Neural Network Training With Gradient Descent

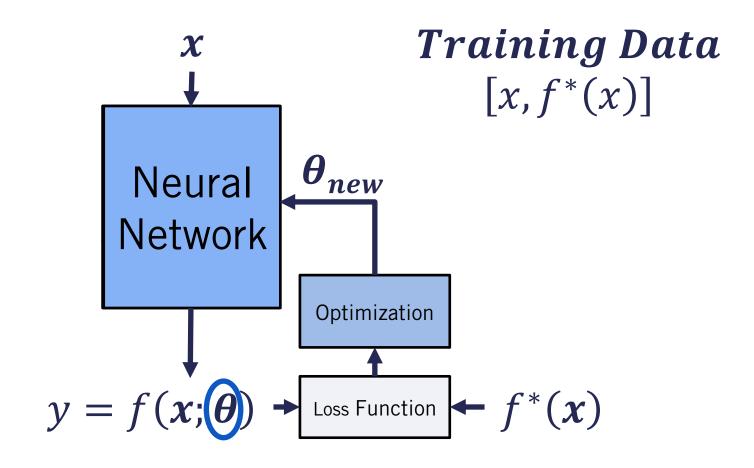
Course 3, Module 3, Lesson 3



Learning Objectives

- Learn how to train a neural network using the iterative optimization algorithm: gradient descent
- Learn how to initialize parameters at the start of the optimization process

Artificial Neural Networks



Neural Network Loss Functions

- Thousands of training example pairs $[x, f^*(x)]$
- The **Loss function** computed over all **N** training examples is termed the **Training Loss** and can be written as:

$$J(\theta) = \frac{1}{N} \sum_{i=1}^{N} L[f(x_i, \theta), f^*(x_i)]$$

• The gradient of the training loss with respect to the parameters θ can be written as:

$$\nabla_{\theta} J(\theta) = \nabla_{\theta} \left[\frac{1}{N} \sum_{i=1}^{N} L[f(x_i, \theta), f^*(x_i)] \right] = \frac{1}{N} \sum_{i=1}^{N} \nabla_{\theta} L[f(x_i, \theta), f^*(x_i)]$$

Batch Gradient Descent

Batch Gradient Descent is an iterative first order optimization procedure

Batch Gradient Descent Algorithm:

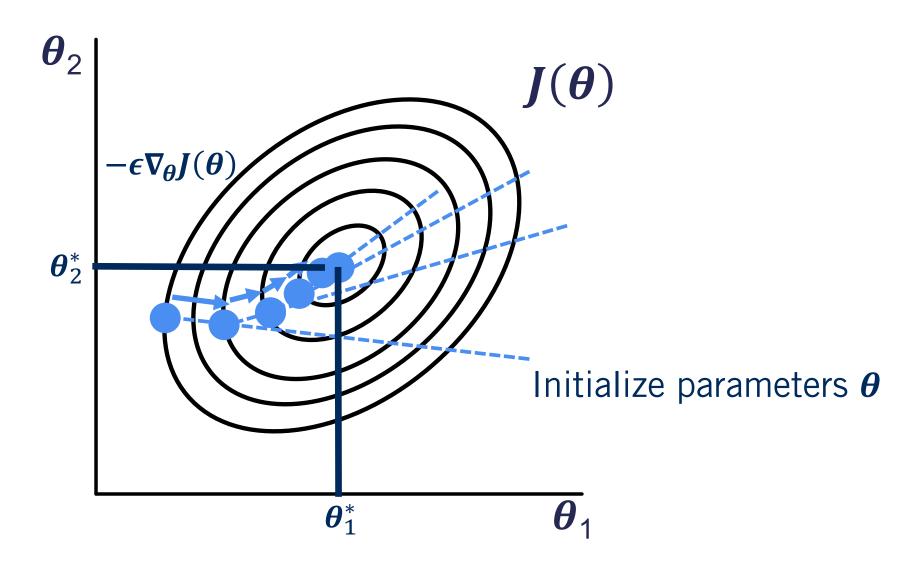
- \circ Initialize parameters θ
- While Stopping Condition is Not Met:
 - Compute gradient of loss function over all training examples:

$$\nabla_{\theta} J(\theta) = \frac{1}{N} \sum_{i=1}^{N} \nabla_{\theta} L[f(x_i, \theta), f^*(x_i)]$$

Update parameters according to:

$$\theta \leftarrow \theta - \epsilon \nabla_{\theta} J(\theta)$$

Batch Gradient Descent



Parameter Initialization and Stopping Conditions

Parameter Initialization:

- Weights: initialized by randomly sampling from a standard normal distribution
- Biases: initialized to 0
- Other heuristics exist

Stopping Conditions:

- Number of iterations: How many training iterations the neural network has performed
- \circ Change In θ value: Stop if $\theta_{new} \theta_{old} <$ Threshold
- o Change In $J(\theta)$ value: Stop if $J(\theta_{new}) J(\theta_{old}) <$ Threshold

Batch Gradient Descent

• Backpropagation used to compute $\nabla_{\theta} J(\theta)$ is very expensive to compute over the whole training dataset.

$$\nabla_{\boldsymbol{\theta}} \boldsymbol{J}(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i}^{N} \nabla_{\boldsymbol{\theta}} L \left[f_i(x, \boldsymbol{\theta}), f_i^*(x) \right]$$
 is a mean!

- Standard error of the mean estimated from N samples is $\frac{\sigma}{\sqrt{N}}$, where σ is the standard deviation of the value of the samples
- Using all samples to estimate the gradient results in less than linear return in accuracy of this estimate
- Use a **small subsample (Minibatch)** of the training data to estimate the gradient!

Stochastic (minibatch) Gradient Descent

• Stochastic (minibatch) Gradient Descent Algorithm:

- \circ Initialize parameters $\boldsymbol{\theta}$
- While Stopping Condition is False:
 - 1. Sample a preset number N' of examples (minibatch) from the training data
 - 2. Compute gradient of Loss Function Over **all** training examples:

$$\nabla_{\theta} J(\theta) = \frac{1}{N'} \sum_{i}^{N'} \nabla_{\theta} L \left[f_i(x, \theta), f_i^*(x) \right]$$

3. Update parameters according to:

$$\theta \leftarrow \theta - \epsilon \nabla_{\theta} J(\theta)$$

What Minibatch Size To Use?

- GPUs work better with powers of 2 batch sizes
- Large batch sizes > 256:
 - Hardware underutilized with very small batch sizes.
 - More accurate estimate of the gradient, but with less than linear returns
- Small batch size < 64
 - Small batches can offer a regularizing effect. The best generalization error is often achieved with batch size of 1.
 - Small batch sizes allow for faster convergence, as the algorithm can compute the parameter updates rapidly
- Always make sure dataset is shuffled before sampling minibatch

SGD Variations

- Many variations of SGD exist
 - Momentum SGD, Nestrove Momentum SGD
 - o Ada-Grad, RMS-Prop
 - ADAM (Adaptive Moment Estimation)
- Which one to use?
 - ADAM: Implemented in most deep neural network libraries, fairly robust to the choice of the learning rate and other hyperparameters
- http://deeplearningbook.org

Summary

- You can optimize for neural network parameters using batch gradient descent
- When the number of training examples is extremely large, you can use minibatch (stochastic) gradient descent
- State-of-the-art optimization algorithms built on top of SGD are implemented in most neural network libraries
- Next: Dataset Splits and Neural Network Performance Evaluation