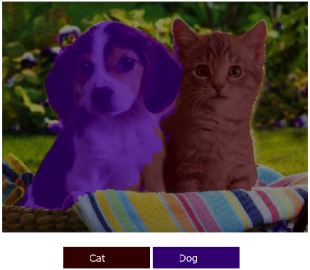
Neural Networks

Today

- Multi-layer Perceptron
- Forward propagation
- Backward propagation

Motivating Examples



Limitations of Linear Classifiers

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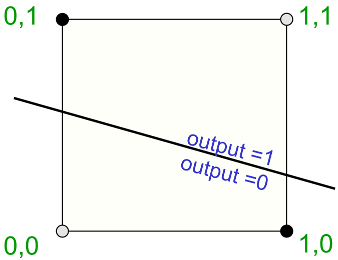

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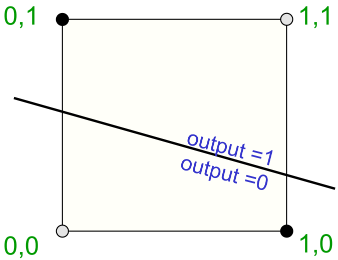

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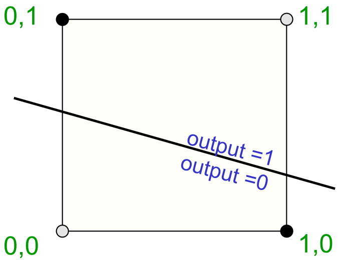

- The positive and negative cases cannot be separated by a plane
- What can we do?

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- We would like to construct non-linear discriminative classifiers that utilize functions of input variables
- Use a large number of simpler functions
  - If these functions are fixed (Gaussian, sigmoid, polynomial basis functions), then optimization still involves linear combinations of (fixed functions of) the inputs
  - Or we can make these functions depend on additional parameters $\rightarrow$ need an efficient method of training extra parameters

Inspiration: The Brain

- Many machine learning methods inspired by biology, e.g., the (human) brain
- Our brain has $\sim 10^{11}$ neurons, each of which communicates (is connected) to $\sim 10^{4}$ other neurons

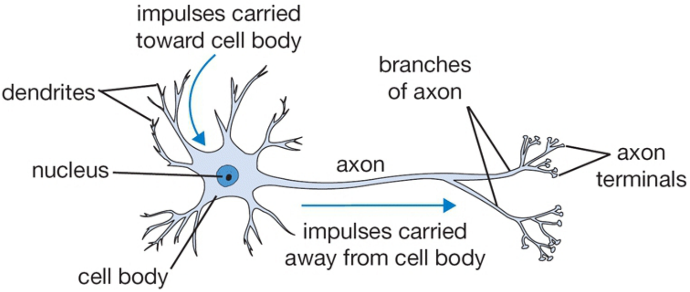


Figure : The basic computational unit of the brain: Neuron

[Pic credit: http://cs231n.github.io/neural-networks-1/]

Mathematical Model of a Neuron

- Neural networks define functions of the inputs (hidden features), computed by neurons
- Artificial neurons are called units

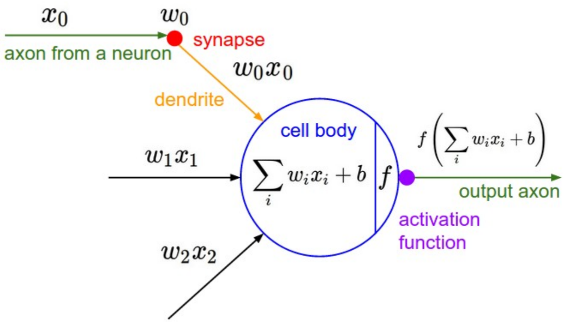


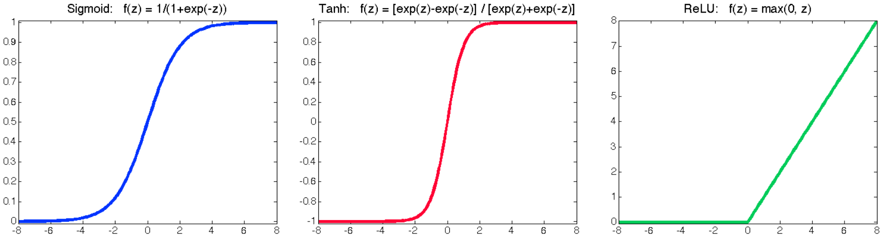
Figure : A mathematical model of the neuron in a neural network

[Pic credit: http://cs231n.github.io/neural-networks-1/]

Activation Functions

Most commonly used activation functions:

- Sigmoid: $\sigma(z) = \frac{1}{1+\exp(-z)}$
- Tanh: $\tanh(z) = \frac{\exp(z)-\exp(-z)}{\exp(z)+\exp(-z)}$
- ReLU (Rectified Linear Unit): $\mathrm{ReLU}(z) = \max(0, z)$



Neuron in Python

- Example in Python of a neuron with a sigmoid activation function

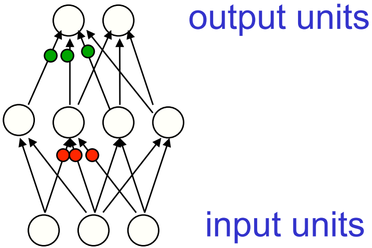
```
class Neuron(object):
  # ...
  def forward(inputs):
    """ assume inputs and weights are 1-D numpy arrays and bias is a number """
    cell_body_sum = np.sum(inputs * self.weights) + self.bias
    firing_rate = 1.0 / (1.0 + math.exp(-cell_body_sum)) # sigmoid activation function
    return firing_rate
```

Figure : Example code for computing the activation of a single neuron

[http://cs231n.github.io/neural-networks-1/]

Neural Network Architecture (Multi-Layer Perceptron)

- Network with one layer of four hidden units:



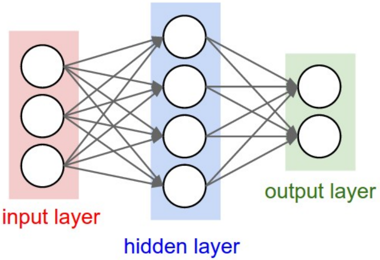


Figure : Two different visualizations of a 2-layer neural network. In this example: 3 input units, 4 hidden units and 2 output units

- Each unit computes its value based on linear combination of values of units that point into it, and an activation function

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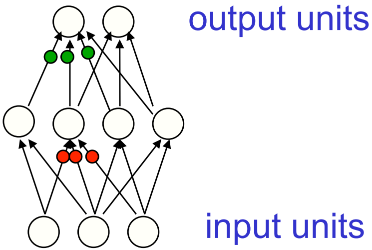

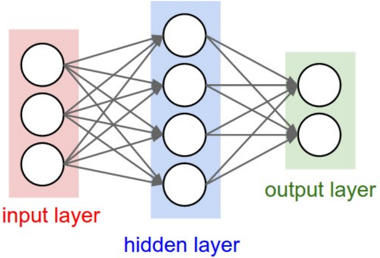

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- Naming conventions; a 2-layer neural network:
  - One layer of hidden units
  - One output layer
    (we do not count the inputs as a layer)

[http://cs231n.github.io/neural-networks-1/]

Neural Network Architecture (Multi-Layer Perceptron)

- Going deeper: a 3-layer neural network with two layers of hidden units

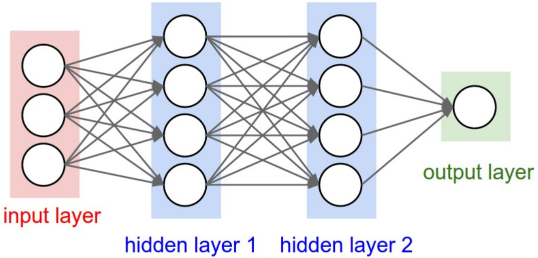

Figure : A 3-layer neural net with 3 input units, 4 hidden units in the first and second hidden layer and 1 output unit

- Naming conventions; a N-layer neural network:
  - $N - 1$ layers of hidden units
  - One output layer

[http://cs231n.github.io/neural-networks-1/]

Representational Power

- Neural network with at **least one hidden layer** is a universal approximator (can represent any function).

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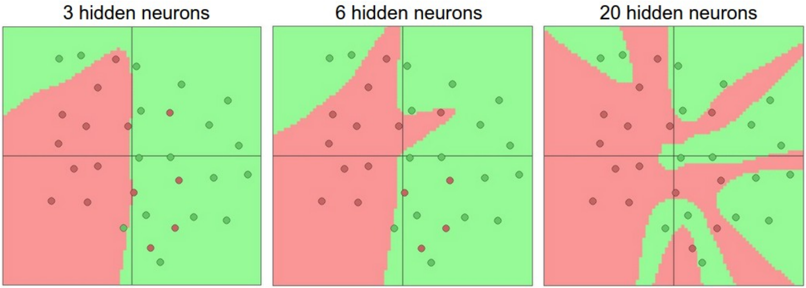

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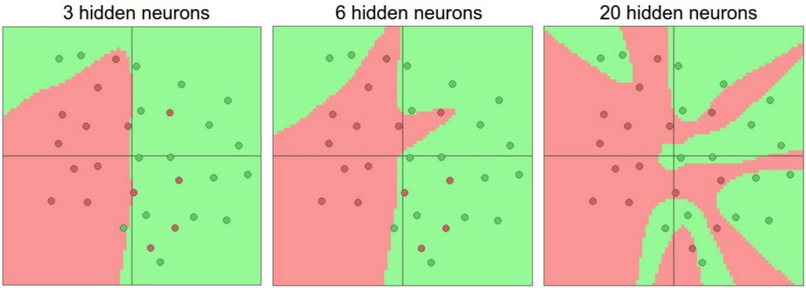

- The capacity of the network increases with more hidden units and more hidden layers
- Why go deeper? Read e.g.,: Do Deep Nets Really Need to be Deep? Jimmy Ba, Rich Caruana, Paper: paper]

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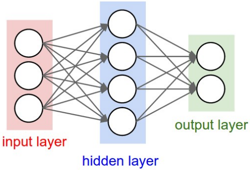
- We only need to know two algorithms
  - Forward pass: performs inference
  - Backward pass: performs learning

Forward Pass: What does the Network Compute?



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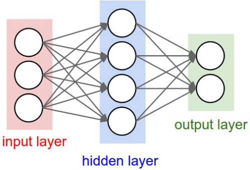

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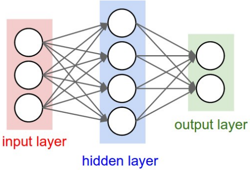

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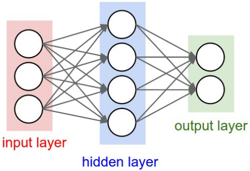

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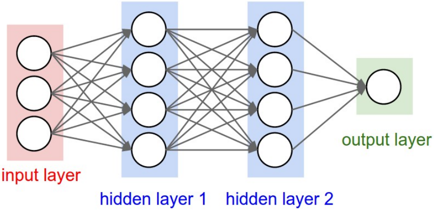
- Activation functions f, g: sigmoid/logistic, tanh, or rectified linear (ReLU)

$$\sigma(z) = \frac{1}{1+\exp(-z)}, \quad \tanh(z) = \frac{\exp(z) - \exp(-z)}{\exp(z) + \exp(-z)}, \quad \mathrm{ReLU}(z) = \max(0, z)$$

Forward Pass in Python

- Example code for a forward pass for a 3-layer network in Python:




```python
# forward-pass of a 3-layer neural network:
f = lambda x: 1.0/(1.0 + np.exp(-x)) # activation function (use sigmoid)
x = np.random.randn(3, 1) # random input vector of three numbers (3x1)
h1 = f(np.dot(W1, x) + b1) # calculate first hidden layer activations (4x1)
h2 = f(np.dot(W2, h1) + b2) # calculate second hidden layer activations (4x1)
out = np.dot(W3, h2) + b3 # output neuron (1x1)
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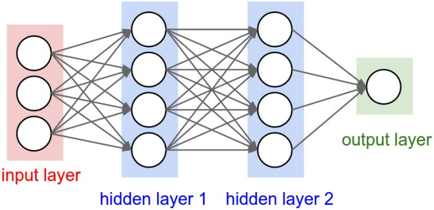


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- Example above: W_1 is matrix of size 4×3, W_2 is 4×4. What about biases and W_3?

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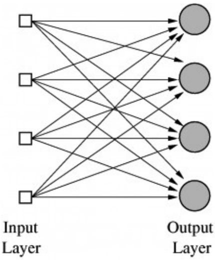
Special Case

- What is a single layer (no hiddens) network with a sigmoid act. function?



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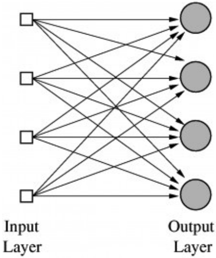

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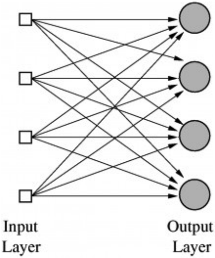

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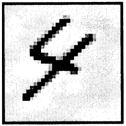
- Logistic regression!

Example Application

- Classify image of handwritten digit (32x32 pixels): 4 vs non-4



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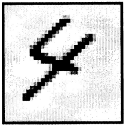

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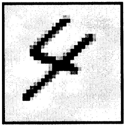

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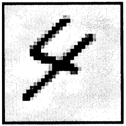

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- How can we train the network, that is, adjust all the parameters $\mathbf{w}$?

Training Neural Networks

- Find weights:

$$\mathbf{w}^* = \underset{\mathbf{w}}{\mathrm{argmin}} \sum_{n=1}^{N} \mathrm{loss}(\mathbf{o}^{(n)}, \mathbf{t}^{(n)})$$

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- Gradient descent:

$$\mathbf{w}^{t+1} = \mathbf{w}^t - \eta \frac{\partial E}{\partial \mathbf{w}^t}$$

  where η is the learning rate (and E is error/loss)

Useful Derivatives

name	function	derivative
Sigmoid	$\sigma(z) = \frac{1}{1+\exp(-z)}$	$\sigma(z) \cdot (1 - \sigma(z))$
Tanh	$\tanh(z) = \frac{\exp(z)-\exp(-z)}{\exp(z)+\exp(-z)}$	$1/\cosh^2(z)$
ReLU	$\mathrm{ReLU}(z) = \max(0, z)$	$\begin{cases} 1, & \text{if } z > 0 \\ 0, & \text{if } z \leq 0 \end{cases}$

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- Given any error function E, activation functions $g()$ and $f()$, just need to derive gradients

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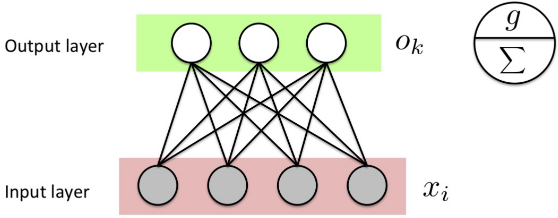
  - We can compute error derivatives for all the hidden units efficiently
  - Once we have the error derivatives for the hidden activities, its easy to get the error derivatives for the weights going into a hidden unit
- This is just the chain rule!

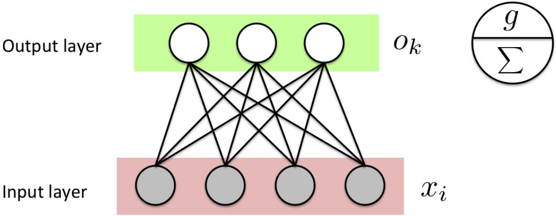
Computing Gradients: Single Layer Network

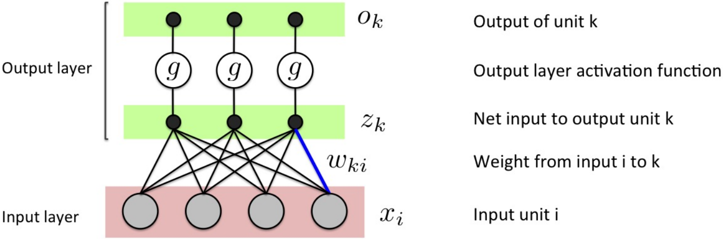
- Let's take a single layer network



Computing Gradients: Single Layer Network

- Let's take a single layer network and draw it a bit differently





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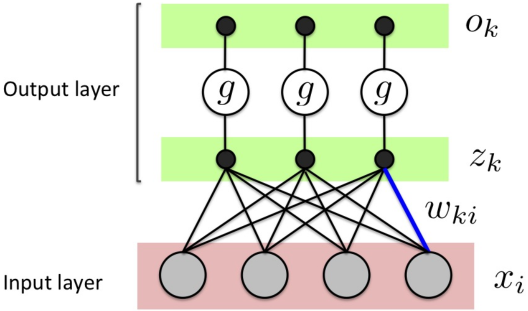

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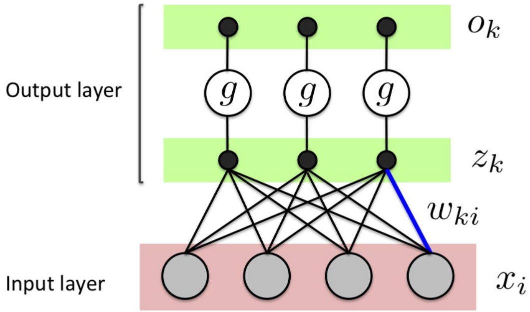

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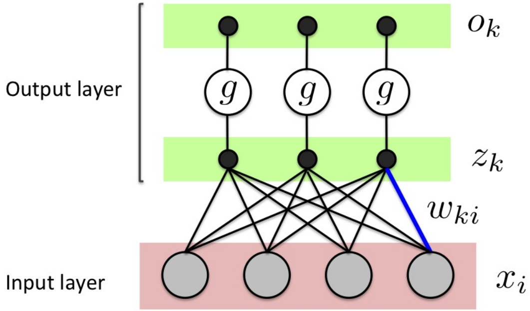
Computing Gradients: Single Layer Network



- Error gradients for single layer network:

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- Error gradient is computable for any continuous activation function $g()$, and any continuous error function

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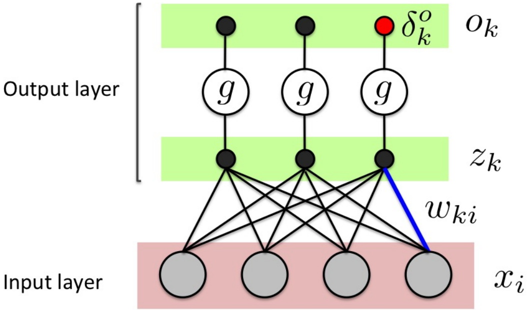

$$\delta_k^o = \frac{\partial E}{\partial o_k}$$

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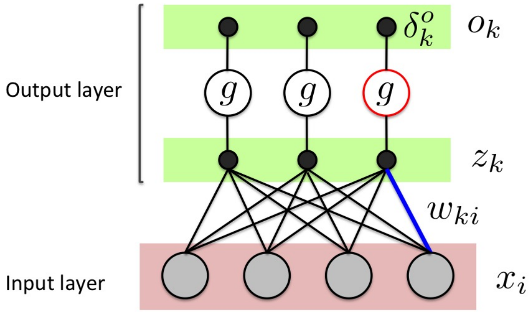

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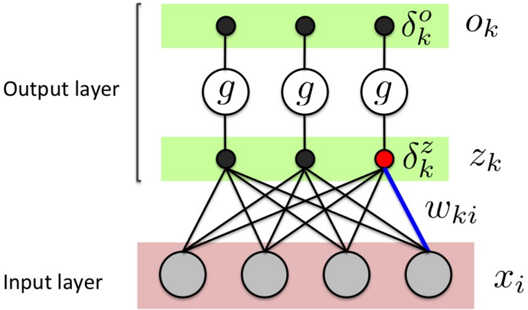

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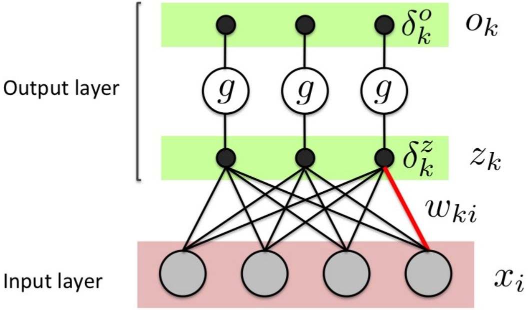

$$\frac{\partial z_k}{\partial w_{ki}}$$

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$$\frac{\partial E}{\partial w_{ki}} = \frac{\partial E}{\partial o_k}\frac{\partial o_k}{\partial z_k}\frac{\partial z_k}{\partial w_{ki}} = \delta_k^z \frac{\partial z_k}{\partial w_{ki}} = \delta_k^z \cdot x_i$$

Gradient Descent for Single Layer Network

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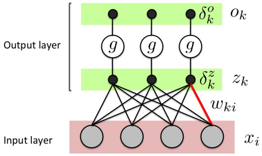

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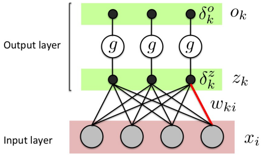

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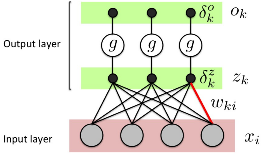

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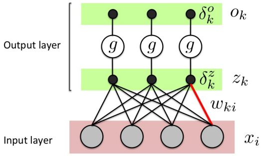

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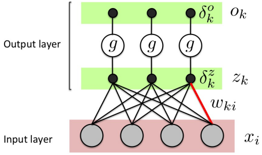

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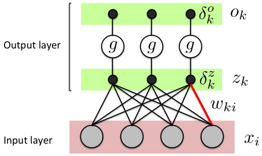

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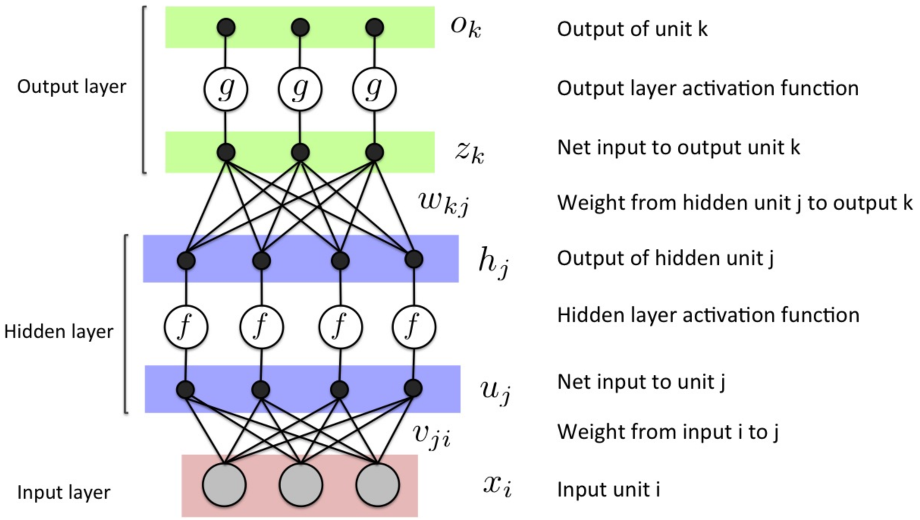
Multi-layer Neural Network



Back-propagation: Sketch on One Training Case

- Convert discrepancy between each output and its target value into an error derivative

$$E = \frac{1}{2}\sum_k (o_k - t_k)^2; \qquad \frac{\partial E}{\partial o_k} = o_k - t_k$$

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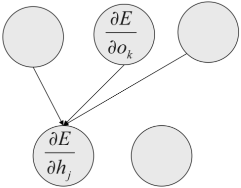

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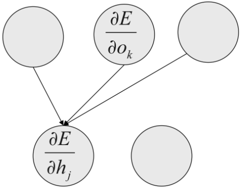
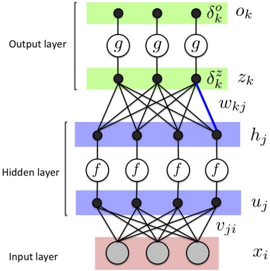


- Use error derivatives w.r.t. activities to get error derivatives w.r.t. the weights.

Gradient Descent for Multi-layer Network



- The output weight gradients for a multi-layer network are the same as for a single layer network

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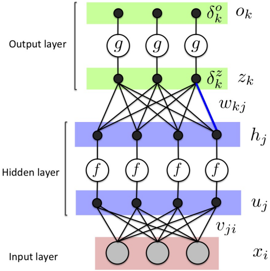

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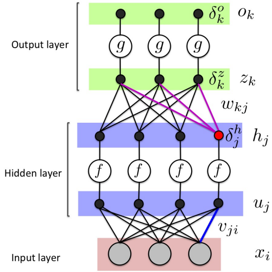

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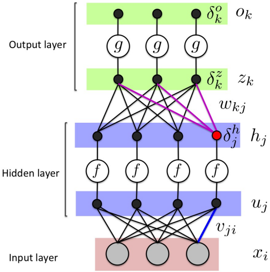

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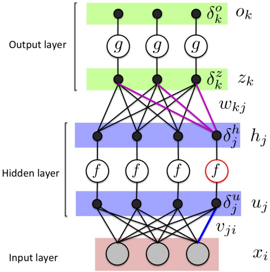

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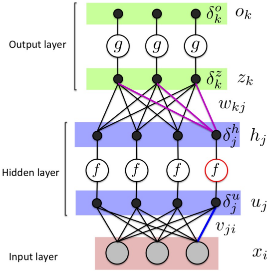
Gradient Descent for Multi-layer Network



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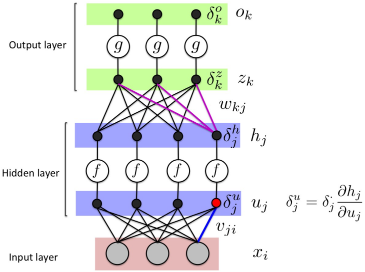

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- For classification, if it is a binary (2-class) problem, then cross-entropy error function often does better (as we saw with logistic regression)

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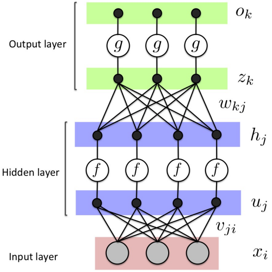
- We can then compute via the chain rule

$$\frac{\partial E}{\partial o} = (o - t)/(o(1 - o))$$

$$\frac{\partial o}{\partial z} = o(1 - o)$$

$$\frac{\partial E}{\partial z} = \frac{\partial E}{\partial o}\frac{\partial o}{\partial z} = (o - t)$$

Multi-class Classification



- For multi-class classification problems, use cross-entropy as loss and the softmax activation function

$$E = -\sum_n \sum_k t_k^{(n)} \log o_k^{(n)}$$

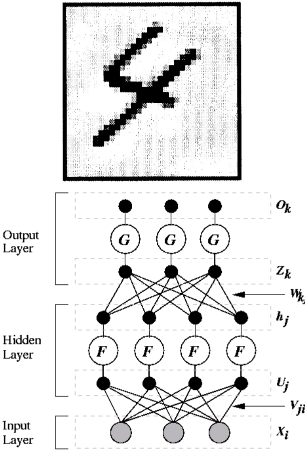
$$o_k^{(n)} = \frac{\exp(z_k^{(n)})}{\sum_j \exp(z_j^{(n)})}$$

- And the derivatives become

$$\frac{\partial o_k}{\partial z_k} = o_k(1 - o_k)$$

$$\frac{\partial E}{\partial z_k} = \sum_j \frac{\partial E}{\partial o_j} \frac{\partial o_j}{\partial z_k} = (o_k - t_k)o_k(1 - o_k)$$

Example Application



- Now trying to classify image of handwritten digit: 32x32 pixels
- 10 output units, 1 per digit
- Use the softmax function:

$$
\begin{aligned}
o_k &= \frac{\exp(z_k)}{\sum_j \exp(z_j)} \\
z_k &= w_{k0} + \sum_{j=1}^{J} h_j(\mathbf{x}) w_{kj}
\end{aligned}
$$

- What is J ?

Ways to Use Weight Derivatives

- How often to update

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- How often to update
  - after a full sweep through the training data (batch gradient descent)

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  - after each training case (stochastic gradient descent)
  - after a mini-batch of training cases
- How much to update
  - Use a fixed learning rate

Ways to Use Weight Derivatives

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  - after a full sweep through the training data (batch gradient descent)

$$w_{ki} \leftarrow w_{ki} - \eta \frac{\partial E}{\partial w_{ki}} = w_{ki} - \eta \sum_{n=1}^{N} \frac{\partial E(\mathbf{o}^{(n)}, \mathbf{t}^{(n)}; \mathbf{w})}{\partial w_{ki}}$$

  - after each training case (stochastic gradient descent)
  - after a mini-batch of training cases
- How much to update
  - Use a fixed learning rate
  - Adapt the learning rate

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- How much to update
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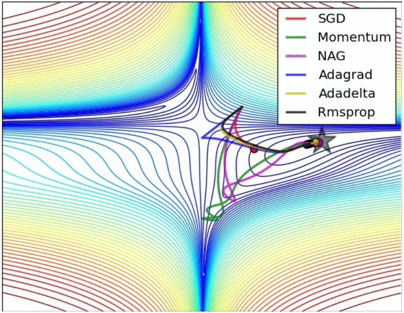
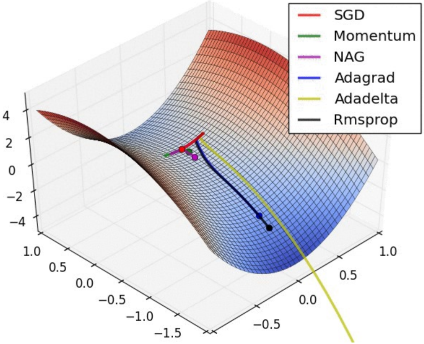
  - Adapt the learning rate
  - Add momentum

$$\begin{aligned} w_{ki} &\leftarrow w_{ki} - v \\ v &\leftarrow \gamma v + \eta \frac{\partial E}{\partial w_{ki}} \end{aligned}$$

Comparing Optimization Methods





[http://cs231n.github.io/neural-networks-3/, Alec Radford]

Monitor Loss During Training

- Check how your loss behaves during training, to spot wrong hyperparameters, bugs, etc

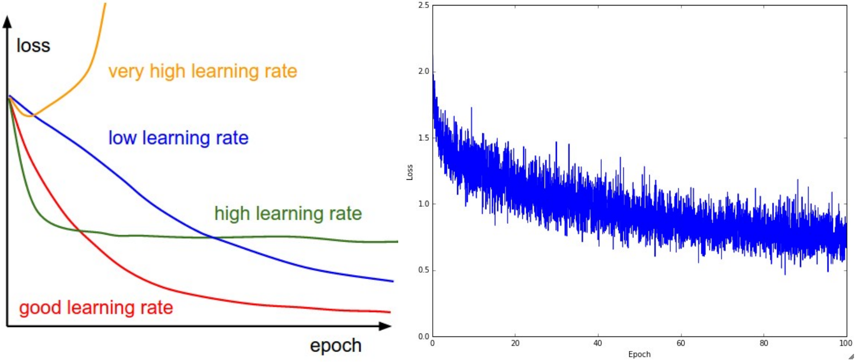
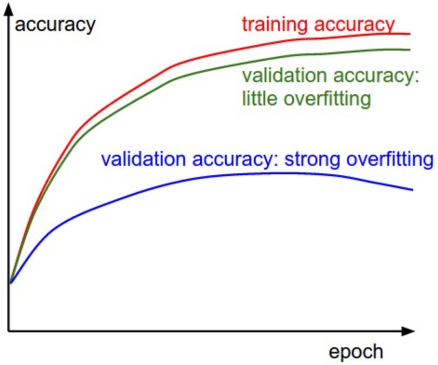


Figure : **Left:** Good vs bad parameter choices, **Right:** How a real loss might look like during training. What are the bumps caused by? How could we get a more smooth loss?

Monitor Accuracy on Train/Validation During Training

- Check how your desired performance metrics behaves during training



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