DEEP LEARNING FOR TABULAR DATA

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Material

https://github.com/tengku-hanis/applied_ml_seberangjaya.git

Contents

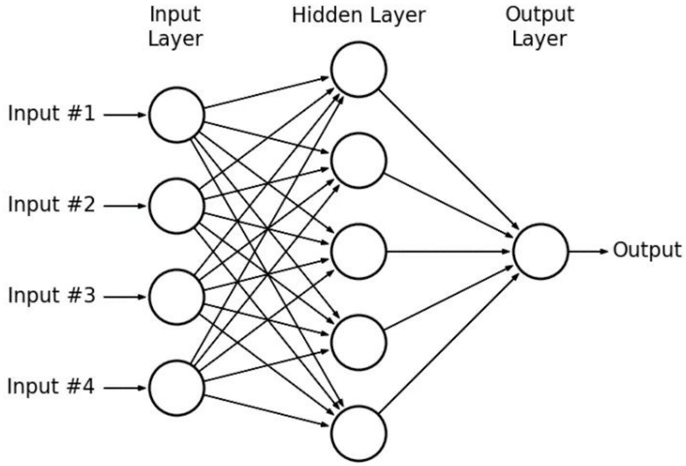
Deep learning

- Deep learning is a subfield of machine learning
- Some consider it as a separate field
- Deep learning is not always a solution to every problem
- Most common/basic architecture based on the source of data:
    - **Tabular data: Deep Neural Network (DNN)**
    - Imaging data: Convolutional Neural Network (CNN)
    - Video data: CNN, Recurrent Neural Network (RNN)
    - Time series data: RNN, Long Short-Term Memory (LSTM), Gated Recurrent Units (GRU)
    - Text data: RNN, LSTM, GRU, Transformer-based models (e.g., BERT, GPT)

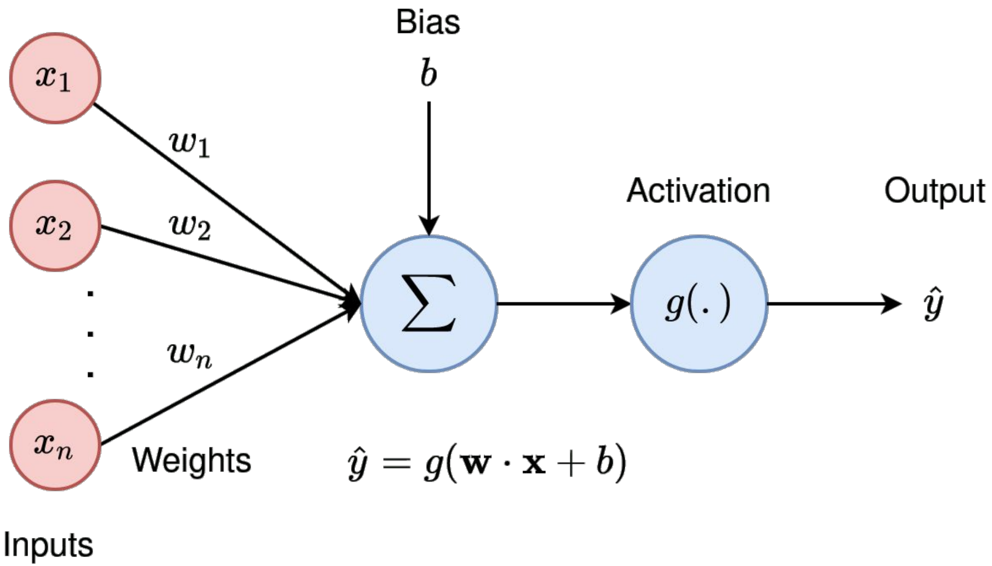
- Classification and regression in DL:
    - Binary classification
    - Multiclass classification
    - Single label classification
    - Multilabel classification
    - Scalar regression
    - Vector regression

Revision - ANN

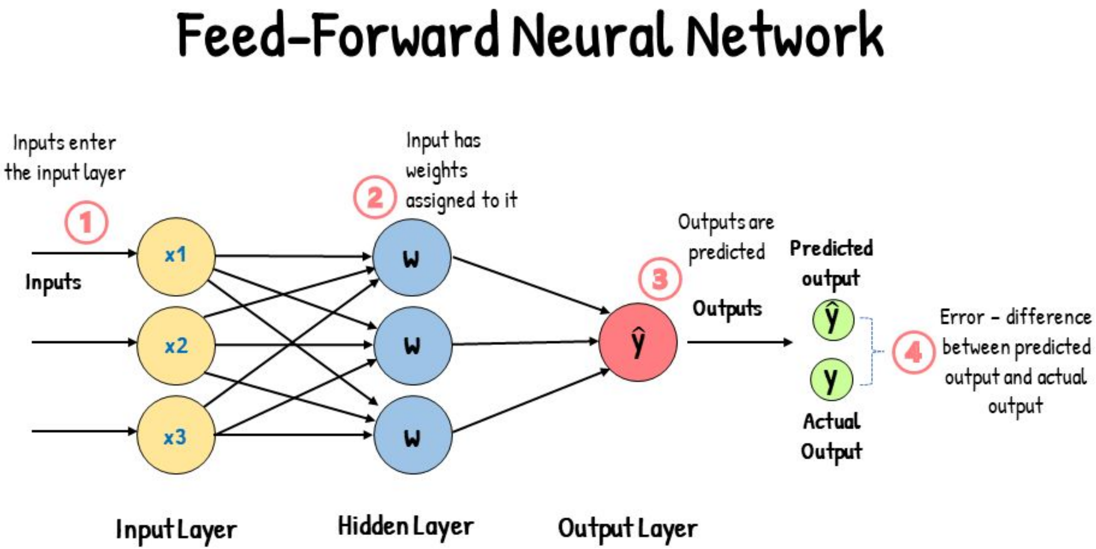
- Neural network is the basis of deep learning
- ANN can be used for regression and classification
- Simple ANN = single layer, feed-forward neural network = multilayer perceptron (MLP) = shallow neural network
- ANN is formed of:
  - Input layer
  - Hidden layer
  - Output layer



- Breakdown of ANN:

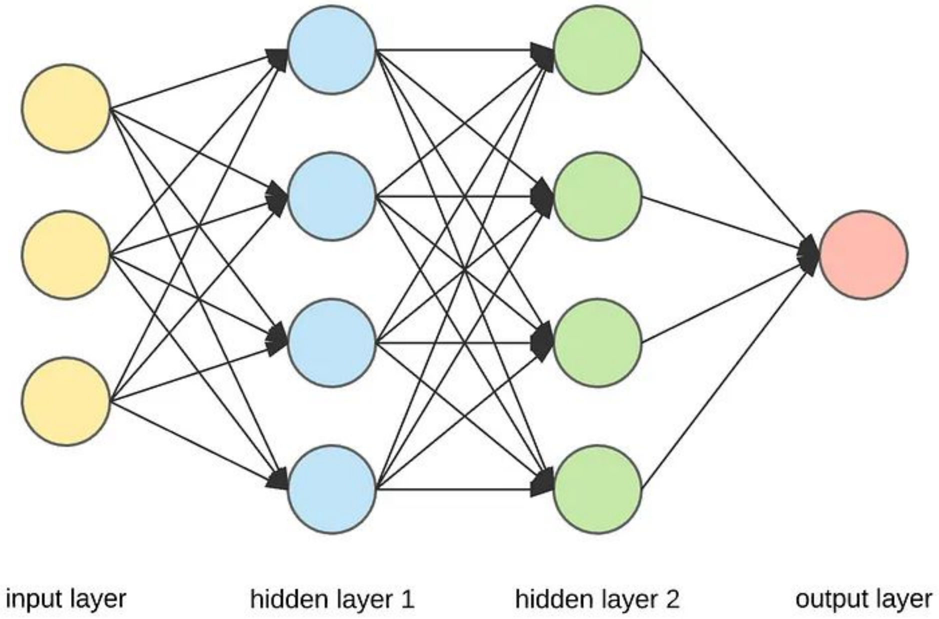


- Simple ANN uses feed-forward neural network approach



Deep Neural Network (DNN)

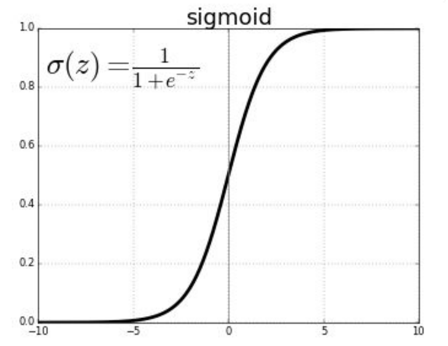
- Shallow neural network/ simple ANN, at most has 3 layers (input, output, and hidden layer)
- DNN has more than 3 layers:
  - “Deep” ≈ more layers

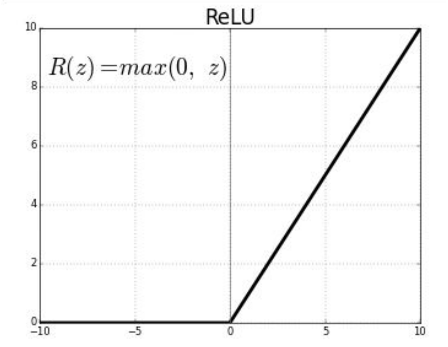


Basic concepts in DNN

Activation function

- To restrict the overall output values
- Example:
    - Sigmoid: for binary classes
    - Softmax: for multiclass
    - Rectified linear unit (ReLU)
        - Solve the issue of vanishing gradient (faster convergence)
        - Introduce non-linearity into the network - enabling the network to learn a complex pattern in the data





Loss/cost function

- A value to be minimised during the training process

Table 9.1: Loss functions, by type of data they work on (binary vs. multi-class) and expected input (raw scores, probabilities, or log probabilities).

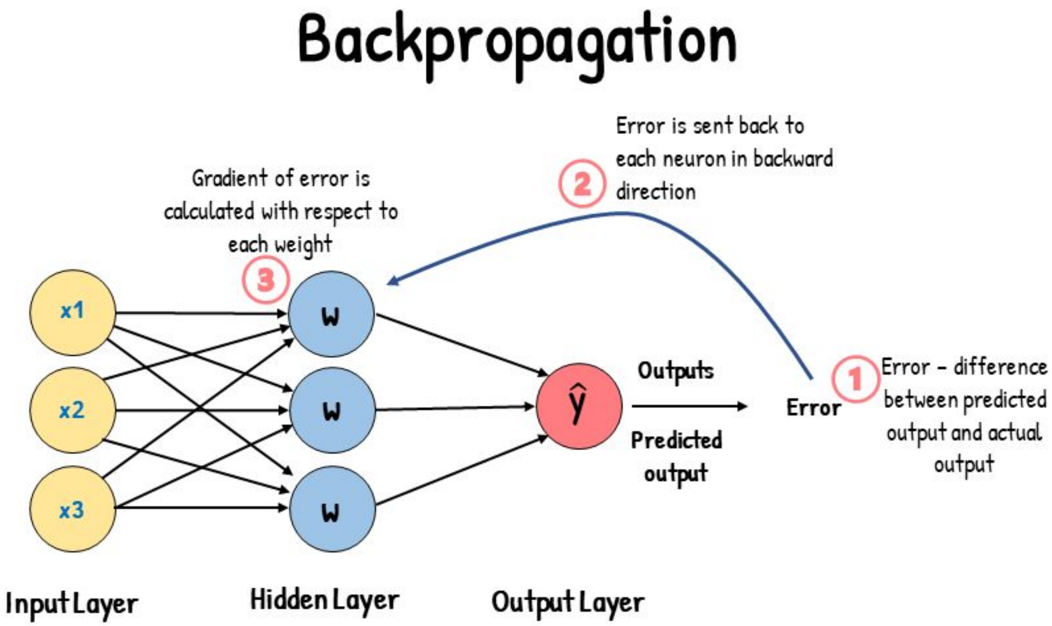
	Data		**Input**		
	binary	multi-class	raw scores	probabilities	log probs
BCeL	Y		Y		
Ce		Y	Y		
BCe	Y			Y	
Nll		Y			Y

Table 9.2: Abbreviations used to refer to `torch` loss functions.

BCeL	`nnf_binary_cross_entropy_with_logits()`
Ce	`nnf_cross_entropy()`
BCe	`nnf_binary_cross_entropy()`
Nll	`nnf_nll_loss()`

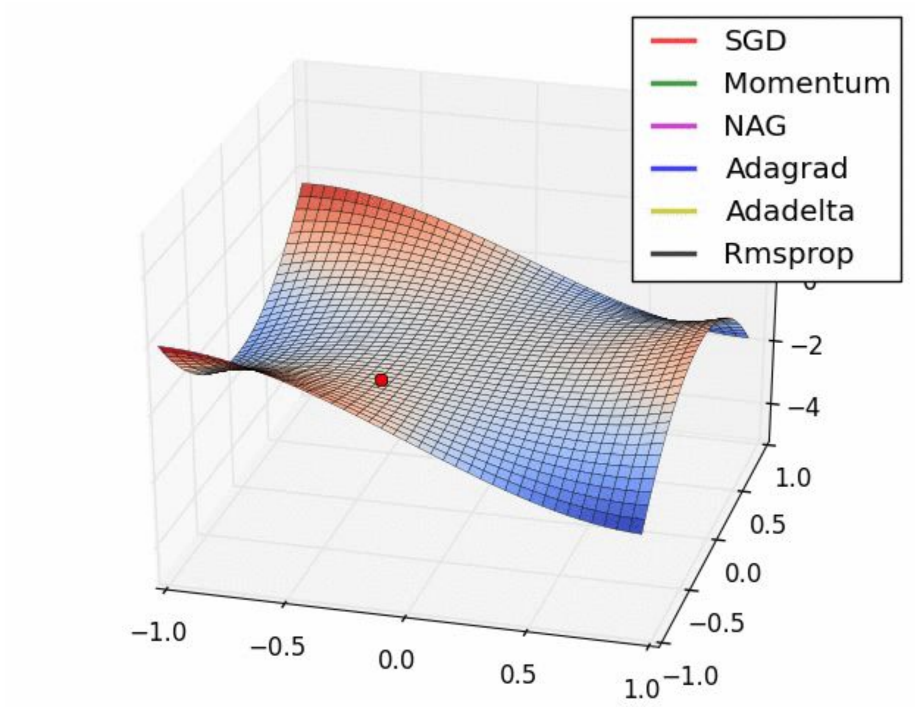
Backpropagation

- This an iterative process of fine-tuning the weights of the network using gradient descent (an optimisation algorithm)
- Process: It operates in two phases:
    - Forward Pass:
        - The input data is passed forward through the network, layer by layer, producing an output
        - The output is compared with the desired output to compute the error
    - Backward Pass:
        - The error is propagated backward through the network, adjusting the weights to minimize it


Backpropagation
Error is sent back to each neuron in backward direction
2
Gradient of error is calculated with respect to each weight
3
x1
x2
x3
w
w
w
ŷ
Outputs
Predicted output
Error
1
Error - difference between predicted output and actual output
Input Layer
Hidden Layer
Output Layer

Gradient descent

- An optimization algorithm used in DL to minimize the error between predicted and actual results
- Example:
    - RMSprop (Root Mean Square Propagation)
        - Usually works for most tasks
        - Some suggestion: γ to be set to 0.9, while a good default value for the learning rate η is 0.001
    - ADAM (Adaptive Moment Estimation)
        - Some suggest to always use ADAM (Adam usually outperforms the rest)
        - Some suggestion: 0.9 for β_1, 0.999 for β_2, and 10^{-8} for ε

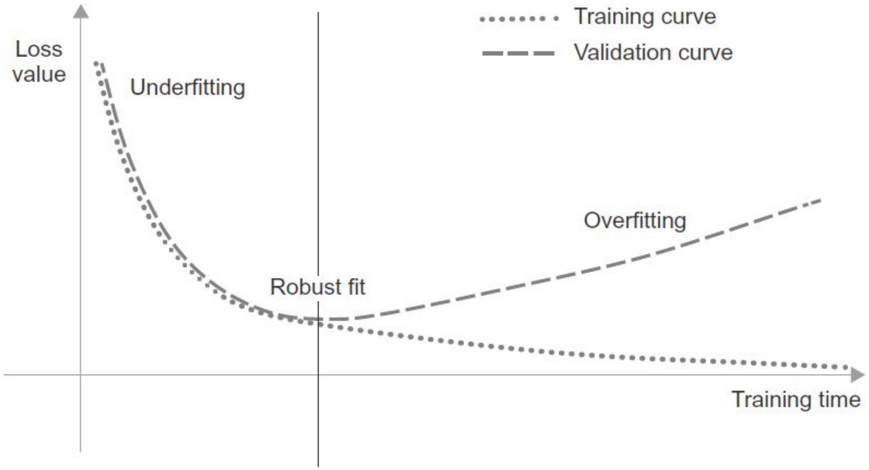

SGD
Momentum
NAG
Adagrad
Adadelta
Rmsprop
−2
−4
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0

Validation approaches

- Hold-out validation - when we have a large dataset
- k-fold cross-validation - when we have a small dataset
- Iterated k-fold cross-validation with shuffling - when we have a small dataset and we need to evaluate the model as precise as possible

Approach to DL

- Set a baseline to beat
- Overfit the network on the training data first
- Then, reduce the overfitting by improving the generalisation



- How to overfit?
    - Add more layers
    - Make the layers bigger
    - Train for more epochs
- How to improve generalisation?
    - Reduce the layers
    - Use regularisation methods
    - Improve the data:
        - Develop better features - feature engineering
        - Remove uninformative features
        - Collect more data

Regularisation methods

- Regularisation methods are applied to avoid overfitting
- Methods:
  - Reduce the network size
  - Weight regularisation - for small deep learning model
    - L1 regularisation
    - L2 regularisation
  - Dropout layer - for large deep learning model
    - Usually between 0.2 - 0.5

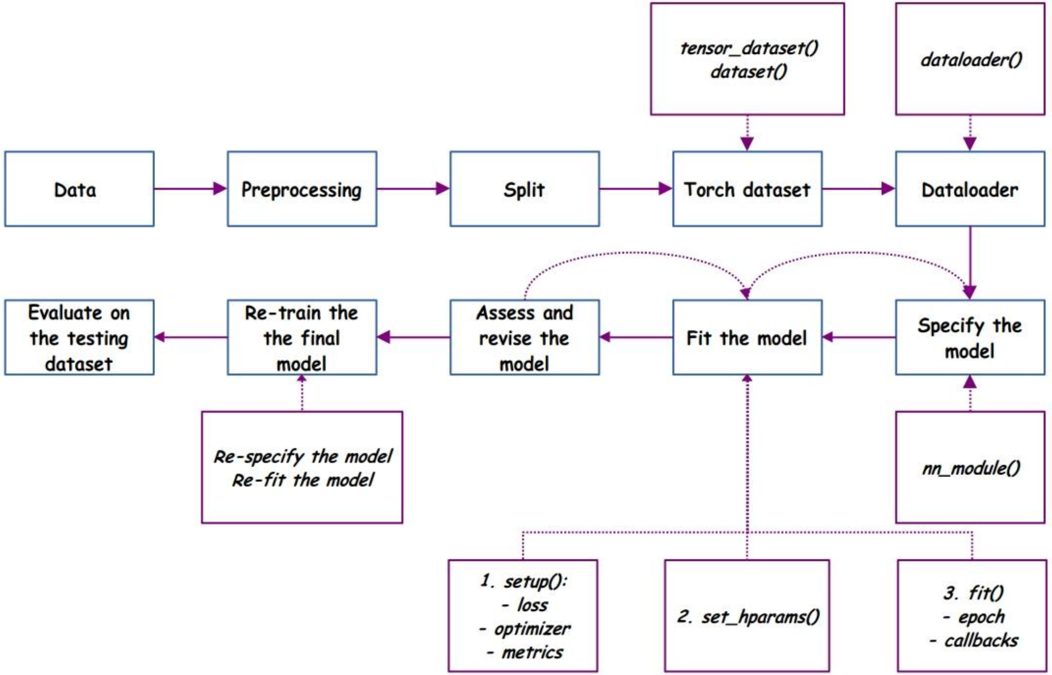
Speed up the training

- Batch normalisation
- Dynamic learning rates
- Transfer learning (for imaging data)

DL packages in R

- Main/core packages:
  - Tensorflow (low level) and Keras (high level)
  - **Torch (low level) and Luz (high level)**
- Some other packages that use Torch for backend:
  - Tabnet (basic):
    - Works well with tidymodels
    - For regression, classification, and time series
  - Brulee (basic):
    - Works well with tidymodels
    - For regression and classification

DNN workflows in torch and luz



Why we need to use luz

- Luz translate this:

```
fitted <-
  model %>%
  setup(optimizer = optim_adam, loss = nn_mse_loss()) %>%
  fit(train_dl, epochs = 10, valid_data = valid_dl)
```

- From this torch low level codes:

```r
# Setup
device <- if (cuda_is_available()) "cuda" else "cpu"
model$to(device = device)
optimizer <- optim_adam(model$parameters)
criterion <- nn_mse_loss()
epochs <- 10

for (epoch in 1:epochs) {

  # --- TRAINING PHASE ---
  model$train()
  train_losses <- c()

  coro::loop(for (b in train_dl) {
    optimizer$zero_grad()

    # Move data to device
    x <- b[[1]]$to(device = device)
    y <- b[[2]]$to(device = device)

    # Forward pass
    output <- model(x)
    loss <- criterion(output, y)

    # Backward pass
    loss$backward()
    optimizer$step()

    train_losses <- c(train_losses, loss$item())
  })
```

```r
  # --- VALIDATION PHASE ---
  model$eval()
  valid_losses <- c()

  # Disable gradient tracking for speed/memory
  torch_no_grad({
    coro::loop(for (b in valid_dl) {
      x <- b[[1]]$to(device = device)
      y <- b[[2]]$to(device = device)

      output <- model(x)
      loss <- criterion(output, y)
      valid_losses <- c(valid_losses, loss$item())
    })
  })

  cat(sprintf("Epoch %d - Train Loss: %.4f | Valid Loss: %.4f\n",
              epoch, mean(train_losses), mean(valid_losses)))
}
```

Running a DL analysis

- Bigger data
- Computational resources:
    - Laptop/PC with GPU
    - Cloud
        - SaturnCloud
        - AWS Amazon
        - Google Colab
        - Etc

“We’ve got a problem. I’ve turned it on but I can’t turn it off again.”

Suggested readings/references

- Chollet, F., Kalinowski, T., & Allaire, J. J. (2022). Deep learning with R (Second edition). Manning.
- Keydana, S. (2023). Deep Learning and Scientific Computing with R Torch. Chapman and Hall/CRC.
- Kalirane, M. (2023, April 5). Gradient Descent vs. Backpropagation: What's the Difference? Analytics Vidhya. https://www.analyticsvidhya.com/blog/2023/01/gradient-descent-vs-backpropagation-whats-the-difference/
- Ruder, S. (2020, March 20). An overview of gradient descent optimization algorithms. Ruder.Io. https://www.ruder.io/optimizing-gradient-descent/

Any question?

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