CSC 411: Lecture 10: Neural Networks I

Class based on Raquel Urtasun & Rich Zemel's lectures

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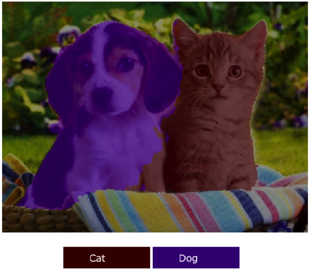
Feb 10, 2016

Today

- Multi-layer Perceptron
- Forward propagation
- Backward propagation

Motivating Examples



Are You Excited about Deep Learning?

Limitations of Linear Classifiers

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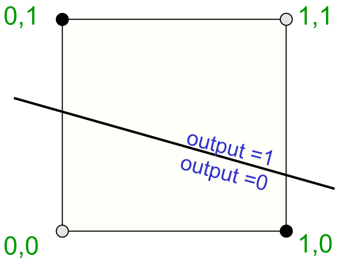

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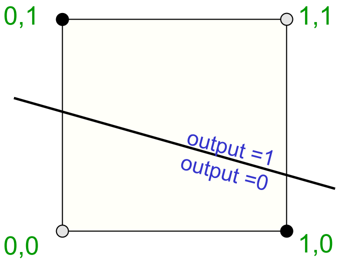

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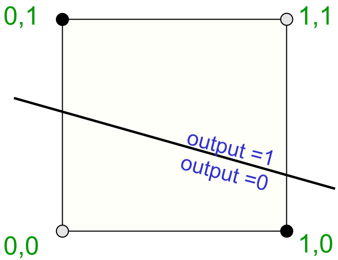

- The positive and negative cases cannot be separated by a plane
- What can we do?

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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

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

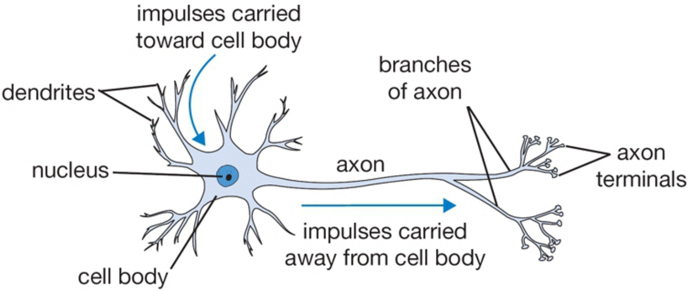


Figure: The basic computational unit of the brain: Neuron

[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

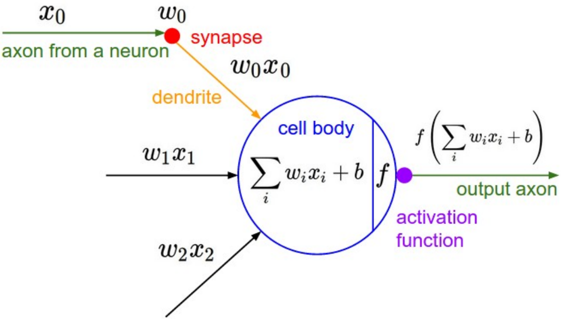


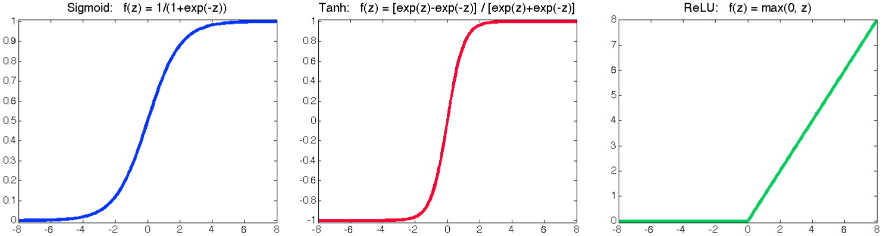
Figure: A mathematical model of the neuron in a neural network

[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

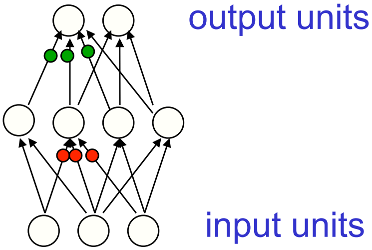
```
class Neuron(object):
  # ...
  def forward(inputs):
    """ assume inputs and weights are 1-D numpy arrays and bias is a number """
    cell_body_sum = np.sum(inputs * self.weights) + self.bias
    firing_rate = 1.0 / (1.0 + math.exp(-cell_body_sum)) # sigmoid activation function
    return firing_rate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

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:



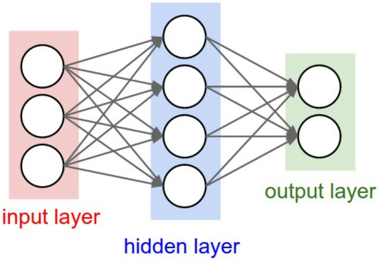


Figure: Two different visualizations of a 2-layer neural network. In this example: 3 input units, 4 hidden units and 2 output units

- 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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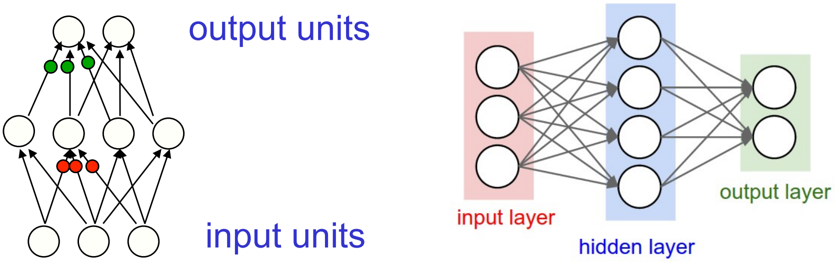

Figure: Two different visualizations of a 2-layer neural network. In this example: 3 input units, 4 hidden units and 2 output units

- 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

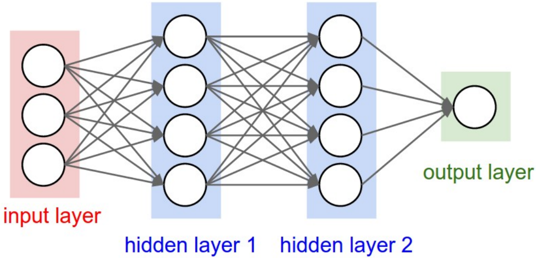

Figure: A 3-layer neural net with 3 input units, 4 hidden units in the first and second hidden layer and 1 output unit

- 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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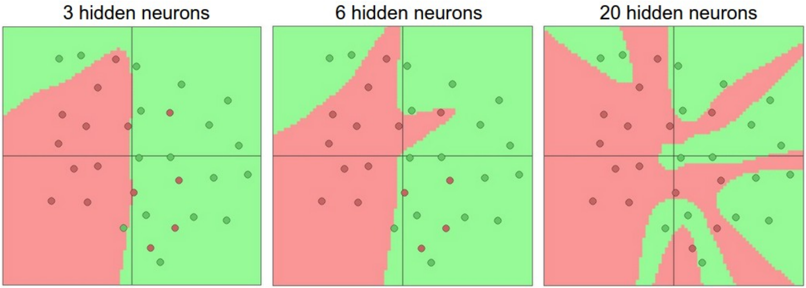

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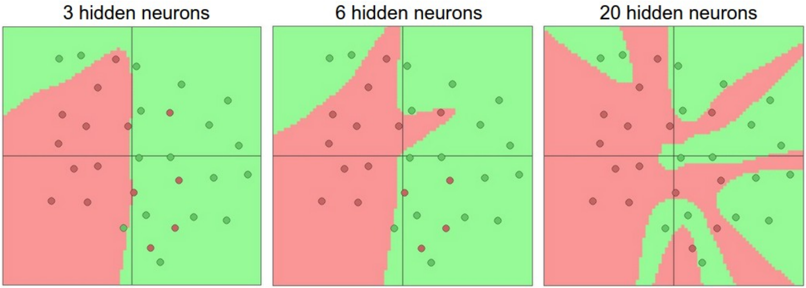

- The capacity of the network increases with more hidden units and more hidden layers
- Why go deeper? Read eg: Do Deep Nets Really Need to be Deep? Jimmy Ba, Rich Caruana, Paper: paper]

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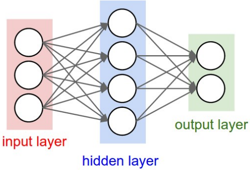
Neural Networks

- 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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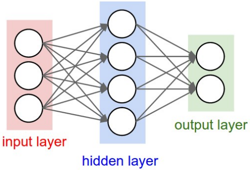

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$$h_j(\mathbf{x}) = f(v_{j0} + \sum_{i=1}^{D} x_i v_{ji})$$

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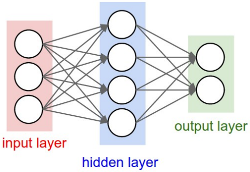

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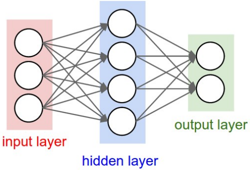

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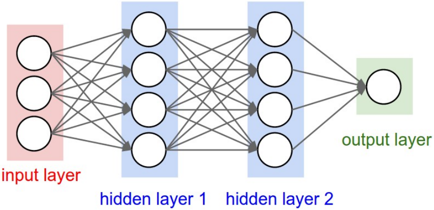
- Activation functions f, g: sigmoid/logistic, tanh, or rectified linear (ReLU)

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

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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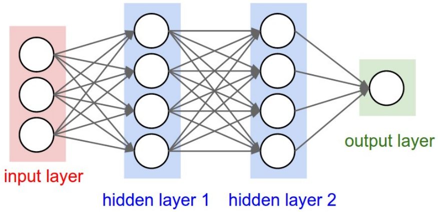


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- Example above: W_1 is matrix of size 4×3, W_2 is 4×4. What about biases and W_3?

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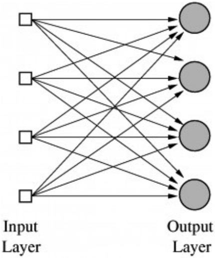
Special Case

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



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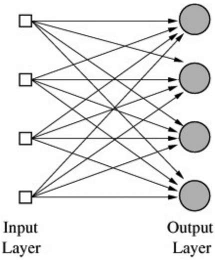

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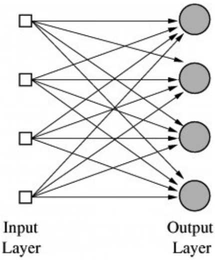

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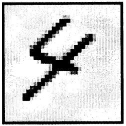
- Logistic regression!

Example Application

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



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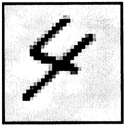

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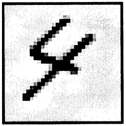

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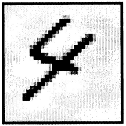

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- How can we train the network, that is, adjust all the parameters **w**?

Training Neural Networks

- Find weights:

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

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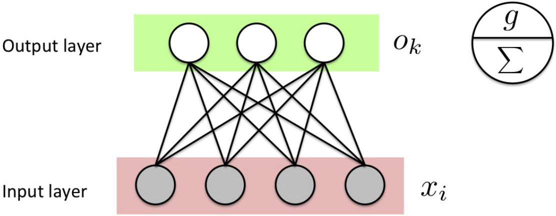
  - We can compute error derivatives for all the hidden units efficiently
  - Once we have the error derivatives for the hidden activities, its easy to get the error derivatives for the weights going into a hidden unit
- This is just the chain rule!

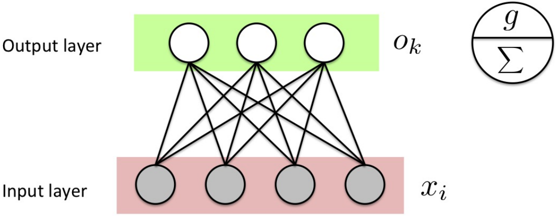
Computing Gradients: Single Layer Network

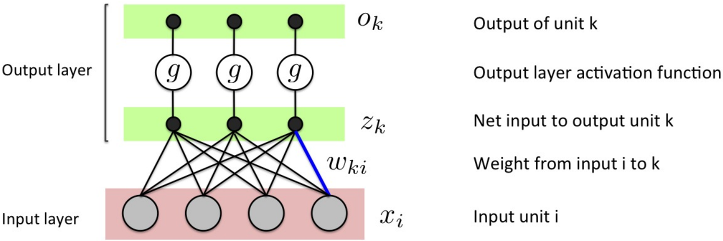
- Let's take a single layer network



Computing Gradients: Single Layer Network

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





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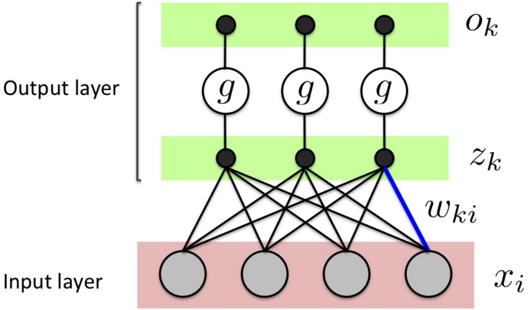

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$$\frac{\partial E}{\partial w_{ki}} =$$

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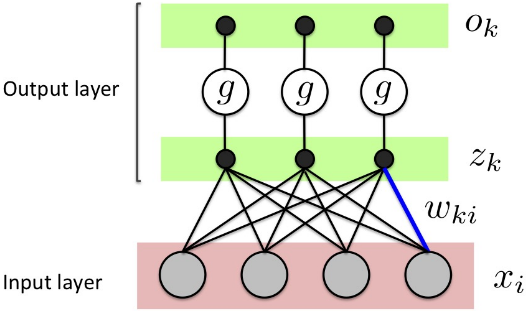

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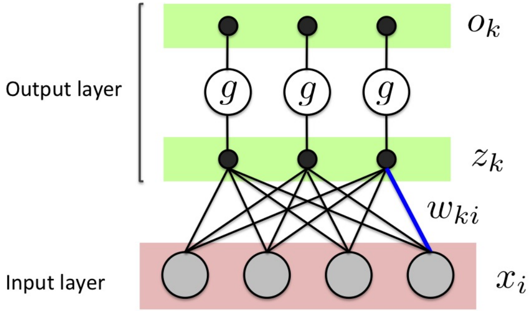

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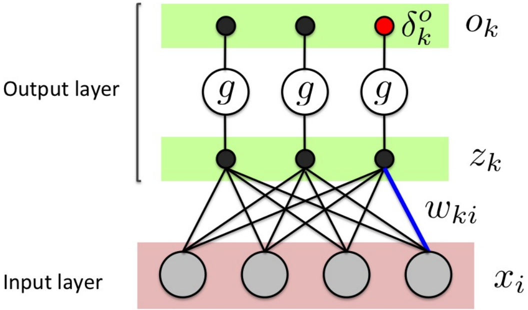
- Error gradient is computable for any continuous activation function $g()$, and any continuous error function

Computing Gradients: Single Layer Network



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

- Error gradients for single layer network:

$$\frac{\partial E}{\partial w_{ki}} = \underbrace{\frac{\partial E}{\partial o_k}}_{\delta_k^o} \frac{\partial o_k}{\partial z_k} \frac{\partial z_k}{\partial w_{ki}}$$

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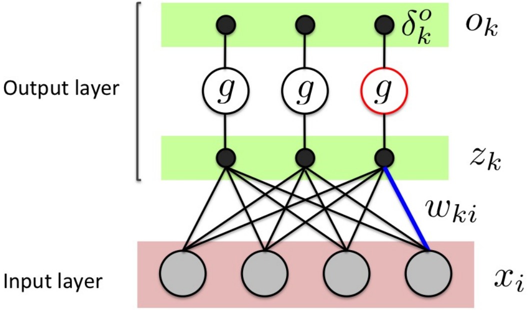

$$\frac{\partial o_k}{\partial z_k}$$

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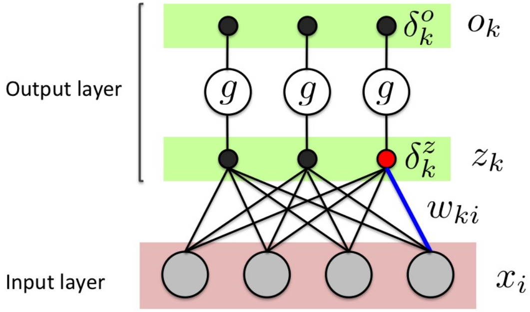

$$\delta_k^z = \delta_k^o \cdot \frac{\partial o_k}{\partial z_k}$$

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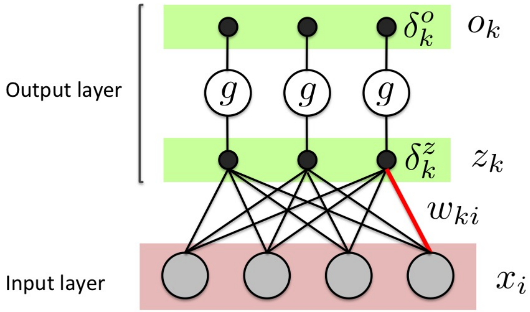

$$\frac{\partial z_k}{\partial w_{ki}}$$

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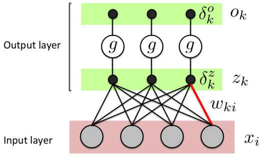
Gradient Descent for Single Layer Network

- Assuming the error function is mean-squared error (MSE), on a single training example n, we have

$$\frac{\partial E}{\partial o_k^{(n)}} = o_k^{(n)} - t_k^{(n)} := \delta_k^o$$



Using logistic activation functions:

$$\begin{aligned} o_k^{(n)} &= g(z_k^{(n)}) = (1 + \exp(-z_k^{(n)}))^{-1} \\ \frac{\partial o_k^{(n)}}{\partial z_k^{(n)}} &= o_k^{(n)}(1 - o_k^{(n)}) \end{aligned}$$

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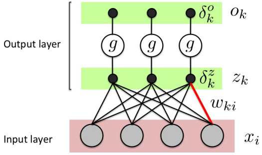

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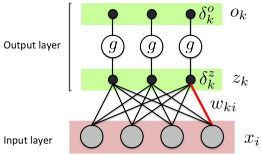

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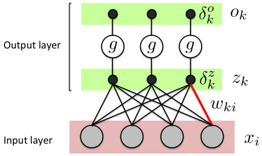

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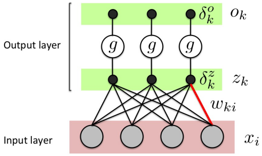

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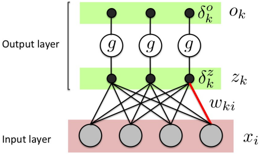

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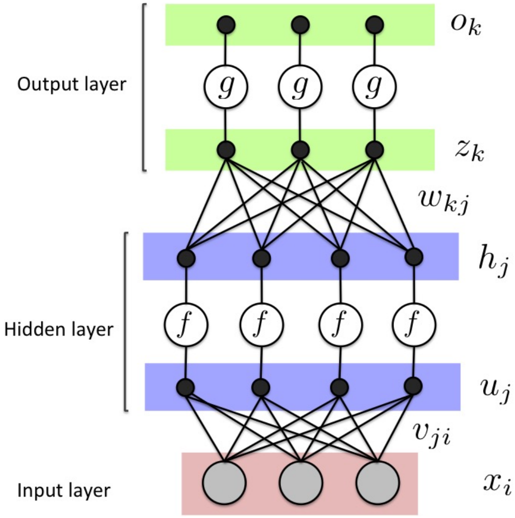
Multi-layer Neural Network



o_k	Output of unit k
	Output layer activation function
z_k	Net input to output unit k
w_{kj}	Weight from hidden unit j to output k
h_j	Output of hidden unit j
	Hidden layer activation function
u_j	Net input to unit j
v_{ji}	Weight from input i to j
x_i	Input unit i

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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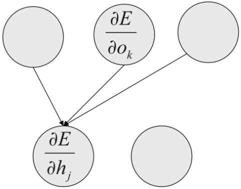

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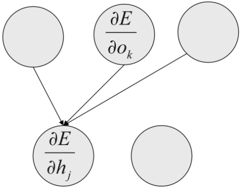
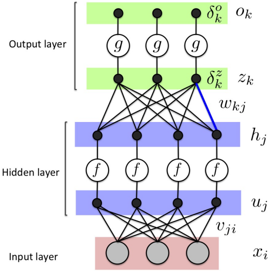


- Use error derivatives w.r.t. activities to get error derivatives w.r.t. the weights.

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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where δ_k is the error w.r.t. the net input for unit k

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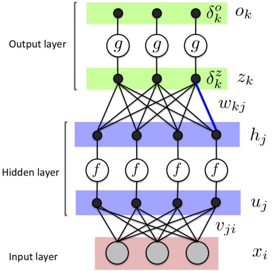

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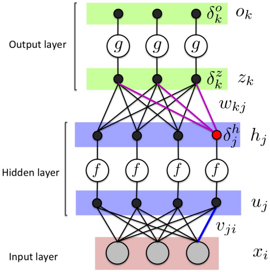

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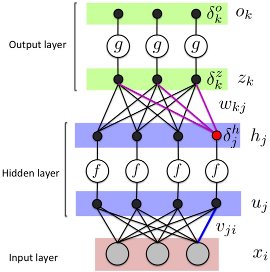

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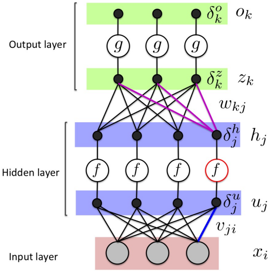

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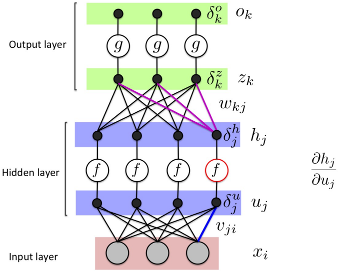

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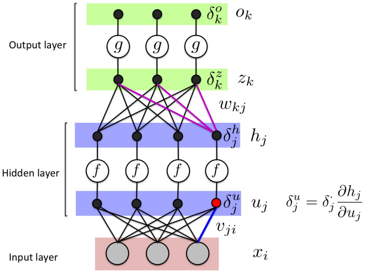

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- For classification, if it is a binary (2-class) problem, then cross-entropy error function often does better (as we saw with logistic regression)

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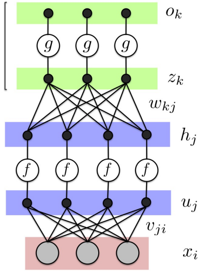
- We can then compute via the chain rule

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

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

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

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

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

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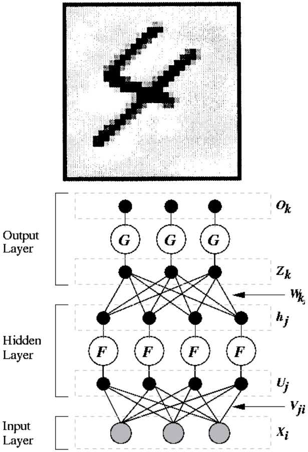

- Now trying to classify image of handwritten digit: 32x32 pixels
- 10 output units, 1 per digit
- Use the softmax function:

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

$$z_k = w_{k0} + \sum_{j=1}^{J} h_j(\mathbf{x}) w_{kj}$$

- What is J ?

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- How often to update

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  - Adapt the learning rate

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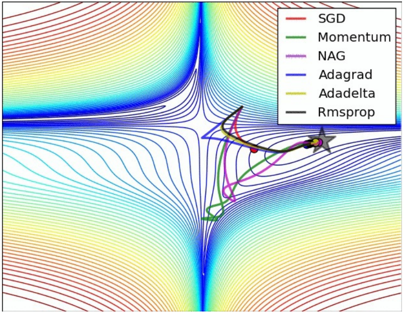
- How often to update
  - after a full sweep through the training data (batch gradient descent)

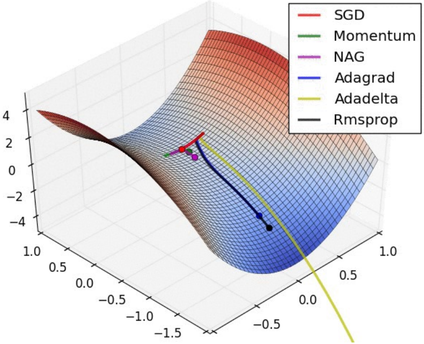
$$w_{ki} \leftarrow w_{ki} - \eta \frac{\partial E}{\partial w_{ki}} = w_{ki} - \eta \sum_{n=1}^{N} \frac{\partial E(\mathbf{o}^{(n)}, \mathbf{t}^{(n)}; \mathbf{w})}{\partial w_{ki}}$$

  - 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
  - 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

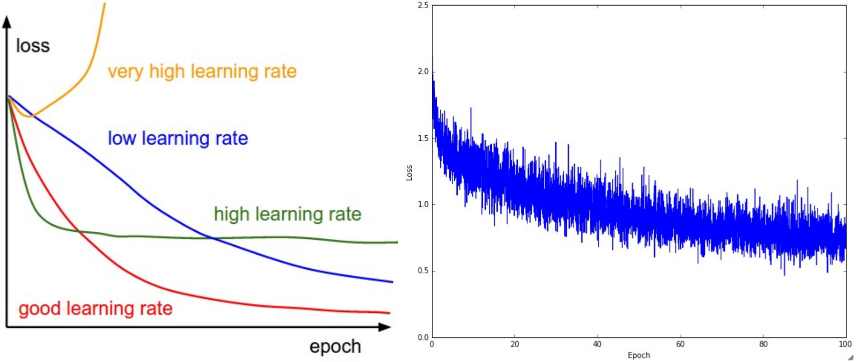
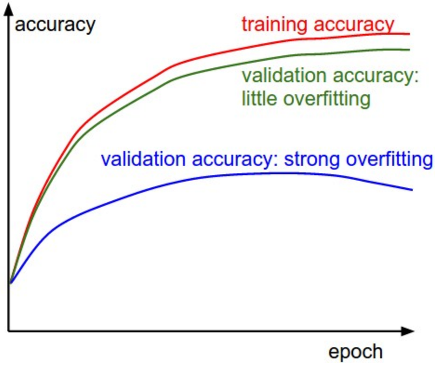


Figure: **Left:** Good vs bad parameter choices, **Right:** How a real loss might look like during training. What are the bumps caused by? How could we get a more smooth loss?

Monitor Accuracy on Train/Validation During Training

- Check how your desired performance metrics behaves during training



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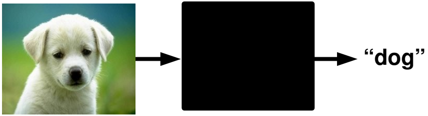
Supervised Learning: Examples

Classification

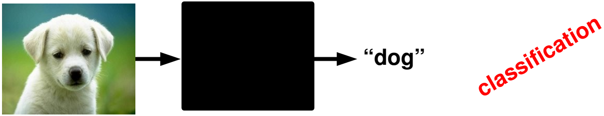


classification

Why "Deep"?

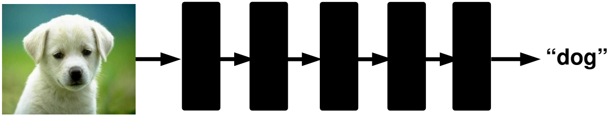
Supervised Learning: Examples

Classification



Supervised Deep Learning

Classification



[Picture from M. Ranzato]

Neural Networks

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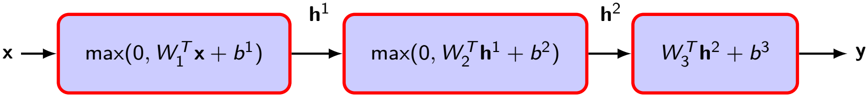

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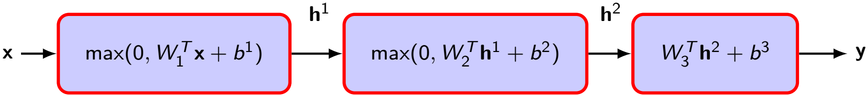

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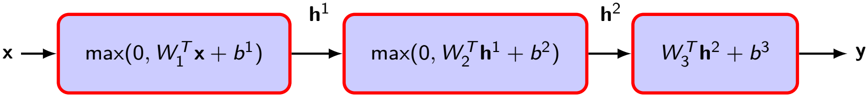

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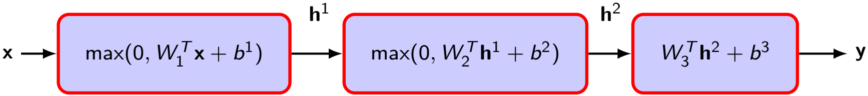

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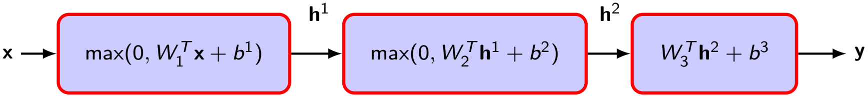

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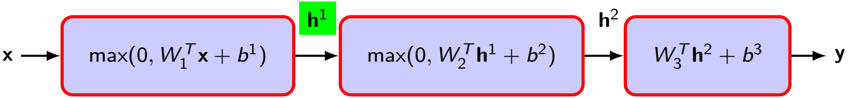
  - W_i are the parameters of the i-th layer

Evaluating the Function

- Assume we have learn the weights and we want to do inference
- Forward Propagation: compute the output given the input



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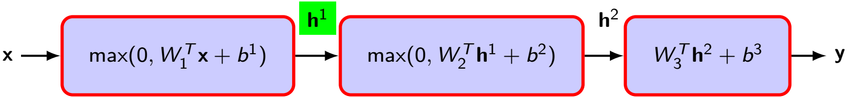

- Do it in a compositional way,

$$\mathbf{h}^1 = \max(0, W_1^T\mathbf{x} + b^1)$$

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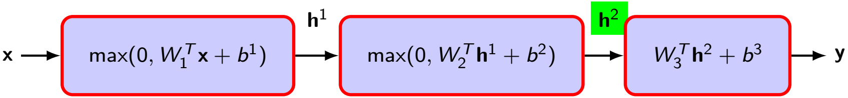

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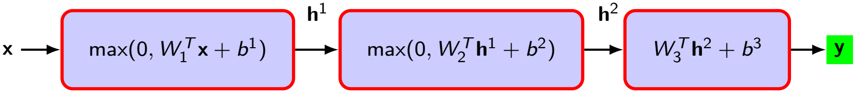

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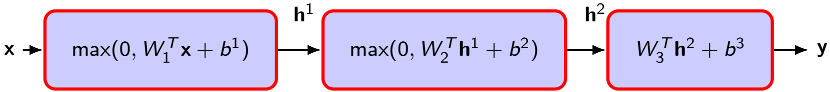
\mathbf{y} &= \max(0, W_3^T \mathbf{h}^2 + b_3)
\end{aligned}$$

Learning



- We want to estimate the parameters, biases and hyper-parameters (e.g., number of layers, number of units) such that we do good predictions
- Collect a training set of input-output pairs $\{\mathbf{x}^{(n)}, \mathbf{t}^{(n)}\}$

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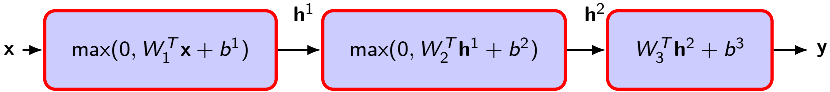

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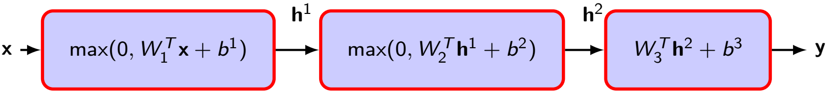

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- Collect a training set of input-output pairs $\{\mathbf{x}^{(n)}, \mathbf{t}^{(n)}\}$
- For classification: Encode the output with 1-K encoding $\mathbf{t} = [0, .., 1, .., 0]$
- Define a loss per training example and minimize the empirical risk

$$\mathcal{L}(\mathbf{w}) = \frac{1}{N} \sum_n \ell(\mathbf{w}, \mathbf{x}^{(n)}, \mathbf{t}^{(n)})$$

with N number of examplesand $\mathbf{w}$ contains all parameters

Loss Function: Classification

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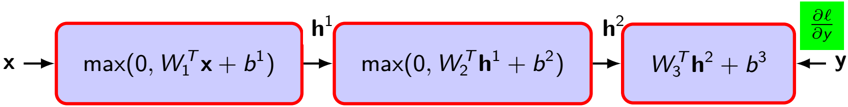
$$\ell(\mathbf{w}, \mathbf{x}^{(n)}, \mathbf{t}^{(n)}) = -\sum_k t_k^{(n)} \log p(c_k|\mathbf{x})$$

- Use gradient descent to train the network

$$\min_{\mathbf{w}} \frac{1}{N}\sum_n \ell(\mathbf{w}, \mathbf{x}^{(n)}, \mathbf{t}^{(n)})$$

Backpropagation

- Efficient computation of the gradients by applying the chain rule



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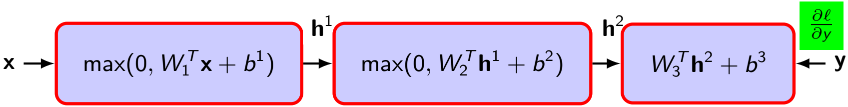

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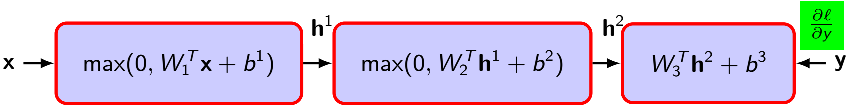

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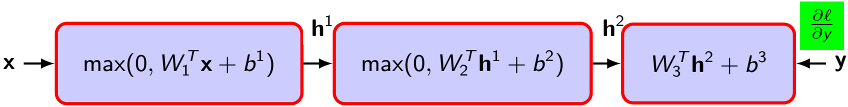

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$$\frac{\partial \ell}{\partial y} = p(c|\mathbf{x}) - t$$

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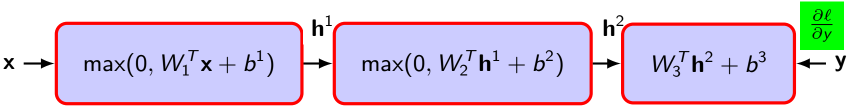

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- Note that the forward pass is necessary to compute $\frac{\partial \ell}{\partial y}$

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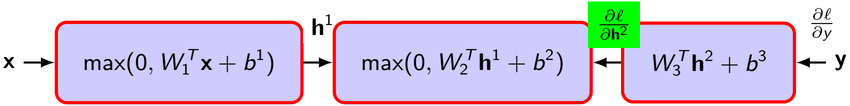

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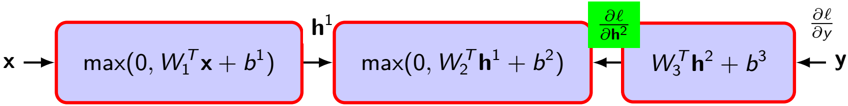

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$$\frac{\partial \ell}{\partial y} = p(c|\mathbf{x}) - t$$

- Given $\frac{\partial \ell}{\partial y}$ if we can compute the Jacobian of each module

Backpropagation

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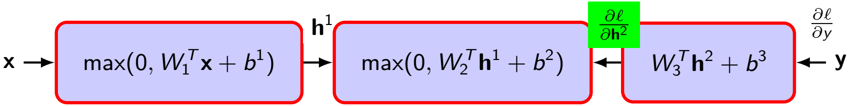

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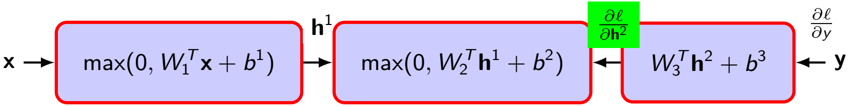

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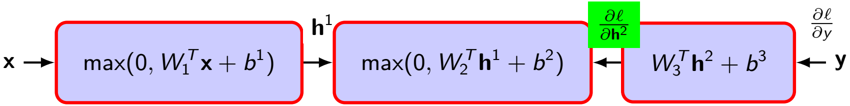

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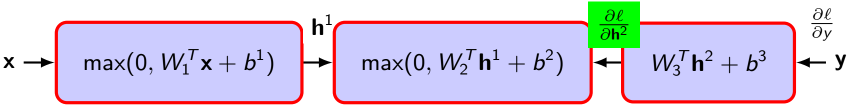

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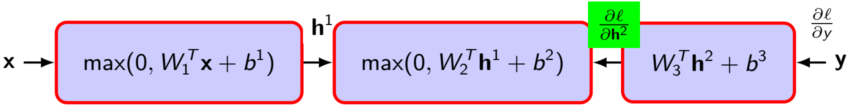

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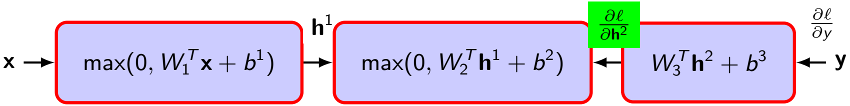

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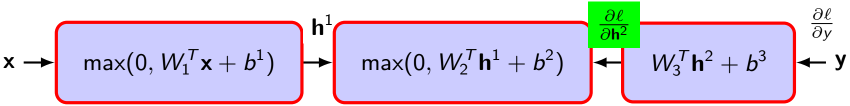

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- Need to compute gradient w.r.t. inputs and parameters in each layer

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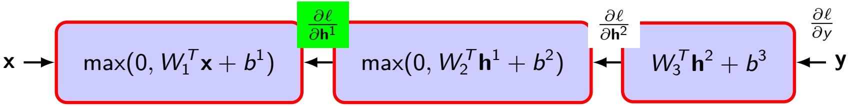

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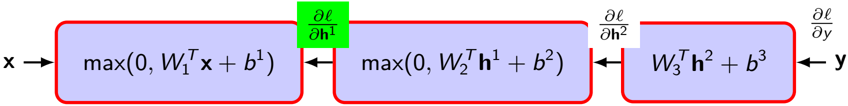

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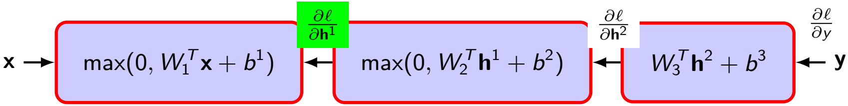

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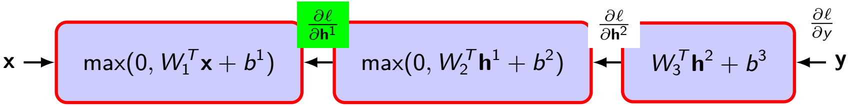

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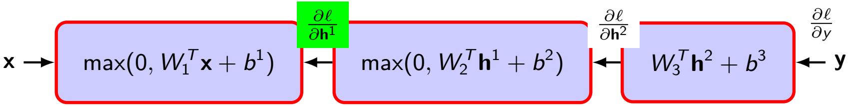

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Toy Code (Matlab): Neural Net Trainer

```
% F-PROP
for i = 1 : nr_layers - 1
  [h{i}  jac{i}]  =  nonlinearity(W{i} * h{i-1} +  b{i});
end
h{nr_layers-1}  =  W{nr_layers-1} * h{nr_layers-2}  +   b{nr_layers-1};
prediction  =  softmax(h{l-1});


% CROSS ENTROPY LOSS
loss  =  -  sum(sum(log(prediction)  .*  target)) / batch_size;


% B-PROP
dh{l-1}  =  prediction  -  target;
for i = nr_layers - 1 : -1 : 1
  Wgrad{i}  =  dh{i} * h{i-1}';
  bgrad{i}  =  sum(dh{i}, 2);
  dh{i-1}  =  (W{i}' * dh{i})  .*  jac{i-1};
end


% UPDATE
for i = 1 : nr_layers - 1
  W{i}  =  W{i}  -  (lr / batch_size)  *  Wgrad{i};
  b{i}  =  b{i}  -  (lr / batch_size)  *  bgrad{i};
end
```

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This code has a few bugs with indices...

Ranzato

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  - So it fits both kinds of regularity.
  - If the model is very flexible it can model the sampling error really well. This is a disaster.

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  - Limit the norm of the weights.
  - Stop the learning before it has time to overfit.

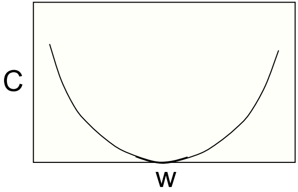
Limiting the size of the Weights

- Weight-decay involves adding an extra term to the cost function that penalizes the squared weights.

$$C = \ell + \frac{\lambda}{2} \sum_i w_i^2$$

- Keeps weights small unless they have big error derivatives.

$$\frac{\partial C}{\partial w_i} = \frac{\partial \ell}{\partial w_i} + \lambda w_i$$



when $\frac{\partial C}{\partial w_i} = 0, \quad w_i = -\frac{1}{\lambda} \frac{\partial \ell}{\partial w_i}$

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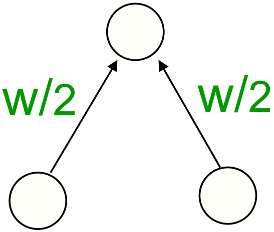
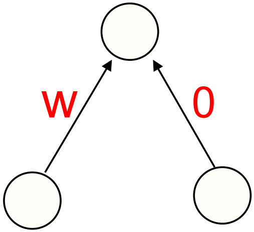
  - This can often improve generalization a lot.
  - It helps to stop it from fitting the sampling error.
  - It makes a smoother model in which the output changes more slowly as the input changes.
- But, if the network has two very similar inputs it prefers to put half the weight on each rather than all the weight on one $\rightarrow$ other form of weight decay?





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- So use a separate validation set to do model selection.

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  - Test data is used to get a final, unbiased estimate of how well the network works. We expect this estimate to be worse than on the validation data
- We could then re-divide the total dataset to get another unbiased estimate of the true error rate.

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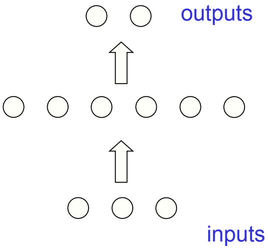
- The capacity of the model is limited because the weights have not had time to grow big.

Why Early Stopping Works



- When the weights are very small, every hidden unit is in its linear range.
  - So a net with a large layer of hidden units is linear.
  - It has no more capacity than a linear net in which the inputs are directly connected to the outputs!
- As the weights grow, the hidden units start using their non-linear ranges so the capacity grows.