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.

For regression, the last layer is just linear:

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

Nonlinearities

Commonly used nonlinearities:

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

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

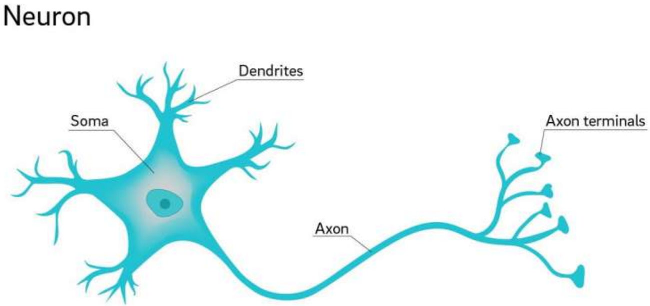
$$\phi(u) = \text{relu}(u) = \max(u, 0)$$

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?

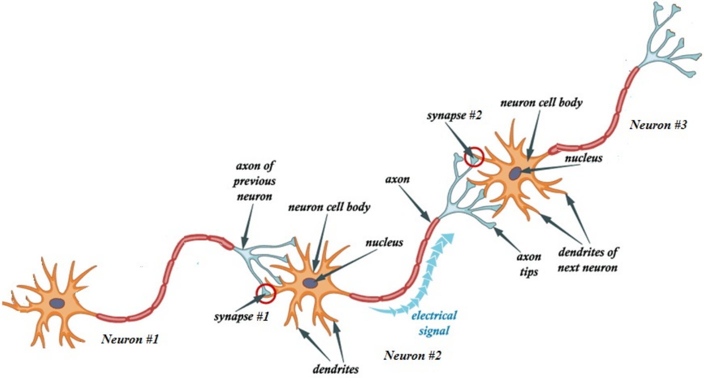
Biological Analogy

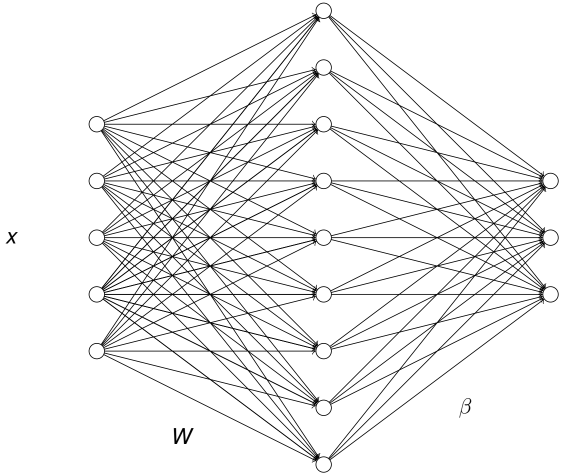


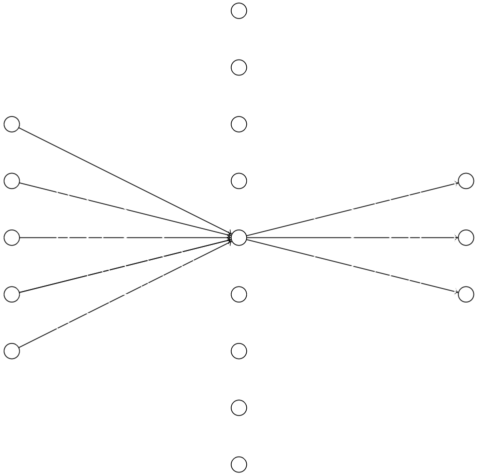
Biological Analogy

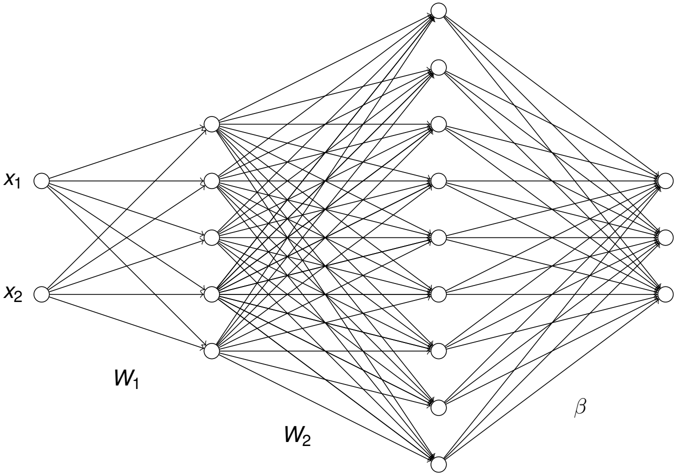
- The dendrites play the role of inputs, collecting signals from other neurons and transmitting them to the soma, which is the “central processing unit.”
- If the total input arriving at the soma reaches a threshold, an output is generated.
- The axon is the output device, which transmits the output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

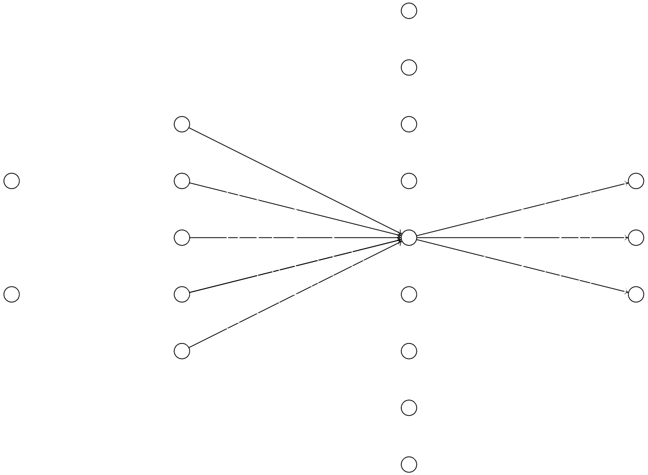
Biological Analogy




x
W
β




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.

Training

- For the last layer, $\mathcal{L} = \frac{1}{2}(y - f)^2$ and

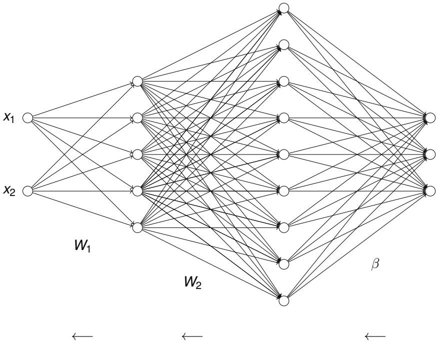
$$\frac{\partial \mathcal{L}}{\partial f} = -(y - f)$$

- Next, we compute

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

We'll go further today

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

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

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

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

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

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

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

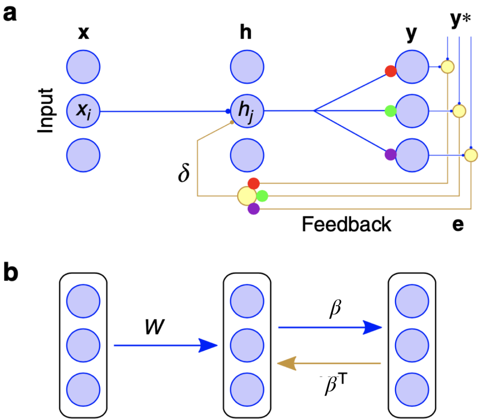
So, we have

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

Examples

Let's go to the notebooks!

Proposal from DeepMind



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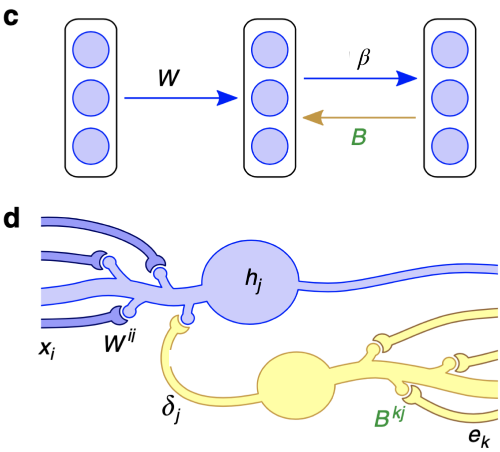

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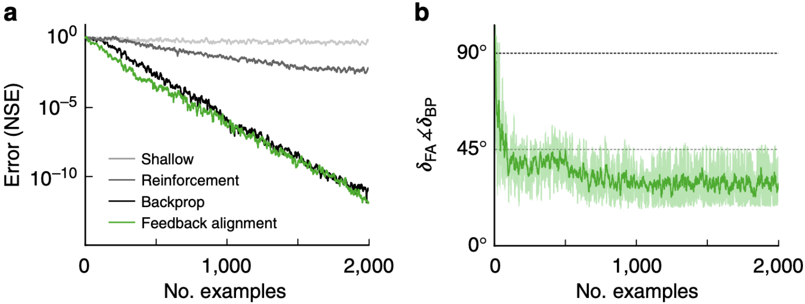

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Feedback alignment

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!)