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

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

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

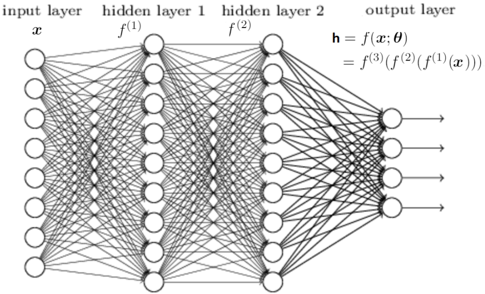
- Next lecture: $\mathbf{h} = f(\mathbf{x})$ as a **convolutional neural network (CNN or ConvNet)**.

Outline

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



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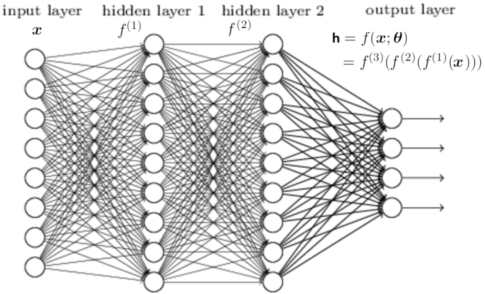

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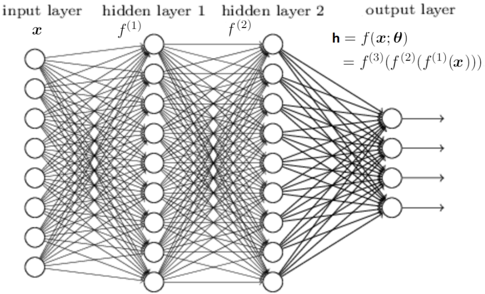

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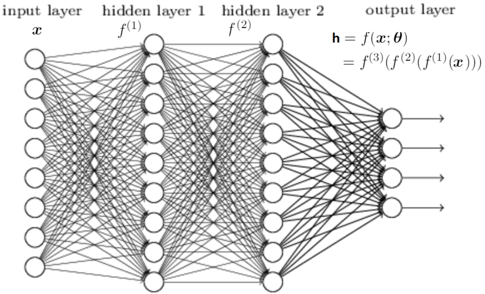

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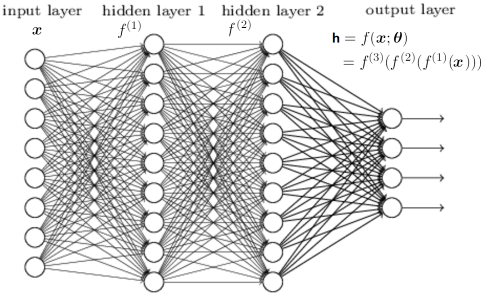

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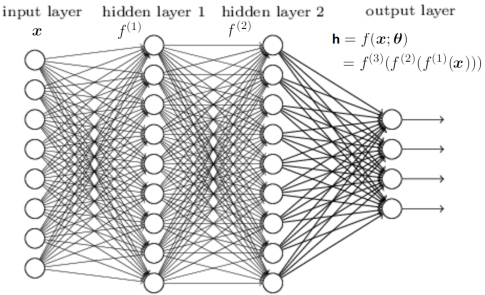

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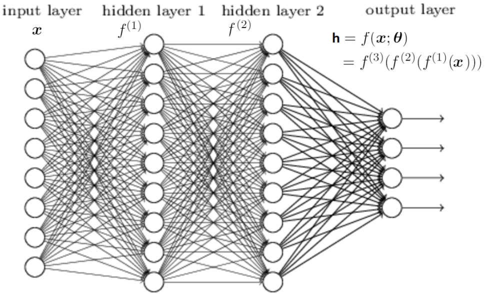

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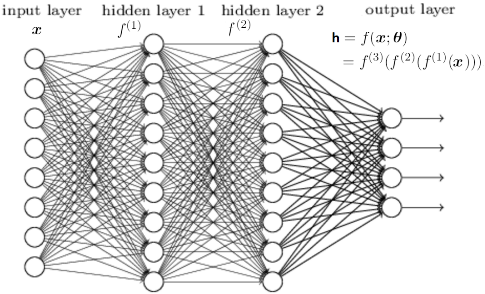

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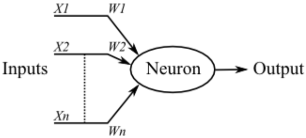
The Units



- 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.

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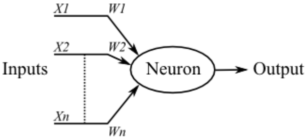

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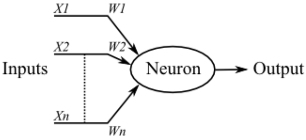

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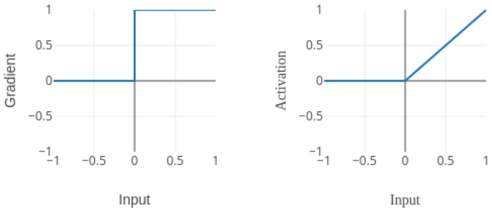
- applies nonlinear **activation function** $g(z)$, and
- gives output $g(z) = g(\mathbf{W}^\top \mathbf{x} + b)$

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

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.

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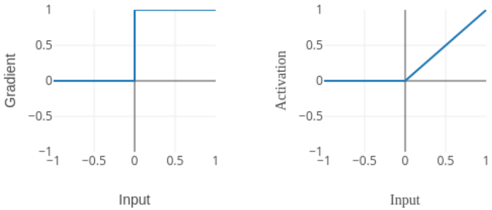

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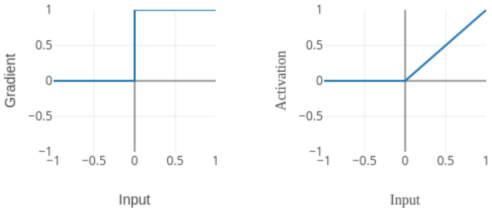

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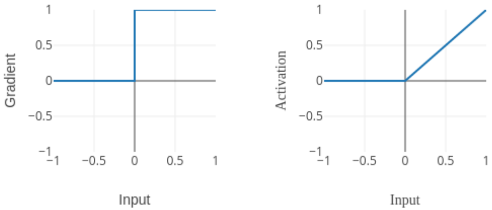

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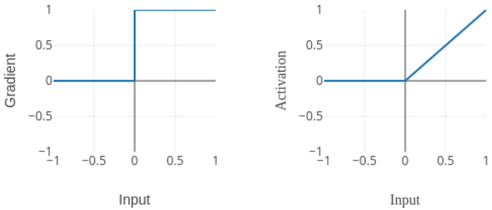

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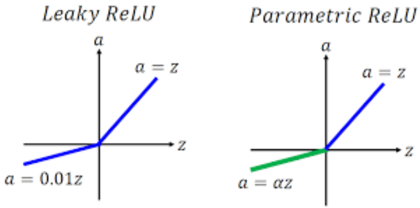
- Zero gradient when $z < 0$. The neuron is **dead** if $z < 0$ for all training examples. Dead neurons cannot be revived.
  - To mitigate the problem somewhat, initialize b to be small positive value, e.g. 0.1, so that the unit is initially active ($z > 0$).

Variations of ReLU



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

- **Absolute value rectification**: $\alpha = -1$,
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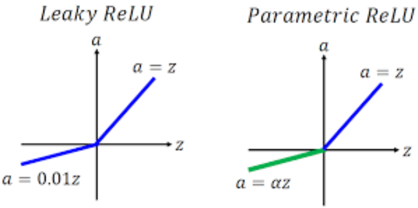

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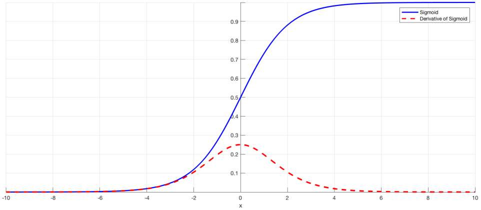
Sigmoid



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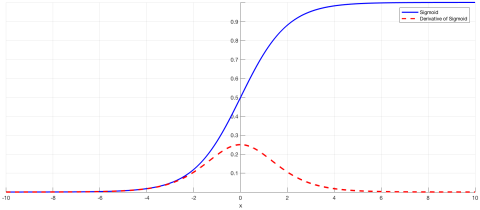

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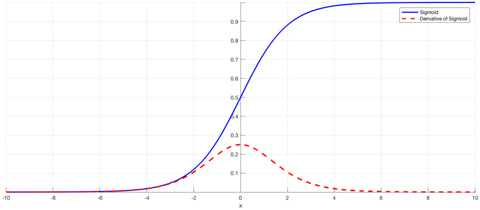

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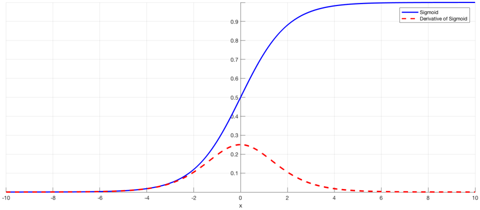

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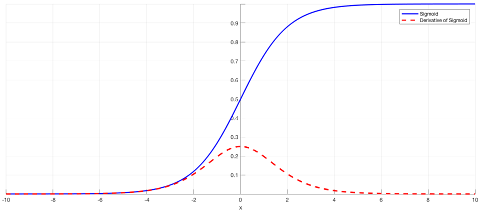

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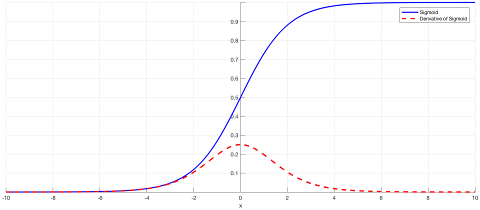

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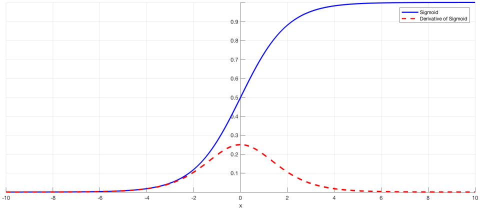

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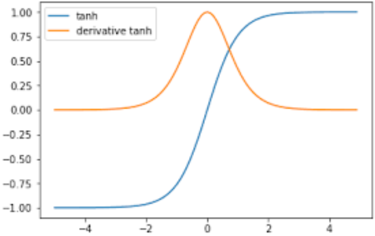
- Not recommended as internal unit.

Hyperbolic Tagent



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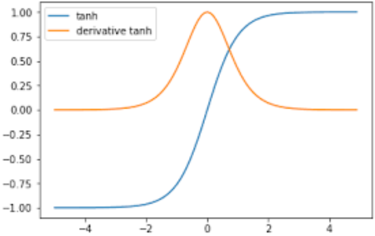

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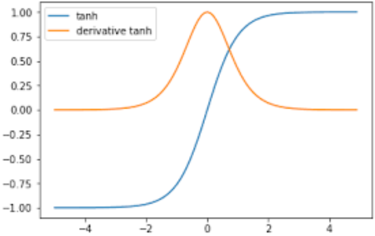

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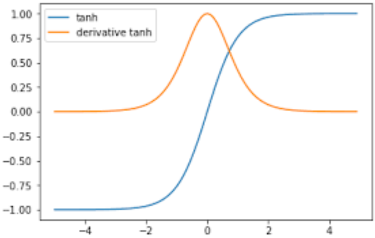

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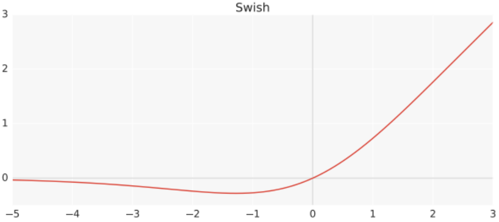
- A popular choice in practice.

Swish



- **Swish activation** was proposed in 2017:

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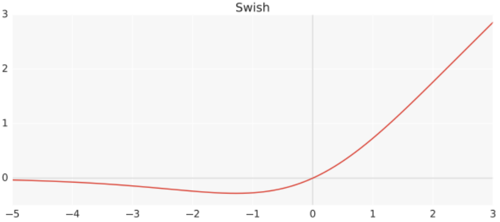

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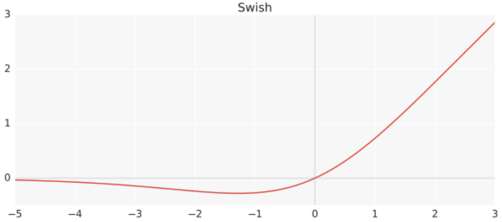

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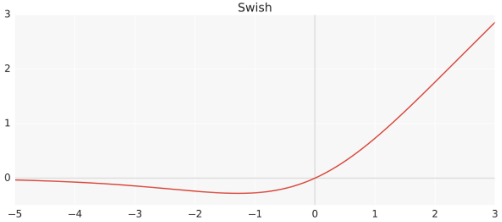

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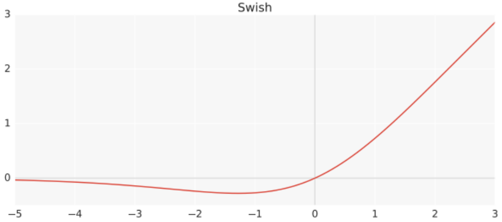

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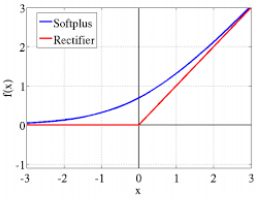
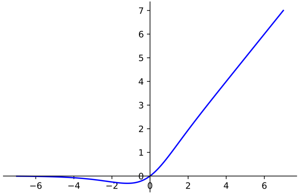
- Unbounded above, which avoids saturation.
- Outperforms ReLU in deep networks.

Softplus and Mish





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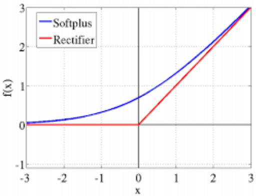
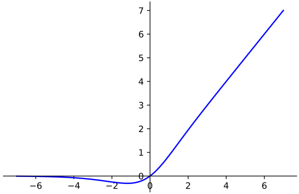




- **Softplus activation function**:

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

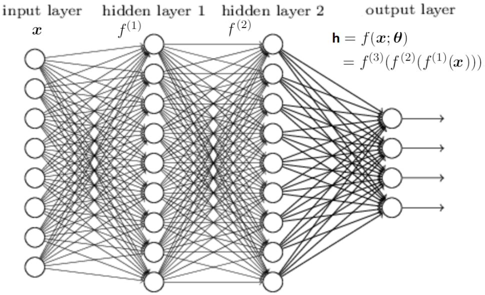
  - Softplus is a smooth version of ReLU, empirically not as good as ReLU.

- **Mish activation function**:

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

  - Recently proposed.Similar to Swish, and better.

Computation by Feedfoward Neural Network



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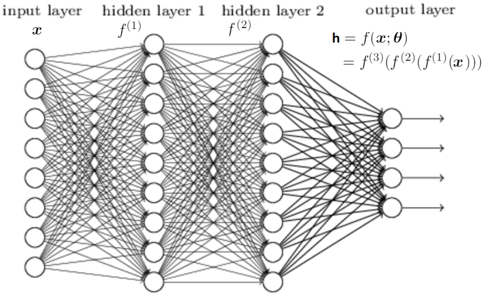

- $\mathbf{h}^{(i)}$ — Column vector for units on layer i; $\mathbf{b}^{(i)}$ — Biases for units on layer i; $g^{(i)}$ — Activation functions for units on layer i.
- $\mathbf{W}^{(i)}$ — Matrix of weights for units on layer i, with weight for unit j at the j-th column.

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

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.

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Deep learning useful when you:

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

Outline

An FNN can be used to define a probabilistic model

$$\underbrace{\underset{\bar{x}}{[\;]} \Rightarrow [\;] \Rightarrow \cdots \Rightarrow \underset{\bar{h}}{[\;]} \xrightarrow{\bar{W}^T \bar{h} + \bar{b}} \bar{z} \qquad p(\bar{y} \mid \bar{z})}_{P(\bar{y} \mid \bar{x}, \theta)}$$

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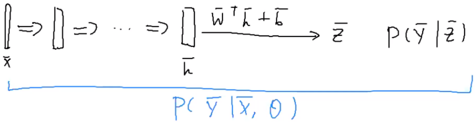

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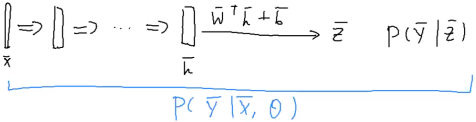

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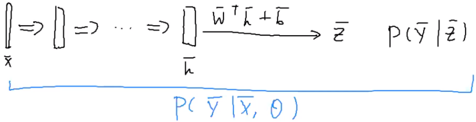

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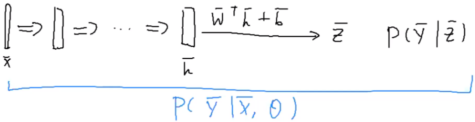

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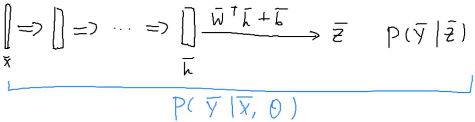

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  where θ consists of weights in f and parameters in $P(\mathbf{y}|\mathbf{h})$.

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

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Linear-Gaussian Output Unit

$$\bar{x} \Rightarrow [\;] \Rightarrow \cdots \Rightarrow \bar{h} \xrightarrow{\bar{W}^T \bar{h} + \bar{b}} \bar{z} \qquad p(\bar{y} \mid \bar{z})$$

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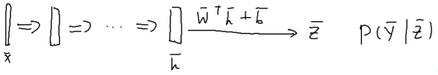

- When $\mathbf{y}$ is real-valued vector, we can assume that $\mathbf{y}$ follows a Gaussian distribution with mean $\mathbf{z}$ and identity covariance matrix $\mathbf{I}$:

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

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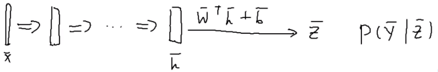

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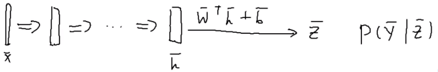

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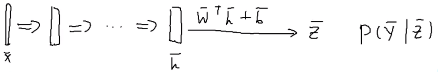

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- They are fine as output units because the negative log-likelihood in the cost function helps to avoid the problem.
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  In words, saturation occurs only when the model already has the right answer: When $y = 1$ and z is very positive, or $y = 0$ and z is very negative.

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Outline

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:

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

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- Algorithm: Stochastic gradient descent (SGD)
  - Initialize θ
  - Repeat for a predetermined number of epochs
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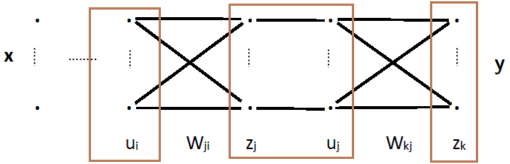
- Question: How to compute the gradient $\nabla L(\mathbf{x}_i, y_i, \theta)$ for each training example?
- Answer: Backpropagation.

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:

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

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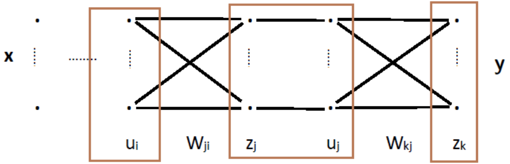

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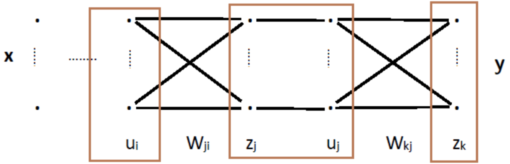

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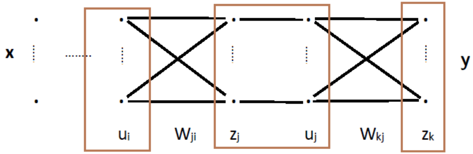
- Let $L = L(\mathbf{x}, \mathbf{y}, \theta)$ for a particular training example $(\mathbf{x}, \mathbf{y})$. The partial derivative of L w.r.t a weigh in the last layer:

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

Backpropagation: Hidden Layer



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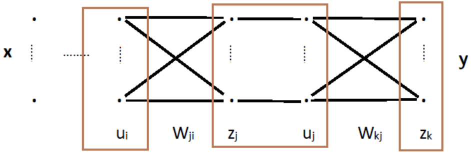


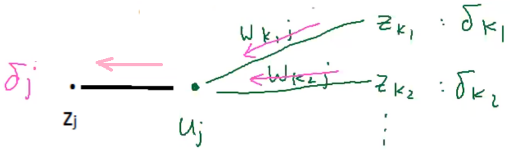
$$z_k = \sum_j u_j W_{kj}, \quad u_j = g(z_j), \quad z_j = \sum_i u_i W_{ji}$$

- 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

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



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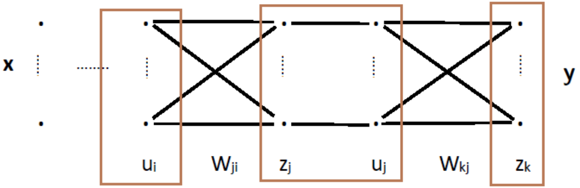
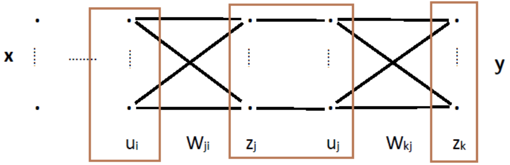


Summary:

- 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



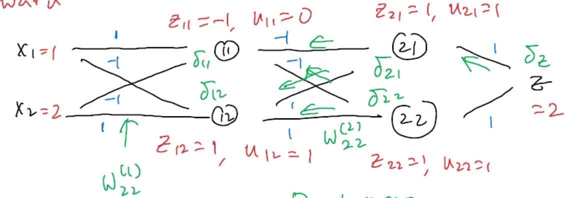
- Objective: Compute $\frac{\partial L}{\partial W_{ji}}$ for all weights (and biases) for each training example:

1. **Propagate forward** to compute the net input and output of each unit (i.e, u_i, u_j, $\ldots$).
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

Backprop Example

Forward



hidden unit: ReLU

$$P(Y|z) = \begin{cases} \sigma(z) & Y=1 \\ 1-\sigma(z) & Y=0 \end{cases}$$

Example

x_1	x_2	Y
1	2	0

$$\delta_{11} = 0$$

Back prop

$$\delta_{21} = \frac{\partial u_{21}}{\partial z_{21}} \, 1 \cdot \delta_z = 0.88$$

$$\delta_z = \sigma(2) - 0 \approx 0.88$$

$$\delta_{12} = \frac{\partial u_{12}}{\partial z_{12}} \cdot (1 \cdot \delta_{21} + 1 \cdot \delta_{22}) = 1.76$$

$$\delta_{22} = 0.88$$

$$\frac{\partial L}{\partial W^{(1)}_{22}} = 2 \times 1.76$$

$$\frac{\partial L}{\partial W^{(2)}_{22}} = 1 \times 0.88$$

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/`

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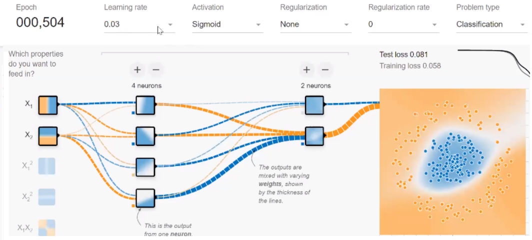
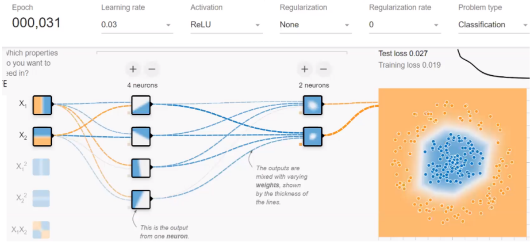
- ReLU units are easier to learn than Sigmoid and Tanh units





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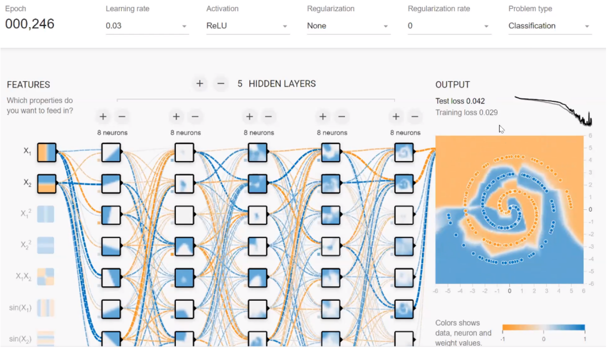
Demonstrations http://playground.tensorflow.org/

- Deep structure helps



- Need to adjust learning rate during training.

Outline

Introduction

- DL models are complex. Overfitting is an important issue.

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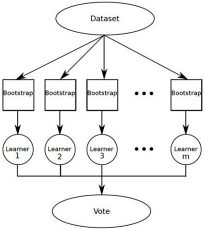
  Almost always do this.

- 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.



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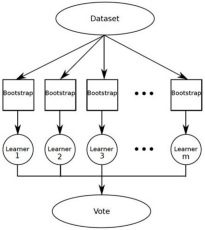

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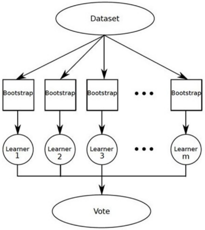

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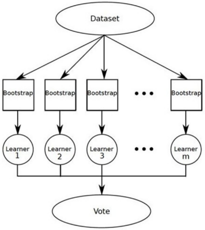

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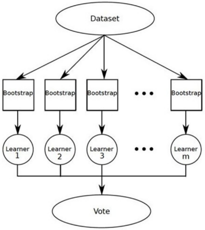

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One Way to Use Bagging for Feedforward Networks

- Start with a large network.
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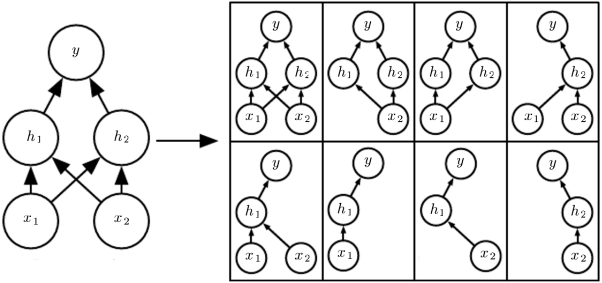
One Way to Use Bagging for Feedforward Networks

- 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.

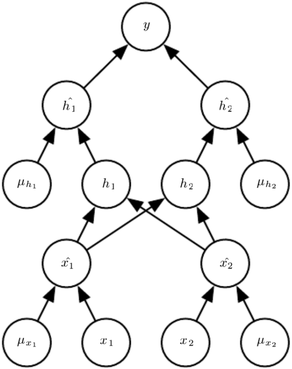


Base network

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).

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See example in CNN code.

Outline

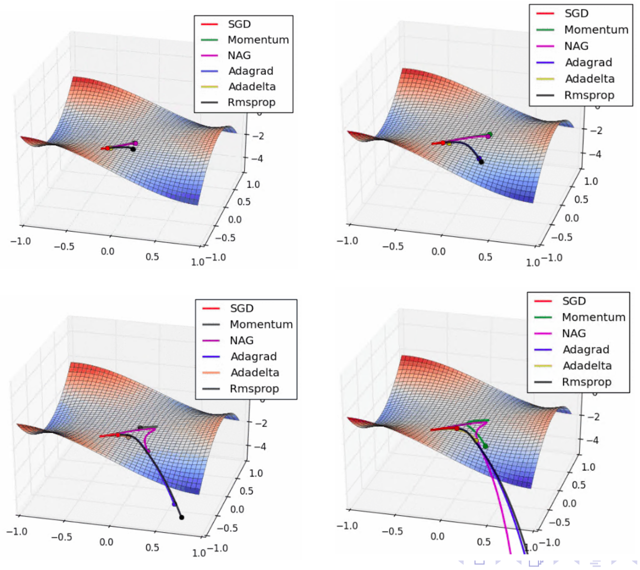
- Our task is: Find θ to minimize the loss function $J(\theta)$.
- There are multiple algorithms that we can use. Stochastic gradient descent is one of them.

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

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

SGD

Compute gradient estimate: $\hat{\boldsymbol{g}} \leftarrow +\frac{1}{m}\nabla_{\boldsymbol{\theta}}\sum_i L(f(\boldsymbol{x}^{(i)};\boldsymbol{\theta}),\boldsymbol{y}^{(i)})$
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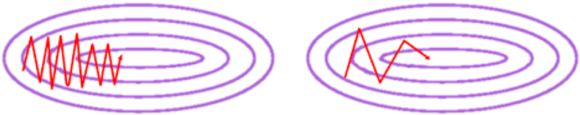
SGD with Momentum

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.



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 (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 (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

AdaGrad vs RMSProp

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

"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

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

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	$(1-\rho)(\underline{\rho^2} g_1^2 + \underline{\rho} g_2^2 + g_3)$	

Exponentially decaying weights

Adam (Adaptive Moments)

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

Momentum

$$\bar{v} \leftarrow \alpha \bar{v} - \epsilon \bar{g} \qquad \Delta\bar{\theta} = \bar{v}$$

$$\bar{\mu} = -\bar{v}$$

$$\bar{\mu} \leftarrow \alpha \bar{\mu} + \epsilon \bar{g} \qquad \Delta\bar{\theta} = -\bar{\mu}$$

RMS Prop

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

$$\Delta\theta = -\frac{\epsilon}{\delta + \sqrt{r}} \odot \bar{g}$$

Adam

$$\bar{s} \leftarrow \rho_1 \bar{s} + (1-\rho_1)\bar{g} \qquad \bar{r} \leftarrow \rho_2 \bar{r} + (1-\rho_2)\, \bar{g} \odot \bar{g}$$

Bias correction

t: iteration number

$$\bar{s} \leftarrow \frac{\bar{s}}{1-\rho_1^t} \qquad \bar{r} \leftarrow \frac{\bar{r}}{1-\rho_2^t}$$

$$\Delta\bar{\theta} = -\frac{\epsilon}{\delta + \sqrt{\bar{r}}} \odot \bar{s}$$

Adam: Bias Correction

Adam: Bias Correction

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

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

r_t

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

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

Expectation

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

2nd order moment

Prob distribution

Adam (Adaptive Moments)

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