Statistical Learning for Public Policy

Introduction to Neural Networks

Stephen Hansen
University College London

Reading:
[Chollet, 2021], Chapters 2/4; [James et al., 2023], Chapter 10.

Introduction

Neural network models have driven many of the important breakthroughs in machine learning and AI over the last ten years.

They were already well-known and popular in the 1990s.

Several interrelated drivers of their recent growth:

1. Availability of large datasets for training
2. Hardware advances: GPU/TPU, cloud infrastructure
3. Software advances: high-level frameworks for model estimation that hide many details from the user
4. Algorithmic advances: efficient gradient computation

In this lecture, we describe the structure of the simplest class of neural networks: feed-forward neural networks.

Basic Architecture of a Neural Network

A neuron

As usual, suppose that each data observation i has J associated covariates which we stack in $\mathbf{x}_i$.

As in linear regression, we can linearly combine covariates and add a constant:

$$z_i = \theta_0 + \sum_{j=1}^{J} \theta_j x_{i,j}.$$

In neural network jargon, the $\{\theta_j\}_{j=1}^{J}$ terms are sometimes called *weights* and θ_0 is called a *bias*.

We can transform the linear combination via an *activation function* ϕ.

Activation Functions

Traditionally:

1. A sigmoid function (logistic regression):

$$\phi(z_i) = \frac{1}{1 + e^{-z_i}}$$

2. A particular limiting case: step function.
3. Hyperbolic tangent.
4. Identity function (linear regression): $\phi(z_i) = z_i$.

Other activation functions have gained popularity recently:

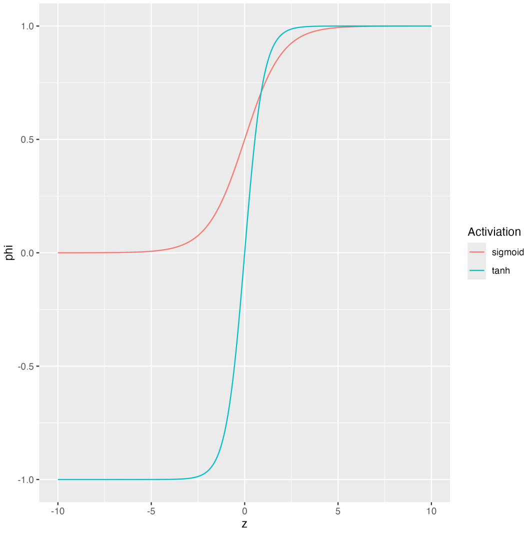
1. Rectified linear unit (ReLU):

$$\phi(z_i) = max(0, z_i)$$

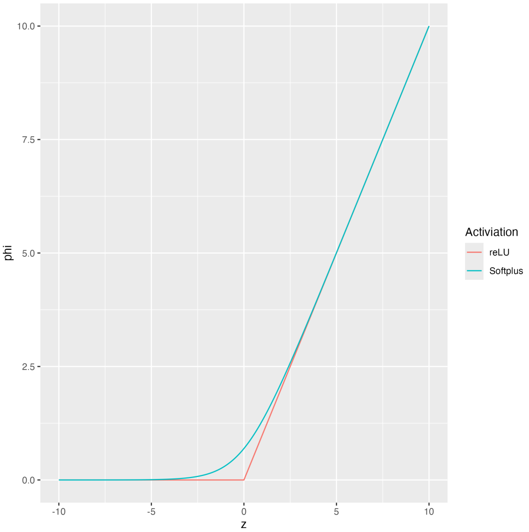
2. Softplus:

$$\phi(z_i) = log(1 + e^{z_i})$$

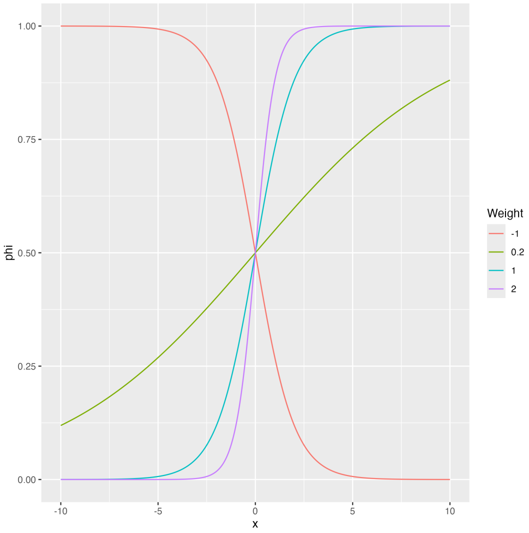
Activation Function Plots I



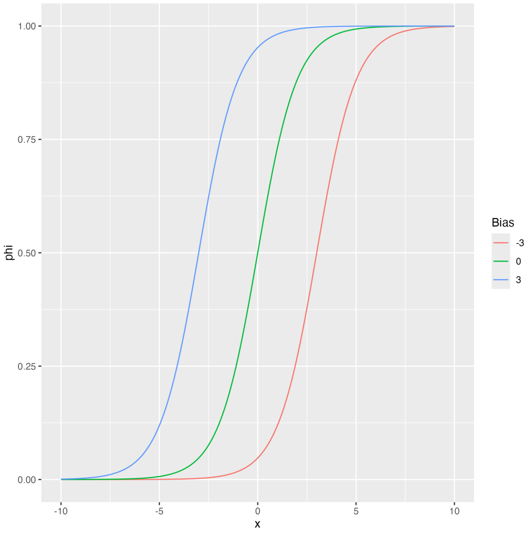
Activation Function Plots II



Effect of Varying Weight (Sigmoid)



Effect of Varying Bias (Sigmoid)



Combining Neurons into a Neural Network

Now suppose we have K separate activation functions operating over the same input $\mathbf{x}_i$.

We first obtain K separate linear combinations of covariates

$$z_{i,k} = \theta_{0,k} + \sum_{j=1}^{J} \theta_{j,k} x_{i,j} \quad \forall k = 1, \ldots, K \qquad \text{(Hidden Layer)}$$

Next we linearly combine each separate neuron to create a final output

$$f(\mathbf{x}_i \mid \boldsymbol{\theta}) = \theta_0 + \sum_{k} \theta_k \phi(z_{i,k}) \qquad \text{(Output Layer)}$$

This is known as a single layer network.

Consists of K non-linear transformations of linear combinations of input variables.

Classic Result I

Result

Universal approximation theorem: [Hornik et al., 1989] A neural network with at least one hidden layer can approximate any Borel measurable function mapping finite-dimensional spaces to any desired degree of accuracy.

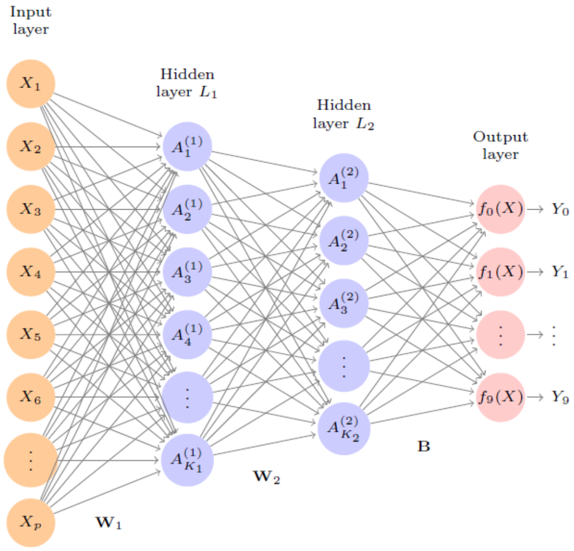
Adding Layers

Additional layers can easily be added as follows:

$$
\begin{aligned}
z_{i,k}^{(1)} &= \theta_{0,k}^{(1)} + \sum_{j=1}^{J} \theta_{j,k}^{(1)} x_{i,j} \qquad k = 1, \ldots, K_1 && \text{(Hidden Layer 1)} \\
z_{i,k}^{(2)} &= \theta_{0,k}^{(2)} + \sum_{k'=1}^{K_1} \theta_{k',k}^{(2)} \phi\left(z_{i,k'}^{(1)}\right) \quad k = 1, \ldots, K_2 && \text{(Hidden Layer 2)} \\
z_{i,k}^{(3)} &= \theta_{0,k}^{(3)} + \sum_{k'=1}^{K_2} \theta_{k',k}^{(3)} \phi\left(z_{i,k'}^{(2)}\right) \quad k = 1, \ldots, K_3 && \text{(Hidden Layer 3)} \\
&\ldots \\
f_m(\mathbf{x_i} \mid \boldsymbol{\theta}) &= \theta_{0,m}^{(L+1)} + \sum_{k'=1}^{K_{L-1}} \theta_{k',m}^{(L+1)} \phi\left(z_{i,k'}^{(L)}\right) \; m = 1, \ldots, M && \text{(Output Layer)}
\end{aligned}
$$

Overall structure is called a *feed-forward neural network*.

Graphical Representation



Feed-Forward Networks

Multiple layers allow for complex downstream structures to develop by combining simpler upstream structures.

Typical to have $K_l < K_{l-1}$, e.g. fewer units as we move along network.

Output layer can generate class probabilities via the softmax function:

$$P_m(\mathbf{x_i} \mid \boldsymbol{\theta}) = \frac{\exp(f_m)}{\sum_{m=1}^{M} \exp(f_m)}$$

where M is the number of classes to predict.

Estimation

Objective Function

The first step in estimating a neural network is to define an objective (loss) function to target of the form $L(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N} L'(y_i, f(\mathbf{x_i} \mid \boldsymbol{\theta}))$.

Typical choices:

1. Continuous, scalar y_i: $-(y_i - f(\mathbf{x_i} \mid \boldsymbol{\theta}))^2$
2. Categorical y_i: $-\sum_{m=1}^{M} y_i \log\left(P_m(\mathbf{x_i} \mid \boldsymbol{\theta})\right)$

Idea of gradient descent algorithm:

1. Randomly initialize $\boldsymbol{\theta} = \boldsymbol{\theta}^0$.
2. For all $i = 1, \ldots, I$: update $\boldsymbol{\theta}^i = \boldsymbol{\theta}^{i-1} - r\nabla L\left(\boldsymbol{\theta}^{i-1}\right)$.

r is the *learning rate* and is set to small number.

Stochastic Gradient Descent

For large datasets, computing the gradient over all data points is expensive.

Stochastic gradient descent forms an unbiased estimate of the gradient by randomly sampling a data point.

Mini-batch stochastic gradient descent instead uses a random draw of N_B data points where N_B is the *batch size*.

In practice, data is often randomly shuffled once and then cycled through N_B-sized-chunk-by-N_B-sized-chunk.

An *epoch* is a single pass through all of the training data.

Gradient Computation

Analytically deriving the gradient is in most cases straightforward and involves repeated application of the chain rule.

Efficiently evaluating the gradient on a computer requires some care and is typically done via *backpropagation* which avoids repeated evaluation of the same expression.

The combination of efficient gradient computation with modern hardware (GPU/TPU) allows for the estimation of large models.

Regularization

As with other machine learning algorithms, overfitting can be controlled via regularization.

The first approach is to add a ridge (or LASSO) penalty to the loss function which adds minimal computational overhead.

The second is *dropout* whereby a random fraction of nodes is left out of the network when it is being trained.

There is also a large number of parameters to tune in a network which can contribute substantially to performance.

Conclusion

Conclusion

Neural networks, in particular those with many layers, have generated important recent advances in machine learning.

They reach their full potential when trained on enormous datasets and powerful modern hardware.

Not clear that these conditions hold in many applied problems relevant for economics and social science.

Neural networks also require more fine-tuning than more “off-the-shelf” regression models.

One domain in which they are clearly valuable is modeling unstructured data, which we cover next.

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