Machine Learning applied to Planetary Sciences

PTYS 595B/495B

Leon Palafox

https://leonpalafox.github.io/MLClass/

Google DeepMind teams up with London hospitals to put machine learning to work against head and neck cancers

The artificial intelligence subsidiary launched a new research partnership to reduce the amount of time it takes to plan radiotherapy treatment for certain cancers.

By Bill Siwicki | August 31, 2016 | 03:13 PM

SHARE 116

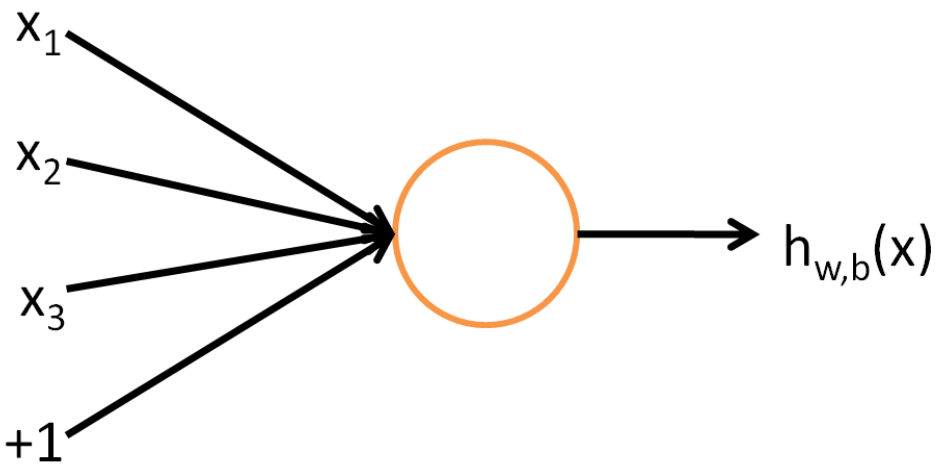
Google's machine learning subsidiary DeepMind has kicked off a new research partnership with the radiotherapy department at the University College London Hospitals NHS Foundation Trust, a provider organization that specializes in cancer treatment.

DeepMind and clinicians in UCLH's radiotherapy team are exploring whether machine learning methods can reduce the amount of time it takes to plan radiotherapy treatment for cancers of the head and neck.

http://www.healthcareitnews.com/news/google-deepmind-teams-london-hospitals-put-machine-learning-work-against-head-and-neck-cancers

Perceptron

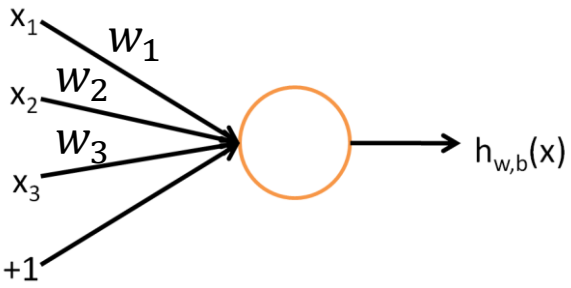
- Tries to mimic a real NN, since it has a nucleus that processes some inputs and give an output.



- $h_{w,b}(x)$ is a function of all the inputs, and is composed of two terms.

Perceptron

$$h_{w,b}(x) = f\left(\sum_{i=1}^{3} W_i x_i + b\right)$$



f is called the activation function, and it works as a way to discretize the outputs of the perceptron.

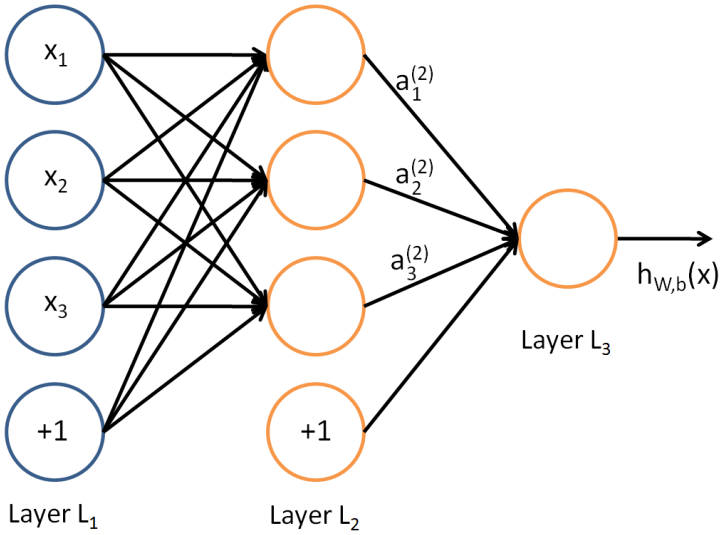
One of the most common activations functions is the sigmoid function:

$$f(z) = \frac{1}{1 + \exp(z)}$$

This looks very familiar

Neural Network

- Naturally, a NN is going to be a set of perceptrons interconnected within each other.

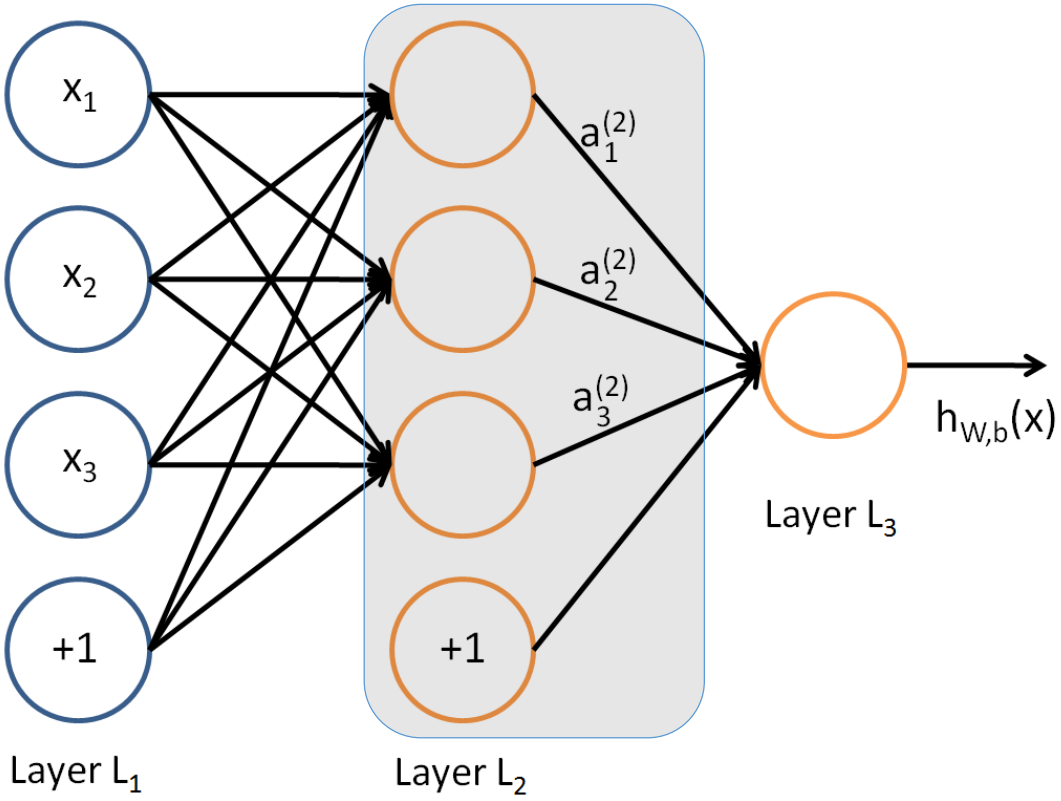


$$
\begin{aligned}
a_1^{(2)} &= f(W_{11}^{(1)}x_1 + W_{12}^{(1)}x_2 + W_{13}^{(1)}x_3 + b_1^{(1)}) \\
a_2^{(2)} &= f(W_{21}^{(1)}x_1 + W_{22}^{(1)}x_2 + W_{23}^{(1)}x_3 + b_2^{(1)}) \\
a_3^{(2)} &= f(W_{31}^{(1)}x_1 + W_{32}^{(1)}x_2 + W_{33}^{(1)}x_3 + b_3^{(1)}) \\
h_{W,b}(x) &= a_1^{(3)} = f(W_{11}^{(2)}a_1^{(2)} + W_{12}^{(2)}a_2^{(2)} + W_{13}^{(2)}a_3^{(2)} + b_1^{(2)})
\end{aligned}
$$

Training of Neural Networks

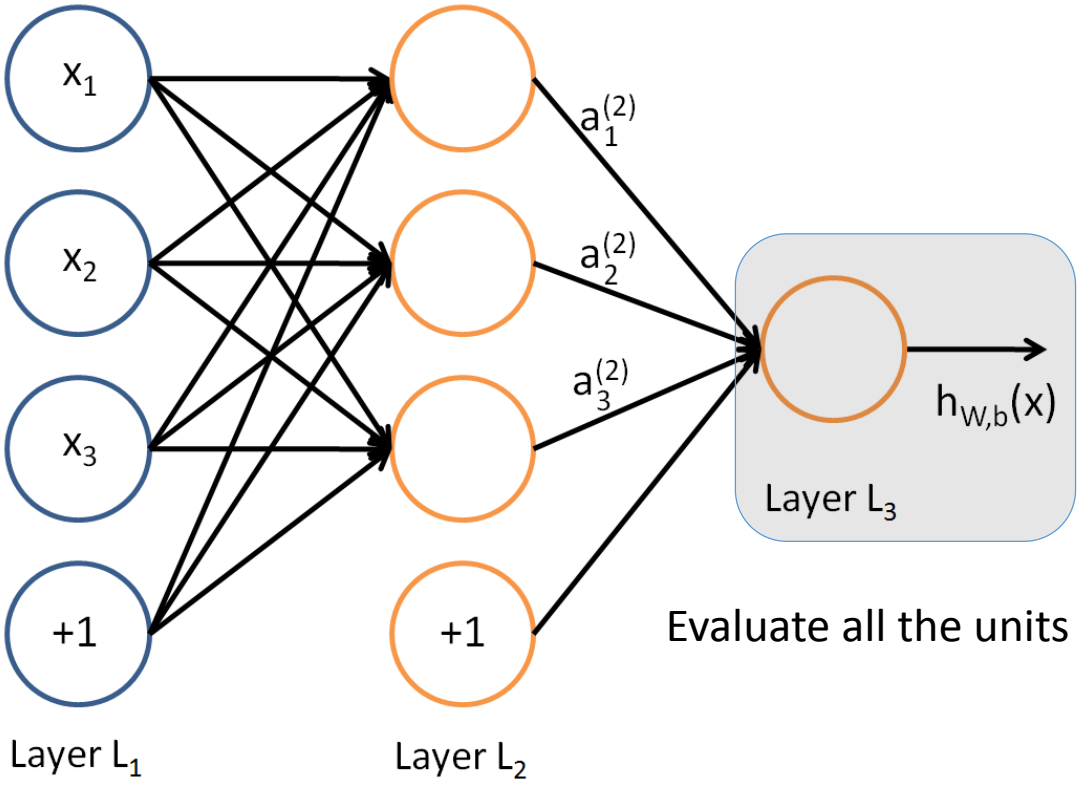
- The basic principle to train Neural Networks is Error Backpropagation.
  - We can find an error for a given input using the equations in the slide 11.
  - Next we go backwards in the network, and find the “share” of error each individual neuron has.
  - We calculate the derivative of this error to use Gradient Based techniques, like Gradient Descent.

Feedforward-Backpropagation



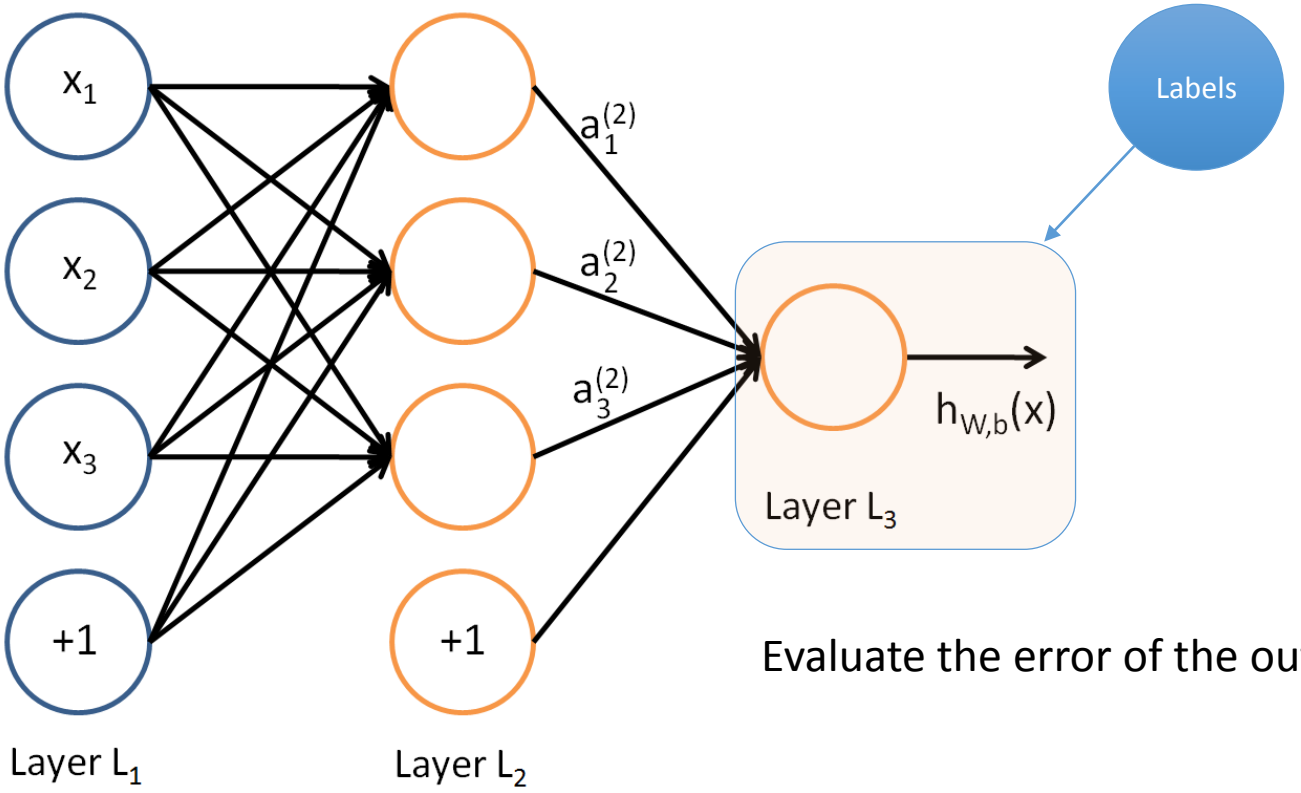
Evaluate all the units in Layer L2

Feedforward-Backpropagation



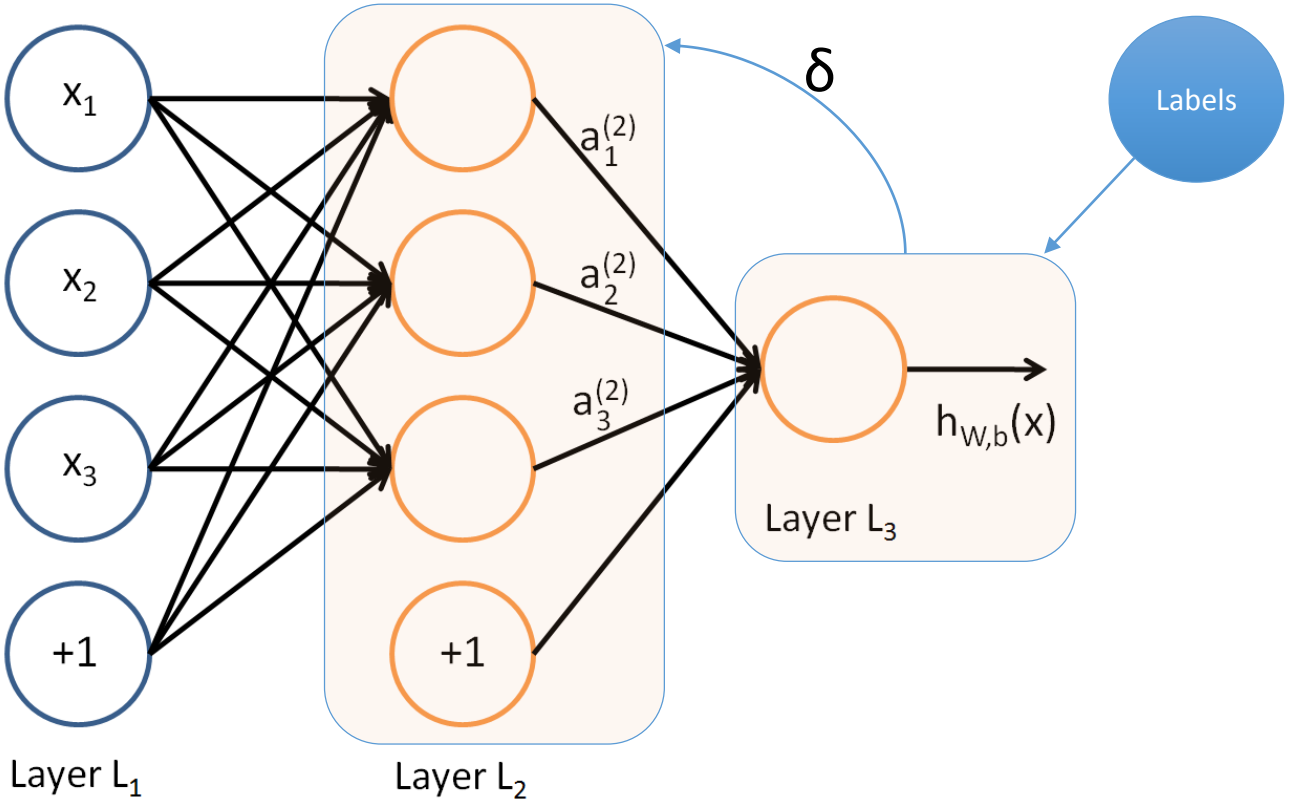
Evaluate all the units in Layer L3

Feedforward-Backpropagation



Evaluate the error of the output node (δ)

Feedforward-Backpropagation



Evaluate the errors of the middle layer nodes (δ)

Gradient Descent

- Given a cost function

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

- m is the number of examples and h some function of parameter θ.
- Gradient descent updates the parameter in steps:

$$\theta_j = \theta_j - \alpha\frac{\delta}{\delta\theta_j}J(\theta)$$

Gradient Descent for NNs

- The cost function for the overall network is:

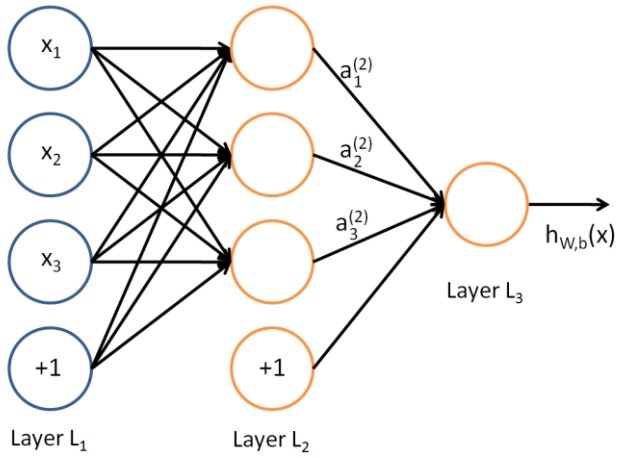
$$J(W,b) = \left[\frac{1}{m}\sum_{i=1}^{m}\left(\frac{1}{2}\left\|h_{W,b}(x^{(i)}) - y^{(i)}\right\|^2\right)\right] + \frac{\lambda}{2}\sum_{l=1}^{n_l-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_{l+1}}\left(W_{ji}^{(l)}\right)^2$$

- Given the compact representation of the network:

$$z^{(2)} = W^{(1)}x + b^{(1)}$$
$$a^{(2)} = f(z^{(2)})$$
$$z^{(3)} = W^{(2)}a^{(2)} + b^{(2)}$$
$$h_{W,b}(x) = a^{(3)} = f(z^{(3)})$$

In General

$$z^{(l+1)} = W^{(l)}a^{(l)} + b^{(l)}$$
$$a^{(l+1)} = f(z^{(l+1)})$$



Gradient Descent for NNs

- Gradient Descent: (Per Layer)

$$W_{ij}^{(l)} = W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W, b)$$

$$b_i^{(l)} = b_i^{(l)} - \alpha \frac{\partial}{\partial b_i^{(l)}} J(W, b)$$

With:

$$\frac{\partial}{\partial W_{ij}^{(l)}} J(W, b) = \left[\frac{1}{m} \sum_{i=1}^{m} \frac{\partial}{\partial W_{ij}^{(l)}} J(W, b; x^{(i)}, y^{(i)}) \right] + \lambda W_{ij}^{(l)}$$

$$\frac{\partial}{\partial b_i^{(l)}} J(W, b) = \frac{1}{m} \sum_{i=1}^{m} \frac{\partial}{\partial b_i^{(l)}} J(W, b; x^{(i)}, y^{(i)})$$

Gradient Descent for NNs

- We want to compute an “error term” δ, that will measure the error of a node I in layer ‘l’.

For the output layer:

$$\delta_i^{(n_l)} = \frac{\partial}{\partial z_i^{(n_l)}} \frac{1}{2} \|y - h_{W,b}(x)\|^2 = -(y_i - a_i^{(n_l)}) \cdot f'(z_i^{(n_l)})$$

For the middle layers

$$\delta_i^{(l)} = \left(\sum_{j=1}^{s_{l+1}} W_{ji}^{(l)} \delta_j^{(l+1)} \right) f'(z_i^{(l)})$$

Is a weighted average of all the errors related to this node

$$\frac{\partial}{\partial W_{ij}^{(l)}} J(W, b; x, y) = a_j^{(l)} \delta_i^{(l+1)}$$

$$\frac{\partial}{\partial b_i^{(l)}} J(W, b; x, y) = \delta_i^{(l+1)}.$$

Rule of thumb

- In general is a bad idea to just use a range between 0 and 1.
  - Since there are many parameters, it can take a long time if we use a random initialization.
- For training, a good initialization range is:

$$\left[-\sqrt{\frac{6}{n_{\text{in}}+n_{\text{out}}+1}}, \sqrt{\frac{6}{n_{\text{in}}+n_{\text{out}}+1}}\right]$$

Problems of NNs

- We need to answer two questions:
  - How many layers are enough to solve a problem?
  - How many hidden units should we use per layer?
- As you can imagine, training complexity increases as we increase hidden units.
  - This can be reduced by avoiding a full interconnection.
- The elephant in the room is called “Vanishing Gradient”

Vanishing Gradient

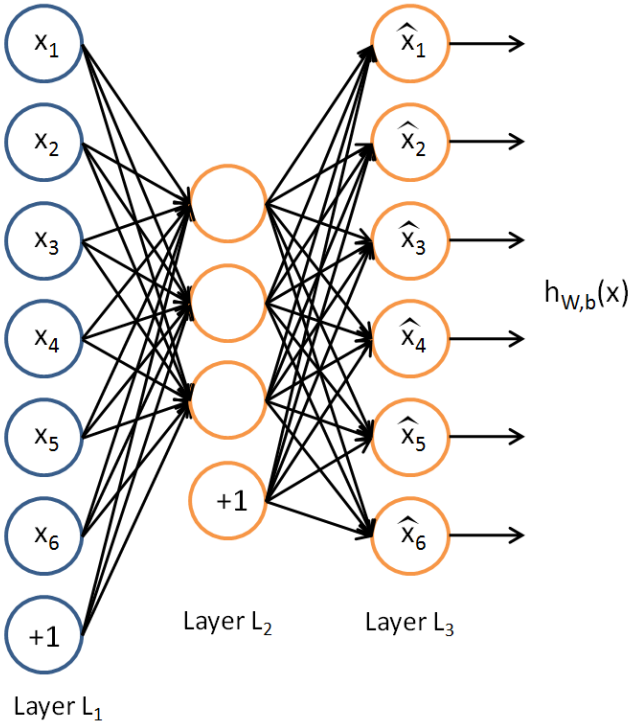
- A problem of NNs, is that our small δs, will become even smaller as we go back in our layers.
- If we have many layers, we are going to end up with really small gradients.
- This will show as negligible updates in the gradient descent equations.
- For many years, before 2006, this was the main reason few people used classic NNs.
  - What is the point of having the power that comes from many layers, if we cannot train it properly anyways?
  - The solution: Pre-training of the individual layers.

The Autoencoder

- The autoencoder is one of many architectures of NNs.
- In the autoencoder we do not use the labels in the dataset.
- Is an unsupervised learning algorithm.
- We do not run things like testing and training datasets.

Autoencoders

- An autoencoder is a NN where the output and the input are the same.



MNIST Dataset

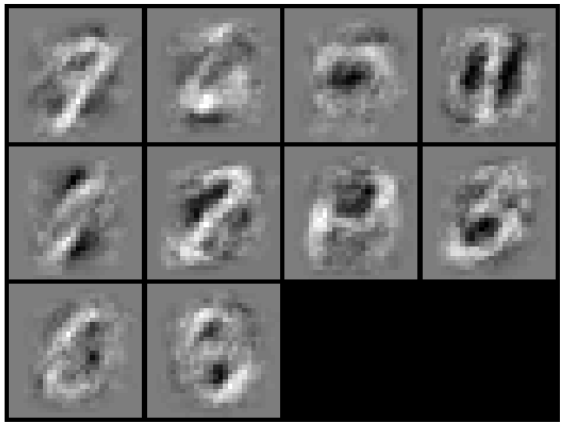
- Dataset of handwritten digits
- Has a training set of 60,000 examples, and a test set of 10,000 examples.
- Each digit is an 28x28 image (784 pixels)
- Each digit has a label that identifies which digit it represents. (9 labels)

MNIST Dataset

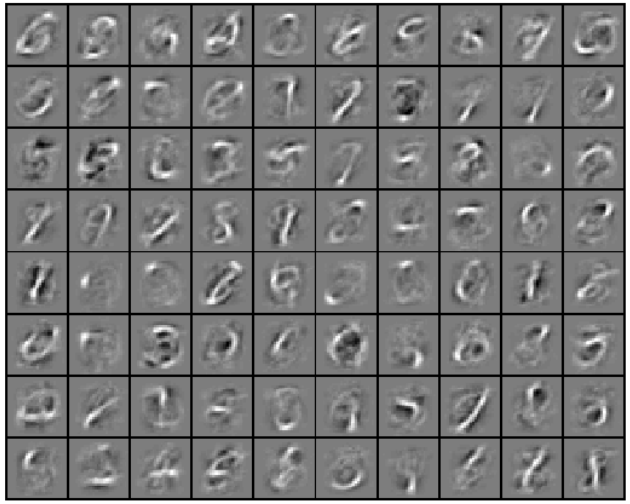
- http://yann.lecun.com/exdb/mnist/
- Is very good for learning:
  - All of the images have the same size (8x8)
  - It's black and white, which means we do need to modify activation functions.
  - All the numbers have the same orientation.
- http://yann.lecun.com/exdb/lenet/scale.html

Autoencoder

- Why would I want both the input and the output to be the same.
- MNIST dataset as an example (28x28 input images)



10 hidden units in Autoencoder



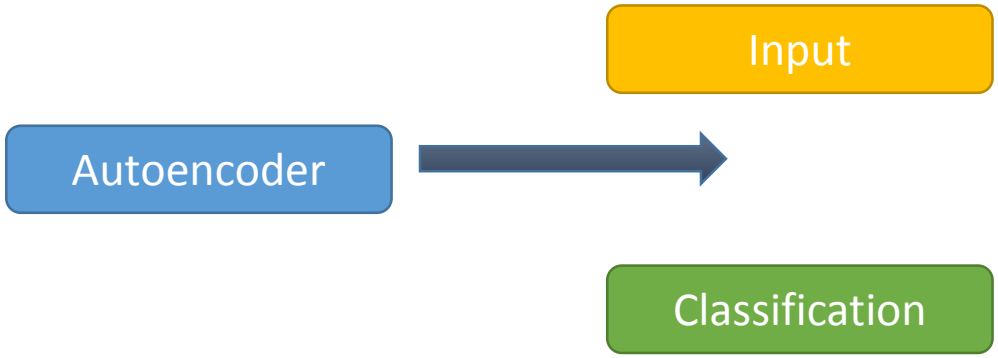
80 hidden units in Autoencoder

Autoencoders & Deep Nets

- Remember we mentioned that initializing Neural Networks is tricky.
- The Vanishing gradient makes it hard to train large NNs.
- Autoencoders (and RBMs) are a solution to this problem.
- We use the autoencoder as an initializing step.

Autoencoder & Deep Nets

- If we train an autoencoder, and plug it in a NN then train. Things just work



Deep Nets

- Train Autoencoder using a subset of MNSIT (10,000)
- Plug the autoencoder as the hidden layer of the NN.
- Do what we call a “fine tuning”, which is just a fast training to get the labeled part. (supervised)
- Now you can break ReCaptcha

Deep Nets

- They are supposed to be deep so: