Optimization

Reading

- Deep Learning: chapters 4.3, 6.5, 8
  - https://www.deeplearningbook.org/contents/optimization.html

- Optimization overview, with a deep learning bias

Optimization Overview

- Optimization is a very large research field (typically taught/studied in engineering departments)
- Many tasks can be formulated as an optimization problem
  - Allocating different people to different jobs to maximize productivity
  - Choosing the best control action for your autonomous car
  - Finding the best parameters for your neural network
- Standard form

$$\begin{aligned} \underset{\boldsymbol{x}}{\text{minimize}} \quad & f(\boldsymbol{x}) \\ subject\ to \quad & g(\boldsymbol{x}) \leq C \end{aligned}$$

- Optimization is either minimization or maximization

Optimization in ML

- The optimization problem in ML is indirect
  - Want to perform well according to metric P (e.g., classification accuracy) but optimize some loss L (e.g., least squares)
  - Want to maximize performance on true data distribution but can only maximize performance on sampled data

Empirical Risk Minimization

- Expected value of loss function is called **risk** in ML

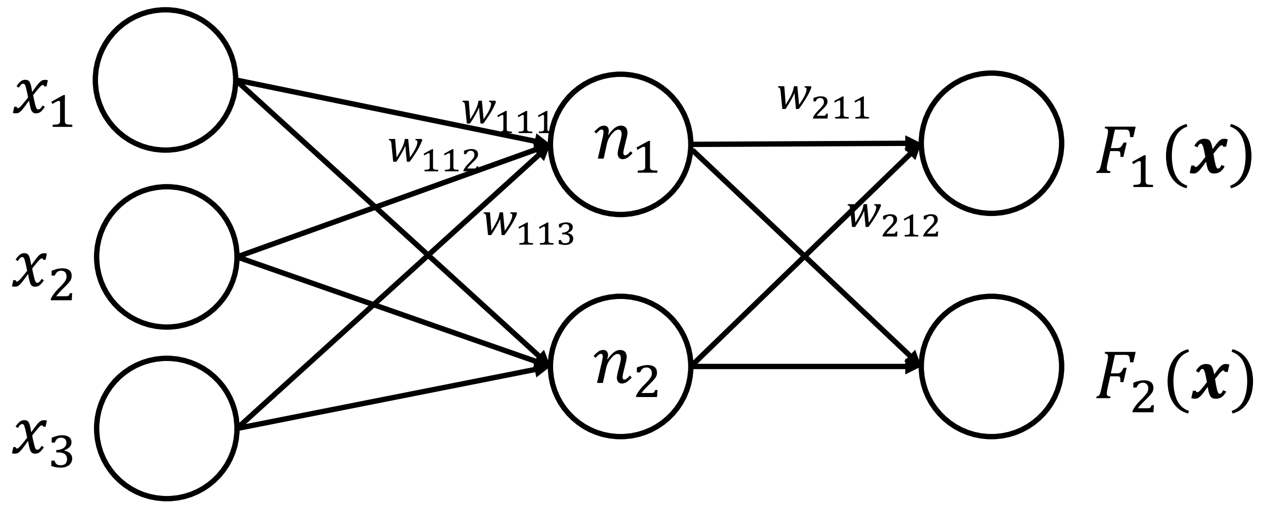
$$J(\boldsymbol{\theta}) = \mathbb{E}_{(\boldsymbol{X},Y)\sim\mathbb{P}_{population}} L(f(\boldsymbol{X};\boldsymbol{\theta}),Y)$$

- **Empirical risk** is the average of the loss function over dataset

$$\mathbb{E}_{(\boldsymbol{X},Y)\sim\mathbb{P}_{data}} L(f(\boldsymbol{X};\boldsymbol{\theta}),Y) = \frac{1}{N}\sum_{i=1}^{N} L(f(\boldsymbol{x}_i;\boldsymbol{\theta}),y_i)$$

- ML is all about empirical risk minimization
- 2 challenges
  - Formulating the right minimization problem
    - Pick the architecture, loss, regularization, etc.
  - Solving the minimization problem
    - Find global optimum, scale well with more data, complex models

Setup



- A 3-input, 2-output network
  - The inputs are $\boldsymbol{x} = [x_1 \ \ x_2 \ \ x_3]$
  - The parameters are $\boldsymbol{\theta} = [w_{111}, w_{112}, w_{113}, w_{121}, w_{122}, w_{123}, w_{211}, w_{212}, w_{221}, w_{222}]$
  - No offsets in this example

Some losses are better than others

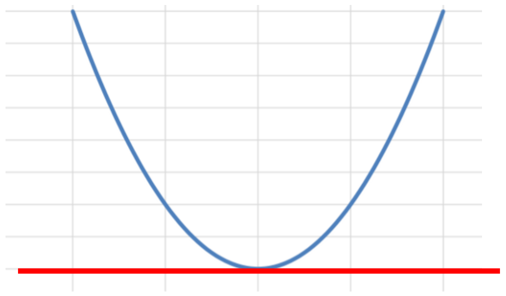
- In classification, one is tempted to choose weights that minimize a 0-1 loss (1 for incorrect classification, 0 for correct)
  - However, picking the weights that minimize 0-1 loss is a hard computational task
- Other losses often more efficient
  - E.g., NLL is a smooth function of the data, which makes it easier to minimize
- Cannot compute solution in closed form for any loss, e.g.,

$$min_{\boldsymbol{\theta}} \frac{1}{N} \sum_{i=1}^{N} (y_i - f(\boldsymbol{x}_i; \boldsymbol{\theta}))^2$$

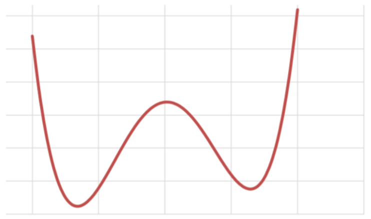
  - Also, NN makes the loss functions non-convex
  - Why would convexity be a nice property?

Gradient Descent Idea

- Section 4.3 in the book
  - Gradient is the word for derivate in higher dimensions
- Some functions can be minimized in closed form
  - E.g., convex functions are minimized when derivative is 0

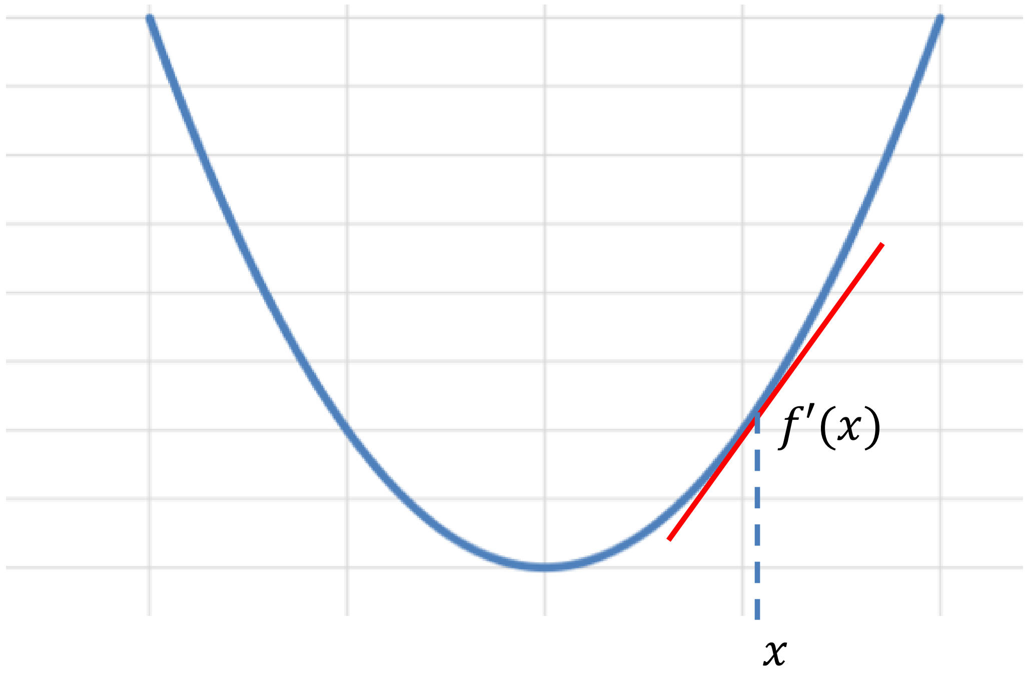


- Hard to find root of derivative in most cases
- Also, most functions are not convex (including neural nets)



Gradient Descent, cont'd

- If you can't find the root of the derivative, you can try to iteratively minimize the function
  - Start from some x, compute $f'(x)$ and make a step in the opposite direction
  - We know that $f\left(x - \epsilon f'(x)\right) < f(x)$ for small ϵ
    - ϵ is learning rate



Gradient Descent, cont'd

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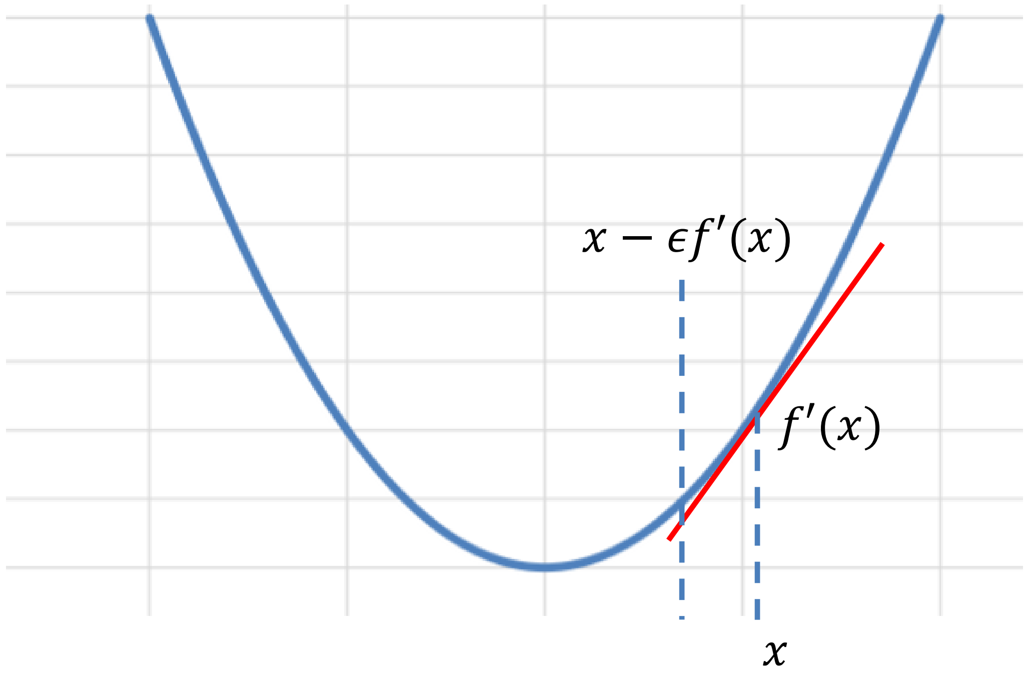


Aside: Vector Calculus

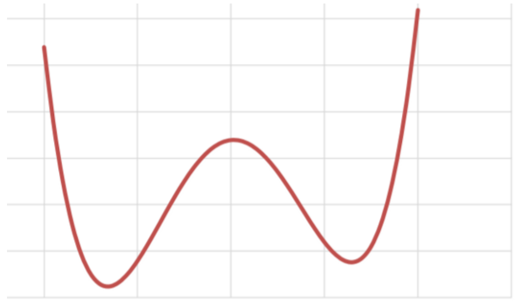
- Suppose we are given a function $f: \mathbb{R}^n \rightarrow \mathbb{R}$
- What is the derivative of f?
- When $n = 1$, it is just the partial derivative $f' = \frac{\partial f}{\partial x}$
- When $n > 1$, the derivative is a vector of all partial derivatives:

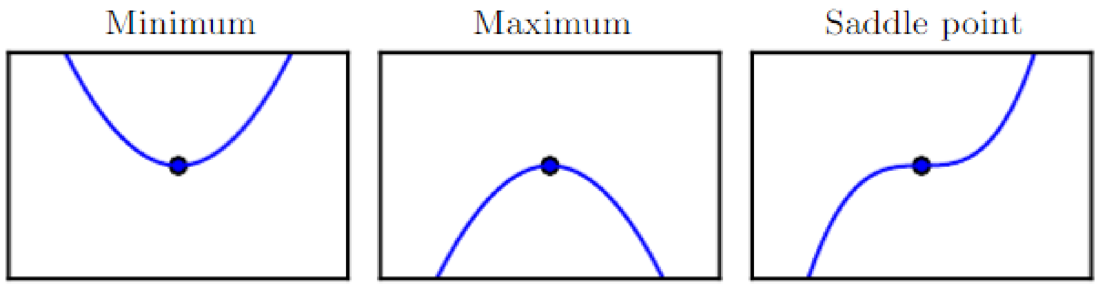
$$\nabla_{\boldsymbol{x}} f = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \cdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix}$$

  – This is called the "gradient" of f
  – The gradient is the multi-dimensional extension of the derivative

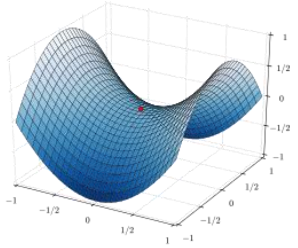
Gradient Descent, cont'd

- What about non-convex functions?
  - Can easily get stuck in a local min
- What about saddle points?
  - Derivative can be very small
  - Major concern in high-dimensional spaces





Source: wikipedia



- Despite all these limitations, neural network training usually finds a good local minimum
  - Beware: larger networks can easily minimize the loss and overfit (more on this next)

Back Propagation

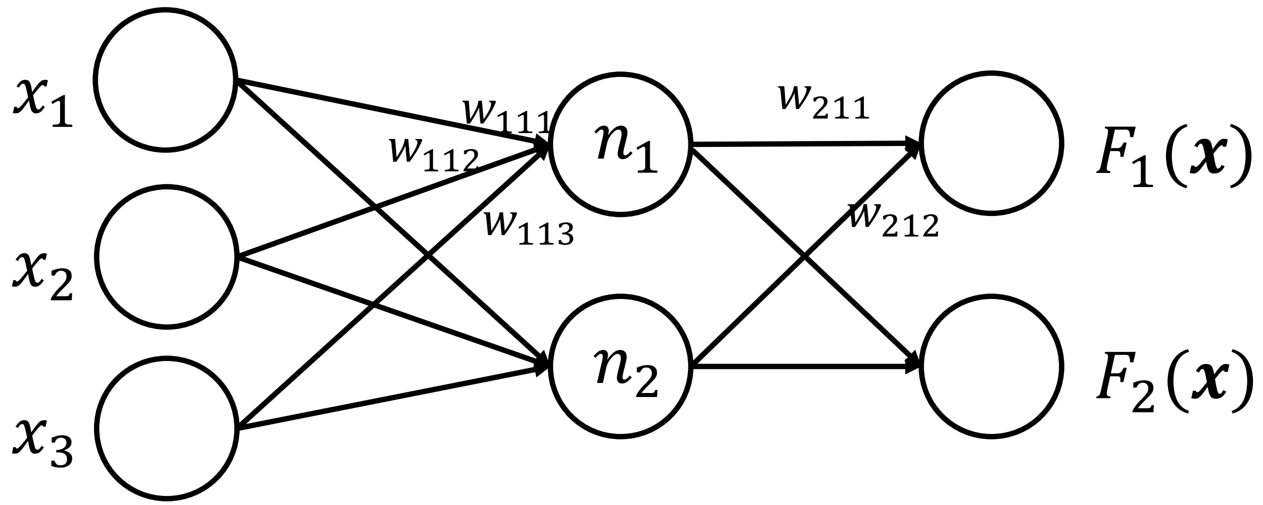
- An algorithm for computing gradients quickly
  - This is what makes deep learning so efficient
  - No need to worry about it too much – implemented in deep learning libraries
  - But good to understand it when choosing an architecture/loss combination
- Computing NN derivatives involves multiple repeated expressions
  - Backprop is an efficient way of reusing previously computed values

Computing NN derivatives is a massive chain rule

Rensselaer

- Most derivates have interesting properties
    - $\sigma'(x) = \sigma(x)\big(1 - \sigma(x)\big)$
    - $\tanh'(x) = 1 - \tanh^2(x)$
    - $ReLU'(x) = Step(x) := \begin{cases} 0 \; if \; x \leq 0 \\ 1 \; if \; x > 0 \end{cases}$
- Most derivatives can be expressed in terms of the original function
    - Also appear multiple times

Example



- Suppose we have a two-neuron neural network with 3 inputs and 2 outputs
  - ReLU activation in hidden layer and linear last layer
- Suppose loss is least squares (assume $y_i \in \{0,1\}$)

$$\frac{1}{N}\sum_{i=1}^{N}(y_i - F_1(\boldsymbol{x}_i))^2 + \left((1 - y_i) - F_2(\boldsymbol{x}_i)\right)^2$$

Example, cont'd

Rensselaer

- To compute the gradient, need to compute partial derivative w.r.t. each weight
- Start with w_{111}
- The partial derivative of the first term in the sum is

$$\frac{\partial (y_i - F_1(\boldsymbol{x}_i))^2}{\partial w_{111}} = -2(y_i - F_1(\boldsymbol{x}_i))\frac{\partial F_1(\boldsymbol{x}_i)}{\partial w_{111}}$$

$$\frac{\partial F_1(\boldsymbol{x}_i)}{\partial w_{111}} = \frac{\partial (w_{211} n_1(\boldsymbol{x}_i) + w_{212} n_2(\boldsymbol{x}_i))}{\partial w_{111}} = w_{211}\frac{\partial n_1(\boldsymbol{x}_i)}{\partial w_{111}}$$

Example, cont'd

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$$\frac{\partial n_1}{\partial w_{111}} = \frac{\partial ReLU(w_{111} x_{i1} + w_{112} x_{i2} + w_{113} x_{i3})}{\partial w_{111}}$$

$$= x_{i1} Step(w_{111} x_{i1} + w_{112} x_{i2} + w_{113} x_{i3})$$

Example, cont'd

- Thus, the partial derivative of the 1st term w.r.t. w_{111} is
  $-2(y_i - F_1(\boldsymbol{x}_i))w_{211}x_{i1}Step(w_{111}x_{i1} + w_{112}x_{i2} + w_{113}x_{i3})$
- The partial derivative of the 1st term w.r.t. w_{112} is
  $-2(y_i - F_1(\boldsymbol{x}_i))w_{211}x_{i2}Step(w_{111}x_{i1} + w_{112}x_{i2} + w_{113}x_{i3})$
- …
- Thus, the partial derivative of the 2nd term w.r.t. w_{111} is

$-2((1 - y_i) - F_2(\boldsymbol{x}_i))w_{221}x_{i1}Step(w_{111}x_{i1} + w_{112}x_{i2} + w_{113}x_{i3})$

- …
- Need to do this for all weights and for all datapoints
  - Many repeated terms, especially for big NNs

General setup: one-hot encoding

- To make writing losses easier, the training labels are often stored as one-hot encodings
- Suppose we have a label y_i
  - The one-hot encoding is $\boldsymbol{y}_i = [0\ \ 0\ \ \ldots\ \ 1\ \ 0\ \ \ldots\ \ 0]$
  - With a 1 in position y_i
- Thus, $\boldsymbol{y}_i$ has the same dimension as the NN output layer
- Can now write least squares as:

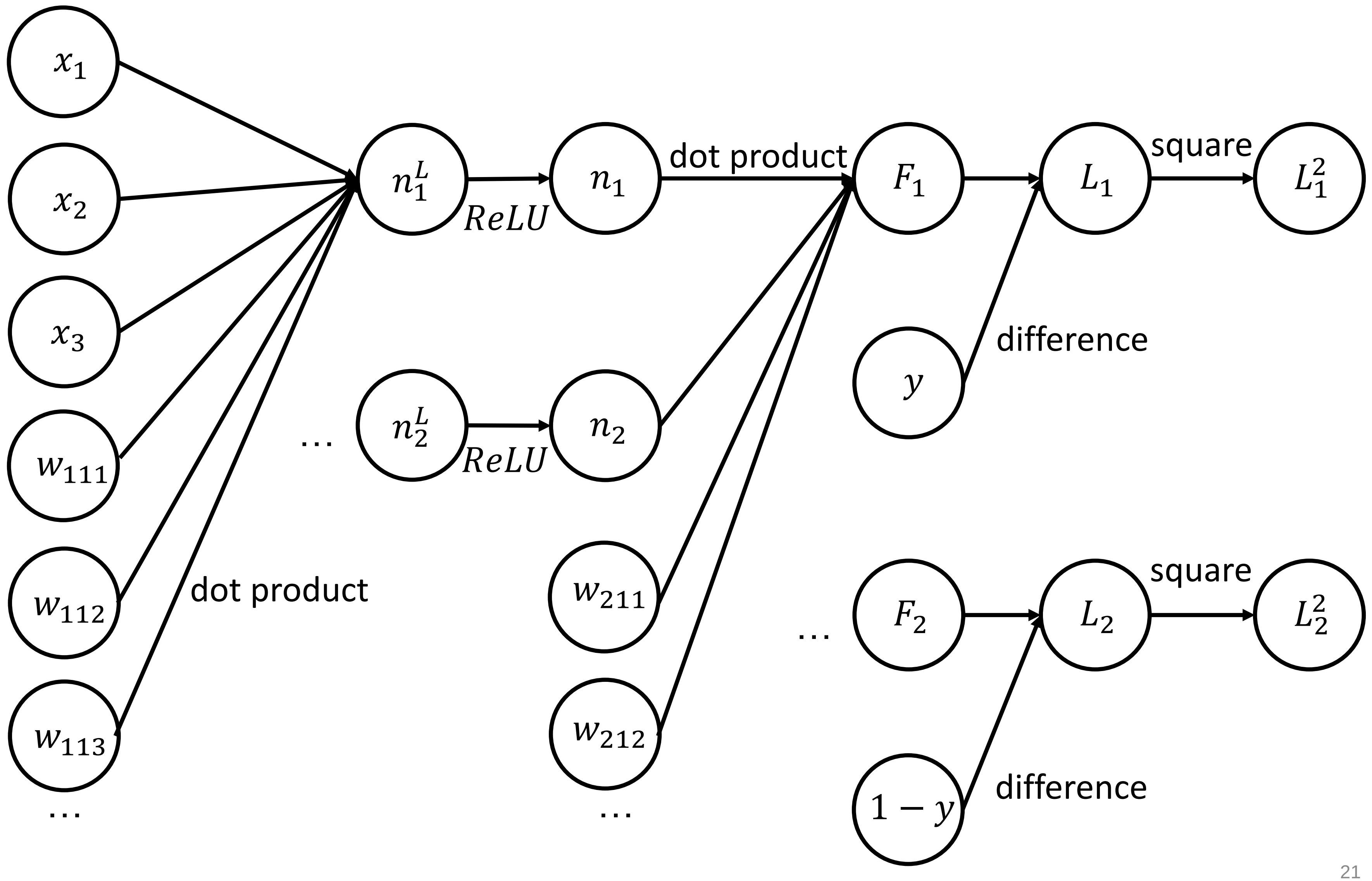
$$\sum_{i=1}^{N} ||\boldsymbol{F}(x_i) - \boldsymbol{y}_i||_2^2 = \sum_{i=1}^{N} (\boldsymbol{F}(x_i) - \boldsymbol{y}_i)^T (\boldsymbol{F}(x_i) - \boldsymbol{y}_i)$$

- Other losses can be written similarly

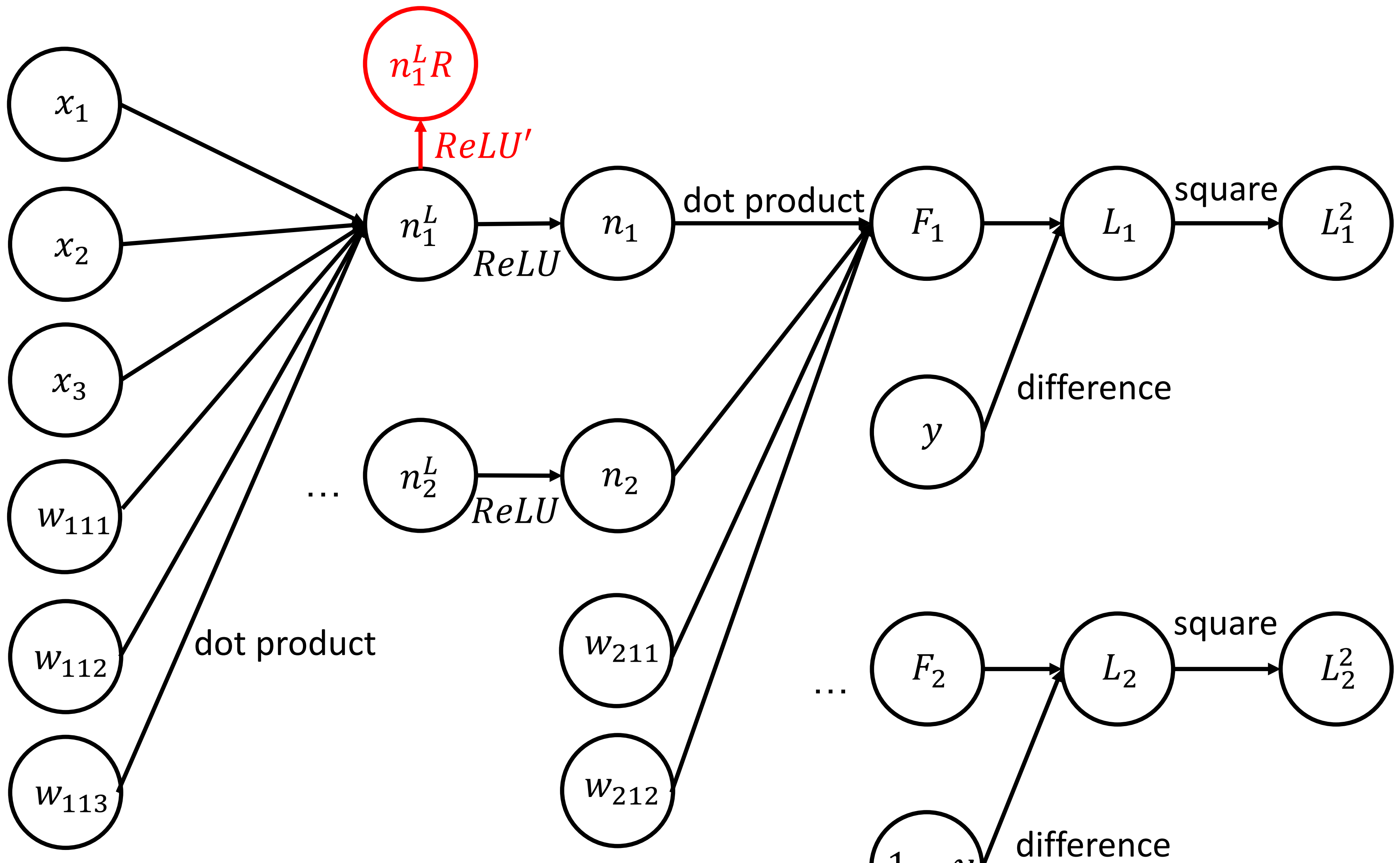
Computational Graphs

- Store all operations in a graph to be reused later
  - Nodes represent intermediate variables
  - Edges represent operations on variables
- Most derivatives appear multiple times
  - Graph representation can save a lot of time
  - Same idea as dynamic programming
- Gradient computation really involves two computations
  - Forward propagation: compute the actual value of the loss
  - Backward propagation: compute the gradient using the chain rule

Example, forward propagation



Example, backward propagation (start)



$-2(y_i - F_1(\boldsymbol{x}_i))w_{211}x_{i1}Step(w_{111}x_{i1} + w_{112}x_{i2} + w_{113}x_{i3})$

Implementation

- Many optimizations to make gradient computation fast
  - Linear operations performed on GPUs (gamers know why)
  - Variables stored as tensors (high-dimensional matrices)
- Several popular deep learning libraries
  - Mostly in python
  - Tensorflow – a bit clunky, but fairly flexible
  - Pytorch – a bit less flexible, but very easy to use
- You don’t need to worry about most of the low-level details in this lecture when implementing NNs
  - However, you need to have a good working knowledge of the low-levels if you want your code to work

Minibatch Algorithms

- A major reason for the success of deep learning
- Computing the gradient over all examples each time is too expensive
- What if use just a few examples per gradient computation?
- Randomly sample a few examples each time
  - Sample called a minibatch
  - Compute gradient on minibatch
  - Algorithm called **stochastic gradient descent (SGD)**

SGD Properties

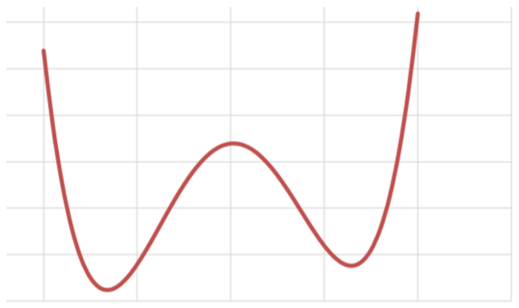
- Standard error of the gradient is $\frac{\sigma}{\sqrt{n}}$
    - σ is the true standard deviation for one example
    - n is the number of examples in the minibatch
  - Standard error decreases slowly $O\left(1/\sqrt{n}\right)$
    - Larger minibatches don't bring significant benefits
- Using minibatches also useful when data has low natural variance (why?)
  - Not usually true, but many examples may be similar
- Entire minibatch can be processed in parallel on GPU
  - The bottleneck is fitting all data in memory
- Overall, computation speedup offsets noise due to using a minibatch

Epochs

- Ideally, each minibatch is selected randomly every time
  - Nearby examples may often be correlated
  - Impractical for big datasets
- Instead, we shuffle the dataset before training and then process minibatches in order
  - Each pass of the full dataset is called an **epoch**
  - Other hyper-parameters may also change in between epochs
    - E.g., learning rate, regularization, etc.

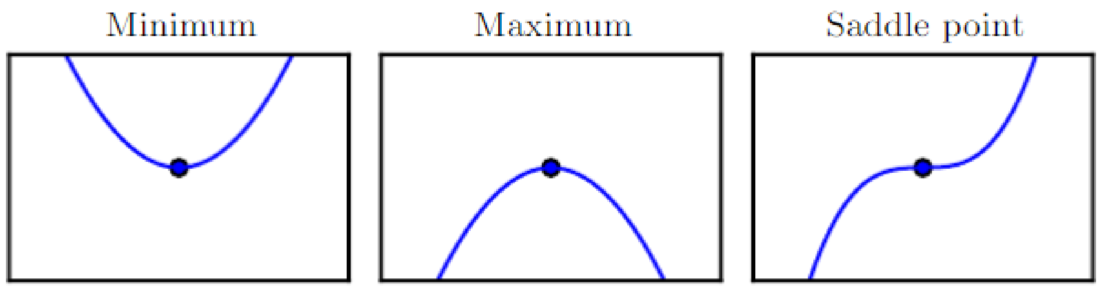
Optimization Challenges

- Local Minima
- Gradient is ~0, so no progress can be made
- Local minima are very common
  - One of the most impressive achievements of NNs is that they are able to generalize well despite using suboptimal weights
  - A possible explanation for this phenomenon is that all local minima have similar values
  - An active research area



Optimization Challenges, cont’d

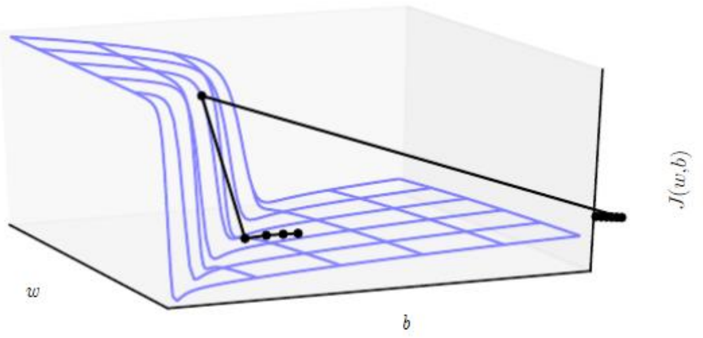
- Plateaus, saddles



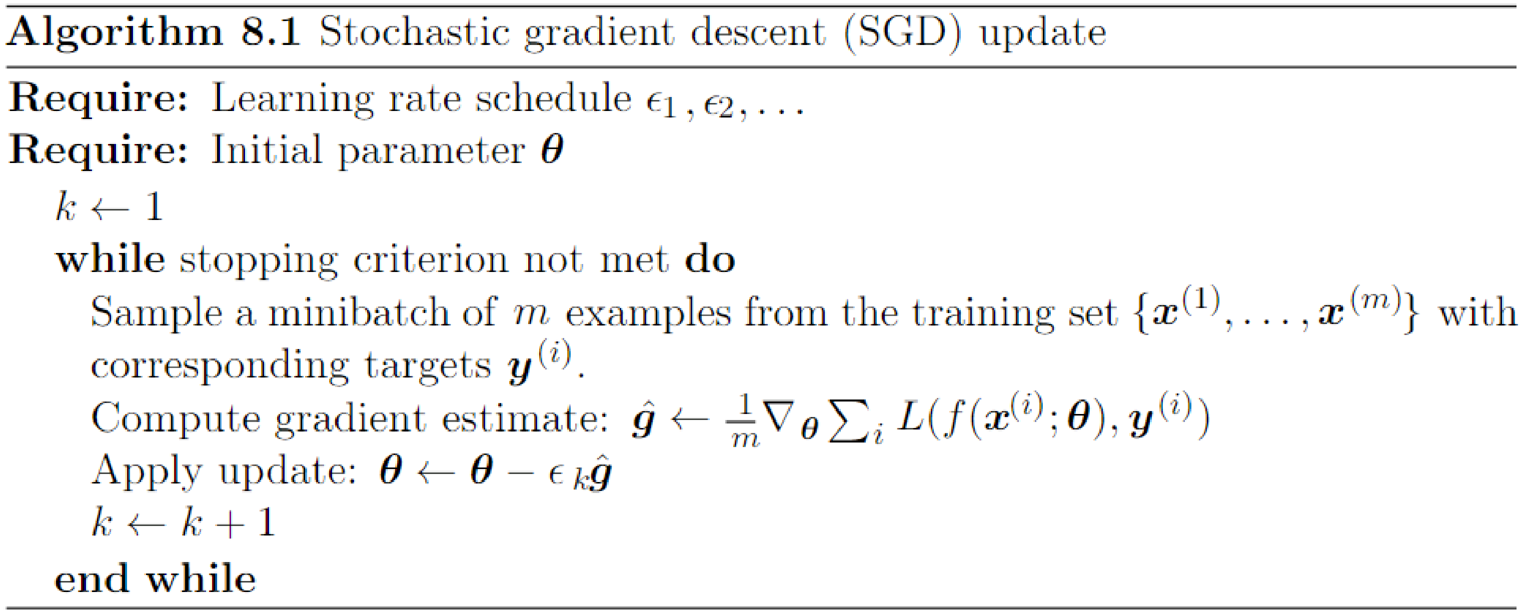
- More problematic than local minima
  - Gradient is also ~0, but loss is not low
  - Very common in high-dimensional spaces and in NN optimization
  - However, gradient descent is usually able to escape

Optimization Challenges, cont'd

- Exploding gradients
- Gradients can get very large when reaching a cliff in loss function
  - Can destabilize training (parameters jumping around)
  - Can also cause numerical issues
- Disaster can be avoided by using gradient clipping
  - If gradient norm above some threshold, reduce learning rate



SGD Summary



```
Algorithm 8.1 Stochastic gradient descent (SGD) update
Require: Learning rate schedule $\epsilon_1, \epsilon_2, \dots$
Require: Initial parameter $\boldsymbol{\theta}$
  $k \leftarrow 1$
  while stopping criterion not met do
    Sample a minibatch of $m$ examples from the training set $\{\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient estimate: $\hat{\boldsymbol{g}} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \epsilon_k \hat{\boldsymbol{g}}$
    $k \leftarrow k + 1$
  end while
```

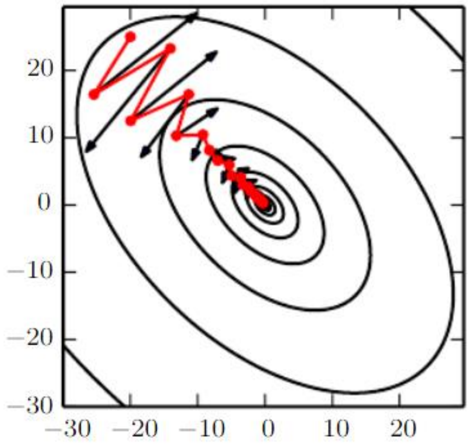
- Learning rate is usually gradually decreased to some final value
  - Linear, exponential rates of decay both work
  - Typically, you can also just keep it constant
  - What are the trade-offs between small/large learning rate?

Momentum

Algorithm 8.2 Stochastic gradient descent (SGD) with momentum

```
Require: Learning rate $\epsilon$, momentum parameter $\alpha$
Require: Initial parameter $\boldsymbol{\theta}$, initial velocity $\boldsymbol{v}$
  while stopping criterion not met do
    Sample a minibatch of $m$ examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with
    corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient estimate: $\boldsymbol{g} \leftarrow \frac{1}{m}\nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$.
    Compute velocity update: $\boldsymbol{v} \leftarrow \alpha\boldsymbol{v} - \epsilon\boldsymbol{g}$.
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}$.
  end while
```

- Descent direction is smoothed out over time in order to filter out noise due to minibatch variance
  - Essentially a low-pass filter (in signal processing terms)
  - Allows you to increase the learning rate somewhat



Parameter Initialization

- Parameter initialization may have a serious impact on training
- Unlikely to be a major issue but it could slow down training significantly
  - If you try hard, you could also find unstable initializations
- Initialization strategies are heuristics
  - Not fully clear why they work and when
  - There is also a difference between what weights are good for optimization and for generalization
  - The only thing we know for certain is to avoid the same weights across units (why?)
    - Gradients will be the same; weights will always remain the same
    - “break symmetry”

Parameter Initialization, cont'd

- Usually, we select initial weights from a Gaussian or Uniform distribution
  - Larger weights avoid the "symmetry" problem
  - Too large weights can result in exploding gradients
- Standard choices are initial uniform distributions

$$U\left(-\frac{1}{\sqrt{m}},\frac{1}{\sqrt{m}}\right),U\left(-\frac{6}{\sqrt{n+m}},\frac{6}{\sqrt{n+m}}\right)$$

  - where n is number of neurons in the layer, m is number of inputs
- Biases are initialized similarly

Batch Normalization

- Another important factor for the success of deep learning
- It is common practice to normalize all training data to be 0-mean and bounded between [-0.5, 0.5]

$$\frac{\boldsymbol{X} - \boldsymbol{\mu}}{\boldsymbol{\sigma}}$$

  – Can do the same for inputs to all hidden layers also
- Gradient descent can be brittle for deep networks
  – Updates all layers simultaneously, using a local linear approximation
  – However, the output of the NN is a non-linear (composite) function of the weights
  – Complex non-linear relationships may make it hard to choose the right learning rate

Batch Norm, cont'd

- For a given minibatch, let $\boldsymbol{H}_l$ be the output of layer l
- We can normalize it as follows

$$\boldsymbol{H}'_l = \frac{\boldsymbol{H}_l - \boldsymbol{\mu}}{\boldsymbol{\sigma}}$$

  – where $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}$ are the (element-wise) mean and variance of $\boldsymbol{H}_l$ over the minibatch
- Crucially, we backpropagate through this operation in order to stabilize the gradients across layers
- At test time, we can use a running average of $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}$ accumulated during training

Batch Norm Summary

- In practice, we introduce learned parameters $\boldsymbol{\gamma}$ and $\boldsymbol{\beta}$ such that the output of the batch norm layer is

$$\boldsymbol{\gamma} \boldsymbol{H}' + \boldsymbol{\beta}$$

- Seems a bit counter-intuitive since we are adding back a mean and a variance
  - The hope is that gradient descent finds suitable parameters that make training more stable
- Batch normalization most useful for deep convolutional NNs
  - It may be useful in the big deep learning homework