An introduction to conditional density estimation using the R interface to Keras

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Outline

What is Keras?

- Keras is a **high-level API** for fast deep learning developed by **Google** and written primarily in **Python**, released in 2015
- Whilst it used to support a number of different **back-ends** (Theano, MILA; CNTK, Microsoft) it now solely runs on top of **Tensorflow**
- Tensorflow is a free open-source machine learning (not just DL) library written in Python, C++ and CUDA (for **GPUs**) that does all of the lower-level computations for Keras
- Keras is the **most popularly applied deep learning software** due to its simple yet powerful framework, followed closely by Facebook's PyTorch. This can also be used in R (see `https://www.rstudio.com/blog/torch/`)

What is (parametric) conditional density estimation?

Let's say you have a **response** variable Y with **covariates/predictors $\mathbf{X}$**:

- Conditional density estimation is a **generalisation** of normal (mean/least-squares) regression
- In mean regression, we model $\mathbb{E}[Y|\mathbf{X}]$ as a function m of predictors. For CDF, we model the **entire conditional density** $f(Y|\mathbf{X})$
- In a **parametric framework**, we let $Y|\mathbf{X} \sim \mathcal{F}(\boldsymbol{\theta})$ for a parameter set $\boldsymbol{\theta}$ and then let $\boldsymbol{\theta}$ be a function m of observations $\mathbf{x}$ of $\mathbf{X}$
- Prediction $\Leftrightarrow$ Gaussian density estimation (with fixed $\sigma = 1$). Classification problems $\Leftrightarrow$ Multinomial density estimation
- We are going to estimate $m(\mathbf{x})$ using **Deep Learning**

Objectives

The objectives of this short-course are:

- Understand the basics of deep learning and neural networks
- Build and train simple feed-forward prediction and regression models using the R interface to Keras
- Perform conditional density estimation using neural networks

Some suggested reading

For deep learning:

- Chollet, F. with Allaire, J. J. (2018). Deep learning with R
- Any of the multitude of Keras for R blogs, see e.g., blogs.rstudio.com, r-bloggers.com, towardsdatascience, analaticsvidyha. (Even those that give code written in Python as it's very easy to translate!)
- Rodrigeus, F., Pereira, F. C., (2022). Beyond expectation: Deep joint mean and quantile regression for spatiotemporal problems (Nice introduction to CNNLSTMs for quantile regression)
- There's some really good `https://www.coursera.org/coursera` courses for deep learning, particularly with Python

Some suggested reading

For CDE (tailored towards extremes):

- Cannon, A. J. (2010). A flexible nonlinear modelling framework for nonstationary generalized extreme value analysis in hydroclimatology
- Cannon, A. J. (2011). GEVcdn R package
- Carreau, J., Bengio, Y. (2007). A hybrid Pareto model for asymmetric fat-tailed data
- Richards, J., Huser, R., (2022). High-dimensional extreme quantile regression using partially-interpretable neural networks: With application to U.S. wildfires

Installation

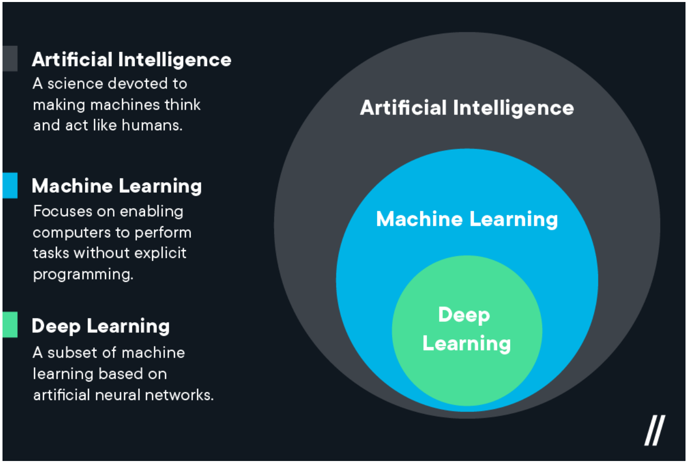
First thing's first, let's get Keras installed

- Open *installation.R*
- Download and install Python 3.8.4 from `https://www.python.org/downloads/macos/` (unless you already have a working version of Python ≥ 3.5)
- Install the `keras` and `tensorflow` R packages
- Create a virtual Python environment
- Configure the Rstudio Python interpreter (you will need to restart the R session for this)
- Install the latest versions of the Python libraries *tensorflow* and *keras*

Don't touch any Python2 installations!

Deep learning

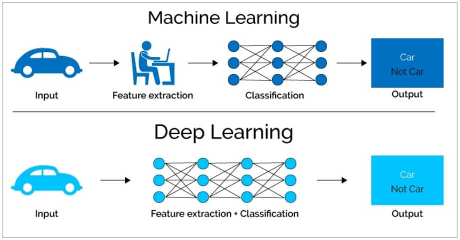
What is deep learning?[1]


Artificial Intelligence
A science devoted to making machines think and act like humans.
Machine Learning
Focuses on enabling computers to perform tasks without explicit programming.
Deep Learning
A subset of machine learning based on artificial neural networks.
Artificial Intelligence
Machine Learning
Deep Learning

[1]Copyright belongs to https://flatironschool.com/blog/deep-learning-vs-machine-learning/

Deep learning vs. machine learning[2]

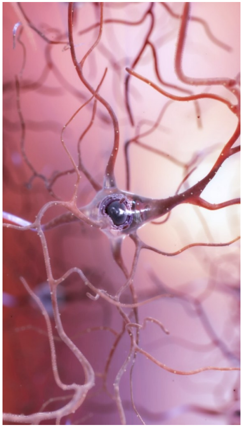
- Specifically uses **artificial neural networks** (ANNs)
- Algorithms are much **more complex** and require **less human intervention** $\Rightarrow$ no manual feature extraction/engineering required
- Typically requires substantially more data to train. Gives rise to the concept of **transfer learning**, i.e., using pre-trained models



[2]Copyright belongs to
`https://levity.ai/blog/difference-machine-learning-deep-learning`

Basics of neural networks

- A neural network is an algorithm designed to mimic the **human brain**.
- It can be constructed as a **directed graph** with a single input and a single output, with a dense network of **interconnected nodes** in-between
- Data is input into the graph and information is extracted at each node, a.k.a **perceptron**. An output is provided at the end of the network.
- Similarly brain activity occurs when a stimuli enters the system, information is based through the network via **neurons** that extra relevant information and this information passes to some area of the brain that forces a response (output)

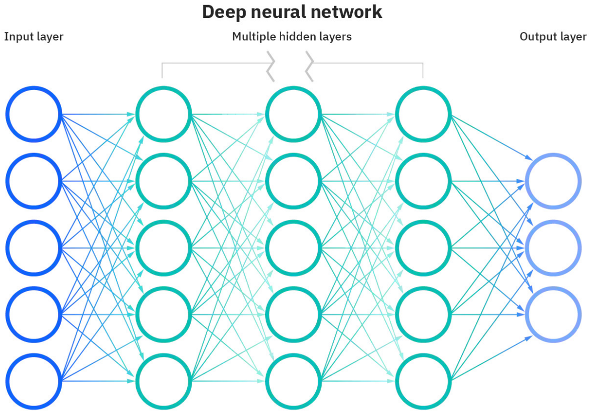


Nodes in a neural network are arranged in layers:

- A single node may be connected to several nodes in the layer above, from which it **receives information**, and to the layer below, which it **feeds information**
- Most neural networks are **“feed forward"** - information is passed forward, layer-to-layer, in one direction only
- Different information is extracted at each layer in a **hierarchical** fashion, i.e., the most important aspects first
- The “deep" in deep learning refers to the depth of layers in a neural network as well as its hierarchical nature

Architecture

Typical structure[3]



[3]Copyright belongs to `https://www.ibm.com/cloud/blog/ai-vs-machine-learning-vs-deep-learning-vs-neural-networks`

Typical structure

- A **single input layer**. Each input would be a single predictor variable in the form of a scalar value, a sequence or an image (or even a sequence of images!).
- **A single output layer**. For prediction or classification problems, we would have a single node here. For CDE, we would have $|\boldsymbol{\theta}|$ nodes.
- A collection of **hidden layers**. Preferably more than one! In the previous example, each hidden layer has a **width** of five.
- Calculations are completed at each node in the hidden layer. These are parameterised by **weights and biases**.
- The calculations within a layer are of a certain “type". We will consider standard, convolution and recurrent layers.

We refer to the structure of a neural network as its **architecture**.

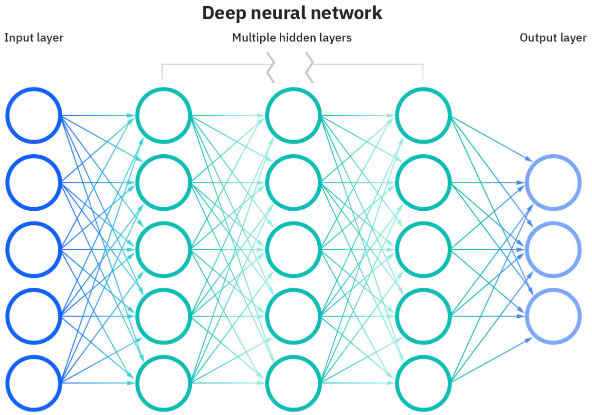
Standard “vanilla" MLPs

A standard multi-layered perception uses `layer_dense` in `Keras` and takes in a vector of values, i.e., a scalar for each input node. Let's say that $\mathbf{x} \in \mathbb{R}^d$ is our input - so the previous layer had d outputs! We take some

- Weights: $w_i \in \mathbb{R}$ for $i = 1, \ldots, d$
- Bias: $b \in \mathbb{R}$
- Calculate $\sum_{i=1}^{d} w_i x_i + b$
- And apply an **activation function** a to get:

$$a\left(\sum_{i=1}^{d} w_i x_i + b\right).$$

And that's it!


Deep neural network
Input layer
Multiple hidden layers
Output layer

Activation function[4]

The activation function defines the **output of the node**. There's a range of different functions that you can use (see `https://keras.rstudio.com/reference/activation_relu.html`), but typically they must satisfy two properties:

- **Nonlinear**! If all nodes had linear activation, this would just be a linear regression model. A two-layered NN with non-linear activations is a **universal function approximator**.
- **Continuously differentiable**. Needed for gradient-based optimisation.

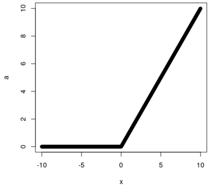
You can think of the activation function as an analogue to the link function in regression. In fact, a single-layered NN is simply a **generalised linear regression model**. We can think of CDE using NNs as a**hierarchical generalised linear model**.

[4] `https://en.wikipedia.org/wiki/Activation_function`

ReLu activation

An activation function that's popularly applied is the **rectified linear unit**:

- Older neural networks relied on sigmoid or tanh activation functions
- These suffered from the *vanishing gradient problem*[5], which made it difficult to efficiently train deep networks
- The Relu replaced these. It has the form $a(x) = \max\{x, 0\}$.

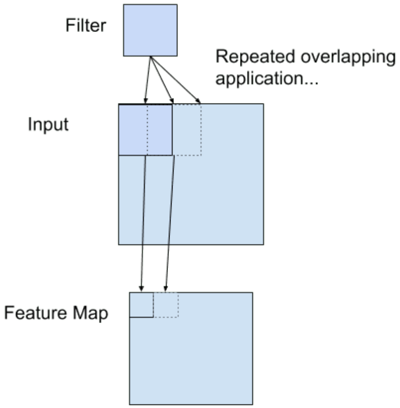


- The neuron "activates" only if **enough information passes through** (think pain receptors)
- One drawback: not differentiable at zero

[5]The networks we will be considering will not be overly deep, so this problem does not occur. For details, see `https://machinelearningmastery.com/rectified-linear-activation-function-for-deep-learning-neural-networks/`

Convolution layers[6]

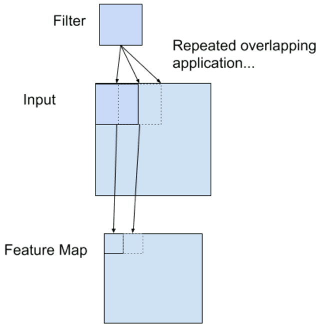
A **convolution layer** acts on an image, not a vector of inputs. The image can be 1D (e.g., text), 2D or 3D (e.g., a video or 3D model)



- A convolution filter/kernel of a certain dimension is passed over the image
- The filter starts in a corner of the image. A convolution is performed, and then the filter moves one horizontal “stride". Once it reaches the edge, it moves one vertical stride down.

[6] Copyright belongs to `https://machinelearningmastery.com/convolutional-layers-for-deep-learning-neural-networks/`

Convolution layers[7]



- After the filter has passed over the entire image, a **feature map** will be produced. The dimension of the feature map will be determined by the filter dimension and the strides
- An image can have multiple “channels", i.e., different colours, inputs, each with its own filter
- The feature maps for the different channels are added, a bias is introduced and then *a* is applied
- A layer can have **multiple filters**, similar to nodes in a densely-connected network

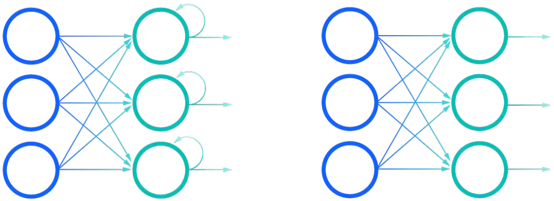
[7] Copyright belongs to `https://machinelearningmastery.com/convolutional-layers-for-deep-learning-neural-networks/`

Convolutions

- Each filter has an array of weights corresponding to its dimension. A 3×4 filter will have a 3×4 matrix of weights
- A convolution is simply the **dot product** of the filter weights and the image values
- Unless the filter has all dimensions one and a stride of one (**this is just a dense layer!**), the outputted feature map will have a smaller dimension that the input images. This can be rectified using **padding**, i.e., adding zeroes to the boundaries of the image
- Very good for capturing spatial characteristics in data

Recurrent layers[8]

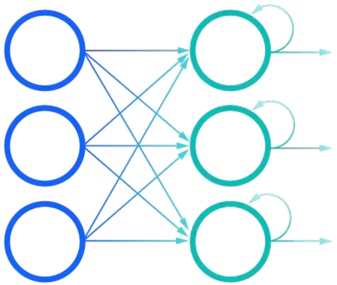
A recurrent layer takes in as input a sequence of vectors/images. Let's say that the input is the sequence of vectors $\{\mathbf{x}_t : t = 1, \ldots, T\}$ where $\mathbf{x}_t \in \mathbb{R}^d$ for all t.

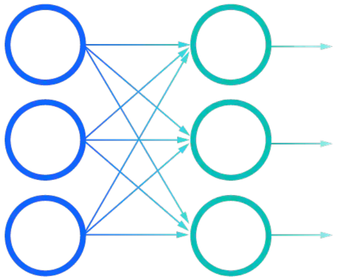


Once an input enters the layer, it becomes stuck in a **recurrence loop** - the output from the computation using the first input vector $\mathbf{x}_1$ becomes an input for the computation on $\mathbf{x}_2$ (and so on...).

[8]Copyright belongs to
`https://www.ibm.com/cloud/learn/recurrent-neural-networks`

Recurrent layers[9]





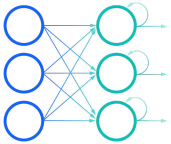
[9]Copyright belongs to
https://www.ibm.com/cloud/learn/recurrent-neural-networks

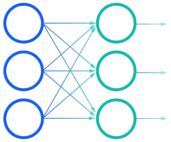
Recurrent layers[10]

Let's consider a very basic example of a recurrent layer and just look at the computations at a single recurrent node. The output from the first vector in the sequence $\mathbf{x}_1$ is $a(m_1 + b)$ where

$$m_1 = \sum_{i=1}^{d} x_{i,1} w_i.$$

The output $a(m_1 + b)$ moves to the next layer, but the information m_1 returns back into the same layer.





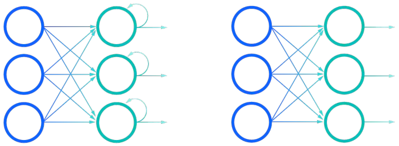
[10] Copyright belongs to https://www.ibm.com/cloud/learn/recurrent-neural-networks

Recurrent layers[11]

The output from the second input $\mathbf{x}_2$ is $a(m_2 + b)$ where

$$m_2 = \sum_{i=1}^{d} x_{2,1} w_i + m_1 + b.$$

So now the output $a(m_2 + b)$ contains information from the previous vector in the sequence! And this procedure is repeated for the **entire sequence** and for all nodes.



[11]Copyright belongs to
`https://www.ibm.com/cloud/learn/recurrent-neural-networks`

Some points...

- These simple layers can be implemented using `layer_simple_rnn`
- Generally these are not used anymore due to numerical stability problems. People now use **Long Short-Term Memory** layers[12], implementable by `layer_lstm`.
- The intuition is the same, but these layers have “forget gates" which allow them to forget **useless information** and avoids numerical instability, i.e., vanishing/exploding gradients

[12] S. Hochreiter; J. Schmidhuber (1997). "Long short-term memory". Neural Computation. 9 (8): 1735–1780.

Some points...

- We considered a dense “vanilla" recurrent layer. We can have recurrent convolutional layers instead (see e.g., `layer_conv_lstm_2d`), which captures temporal structure within sequences of images
- The introduction of a recurrent layer means that the NN is no longer “feed-forward"; unlike like the previous layers, computations for recurrent layers cannot be done in parallel. This makes training more computationally demanding and not suitable for laptop-based work. I've not included an explanation of their implementation in `Keras`, but I can provide **help/code on request**.

Training

Loss

Training a neural network, i.e., estimating the weights and biases, is done by optimizing some **loss function**. Let's say we have N observations of the response $y_1, y_2, \ldots$ and the neural network predicts some output $\hat{\mathbf{y}}_1, \hat{\mathbf{y}}_2, \ldots$ (could be a vector!). We write the loss function as $l(y, \hat{\mathbf{y}})$.

Loss

Whilst the NN architecture can be standard for any task, the loss function must be **very specific**! Examples include:

- MSE: $(1/N)\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$ (mean prediction)
- MAE: $(1/N)\sum_{i=1}^{N}|y_i - \hat{y}_i|$ (median prediction)
- Binary cross-entropy (if $\hat{y}_i \in (0,1)$ and $y_i = 0$ or 1): $-(1/N)\sum_{i=1}^{N}(y_i \log \hat{y}_i + (1-y_i)\log(1-\hat{y}_i))$. Two-class Classification, but can be extended to more than two classes.

For CDE, we will use the negative log-likelihood as the loss function. Here $\hat{\mathbf{y}}$ will be the parameters for distribution we are fitting.

Training

The loss function is minimised using a form of **gradient descent**. Neural networks are trained for a **finite number of epochs** (iterations). Let's say all of the trainable weights and parameters for our NN are contained in some set $\boldsymbol{\Theta}$. For epoch i:

1. We go forward through the network to compute $\hat{y}$ given the current state of the network. This allows us to evaluate $l(y, \hat{\mathbf{y}})$.
2. We move back through the network to compute (exactly) $\nabla l(y, \hat{\mathbf{y}})$ w.r.t $\boldsymbol{\Theta}$.
3. We update the parameters using

$$\boldsymbol{\Theta}^{(i+1)} = \boldsymbol{\Theta}^{(i)} - \boldsymbol{\lambda}^{(i)} \nabla l(y, \hat{\mathbf{y}}),$$

with the product taken componentwise and where $\boldsymbol{\lambda}^{(i)}$ are a set of learning rates.

Training (cont.)

- The learning rates are **quite important**. Large rates will cause the optimization to diverge; small rates may cause convergence to local minima. Algorithms exist for adaptive tuning of $\boldsymbol{\lambda}$ (hence the superscript (i)), most notably RMSprop[13] and ADAM[14]
- Training using gradient descent can be inefficient. Instead we would use **Mini-batch gradient descent** (MbGD). First split the data into batches of pre-determined size. Within an epoch, parameters are updated for each batch; the partial derivatives of the loss are computed exactly for the batch (which gives an approximation to the true ∇ vector)

[13] Unpublished Coursera course by Geoff Hinton `https://www.cs.toronto.edu/~tijmen/csc321/slides/lecture_slides_lec6.pdf`

[14] `https://arxiv.org/abs/1412.6980` with over 111000 citations!

Training (cont.)

- Training using MbGD is more efficient, but the loss is not guaranteed to decrease for each epoch (we will see this later!)
- The extreme case with a batch size of 1 is Stochastic Gradient Descent (although the names are used interchangeably)
- I would recommend using **a large a batch-size as feasible** for CDE, particularly if you have highly non-stationary data

Backpropagation

In statistical modelling, we often need to approximate the partial derivatives when optimising particularly complicated function. For neural networks, we compute $\nabla l(y, \hat{\mathbf{y}})$ through a procedure called **backpropagation**. This involves moving backwards through the network and using the chain rule to calculate (exactly) the partial derivatives at each layer. As we have constructed the neural network output as a function of differentiable functions with known derivatives, this is very quick and easy to do!

Illustrating back propagation

Let's take a simple illustration. Say we have a network with two hidden layers with widths four, all of the biases are equal to zero and a single output. Then we can construct

$$\begin{aligned}\hat{y} = a_3\left(\sum_{i=1}^{4} w_{3,i} m_{2,i}\right) &= a_3\left(\sum_{i=1}^{4} w_{3,i} a_2\left\{\sum_{i=1}^{4} w_{2,i} m_{1,i}\right\}\right)\\ &= a_3\left(\sum_{i=1}^{4} w_{3,i} a_2\left\{\sum_{i=1}^{4} w_{2,i} a_1\left[\sum_{i=1}^{d} w_{1,i} x_i\right]\right\}\right)\end{aligned}$$

The goal is to calculate all $\partial l(y,\hat{y})/\partial w_{3,i}$, $\partial l(y,\hat{y})/\partial w_{2,i}$ and $\partial l(y,\hat{y})/\partial w_{1,i}$.

Illustrating back propagation

Start at the beginning. We know that

$$\partial dl(y, \hat{y})/\partial d\hat{y}$$

will be simple to compute (especially if standard) if we have constructed $l(y, \hat{y})$ from differentiable functions. Similarly we should also know

$$a_3^{'}(x) = \partial a_3(x)/\partial x, \quad a_2^{'}(x) = \partial a_2(x)/\partial x, \quad \text{and} \quad a_1^{'}(x) = \partial a_1(x)/\partial x,$$

as these are standard.

Illustrating back propagation

Recall that

$$\hat{y} = a_3\left(\sum_{i=1}^{4} w_{3,i} m_{2,i}\right).$$

Now move back through the network. From the final layer, we have

$$\frac{\partial l(y,\hat{y})}{\partial w_{3,i}} = \frac{\partial l(y,\hat{y})}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial w_{3,i}} = \frac{\partial l(y,\hat{y})}{\partial \hat{y}} m_{2,i} a_3^{'}\left(\sum_{i=1}^{4} w_{3,i} m_{2,i}\right).$$

Illustrating back propagation

Recall that

$$\hat{y} = a_3\left(\sum_{i=1}^{4} w_{3,i} m_{2,i}\right), \quad \text{where}$$

$$m_{2,i} = a_2\left\{\sum_{i=1}^{4} w_{2,i} m_{1,i}\right\}.$$

For the second layer, we have

$$\frac{\partial l(y,\hat{y})}{\partial w_{2,i}} = \frac{\partial l(y,\hat{y})}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial m_{2,i}} \frac{\partial m_{2,i}}{\partial w_{2,i}} = \frac{\partial l(y,\hat{y})}{\partial \hat{y}} w_{3,i} a_3^{'}\left(\sum_{i=1}^{4} w_{3,i} m_{2,i}\right) \frac{\partial m_{2,i}}{\partial w_{2,i}}$$

$$= \frac{\partial l(y,\hat{y})}{\partial \hat{y}} w_{3,i} a_3^{'}\left(\sum_{i=1}^{4} w_{3,i} m_{2,i}\right) \frac{\partial m_{2,i}}{\partial w_{2,i}} m_{1,i} a_2^{'}\left(\sum_{i=1}^{4} w_{2,i} m_{1,i}\right),$$

and so on and so forth.

As long as we choose **differentiable loss and activation functions**, backpropagation can be performed very efficiently!
When writing custom functions for `Keras`, we **must use the** `tensorflow` or `Keras` backend functions; these have **known derivatives** that `tensorflow` can easily call.

Overfitting

Training/validation/testing

Due to their large number of parameters, neural networks are prone to overfitting. It's necessary to use **validation/testing** to assess any overfitting.

- First, we subset the data into training, validation and testing. Opinions differ, but the standard is 80/10/10
- Each set has a different purpose:
  - The model is **trained** on the training data. This is used to optimise the weights, biases and other hyper-parameters
  - We then **validate** the model by getting predictions for the validation set and evaluating validation loss. This will give us some insight as to whether or not overfitting is occurring. Typically the validation loss is used for model selection
  - To get a truly unbiased evaluation of the model fit and to compare amongst different models, we should **test** the model on previously unseen data

Mitigation

- Some literature uses **test** and **validation** interchangeably, e.g., in cross-validation, the validation (hold-out) set is actually a test set because the model never sees it for training
- Overfitting in neural networks is **inevitable** if a network is trained **indefinitely**.
- However, you can mitigate the risk of fitting using forms of regularisation. We will discuss these in the practical.

That's the end of the first session.
Thanks for listening!

Building a Keras model

Please download the R markdown file from `https://github.com/Jbrich95/cde-RKeras-intro/tree/main/keras_build`

and follow my GitHub while you're at it

Practicals

Overview

We will now put your new practical skills to the test!

- I have simulated 10000 observations of a response Y on a 10×12 grid. The distribution of the response is dependent on a predictor set $\mathbf{X} \in \mathbb{R}^{10}$. Observations are replicates from a GP on the same 10×12 grid. The unknown function that connects the predictors to the parameters of the response distribution is highly non-linear.
- You will build and train a neural network to estimate the conditional density $f(Y|\mathbf{X})$. Choose your own architecture, optimisation scheme, validation sets and try to build the best predictive model possible
- 1000 observations of Y and $\mathbf{X}$ have been left out for testing. At the end we will test everyone's models using this hold-out set, and see who has the best model!

Some notes:

- There's no temporal structure in the data, so using an RNN is unnecessary. This also means a simple validation scheme will be sufficient!
- There is spatial structure in the predictor set, so convolution layers will perform well here. However, you will have to consider the extra time/difficulty in training due to the increased number of parameters, as well as the increased risk of overfitting (and hence poor extrapolation)
- You will have to write your own custom loss function to perform both quantile and GPD regression
- Training data can be downloaded from `https://github.com/Jbrich95/cde-RKeras-intro/tree/main/Data`

Logistic regression

- Load `logistic_train_df.Rdata`
- Build a model to estimate $\Pr\{Y = 1\}$ for the response using the binary cross-entropy loss
- At the end, we will load the test data in `logistic_test_df.Rdata`
- Use your model to predict the probabilities for the test data and then evaluate the binary cross-entropy loss given those predictions

Non-parametric quantile regression

- Load `qregress_train_df.Rdata`
- Build a model to estimate the 90% quantile for the response using the tilted loss function. For the $\tau-$quantile, this is

$$l(y,\hat{y}) = (1/N)\sum_{i=1}^{N}\max\{\tau(y_i-\hat{y}_i),(\tau-1)(y_i-\hat{y}_i)\}.$$

- At the end, we will load the test data in `qregress_test_df.Rdata`
- Use your model to predict the quantile for the test data and then evaluate the tilted loss given those predictions
- Save the train/test quantile estimates as `pred_u_train`/`pred_u_test` (We will use these for fitting a GPD later!)

GPD regression

- For the data from `qregress_train_df.Rdata`, build a model to fit a GPD above your estimated 90% quantile
- The predicted scale and shape parameters will be used to evaluate the TWCRPS for the test data. For a sequence of increasing thresholds $\{v_1, \dots, v_{n_v}\}$ and weight function $w(x)$, the TWCRPS is

$$\sum_{i=1}^{N} \sum_{j=1}^{n_v} w(v_j)[\mathbb{I}\{y_i \leq v_j\} - \hat{p}_i(v_j)]^2,$$

  where $\hat{p}_i(v_j)$ denotes the predicted probability $\Pr\{Y_i < v_j\}$. The weight function is $w(x) = 1 - (1 + (x+1)^2)^{-1/6}$ and puts more weight on extreme values.

GPD regression

- As the GPD model provides a characterisation of the distribution of Y_i above the exceedance threshold u_i only, the TWCRPS function in `qres_twcrps.R` will use the empirical distribution (of all data) for probabilities $\Pr\{Y_i \leq u_i\}$. This function can also be downloaded from the GitHub.
- I have also assumed that u_i is perfectly estimated as the 90% quantile of Y_i. If this is not the case, we could improve our predictions by modelling $\Pr\{Y_i \leq u_i\}$ using logistic regression (with deep learning!), but that's beyond the scope of this exercise.

Thanks for your attention!