CS 179: LECTURE 14

NEURAL NETWORKS AND BACKPROPAGATION

LAST TIME

- Intro to machine learning
- Linear regression
  - https://en.wikipedia.org/wiki/Linear_regression
- Gradient descent
  - https://en.wikipedia.org/wiki/Gradient_descent
- (Linear classification = minimize cross-entropy)
  - https://en.wikipedia.org/wiki/Cross_entropy

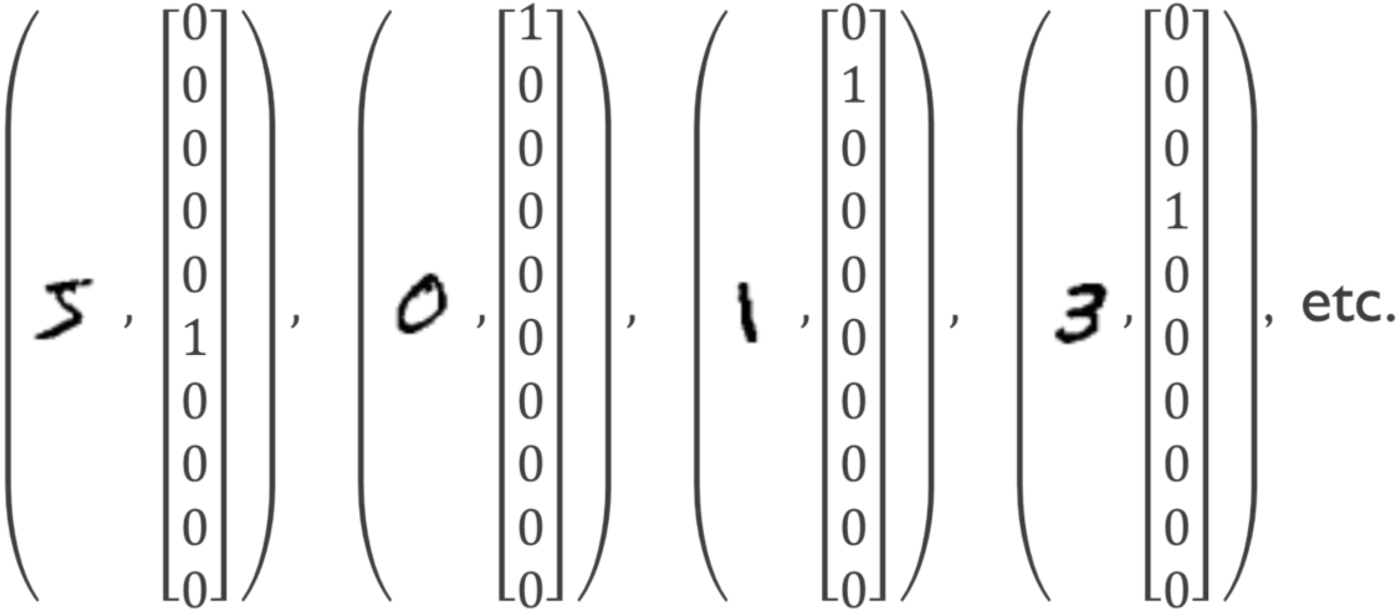
TODAY

- Derivation of gradient descent for **linear classifier**
  - https://en.wikipedia.org/wiki/Linear_classifier
- Using linear classifiers to build up neural networks
- Gradient descent for neural networks (**Back Propagation**)
  - https://en.wikipedia.org/wiki/Backpropagation

REFRESHER ON THE TASK

- We are given $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(N)}, y^{(N)})\}$ as training data
- We want to classify each input x into one of m classes
- Each $x^{(n)}$ is a d-dimensional column vector $\left(x_1^{(n)}, \ldots, x_d^{(n)}\right)^T$
- Each $y^{(n)}$ is a m-dimensional column vector $\left(y_1^{(n)}, \ldots, y_m^{(n)}\right)^T$
- $y_k^{(n)} = 1$ iff $\text{class}(x^{(n)}) = k$; otherwise, $y_k^{(n)} = 0$

EXAMPLE OF (x, y) PAIRS



- Note "Grandmother Cell" representation for {x,y} pairs. See https://en.wikipedia.org/wiki/Grandmother_cell

REFRESHER ON THE TASK

- Our model is parametrized by a matrix $\mathbf{W} \in \mathbb{R}^{(d+1)\times m}$
- Given a d-dimensional input vector $x = (x_1, \ldots, x_d)^T$ and denoting $x' = (1, x_1, \ldots, x_d)^T$, we compute an m-dimensional output vector $z = \mathbf{W}^T x'$
- We then classify x as the class corresponding to the index of z with the largest value
- Find i for z_i: "Best-index" -- estimated "Grandmother Cell" Neuron
- Can use <u>**parallel GPU reduction**</u> to find "i" for largest value.

LINEAR CLASSIFIER GRADIENT

- We will be going through some extra steps to derive the gradient of the linear classifier --
- We'll be using the **"Softmax function"**
  - https://en.wikipedia.org/wiki/Softmax_function
- Similarities will be seen when we start talking about neural networks

LINEAR CLASSIFIER J & GRADIENT

- Define intermediate variables

$$z = \mathbf{W}^T x'$$

- $$p_k = \frac{\exp(z_k)}{\sum_{j=1}^{m} \exp(z_j)}; \; p = (p_1, \dots, p_m)^T$$

$$J = -\sum_{k=1}^{m} y_k \ln(p_k)$$

LINEAR CLASSIFIER GRADIENT

- Simplify derivatives using the multivariate chain rule and the fact that $z_j = \sum_{i=0}^{d} \mathbf{W}_{ij}\, x_i$ (with $x_0 = 1$)

- $$\frac{\partial J}{\partial \mathbf{W}_{ij}} = \sum_{k=1}^{m} \frac{\partial J}{\partial z_k} \frac{\partial z_k}{\partial \mathbf{W}_{ij}} = x_i \frac{\partial J}{\partial z_j}$$

$$\frac{\partial J}{\partial z_j} = -\sum_{i=1}^{m} \frac{y_i}{p_i} \frac{\partial p_i}{\partial z_j}$$

LINEAR CLASSIFIER GRADIENT

- Compute the gradient of the softmax function

$$\frac{\partial p_j}{\partial z_i} = \begin{cases} p_i(1 - p_j) & i = j \\ -p_i \cdot p_j & \text{otherwise} \end{cases}$$

-
- Substituting this into the previous gradient, we can show

$$\boxed{\frac{\partial J}{\partial z_i} = p_i - y_i = \begin{cases} p_i - 1 & \text{class}(x) = i \\ p_i & \text{otherwise} \end{cases}}$$

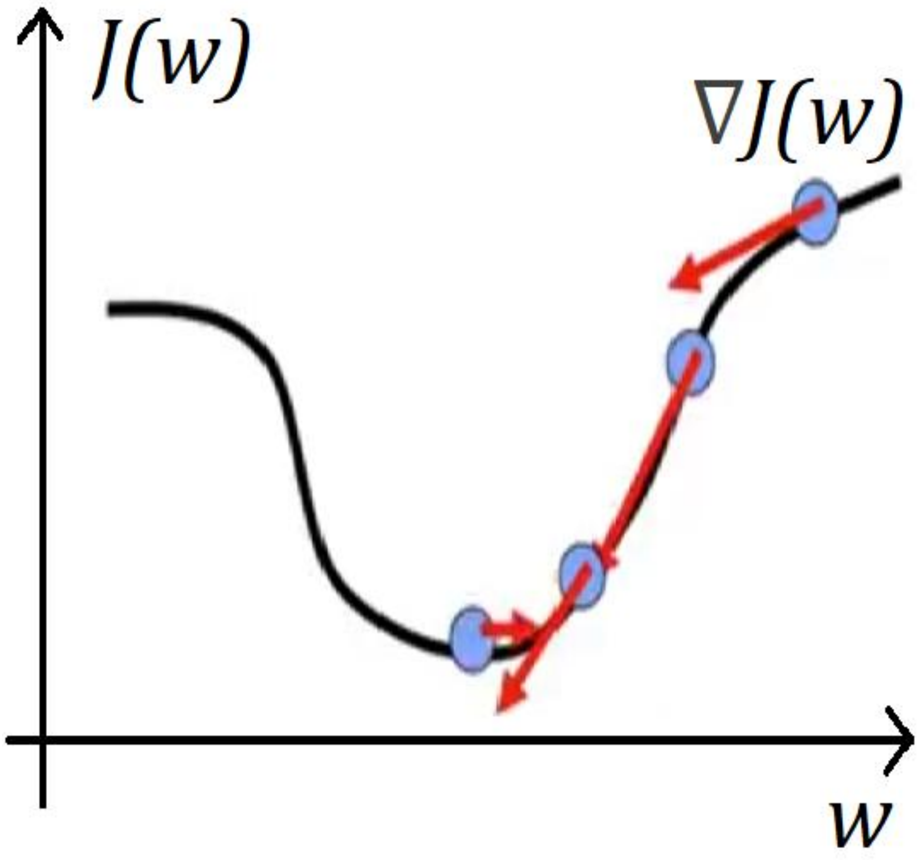
LINEAR CLASSIFIER GRADIENT

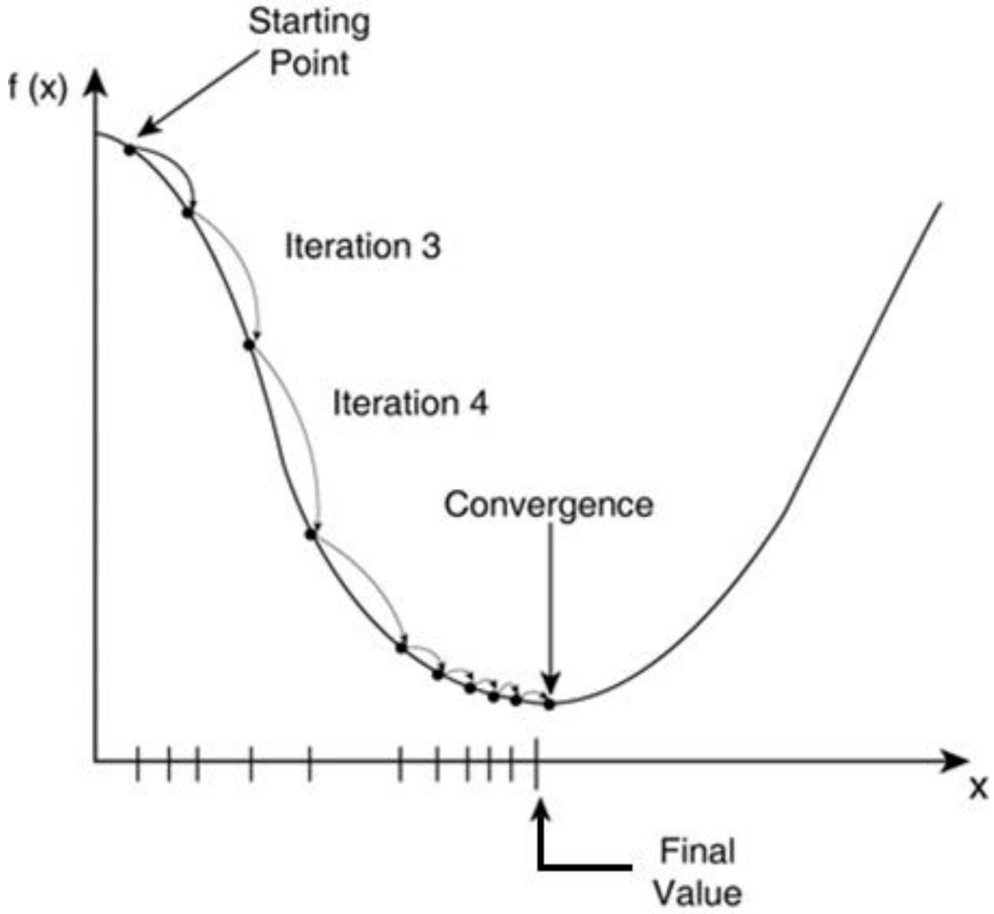
- Then, the gradient of the linear classifier's loss function wrt its parameters is
- $$\frac{\partial J}{\partial \mathbf{W}_{ij}} = \frac{\partial J}{\partial z_i}\frac{\partial z_i}{\partial \mathbf{W}_{ij}} = x_i(p_j - y_j)$$
  $$\nabla_{\mathbf{W}}[J] = x'(p-y)^T$$
- More linear algebra! Again, GPU's are great for this stuff ☺

GRADIENT DESCENT

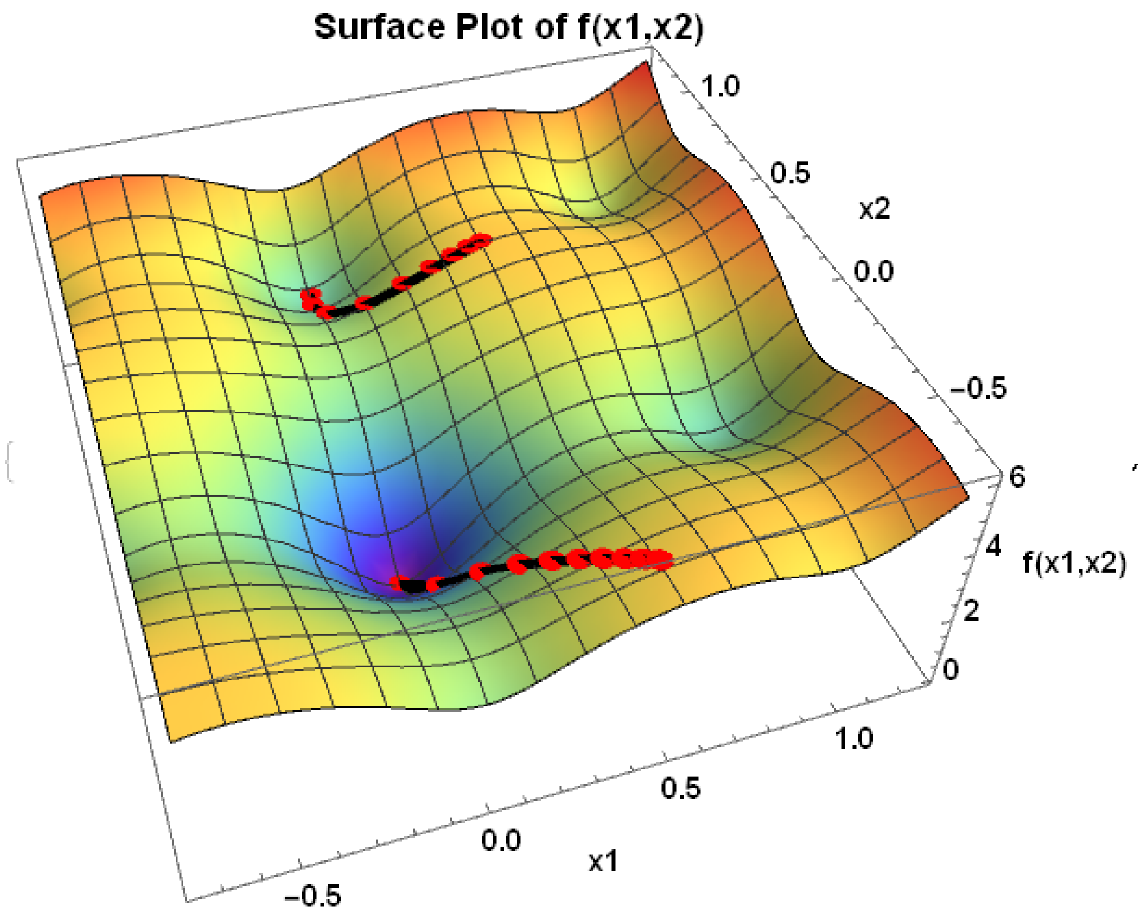
- How do we find $w^* = \underset{w \in \mathbb{R}^{d+1}}{\operatorname{argmin}} J(w; \mathbf{X}, \mathbf{Y})$?
- A function's gradient points in the direction of steepest ascent, and its negative in the direction of steepest descent
- Following the gradient downhill will cause us to converge to a local minimum!

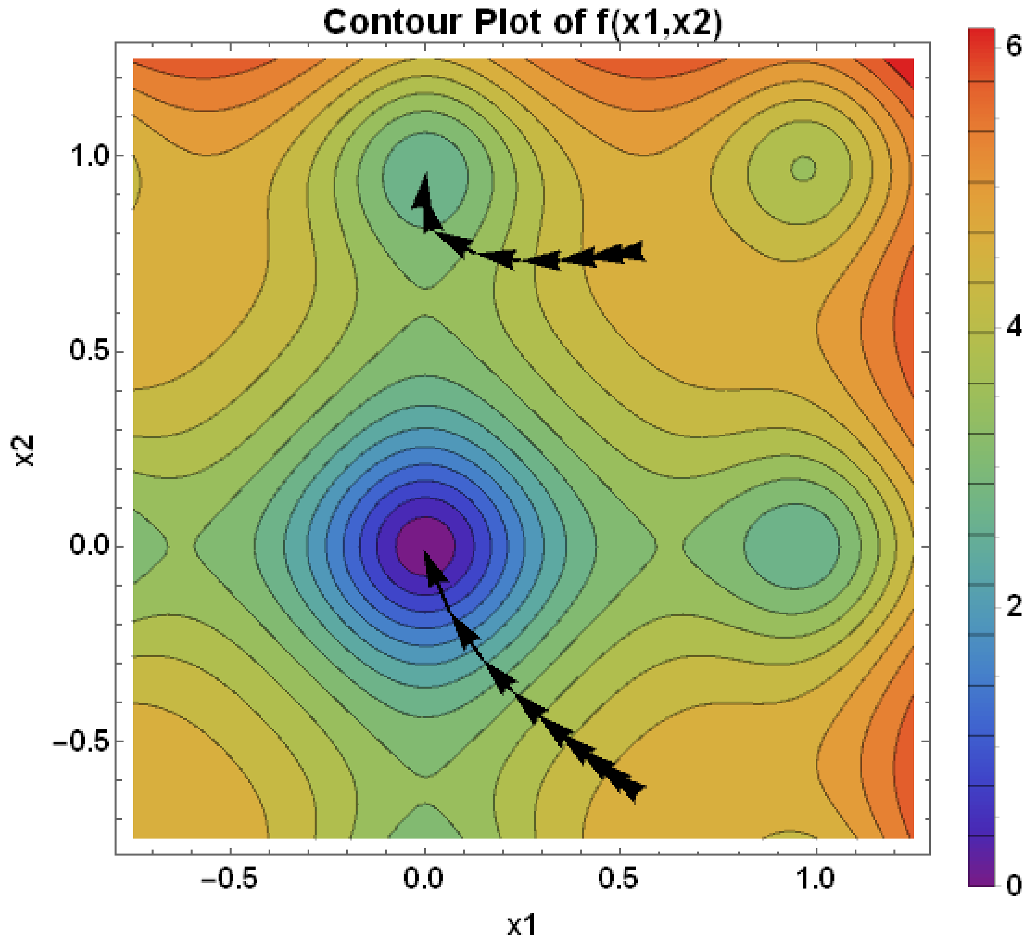
GRADIENT DESCENT, REVIEW





GRADIENT DESCENT IN N^D





GRADIENT DESCENT

- Fix some constant learning rate η (0.03 is usually a good place to start)
- Initialize w randomly
  - Typically select each component of w independently from some standard distribution (uniform, normal, etc.)
- While w is still changing (hasn't converged)
  - Update $w \leftarrow w - \eta \nabla J(w; \mathbf{X}, \mathbf{Y})$

STOCHASTIC GRADIENT DESCENT

- The previous algorithm computes the gradient over the entire data set before stepping.
  - Called batch gradient descent
- What if we just picked a single data point $(x^{(i)}, y^{(i)})$ at random, computed the gradient for that point, and updated the parameters?
  - Called stochastic gradient descent

STOCHASTIC GRADIENT DESCENT

- Advantages of SGD
  - Easier to implement for large datasets
  - Works better for non-convex loss functions
  - Sometimes faster
- Often use SGD on a "mini-batch" of k examples rather than just one at a time
  - Allows higher throughput and more parallelization

STOCHASTIC GRADIENT DESCENT, FOR W

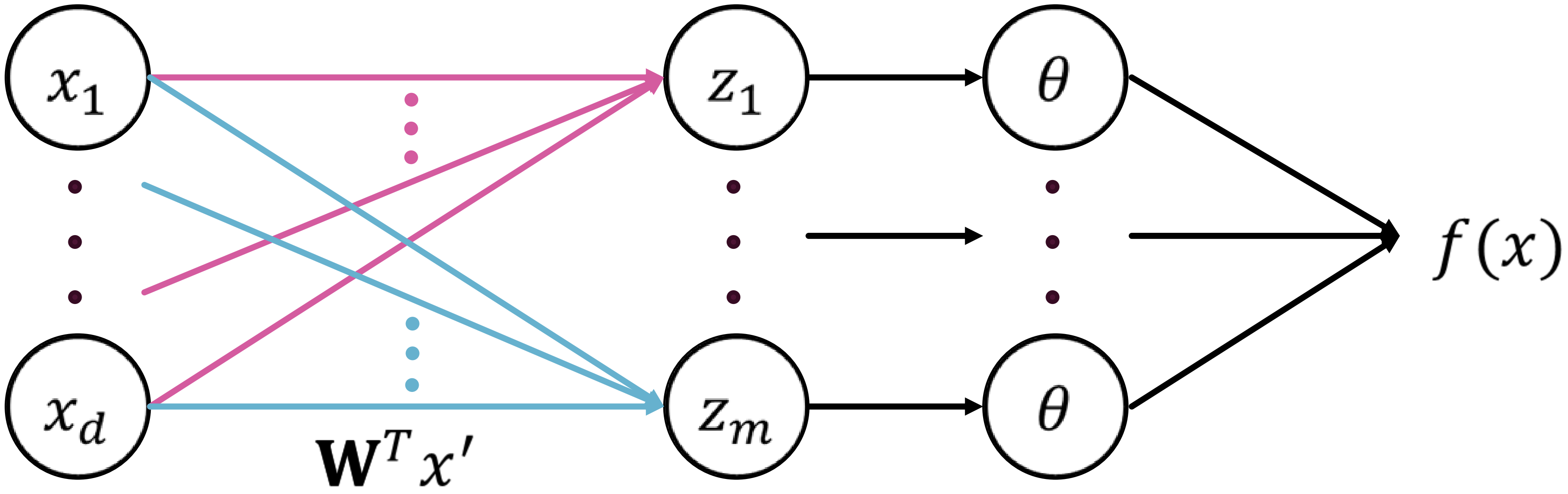
- While $\mathbf{W}$ has not converged
  - For each data point (x, y) in the data set
    - Compute $z = \mathbf{W}^T x'$
-
    - Compute $p = \frac{\exp(z)}{\sum_{k=1}^{m} \exp(z_k)}$
    - Update $\mathbf{W} \leftarrow \mathbf{W} - \eta\, x'(p - y)^T$
- Alternatively, update per mini-batch instead of per data point

LIMITATIONS OF LINEAR MODELS

- Most real-world data is not separable by a linear decision boundary
  - Simplest example: XOR gate
- What if we could combine the results of multiple linear classifiers?
  - Combine two OR gates with an AND gate to get a XOR gate

ANOTHER VIEW OF LINEAR MODELS

- Combine all the components x_i of our input x in different ways in order to get different outputs z_j
- Push z through some nonlinear function θ (e.g. softmax)



NEURAL NETWORKS

- What if we used each $\theta(z_j)$ as the input to another classifier?
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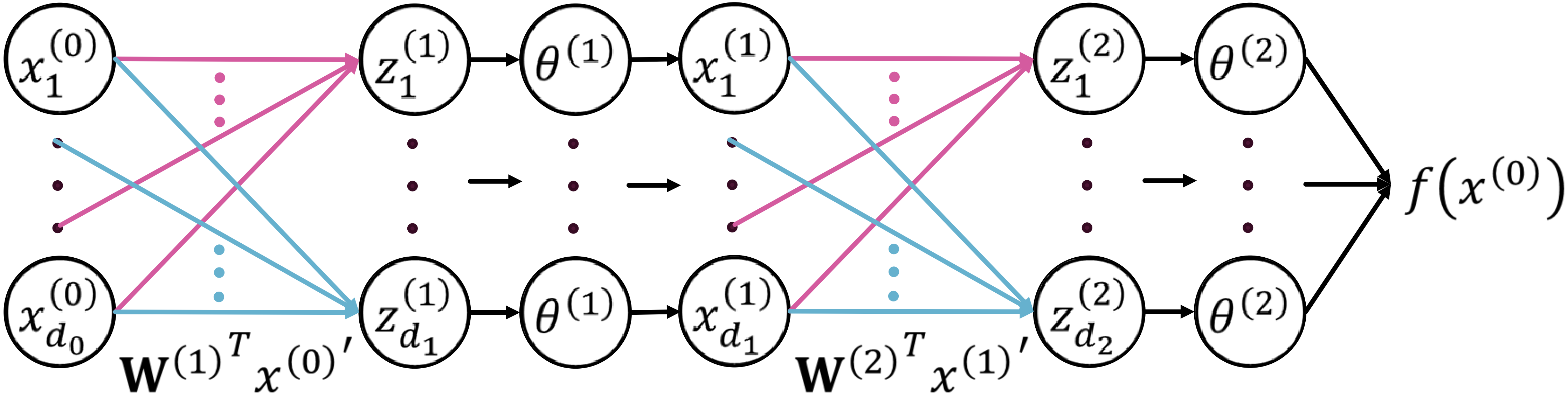
- This lets us compose multiple linear decision boundaries!



NEURAL NETWORKS

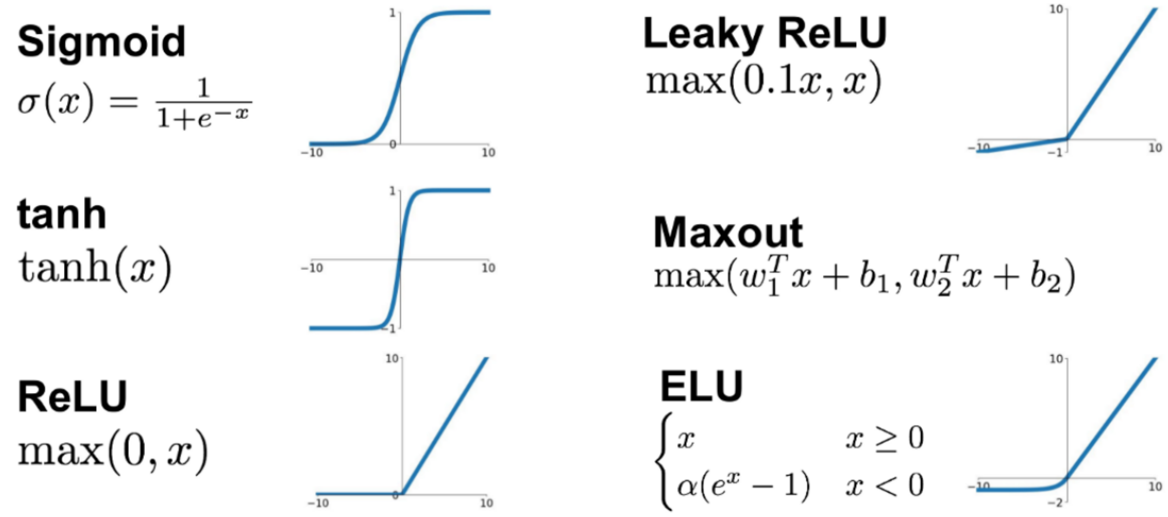
- Why the nonlinearity θ?
  - $\mathbf{W}^{(2)^T}\left(\mathbf{W}^{(1)^T}x'\right)$ is still a linear function x
  - $\mathbf{W}^{(2)^T}\theta\left(\mathbf{W}^{(1)^T}x'\right)$ is no longer a linear function in x
  - θ makes the model more expressive
- The nonlinearity θ is also known as an **activation function**

EXAMPLES OF ACTIVATION FNS

- $\theta(z) = \max(0, z)$ (**ReLU activation**) is most common
- $\theta(z) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$ (**tanh function**) is occasionally used as well
- Note that most derivatives of tanh function will be zero! Makes for much needless computation in gradient descent!

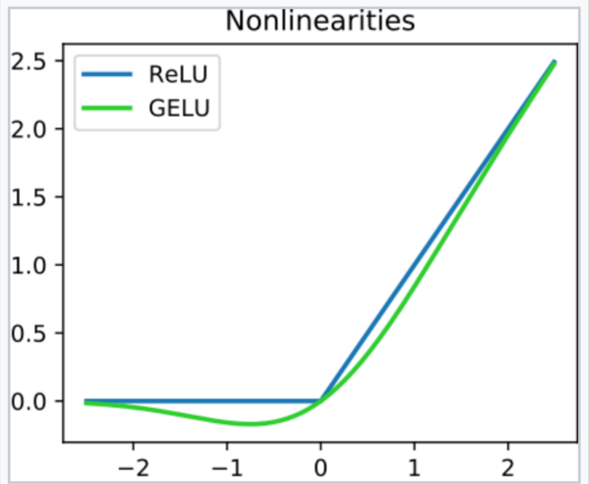
MORE ACTIVATION FUNCTIONS

- https://medium.com/@shrutijadon10104776/survey-on-activation-functions-for-deep-learning-9689331ba092
- Tanh and sigmoid used historically. Many zero gradient values – inefficient.

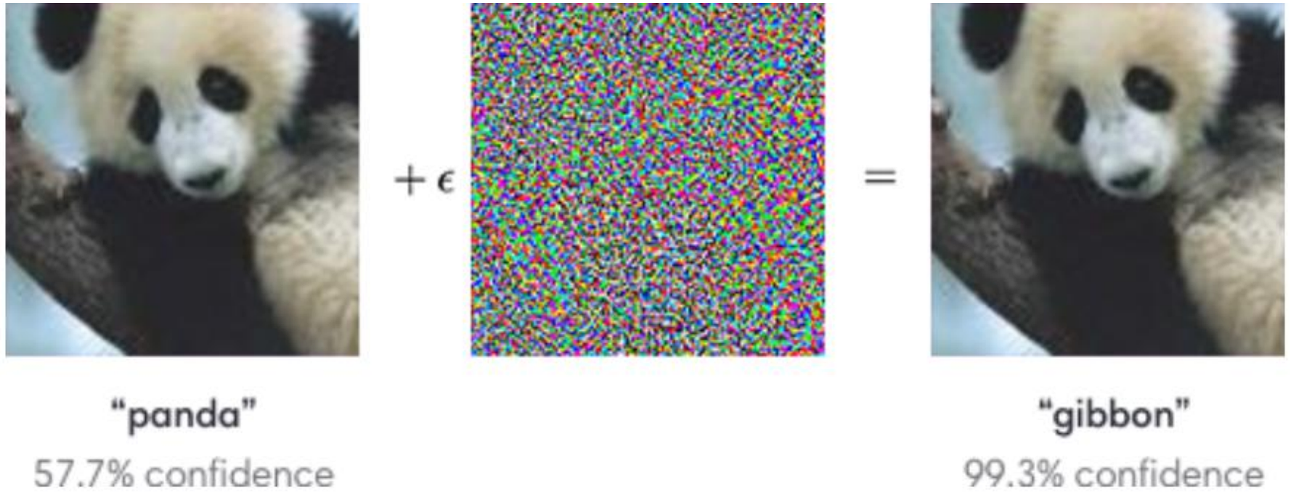


RELU (RECTIFIED LINEAR) ACTIVATION FUNCTION

- https://en.wikipedia.org/wiki/Rectifier_(neural_networks)
- Good, many nonzero derivatives! More "signal" than tanh.
- Oops, leads to other problems, requiring "adversarial networks!"



Plot of the ReLU rectifier (blue) and GELU (green) functions near $x = 0$



An adversarial input, overlaid on a typical image, can cause a classifier to miscategorize

ZEBRA STRIPES CONFUSE FLY VISION!

- https://www.theguardian.com/science/2019/feb/20/why-the-zebra-got-its-stripes-to-deter-flies-from-landing-on-it

Pattern seems to confuse flies, researchers who dressed horses up as zebras find

OTHER ACTIVATION FUNCTIONS FOR NNS…

- https://en.wikipedia.org/wiki/Activation_function
- Tanh activation

- Linear activation: $\phi(\mathbf{v}) = a + \mathbf{v}'\mathbf{b}$,
- ReLU activation: $\phi(\mathbf{v}) = \max(0, a + \mathbf{v}'\mathbf{b})$,
- Heaviside activation: $\phi(\mathbf{v}) = 1_{a+\mathbf{v}'\mathbf{b}>0}$,
- Logistic activation:

$$\phi(\mathbf{v}) = (1 + \exp(-a - \mathbf{v}'\mathbf{b}))^{-1}.$$

UNIVERSAL APPROXIMATOR THM

- It is possible to show that if your neural network is big enough, it can approximate any continuous function arbitrarily well! (Hornik 1991)
- This is why neural nets are important. Can learn almost "anything!"
- Lapedes Theorem shows you only "need" two hidden layers.
  - https://dl.acm.org/doi/10.5555/2969644.2969691 (1987)

NEURAL NETWORKS

- But why stop at just 2 layers of linear function/nonlinearity?
- We can have arbitrarily many L layers!
  - $x^{(\ell-1)}$ is the input to layer ℓ ($x^{(0)}$ is the data given)
  - $x^{(\ell)} = \theta^{(\ell)}\left(\mathbf{W}^{(\ell)^T} x^{(\ell-1)'}\right)$ is the output of layer ℓ
  - The loss function is applied to $x^{(L)} = \theta^{(L)}\left(z^{(L)}\right)$ (the final output), though it is sometimes easier to apply it to $z^{(L)}$ directly (e.g. softmax cross-entropy loss w/ linear classifier)

BACK PROPAGATION GRADIENT

- So how do we take the gradient of a neural network with respect to every parameter matrix $\mathbf{W}^{(1)}, \ldots, \mathbf{W}^{(L)}$?
- Define $z^{(\ell)} = {\mathbf{W}^{(\ell)}}^T x^{(l-1)'}$ and $\delta^{(\ell)} = \nabla_{z^{(\ell)}}[J]$. By chain rule,
- $$\frac{\partial J}{\partial \mathbf{W}_{ij}^{(\ell)}} = \sum_{k=1}^{d_\ell} \frac{\partial J}{\partial z_k^{(\ell)}} \frac{\partial z_k^{(\ell)}}{\partial \mathbf{W}_{ij}^{(\ell)}} = x_i^{(\ell-1)} \frac{\partial J}{\partial z_j^{(\ell)}} = x_i^{(\ell-1)} \delta_j^{(\ell)}$$

$$\boxed{\nabla_{\mathbf{W}^{(\ell)}}[J] = x^{(\ell-1)'} {\delta^{(\ell)}}^T}$$

BACK PROPAGATION TERM

- To find $\delta^{(\ell)} = \nabla_{z^{(\ell)}}[J]$, apply the chain rule again:

$$\frac{\partial J}{\partial z_i^{(\ell-1)}} = \frac{\partial J}{\partial x_i^{(\ell-1)}} \frac{\partial x_i^{(\ell-1)}}{\partial z_i^{(\ell-1)}} = \frac{\partial J}{\partial x_i^{(\ell-1)}} \theta^{(\ell-1)'}\left(z_i^{(\ell-1)}\right)$$

- $$\frac{\partial J}{\partial x_i^{(\ell-1)}} = \sum_{j=0}^{d_\ell} \frac{\partial J}{\partial z_j^{(\ell)}} \frac{\partial z_j^{(\ell)}}{\partial x_i^{(\ell-1)}} = \sum_{j=0}^{d_\ell} \delta_j^{(\ell)} \mathbf{W}_{ij}^{(\ell)} = \left(\mathbf{W}^{(\ell)} \delta^{(\ell)}\right)_i$$

$$\boxed{\delta_i^{(\ell-1)} = \theta^{(\ell-1)'}\left(z_i^{(\ell-1)}\right)\left(\mathbf{W}^{(\ell)} \delta^{(\ell)}\right)_i}$$

BACK PROPAGATION ALGORITHM

- We know $x^{(0)}$ and the current values of $\mathbf{W}^{(1)}, \dots, \mathbf{W}^{(L)}$
- If we do a forward pass through the neural network, we will compute every $x^{(1)}, \dots, x^{(L)}$ and $z^{(1)}, \dots, z^{(L)}$
- From the linear classifier, we know that $\delta^{(L)} = x^{(L)} - y$
- $\theta^{(\ell-1)'}\left(z_i^{(\ell-1)}\right)$ is easy to compute
- We have all we need to do stochastic gradient descent!

BACK PROPAGATION ALGORITHM

- Fix a learning rate η and initialize $\mathbf{W}^{(1)}, \ldots, \mathbf{W}^{(L)}$ randomly
- For each data point $(x^{(0)}, y)$ in the data set
  - Compute each $z^{(\ell)} = \mathbf{W}^{(\ell)^T} x^{(\ell-1)'}$ and $x^{(\ell)} = \theta^{(\ell)}\left(z^{(\ell)}\right)$
  - Initialize $\delta^{(L)} = x^{(L)} - y$
  - For each ℓ counting down from L to 1
    - Calculate $\alpha^{(\ell)} = \nabla_{x^{(\ell-1)}}[J] = \mathbf{W}^{(\ell)}\delta^{(\ell)}$
    - Set $\delta_i^{(\ell-1)} = \alpha_i^{(\ell)}\theta^{(\ell-1)'}\left(z_i^{(\ell-1)}\right)$ for each $i = 1, \ldots, d_{\ell-1}$
    - Update $\mathbf{W}^{(\ell)} \leftarrow \mathbf{W}^{(\ell)} - \eta\left(x^{(\ell-1)}\delta^{(\ell)^T}\right)$

BACKPROPAGATION

- Forward pass
  - We are given $x^{(0)}$
  - $x^{(\ell+1)}$ depends on $z^{(\ell+1)}$, which depends on $x^{(\ell)}$
- Backward pass
  - We have $\delta^{(L)}$ from the forward pass
  - $\delta^{(\ell-1)}$ depends on $\delta^{(\ell)}$
  - We need $\delta^{(\ell)}$ because $\nabla_{\mathbf{W}^{(\ell)}}[J]$ depends on $\delta^{(\ell)}$

BACKPROPAGATION

- This is stochastic gradient descent for a neural network!
- In Homework #5, you will:
  - Implement a linear classifier
  - Extend it to a 2-layer neural network using "minibatch" SGD
- Before discussing implementation details, let's talk about parallelizing the backpropagation algorithm

PARALLELIZATION

- By its nature, the backpropagation algorithm seems fundamentally sequential
- However, each sequential step is a linear algebra operation
  - Parallelize with cuBLAS
- Minibatch stochastic gradient descent
  - Compute the gradient for each data point in the minibatch
  - Use a parallel reduction to take the average at the end

USING MINIBATCHES

- Consider a minibatch size of k
  - Construct a $d_\ell \times k$ matrix $\mathbf{X}^{(\ell)}$ where column i is the $x^{(\ell)}$ corresponding to data point i in the mini-batch
  - Construct a $d_\ell \times k$ matrix $\Delta^{(\ell)}$ where column i is the $\delta^{(\ell)}$ corresponding to data point i in the mini-batch
  - Define $\mathbf{Z}^{(\ell)} = \mathbf{W}^{(\ell)^T} \mathbf{X}^{(\ell-1)'}$
- After fixing a learning rate η and initializing $\mathbf{W}^{(1)}, \ldots, \mathbf{W}^{(\ell)}$ randomly, we have the following algorithm:

USING MINIBATCHES

- For each minibatch $(\mathbf{X}^{(0)}, \mathbf{Y})$ of size k in the data set
  - Compute each $\mathbf{Z}^{(\ell)} = {\mathbf{W}^{(\ell)}}^T \mathbf{X}^{(\ell-1)}$ and $\mathbf{X}^{(\ell)} = \theta^{(\ell)}\left(\mathbf{Z}^{(\ell)}\right)$
  - Initialize $\Delta^{(L)} = \mathbf{X}^{(L)} - \mathbf{Y}$
  - For each ℓ counting down from L to 1
    - Calculate $\mathbf{A}^{(\ell)} = \nabla_{\mathbf{X}^{(\ell-1)}}[J] = \mathbf{W}^{(\ell)} \Delta^{(\ell)}$
    - Set $\Delta_{ij}^{(\ell-1)} = \mathbf{A}_{ij}^{(\ell)} \theta^{(\ell-1)'}\left(\mathbf{Z}_{ij}^{(\ell-1)}\right)$ for all $i = 1, \ldots, d_{\ell-1}$ and $j = 1, \ldots, k$
    - Update $\mathbf{W}^{(\ell)} \leftarrow \mathbf{W}^{(\ell)} - \frac{1}{k}\eta\left(\mathbf{X}^{(\ell-1)'} {\Delta^{(\ell)}}^T\right)$

IMPLEMENTATION

- You can do all the matrix multiplications using cuBLAS
- The only new computation is $\Delta_{ij}^{(\ell-1)} = \mathbf{A}_{ij}^{(\ell)} \theta^{(\ell-1)'} \left(\mathbf{Z}_{ij}^{(\ell-1)}\right)$
- This differentiation and pointwise multiplication step (and much more) is done for you for free by another CUDA package called cuDNN (Deep Neural Nets)
- Next time, you will learn the basics of cuDNN