

Machine Learning

Module 3.3 - Models: Neural Networks

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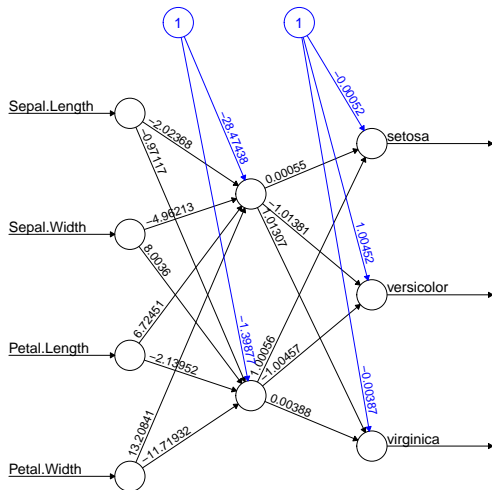
Artificial Neural Network

Artificial Neural networks are models used for classification and for regression based on combining several predictions of small nodes. To illustrate the method we are applying it on the iris data set, without splitting between training and test sets.

Example: iris data with 3 possible classes, Setosa, Virginica, and Versicolor to be predicted from 4 features Sepal.Length (x_1), Sepal.Width (x_2), Petal.Length (x_3), and Petal.Width (x_4).

Example

A neural network looks like this



Error: 1.900926 Steps: 10811

- 4 input **nodes** (circles)
- Arrows with **weights**.
- One middle **layer** made of 2 (+1) nodes.
- 3 output nodes: one for each class (species).

Parameters

In the context of NN, people use the term **weights** to talk about the parameters of the model, θ .

E.g., on the middle layer, coefficients are associated to the arrows. The first (upper) node is the destination of 5 arrows

- Constant terms (node "1") called the **bias**:

$$\theta_{11}^{(0)} = -28.47,$$

- Coefficients for each feature:

$$\theta_{11}^{(1)} = -2.02, \theta_{11}^{(2)} = -4.96, \theta_{11}^{(3)} = 6.72, \theta_{11}^{(4)} = 13.21.$$

Node value

Arrows pointing toward a node indicate a weighted sum. E.g., consider the top node of the middle layer, its linear predictor is η_{11} :

$$\begin{aligned}\eta_{11} &= \theta_{11}^{(0)} + \theta_{11}^{(1)}x_1 + \cdots + \theta_{11}^{(4)}x_4 \\ &= -28.47 - 2.02x_1 - 4.96x_2 + 6.72x_3 + 13.21x_4\end{aligned}$$

Then, the **sigmoid function**¹ is applied to obtain its value:

$$Z_{11} = \sigma(\eta_{11}) = \frac{e^{\eta_{11}}}{1 + e^{\eta_{11}}}$$

This is repeated at the second middle node:

$$\begin{aligned}\eta_{12} &= \theta_{12}^{(0)} + \theta_{12}^{(1)}x_1 + \cdots + \theta_{12}^{(4)}x_4 \\ &= -1.40 - 0.97x_1 + 8.00x_2 + -2.14x_3 - 11.72x_4 \\ Z_{12} &= \sigma(\eta_{12}) = \frac{e^{\eta_{12}}}{1 + e^{\eta_{12}}}\end{aligned}$$

¹See logistic regression.

The output

The Z values are **passed forward** to the outcome nodes. E.g., at setosa:

$$\begin{aligned}\eta_{12} &= \theta_{12}^{(0)} + \theta_{12}^{(1)} Z_{11} + \theta_{12}^{(1)} Z_{21} \\ &= -5.2 \times 10^{-4} + 5.5 \times 10^{-4} Z_{11} + 1.0 Z_{21}\end{aligned}$$

The calculation is repeated for each node giving $\eta_{12}, \eta_{22}, \eta_{32}$. Then, the value of the node is obtained applying the **softmax function**:

$$\begin{aligned}Z_{12} &= \frac{e^{\eta_{12}}}{e^{\eta_{12}} + e^{\eta_{22}} + e^{\eta_{32}}}, \\ Z_{22} &= \frac{e^{\eta_{22}}}{e^{\eta_{12}} + e^{\eta_{22}} + e^{\eta_{32}}}, \\ Z_{32} &= \frac{e^{\eta_{32}}}{e^{\eta_{12}} + e^{\eta_{22}} + e^{\eta_{32}}}.\end{aligned}$$

The prediction formula

The values at the output are the probabilities of each class predicted for the input x :

$$p_c(x; \theta) = Z_{c2}, \quad c = 1, 2, 3.$$

Indeed, the softmax function guaranties that

$$0 < Z_{c2} < 1, \quad Z_{12} + Z_{22} + Z_{32} = 1.$$

The prediction for x is the class with maximum probability:

$$f(x; \theta) = \arg \max_{c=1, \dots, C} p_c(x; \theta).$$

The regression case

For the regression, the main difference is that the output layer is made of just one node whose value is the final prediction. In the example,

$$f(x; \theta) = \theta_{12}^{(0)} + \theta_{12}^{(1)} Z_{11} + \theta_{12}^{(2)} Z_{21}$$

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Number of nodes and layers

Building a NN is kind of an art. Two important parameters are

- The number of middle layers called **hidden** layers,
- For each hidden layer, the number of nodes.

There is no general rule for this choice. One has to try and see if the quality follows.

Empirical rules are

- Hidden layers with more nodes help creating new features (new dimensions).
- Hidden layers with less nodes help combining the previous features to create strong features (dimension reduction).

Activation functions

In the example, the sigmoid function was applied at each hidden layer node. This is not the only available choice: other functions can be used. These functions are called **activation functions**.

For the hidden layers, usual choices are

- (so-called) **Linear**; meaning no function (identity).

$$g(x) = x$$

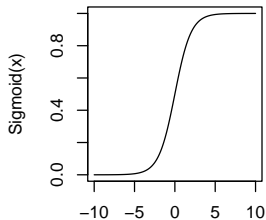
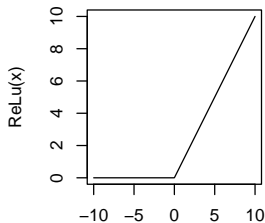
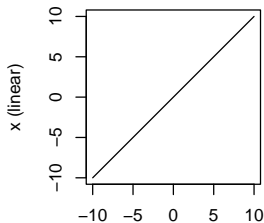
- Rectified Linear Activation **ReLU**

$$g(x) = \max(0, x)$$

- **Sigmoid**

$$g(x) = \frac{e^x}{1 + e^x} = \frac{1}{1 + e^{-x}}$$

Activation functions



Activation functions

For the output layer, choices are

- Classification: **softmax**

$$g(x_c) = \frac{e^{x_c}}{\sum_{j=1}^C e^{x_j}}.$$

- Regression: same as for hidden layers.

Activation functions

There is not a single way to choose them, but there are plenty of errors that can be avoided:

- **Use non-linearity:** using only the linear activation function in the hidden layer creates a very simple NN. In particular,
 - For regression: linear for hidden layers + linear for output layer = linear regression.
 - For binary classification: linear for hidden layers + sigmoid for the output layer = logistic regression.
- Watch the **range of the output**. E.g., if y is positive, then using a ReLu activation function close to the output may be good, whereas using a sigmoid on the output layer will prevent the NN to predict values larger than 1.
- **Mix activation functions** along the hidden layers: helps too learn non-linearities.

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Loss functions

The most common loss functions are

- For regression, the MSE

$$\bar{\mathcal{L}}(\theta) = \frac{1}{n} \sum_{i=1}^n \{y_i - f(x_i; \theta)\}^2.$$

- For classification, the cross-entropy

$$\bar{\mathcal{L}}(\theta) = - \sum_{i=1}^n \sum_{c=1}^C 1_{\{y_i=c\}} \log p_c(x_i; \theta).$$

Here, θ denotes all the NN parameters (weights).

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Gradient Descent

The training is done by minimizing $\bar{\mathcal{L}}(\theta)$, which is an intensive computation.

The most used algorithm is the **gradient descent**.

- Start at a random set of weights θ ,
- Update the weights using a descent direction (i.e., a direction guaranteeing a diminution of the loss), usually the negative gradient

$$\theta \leftarrow \theta - \eta \nabla \bar{\mathcal{L}}(\theta),$$

- Iterate until convergence.

Above, η controls the learning rate. Its choice is crucial. It varies from iterations and can be a vector, i.e., one learning rate per weight (AdaGrad, RMSProp, Adam).

Backpropagation

The computation of the gradient $\nabla \tilde{\mathcal{L}}(\theta)$ can be very heavy on a NN.

Backpropagation is a method exploiting the iterative structure of the network to compute this gradient.

Stochastic Gradient Descent

If n is large (lots of instances)

$$\nabla \bar{\mathcal{L}}(\theta) = \sum_{i=1}^n \nabla \bar{\mathcal{L}}_i(\theta)$$

is heavy to compute. It can be approximated by a partial sum over a random subset of instances $S \subseteq \{1, \dots, n\}$:

$$\nabla \bar{\mathcal{L}}(\theta) = \sum_{i=1}^n \nabla \bar{\mathcal{L}}_i(\theta) \approx \sum_{i \in S} \nabla \bar{\mathcal{L}}_i(\theta)$$

This is called **stochastic gradient descent** (SDG).

SDG: batches and epochs

For SGD, the practice is to

- Split the set $\{1, \dots, n\}$ randomly into m **batches** of the same size: b_1, \dots, b_m ,
- Apply the gradient descent update step sequentially along the batches (in a random order):

$$\theta \leftarrow \theta - \eta \sum_{i \in b_j} \nabla \bar{\mathcal{L}}_i(\theta).$$

- One pass through all the m batches, b_1, \dots, b_m , is called an **epoch**.

SDG: batches and epochs

The choice of the size of the batch is a compromise between computation time and the quality of the gradient approximation:

- A large batch size (at the limit n) makes the gradient approximation, $\sum_{i \in b} \nabla \bar{\mathcal{L}}_i(\theta)$, long to compute. However, $\sum_{i \in b} \nabla \bar{\mathcal{L}}_i(\theta)$ is an accurate approximation of $\sum_{i=1}^n \nabla \bar{\mathcal{L}}_i(\theta)$ because $b \approx \{1, \dots, n\}$.
 \Rightarrow Each epoch has few long iterations.
- A small batch size makes the gradient approximation, $\sum_{i \in b} \nabla \bar{\mathcal{L}}_i(\theta)$, fast to compute because b is small. However, $\sum_{i \in b} \nabla \bar{\mathcal{L}}_i(\theta)$ is not an accurate approximation of $\sum_{i=1}^n \nabla \bar{\mathcal{L}}_i(\theta)$.
 \Rightarrow Each epoch has a lot of short iterations.

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Interpretation

NN are not interpretable. They are large model combining variables along several non-linear activation function layers. Specific methods can be used (see later in the course).

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Model complexity

By construction NN are complex models: they have a lot of weights. E.g., even a small model with 10 features, 2 hidden layers with (16, 8) nodes, and 3 classes has

$$(10 + 1) \times 16 + (16 + 1) \times 8 + (8 + 1) \times 3 = 339$$

weights.

With such a large number of parameters, the model is at risk of overfitting the training set by learning too much. One can regularize the model in a similar way to linear and logistic regressions.

Regularization

The idea is to use L_1 and/or L_2 penalties on the loss during the training

$$\bar{\mathcal{L}}(\theta) + \lambda_1 \sum_j |\theta_j| + \lambda_2 \sum_j \theta_j^2.$$

Again there is no simple way to set the penalty parameters λ_1 and λ_2 . Note that it is possible to have different penalty parameters in different layers.