S&DS 265 / 565

Introductory Machine Learning

Neural Networks (continued)

November 15

Yale

Reminders

- Quiz 5 this Thursday, November 17: Topic models, neural nets
- Assn 5 is out; start early! Due Dec. 1

Last time

- Basic architecture of feeforward neural nets
- Biological analogy and inspiration
- Backpropagation — high level

Today

- Examples: Regression, Tensorflow
- Backpropagation — more detail
- Examples: Classification

Starting with regression

For linear regression, our loss function for an example (x, y) is

$$\begin{aligned}\mathcal{L} &= \frac{1}{2}(y - \beta^T x - \beta_0)^2 \\ &= \frac{1}{2}(y - f)^2\end{aligned}$$

where $f(x) = \beta^T x + \beta_0$.

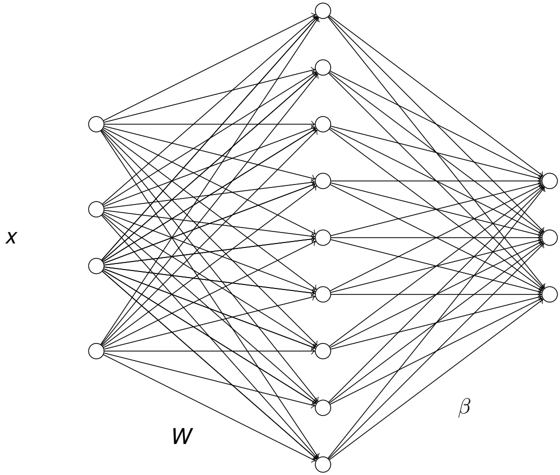
Adding a layer

Loss is

$$\mathcal{L} = \frac{1}{2}(y - f(x))^2$$

where now $f(x) = \beta^T h(x) + \beta_0$ where $h(x) = Wx + b$.

This can be viewed graphically.


x
W
β

Equivalent to linear model

But this is just a linear model

$$f = \widetilde{\beta}^T x + \widetilde{\beta}_0$$

We get a reparameterization of a linear model; nothing new.

Need to add *nonlinearities*

Nonlinearities

Add nonlinearity

$$h = \varphi(Wx + b)$$

fixed and *applied component-wise*

Typically the last layer is just linear (for both classification and regression):

$$f = \beta^T h + \beta_0$$

Nonlinearities

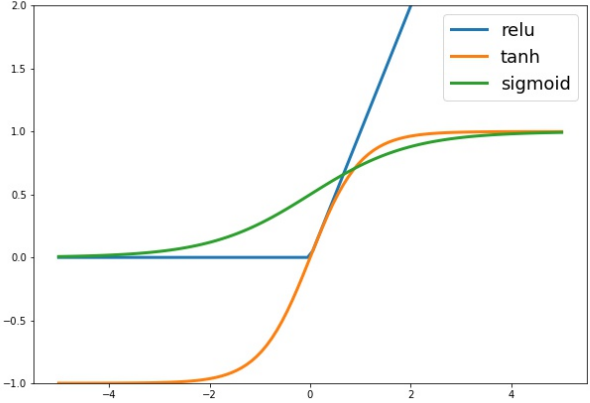
Commonly used nonlinearities:

$$\varphi(u) = \tanh(u) = \frac{e^u - e^{-u}}{e^u + e^{-u}}$$

$$\varphi(u) = \mathrm{sigmoid}(u) = \frac{1}{1 + e^{-u}}$$

$$\varphi(u) = \mathrm{relu}(u) = \max(u, 0)$$

Nonlinearities

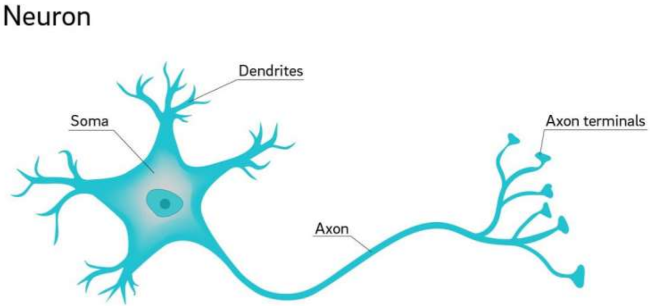


Nonlinearities

So, a neural network is nothing more than a parametric regression model with a restricted type of nonlinearity

Why are they called neural networks?

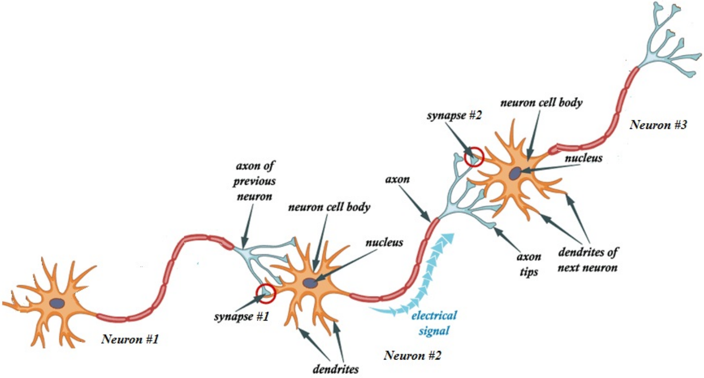
Biological Analogy

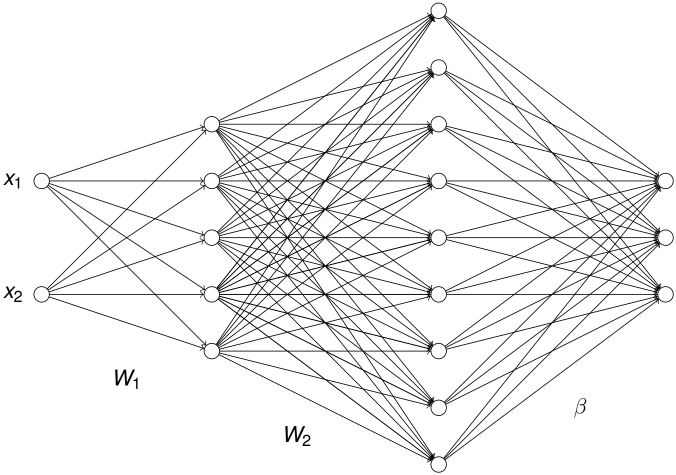


Biological Analogy

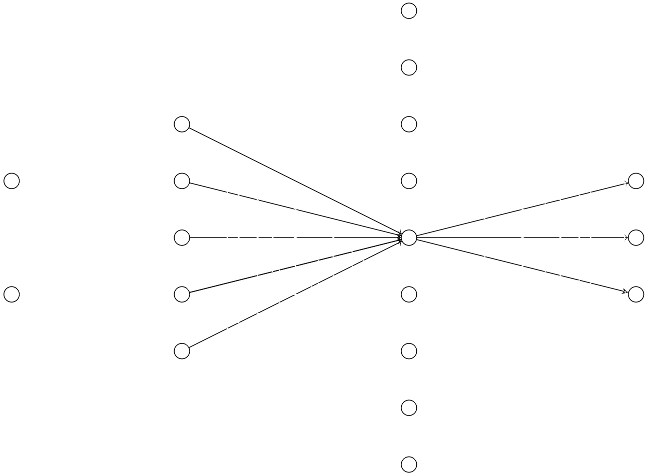
- The dendrites play the role of inputs, collecting signals from other neurons and transmitting them to the soma, which is the “central processing unit.”
- If the total input arriving at the soma reaches a threshold, an output is generated.
- The axon is the output device, which transmits the output signal to the dendrites of other neurons.

Biological Analogy





x_1
x_2
W_1
W_2
β



Sanity check

Let's work through a toy example to be sure we understand the "mechanics" of the neural net

2-dimensional inputs $x = (x_1, x_2)^T$ and a binary classification

We have 2-layer neural net with three hidden neurons

$$h(x) = \varphi\left(Wx + b\right)$$
$$\beta^T h(x) = \log\left(\frac{p(Y = 1 \mid x)}{p(Y = 0 \mid x)}\right)$$

with $\varphi(u) = relu(u) = \max(u, 0)$

Sanity check

Let's work through a toy example to be sure we understand the "mechanics" of the neural net

2-dimensional inputs $x = (x_1, x_2)^T$ and a binary classification

Suppose that the parameters (weights) of the network are

$$b = (1, 0, -1)^T$$
$$W = \begin{pmatrix} 1 & -1 \\ -2 & 1 \\ 0 & 1 \end{pmatrix}$$
$$\beta = (1, 2, -1)^T$$

What is the prediction of the network if $x = (1, -1)^T$ or $x = (-1, 1)^T$?

Sanity check

Let's work through a toy example to be sure we understand the "mechanics" of the neural net

2-dimensional inputs $x = (x_1, x_2)^T$ and a binary classification

Suppose that the parameters (weights) of the network are

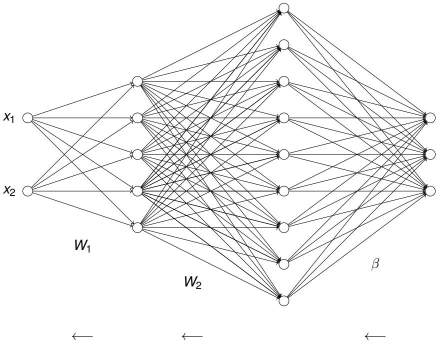
$$b = (1, 0, -1)^T$$
$$W = \begin{pmatrix} 1 & -1 \\ -2 & 1 \\ 0 & 1 \end{pmatrix}$$
$$\beta = (1, 2, -1)^T$$

How do the predictions change if $\varphi = \tanh$?

Training

- The parameters are trained by stochastic gradient descent.
- To calculate derivatives we just use the chain rule, working our way backwards from the last layer to the first.

High level idea



Start at last layer, send error information back to previous layers

Start simple

Loss is

$$\mathcal{L} = \frac{1}{2}(y - f)^2$$

The change in loss due to making a small change in output f is

$$\frac{\partial \mathcal{L}}{\partial f} = (f - y)$$

We now send this backward through the network

Start simple

Loss is

$$\mathcal{L} = \frac{1}{2}(y - f)^2$$

Now suppose that $f = ab$:

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial a} &= \frac{\partial \mathcal{L}}{\partial f} \frac{\partial f}{\partial a} \\ &= \frac{\partial \mathcal{L}}{\partial f} \cdot b \\ &= (f - y) \cdot b \end{aligned}$$

Start simple

Loss is

$$\mathcal{L} = \frac{1}{2}(y - f)^2$$

Now suppose that $f = ab$:

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial b} &= \frac{\partial f}{\partial b}\frac{\partial \mathcal{L}}{\partial f} \\ &= a \cdot \frac{\partial \mathcal{L}}{\partial f} \\ &= a \cdot (f - y) \end{aligned}$$

Fancy verison

We need a matrix version of this. If $A = BC$, then

$$\frac{\partial \mathcal{L}}{\partial B} = \frac{\partial \mathcal{L}}{\partial A} C^T$$

$$\frac{\partial \mathcal{L}}{\partial C} = B^T \frac{\partial \mathcal{L}}{\partial A}$$

Check that the dimensions match up!

Example

So if $f = Wx + b$ then

$$\frac{\partial \mathcal{L}}{\partial W} = \frac{\partial \mathcal{L}}{\partial f} \; x^T$$

$$= (f - y) \; x^T$$

Example

So if $f = Wx + b$ then

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{\partial \mathcal{L}}{\partial f}$$
$$= (f - y)$$

Two layers

Now add a layer:

$$
\begin{aligned}
f &= W_2 h + b_2 \\
h &= W_1 x + b_1
\end{aligned}
$$

Then we have

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial W_2} &= \frac{\partial \mathcal{L}}{\partial f}\ h^T \\
&= (f - y)\ h^T
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial h} &= W_2^T\ \frac{\partial \mathcal{L}}{\partial f} \\
&= W_2^T\ (f - y)
\end{aligned}
$$

Two layers

Now send this back (backpropagate) to the first layer:

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial W_1} &= \frac{\partial \mathcal{L}}{\partial h}\, x^T \\ &= W_2^T\, \frac{\partial \mathcal{L}}{\partial f}\, x^T \\ &= W_2^T\, (f - y)\, x^T\end{aligned}$$

Adding a nonlinearity

Remember, this just gives a linear model! Need a nonlinearity:

$$h = \varphi(W_1 x + b_1)$$

$$f = W_1 h + b_2$$

Adding a nonlinearity

If $\varphi(u) = \mathit{relu}(u) = \max(u, 0)$ then this just becomes

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial W_1} &= \mathbb{1}(h > 0)\ \frac{\partial \mathcal{L}}{\partial h}\ x^T \\ &= \mathbb{1}(h > 0)\ W_2^T\ \frac{\partial \mathcal{L}}{\partial f}\ x^T \\ &= \mathbb{1}(h > 0)\ W_2^T\ (f - y)\ x^T\end{aligned}$$

where

$$\mathbb{1}(u) = \begin{cases} 1 & u > 0 \\ 0 & \text{otherwise} \end{cases}$$

See notes on backpropagation for details

Classification

For classification we use softmax to compute probabilities

$$(p_1, p_2, p_3) = \frac{1}{e^{f_1} + e^{f_2} + e^{f_3}} \left(e^{f_1}, e^{f_2}, e^{f_3} \right)$$

The loss function is

$$\mathcal{L} = -\log P(y \mid x) = \log \left(e^{f_1} + e^{f_2} + e^{f_3} \right) - f_y$$

So, we have

$$\frac{\partial \mathcal{L}}{\partial f_k} = p_k - \mathbb{1}(y = k)$$

Examples

Let’s go to the notebooks!

np-complete demo

Minimal neural network implementation

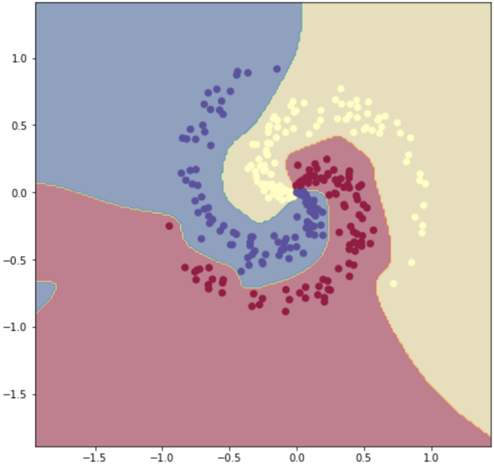
This is a "bare bones" implementation of a 2-layer neural network for classification, using rectified linear units as activation functions. The code is from Andrej Karpathy; please see [this page] for an annotated description of the code.

In assignment 7 you will extend this and experiment with some different settings of the parameters.

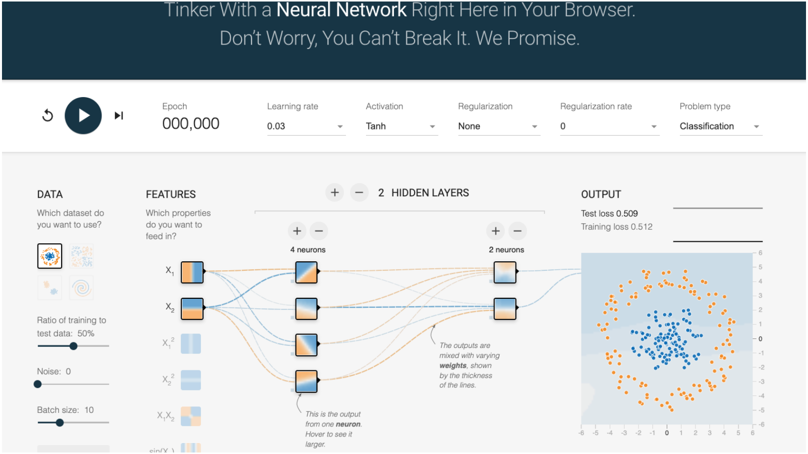
```
import numpy as np
import matplotlib.pyplot as plt

%matplotlib inline
plt.rcParams['figure.figsize'] = (10.0, 8.0) # set default size of plots
plt.rcParams['image.interpolation'] = 'nearest'
plt.rcParams['image.cmap'] = 'gray'
plt.rcParams['axes.facecolor'] = 'lightgray'
```

np-complete demo



playground.tensorflow.org



Summary

- In neural networks, “features” are linear operations followed by an activation function
- Based on a crude analogy with neurons in biological brains
- Neurons are deterministic functions of input; not latent variables
- A special type of (parametric) nonlinear regression model
- Trained using stochastic gradient descent
- Backpropagation is just the chain rule from calculus
- Applied iteratively from the last layer forwards