S&DS 265 / 565

Introductory Machine Learning

Neural Networks (continued)

Tuesday, November 16

Yale

Reminders

- Quiz 3 available at noon today: LMs, embeddings, Bayes, TMs
- Assn 6 posted; start early! Due Nov. 30

Last time

- Basic architecture of feeforward neural nets
- Biological analogy and inspiration
- Backpropagation — high level
- Examples: Regression, Tensorflow

Today

- Backpropagation — more detail
- Examples: Classification

Nonlinearities

Add nonlinearity

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

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:

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

$$\phi(u) = \text{sigmoid}(u) = \frac{e^u}{1 + e^u}$$

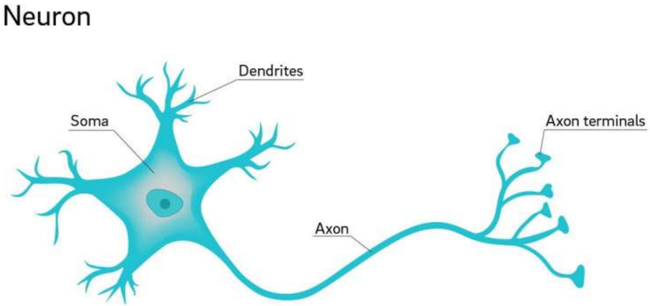
$$\phi(u) = \text{relu}(u) = \max(u, 0)$$

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?

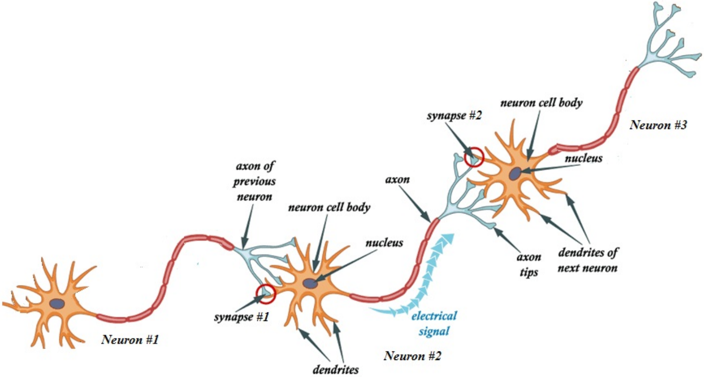
Biological Analogy

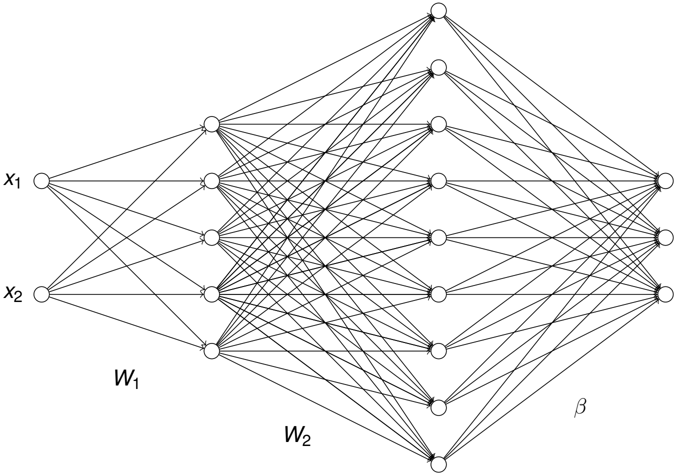


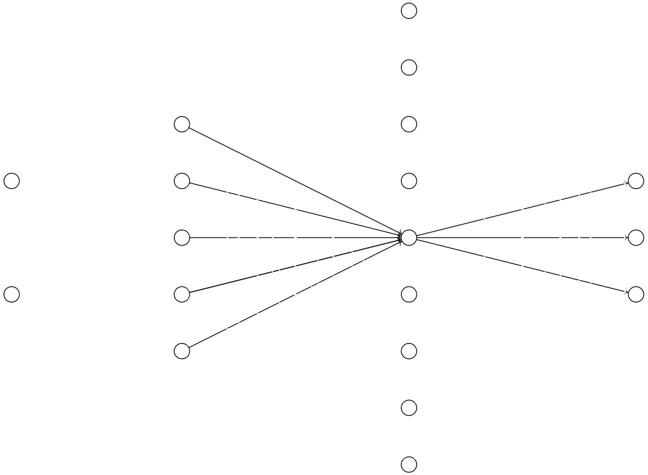
Biological Analogy

- 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



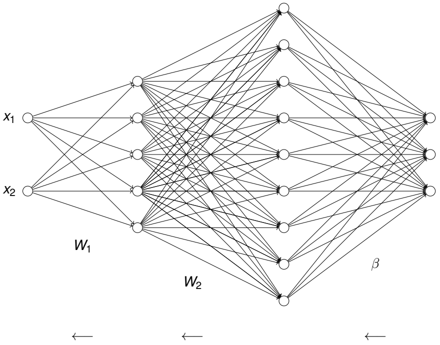

x_1
x_2
W_1
W_2
β



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

$$\frac{\partial \mathcal{L}}{\partial W} = \frac{\partial \mathcal{L}}{\partial f}\, x^T$$
$$= (f - y)\, x^T$$

Recall last problem on the midterm...

Example

So if $f = Wx + b$ then

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

Recall last problem on the midterm...

Two layers

Now add a layer:

$$f = W_2 h + b_2$$
$$h = W_1 x + b_1$$

Then we have

$$\frac{\partial \mathcal{L}}{\partial W_2} = \frac{\partial \mathcal{L}}{\partial f} \; h^T$$
$$= (f - y) \; h^T$$

$$\frac{\partial \mathcal{L}}{\partial h} = W_2^T \; \frac{\partial \mathcal{L}}{\partial f}$$
$$= W_2^T \; (f - y)$$

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 $\varphi(u) = ReLU(u) = \max(u, 0)$ 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

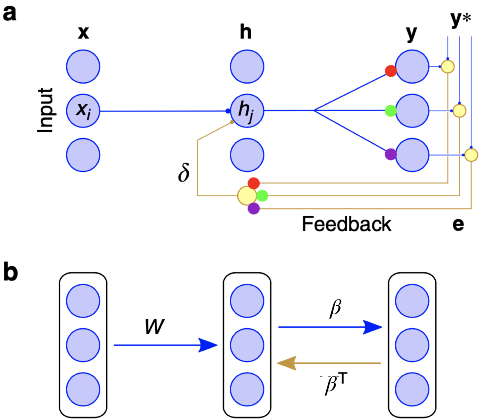
$$\frac{\partial \mathcal{L}}{\partial f_k} = p_k - \mathbb{1}(y = k)$$

Further reading: http://neuralnetworksanddeeplearning.com/ Disclaimer, I haven't "vetted" this online book.

Examples

Let's go to the notebooks!

Proposal from DeepMind



Lillicrap et al., Nature Comm. (2016), Bartunov et al., (2018), Lillicrap et al, "Backpropagation and the brain," Nature Reviews, Neuroscience (2020).

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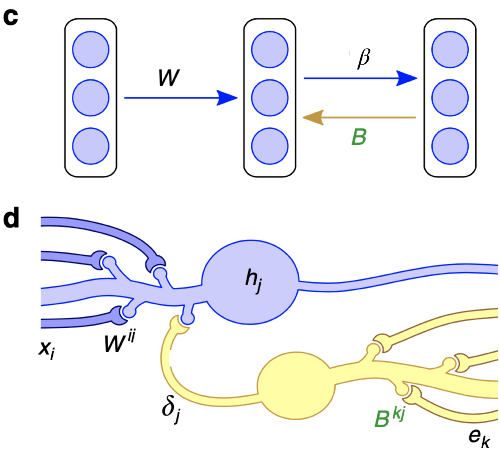

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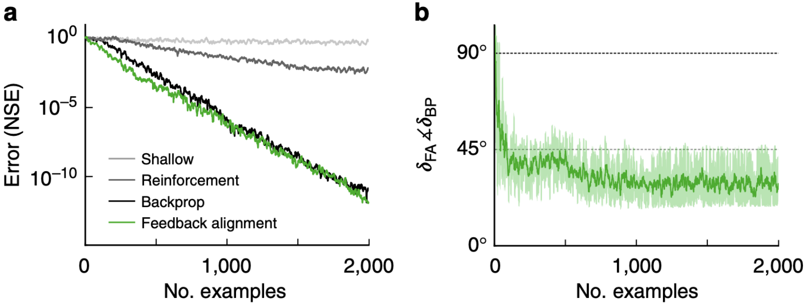

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Feedback alignment

We have recently shown that this converges:
`https://arxiv.org/abs/2106.06044`

Summary

- Neural nets are trained using stochastic gradient descent
- Implemented using backpropagation
- Can be automated to train complex networks (with no math!)