

INF 5860 Machine learning for image classification Lecture : Backpropagation – learning in neural nets Anne Solberg March 3, 2017 ifi



Reading material

– Reading material:

- http://cs231n.github.io/optimization-2/
- Additional optional material:
- Lecture on backpropagation in Coursera Course on Machine Learning (Andrew Ng) CS 231n on youtube: lecture 4
- <u>http://yann.lecun.com/exdb/publis/pdf/lecun-98b.pdf</u>
- <u>http://colah.github.io/posts/2015-08-Backprop/</u>
- <u>http://neuralnetworksanddeeplearning.com/chap2.html</u>

Notation- forward propagation

Assume that the input is layer 0

 $a_i^{(j)}$ - activation of unit *i* and layer *j*

 $\Theta^{(j)}$ - matrix of weights controlling function mapping from layer j-1 to j

 $\Theta^{(j)}$ has dimension (nodes in layer (j)) × (nodes in layer (j-1)+1)

$$s_{j-1} \text{ nodes in layer } j-1, s_{j} \text{ nodes in layer } j: \Theta^{(j)} \text{ has size } s_{j} \times (s_{j-1}+1)$$

$$a_{1}^{(1)} = g \left(\Theta_{10}^{(1)} x_{0} + \Theta_{11}^{(1)} x_{1} + \Theta_{12}^{(1)} x_{2} + \Theta_{13}^{(1)} x_{3} \right)$$

$$a_{2}^{(1)} = g \left(\Theta_{20}^{(1)} x_{0} + \Theta_{21}^{(1)} x_{1} + \Theta_{22}^{(1)} x_{2} + \Theta_{23}^{(1)} x_{3} \right)$$

$$a_{3}^{(1)} = g \left(\Theta_{30}^{(1)} x_{0} + \Theta_{31}^{(1)} x_{1} + \Theta_{32}^{(1)} x_{2} + \Theta_{33}^{(1)} x_{3} \right)$$

$$h_{\Theta}(x) = a_{1}^{(2)} = g \left(\Theta_{10}^{(2)} a_{0}^{(1)} + \Theta_{11}^{(2)} a_{1}^{(1)} + \Theta_{12}^{(2)} a_{2}^{(1)} + \Theta_{13}^{(2)} a_{3}^{(1)} \right)$$

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Example feed-forward computation



• Input x: 3x1 vector

 $\Theta^{(1)}$: 4×4 (nof. hidden nodes in layer 1× nof. inputs +1) $\Theta^{(2)}$: 2×5 (nof. classes × nof. hidden nodes in layer 1+1) If we have N training samples we can predict all n = 1....N at one time :

$$\mathbf{X} = \begin{bmatrix} 1 & x_{pixel1}(n=1) & x_{pixel2}(1) & x_{pixel3}(1) \\ 1 & x_{pixel1}(n=2) & x_{pixel2}(2) & x_{pixel3}(2) \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_{pixel1}(n=N) & x_{pixel2}(N) & x_{pixel3}(N) \end{bmatrix}$$

z1 = Theta1.dot(X)
a1 = sigmoid(z1)
#Append 1 to a1 before computing z2
Continue with layer 2.....

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Cost function for one-vs-all neural networks

For a neural nets with one-vs-all : $\begin{aligned}
\text{Output}: a^{L} &= h_{\Theta}(x) \in \mathbb{R}^{K} \\
J(\Theta) &= -\frac{1}{m} \left[\sum_{i=1}^{m} \sum_{k=1}^{K} y_{k}(i) \log h_{\theta k}(X(i,:)) + (1 - y_{k}(i)) \log(1 - h_{\theta k}(X(i,:))) \right] + \frac{\lambda}{2m} \sum_{l=1}^{L-1} \sum_{i=1}^{s_{l}} \sum_{j=1}^{s_{l}+1} (\Theta_{ji}^{(l)})^{2} \\
\text{L: number of layers} \\
s_{1}: \text{Number of units (without bias) in layer 1}
\end{aligned}$

 $J(\Theta) = \text{LossTerm} + \lambda * \text{RegularizationTerm}$

Remark: two variations are common:

- Regularize all weights including the bias terms (sum from 0)
- Avoid regularizing the bias terms (sum from 1)

In practise, this choice do not matter.

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Cost function for softmax neural networks

For a neural net with softmax loss function :

Output :
$$\mathbf{a}^{L} = \mathbf{h}_{\Theta}(\mathbf{x}) = \begin{bmatrix} \mathbf{P}(\mathbf{y} = 1 | \mathbf{x}, \Theta) \\ \mathbf{P}(\mathbf{y} = 2 | \mathbf{x}, \Theta) \\ \vdots \\ \mathbf{P}(\mathbf{y} = \mathbf{K} | \mathbf{x}, \Theta) \end{bmatrix} = \frac{1}{\sum_{k=1}^{K} e^{\Theta_{k}^{T} \mathbf{x}}} \begin{bmatrix} e^{\Theta_{1}^{T} \mathbf{x}} \\ e^{\Theta_{2}^{T} \mathbf{x}} \\ \vdots \\ e^{\Theta_{k}^{T} \mathbf{x}} \end{bmatrix}$$

$$J(\Theta) = -\frac{1}{m} \begin{bmatrix} \sum_{i=1}^{m} \sum_{k=1}^{K} 1\{y_{i} = k\} \log\left(\frac{e^{\Theta_{k}^{T} x_{i}}}{\sum_{k=1}^{K} e^{\Theta_{k}^{T} x_{i}}}\right) \end{bmatrix} + \frac{\lambda}{2m} \sum_{l=1}^{L-1} \sum_{i=1}^{s_{l}} \sum_{j=1}^{s_{l}+1} (\Theta_{ji}^{(l)})^{2}$$

Remark: two variations are common, See previous slide:
 $J(\Theta) = \text{LossTerm} + \lambda * \text{RegularizationTerm}$

Introduction to backpropagation and computational graphs

- We now have a network architecture and a cost function.
- A learning algorithm for the net should give us a way to change the weights in such a manner that the output is closer to the correct class labels.
- The activation function should assure that a small change in weights results in a small change in ouputs.
- Backpropagation use partial derivatives to compute the derivative of the cost function J with respect to all the weights.



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Green numbers: forward propagation Red numbers: backwards propagation



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A more complicated graph example

$$f(w,x)=rac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

$$egin{aligned} f(x) &= rac{1}{x} & o & rac{df}{dx} &= -1/x^2 \ f_c(x) &= c+x & o & rac{df}{dx} &= 1 \ f(x) &= e^x & o & rac{df}{dx} &= e^x \ f_a(x) &= ax & o & rac{df}{dx} &= a \end{aligned}$$

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$$egin{aligned} f(x) &= rac{1}{x} & o & rac{df}{dx} &= -1/x^2 \ f_c(x) &= c + x & o & rac{df}{dx} &= 1 \ f(x) &= e^x & o & rac{df}{dx} &= e^x \ f_a(x) &= ax & o & rac{df}{dx} &= a \end{aligned}$$

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The sigmoid gate

$$\sigma(x) = rac{1}{1+e^{-x}}
onumber \ rac{d\sigma(x)}{dx} = rac{e^{-x}}{(1+e^{-x})^2} = \left(rac{1+e^{-x}-1}{1+e^{-x}}
ight) \left(rac{1}{1+e^{-x}}
ight) = (1-\sigma(x))\,\sigma(x)$$

Output: 0.73 Derivative of the sigmoid gate: (1-0.73)0.73=0.20 This is the same result as above.

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Forward and backward for a single neuron

```
w = [2,-3,-3] # assume some random weights and data
x = [-1, -2]
# forward pass
dot = w[0]*x[0] + w[1]*x[1] + w[2]
f = 1.0 / (1 + math.exp(-dot)) # sigmoid function
# backward pass through the neuron (backpropagation)
ddot = (1 - f) * f # gradient on dot variable, using the sigmoid gradient derivation
dx = [w[0] * ddot, w[1] * ddot] # backprop into x
dw = [x[0] * ddot, x[1] * ddot, 1.0 * ddot] # backprop into w
# we're done! we have the gradients on the inputs to the circuit
```

Remark: an efficient implemetation will store inputs and intermediates during forward, so that they are available for backprop.

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A more tricky example

$$f(x,y)=rac{x+\sigma(y)}{\sigma(x)+(x+y)^2}$$

• Stage the forward pass into simple operations that we now the derivative of:

x = 3 # example values	
y = -4	
# forward pass	
<pre>sigy = 1.0 / (1 + math.exp(-y)) # sigmoid in numerator</pre>	#(1)
num = x + sigy # <i>numerator</i>	#(2)
<pre>sigx = 1.0 / (1 + math.exp(-x)) # sigmoid in denominator</pre>	#(3)
x p y = x + y	#(4)
xpysqr = xpy**2	#(5)
den = sigx + xpysqr # denominator	#(6)
invden = 1.0 / den	#(7)
f = num * invden # done!	#(8)

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A more tricky example

 $f(x,y)=rac{x+\sigma(y)}{\sigma(x)+(x+y)^2}$

• In the backwards pass: compute the derivative of all these terms:

	# backprop f = num * invden	
	dnum = invden # gradient on numerator	#(8)
	dinvden = num	#(8)
	# backprop invden = 1.0 / den	
	dden = (-1.0 / (den**2)) * dinvden	#(7)
	# backprop den = sigx + xpysqr	
	dsigx = (1) * dden	#(6)
	dxpysqr = (1) * dden	#(6)
	# backprop xpysqr = xpy**2	
	dxpy = (2 * xpy) * dxpysqr	#(5)
	<pre># backprop xpy = x + y</pre>	
	dx = (1) * dxpy	#(4)
	dy = (1) * dxpy	#(4)
	# backprop sigx = 1.0 / (1 + math.exp(-x))	
	<pre>dx += ((1 - sigx) * sigx) * dsigx # Notice += !! See notes below</pre>	#(3)
	# backprop num = x + sigy	
	dx += (1) * dnum	#(2)
	dsigy = (1) * dnum	#(2)
	# backprop sigy = 1.0 / (1 + math.exp(-y))	
2	dy += ((1 - sigy) * sigy) * dsigy	#(1)
2	<i>H</i> T J T	

Patterns in backward flow

add gate: gradient distributor max gate: gradient router mul gate: be careful

> f=x*y means that df/dx=y and df/dy=x

Remark on multiplier gate: If a gate get one large and one small input, backprop will use the big input to cause a large change on the small input, and vice versa. This is partly why feature scaling is important



The optimization problem

Given a loss function J and a feed - forward net with L layers with weights $\Theta^{(l)}$

We want to minimize J using gradient descent

Need the derivatives of J with respect to every $\Theta_{m,n}^{(l)}$

Backpropagation: recursive application of the chain rule on a computational graph to compute the gradients of all input/parameters/intermediates

Implementation:

- Forward: compute the result of the node operation and save the intermediates needed for gradient computation
- Backwards: apply the chain rule to compute the gradients of the loss function with respect to the input of each node.

A very simple net with one input



Assume that we want to minimize the square error between the output $a^{(2)}$ and the true class y

E=1/2(y-a⁽²⁾)² (Mean square error in this example) Compute the partial derivatives with respect to $\theta^{(1)}$ and $\theta^{(2)}$, $\frac{\partial E}{\partial \theta^{(1)}}$ and $\frac{\partial E}{\partial \theta^{(2)}}$ and use use gradient descent to update $\theta^{(1)}$

and $\theta^{(2)}$

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$$a^{(2)}$$
 applies the sigmoid function $g(z)$ so $\frac{\partial a^{(2)}}{\partial z^{(2)}} = g'(z^{(2)}) = g(z^{(2)})(1 - g(z^{(2)}))$

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$$\begin{aligned} \frac{\partial E}{\partial \theta^{(1)}} &= \frac{\partial E}{\partial a^{(2)}} \frac{\partial a^{(2)}}{\partial \theta^{(1)}} = \left(a^{(2)} - y\right) \frac{\partial a^{(2)}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial \theta^{(1)}} \\ &= \left(a^{(2)} - y\right)g(z^{(2)})\left(1 - g(z^{(2)})\right) \frac{\partial z^{(2)}}{\partial a^{(1)}} \frac{\partial a^{(1)}}{\partial \theta^{(1)}} \\ &= \left(a^{(2)} - y\right)g(z^{(2)})\left(1 - g(z^{(2)})\right) \theta^{(2)} \frac{\partial a^{(1)}}{\partial z^{(1)}} \frac{\partial z^{(1)}}{\partial \theta^{(1)}} \\ &= \left(a^{(2)} - y\right)g(z^{(2)})\left(1 - g(z^{(2)})\right) \theta^{(2)}g(z^{(1)})\left(1 - g(z^{(1)})\right) \frac{\partial z^{(1)}}{\partial \theta^{(1)}} \\ &\left(a^{(2)} - y\right)g(z^{(2)})\left(1 - g(z^{(2)})\right) \theta^{(2)}g(z^{(1)})\left(1 - g(z^{(1)})\right) x \\ &a^{(1)} \text{ applies the sigmoid function } g(z) \text{ so } \frac{\partial a^{(1)}}{\partial z^{(1)}} = g'(z^{(1)}) = g(z^{(1)})\left(1 - g(z^{(1)})\right) \end{aligned}$$

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From scalars to vectors

- In the example x was a scalar, and $\frac{\partial E}{\partial \theta}$ was a vector with one element pr. weight.
- When working with vector input, for each layer $\frac{\partial E}{\partial \Theta^l}$ will be a matrix.
- Deriving the vector/matrix version of backpropagation is more tedious, but follows the same principle.
- A good source is

http://neuralnetworksanddeeplearning.com/chap2.html

• We now present the vector algorithm

Backpropagation algorithm for a single training sample (x_i, y_i)

For now, ignore the regularization (set $\lambda = 0$)

For a 3 - layer net :

Let
$$\delta_j^{(3)} = a_j^{(3)} - y_j$$

Let $\delta^{(3)} = a^{(3)} - y$ be the vector of $\delta_j^{(3)} j = 1, ... s_j$, where s_j is the number of nodes in layer j
Compute $\delta^{(2)} = \left(\left(\Theta^{(3)} \right)^T \delta^{(3)} \right) \cdot *g'(z^{(2)})$
 $\delta^{(1)} = \left(\left(\Theta^{(2)} \right)^T \delta^{(2)} \right) \cdot *g'(z^{(1)})$

Note that this is the elementwise product, or Hadamard-product of two vectors

With this notation,
$$\frac{\partial \mathbf{J}}{\partial \Theta_{ij}^{(l)}} = a_j^{(l)} \delta_i^{l+1}$$

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Derivative of loss function

- In backpropagation, we need the derivative of the loss functions with respect to the activation of the output layer a^L_i.
- If we ignore the regularization term, the derivative of the logistic loss function for sample *i* can be shown to be (a_i^L-y_i)
 - See <u>http://stats.stackexchange.com/questions/219241/gradient-for-logistic-loss-function</u>
- For softmax, ignoring the regularization term, the derivative of the softmax loss is also (a_i^L-y_i)
 - See http://math.stackexchange.com/questions/945871/derivativeof-softmax-loss-function

NOTE: a_i^L is computed differently

Notice that the bias nodes do not receive input from previous layer. Thus, they should NOT be used in backpropagation



Including the regularization term

$$J(\Theta) = -\frac{1}{m} \left[\sum_{i=1}^{m} \sum_{k=1}^{K} y_{k}(i) \log h_{\theta k}(X(i,:)) + (1 - y_{k}(i)) \log(1 - h_{\theta k}(X(i,:))) \right] + \frac{\lambda}{2m} \sum_{l=1}^{L-1} \sum_{i=1}^{s_{l}} \sum_{j=1}^{s_{j}+1} (\Theta_{ji}^{(l)})^{2}$$

 $J(\Theta) = \text{LossTerm} + \lambda * \text{RegularizationTerm}$

Backpropagation update including the regularization :

 $\frac{\partial J}{\partial \Theta_{ij}^{(l)}} = D_{ij}^{(l)} = \frac{1}{m} \Delta_{ij}^{(l)} \quad \text{for } j = 0 \text{, here the convention is that we do not regularize the bias terms}$ $\frac{\partial J}{\partial \Theta_{ij}^{(l)}} = D_{ij}^{(l)} = \frac{1}{m} \Delta_{ij}^{(l)} + \frac{\lambda}{m} \Theta_{ij}^{(l)} \quad \text{for } j = \ge 1$

Note that i is indexed from 1, and j from 0 (it gets input from the bias in the previous layer)

Remark: softmax will have the same regularization term

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Backpropagation with a loop over training data

Training set $\{(\mathbf{x}_1, \mathbf{y}_1), \dots, (\mathbf{x}_m, \mathbf{y}_m)\}$ Set $\Delta_{ij}^{(l)} = 0$ for all i, j, 1 for i = 1 : m Set $\mathbf{a}^{(0)} = \mathbf{x}_i$ Do forward propagation to compute $\mathbf{a}^{(l)}, l = 1, \dots L - 1$ Compute $\delta_k^{(L-1)} = a_k^{(L-1)} - yind(k)_i$, yind is an indicator function, = 1 if $\mathbf{y}_i = \mathbf{k}$ and 0 otherwise Compute $\delta^{(L-2)}, \dots, \delta^{(1)}as \ \delta^{(l)} = \left((\Theta^{(l)})^T \delta^{(l+1)} \right) \cdot *g'(z^{(l)})$ Set $\Delta_{ij}^{(l)} = \Delta_{ij}^{(l)} + \mathbf{a}_j^{(l)} \delta_i^{(l+1)}$

$$D_{ij}^{(l)} = \frac{1}{m} \Delta_{ij}^{(l)} + \lambda \Theta_{ij}^{(l)}, \text{ if } j \neq 0$$
$$D_{ij}^{(l)} = \frac{1}{m} \Delta_{ij}^{(l)}, \qquad \text{ if } j = 0$$
$$\text{Here, } \frac{\partial J}{\partial \Theta_{ij}^{(l)}} = D_{ij}^{(l)}$$

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Checking dimensions

 $\delta^{(1)} = \left(\left(\Theta^{(2)} \right)^T \delta^{(2)} \right) \cdot *g'(z^{(1)})$

- Note that in backpropagation, we use Θ^T
- When implementing this shape() is your best friend ③
- Think of a net with one hidden layer (layer 1) with 25 nodes + bias, and output layer with 10 nodes (10 classes)
- $\Theta^{(2)}$ has dimension 10x26 including bias, and $(\Theta^{(2)})^T$ is 26x10
- $\delta^{(2)}$ has dimension 10x1
- REMARK: we can either ignore the bias terms in backpropagation, or compute $\delta_0^{(1)}$ also (resulting in a 26x1 vector), but later ignore the $\delta_0^{(1)}$ values
 - When doing backpropagation from layer 2 to layer 1, ignore the bias in (index 0 of layer 2) and backpropagate $(\Theta^{(2)})^T(1:25,0:9)$
- $\delta^{(1)}$ then has dimension [(25x10)x(10x1)]·*(25x1) = 25x1

Assumptions behind backpropragation

- 1. The loss function should be expressed as a sum or average over all training samles.
 - This is true for all the functions we have studied so far
 - We will be able to compute $\frac{\partial L}{\partial \Theta_{ij}^{l}}$ for a single training example, and then average over all samples.

Output :
$$h_{\Theta}(x) \in \mathbb{R}^{K}$$

$$J(\Theta) = -\frac{1}{m} \left[\sum_{i=1}^{m} \sum_{k=1}^{K} y_{k}(i) \log h_{\theta_{k}}(X(i,:)) + (1 - y_{k}(i)) \log(1 - h_{\theta_{k}}(X(i,:))) \right] + \frac{\lambda}{2m} \sum_{l=1}^{L-1} \sum_{i=1}^{s_{l}} \sum_{j=1}^{s_{l}+1} (\Theta_{ji}^{(l)})^{2}$$

L:number of layers

 s_1 : Number of units (without bias) in layer 1

Assumptions behind backpropragation

- 2. The loss function must be expressed as a function of the outputs of the net.
 - This allows us to change the weights and measure how similar y_i and the output $h_{\Theta}(x)$ is.

Output :
$$h_{\Theta}(x) \in \mathbb{R}^{K}$$

$$L(\Theta) = -\frac{1}{m} \left[\sum_{i=1}^{m} \sum_{k=1}^{K} y_{k}(i) \log h_{\theta_{k}}(X(i,:)) + (1 - y_{k}(i)) \log(1 - h_{\theta_{k}}(X(i,:))) \right] + \frac{\lambda}{2m} \sum_{l=1}^{L-1} \sum_{i=1}^{s_{l}} \sum_{j=1}^{s_{l}+1} (\Theta_{ji}^{(l)})^{2}$$

L : number of layers

 s_1 : Number of units (without bias) in layer l

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Gradient checking

- When implementing backpropagation, we use gradient checking to verify the implementation.
- When the code works, we turn off gradient checking.
- But what is it?

Gradient checking: numerical estimation of the gradient

• The gradient of a function is defined as:

$$\frac{d}{d\theta}J(\theta) = \lim_{\varepsilon \to 0} \frac{J(\theta + \varepsilon) - J(\theta - \varepsilon)}{2\varepsilon}$$

• When we have the cost function implemented, we can easily approximate the gradient θ as

$$\frac{J(\theta + \varepsilon) - J(\theta - \varepsilon)}{2\varepsilon}$$

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Procedure for gradient checking

- 'Unroll' $\Theta_1, \Theta_2,...$ into a 1-d vector $\theta = [\theta_1,..., \theta_n]$
- Approximate

$$\frac{\partial J}{\partial \theta_1} = \frac{J(\theta_1 + \varepsilon, \theta_2, \dots, \theta_n) - J(\theta_1 - \varepsilon, \theta_2, \dots, \theta_n)}{2\varepsilon}$$
$$\frac{\partial J}{\partial \theta_2} = \frac{J(\theta_1, \theta_2 + \varepsilon, \dots, \theta_n) - J(\theta_1, \theta_2 - \varepsilon, \dots, \theta_n)}{2\varepsilon}$$
$$\vdots$$
$$\frac{\partial J}{\partial \theta_n} = \frac{J(\theta_1, \theta_2, \dots, \theta_n + \varepsilon) - J(\theta_1, \theta_2, \dots, \theta_n - \varepsilon)}{2\varepsilon}$$

• Check that the difference between this partial derivative and the one from backpropagation is smaller than a threshold.

Regarding gradient checking:

- Computing the approximated gradient is computationally much slower than backpropagation:
 - Use gradient checking for a small example when debugging the backpropagation code.
 - Once it works, turn off gradient checking and proceed with training the entire data set.

Random initialization of weights

- All weights must be initialized to small, but different random numbers.
 - More on why next week.

Training a neural network

- Choose an architecture:
 - Number of inputs: dimension of feature vector or image
 - Number of outputs: number of classes
 - 1-2 hidden layers.
 - For simplicity: use the same number of nodes in each hidden layer
 - More on practial details in the next two lectures.

Training a network

- 1. Randomly initialize each weight to small numbers
- 2. Implement forward propagation to get the output
- 3. Implement code to compute the cost function $J(\theta)$
- Implement backprop to compute the partial derivatives for i=1:m

Perform forward propagation and backpropagation for sample x_i, y_i

- 5. Use gradient checking to compate numerical estimates and backpropagation gradients. Afterward, disable gradient checking.
- 6. Use gradient descent (or optimization methods) with backpropagation to minimize J.

Weekly exercise:

- A detailed programming exercise, with descriptions on the operations, will be available.
- Implementing backpropagation is central to Mandatory exercise 1
 - No solution in python will be given, but test data with known results.

Next weeks:

- Training in practice, useful tricks.
- Babysitting the training process
- Parameter updates
- Activation functions
- Weight initialization
- Preprocessing
- Evaluation

Main reading material: http://cs231n.github.io/neuralnetworks-3/