function of the weights *w.*
- Use the gradient (slope) of the error surface to guide the search towards appropriate weights:

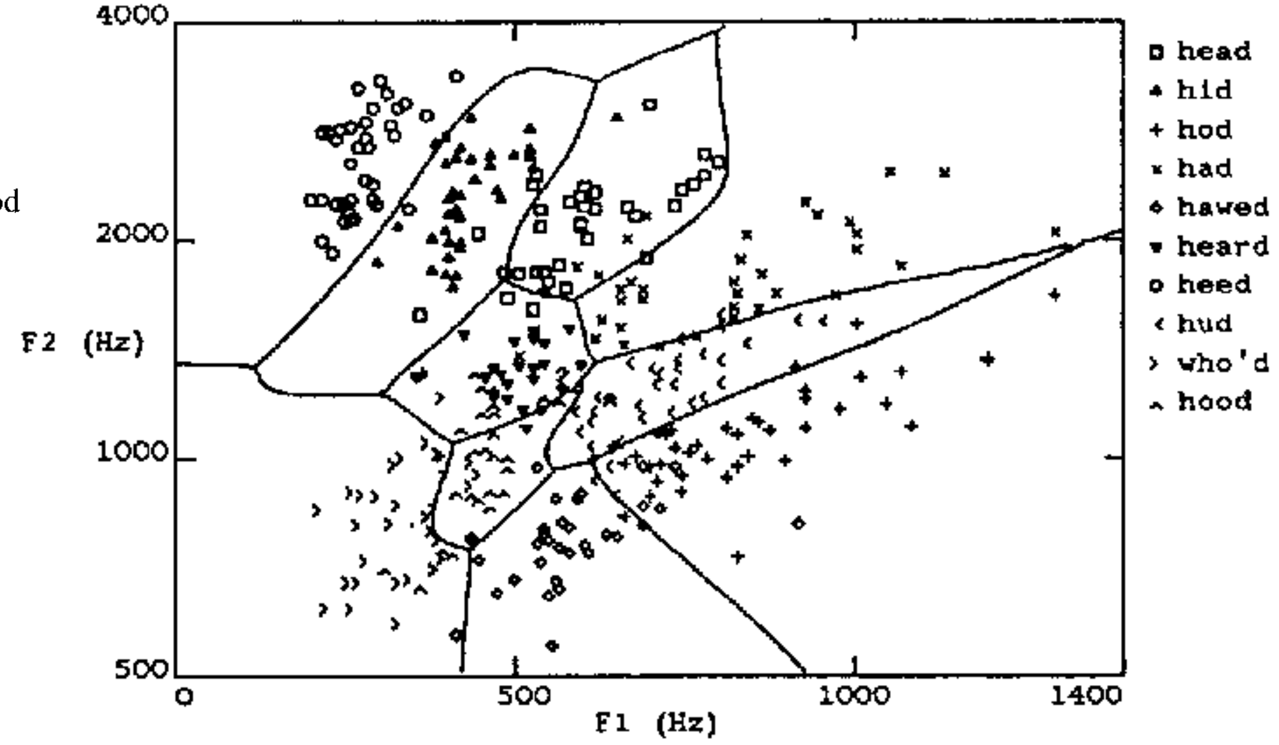


$$\Delta w_k = -\eta \frac{\partial \Delta_x}{\partial w_k}$$

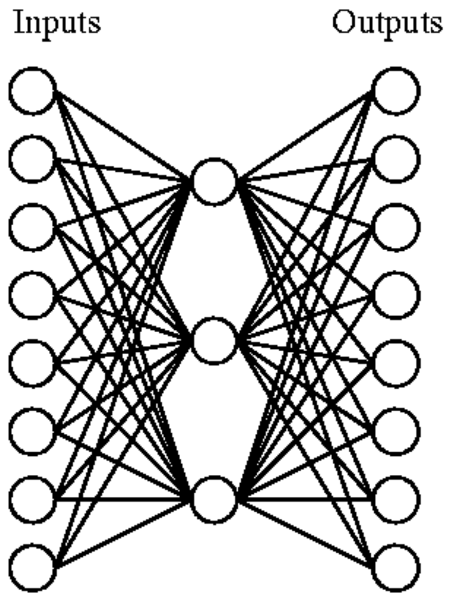
Representational Power

- Every bounded continuous function can be approximated with arbitrarily small error by a network with one hidden layer.
- Any function can be approximated to arbitrary accuracy by a network with two hidden layers.





Hidden Layer Representations

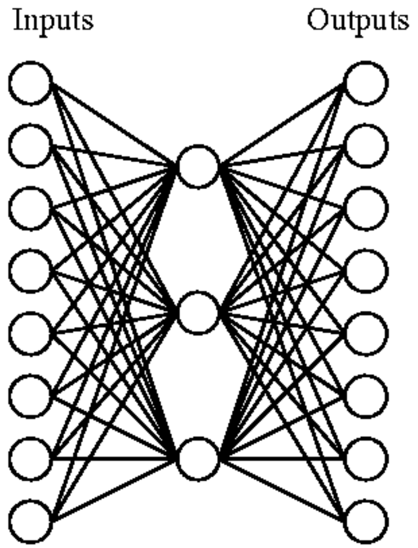


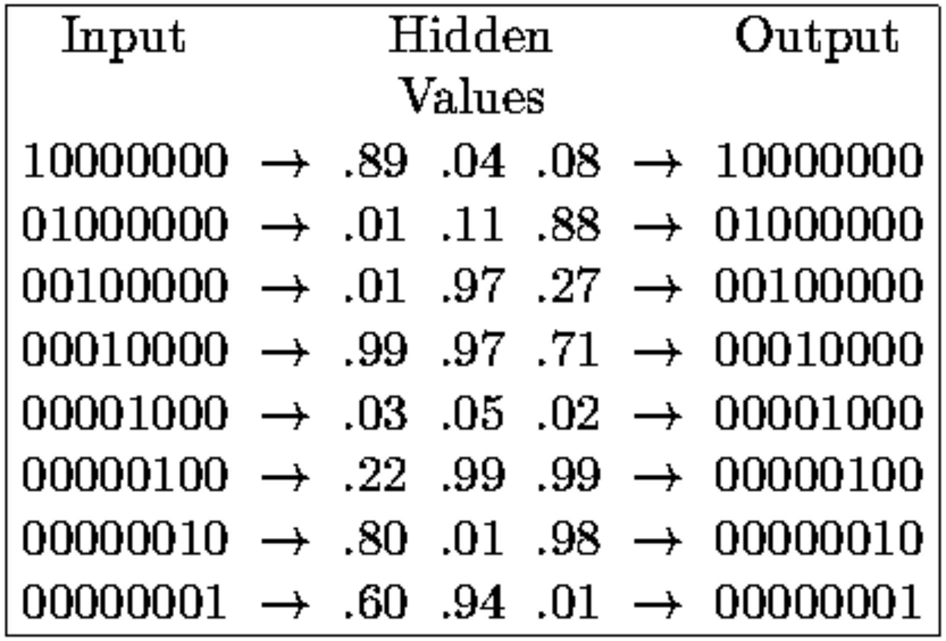
Target Function:

Input		Output
10000000	$\rightarrow$	10000000
01000000	$\rightarrow$	01000000
00100000	$\rightarrow$	00100000
00010000	$\rightarrow$	00010000
00001000	$\rightarrow$	00001000
00000100	$\rightarrow$	00000100
00000010	$\rightarrow$	00000010
00000001	$\rightarrow$	00000001

Can this be learned?

Hidden Layer Representations





Input		Hidden Values				Output
10000000	→	.89	.04	.08	→	10000000
01000000	→	.01	.11	.88	→	01000000
00100000	→	.01	.97	.27	→	00100000
00010000	→	.99	.97	.71	→	00010000
00001000	→	.03	.05	.02	→	00001000
00000100	→	.22	.99	.99	→	00000100
00000010	→	.80	.01	.98	→	00000010
00000001	→	.60	.94	.01	→	00000001

1	0	0
0	0	1
0	1	0
1	1	1
0	0	0
0	1	1
1	0	1
1	1	0

Hidden layers allow a network to invent appropriate internal representations.

MLPClassifier

```
import pandas as pd
from sklearn.neural_network import MLPClassifier
from sklearn.model_selection import cross_val_score
from sklearn.metrics import accuracy_score
from sklearn.metrics import confusion_matrix

# get data
df = pd.read_csv(”wdbc.csv")
df = df.drop(["ID'],axis=1)
X  = df.drop([’Diagnosis'],axis=1)
y = df[’Diagnosis']


# neural network
model = MLPClassifier(hidden_layer_sizes=(15,))

# do the 5-fold cross validation
scores = cross_val_score(model, X, y, cv=5)
print("Fold Accuracies: {}".format(scores))
print("Accuracy: {}".format(scores.mean()))
```

```
Fold Accuracies: [ 0.87591241
0.95620438  0.95620438  0.98540146
0.98518519]

Accuracy: 0.9517815625844823
```

MLP Grid Search

We can also perform a grid search

BEWARE: a grid search over all possible parameters of an MLP is almost impossible - combinatoric explosion, too many different combinations possible.

Here we only perform a grid over the *number of nodes in a single hidden layer.*

MLP Grid Search

```
# neural network
model = MLPClassifier(max_iter=2000)

# grid search
param_grid = {'hidden_layer_sizes': [ (5,), (6,), (7,), (8,), (9,), (10,),
                                      (11,), (12,), (13,), (14,), (15,), (16,),
                                      (17,), (18,), (19,), (20,)]}
grid = GridSearchCV(model, param_grid, cv=5)
grid.fit(X, actual_y)
print("Grid Search: best parameters: {}".format(grid.best_params_))

# evaluate the best model
best_model = grid.best_estimator_

predict_y = best_model.predict(X)
print("Accuracy: {}".format(accuracy_score(actual_y, predict_y)))

# build the confusion matrix
labels = ['benign', 'malignant']
cm = confusion_matrix(actual_y, predict_y, labels=labels)
cm_df = pd.DataFrame(cm, index=labels, columns=labels)
print("Confusion Matrix:\n{}".format(cm_df))

# boostrapped confidence interval
print("Confidence interval best MLP: {}".format(bootstrap(best_model,df,'class')))
```

MLP Grid Search

```
Grid Search: best parameters: {'hidden_layer_sizes': (9,)}
Accuracy: 0.9707174231332357
Confusion Matrix:
           benign  malignant
benign        435          9
malignant      11        228
Confidence interval best MLP: (0.93412408759124088, 0.9928832116788322)
```

Team Exercise

Use the Crohn's Disease dataset: CrohnD

https://vincentarelbundock.github.io/Rdatasets/datasets.html

You will need to preprocess this before you can use it:

c1 -> 0, c2 -> 1, F -> 0, M -> 1

Build a ANN/MLP with the best cross-validated performance you can find.

Compare it to either a tree or a KNN (or both).

Report if the difference between the models is statistically significant.

Teams:

Team 0: Shehjar Harout Geron
Team 1: Aakash Cory Christopher
Team 2: Maurice Kevin Ben
Team 3: Najib Aguilar Ronil
Team 4: Joe Shamal Gabe
Team 5: Kermalyn Peter David_M
Team 6: Matt Alexander Alber
Team 7: Evelyn Susallin David_P