## Section 5: Forward-Backward Propagation

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• Why do we need neural networks?

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Intro ●0

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  - This transformation, often, is guided by domain-specific knowledge.
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  - This transformation, often, is guided by domain-specific knowledge.
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- What is the forward-backward propogation?
  - forward propagation: the algorithm that pushes our inputs through the hidden layers (weight matrices, activation functions) NN to get the final outputs

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  - This transformation, often, is guided by domain-specific knowledge.
  - Neural networks simultaneously solve for our model parameters and the best basis transformations.
- What is the forward-backward propogation?
  - forward propagation: the algorithm that pushes our inputs through the hidden layers (weight matrices, activation functions) NN to get the final outputs
  - backward-propagation: the algorithm that finds the best-suited weight matrices that would minimize the errors in the final outputs.

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- A schematic review of what NN is doing
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- Some coding exercise (Rmd file available on course website)

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### Feed-Forward Network

• The feed-forward neural network is a basic setup for a NN



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 $\bullet$  Input layer is design matrix  ${\boldsymbol X}$  which includes our usual vector of 1s

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- Hidden layers are intermediate design matrices between inputs and outputs (Deep learning is just a neural network with multiple hidden layers)
- d features, then d + 1 input nodes
- k possible classes, then k-1 output nodes
- h nodes in the hidden layer plus an intercept, where each of these nodes is a linear combination of the inputs, passed through an activation function (though note the intercept is always active and doesn't depend on nodes in the previous layer)

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## More on the Activation Function

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### More on the Activation Function

• Many possible choices (as seen in lecture). A common choice is the sigmoid function:

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• Notice that this is the inverse of the logit function:

$$\operatorname{logit}(x) = \log\left(\frac{x}{1-x}\right)$$

, where x is probability of an event, and logit(x) is its log odds.

Steps

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Note, when h = 1 there is only one linear combination of predictors. What does this become? Without the nonlinearity in the hidden layer, the neural network reduces to a GLM.

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1. Compute linear combination of features using weight matrix

$$\textbf{z}_1 = \textbf{X} \textbf{W}_{\mathsf{in}} \ = \begin{bmatrix} \ 1 & \textbf{x} \end{bmatrix} \quad \textbf{W}_{\mathsf{in}} \ , \ \mathsf{where} \ \textbf{W}_{\mathsf{in}} \ \in \mathbb{R}^{(d+1) \times h}$$

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2. Apply activation fn to get nodes in hidden layer

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$$\mathbf{H} = \begin{bmatrix} 1 & \mathbf{h} \end{bmatrix} = \begin{bmatrix} 1 & \sigma(\mathbf{z}_1) \end{bmatrix} = \begin{bmatrix} 1 & \sigma(\mathbf{XW}_{in}) \end{bmatrix}$$

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5. Put it all together:  $\hat{\mathbf{y}} = \sigma (\mathbf{HW}_{out}) = \sigma (\begin{bmatrix} 1 & \sigma (\mathbf{XW}_{in}) \end{bmatrix}_{a} \mathbf{W}_{out})$ 

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• Optimize  $-\mathcal{L} = f(\mathbf{W})$  via gradient descent by iterating the formula: where  $\mathbf{W}_{t+1} = \mathbf{W}_t - \gamma \cdot \nabla f(\mathbf{W}_t) \mathbf{W}$  and  $\gamma$  is 'learning rate'.

How do we get the gradient of the objective function?

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How do we get the gradient of the objective function?

• With respect to the output weights is:

$$\frac{-\partial \mathcal{L}}{\partial \mathbf{W}_{\mathsf{out}}} = \frac{-\partial \mathcal{L}}{\partial \hat{\mathbf{y}}} \frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{W}_{\mathsf{out}}}$$

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, where

$$\begin{aligned} \frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{H}} &= \sigma \left( \mathbf{H} \mathbf{W}_{\text{out}} \left( 1 - \sigma \left( \mathbf{H} \mathbf{W}_{\text{out}} \right) \right) \right) \mathbf{W}_{\text{out}}^{\top} = \hat{\mathbf{y}} (1 - \hat{\mathbf{y}}) \mathbf{W}_{\text{out}}^{\top} \\ \frac{\partial \mathbf{H}}{\partial \mathbf{W}_{\text{in}}} &= \mathbf{X}^{\top} \begin{bmatrix} 1 & \sigma \left( \mathbf{X} \mathbf{W}_{\text{in}} \right) \left( 1 - \sigma \left( \mathbf{X} \mathbf{W}_{\text{in}} \right) \right) \end{bmatrix} \end{aligned}$$

# Putting Everything Together

#### Training a NN using forward-backward propagation

- 1. Initialize weights
- 2. Propagate forward to get output estimates
- 3. Propagate error backward to update the weights toward a better solution
- 4. Iterate forward and back propagation until stopping criterion
  - Coding exercise available on the course website (Rmd)

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