ECE 417 Fall 2018 Lecture 17: Neural Networks

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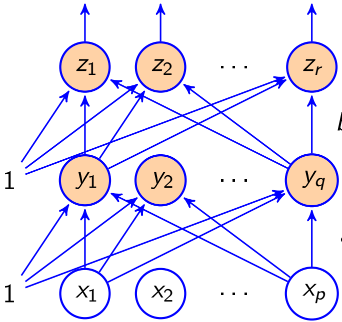
Outline

Two-Layer Feedforward Neural Network



$$\vec{z} = h(\vec{x}, U, V)$$

which is decomposed as. . .

$z_\ell = g(b_\ell)$	$\vec{z} = g(\vec{b})$
$b_\ell = v_{k0} + \sum_{k=1}^{q} v_{\ell k} y_k$	$\vec{b} = V\vec{y}$
$y_k = f(a_k)$	$\vec{y} = f(\vec{a})$
$a_k = u_{k0} + \sum_{j=1}^{p} u_{kj} x_j$	$\vec{a} = U\vec{x}$

$\vec{x}$ is the input vector

A Neural Net is Made Of. . .

- Linear transformations: $\vec{a} = U\vec{x}$, $\vec{b} = V\vec{y}$, one per layer.
- Scalar nonlinearities: $\vec{y} = f(\vec{a})$ means that, element-by-element, $y_k = f(a_k)$ for some nonlinear function $f(\cdot)$.
- The nonlinearities can all be different, if you want. For today, I'll assume that all nodes in the first layer use one function $f(\cdot)$, and all nodes in the second layer use some other function $g(\cdot)$.
- Networks with more than two layers are called "Deep Neural Networks" (DNN). I won't talk about them today.

Andrew Barron (1993) proved that combining two layers of linear transforms, with one scalar nonlinearity between them, is enough to model **any** multivariate nonlinear function $\vec{z} = h(\vec{x})$.

Neural Network = Universal Approximator

Assume...

- Linear Output Nodes: $g(b) = b$
- Smoothly Nonlinear Hidden Nodes: $f'(a) = \frac{df}{da}$ finite
- Smooth Target Function: $\vec{z} = h(\vec{x}, U, V)$ approximates $\vec{\zeta} = h^*(\vec{x}) \in \mathcal{H}$, where $\mathcal{H}$ is some class of sufficiently smooth functions of $\vec{x}$ (functions whose Fourier transform has a first moment less than some finite number C)
- There are q hidden nodes, y_k, $1 \le k \le q$
- The input vectors are distributed with some probability density function, $p(\vec{x})$, over which we can compute expected values.

Then (Barron, 1993) showed that...

$$\max_{h^*(\vec{x})\in\mathcal{H}} \min_{U,V} E\left[h(\vec{x}, U, V) - h^*(\vec{x})|^2\right] \le \mathcal{O}\left\{\frac{1}{q}\right\}$$

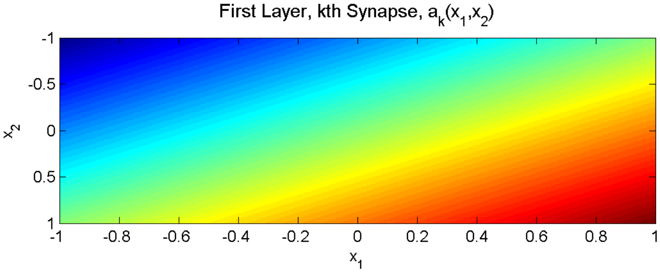
Neural Network Problems: Outline of Remainder of this Talk

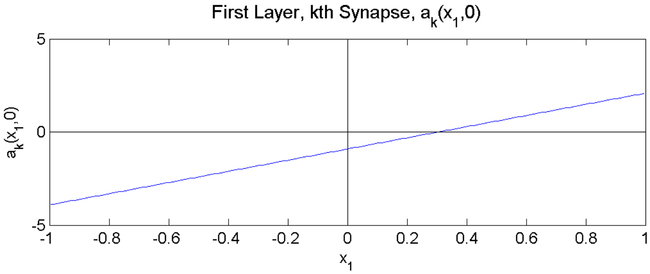
1. **Knowledge-Based Design.** Given U, V, f, g, what kind of function is $h(\vec{x}, U, V)$? Can we draw $\vec{z}$ as a function of $\vec{x}$? Can we heuristically choose U and V so that $\vec{z}$ looks kinda like $\vec{\zeta}$?
2. **Nonlinearities.** They come in pairs: the test-time nonlinearity, and the training-time nonlinearity.
3. **Error Metric.** In what way should $\vec{z} = h(\vec{x})$ be "similar to" $\vec{\zeta} = h^*(\vec{x})$?
4. **Training: Gradient Descent with Back-Propagation.** Given an initial U, V, how do I find $\hat{U}$, $\hat{V}$ that more closely approximate $\vec{\zeta}$?

Outline

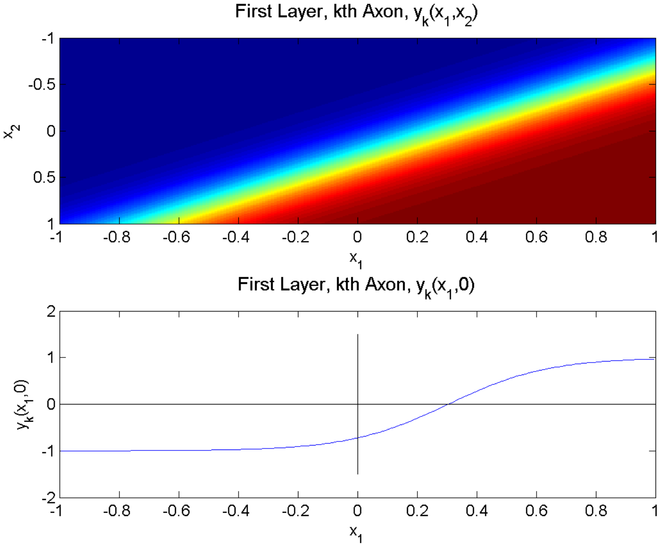
1. What is a Neural Net?
2. Knowledge-Based Design
3. Nonlinearities
4. Error Metric
5. Gradient Descent

Synapse, First Layer: $a_k = u_{k0} + \sum_{j=1}^{2} u_{kj} x_j$

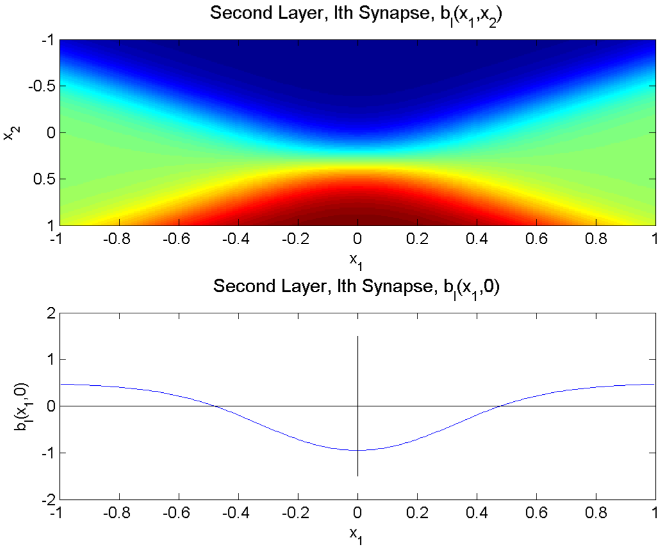




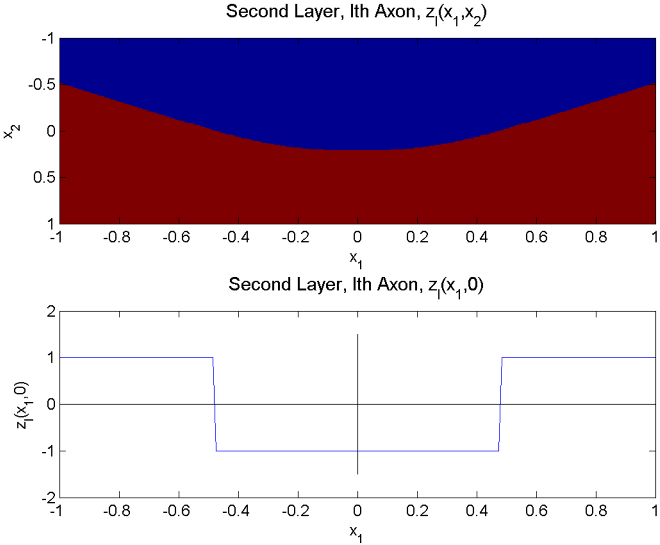
Axon, First Layer: $y_k = \tanh(a_k)$



Synapse, Second Layer: $b_\ell = v_{\ell 0} + \sum_{k=1}^{2} v_{\ell k} y_k$



Axon, Second Layer: $z_\ell = \mathrm{sign}(b_\ell)$



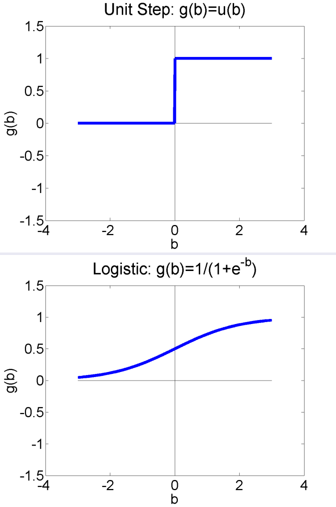
Outline

Differentiable and Non-differentiable Nonlinearities

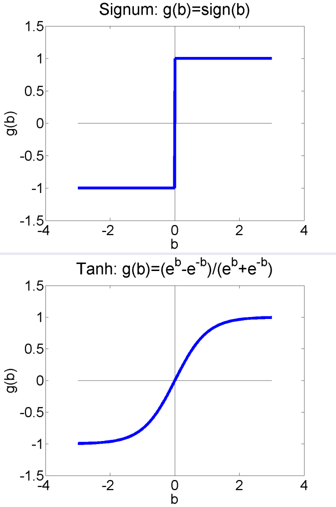
The nonlinearities come in pairs: (1) the **test-time nonlinearity** is the one that you use in the **output layer** of your **learned classifier**, e.g., in the app on your cell phone (2) the **training-time nonlinearity** is used in the output layer during training, and in the hidden layers during both training and test.

Application	Test-Time Output Nonlinearity	Training-Time Output & Hidden Nonlinearity
$\{0, 1\}$ classification	step	logistic or ReLU
$\{-1, +1\}$ classification	signum	tanh
multinomial classification	argmax	softmax
regression	linear	(hidden nodes must be nonlinear)

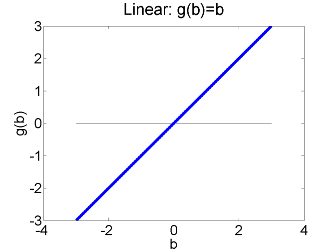
Step and Logistic nonlinearities

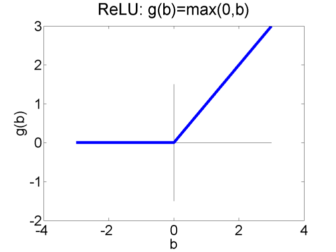


Signum and Tanh nonlinearities



"Linear Nonlinearity" and ReLU





Argmax and Softmax

Argmax:

$$z_\ell = \begin{cases} 1 & b_\ell = \max_m b_m \\ 0 & \text{otherwise} \end{cases}$$

Softmax:

$$z_\ell = \frac{e^{b_\ell}}{\sum_m e^{b_m}}$$

Outline

Error Metric: MMSE for Linear Output Nodes

Minimum Mean Squared Error (MMSE)

$$U^*, V^* = \arg\min E = \arg\min \frac{1}{2n} \sum_{i=1}^{n} |\vec{\zeta}_i - \vec{z}(x_i)|^2$$

Why would we want to use this metric?

If the training samples $(\vec{x}_i, \vec{\zeta}_i)$ are i.i.d., then in the limit as the number of training tokens goes to infinity,

$$h(\vec{x}) \rightarrow E\left[\vec{\zeta}|\vec{x}\right]$$

Error Metric: MMSE for Binary Target Vector

Binary target vector

Suppose

$$\zeta_\ell = \begin{cases} 1 & \text{with probability } P_\ell(\vec{x}) \\ 0 & \text{with probability } 1 - P_\ell(\vec{x}) \end{cases}$$

and suppose $0 \le z_\ell \le 1$, e.g., logistic output nodes.

Why does MMSE make sense for binary targets?

$$\begin{aligned} E\left[\zeta_\ell | \vec{x}\right] &= 1 \cdot P_\ell(\vec{x}) + 0 \cdot (1 - P_\ell(\vec{x})) \\ &= P_\ell(\vec{x}) \end{aligned}$$

So the MMSE neural network solution is

$$h(\vec{x}) \rightarrow E\left[\vec{\zeta}|\vec{x}\right] = P_\ell(\vec{x})$$

Softmax versus Logistic Output Nodes

Encoding the Neural Net Output using a "One-Hot Vector"

- Suppose $\vec{\zeta}_i$ is a "one hot" vector, i.e., only one element is "hot" ($\zeta_{\ell(i),i} = 1$), all others are "cold" ($\zeta_{mi} = 0$, $m \neq \ell(i)$).
- Training logistic output nodes with MMSE training will approach the solution $z_\ell = \Pr\left\{\zeta_\ell = 1 | \vec{x}\right\}$, but there's no guarantee that it's a correctly normalized pmf ($\sum z_\ell = 1$) until it has fully converged.
- Softmax output nodes guarantee that $\sum z_\ell = 1$.

Softmax output nodes

$$z_\ell = \frac{e^{b_\ell}}{\sum_m e^{b_m}}$$

Cross-Entropy

The softmax nonlinearity is "matched" to an error criterion called "cross-entropy," in the sense that its derivative can be simplified to have a very, very simple form.

- $\zeta_{\ell,i}$ is the true reference probability that observation $\vec{x}_i$ is of class ℓ. In most cases, this "reference probability" is either 0 or 1 (one-hot).
- $z_{\ell,i}$ is the neural network's hypothesis about the probability that $\vec{x}_i$ is of class ℓ. The softmax function constrains this to be $0 \leq z_{\ell,i} \leq 1$ and $\sum_\ell z_{\ell,i} = 1$.

The average cross-entropy between these two distributions is

$$E = -\frac{1}{n}\sum_{i=1}^{n}\sum_{\ell}\zeta_{\ell,i}\log z_{\ell,i}$$

Cross-Entropy = Log Probability

Suppose token $\vec{x}_i$ is of class ℓ^*, meaning that $\zeta_{\ell^*,i} = 1$, and all others are zero. Then cross-entropy is just the neural net's estimate of the negative log probability of the correct class:

$$E = -\frac{1}{n}\sum_{i=1}^{n} \log z_{\ell^*,i}$$

In other words, E is the average of the negative log probability of each training token:

$$E = -\frac{1}{n}\sum_{i=1}^{n} E_i, \quad E_i = -\log z_{\ell^*,i}$$

Cross-Entropy is matched to softmax

Now let's plug in the softmax:

$$E_i = -\log z_{\ell^*,i}, \quad z_{\ell^*,i} = \frac{e^{b_{\ell^*,i}}}{\sum_k e^{b_{ki}}}$$

Its gradient with respect to the softmax inputs, b_{mi}, is

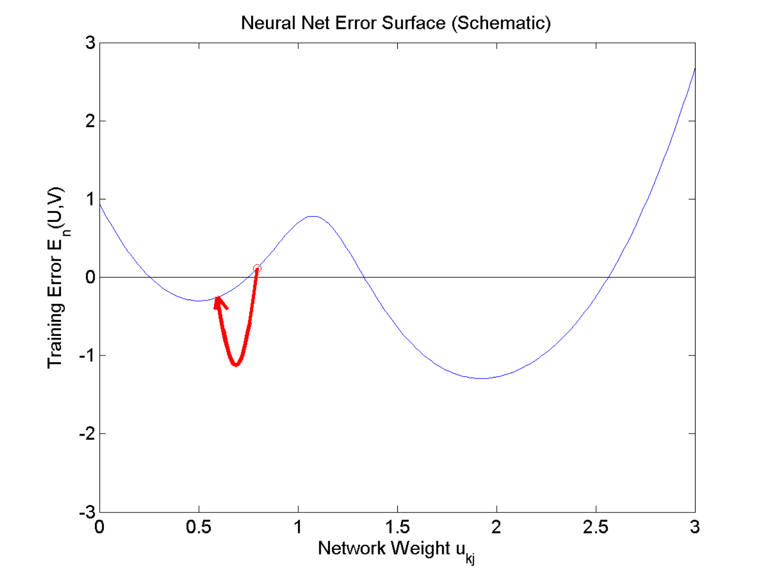
$$\begin{aligned}
\frac{\partial E_i}{\partial b_{mi}} &= -\frac{1}{z_{\ell^*,i}} \frac{\partial z_{\ell^*,i}}{\partial b_{mi}} \\
&= \begin{cases} -\frac{1}{z_{\ell^*,i}} \left(\frac{e^{b_{\ell^*,i}}}{\sum_k e^{b_{ki}}} - \frac{\left(e^{b_{\ell^*,i}}\right)^2}{\left(\sum_k e^{b_{ki}}\right)^2} \right) & m = \ell^* \\ -\frac{1}{z_{\ell^*,i}} \left(-\frac{e^{b_{\ell^*,i}} e^{b_{mi}}}{\left(\sum_k e^{b_{ki}}\right)^2} \right) & m \neq \ell^* \end{cases} \\
&= z_{mi} - \zeta_{mi}
\end{aligned}$$

Error Metrics Summarized

- Use MSE to achieve $\vec{z} = E\left[\vec{\zeta}|\vec{x}\right]$. That's almost always what you want.
- If $\vec{\zeta}$ is a one-hot vector, then use Cross-Entropy (with a softmax nonlinearity on the output nodes) to guarantee that $\vec{z}$ is a properly normalized probability mass function, and because it gives you the amazingly easy formula $\frac{\partial E_i}{\partial b_{mi}} = z_{mi} - \zeta_{mi}$.
- If ζ_ℓ is binary, but not necessarily one-hot, then use MSE (with a logistic nonlinearity) to achieve $z_\ell = \Pr\left\{\zeta_\ell = 1|\vec{x}\right\}$.

Outline

Gradient Descent = Local Optimization



Gradient Descent = Local Optimization

Given an initial U, V, find $\hat{U}$, $\hat{V}$ with lower error.

$$\begin{aligned}\hat{u}_{kj} &= u_{kj} - \eta \frac{\partial E}{\partial u_{kj}} \\ \hat{v}_{\ell k} &= v_{\ell k} - \eta \frac{\partial E}{\partial v_{\ell k}}\end{aligned}$$

η =Learning Rate

- If η too large, gradient descent won't converge. If too small, convergence is slow. Usually we pick $\eta \approx 0.001$, then see whether it converges or not; if not, we tweak η and then try again.
- Second-order methods like Newton's algorithm, L-BFGS, ADAM, and Hessian-free optimization choose an optimal η at each step, so they're MUCH faster.

Computing the Gradient

$$E = \frac{1}{n}\sum_{i=1}^{n} E_i, \quad E_i = \text{cross-entropy or MMSE}$$

$$\frac{\partial E}{\partial v_{\ell k}} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{\partial E}{\partial b_{\ell i}}\right)\left(\frac{\partial b_{\ell i}}{\partial v_{\ell k}}\right) = \frac{1}{n}\sum_{i=1}^{n} \epsilon_{\ell i} y_{ki}$$

where I've used one thing you already know, and one new definition. Here's the thing you already know:

$$b_{\ell i} = \sum_k v_{\ell k} y_{ki}, \quad \text{therefore} \quad \frac{\partial b_{\ell i}}{\partial v_{\ell k}} = y_{ki}$$

Here's the new definition:

$$\epsilon_{\ell i} = \frac{\partial E_i}{\partial b_{\ell i}} = \begin{cases} z_{\ell i} - \zeta_{\ell i} & \text{Cross-Entropy with Softmax} \\ (z_{\ell i} - \zeta_{\ell i}) g'(b_{\ell i}) & \text{MMSE with Nonlinearity } g(b) \end{cases}$$

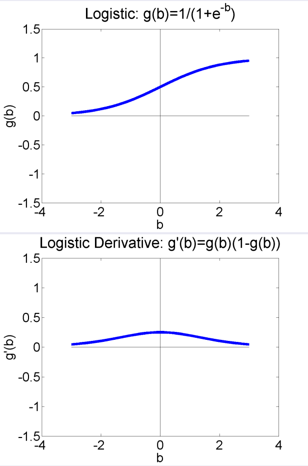
Forward Propagation and Back-Propagation

$$\frac{\partial E}{\partial v_{\ell k}} = \frac{1}{n}\sum_{i=1}^{n} \epsilon_{\ell i} y_{ki}$$

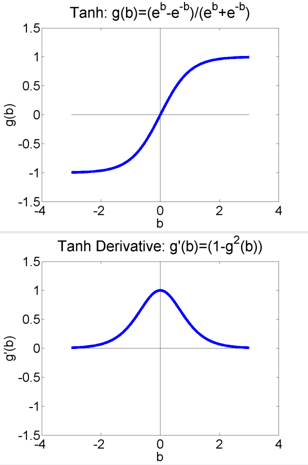
- First, y_{ji} and $z_{\ell i}$ are generated from $\vec{x}_i$ in the forward pass.
- Then $\epsilon_{\ell i}$ is generated from $z_{\ell i} - \zeta_{\ell i}$ in the back-propagation.

$g'(b)$: Derivatives of the Nonlinearities

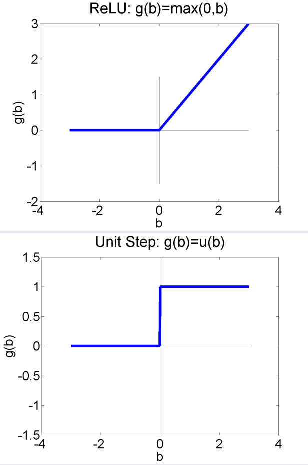
Logistic

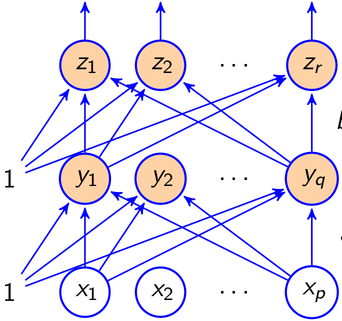


Tanh



ReLU





$$\vec{z} = h(\vec{x}, U, V)$$

which is decomposed as...

$z_\ell = g(b_\ell)$	$\vec{z} = g(\vec{b})$
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$y_k = f(a_k)$	$\vec{y} = f(\vec{a})$
$a_k = u_{k0} + \sum_{j=1}^{p} u_{kj} x_j$	$\vec{a} = U\vec{x}$

$\vec{x}$ is the input vector

Back-Propagating to the First Layer

$$\frac{\partial E}{\partial u_{kj}} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{\partial E}{\partial a_{ki}}\right)\left(\frac{\partial a_{ki}}{\partial u_{kj}}\right) = \frac{1}{n}\sum_{i=1}^{n}\delta_{ki}x_{ji}$$

where... $\delta_{ki} = \frac{\partial E_i}{\partial a_{ki}} = \sum_{\ell=1}^{r}\epsilon_{\ell i} v_{\ell k} f'(a_{ki})$

Forward Propagation and Back-Propagation

$$\frac{\partial E}{\partial v_{\ell k}} = \frac{1}{n}\sum_{i=1}^{n} \epsilon_{\ell i} y_{ki}$$

$$\frac{\partial E}{\partial u_{kj}} = \frac{1}{n}\sum_{i=1}^{n} \delta_{ki} x_{ji}$$

- First, y_{ji} and $z_{\ell i}$ are generated from $\vec{x}_i$ in the forward pass.
- Then $\epsilon_{\ell i}$ and δ_{ki} are generated from $z_{\ell i} - \zeta_{\ell i}$ in the back-propagation.