Machine Learning

Lecture 06: Deep Feedforward Networks

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This set of notes is based on various sources on the internet and Goodfellow, I., Bengio, Y., & Courville, A. (2016). *Deep Learning*. MIT press. www.deeplearningbook.org

Introduction

- So far, probabilistic models for supervised learning

$$\{\mathbf{x}_i, y_i\}_{i=1}^N \rightarrow P(y|\mathbf{x})$$

- Next, **deep learning**:

$$\{\mathbf{x}_i, y_i\}_{i=1}^N \rightarrow \mathbf{h} = f(\mathbf{x}), P(y|\mathbf{h})$$

  - $\mathbf{h} = f(\mathbf{x})$ is a feature transformation represented by a neural network,
  - $P(y|\mathbf{h})$ is a probabilistic model on the transformed features.
  - Regarded as one whole model: $P(y|\mathbf{x})$.

- This lecture: $\mathbf{h} = f(\mathbf{x})$ as a **feedforward neural network (FNN)**.
- Next lecture: $\mathbf{h} = f(\mathbf{x})$ as a **convolutional neural network (CNN or ConvNet)**.

Outline

1 Feedforward Neural Network as Function Approximator

2 Feedforward Neural Network as Probabilistic Model

3 Backpropagation

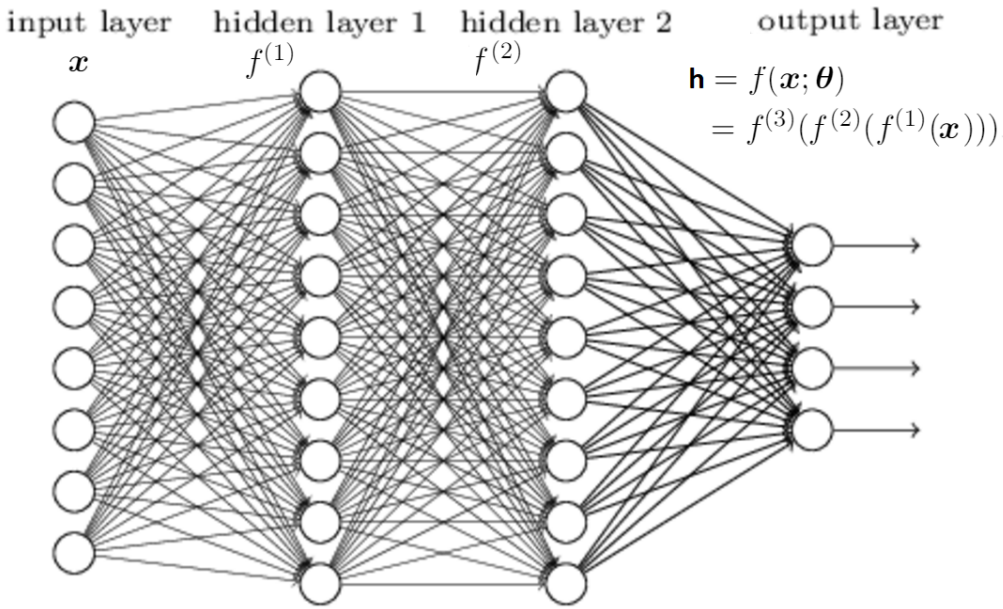
4 Dropout

5 Optimization Algorithms

Deep Feedforward Networks

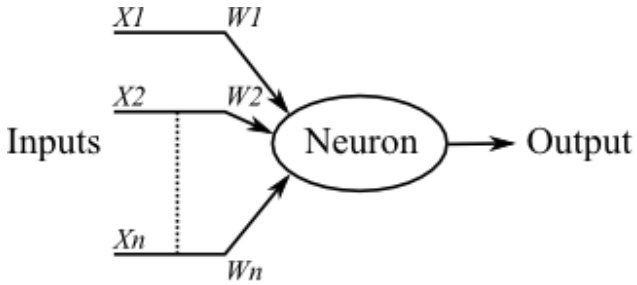
- **Deep feedforward networks**, also often called **feedforward neural networks (FNNs)**,or **multilayer perceptrons(MLPs)**, are the quintessential deep learning models
- A feedforward network defines a function $\mathbf{h} = f(\mathbf{x}, \boldsymbol{\theta})$.
- During learning, the parameters $\boldsymbol{\theta}$ are optimized so that $f(\mathbf{x}, \boldsymbol{\theta})$ approximates some target function $f^*(\mathbf{x})$

Feedforward Neural Networks



- Networks of simple computing elements (**units, neurons**).
  - Each unit is connected to units on the previous layer and units on the next layer
  - Parameters include a **bias** for each unit and a **weight** for each link.
  - Units are divided into: **input units**, **hidden units**, and **output units**
- Feedforward networks:
  - Inputs enter the input units,
  - Propagate through the network to the output units.

The Units



- A unit accepts vector of inputs $\mathbf{x}$,
- computes an affine transformation $z = \mathbf{W}^\top \mathbf{x} + b$, where $\mathbf{W} = (W_1, W_2, \ldots, W_n)^\top$ are the **link weights** and b is the **bias** of the unit. z is sometimes called the **net input** of the unit.
- applies nonlinear **activation function** $g(z)$, and
- gives output $g(z) = g(\mathbf{W}^\top \mathbf{x} + b)$

Different types of units have different activation functions.
Initialize all weights to small random values, and biases to zero or to small positive values.

Weight Initialization

- The *Xavier* initialization method:

$$w \sim U[-\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}]$$

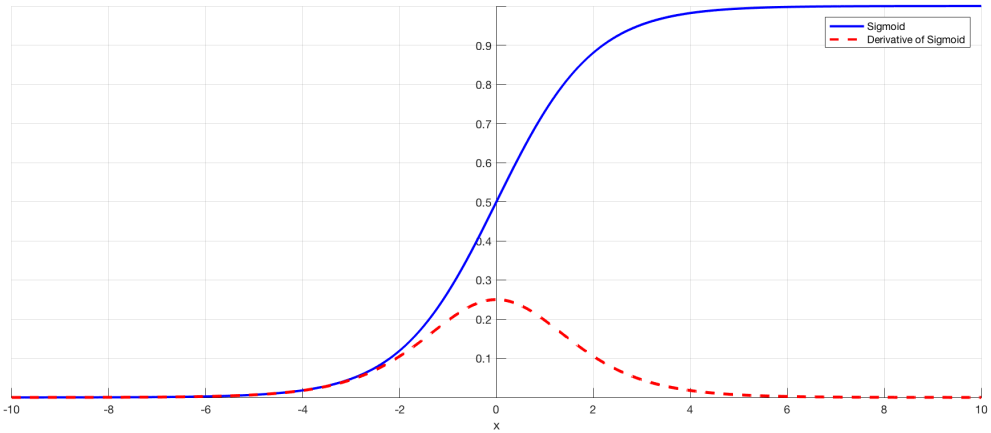
  where n is the number of inputs to the neuron. Usually used for tanh.

- The *He* initialization or *Kaimin* initialization method:

$$w \sim \mathcal{N}[0, \frac{2}{\sqrt{n}}]$$

  where n is the number of inputs to the neuron. Usually used for ReLU.

Sigmoid

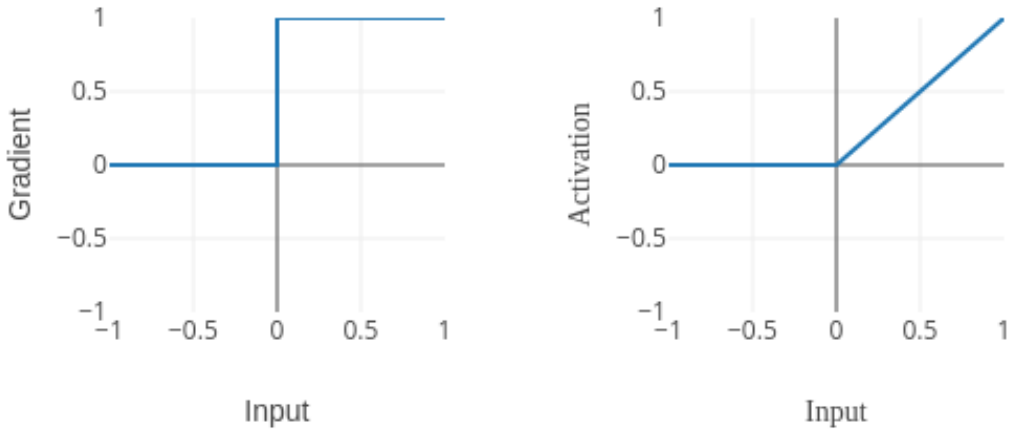


- **Sigmoid activation function**:

$$g(z) = \sigma(z) = \frac{1}{1 + \exp(-z)}$$

- Sigmoidal unit has small gradients across most of its domain (**vanishing gradient**), and hence leads to slow learning, especially in deep models.
  - It is said to saturate easily, where saturation refers to the state in which a neuron predominantly outputs values close to the asymptotic ends of the bounded activation function. Saturation implies slow learning.
- Not recommended as internal unit.

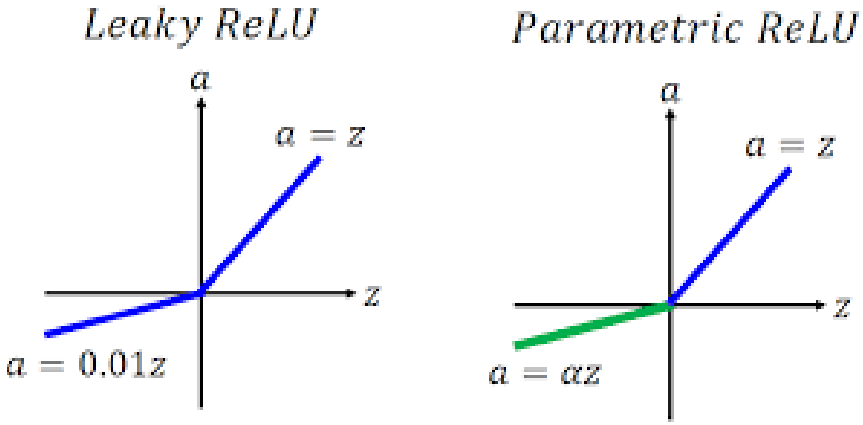
Rectified Linear Units (ReLU)



General form of activation function: $g(z) = g(\mathbf{W}^\top \mathbf{x} + b)$

- **ReLU**: $g(z) = \max\{0, z\}$.
- Constant gradient when $z > 0$, which leads to faster learning. Probably the most commonly used activation function.
- Zero gradient when $z < 0$. The neuron is **dead** if $z < 0$ for all training examples. Dead neurons cannot be revived.
  - To mitigate the problem somewhat, initialize b to be small positive value, e.g. 0.1, so that the unit is initially active ($z > 0$).

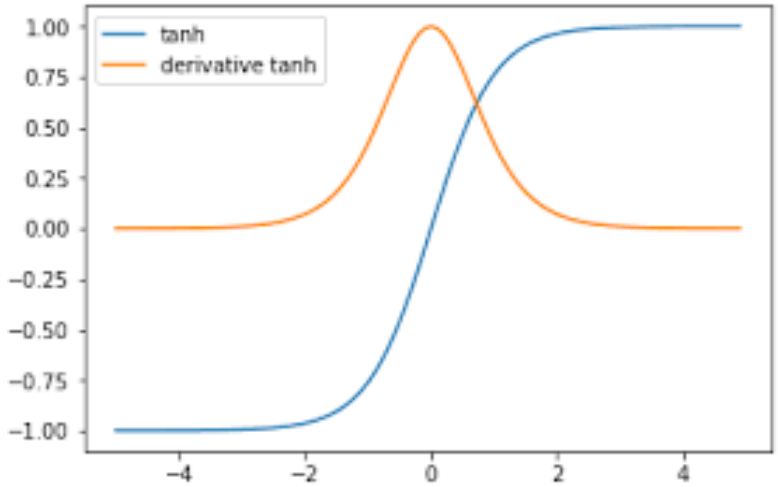
Variations of ReLU



$g(z, \alpha) = \max\{0, z\} + \alpha \min\{0, z\}$:

- **Absolute value rectification**: $\alpha = -1$,
- **Leaky ReLU**: α is small value like 0.01,
- **Parametric ReLU**: Learns α
- Non-zero gradient even when $z < 0$, which mitigates the dead neuron problem.

Hyperbolic Tagent



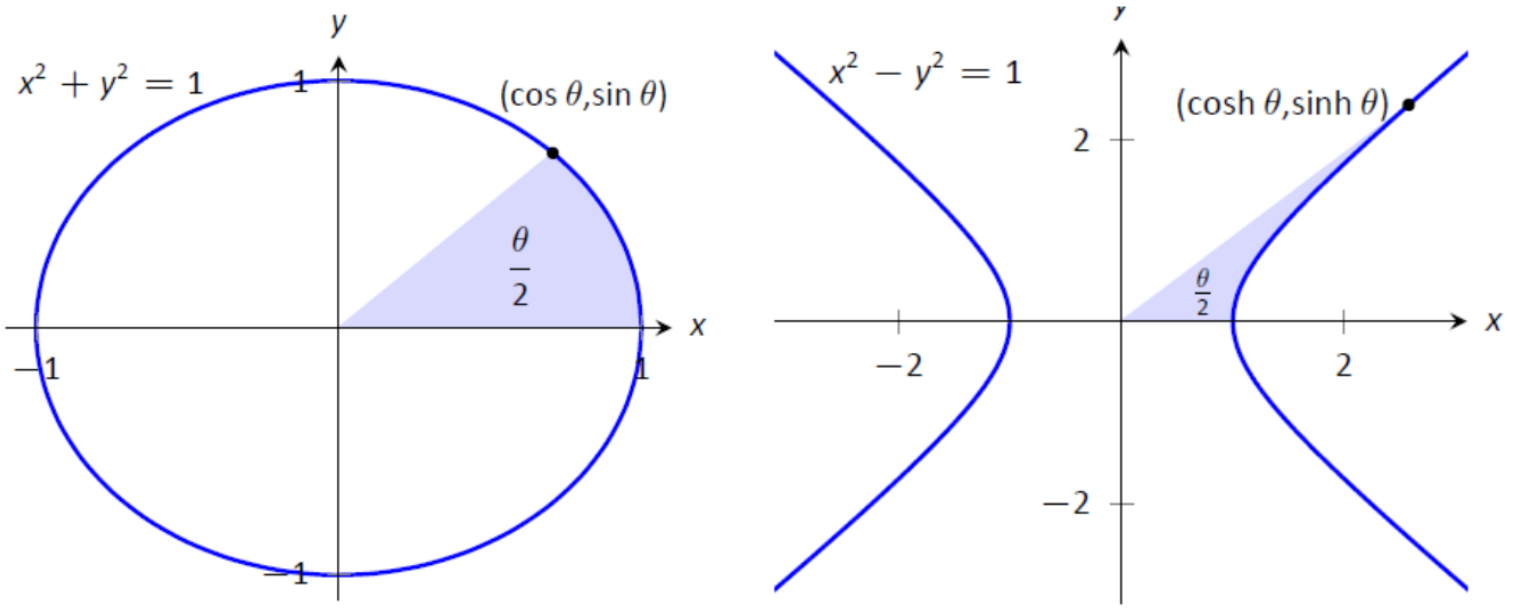
- **Hyperbolic tagent activation function**:

$$g(z) = \tanh(z) = \frac{\exp(z) - \exp(-z)}{\exp(z) + \exp(-z)}$$

- Tanh has larger gradients than sigmoid, and smoother than ReLU. However, it can still saturate.
- A popular choice in practice.

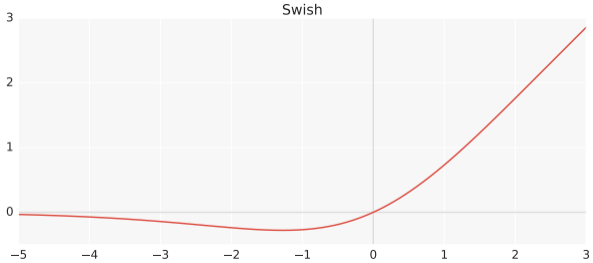
Hyperbolic Tagent

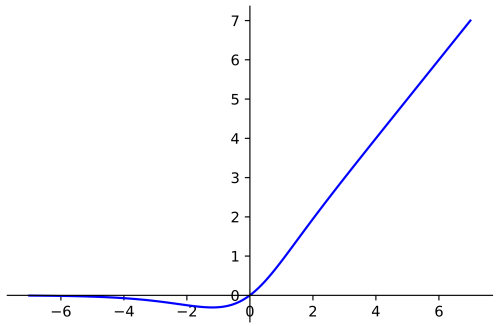
Just as cosine and sine are used to define points on the circle defined by $x^2 + y^2 = 1$, the functions hyperbolic cosine and hyperbolic sine are used to define points on the hyperbola $x^2 - y^2 = 1$:

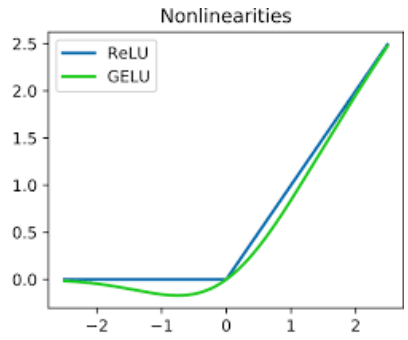


Source: https://math.libretexts.org/

Swish, Mish and GELU







- **Swish activation**:

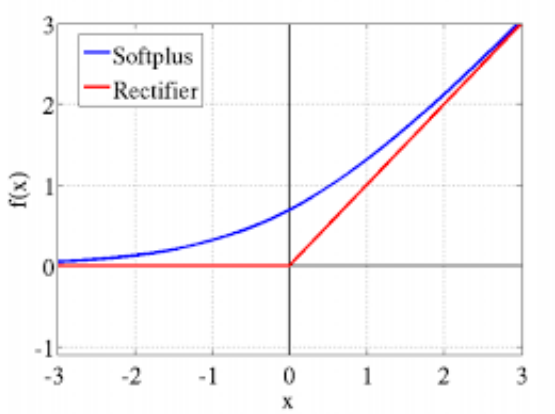
$$g(z) = z\sigma(\beta z),\ \beta \text{ is parameter fixed or learned}$$

- **Mish activation function**:

$$g(z) = z\tanh(\log(1+\exp(z)) = z\tanh(\zeta(z))$$

- **GELU activation function**: $g(z) = z\Phi(z)$ Where $\Phi(z)$ is the standard Gaussian cumulative distribution function.
- Non-zero gradients when $z < 0$, smooth and non-monotonic. Unbounded above, which avoids saturation. Outperform ReLU in deep networks.

Softplus

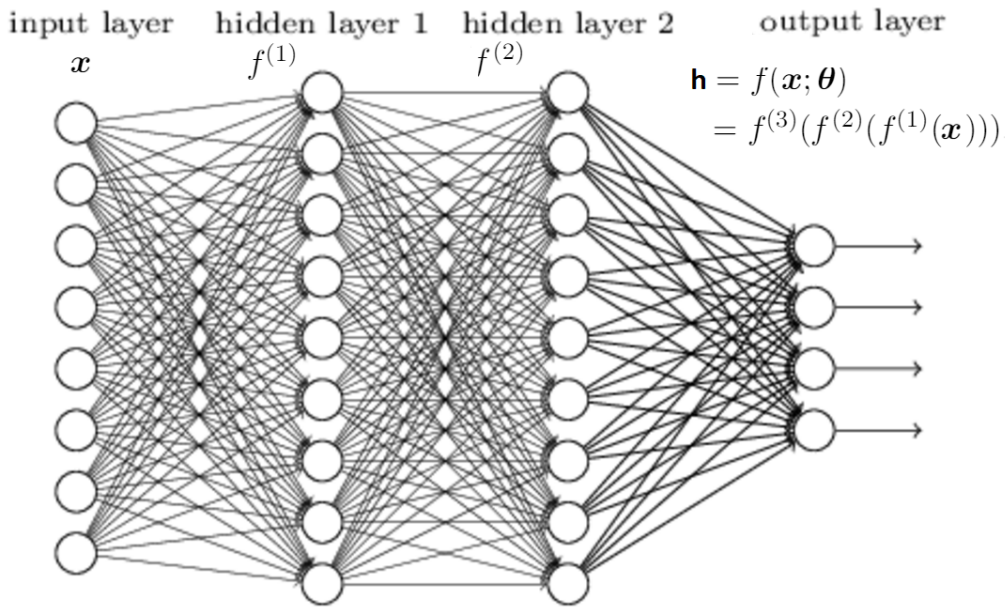


- **Softplus activation function**:

$$g(z) = \zeta(z) = \log(1 + \exp(z))$$

  - Softplus is a smooth version of ReLU, empirically not as good as ReLU.

Computation by Feedfoward Neural Network



- $\mathbf{h}^{(i)}$ — Column vector for units on layer i; $\mathbf{b}^{(i)}$ — Biases for units on layer i; $g^{(i)}$ — Activation functions for units on layer i.
- $\mathbf{W}^{(i)}$ — Matrix of weights for units on layer i, with weight for unit j at the j-th column.

$$\begin{aligned}\mathbf{h}^{(1)} &= g^{(1)}({\mathbf{W}^{(1)}}^{\top}\mathbf{x} + \mathbf{b}^{(1)})\\ \mathbf{h}^{(2)} &= g^{(2)}({\mathbf{W}^{(2)}}^{\top}\mathbf{h}^{(1)} + \mathbf{b}^{(2)})\\ \mathbf{h} &= g^{(3)}({\mathbf{W}^{(3)}}^{\top}\mathbf{h}^{(2)} + \mathbf{b}^{(3)})\end{aligned}$$

Universal Approximation

Theorem

Only one layer of sigmoid hidden units suffices to approximate any well-behaved function (e.g., bounded continuous functions) to arbitrary precision.

Deep learning useful when you:

- Need a complex function, and
- Have abundant data.

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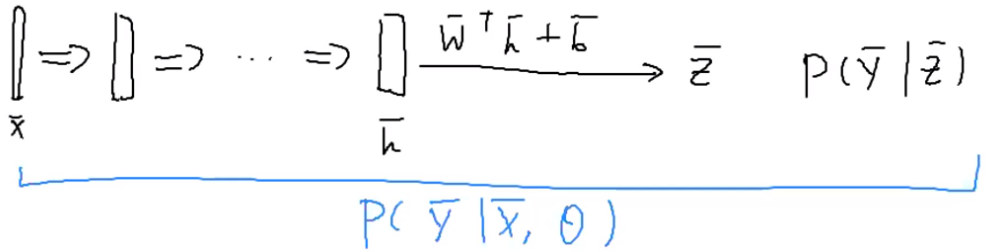
An FNN can be used to define a probabilistic model



- The first-second last layers define a feature transformation:

$$\mathbf{h} = f(\mathbf{x})$$

- The last layer defines a probabilistic model on the features:

$$P(\mathbf{y}|\mathbf{h})$$

Note: Here $\mathbf{y}$ is a vector of output variables, while so far we have been talking about only one output variable y.

- The whole network defines a probabilistic model:

$$P(\mathbf{y}|\mathbf{x},\theta),$$

where θ consists of weights in f and parameters in $P(\mathbf{y}|\mathbf{h})$.

Logits

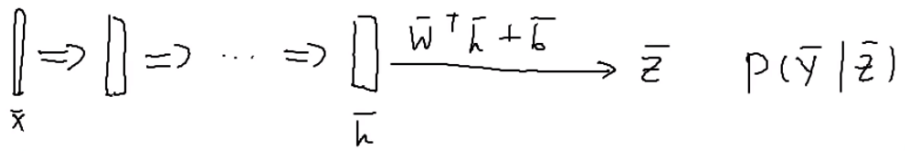
- To define a probabilistic model on the features $\mathbf{h}$, first define a **logit vector**

$$\mathbf{z} = \mathbf{W}^\top \mathbf{h} + \mathbf{b},$$

  where $\mathbf{W}$ is a weight matrix and $\mathbf{b}$ is a bias vector. They are the parameters of the last layer. $\mathbf{z} = (z_1, z_2, \ldots)^\top$.

- Then, we can define various probabilistic models using $\mathbf{z}$, which are viewed as units for the last layer.

Linear-Gaussian Output Unit



- When **y** is real-valued vector, we can assume that **y** follows a Gaussian distribution with mean **z** and identity covariance matrix **I**:

$$p(\mathbf{y}|\mathbf{x}) = \mathcal{N}(\mathbf{y}|\mathbf{z}, \mathbf{I})$$

- In this case, the **per-sample loss** is:

$$L(\mathbf{x}, \mathbf{y}, \theta) = -\log P(\mathbf{y}|\mathbf{x}, \theta) \propto \frac{1}{2}||\mathbf{y} - \mathbf{z}||_2^2 \qquad \text{(See p12 of L02)}$$

- Partial derivative of per-sample loss with respect to logit z_k:

$$\frac{\partial L}{\partial z_k} = z_k - y_k.$$

It is error.

Sigmoid Output Unit

- When there is only one binary output variable $y \in \{0, 1\}$, we can define a distribution $p(y|\mathbf{x})$ using a sigmoid unit:

$$P(y|\mathbf{x}) = Ber(y|\sigma(z)),$$

  where z is a scalar.

- In this case, the **per-sample loss** is:

$$L(\mathbf{x}, \mathbf{y}, \theta) = -[y \log \sigma(z) + (1 - y) \log(1 - \sigma(z))] \qquad \text{(See p10 of L03)}$$

- Partial derivative of per-sample loss with respect to logit z:

  It is error.
$$\frac{\partial L}{\partial z} = \sigma(z) - y. \qquad \text{(See p21 of L03)}$$

Sigmoid Output Unit

- We said earlier that sigmoid units are not recommended for hidden units because they saturates across most of their domains.
- They are fine as output units because the negative log-likelihood in the cost function helps to avoid the problem.
- In fact, $\sigma(z) - y \approx 0$ means:
  - $z \gg 0, y = 1$, or
  - $z \ll 0, y = 0$

  In words, saturation occurs only when the model already has the right answer: When $y = 1$ and z is very positive, or $y = 0$ and z is very negative.

Softmax Output Unit

- When y is a variable with C possible values $\{1, 2, \ldots, C\}$, we can define a distribution $p(y|\mathbf{x})$ using a **softmax unit**.
- Here $\mathbf{z} = \mathbf{W}^\top \mathbf{h} + \mathbf{b}$ is a vector of n components: $\mathbf{z} = (z_1, z_2, \ldots, z_C)^\top$.
- The follow formula gives a distribution over the domain of y:

$$P(y = k|\mathbf{x}) = \frac{\exp(z_k)}{\sum_{j=1}^{C} \exp(z_j)}$$

- Partial derivative of per-sample cross entroyp loss with respect to logit z_k:

$$\frac{\partial L}{\partial z_k} = P(y = k) - \mathbf{1}(y = k). \qquad \text{(See p40 of L03)}$$

It is error.

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Training Feedforward Neural Networks

- Given data $\{\mathbf{x}_i, \mathbf{y}_i\}_{i=1}^N$, we want to learn the parameters θ by minimizing the cross-entropy loss:

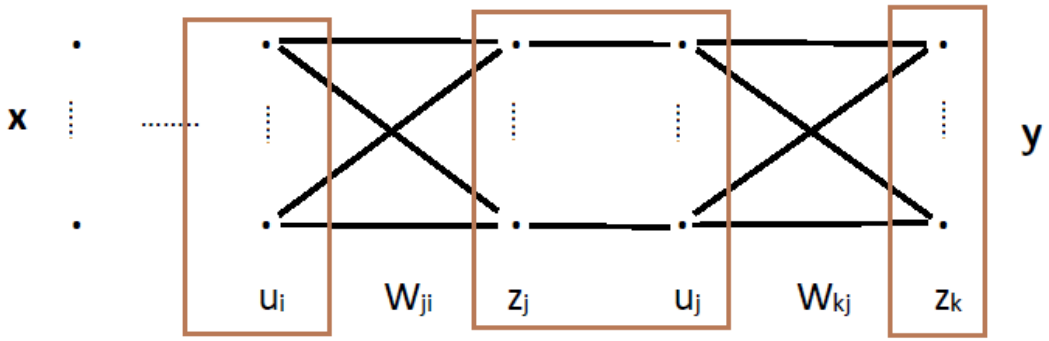
$$J(\theta) = \frac{1}{N}\sum_{i=1}^{N} L(\mathbf{x}_i, y_i, \theta) = \frac{1}{N}\sum_{i=1}^{N}(-\log P(\mathbf{y}_i|\mathbf{x}_i, \theta))$$

- Algorithm: Stochastic gradient descent (SGD)
  - Initialize θ
  - Repeat for a predetermined number of epochs
    - For each minibatch B,

$$\theta \leftarrow \theta - \alpha \frac{1}{|B|}\sum_{i\in B} \nabla L(\mathbf{x}_i, y_i, \theta)$$

- Question: How to compute the gradient $\nabla L(\mathbf{x}_i, y_i, \theta)$ for each training example?
- Answer: Backpropagation.

Backpropagation: Output Layer



- Let y_k, u_j and u_i each be the output of a unit at the last three layers, and z_k, z_j, z_i be the output before applying the activation function:

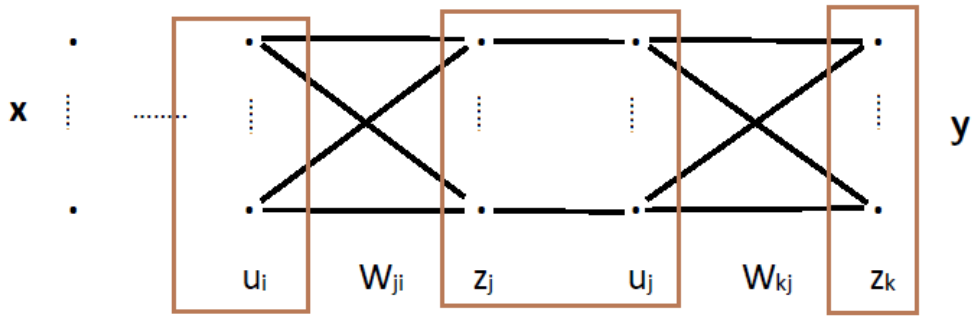
$$z_k = \sum_j u_j W_{kj}, \quad u_j = g(z_j), \quad z_j = \sum_i u_i W_{ji}$$

(Bias ignored for simplicity.)

- Let $L = L(\mathbf{x}, \mathbf{y}, \theta)$ for a particular training example $(\mathbf{x}, \mathbf{y})$. The partial derivative of L w.r.t a weigh in the last layer:

$$\frac{\partial L}{\partial W_{kj}} = \frac{\partial L}{\partial z_k}\frac{\partial z_k}{\partial W_{kj}} = u_j \delta_k, \text{ where } \delta_k = \frac{\partial L}{\partial z_k}$$

Backpropagation: Hidden Layer



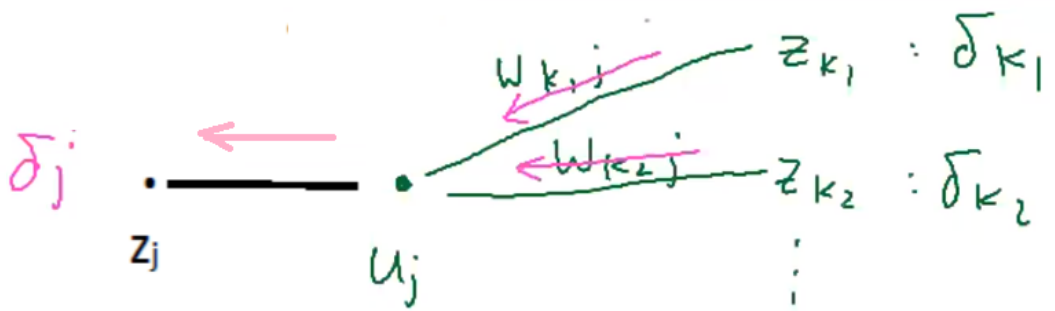
$$z_k = \sum_j u_j W_{kj}, \quad u_j = g(z_j), \quad z_j = \sum_i u_i W_{ji}$$

- The partial derivative of L w.r.t a weigh in the second last layer (similar for weight in other hidden layers):

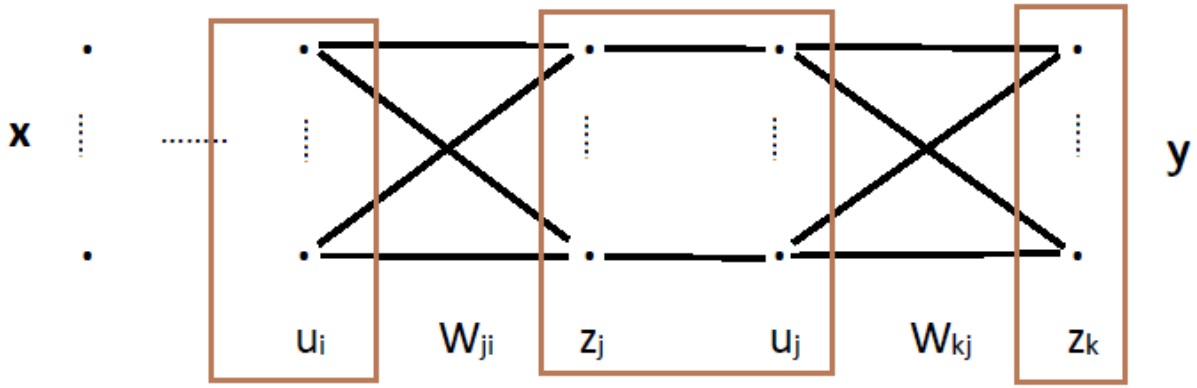
$$\begin{aligned}\frac{\partial L}{\partial W_{ji}} &= \sum_k \frac{\partial L}{\partial z_k}\frac{\partial z_k}{\partial W_{ji}} = \sum_k \delta_k \frac{\partial z_k}{\partial u_j}\frac{\partial u_j}{\partial z_j}\frac{\partial z_j}{\partial W_{ji}} \\ &= \sum_k \delta_k W_{kj}\frac{\partial u_j}{\partial z_j}u_i = u_i\delta_j, \text{ where } \delta_j = \frac{\partial u_j}{\partial z_j}\sum_k W_{kj}\delta_k\end{aligned}$$

Backpropagation of error

$$\delta_j = \frac{\partial u_j}{\partial z_j} \sum_k W_{kj} \delta_k$$



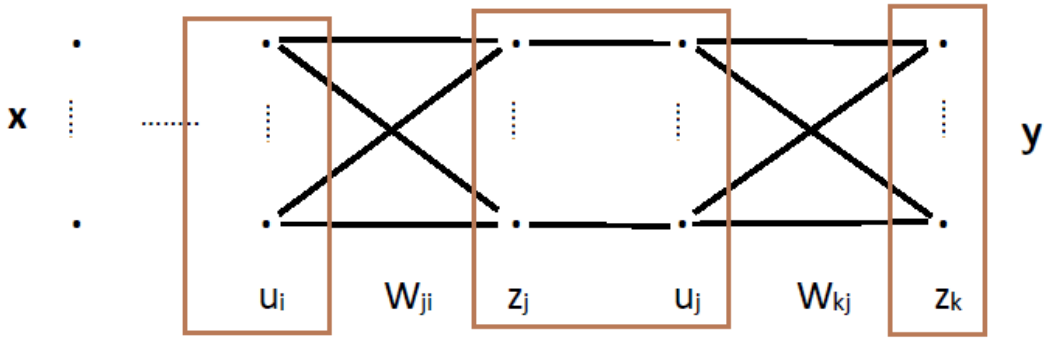
Backpropagation



Summary:

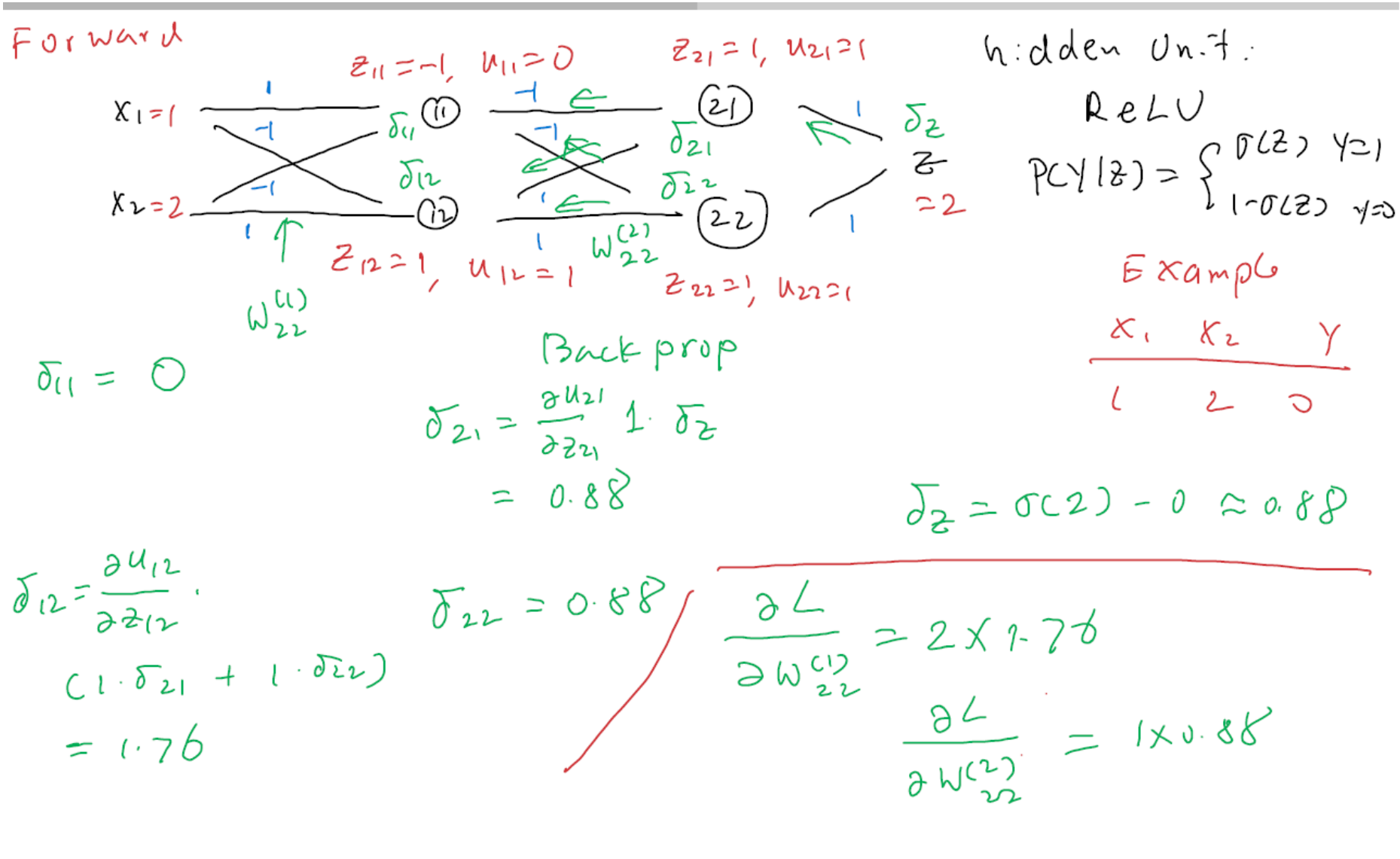
- For a weight W_{kj} the output layer: $\frac{\partial L}{\partial W_{kj}} = u_j \delta_k$, where $\delta_k = \frac{\partial L}{\partial z_k}$
  - u_j is the output of unit j from input $\mathbf{x}$
  - δ_k is the "error value" for unit k obtained by comparing the model output $\mathbf{z} = f(\mathbf{x})$ and the observed output $\mathbf{y}$ in L.
- For a weight W_{ji} in a hidden layer: $\frac{\partial L}{\partial W_{ji}} = u_i \delta_j$, where $\delta_j = \frac{\partial u_j}{\partial z_j} \sum_k W_{kj} \delta_k$
  - u_i is the output of unit i from input $\mathbf{x}$
  - δ_j is the "error value" for unit j obtained by backpropagating the errors (δ_k) from the next layer .

The Backpropagation Algorithm



- Objective: Compute $\frac{\partial L}{\partial W_{ji}}$ for all weights (and biases) for each training example:
  1. **Propagate forward** to compute the net input and output of each unit (i.e, u_i, u_j, ...).
  2. **Propagate "error" backward**
     - For each output unit k: $\delta_k \leftarrow \frac{\partial L}{\partial z_k}$
     - For each hidden unit j: $\delta_j \leftarrow \frac{\partial u_j}{\partial z_j} \sum_k W_{kj}\delta_k$
  3. Get the gradient for each weight: $\frac{\partial L}{\partial W_{ji}} \leftarrow u_i\delta_j$, $\frac{\partial L}{\partial b_j} \leftarrow \delta_j$

Backprop Example

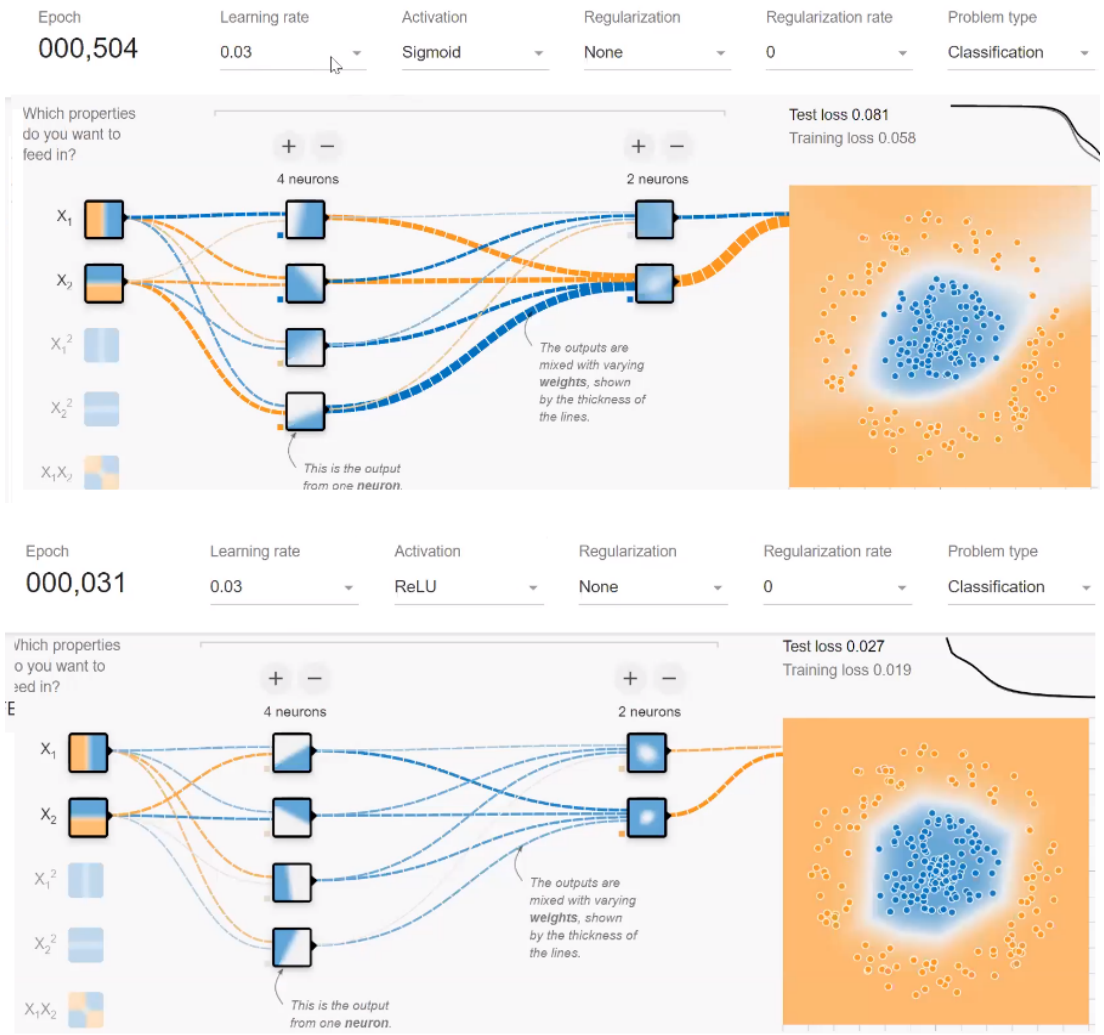


The Backpropagation Algorithm

- The backpropagation algorithm and SGD are implemented in deep learning packages such as Tensorflow.
- Weights are packed into **tensors** ($[a_{ijk}]$) for efficiency
  - A 1-D tensor is a vector
  - A 2-D tensor is a matrix
  - A 3-D tensor is several matrices stacked on top of each other.
- Although you do not need to know everything about backpropagation and SGD, some basic understanding will be very helpful when you work with deep learning.

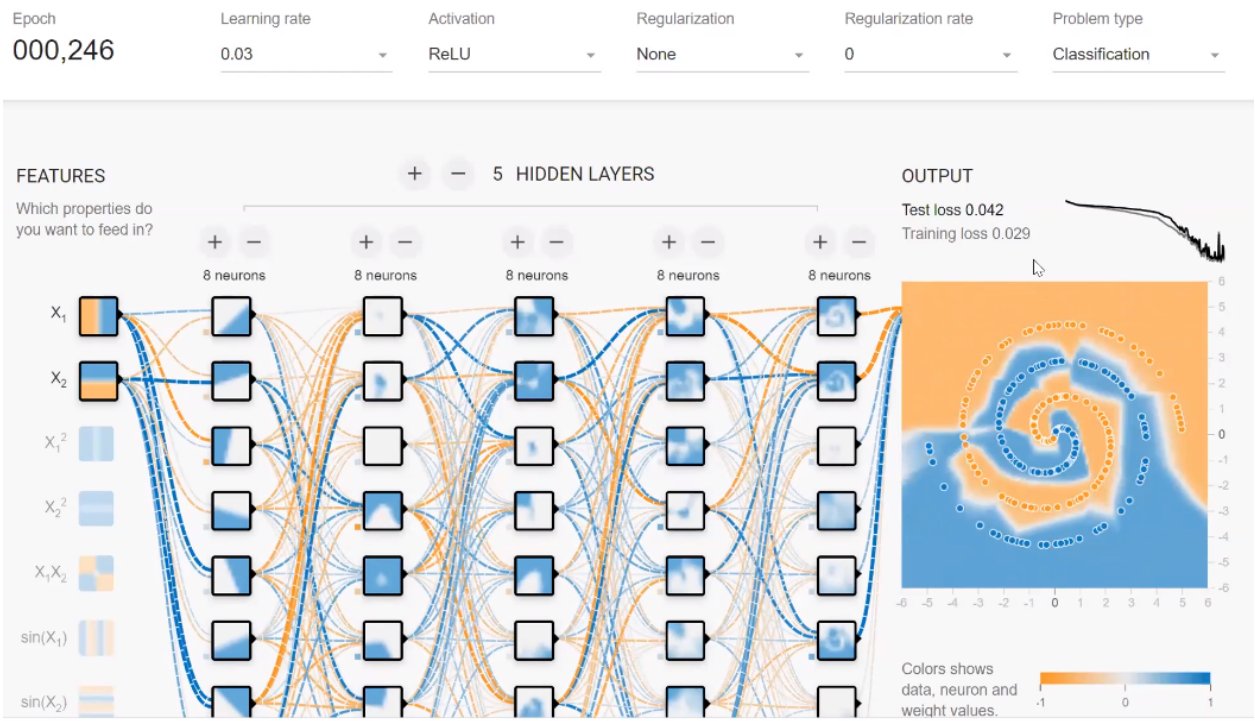
Demonstrations http://playground.tensorflow.org/

- ReLU units are easier to learn than Sigmoid and Tanh units



Demonstrations http://playground.tensorflow.org/

- Deep structure helps



- Need to adjust learning rate during training.

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Introduction

- DL models are complex. Overfitting is an important issue.
- One way to do that is to regularize (weight decay):

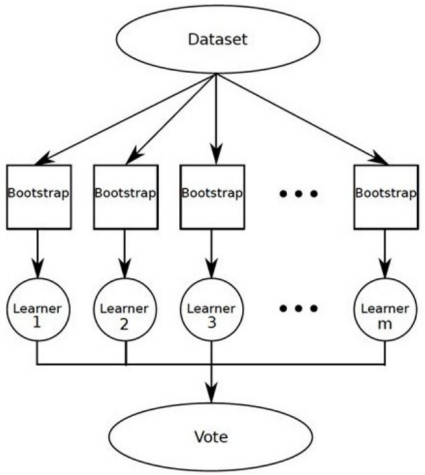
$$\tilde{J}(\theta) = J(\theta) + \lambda ||\theta||_2^2$$

  Almost always do this.

- Dropout is another technique for avoiding overfitting specifically proposed for deep learning.

Bagging (Bootstrap Aggregating)

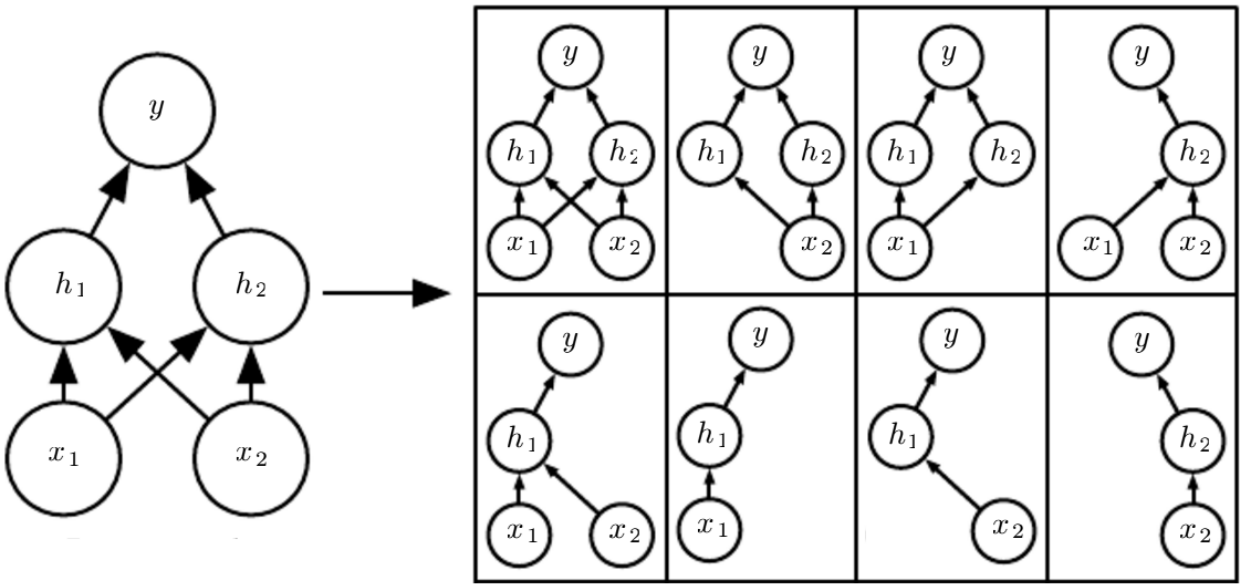
- A technique for reducing generalization error by combining several models
  - Train several different models separately on different randomly selected subsets of data called **bootstrap samples**,
  - Classification: Have all of the models vote on the output for test examples.



- Bagging reduces variance: Variance is error due to randomness. Different bootstrap samples contain different randomness, and hence unlikely to **most** make the same errors on the test set.

One Way to Use Bagging for Feedforward Networks

- Start with a large network.
- Obtain subnetworks and train them separately on different randomly selected subsets of data.
- To classify future examples, let the subnetworks vote.
- **Problem**: Too expensive.
- **Dropout** is an inexpensive approximation of the idea.

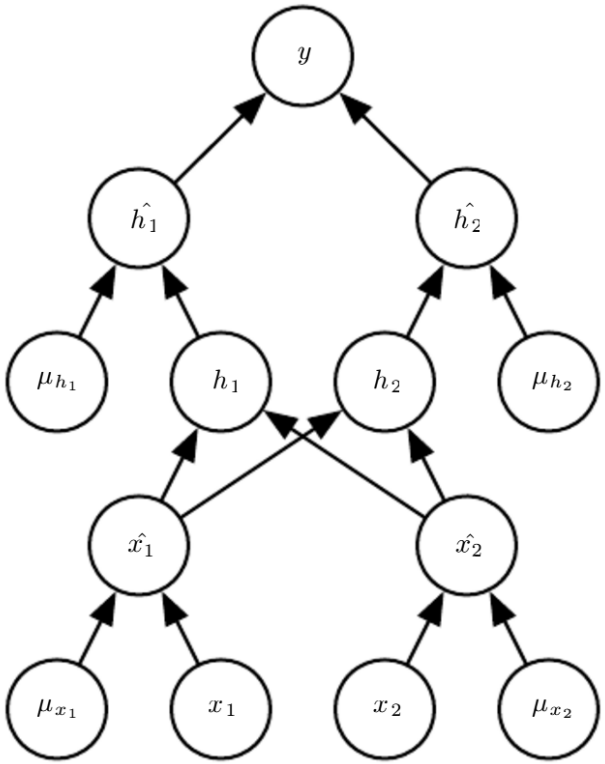


Base network

Ensemble of subnetworks

Subnetwork Selection via Masking

- Associate a **binary mask variable** with each input and hidden unit.
- Sample their values randomly and independently (e.g., with probability 0.5 for hidden units and 0.8 for input units).
- Multiply the output of each unit by its mask value before passing it to the next layer.
- Units with 0 mask values are effectively removed from the network.



Dropout

- To be used with minibatch-based algorithms such as SGD.
- For each minibatch,
  - Randomly sample values for mask variables
  - Carry out one step of gradient descent.
    - (Only parameters for the units with mask value 1 are updated. The others have gradient zero and hence not updated.)
- There is only **one network**, no subnetworks. At each step, training is conducted in a part of the network (a subnetwork).
- Dropout is a widely used regularization method for deep learning. It reduces overfitting by preventing complex co-adaptations of parameters on training data.

See example in CNN code.

Outline

1 Feedforward Neural Network as Function Approximator

2 Feedforward Neural Network as Probabilistic Model

3 Backpropagation

4 Dropout

5 Optimization Algorithms

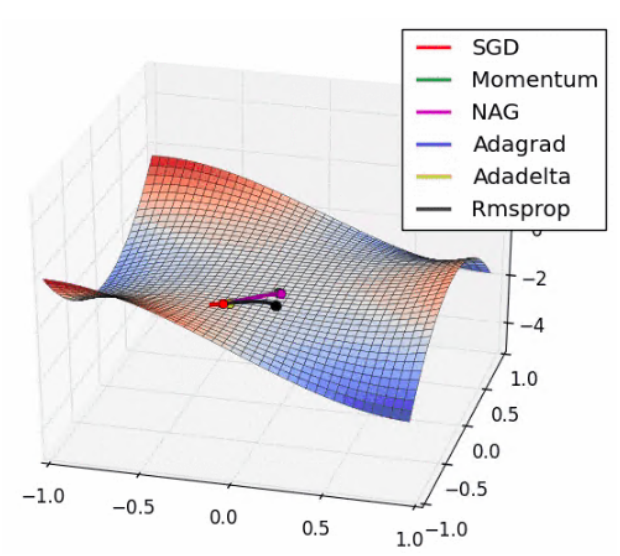
- Our task is: Find θ to minimize the loss function $J(\theta)$.
- There are multiple algorithms that we can use. Stochastic gradient descent is one of them.

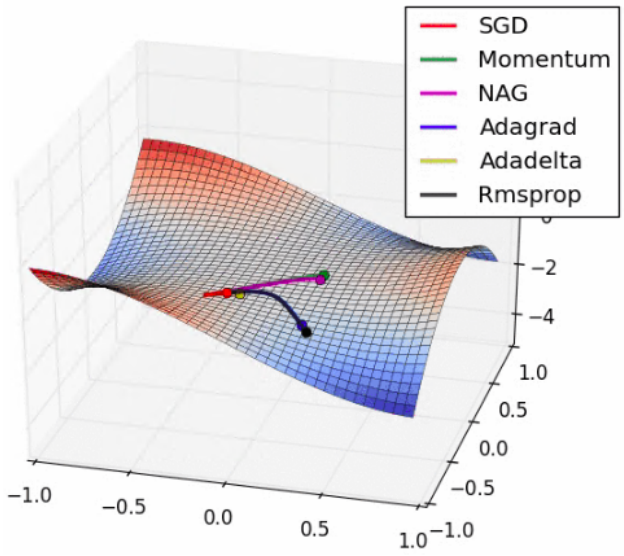
Algorithm 8.1 Stochastic gradient descent (SGD) update at training iteration k

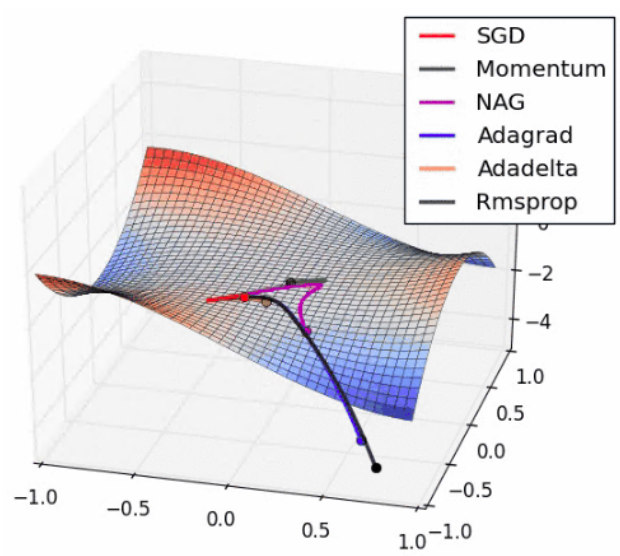
Require: Learning rate ϵ_k.
Require: Initial parameter $\boldsymbol{\theta}$
  while stopping criterion not met **do**
    Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient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

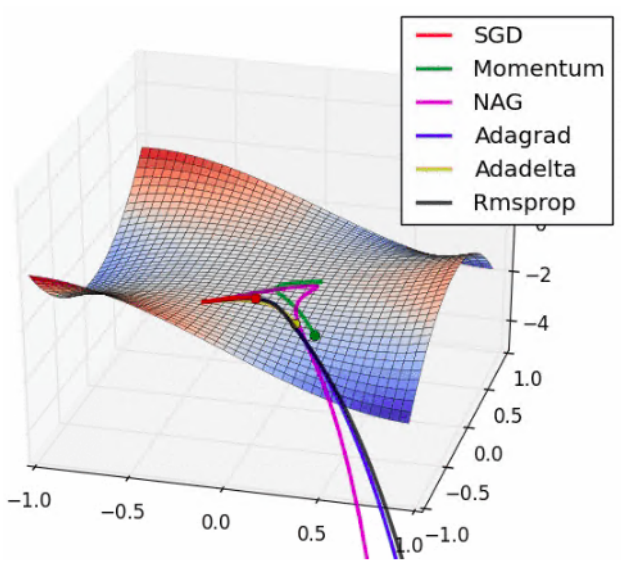
- There are others ....

Performances of Different Optimizers Vary a Lot









Momentum

SGD

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: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \epsilon\hat{\boldsymbol{g}}$

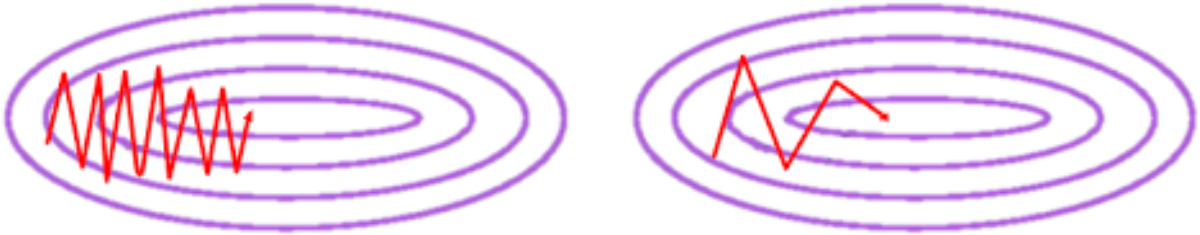
SGD with Momentum

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: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}$

- **Momentum** is a technique to accelerate SGD.
- View θ as a "particle" that travels in the space of parameter values.
- In SGD, its movement is determined by gradient and learning rate.
- In SGD with momentum, the movement is additionally affected by its **velocity** v
  - v is an exponentially decaying average of past negative gradients.
  - The hyperparameter α is usually set at 0.5, 0.9 or 0.99.

Momentum

- The incorporation of momentum into stochastic gradient descent **reduces the variation in overall gradient directions** and **speeds up learning** (larger improvements to parameters at each step).



Online demo: https://medium.com/@ramrajchandradevan/the-evolution-of-gradient-descend-optimization-algorithm-4106a6702d39

Algorithms with Adaptive Learning Rates

- Learning rate should be reduced gradually.
- Several common algorithms:
  - AdaGrad
  - RMSProp
  - Adam
- Key idea: Parameters that have changed a lot should be allowed to change less in future.

AdaGrad (Adaptive Gradient Algorithm)

- AdaGrad scales the learning rates of all model parameters by inversely proportional to the square root of the sum of all of their historical squared gradients.
- The net effect is greater progress in the more gently sloped directions of parameter space.

Algorithm 8.4 The AdaGrad algorithm

Require: Global learning rate ϵ
Require: Initial parameter $\boldsymbol{\theta}$
Require: Small constant δ, perhaps 10^{-7}, for numerical stability
  Initialize gradient accumulation variable $\boldsymbol{r} = \mathbf{0}$
  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: $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
    Accumulate squared gradient: $\boldsymbol{r} \leftarrow \boldsymbol{r} + \boldsymbol{g} \odot \boldsymbol{g}$
    Compute update: $\Delta\boldsymbol{\theta} \leftarrow -\frac{\epsilon}{\delta + \sqrt{\boldsymbol{r}}} \odot \boldsymbol{g}$. (Division and square root applied element-wise)
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \Delta\boldsymbol{\theta}$
  end while

RMSProp (Root Mean Square Propagation)

- RMSProp uses an exponentially decaying average to discard history from the extreme past

Algorithm 8.5 The RMSProp algorithm

Require: Global learning rate ϵ, decay rate ρ.
Require: Initial parameter $\boldsymbol{\theta}$
Require: Small constant δ, usually 10^{-6}, used to stabilize division by small numbers.
Initialize accumulation variables $\boldsymbol{r} = 0$
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: $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
  Accumulate squared gradient: $\boldsymbol{r} \leftarrow \rho \boldsymbol{r} + (1 - \rho) \boldsymbol{g} \odot \boldsymbol{g}$
  Compute parameter update: $\Delta \boldsymbol{\theta} = -\frac{\epsilon}{\sqrt{\delta + \boldsymbol{r}}} \odot \boldsymbol{g}$. ($\frac{1}{\sqrt{\delta + \boldsymbol{r}}}$ applied element-wise)
  Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \Delta \boldsymbol{\theta}$
end while

AdaGrad vs RMSProp

$\bar{\theta} = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \end{bmatrix}$ $\bar{g} = \begin{bmatrix} g_1 \\ g_2 \\ \vdots \end{bmatrix}$

"Sum of past changes"

$\bar{r} = \begin{bmatrix} r_1 \\ r_2 \\ \vdots \end{bmatrix}$

AdaGrad

$\bar{r} \leftarrow \bar{r} + \bar{g} \odot \bar{g}$

t	r_i	
1	g_1^2	g_{i1}
2	$g_1^2 + g_2^2$	
3	$g_1^2 + g_2^2 + g_3^2$	

No decaying

RMSProp

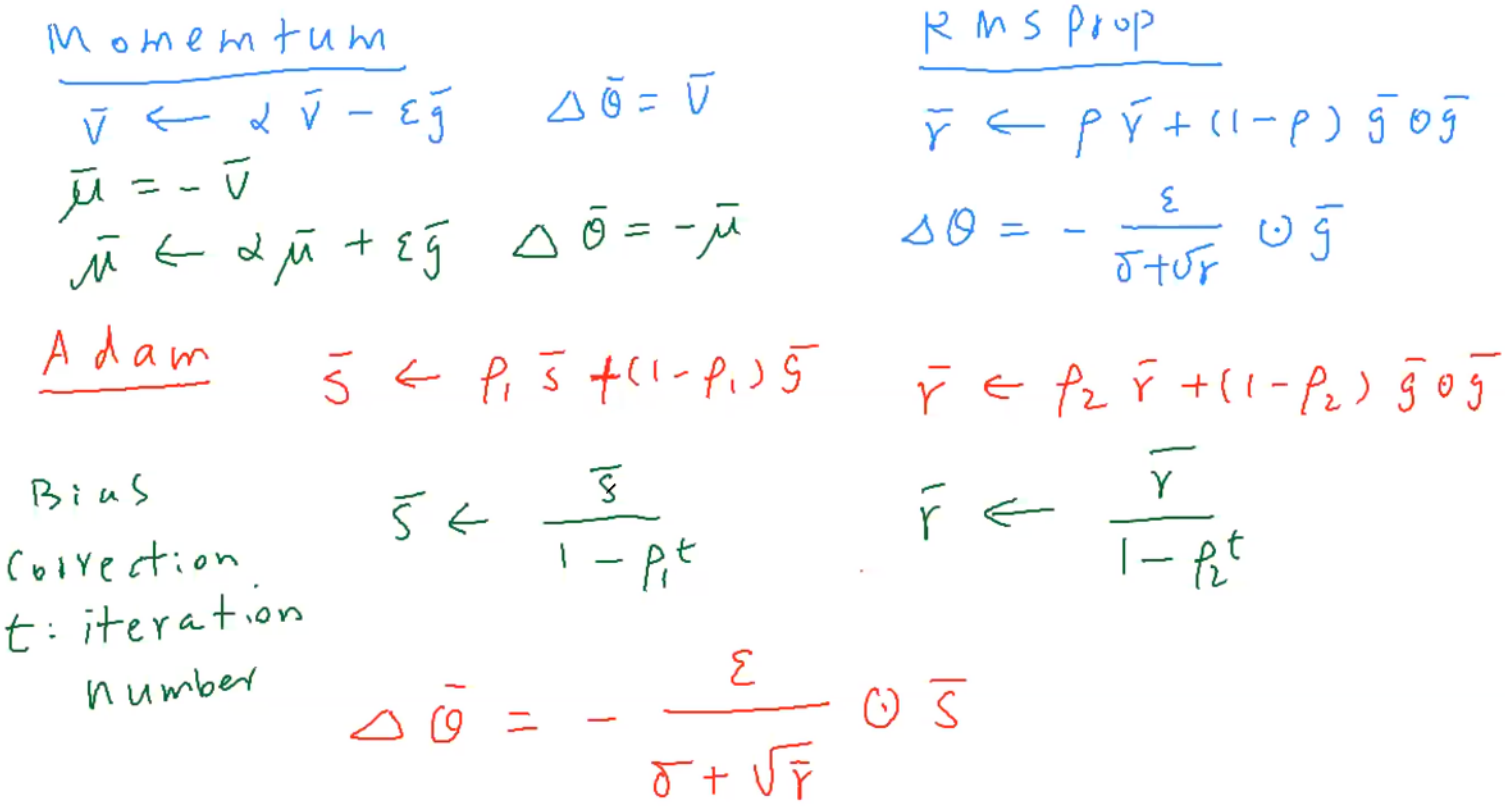
$\bar{r} \leftarrow \rho \bar{r} + (1-\rho)\, \bar{g} \odot \bar{g} \quad 0 < \rho < 1$

t	r_i	
1	$(1-\rho) g_1^2$	(g_{i1})
2	$\rho(1-\rho) g_1^2 + (1-\rho) g_2^2$	
	$= (1-\rho)(\rho g_1^2 + g_2^2)$	
3	$(1-\rho)(\rho^2 g_1^2 + \rho g_2^2 + g_3)$	

Exponentially decaying weights

Adam (Adaptive Moments)

- Roughly a combination of RMSProp and momentum, with bias correction.
- "Insofar, Adam might be the best overall choice."



Adam: Bias Correction

$\bar{r} \leftarrow \rho_2 \bar{r} + (1-\rho_2)\, \bar{g} \odot \bar{g}$ $\quad \hat{r} \leftarrow \frac{r}{1-\rho_2^t}$

t	$\bar{r}$
3	$(1-\rho_2)(\rho_2^2 g_1^2 + \rho_2 g_2^2 + g_3^2)$
t	$(1-\rho_2)(\rho_2^{t-1} g_1^2 + \rho_2^{t-2} g_2^2 + \cdots + g_t^2)$

r_t

$$\hat{r}_t = \frac{r_t}{1-\rho_2^t} = \frac{(1-\rho_2)(\rho_2^{t-1} g_1^2 + \rho_2^{t-2} g_2^2 + \cdots + g_t^2)}{(1-\rho_2)(\rho_2^{t-1} + \rho_2^{t-2} + \cdots + 1)}$$

Expectation

$\int x^2 p(x)\, dx$

$$= \frac{\rho_2^{t-1}}{z} g_1^2 + \frac{\rho_2^{t-2}}{z} g_2^2 + \cdots + \frac{1}{z} g_t^2 \qquad z$$

2nd order moment

Prob distribution

Adam (Adaptive Moments)

Algorithm 8.7 The Adam algorithm

Require: Step size ϵ (Suggested default: 0.001)

Require: Exponential decay rates for moment estimates, ρ_1 and ρ_2 in $[0, 1)$. (Suggested defaults: 0.9 and 0.999 respectively)

Require: Small constant δ used for numerical stabilization. (Suggested default: 10^{-8})

Require: Initial parameters $\boldsymbol{\theta}$

Initialize 1st and 2nd moment variables $\boldsymbol{s} = \mathbf{0}$, $\boldsymbol{r} = \mathbf{0}$

Initialize time step $t = 0$

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: $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$

$t \leftarrow t + 1$

Update biased first moment estimate: $\boldsymbol{s} \leftarrow \rho_1 \boldsymbol{s} + (1 - \rho_1)\boldsymbol{g}$ Momentum

Update biased second moment estimate: $\boldsymbol{r} \leftarrow \rho_2 \boldsymbol{r} + (1 - \rho_2)\boldsymbol{g} \odot \boldsymbol{g}$ RMSProp

Correct bias in first moment: $\hat{\boldsymbol{s}} \leftarrow \frac{\boldsymbol{s}}{1 - \rho_1^t}$

Correct bias in second moment: $\hat{\boldsymbol{r}} \leftarrow \frac{\boldsymbol{r}}{1 - \rho_2^t}$

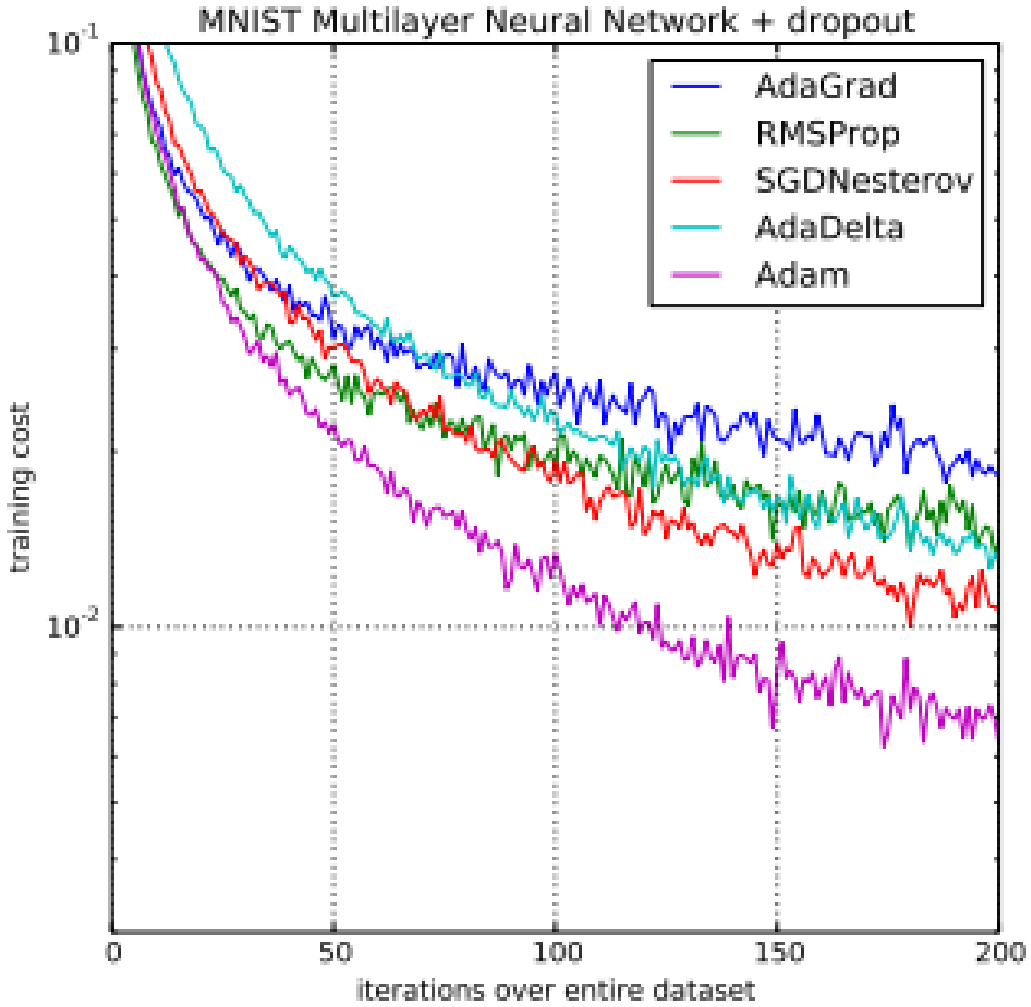
Compute update: $\Delta\boldsymbol{\theta} = -\epsilon \frac{\hat{\boldsymbol{s}}}{\sqrt{\hat{\boldsymbol{r}}} + \delta}$ (operations applied element-wise)

Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \Delta\boldsymbol{\theta}$

end while

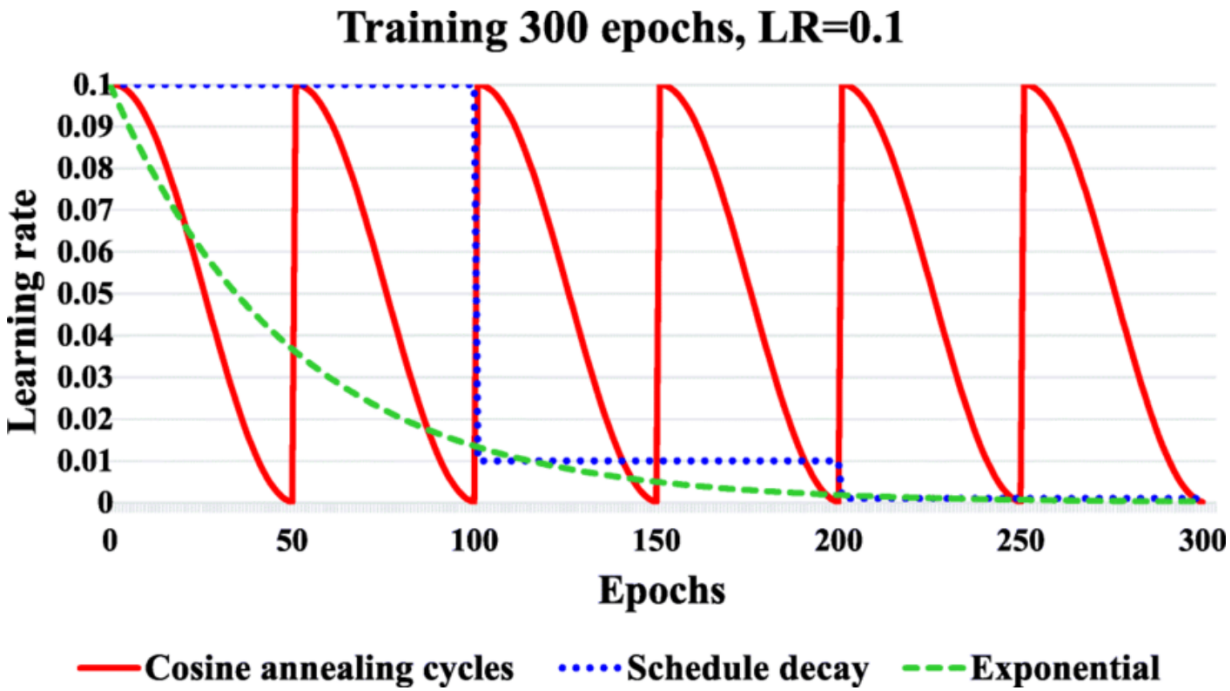
Adam (Adaptive Moments)

Results of different optimizers



Learning Rate Scheduling

- Momentum and Adam are about the use of gradients.
- Here are some ways to schedule the learning rate α



https://www.researchgate.net/figure/Schedule-decay-vs-Cyclic-Cosine-Annealing-vs-Exponential-decay_fig6_336989719

- Cosine Annealing: he resetting of the learning rate acts like a simulated restart of the learning process and the re-use of good weights as the starting point of the restart is referred to as a "warm restart".