Lecture 1: Introduction

Why Deep Learning?

- Hard-coded features are time-consuming, brittle, and not scalable practically
    - Developing heuristics are expensive

Why Now?

1. Big Data

- Larger datasets, easier to access and store

2. Hardware

- GPUs exist, are highly parallizable

3. Software

- Improved techniques, new models, better frameworks

The Fundamental Unit of a Neural Network: Perceptron

- Inputs to a perceptron: $x_1 \dots x_n$
- Each input is weighted: $\theta_1 \dots \theta_n$
- θ_0 is a bias unit
- $g(x)$ is a nonlinear function, called an *activation function*
- Formula to calulate output (non-vectorized):

$\hat{y} = g(\theta_0 + \sum_{i=1}^{m} x_i \theta_i)$

- Vectorized version:

$\hat{y} = g(\theta_0 + X^\top \theta)$

where X is a column vector of inputs and θ is a column vector of weights

- Examples of the nonlinearity $g(z)$ include:

Name	Function	Derivative	TensorFlow Function
Sigmoid	$g(z) = \frac{1}{1+\exp(-z)}$	$g'(z) = g(z)(1 - g(z))$	`tf.nn.sigmoid(z)`
Hyperbolic Tangent	$g(z) = \frac{\exp(z)+\exp(-z)}{\exp(z)+\exp(-z)}$	$g'(z) = 1 - g(z)^2$	`tf.nn.tanh(z)`
Rectified Linear Unit (ReLU)	$g(z) = \max(0, z)$	$g'(z) = 1$ if $x > 0$ or 0 otherwise	`tf.nn.relu(z)`

Why Activation Functions?

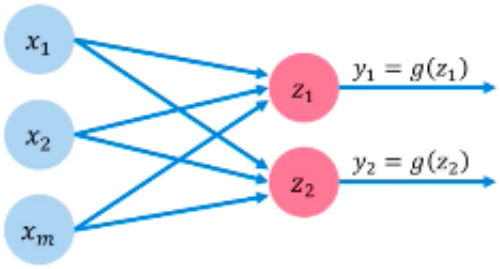
- Introduces non-linearities into the network
- Otherwise the network can only produce linear decisions (regardless of network size)
- Having non-linearities allows modeling of any complex function

Building Neural Networks Using Perceptrons

Simplified Pereptron

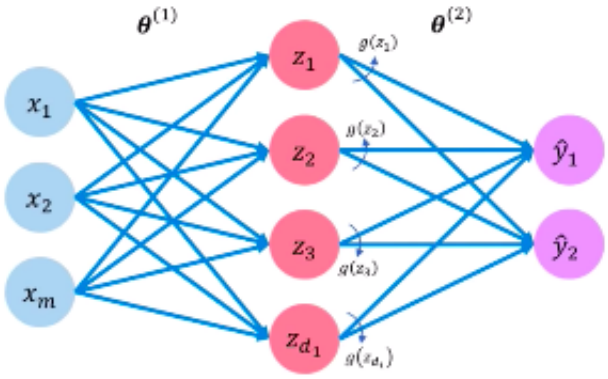
- Remove the bias term, remove weights for simplicity
- $z = \theta_0 + \sum_{j=1}^{m} x_j \theta_j$
- Output of perceptron: $y = g(z)$

Multi-Output Perceptron



- Inputs are still $x_1 \dots x_m$, with each input connected to two units, z_1 and z_2, which produce outputs y_1 and y_2
- Formula for each unit is $z_i = \theta_{0,i} + \sum_{j=1}^{m} x_j \theta_{j,i}$

Single-Layer Neural Network



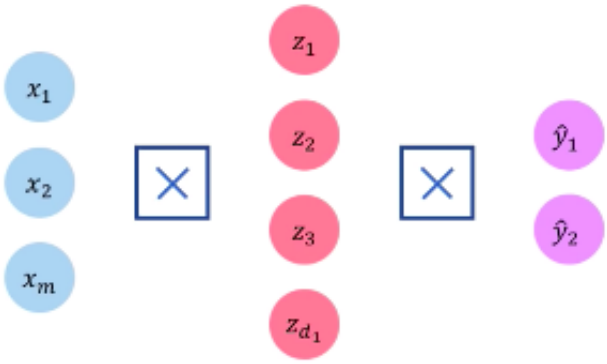
- Not a "deep" NN, it's "shallow"
- Allows for a transformation from input space → hidden unit space → output space
- Formula for hidden units is:

$$z_1 = \theta_{0,i}^{(1)} + \sum_{j=1}^{m} x_j \theta_{j,i}^{(1)}$$

- Formula for output units is:

$$\hat{y}_i = \theta_{0,i}^{(2)} + \sum_{j=1}^{m} x_j \theta_{j,i}^{(2)}$$

- These layers are *fully connected*, meaning every unit in the previous layer is connected to every unit in the next layer
    - Denoted as $\times$, as shown below



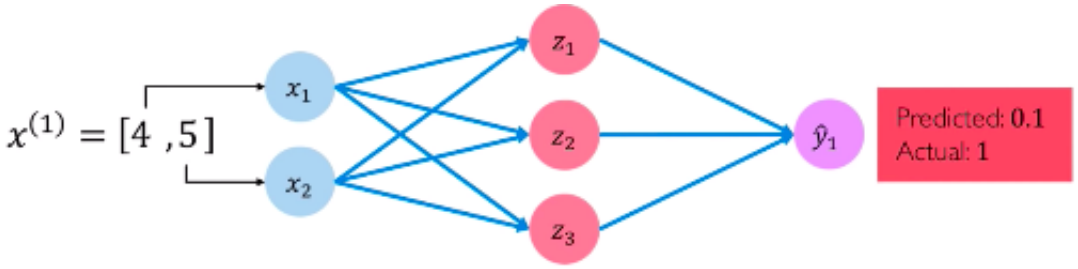
Deep Neural Network

- Just a stack of layers, same method

Applying Neural Networks

Example: Will I Pass This Class?

- Two features: x_1 (# of lectures attended), x_2 (hours spent on final project)
- We want to know if a new person passed or failed the class
- For a feature vector $x^{(1)} = [4, 5]$, we got a prediction 0.1



- Why is this so? This network has never been trained

Quantifying Loss

- We need to find out how "off" we are from the actual
- The *loss* of a network measures the cost incurred from an incorrect prediction
  - Thought of as a "distance" between actual and predicted output
- Denoted as $\mathcal{L}(f(x^{(i)};\theta), y^{(i)})$
- Low loss = close to actual

Empirical Loss

- *Empirical loss* measures total loss over entire dataset.
- Also known as objective function/cost function/empirical risk
- Calculated as $J(\theta) = \frac{1}{n}\sum_{i=1}^{n} \mathcal{L}(f(x^{(i)};\theta), y^{(i)})$

Softmax Cross-Entropy Loss

- A type of loss function that can be used with models that predict a value in $(0, 1)$ (i.e. a probability)
- Calculated as:

$$J(\theta) = \frac{1}{n}\sum_{i=1}^{n} y^{(i)} \log\Big(f(x^{(i)};\theta)\Big) + (1 - y^{(i)}) \log\Big(1 - f(x^{(i)};\theta)\Big)$$

- $y^{(i)}$ is actual, while $f(x^{(i)};\theta)$ is predicted
- In TensorFlow, the loss is found as `loss = tf.reduce_mean( tf.nn.softmax_cross_entropy_with_logits(model.y, model.pred))`

Mean Squared Error Loss

- Can be used wih regression models that produce continuous numbers $y \in \mathbb{R}$
- Calculated as:

$$J(\theta) = \frac{1}{n}\sum_{i=1}^{n} \Big(y^{(i)} - f(x^{(i)};\theta)\Big)^2$$

- In English: average of actual minus predicted squared
- In TensorFlow, MSE loss is found as: `loss = tf.reduce_mean(tf.square(tf.subtract(model.y, model.pred)))`

Training Neural Networks

- We want to find the weights θ that give us the lowest loss
- Our goal: $\theta^* = \text{argmin}_\theta J(\theta)$
- Steps towards gradient descent:
  - Step 1: Randomly initialize θ, usually with distribution $\mathcal{N}(0, 1)$
  - Step 2: Compute gradient $\frac{\partial J(\theta)}{\partial \theta}$ (aka $\nabla J(\theta)$)
    - Tells us the direction of highest descent
  - Step 3: Step in opposite of gradient (negate gradient)
  - Step 4: Repeat Steps 1-3 until convergence
- Psuedocode:

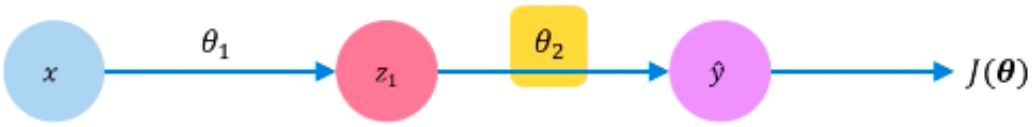
1. Initialize weights randomly ~$\mathcal{N}(0, \sigma^2)$
2. Loop until convergence:
3. Compute gradient $\frac{\partial J(\theta)}{\partial \theta}$
4. Update weights $\theta \leftarrow \theta - \eta \frac{\partial J(\theta)}{\partial \theta}$
5. Return weights

- TensorFlow pseudocode:

```
weights = tf.random_normal(shape, stddev=sigma)
while not converged:
    grads = tf.gradients(ys=loss, xs=weights)
    weights_new = weights.assign(weights - lr * grads)
return weights
```

How to Compute Gradients?

- Let's look at a simplified example:



- Let's calculate the gradient of $J(\theta)$ with respect to θ_2
  - $\frac{\partial J(\theta)}{\partial \theta} = \frac{\partial J(\theta)}{\partial \hat{y}} * \frac{\partial \hat{y}}{\partial \theta_2}$ because of Chain Rule
- Repeat this for every weight in all layers: backprop

Neural Networks in Practice: Optimization

- However, most NN cost functions are actually non-convex, making them susceptible to local minima
- Setting the learning rate η is extremely hard
  - Small learning rates converge slowly and are susceptible to local minima
  - Large learning rates overshoot and may diverge
  - Stable learning rates converge smoothly while avoiding local minima
- Ways to mitigate?
  - Try a bunch of different η, see what works
  - Design an adaptive learning rate that "adapts" to the landscape

Adaptive Learning Rates

- η is not fixed
- Can be adjusted based on:
  - how large gradient is
  - how fast learning is happening
  - size of weights
  - and more
- Examples of Adapting LR Algorithms:
  - Momentum (`tf.train.MomentumOptimizer`)
  - Adagrad (`tf.train.AdagradOptimizer`)
  - Adadelta (`tf.train.AdadeltaOptimizer`)
  - Adam (`tf.train.AdamOptimizer`)
  - RMSProp (`tf.train.RMSPropOptimizer`)
- TODO: Read <ruder.io/optimizing-gradient-descent>

Neural Networks in Practice: Minibatches

- Computing the gradient is computationally expensive on big datasets
- Stochastic GD:

1. Initialize weights randomly ~$\mathcal{N}(0, \sigma^2)$
2. Loop until convergence:
3. Pick single data point i
4. Compute gradient estimate $\frac{\partial J(\theta)}{\partial \theta}$
5. Update weights $\theta \leftarrow \theta - \eta \frac{\partial J(\theta)}{\partial \theta}$
6. Return weights

- While it's easy to compute, it's very noisy (stochastic)
- Minibatch GD:

1. Initialize weights randomly ~$\mathcal{N}(0, \sigma^2)$

2. Loop until convergence:
3. Pick batch of B data points
4. Compute gradient estimate $\frac{\partial J(\theta)}{\partial \theta} = \frac{1}{B} \sum_{k=1}^{B} \frac{\partial J_k(\theta)}{\partial \theta}$
5. Update weights $\theta \leftarrow \theta - \eta \frac{\partial J(\theta)}{\partial \theta}$
6. Return weights

- Minibatches will allow us to:
    - Have an accurate estimation of the gradient with smoother convergence and ability to have higher η
    - Parallelize training to make it faster (especially on GPUs and clusters)

Neural Networks in Practice: Overfitting

- Underfitting = model does not have the capacity to fully learn data
- Ideal fit = model can generalize well on new data
- Overfitting = too complex and does not generalize well
- Regularization = technique that constrains optimization to discourage overly complex models

Regularization Using Dropout

- During training, randomly set some activations to 0
    - Usually "drop" 50% of activations in layer
    - Forces network to not rely on any one node
    - TF code: `tf.nn.dropout(hiddenLayer, p=0.5)`

Regularization Using Early Stopping

- Stop training before overfitting

Acknowledgements

- Diagrams screenshotted from MIT 6.S191 2018 slides