Lecture 07:
Intro a Deep Learning, Redes Neuronales

Aprendizaje y Minería de Datos para los Negocios

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Agenda

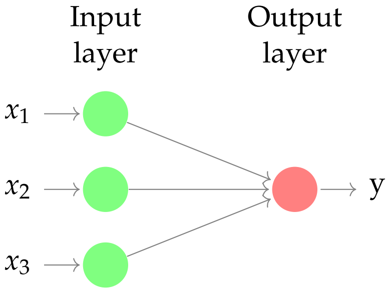
1. Recap
2. Multilayer Perceptrons
    - Worked Example
    - Minimalist Theory
        - Activation Functions
        - Output Functions
        - Architecture Design
        - Numerical Optimization Issues
3. Break
4. `R para ML`

Deep Learning: Recap

- Let's start with a familiar and simple model, the linear model

$$y = f(X) + u \tag{1}$$

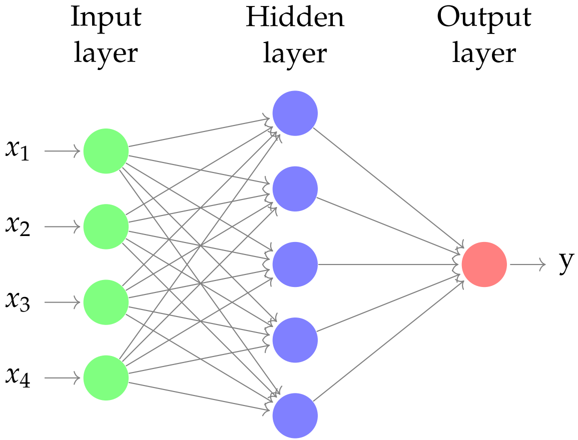
$$y = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + u$$



Multilayer Perceptrons

- Linear Models may be to simple, and miss the nonlinearities that best approximate $f^*(x)$
- We can overcome these limitations of linear models and handle a more general class of functions by incorporating one or more hidden layers.
- Deep feedforward networks, also called feedforward neural networks, or multilayer perceptrons (MLPs), are the quintessential deep learning models
- Feedforward neural networks are called networks because they are typically represented by composing together many different functions.
- The model is associated with a directed acyclic graph describing how the functions are composed together. For example, we might have two functions $f^{(2)}, f^{(1)}$ and connected in a chain to form $f(x) = f^{(2)}(f^{(1)}(x))$ and
- These chain structures are the most commonly used structures of neural networks.

Multilayer Perceptrons



Multilayer Perceptrons

- The overall length of the chain gives the depth of the model. The name “deep learning” arose from this terminology.
- The final layer of a feedforward network is called the output layer
- During neural network training, we try to train $f(x)$ to match $f^*(x)$
- In the training data we observe the first layer, inputs (x), and the last layer, output (y)
- We do not observe the intermediate layers,they are then called hidden layers.
- Finally, these networks are called neural because they are loosely inspired by neuroscience.

Worked Example: The ”Exclusive OR (XOR)” Function

- The exclusive disjunction of a pair of propositions, (p, q), is supposed to mean that p is true or q is true, but not both
- It’s truth table is:

q	p	q v p
0	0	0
0	1	1
1	0	1
1	1	0

- When exactly one of these binary values is equal to 1, the XOR function returns 1. Otherwise, it returns 0

Worked Example: The ”Exclusive OR (XOR)” Function

- Let’s use a linear model

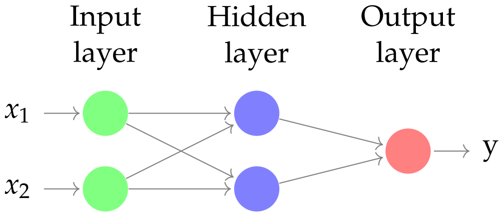
$$y = X\beta + \iota\alpha \tag{2}$$

$$y = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} X = \begin{pmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{pmatrix} \iota = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \tag{3}$$

- Solution $\alpha = \frac{1}{2}$ $\beta = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$
- Prediction $\hat{y} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$

Worked Example: The "Exclusive OR (XOR)" Function

- Let's use multilayer perceptrons (feedforward network) with one hidden layer containing two hidden units



- This network has a vector of hidden units h that are computed by a function $f^{(1)}(x; W, c)$.
- The values of these hidden units are then used as the input for a second layer.
- The second layer is the output layer of the network. The output layer is still just a linear regression model, but now it is applied to h rather than to x
- The network now contains two functions chained together, $f(x; W, c, w, b) = f^{(2)}(f^{(1)}(x))$

Worked Example: The ”Exclusive OR (XOR)” Function

- Which $f^{(1)}$ should we specify?
  - Clearly **not** linear, otherwise it would defeat the entire purpose
  - We are going to use the rectified linear unit or ReLU (it is usually the default recommendation, there are many others (more on this later))
  - ReLU is defined as $g(z) = max\{0, z\}$
- For $f^{(2)}$? For this example, a linear model will suffice

$$f^{(2)} = f^{(1)}w + b \tag{4}$$

- The final model is then

$$f(x, W, C, w, b) = max\{0, XW + c\}\, w + b \tag{5}$$

Worked Example: The ”Exclusive OR (XOR)” Function

- Suppose this is the solution to the XOR problem

$$f(x) = max\{0, XW + c\}\, w + b$$

$$W = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$c = \begin{pmatrix} 0 & -1 \\ 0 & -1 \\ 0 & -1 \\ 0 & -1 \end{pmatrix}$$

$$w = \begin{pmatrix} 1 & -2 \end{pmatrix}$$

$$b = 0$$

Worked Example: The ”Exclusive OR (XOR)” Function

- Lets work out the example step by step

$$f(x) = max\{0, XW + c\}\,w + b \tag{6}$$

$$XW = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 1 \\ 1 & 1 \\ 2 & 2 \end{pmatrix}$$

$$XW + c = \begin{pmatrix} 0 & -1 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{pmatrix}$$

$$max\{0, XW + c\} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{pmatrix}$$

Worked Example: The ”Exclusive OR (XOR)” Function

$$\hat{y} = max\{0, XW + c\}\, w + b = \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{pmatrix} \begin{pmatrix} 1 & -2 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}$$

- The neural network has obtained the correct answer for every data point

Worked Example: The ”Exclusive OR (XOR)” Function

- In this example, we simply specified the solution, then showed that it obtained zero error.
- In a real situation, there might be billions of model parameters and billions of training examples, so one cannot simply guess the solution as we did here.
- Instead, a gradient-based optimization algorithm can find parameters that produce very little error.
- The solution we described to the XOR problem is at a global minimum of the loss function, so gradient descent could converge to this point.
- There are other equivalent solutions to the XOR problem that gradient descent could also find.
- The convergence point of gradient descent depends on the initial values of the parameters.
- In practice, gradient descent would usually not find clean, easily understood, integer-valued solutions like the one we presented here.

Multilayer Perceptrons: Theory

- Why not a linear model?

$$\begin{aligned}\mathbf{H} &= \mathbf{X}\mathbf{W}^{(1)} + \mathbf{b}^{(1)} \\ \mathbf{Y} &= \mathbf{H}\mathbf{W}^{(2)} + \mathbf{b}^{(2)}\end{aligned} \tag{7}$$

- where $\mathbf{X} \in \mathbb{R}^{n \times d}$, n obs. and d inputs (features).
- H is a hidden layer with h hidden units, $\mathbf{H} \in \mathbb{R}^{n \times h}$
- Because the hidden and output layers are both fully connected, we have
  - hidden-layer weights $\mathbf{W}^{(1)} \in \mathbb{R}^{d \times h}$ and biases $\mathbf{b}^{(1)} \in \mathbb{R}^{1 \times h}$
  - output-layer weights $\mathbf{W}^{(2)} \in \mathbb{R}^{h \times q}$ and biases $\mathbf{b}^{(2)} \in \mathbb{R}^{1 \times q}$

Multilayer Perceptrons: Theory

- Why not a linear model?
- Note that after adding the linear hidden layer , we gain nothing for our troubles!

$$\begin{aligned} \mathbf{Y} &= (\mathbf{X}\mathbf{W}^{(1)} + \mathbf{b}^{(1)})\mathbf{W}^{(2)} + \mathbf{b}^{(2)} \\ &= \mathbf{X}\mathbf{W}^{(1)}\mathbf{W}^{(2)} + \mathbf{b}^{(1)}\mathbf{W}^{(2)} + \mathbf{b}^{(2)} \\ &= \mathbf{X}\mathbf{W} + \mathbf{b}. \end{aligned} \tag{8}$$

Multilayer Perceptrons: Theory

- The gain comes from using nonlinear activation function σ
- Note that, with activation functions in place, it is no longer possible to collapse our MLP into a linear model:

$$\begin{aligned} \mathbf{H} &= \sigma(\mathbf{X}\mathbf{W}^{(1)} + \mathbf{b}^{(1)}), \\ \mathbf{Y} &= \mathbf{H}\mathbf{W}^{(2)} + \mathbf{b}^{(2)}. \end{aligned} \tag{9}$$

- Note that we can build more general MLPs, by stacking hidden layers, yielding ever more expressive models.

$$\begin{aligned} \mathbf{H}^{(1)} &= \sigma_1(\mathbf{X}\mathbf{W}^{(1)} + \mathbf{b}^{(1)}) \\ \mathbf{H}^{(2)} &= \sigma_2(\mathbf{H}^{(1)}\mathbf{W}^{(2)} + \mathbf{b}^{(2)}) \\ \mathbf{Y} &= \mathbf{H}^2\mathbf{W}^{(3)} + \mathbf{b}^{(3)}. \end{aligned} \tag{10}$$

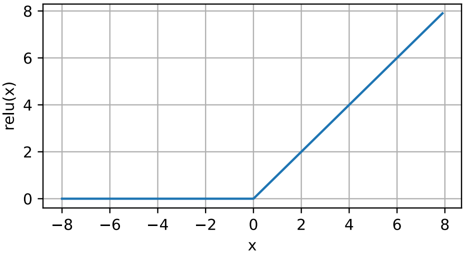
Activation Functions

- Activation functions are fundamental to deep learning, let us briefly survey some common activation functions.
- ReLU Function
  - The most popular choice, due to both simplicity of implementation and its good performance on a variety of predictive tasks, is the rectified linear unit (ReLU).
  - ReLU provides a very simple nonlinear transformation. Given an element x, the function is defined as the maximum of that element and 0:

$$\mathrm{ReLU}(x) = \max\{x, 0\}.$$

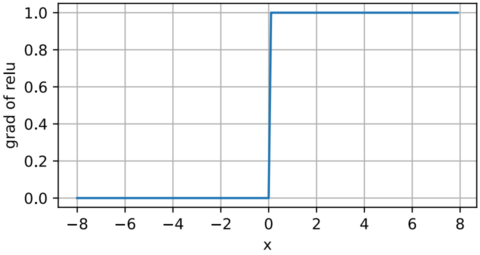
Activation Functions

- ReLU function retains only positive elements and discards all negative elements by setting the corresponding activations to 0.
- It is piecewise linear.



Activation Functions

- Part of the appeal of ReLU has to do with it's well behaved derivative
  - Note that the ReLU function is not differentiable when the input takes value precisely equal to 0. In these cases, we default to the left-hand-side derivative and say that the derivative is 0 when the input is 0. (we may even get away with this because the input may never actually be zero!)
  - This makes optimization better behaved and it mitigates the problem of vanishing gradients



Activation Functions

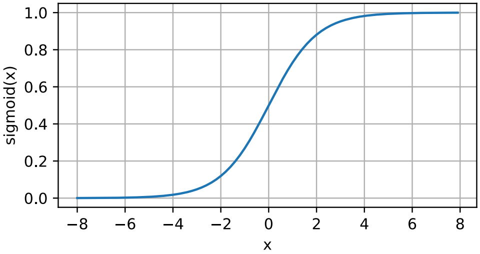
- Sigmoid Function
  - The sigmoid function transforms its inputs, for which values lie in the domain $\mathbb{R}$, to outputs that lie on the interval (0, 1).
  - For that reason, the sigmoid is often called a squashing function: it squashes any input in the range (-inf, inf) to some value in the range (0, 1):

$$\text{sigmoid}(x) = \frac{1}{1 + \exp(-x)}.$$

  - In the earliest neural networks, scientists were interested in modeling biological neurons which either fire or do not fire. Thus the pioneers of this field, going all the way back to McCulloch and Pitts, the inventors of the artificial neuron, focused on thresholding units. A thresholding activation takes value 0 when its input is below some threshold and value 1 when the input exceeds the threshold.
  - When attention shifted to gradient based learning, the sigmoid function was a natural choice because it is a smooth, differentiable approximation to a thresholding unit.

Activation Functions

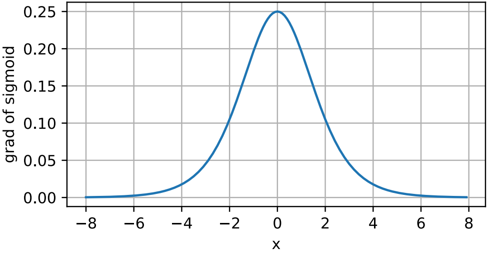
- Sigmoid Function



Activation Functions

- The derivative of the sigmoid function is given by the following equation:

$$\frac{d}{dx}\,\text{sigmoid}(x) = \frac{\exp(-x)}{(1+\exp(-x))^2} = \text{sigmoid}(x)\,(1-\text{sigmoid}(x))\,.$$

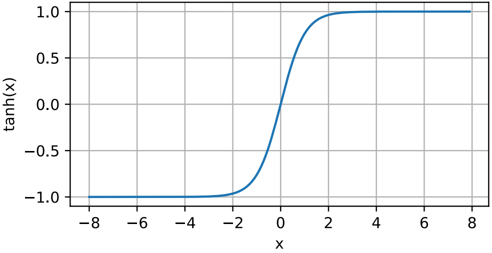


Activation Functions

- *Tanh* Function
  - Like the sigmoid function, the tanh (hyperbolic tangent) function also squashes its inputs, transforming them into elements on the interval between -1 and 1:

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

  - Although the shape of the function is similar to that of the sigmoid function, the *tanh* function exhibits point symmetry about the origin of the coordinate system.

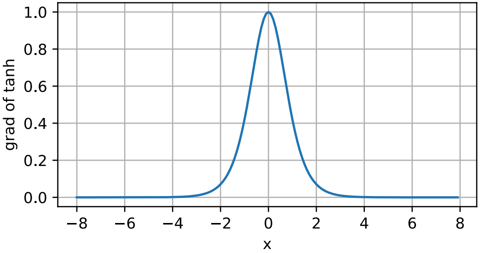


Activation Functions

- The derivative of the *tanh* function is:

$$\frac{d}{dx}\tanh(x) = 1 - \tanh^2(x).$$

- The derivative of *tanh* function is plotted below. As the input nears 0, the derivative of the *tanh* function approaches a maximum of 1. And as we saw with the sigmoid function, as the input moves away from 0 in either direction, the derivative of the *tanh* function approaches 0.



Activation Functions

- Other Activation functions
  - $h = cos(Wx + b)$ Goodfellow et all (2016) claim that on the MNIST dataset they obtained an error rate of less than 1 percent
  - Radial basis function (RBF): $exp\left(\frac{1}{\sigma^2)}||W - x||^2\right)$
  - Softplus: $log(1 + e^x)$
  - Hard tanh: $max(-1, min(1, x))$
- Hidden unit design remains an active area of research, and many useful hidden unit types remain to be discovered

Output Functions

- The choice of cost function is tightly coupled with the choice of output unit.
- Most of the time, we simply use the distance between the data distribution and the model distribution.
  - Linear $y = W'h + b \rightarrow \mathbb{R}$
  - Sigmoid (Logistic)$\frac{1}{1+\exp(-x)}$ $\rightarrow$ classification $\{0, 1\}$
  - Softmax $\frac{exp(x)}{\sum exp(x))}$ $\rightarrow$ classification multiple categories

Architecture Design

- Another key design consideration for neural networks is determining the architecture.
- The word architecture refers to the overall structure of the network: how many units it should have and how these units should be connected to each other.
- In these chain-based architectures, the main architectural considerations are choosing the depth of the network and the width of each layer.
- A multilayer perceptron (feedforward networks) with hidden layers provide a universal approximation framework.
  - The universal approximation theorem (Hornik et al., 1989; Cybenko, 1989) states that a feedforward network with a linear output layer and at least one hidden layer with any "squashing" activation function (such as the logistic sigmoid activation function) can approximate any Borel measurable function from one finite-dimensional space to another with any desired nonzero amount of error, provided that the network is given enough hidden unit.
  - The derivatives of the feedforward network can also approximate the derivatives of the function arbitrarily well (Hornik et al., 1990).

Architecture Design

- The universal approximation theorem means that regardless of what function we are trying to learn, we know that a large MLP will be able to represent this function.
- We are not guaranteed, however, that the training algorithm will be able to learn that function. Even if the MLP is able to represent the function, learning can fail for two different reasons.
    1. The optimization algorithm used for training may not be able to find the value of the parameters that corresponds to the desired function.
    2. The training algorithm might choose the wrong function as a result of overfitting
- A feedforward network with a single layer is sufficient to represent any function, but the layer may be infeasible large and may fail to learn and generalize correctly.
- In many circumstances, using deeper models can reduce the number of units required to represent the desired function and can reduce the amount of generalization error.
- The ideal network architecture for a task must be found via experimentation guided by monitoring the validation set error

Numerical Stability and Initialization

- Vanishing and exploding gradients are common issues in deep networks. Great care in parameter initialization is required to ensure that gradients and parameters remain well controlled.
- Initialization heuristics are needed to ensure that the initial gradients are neither too large nor too small.
- ReLU activation functions mitigate the vanishing gradient problem. This can accelerate convergence.
- Random initialization is key to ensure that symmetry is broken before optimization

Volvemos en 15 mins con R

R para ML

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