Introduction to Neural Networks

Learning like a human

Yordan Darakchiev

Technical Trainer iordan93@gmail.com



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Perceptron The basic unit

Neural Networks

- Neural networks try to mimic the way the human brain works
 - Series of interconnected artificial neurons (perceptrons)
 - Can do classification, regression, unsupervised learning, etc.
- Perceptrons were "invented" in the 1940s
 - Great development in the recent years
- "Deep learning" ML algorithms using neural networks
- Cutting-edge applications
 - Machine translation
 - Speech recognition and generation
 - Image recognition
 - Game playing, etc.
- Some <u>examples</u> of deep learning applications

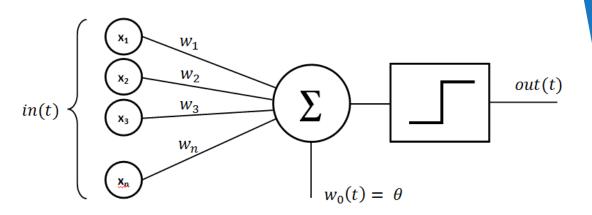
Neural Networks: Pros and Cons

- Can be used to model any datasets
 - Arbitrary dataset complexity
 - One type of algorithm can be used for many applications
- Do not provide any interpretability
 - The classification boundaries are hard to interpret
 - The model is mostly "black box"
 - NNs are not probabilistic (we can't get a confidence metric)
 - "The Dark Secrets at the Heart of AI"
 - Solutions: trying to explain decisions, combining with other algorithms, etc.
- Can be slow
 - Other models usually train a lot faster, even if we use special hardware
- NNs are not a substitute for understanding the problem deeply

Perceptron

- The main "NN unit"
- Algorithm
 - Assign each input a weight
 - Sum all weighted inputs
 - Pass the sum to an activation function
 - Decides whether the neuron will activate (i.e. return 1) → binary output
 - Usually sigmoid function or step function
 - As a result, the perceptron returns 0 or 1
- One perceptron is enough to solve any linearly separable problem
- Usage in scikit-learn

from sklearn.linear_model import Perceptron
perceptron = Perceptron()



Perceptron Learning

- The algorithm definition is not enough
 - We have to update the weights
- Adaline (ADAptive LINear Element) a perceptron that can learn
 - Implements the same linear model: $y = \sum_{j=1}^{n} w_j x_j + \theta$
 - Reformulation: using a bias term $x_{n+1} = 1, \ w_{n+1} = \theta \Rightarrow y = wx$
- Adaline learning update the weights using $w = w + \eta(\tilde{y} y)x$
 - w weights
 - η learning rate (positive constant, model hyperparameter)
 - \tilde{y} model output
 - *y* desired output

Example: Perceptron

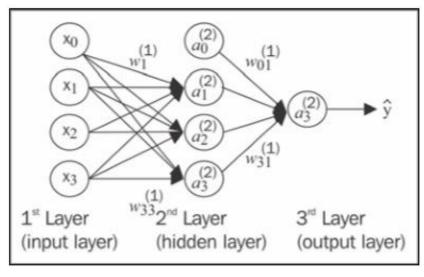
- Generate 2D blobs using scikit-learn
 - Make sure they're linearly separable
 - Make sure you create enough samples, e.g. 10 000
- Use a perceptron to classify samples as belonging to one blob or another
- Test and score the performance
 - Score both in-sample and out-of-sample data
 - It's useful to compare the two metrics this can sometimes detect underfitting or overfitting
 - Print a confusion matrix (and optionally, other metrics, e.g. ROC curve)
 - * Optionally, perform hyperparameter tuning
 - Especially if your blobs are too close

Neural Networks

Combining perceptrons to achieve glory

Neural Network Architecture

- Neural network layout
 - Input(s) (+ bias unit)
 - "Hidden layers" (+ bias units)
 - Output(s)
- Each "node" is a perceptron
- Each arrow carries 0 or 1, and is assigned a weight
- The layers are fully connected
 - There are no connections within layers
- More than 1 hidden layer → "deep learning" (deep NN)
- How many layers? How many units per layer?
 - We don't know :(⇒ hyperparameter tuning



Neural Network Architecture (2)

- Many layers ⇒ the error gradients become too small
 - "Vanishing gradient problem"
 - Small gradient = too slow learning
 - Special algorithms have been developed to deal with this
 - E.g. pre-train the NN one layer at a time using unsupervised learning, use some form of "back-links" (recurrent NNs), use a genetic algorithm instead of gradient descent
 - This is the field of deep learning
- Classification using NNs
 - Two classes: one output (0 or 1)
 - Many classes: use one-hot encoding to represent each class, have as many outputs as there are classes

Neural Network Learning

- The type of NN we look at is called a "feed-forward NN"
 - Data flows only forward, there are no "back-links"
- Learning algorithm:
 - Forward propagation / backpropagation
 - Using the data, propagate the patterns from input to output
 - Based on the output, calculate the error (using a cost function)
 - Backpropagate the error (using derivatives), update the model
- We get the "final" weights after repeating the process for several epochs
- The maths is a bit ugly
 - You can read an explanation <u>here</u>

Neural Network Learning (2)

- Classification: just use one-hot encoding
 - MLP = multi-layer perceptron
 from sklearn.neural_network import MLPClassifier
- Regression: no activation function at the output layer

```
from sklearn.neural_network import MLPRegressor
```

- Regularization: parameter alpha
 - Increasing = less overfitting
 - A <u>visual comparison</u> of regularization parameters
- Tips
 - A neural network is very sensitive to feature scaling
 - [0; 1], [-1; 1] or Z
 - Use a scaler, e.g. StandardScaler
 - Use fine-tuning to optimize alpha
 - Usually in the range 10.0 ** -np.arange(1, 7)

Example: Classifying Handwritten Digits

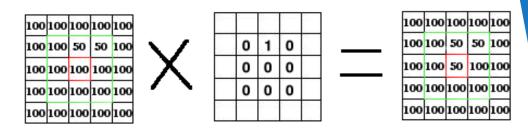
- Obtain the MNIST dataset of handwritten digits
 - This is a famous dataset for learning and comparing neural networks
 - Each data point represents a 28 x 28 image of a digit (0 9)
- Train a simple NN on the MNIST dataset
 - Choose a reasonable number of layers and units per layer, e.g. {3, 3}
- Test, score and evaluate the classification performance
 - E.g. accuracy, precision, recall, F1, confusion matrix, ROC curve
- * Try several other architectures (e.g. more layers, more units per layer, different structure, e.g. 2 + 3 + 2 units, etc.)
- * Compare the results with (an)other classifier(s), e.g. SVM

Convolutional Neural Networks

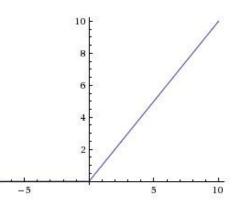
- Feed-forward NNs inspired by the visual cortex
 - Very useful for working on images
 - Recognition and classification
 - Example: https://www.clarifai.com/demo
- Main operations
 - Convolution
 - Non-linearity (ReLU Rectified Linear Units)
 - Pooling (downsampling, subsampling)
 - Classification (fully-connected layer)
- Idea: before proceeding to classification, perform image processing using convolution, pooling and ReLU
 - This process produces the input features of a classical NN

Convolutional Neural Networks (2)

 Convolution: slide a particular matrix (called kernel) over the image

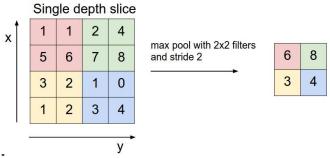


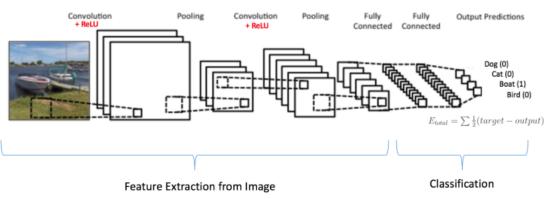
- This produces a new, smaller matrix representing the convolved feature (called feature map)
 - Many filters => "stacked" matrices (3D feature map)
- Rectification (ReLU): $y = \max(0, x)$
 - Performed after each convolution
 - Replaces all negative feature map values with 0 ==
 - Convolution is a linear operation and we want to learn non-linear features; this unit introduces non-linearity
 - It's also possible to use other functions
 - Result from the operation: rectified feature map



Convolutional Neural Networks (3)

- Pooling (downsampling)
 - Reduces the feature map size
 - Types: max, average, sum, etc.
 - The function is applied to a "window" over the image
 - Stride: how many pixels to "skip"
- The combination of convolution, ReLU and pooling layers should output a 1D number vector
 - Represents high-level features of the input image
 - Used as the input to a "standard" feed-forward NN
 - Called a fully-connected layer
 - The NN outputs the final result (e.g. image class)





Summary

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Questions?