Applied Machine Learning (AML)

Neural Networks

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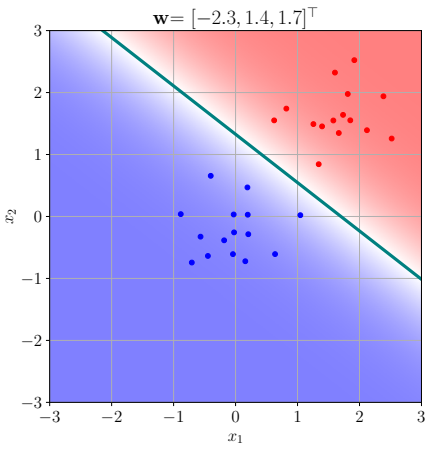
Introduction to Neural Networks

Recap - Linear Classifiers

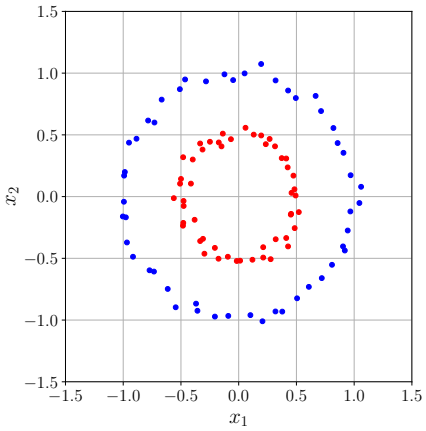
- Logistic regression =
  linear weights + **logistic function**

$$p(y=1|\boldsymbol{x}) = \sigma(\boldsymbol{w}^\intercal \boldsymbol{x} + b)$$



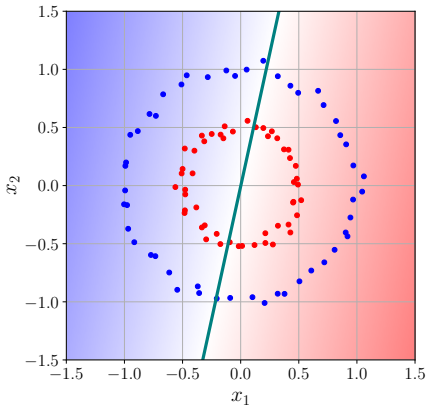
Classifying Non-Linear Data

- There is no linear classifier that will separate the data on the right given these 2D input features.



Classifying Non-Linear Data

- There is no linear classifier that will separate the data on the right given these 2D input features.
- In order to classify it, we can:
  - Use an alternative classifier that can generate *non-linear* decision boundaries.
  - *Transform* our input features so that they are linearly separable.



Neural Networks

- The performance of the classification methods we have explored depend on the input features, i.e. having a good 'representation' of the problem.
- If we do not have good features, many methods will not be effective, e.g. linear classifiers.

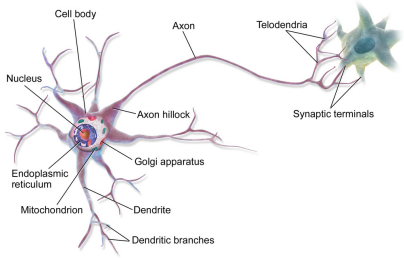
- What if we could *learn* the features from the input data?
- This is what **neural networks** attempt to do.
- We can think of them as a linear method, where we *learn* the features.

Neural Network Intuition

- Neural networks allow us to learn more effective features from the raw input data.
- We can think of them as functions that transform our input into something more useful for our task of interest.

Biological Neurons

- Neural networks are motivated by a *weak* analogy to the human brain, hence the name **artificial neural networks**.
- **Neurons** (also known as nerve cells) are electrically excitable cells in the nervous system that process and transmit information.
- Neurons are the core components of the brain, spinal cord, and nerves of vertebrates.



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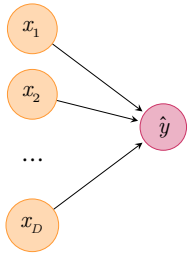
Artificial Neurons

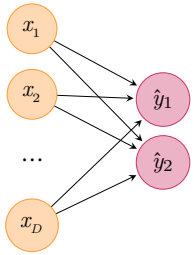
- Each *artificial* neuron is a linear weight vector with a non-linear activation function.
- We compute a neuron's activation as
$\hat{y} = g(\boldsymbol{w}^\intercal \boldsymbol{x} + b)$
- Here, $g()$ is a *non-linear activation* function.
- If we used the logistic function this would just be logistic regression.



Note, we are not depicting the bias term b here.

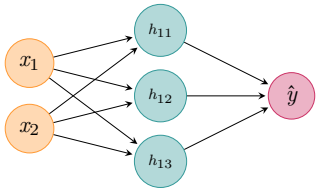
Artificial Neurons

- We can have multiple neurons
$\hat{y}_1 = g(\boldsymbol{w}_1^\intercal \boldsymbol{x} + b_1)$
$\hat{y}_2 = g(\boldsymbol{w}_2^\intercal \boldsymbol{x} + b_2)$
- We can present this using a weight *matrix* $\boldsymbol{W}$ and bias *vector* $\boldsymbol{b}$
$\hat{\boldsymbol{y}} = g(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$



Single Layer Network

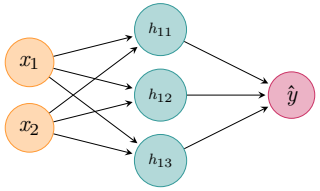
- We can connect multiple neurons (i.e. units) together into a directed acyclic graph.
- This results a **feed-forward neural network**.
- One of the simplest neural networks is a **single layer neural network**.



Single Layer Network

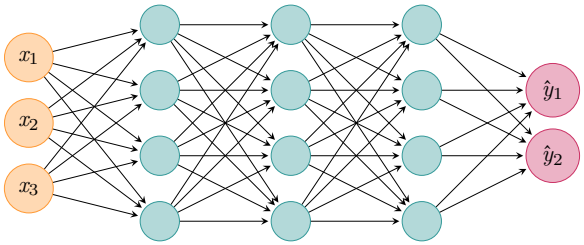
- In a single layer network, we have input units, hidden units, and output units.
- We can represent this function as

$$\hat{y} = g_2(\boldsymbol{w}_2^\intercal g_1(\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{b}_1) + b_2)$$



Multilayer Neural Network

- Individual units in a network are grouped together into **layers**.
- We can stack multiple layers to form a **multilayer network**, i.e. a multilayer perceptron (MLP).
- Here we see a **fully connected network** with three input features, three hidden layers with four hidden units in each, and two output units.



Non-Linear Activation Functions

- Recall our expression for the single layer neural network
  $\hat{y} = g_2(\boldsymbol{w}_2^\intercal g_1(\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{b}_1) + b_2)$
- One might ask why do we need a non-linear activation function $g()$ in $g(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$?
- Any sequence of linear layers can be equivalently represented with a single linear layer, i.e.

$$\begin{aligned}\boldsymbol{y} &= \boldsymbol{W}_1\boldsymbol{W}_2\boldsymbol{W}_3\boldsymbol{x} \\ &\triangleq \boldsymbol{W}'\boldsymbol{x}\end{aligned}$$

Non-Linear Activation Functions - Choices

- Sigmoid i.e. Logistic

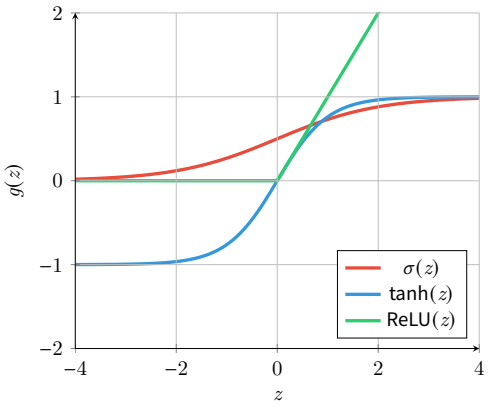
$$\sigma(z) = \frac{1}{1+\exp(-z)}$$

- Hyperbolic tangent

$$\tanh(z) = \frac{\exp(2z)-1}{\exp(2z)+1}$$

- Rectified linear unit

$$\text{ReLU}(z) = \max(z, 0)$$



Neural Networks - Expressive Power

- Feed-forward neural nets with non-linear activation functions are **universal function approximators**, i.e. they can approximate any function arbitrarily well.
- In practice, you may need an exponentially large network.
- If you can learn any function, this can just result in overfitting.

Importance of Network Depth

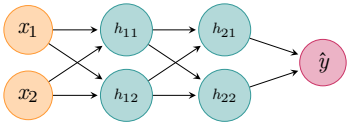
- A fully connected neural network with *one hidden layer* is a universal function approximator.
- This means it can model any sufficiently smooth function given a suitable number of hidden units.

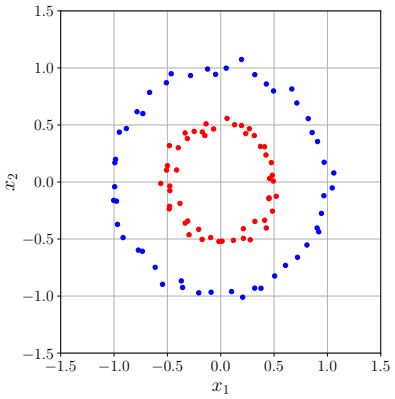
- However, both experimental and theoretical work have shown that *deeper* neural networks (i.e. ones with more layers) are more effective than *shallow* ones.
- In deeper networks, later layers can leverage the features learned by earlier ones.

Non-Linear Classification with Neural Networks

- Here we revisit the non-linear binary classification problem from earlier.
- We will use the following neural network with **two** hidden layers:

$$\begin{aligned}\hat{y} &= g_3(\boldsymbol{w}_3^\intercal\, g_2(\,\boldsymbol{W}_2 g_1(\,\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{b}_1) + \boldsymbol{b}_2) + b_3) \\ &= f(\boldsymbol{x}) = f_3(f_2(f_1(\boldsymbol{x})))\end{aligned}$$



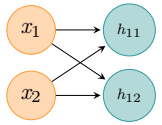


Neural Network Example - Input

- Input $\boldsymbol{x}$

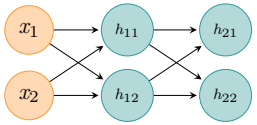
Neural Network Example - First Hidden Layer

- Input $\boldsymbol{x}$
- First hidden layer
  $\boldsymbol{h}_1 = g_1(\,\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{b}_1)$



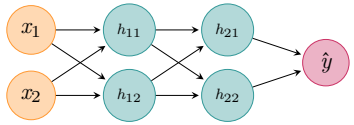
Neural Network Example - Second Hidden Layer

- Input $\boldsymbol{x}$
- First hidden layer
  $\boldsymbol{h}_1 = g_1(\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{b}_1)$
- Second hidden layer
  $\boldsymbol{h}_2 = g_2(\boldsymbol{W}_2\boldsymbol{h}_1 + \boldsymbol{b}_2)$



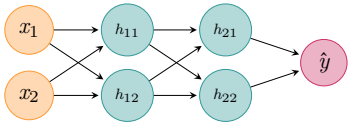
Neural Network Example - Output Layer

- Input $\boldsymbol{x}$
- First hidden layer
  $\boldsymbol{h}_1 = g_1(\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{b}_1)$
- Second hidden layer
  $\boldsymbol{h}_2 = g_2(\boldsymbol{W}_2\boldsymbol{h}_1 + \boldsymbol{b}_2)$
- Output
  $\hat{y} = g_3(\boldsymbol{w}_3^\intercal \boldsymbol{h}_2 + b_3)$



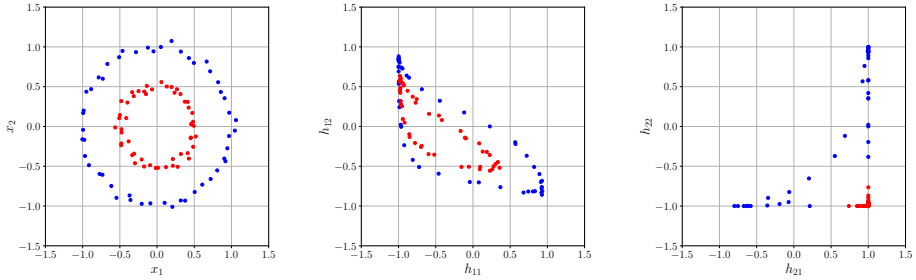
Neural Network Example - Output Layer

- Input $\boldsymbol{x}$
- First hidden layer
  $\boldsymbol{h}_1 = \tanh(\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{b}_1)$
- Second hidden layer
  $\boldsymbol{h}_2 = \tanh(\boldsymbol{W}_2\boldsymbol{h}_1 + \boldsymbol{b}_2)$
- Output
  $\hat{y} = \sigma(\boldsymbol{w}_3^\intercal \boldsymbol{h}_2 + b_3)$



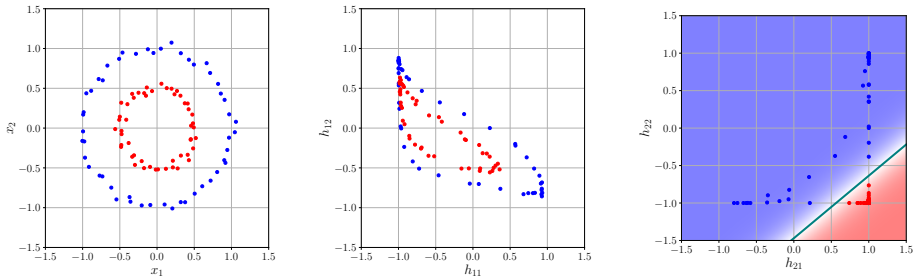
Transforming Features

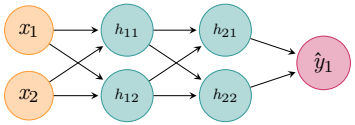
Here we see the outputs from each layer of the network.



Transforming Features

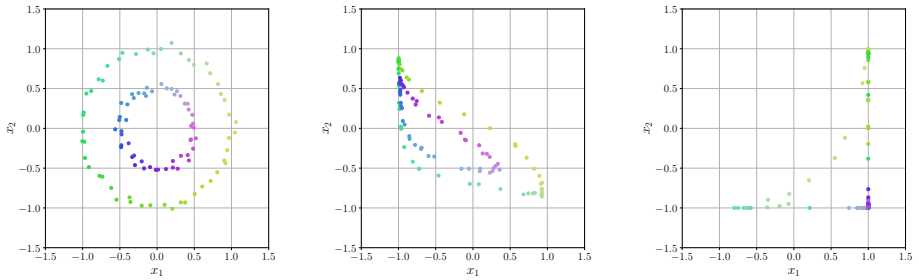
Now we can use a linear classifier on the final hidden features.

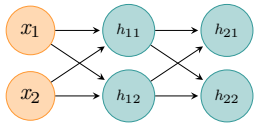




Transforming Features

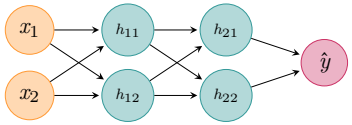
This is the same as previous, but we have colour coded each individual instance.

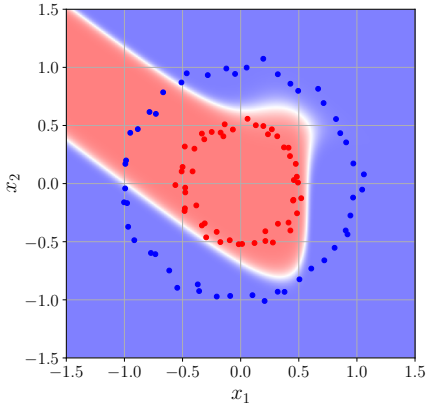




Final Neural Network Predictions

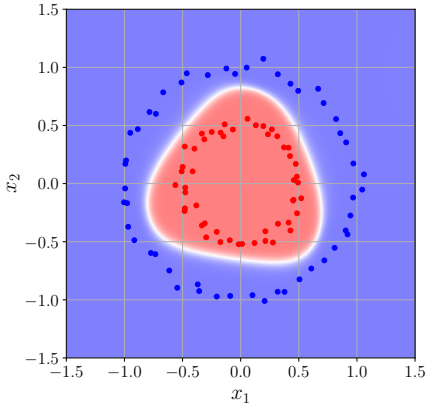
- On the right we see the final network predictions, colour-coded by predicted class.
- Note, in this example we defined a simple, and small, neural network for ease of visualisation.
- Our network did *not* successfully classify *all* the training data.





Final Neural Network Predictions

- With a minor change to the structure of the neural network, we can correctly classify the training data.
- In the example on the right we increased the number of hidden units in the first layer (from two to four).



Training Neural Networks

Neural Network Parameters

- Recall that a multilayer neural network is a nested set of linear functions with non-linear activations.

$$f(\boldsymbol{x}) = f_L(\ldots f_2(f_1(\boldsymbol{x})))$$

- Each layer f_L has its own weight matrix $\boldsymbol{W}_L$ and bias vector $\boldsymbol{b}_L$.
- The concatenation of these terms form the model weights that need to be learned.

$$\boldsymbol{\theta} = (\boldsymbol{W}_1, \boldsymbol{b}_1, \boldsymbol{W}_2, \boldsymbol{b}_2, \ldots, \boldsymbol{W}_L, \boldsymbol{b}_L)$$

Training Neural Networks

- The task of training a neural network involves finding the best parameters (i.e. weights) for each unit.
- We will use a loss function $\mathcal{L}(\boldsymbol{\theta})$ to measure the disagreement between the model prediction $f(\boldsymbol{x})$ and the ground truth target y.

- During optimisation we will try to find the parameters that minimise the loss.
- We will take the gradient of the loss $\nabla_{\boldsymbol{\theta}}\mathcal{L}$ and use gradient descent to update the parameters.
  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \cdot \nabla_{\boldsymbol{\theta}}\mathcal{L}$

Training Multilayer Neural Networks

- Hidden units make optimising the network weights more complicated as we do not have ground truth targets for them.
- Each hidden activity can affect many output units and can therefore have many separate effects on the error.

Backpropagation

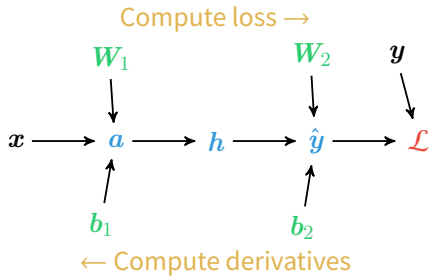
- There is a recursive algorithm for computing the derivatives. It uses the **chain rule** by storing some intermediate terms. This is called **backpropagation**.
- We make use of the layered structure of the network to compute the derivatives, heading backwards from the output layer to the inputs.

Backpropagation Algorithm

- Consists of two main steps:
  - A **forward pass**, in which we compute and store the values at all of the hidden units and the network output.
  - A **backward pass**, in which we calculate the derivatives of each weight, starting at the end of the network, and reusing the previous computation as we move towards the start.

Backpropagation

- We can visualise the computations using a **computation graph**.
- The nodes represent all the inputs and computed quantities, and the edges represent which nodes are computed directly as a function of which other nodes [1].



[1] Example adapted from Ren and MacKay: CSC 411.

Chain Rule of Calculus

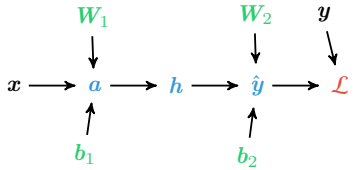
- Suppose we had two functions $u(x)$ and $v(x)$.
- Then $y = u(v(x))$ is a function of a function.

- The **chain rule** of calculus gives us a way to expresses the derivative of the composition of two differentiable functions $u(x)$ and $v(x)$ in terms of their derivatives.

- For example, if we substitute $s = v(x)$, thus $y = u(s)$, and

$$\frac{dy}{dx} = \frac{dy}{ds}\frac{ds}{dx}$$

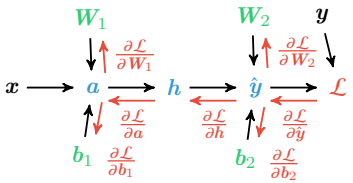
Backpropagation - Forward Pass



Forward Pass

$$\begin{aligned}
\boldsymbol{a} &= \boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{b}_1 \\
\boldsymbol{h} &= g(\boldsymbol{a}) \\
\hat{\boldsymbol{y}} &= \boldsymbol{W}_2\boldsymbol{h} + \boldsymbol{b}_2 \\
\mathcal{L} &= \frac{1}{2}||\hat{\boldsymbol{y}} - \boldsymbol{y}||^2
\end{aligned}$$

Backpropagation - Backward Pass



Forward Pass

$$\begin{aligned}
\boldsymbol{a} &= \boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{b}_1 \\
\boldsymbol{h} &= g(\boldsymbol{a}) \\
\hat{\boldsymbol{y}} &= \boldsymbol{W}_2\boldsymbol{h} + \boldsymbol{b}_2 \\
\mathcal{L} &= \frac{1}{2}||\hat{\boldsymbol{y}} - \boldsymbol{y}||^2
\end{aligned}$$

Backward Pass

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \hat{\boldsymbol{y}}} &= (\hat{\boldsymbol{y}} - \boldsymbol{y}) \\
\frac{\partial \mathcal{L}}{\partial \boldsymbol{W}_2} &= \frac{\partial \mathcal{L}}{\partial \hat{\boldsymbol{y}}}\frac{\partial \hat{\boldsymbol{y}}}{\partial \boldsymbol{W}_2} = \frac{\partial \mathcal{L}}{\partial \hat{\boldsymbol{y}}}\boldsymbol{h}^\top \\
\frac{\partial \mathcal{L}}{\partial \boldsymbol{b}_2} &= \frac{\partial \mathcal{L}}{\partial \hat{\boldsymbol{y}}}\frac{\partial \hat{\boldsymbol{y}}}{\partial \boldsymbol{b}_2} = \frac{\partial \mathcal{L}}{\partial \hat{\boldsymbol{y}}} \\
\frac{\partial \mathcal{L}}{\partial \boldsymbol{h}} &= \frac{\partial \mathcal{L}}{\partial \hat{\boldsymbol{y}}}\frac{\partial \hat{\boldsymbol{y}}}{\partial \boldsymbol{h}} \\
\frac{\partial \mathcal{L}}{\partial \boldsymbol{a}} &= \frac{\partial \mathcal{L}}{\partial \boldsymbol{h}}\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{a}} \\
\frac{\partial \mathcal{L}}{\partial \boldsymbol{W}_1} &= \frac{\partial \mathcal{L}}{\partial \boldsymbol{a}}\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{W}_1} = \frac{\partial \mathcal{L}}{\partial \boldsymbol{a}}\boldsymbol{x}^\top \\
\frac{\partial \mathcal{L}}{\partial \boldsymbol{b}_1} &= \frac{\partial \mathcal{L}}{\partial \boldsymbol{a}}\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{b}_1} = \frac{\partial \mathcal{L}}{\partial \boldsymbol{a}}
\end{aligned}$$

Convergence of Neural Networks

- For *logistic regression*, the loss function is conveniently convex. A convex function has just one minimum.
- Multilayer *neural networks* are **non-convex**, and gradient descent may get stuck in local minima during training and never find the global optimum.
- In practice this is not necessarily an issue and we can still apply gradient-based methods and can obtain good solutions for many practical problems of interest.

Hyperparameters

Network Structure

- There are several elements of the network that you can change e.g.
  - The number of hidden layers.
  - The number of units in each hidden layer.
  - The type of non-linear activation function e.g. ReLU, sigmoid, ...

Training Schedule

- There also are several aspects of the training procedure that can be changed e.g.
  - The learning rate.
  - The type of optimiser e.g. standard gradient descent, ...
  - How the weights are initialised.
  - When to stop training.

Automatic Differentiation

- The **backpropagation algorithm**, which can be used to compute the gradient of a loss function applied to the output of the network wrt the parameters in each layer.
- This gradient can then be used with any gradient-based optimisation, e.g. gradient descent.

- Manually computing these gradients for anything but small toy problems is too time consuming.
- Instead, we can make use **automatic differentiation** (or **autodiff**). This is a set of automatic techniques to evaluate the derivative of a function.

- Many machine learning frameworks have autodiff functionality built in.

Automatic Differentiation Example

The following is an example of using autodiff for binary logistic regression.

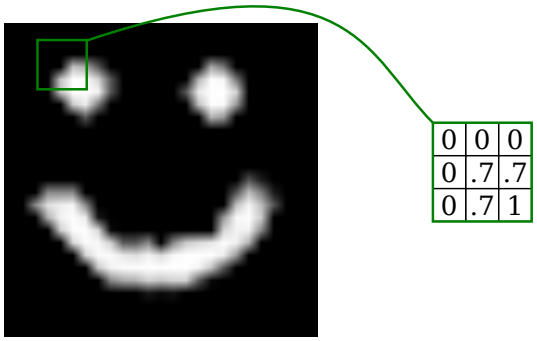
```python
import jax.numpy as jnp
from jax import grad, nn

# Define our loss function
def nll_loss(X, y, w):
    pred = nn.sigmoid(X@w)
    loss_pos = (y==1)*jnp.log(pred)
    loss_neg = (y==0)*jnp.log(1.0 - pred)
    loss = -(loss_pos + loss_neg).mean()
    return loss


# Define our dataset, which has 3 instances
# We have already appended a 1.0 to each row of X
X = jnp.array([[1.0, 0.5,-0.35],
               [1.0, -0.1, 0.1],
               [1.0, -1.2, 1.0]])
y = jnp.array([0.0, 0.0, 1.0])

# This is our initial weight vector w
w = jnp.array([0.0, -1.0, 1.0])

```

```python
# (i) Compute the gradient manually
# Here we use the derived expression
manual_grad = (nn.sigmoid(X@w) - y)@X
manual_grad *= (1.0/X.shape[0])
print('Manual gradient', jnp.round(manual_grad, 3))


# (ii) Compute the gradient automatically
# Evaluate the loss and compute the gradient
loss = nll_loss(X, y, w)
w_grad = grad(nll_loss, (2))(X, y, w)
print('Auto gradient  ', jnp.round(w_grad, 3))


# We can take one step of gradient descent
learning_rate = 3.0
w_update = w - learning_rate*w_grad

```


Alternative Network Architectures

Images as Tensors

- We can represent images as **matrices**, where each entry stores the intensity value of a given pixel.

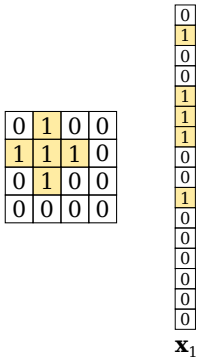


Issues with Fully Connected Neural Networks

- Fully connected networks with high-dimensional inputs have a lot of model weights.
- This results in a very large number of model weights that have to be learned.
- For example, if our input was an image of size 100×100, this would require $10,000$ weights for *each* hidden unit in the first layer.

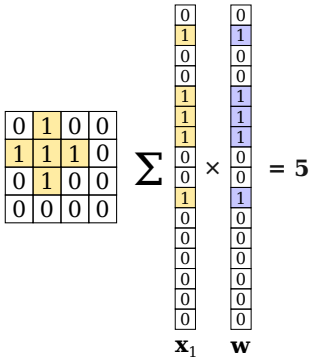
Shift Invariance

- Fully connected networks are sensitive to the position of the signal of interest in an input image.



Shift Invariance

- Fully connected networks are sensitive to the position of the signal of interest in an input image.



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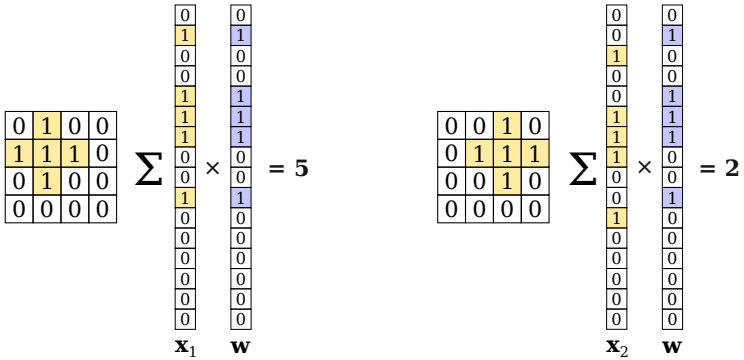


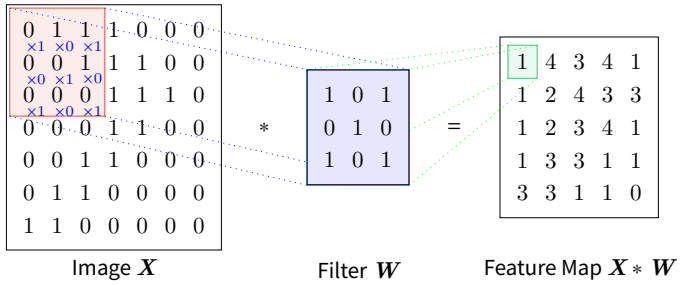
Convolutional Filters

- Constrain each hidden unit to extract features by **sharing** weights across the input.
- For an image $\boldsymbol{X}$ and $K \times K$ weight matrix $\boldsymbol{W}$ (i.e. a filter) we compute the outputs as

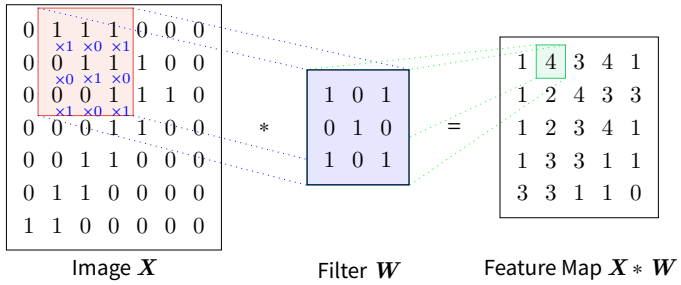
$$h_{ij} = g\left(\sum_{m=1}^{K}\sum_{n=1}^{K} w_{m,n} x_{i+m,j+n} + b\right)$$

- The output is a **feature map**, where each entry h_{ij} is the local response of the filter convolved with the image at that location.
- Multiple weight matrices can be used to produce multiple feature maps.

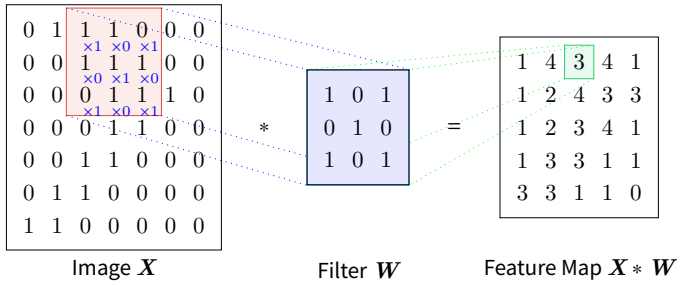
Convolution



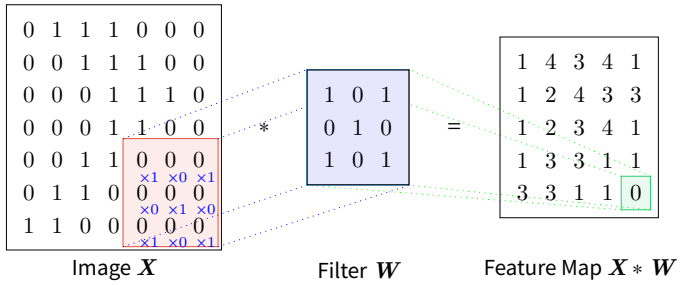
Convolution



Convolution

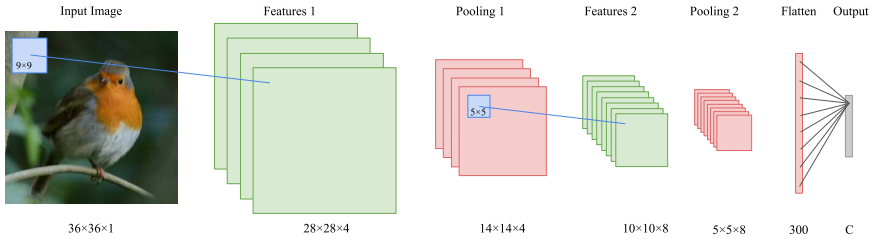


Convolution



Convolutional Neural Network - Example

- A Convolutional Neural Network (CNN) consists of *learnable* convolutional filters and *non-learnable* pooling layers.
- The pooling layers reduce the spatial dimensionality of the feature maps.
- For classification, at the output of the network, we have a fully connected layer which predicts one of C classes.

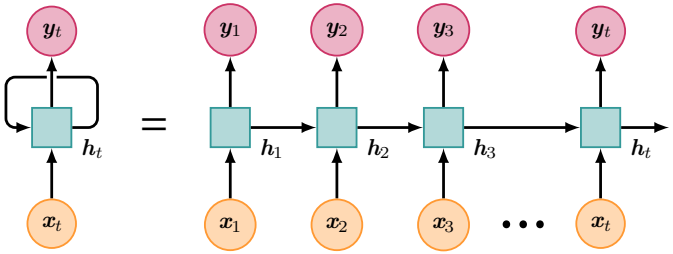


Recurrent Neural Networks

- A model for sequence data (e.g. time series).
- Different network architectures and recurrent units exist, e.g. long short-term-memories (LSTMs).
- In a RNN, each input is processed sequentially, one item at a time.
- Past information is retained through past hidden states.

Recurrent Neural Networks

- In RNNs, the outputs $\boldsymbol{y}_t$ are a function of the current input $\boldsymbol{x}_t$ and the previous hidden state $\boldsymbol{h}_{t-1}$.



Transformers

- Alternative, and more recent, approach for modelling sequential data.
- Unlike RNNs, Transformers process the entire input all at once.
  - Thus training can be performed in parallel.
  - They are also less susceptible to 'forgetting' information from the past, i.e. better suited to capture *long-range* dependencies.
- Transformers have a special type of unit called a **self-attention** unit. This is used to compute similarity scores between inputs in the input sequence.
- They can also be applied to other data types, e.g. images.

Summary

- Artificial neural networks are a powerful non-linear modelling tool for classification and regression.
- They are *not* biologically plausible models.
- The output of the hidden units are a new representation of the original input data. This can be interpreted as learned features.
- Training makes use of the backpropagation algorithm to compute derivatives.
- Beyond standard fully connected networks, alternative architectures exist for learning from structured input data (e.g. images, audio, text, ...).