EMAT31530, Part 4: Neural Networks

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Most of the content this week is in the Colab notebooks. But there's a few pages here introducing neural networks.

So far, we have worked with linear functions, of the form,

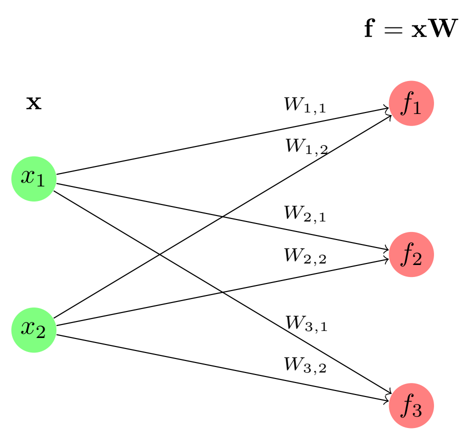
$$\mathbf{f}(\mathbf{x}) = \mathbf{x}\mathbf{W}. \tag{1}$$

And we used this function as the prediction in linear regression (with a squared error loss function), or as the logits in classification (with a maximum-likelihood objective / cross-entropy loss function).

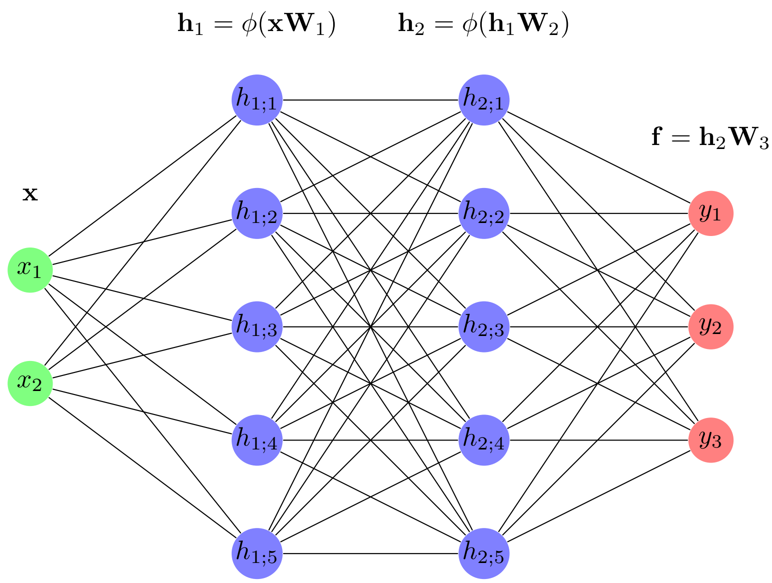
But we can use *any* function here. So what function should we use? Well, there's a few requirements.

- lots of parameters (so we have lots of knobs to twiddle to improve the function).
- doesn't reduce to something simpler.
- fast (e.g. uses matmuls).

We can draw the current setup as,



Now, one way to get a more interesting function is to stack multiple layers (i.e. connect the outputs of one linear layer to the inputs of another layer):



Note that we have included an "nonlinearity", ϕ. This nonlinearity is necessary, because without it (or if we set $\phi(\mathbf{h}) = \mathbf{h}$), we end up with,

$$\mathbf{h}_1 = \mathbf{x}\mathbf{W}_1 \tag{2a}$$
$$\mathbf{h}_2 = \mathbf{h}_1\mathbf{W}_2 \tag{2b}$$
$$\mathbf{f} = \mathbf{h}_2\mathbf{W}_3 \tag{2c}$$

If we substitute $\mathbf{h}_1$ into the expression for $\mathbf{h}_2$, and $\mathbf{h}_2$ into the expression for $\mathbf{f}$, we end up with,

$$\mathbf{f} = \mathbf{x}\underbrace{\mathbf{W}_1\mathbf{W}_2\mathbf{W}_3}_{=\mathbf{W}} = \mathbf{x}\mathbf{W}. \tag{3}$$

This is again just a linear combination of the inputs, $\mathbf{x}$, so offers no advantages over the original linear model.

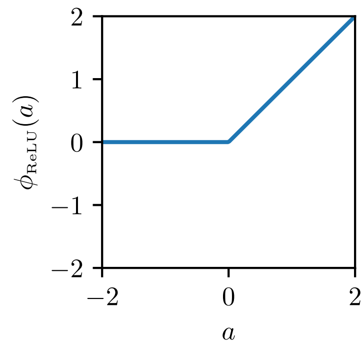
Including a nonlinearity prevents the collapse back to a linear model, giving us a strictly more powerful class of models.

$$\mathbf{h}_1 = \phi(\mathbf{x}\mathbf{W}_1) \tag{4a}$$
$$\mathbf{h}_2 = \phi(\mathbf{h}_1\mathbf{W}_2) \tag{4b}$$
$$\mathbf{f} = \mathbf{h}_2\mathbf{W}_3 \tag{4c}$$

There are lots of different choices for the nonlinearity. Perhaps the most common is the "rectified linear unit" or ReLU,

$$\phi_{\text{ReLU}}(a) = \begin{cases} a & \text{if } a > 0 \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

This is commonly known as a 3-layer network, as there are three weight-matrices.



Q: Why don't we have a nonlinearity in the final layer (i.e. for producing the output, f)? Nonlinearities can impose constraints on their outputs. For instance, ReLU can't return negative numbers. Alternatively, people sometimes use a sigmoid as a nonlinearity, but that can only output numbers between 0 and 1. We don't want to impose such constraints on our outputs, which is why we don't apply the output at the final layer.

Q: Is there a better way of understanding what nonlinearities are doing? Yes ... but you need quite a bit of theory to get there.

Q: Why is relu far more commonly used than e.g. sigmoid? This is to do with propagation of the gradients (we'll see some of this in the next part on backprop).