Machine Learning

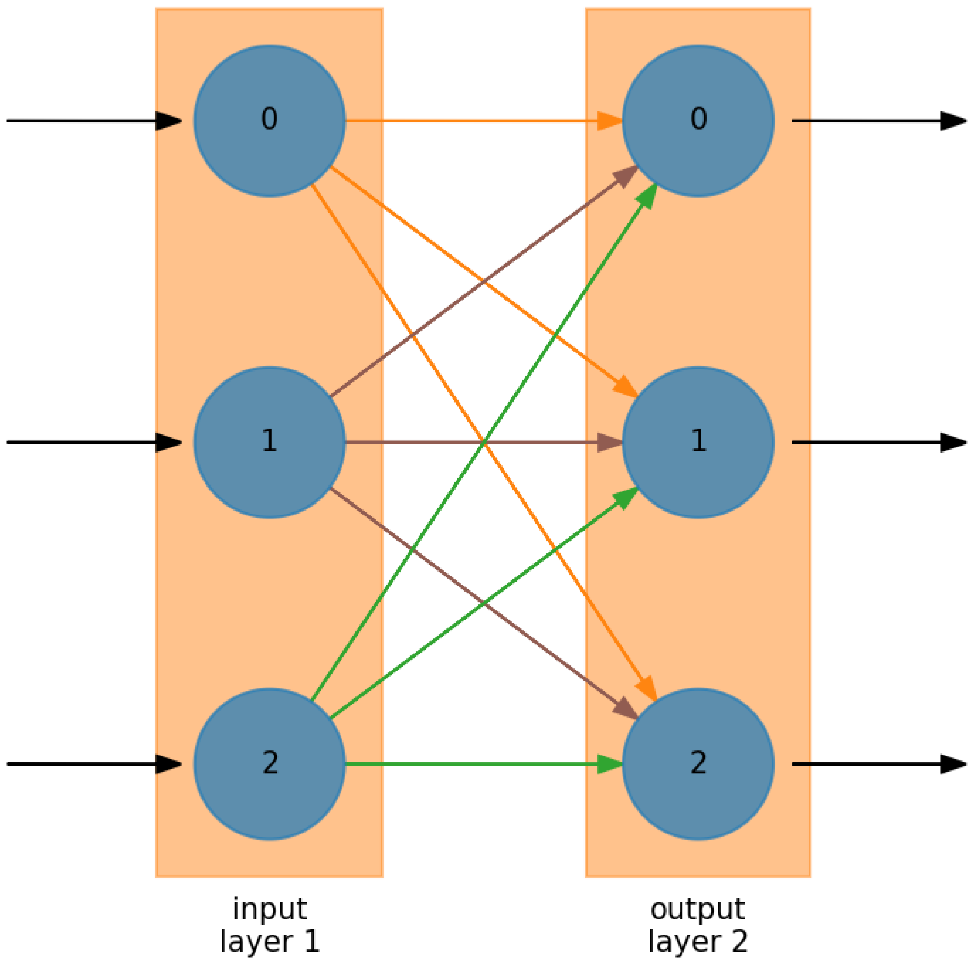
Neural Network Overview

- Computers are good at arithmetic but not great at pattern recognition
  - Neural nets attempt to model how neurons transmit information

(original source unknown)

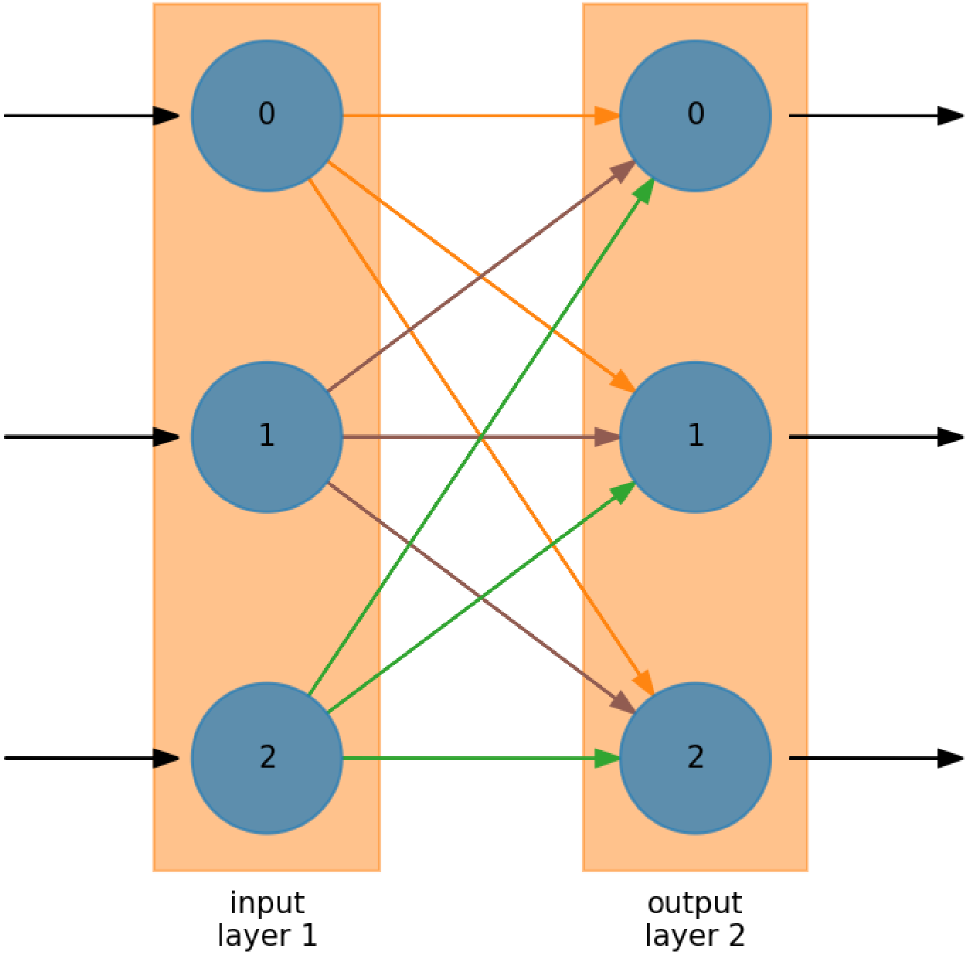
Neural Network Overview

- Some nomenclature:
  - Neural networks are divided into *layers*
    - There is always an input layer—it doesn't do any processing—just accepts the input
    - There is always an output layer
  - Within a layer, there are neurons or *nodes*
    - For input, there will be one node for each input variable
  - Every node in the first layer connects to every node in the next layer
    - The *weight* associated with the *connection* can vary—these are the matrix elements
  - In this example, the processing is done in layer 2 (output)



Neural Network Overview

- When you train a neural network, you are adjusting the weights connecting the nodes
- Some connections may have zero weight
- This mimics nature—a single neuron can connect to several (or lots) of other neurons
- Linear algebra problem:
  - Inputs: $\mathbf{x} \in \mathbb{R}^n$
  - Outputs: $\mathbf{z} \in \mathbb{R}^m$
  - Neutral network is a map, $\mathbb{R}^n \rightarrow \mathbb{R}^m$ that can be expressed as a matrix, **A**
    - $\mathbf{z} = \mathbf{A}\mathbf{x}$
  - Given enough input, we could know all the matrix elements in **A**



Nonlinear Model

- We'll use a nonlinear function, g(p), that acts on a vector:

$$g(\mathbf{x}) = \begin{pmatrix} g(x_0) \\ g(x_1) \\ \vdots \\ g(x_{n-1}) \end{pmatrix}$$

  – then **z** = g(**A x**)

- New procedure: set the entries of **A** via training, using a simple, nonlinear, g(p) that fits our training data
- From the graphical representation, the nonlinear function is applied on the output layer

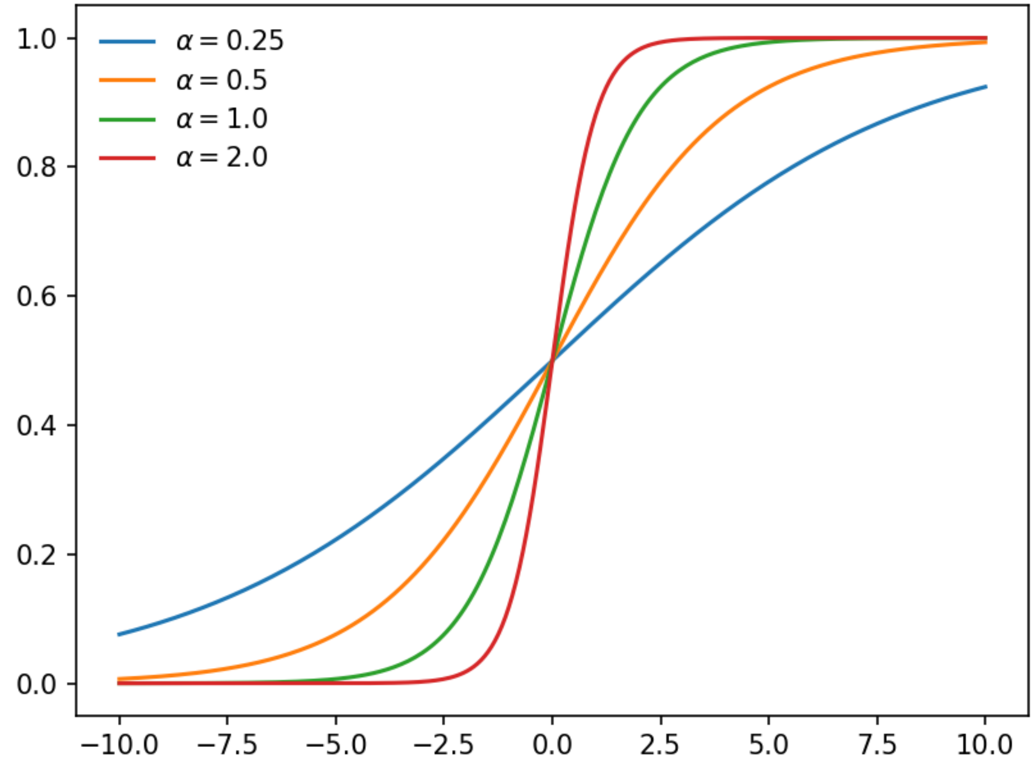
Nonlinear Model

- Again, this mirrors biology
  - Neurons don't act linearly
  - There is a threshold that needs to be reached before a neuron "fires"
- A step function would work, but we want something differentiable
- There are a lot of different choices in the literature

Sigmoid Function

- Common choice: sigmoid function

$$g(p) = \frac{1}{1 + e^{-\alpha p}}$$



- Note, all outputs are scaled to be $z_j \in (0, 1)$
- We'll take $\alpha = 1$

Scaling Output

- Note that since the sigmoid maps all output to (0, 1), we need to make sure that the output in our training set is likewise mapped to (0, 1)
  - If the data doesn't already fall in (0, 1), we can just use a linear transformation:

$$\tilde{x} = 0.9 \, \frac{x - \min x_i}{\Delta x} + 0.05$$

    - here, Δx is the largest possible range of x_i in the inputs

Actually, (0, 1] works fine—we just need to avoid a 0, since that cancels out weights in the matrices

Implementation

- Basic operation
  - Train the model with known input/output to get all A_{ij}
  - Use $\mathbf{z} = g(\mathbf{A}\,\mathbf{x})$ to get output for a new input $\mathbf{x}$
- Training:
  - We have T pairs $(\mathbf{x}^k, \mathbf{y}^k)$ for k = 1, …, T
    - Important: remember that our **y**'s have to be scaled to be in (0, 1), so they are in the same range that our function g(p) maps to
  - We require that $g(\mathbf{A}\,\mathbf{x}^k) = \mathbf{y}^k$ for all k
    - Recall, that g(p) is a scalar function that works element-by-element:

$$z_i = g([\mathbf{A}\mathbf{x}]_i) = g\left(\left[\sum_j A_{ij} x_j\right]\right)$$

Implementation

- Training (cont.)
  - We find the elements of **A**
    - This can be expressed as a minimization problem, where we alter the matrix elements to achieve this agreement
    - There may not be a unique set of A_{ij}, so we will loop randomly over all training data multiple times to optimize **A**

$$f(A_{ij}) = \|g(\mathbf{A}\mathbf{x}^k) - \mathbf{y}^k\|^2$$

      - This looks like a least-squares minimization
- The function we minimize is called the *cost function*
  - There are other choices than the square of the error

Implementation

- Minimization
  - A common technique for minimization is *gradient descent* (sometimes called steepest descent)
    - This looks at the local derivative of the function f with respect to the parameters A_{ij} and moves a small distance *downhill*, and iterates…
  - We'll also compare to an external library for minimization
- Caveats
  - When you minimize with one set of training data, there is no guarantee that you are still minimized with respect to the previous sets
  - In practice, you feed the training data multiple times, in random order, to the minimizer—each pass is called an *epoch*

Aside: Minimization

- Steepest descent minimization
  - Start at a point $\mathbf{x}_0$ and evaluate the gradient
  - Move *downhill* by following the gradient by some amount η
  - Correct our initial guess and iterate

$$\mathbf{x} \leftarrow \mathbf{x} - \eta \frac{\partial u}{\partial \mathbf{x}}$$

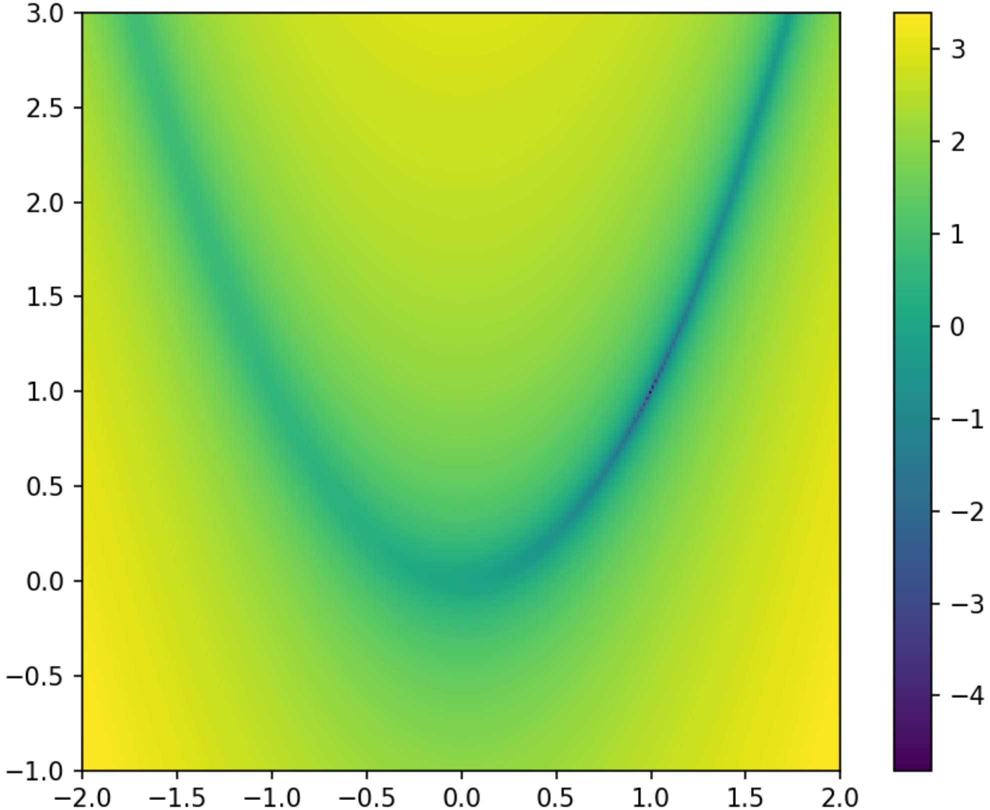
- Need to choose the amount to move each iteration
  - Sometimes we instead define a unit vector in the direction of the local gradient, and then η represents the distance to travel in that direction
- You can think about this as what happens if you put a marble on a surface—it rolls to a minimum
  - May not be the global minimum—we can get stuck in a local minimum

Aside: Minimization

- Example: Rosenbrock (banana) function

$$f(x, y) = (a - x)^2 + b(y - x^2)^2$$

  - This is a hard problem for optimization
  - Global minimum is at (a, a^2)

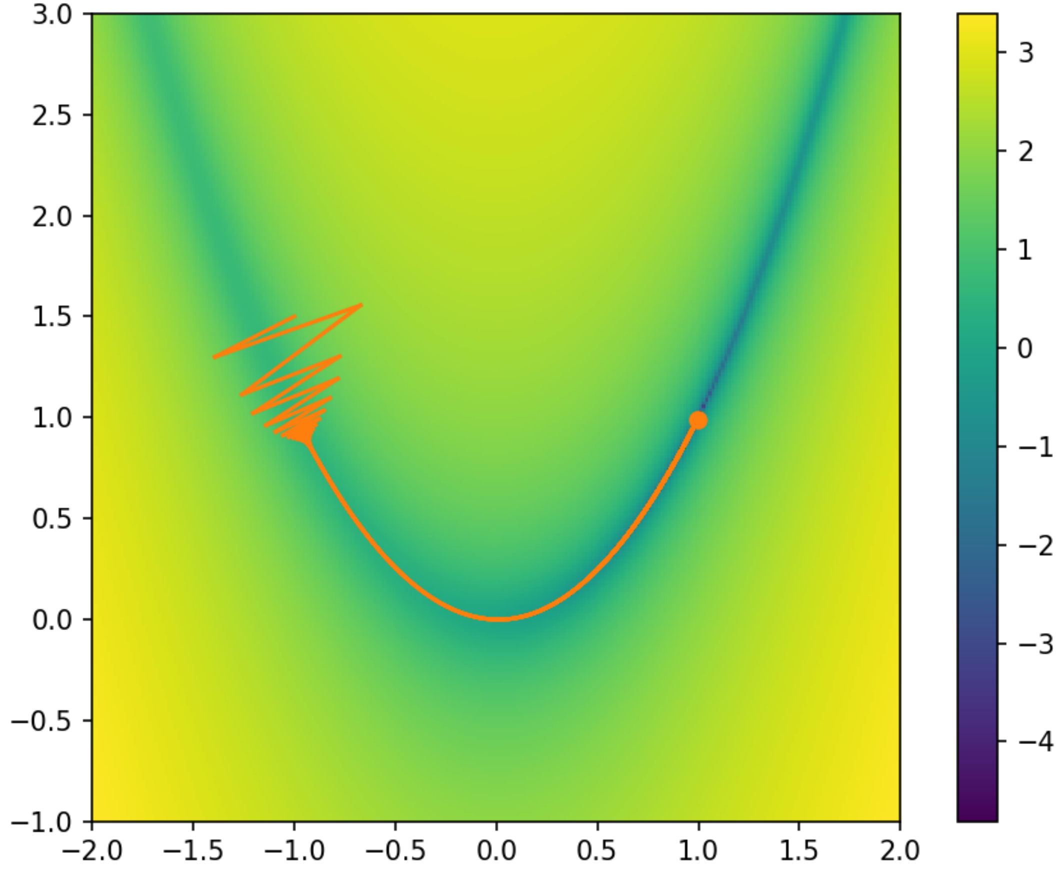


Note: this is the log of the function plotted

code: steepest_descent.py

Aside: Minimization

- Minimization with gradient descent is very sensitive to choice of η
  - Too large and you may shoot off far from the minimum
  - Too small and you do a lot of extra work



code: steepest_descent.py

Neural Net Minimization

- For our function,

$$f(A_{ij}) = \|g(\mathbf{A}\mathbf{x}^k) - \mathbf{y}^k\|^2$$

  - Note, this definition is for a single training pair, ($\mathbf{x}^k$, $\mathbf{y}^k$)

$$(\mathbf{x}^k, \mathbf{y}^k) = (\{x_1^k, x_2^k, \ldots, x_n^k\}, \{y_1^k, y_2^k, \ldots, y_m^k\})$$

  - Our update would be

$$A_{pq} = A_{pq} - \eta \frac{\partial f}{\partial A_{pq}}$$

  - where

$$f(A_{ij}) = \sum_{i=1}^{m} \left[g\left(\sum_{j=1}^{n} A_{ij} x_j \right) - y_i \right]^2$$

Neural Net Minimization

- Working out the derivative:

$$\frac{\partial f}{\partial A_{pq}} = 2(z_p - y_p)\alpha z_p(1 - z_p)x_q$$

  - We could then use steepest descent, looping over the matrix elements and doing the minimization on them one by one, iterating until we converge
    - Instead, we just do one push “downhill” following the gradient for a single training set and then move to the next.
    - η is often called the *learning rate*
- Gradient descent is often used for neural nets because it only requires the first derivative
  - Newton’s method would require the second derivatives (Hessian matrix)

Neural Net Minimization

- Recall,
  - **A** is m × n matrix
  - **x** is n × 1 vector
  - **y** (and hence **z**) is m × 1 vector
- We can write our derivative as:

$$\frac{\partial f}{\partial \mathbf{A}} = \underbrace{2(\mathbf{z} - \mathbf{y}) \circ \alpha \mathbf{z} \circ (1 - \mathbf{z})}_{m \times 1} \cdot \underbrace{\mathbf{x}^\mathsf{T}}_{1 \times n}$$

- Then the correction to our matrix is:

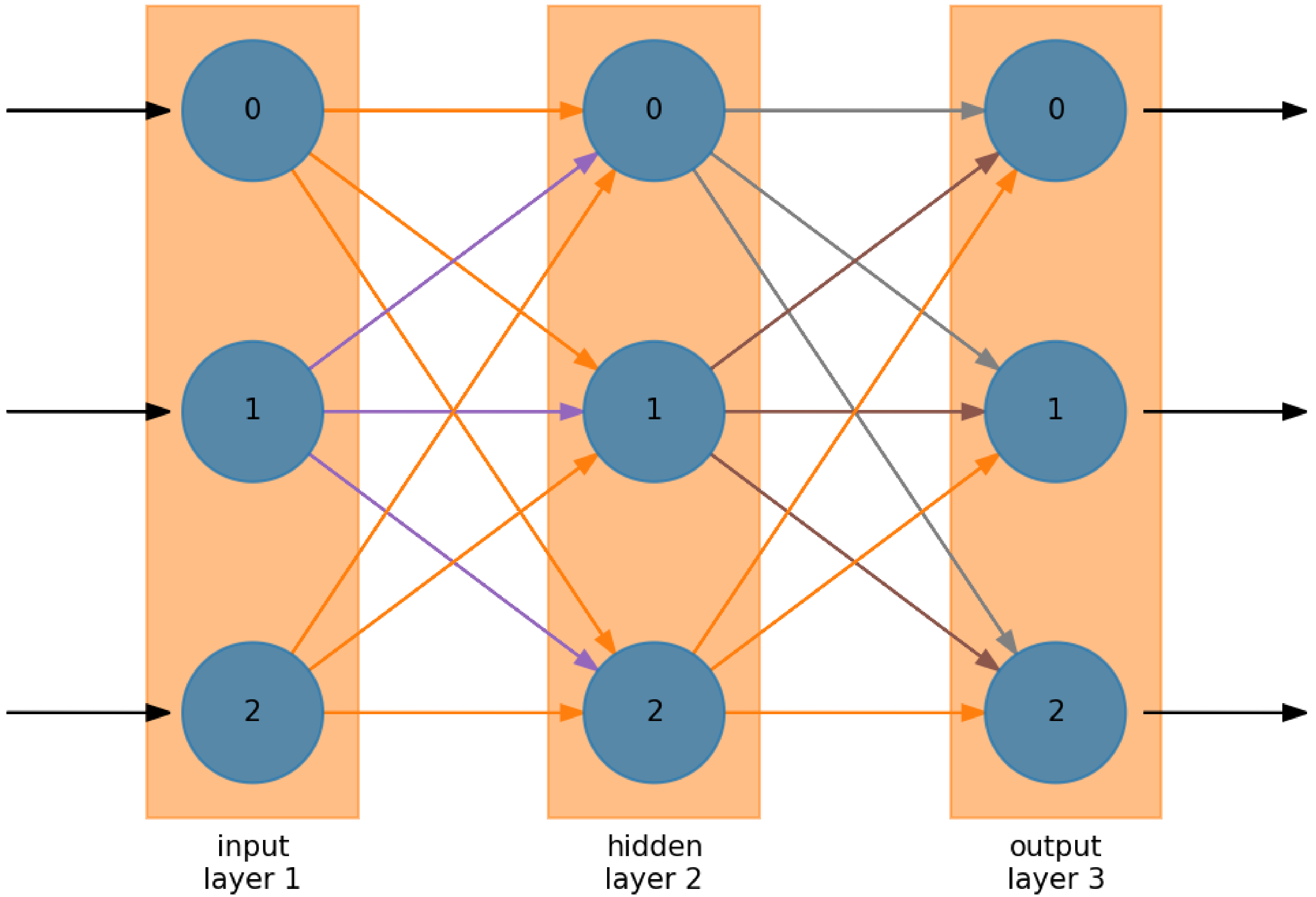
$$\Delta \mathbf{A} = -2\eta \left(\mathbf{z} - \mathbf{y}\right) \circ \alpha \mathbf{z} \circ \left(1 - \mathbf{z}\right) \cdot \mathbf{x}^\mathsf{T}$$

$$\mathbf{A} \leftarrow \mathbf{A} + \Delta \mathbf{A}$$

Here, **a** ∘ **b** is an element-wise product

Hidden Layers

- We can add more more parameters by another layer of nodes/neurons



Hidden Layers

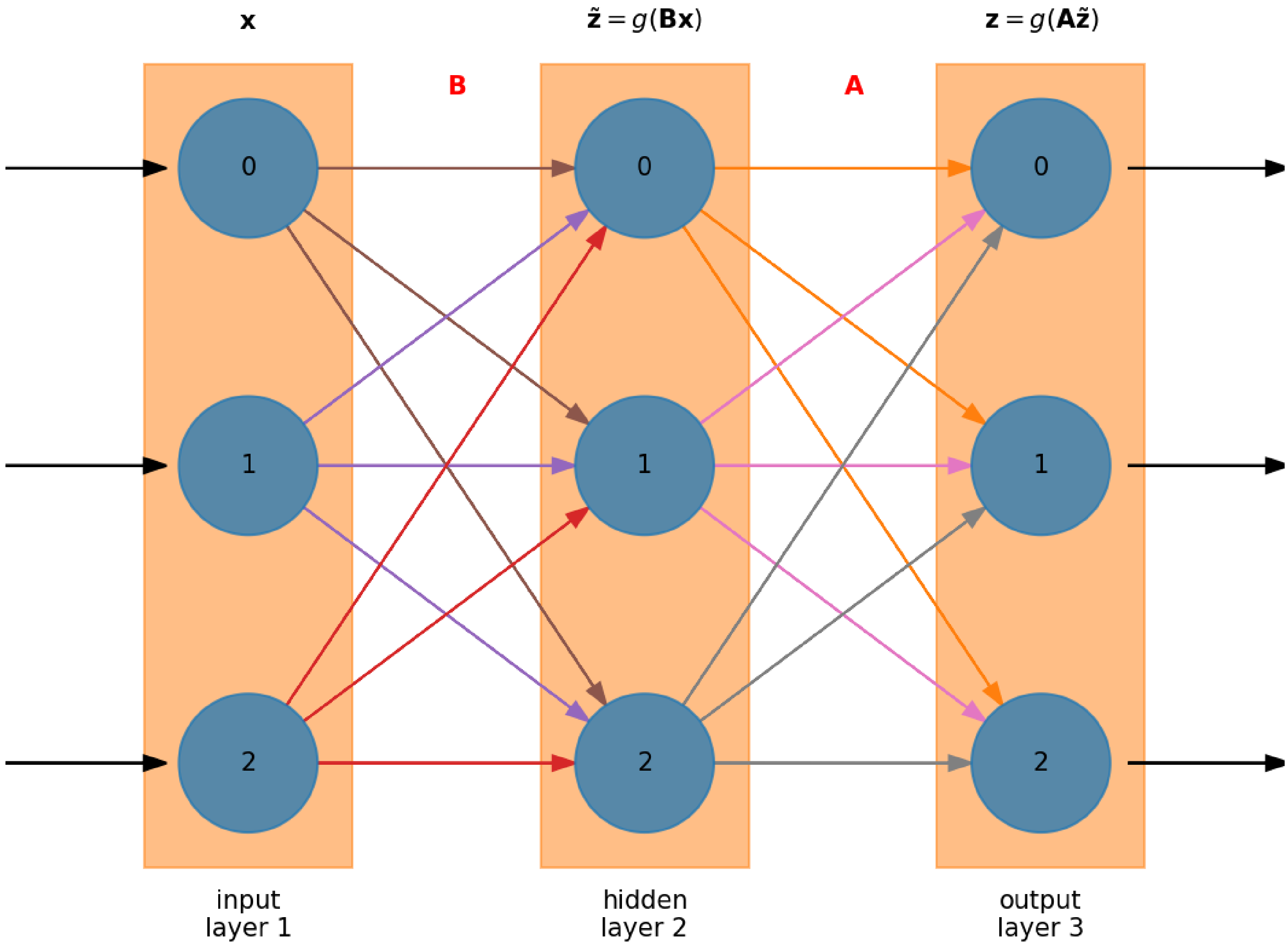
- *Hidden layers* sit between the input and output
- For hidden layer of dimension k:
  - Inputs: $\mathbf{x} \in \mathbb{R}^n$
  - Outputs: $\mathbf{z} \in \mathbb{R}^m$
  - **A** is an m × k matrix
  - **B** is an k × n matrix
  - The product **AB** is m × n, as we had before
- *Universal approximation theorem*: single layer network can represent any continuous function
- We transform the input in two steps:

$$\tilde{\mathbf{z}} = g(\mathbf{B}\mathbf{x})$$

$$\mathbf{z} = g(\mathbf{A}\tilde{\mathbf{z}})$$

Hidden Layers

- Graphically this appears as:



Hidden Layers

- Now we minimize:

$$f(A_{ls}, B_{ij}) = \sum_{l=1}^{m} (z_l - y_l)^2$$

$$\tilde{z}_i = g\left(\sum_{j=1}^{n} B_{ij} x_j\right)$$

$$z_l = g\left(\sum_{s=1}^{k} A_{ls} \tilde{z}_s\right)$$

Minimization

- We need to do the minimization now for both sets of weights (matricies)
- In practice, we do them one at a time, with each seeing the result from its layer
  - This process is also called *backpropagation* in neural networks—we are using the errors at the end to change the weights that came earlier in the network

Gradient Descent

- We can do our gradient descent on **A** and **B** separately now
  - This is the strength of backpropagation and gradient descent vs. some "canned" minimization routine—we are not optimizing the entire system all together
- Differentiating our error and lots of chain rule gives:

$$\Delta A = -2\eta\, \mathbf{e} \circ \mathbf{z} \circ (1 - \mathbf{z}) \cdot \tilde{\mathbf{z}}^\intercal$$
$$\Delta B = -2\eta\, \tilde{\mathbf{e}} \circ \tilde{\mathbf{z}} \circ (1 - \tilde{\mathbf{z}}) \cdot \mathbf{x}^\intercal$$

Note: this is a single dot product, the combination of vectors on the left are multiplied element-by-element (the Hadamard product)

  - With

$$\tilde{\mathbf{e}} = \mathbf{A}^\intercal \mathbf{e} \circ \mathbf{z} \circ (1 - \mathbf{z}) \approx \mathbf{A}^\intercal \mathbf{e}$$

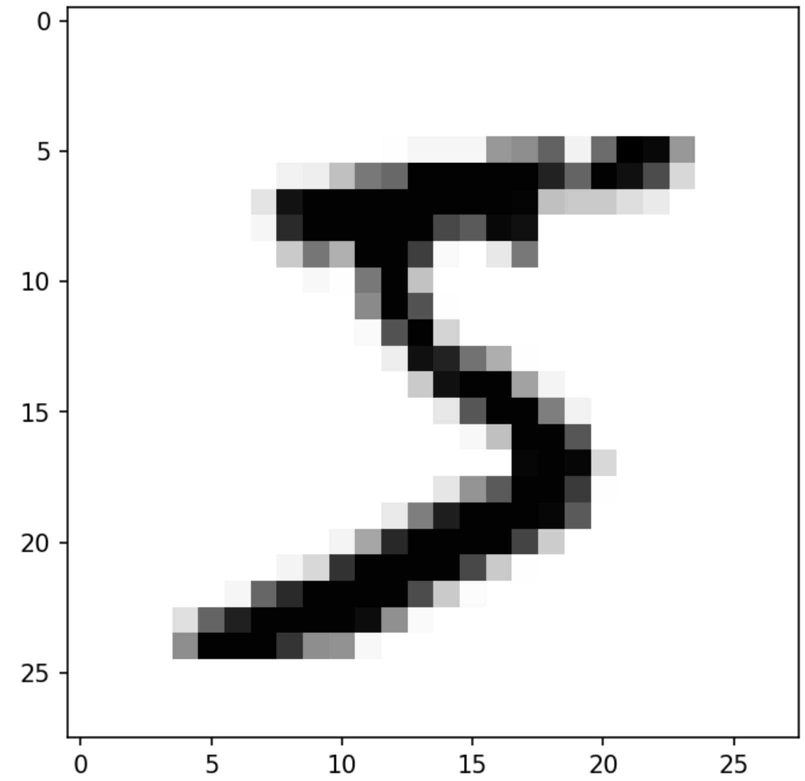
This approximation seems to be commonly made and supposedly doesn't affect convergence much

Image Classification

- We'll try to recognize a digit (0 – 9) from an image of a handwritten digit.
  - MNIST dataset (http://yann.lecun.com/exdb/mnist/)
    - Popular dataset for testing out maching learning techniques
    - Training set is 60,000 images
      - Approximately 250 different writers
    - Test set is 10,000 images
    - Correct answer is know for both sets so we can test our performance
- Image details:
  - 28×28 pixels, grayscale (0 – 255 intensity)
- The best learning algorithms can get accuracy > 99%

Image Classification

- Neural network characteristics:
  - Input layer will be 784 nodes
    - One for each pixel in the input image
  - Output layer will be 10 nodes
    - An array with an entry for each possible digit
    - "3" would be represented as: [0, 0, 0, 1, 0, 0, 0, 0, 0, 0]
  - We'll start with a hidden layer size of 100
- We'll train on the training set, using up to 60000 images
  - Rescale the input to be in [0.01, 1]
- We'll test on the test set of 10000 images



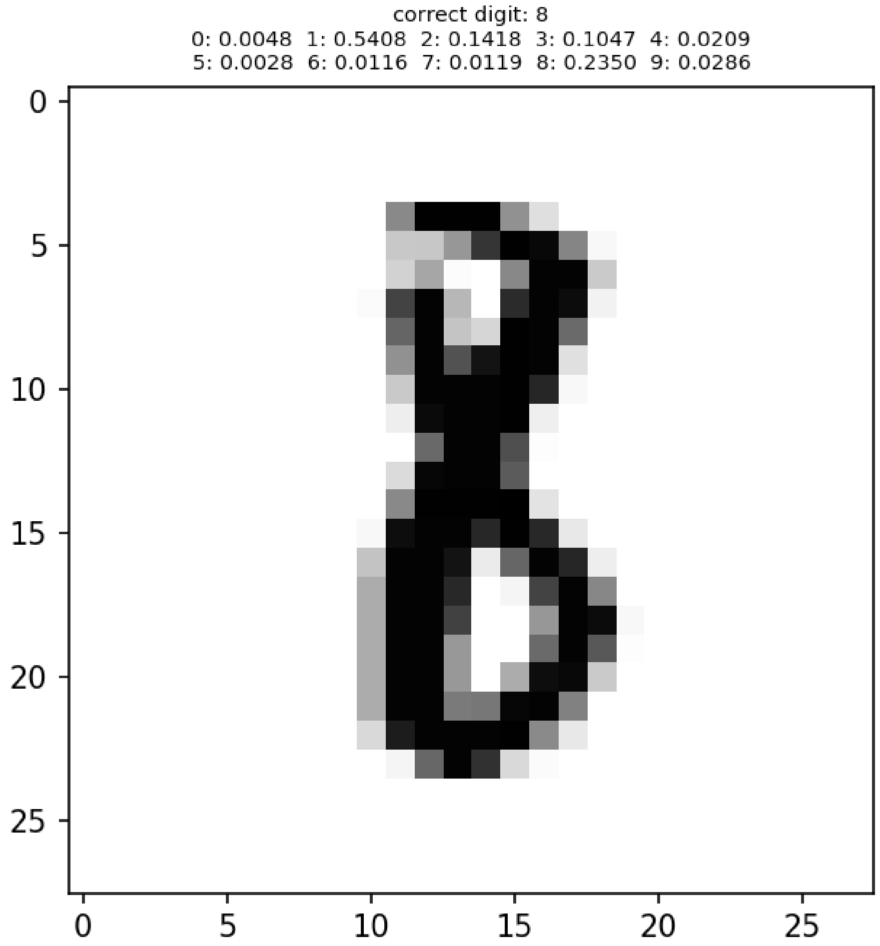
First digit MNIST in the training set

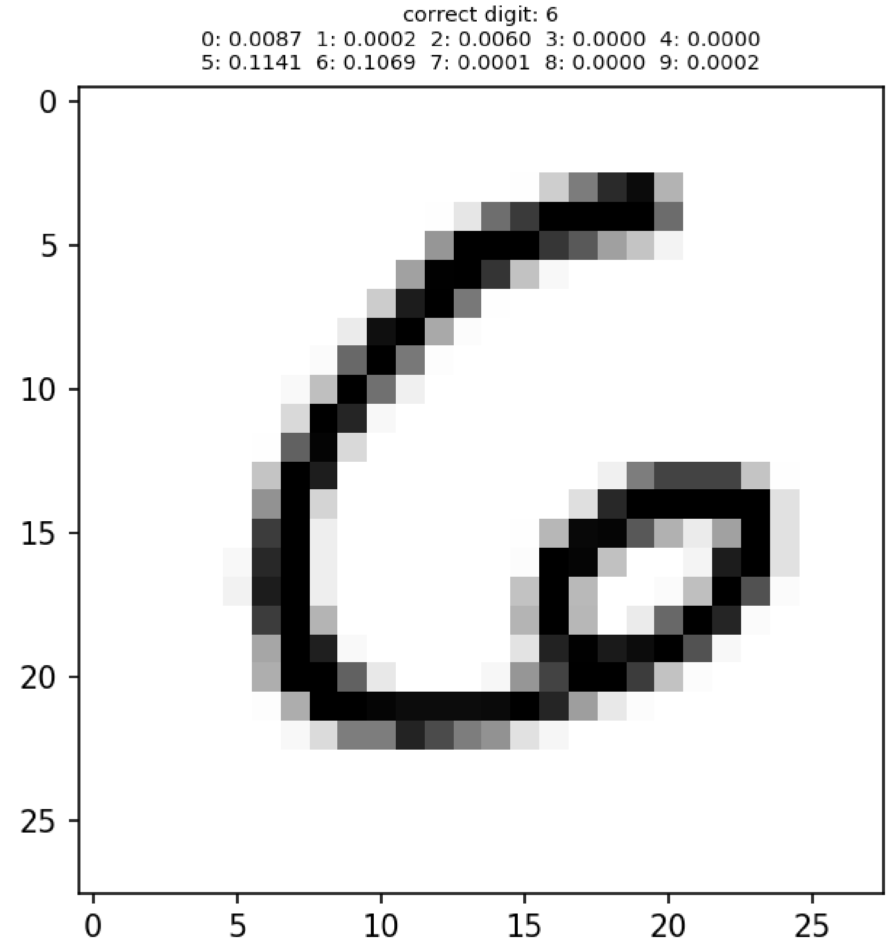
Image Classification

- Default configuration:
  - The full training set (60000 images)
  - Hidden layer of 100 nodes
  - 5 epochs of training
  - Learning rate of 0.1
- We achieve 95 – 96% accuracy

code: char_recognition.py

Some Image Classification Failures





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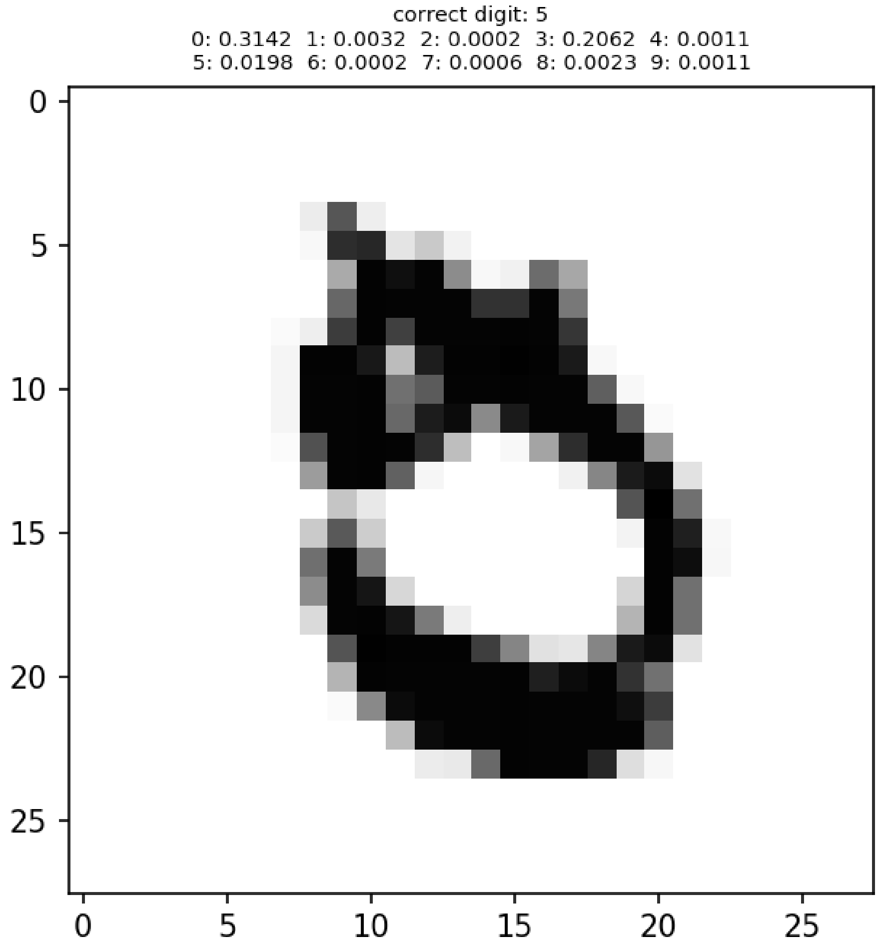

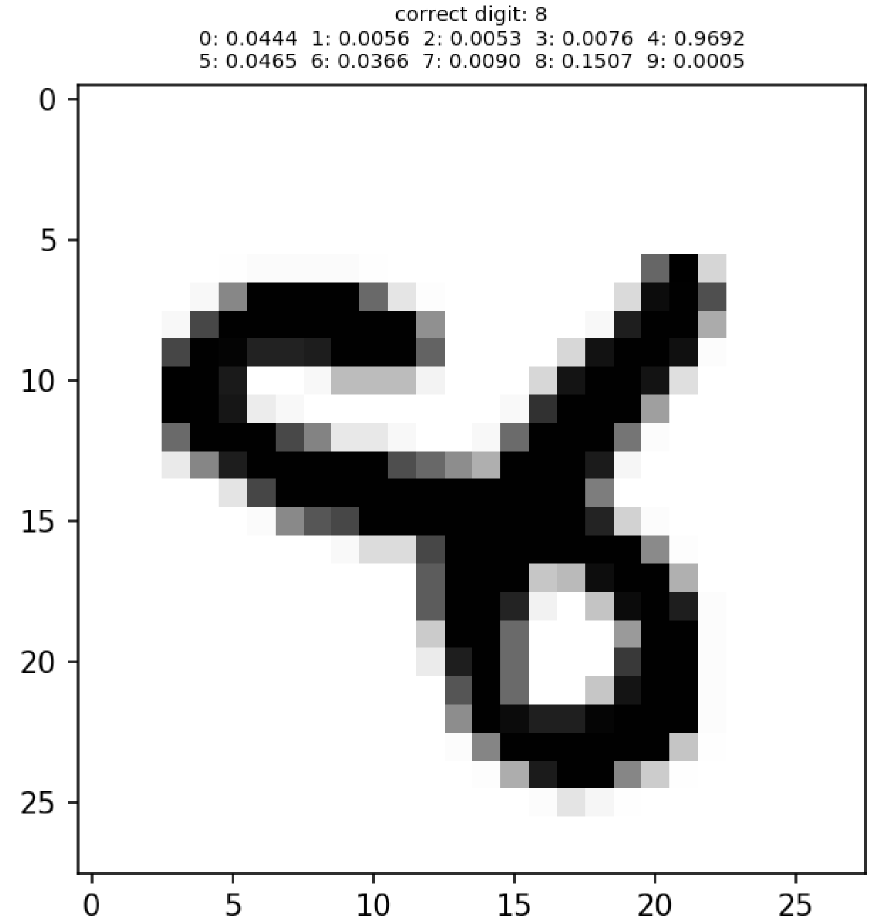

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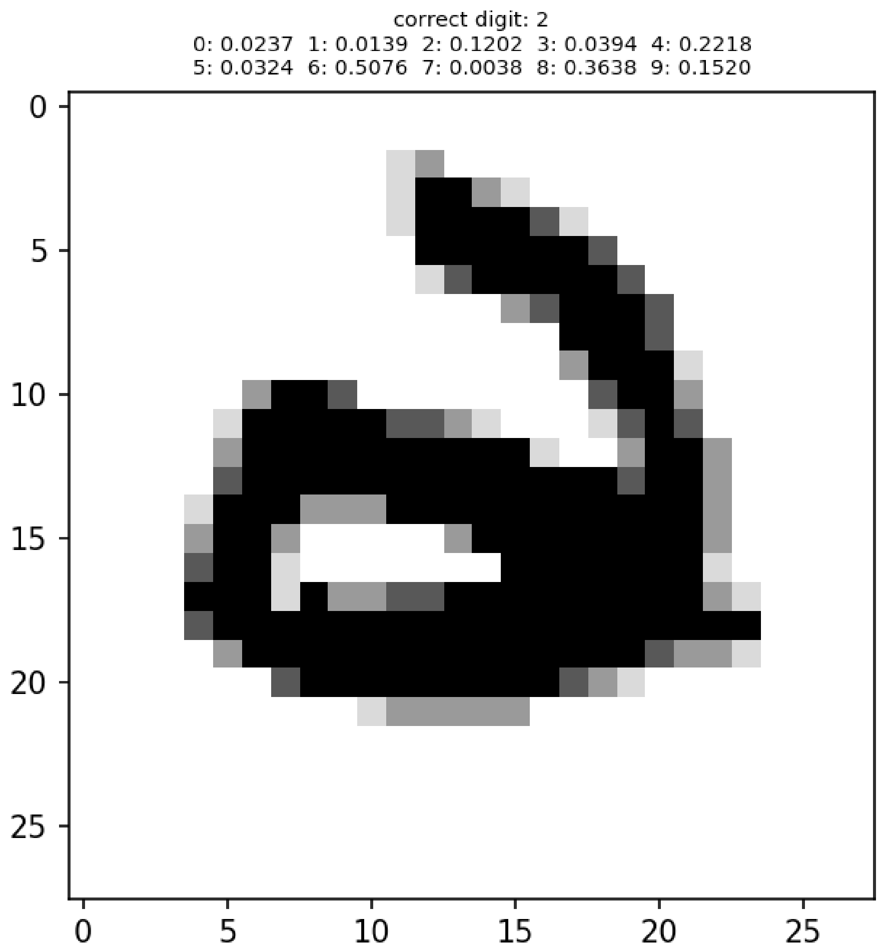


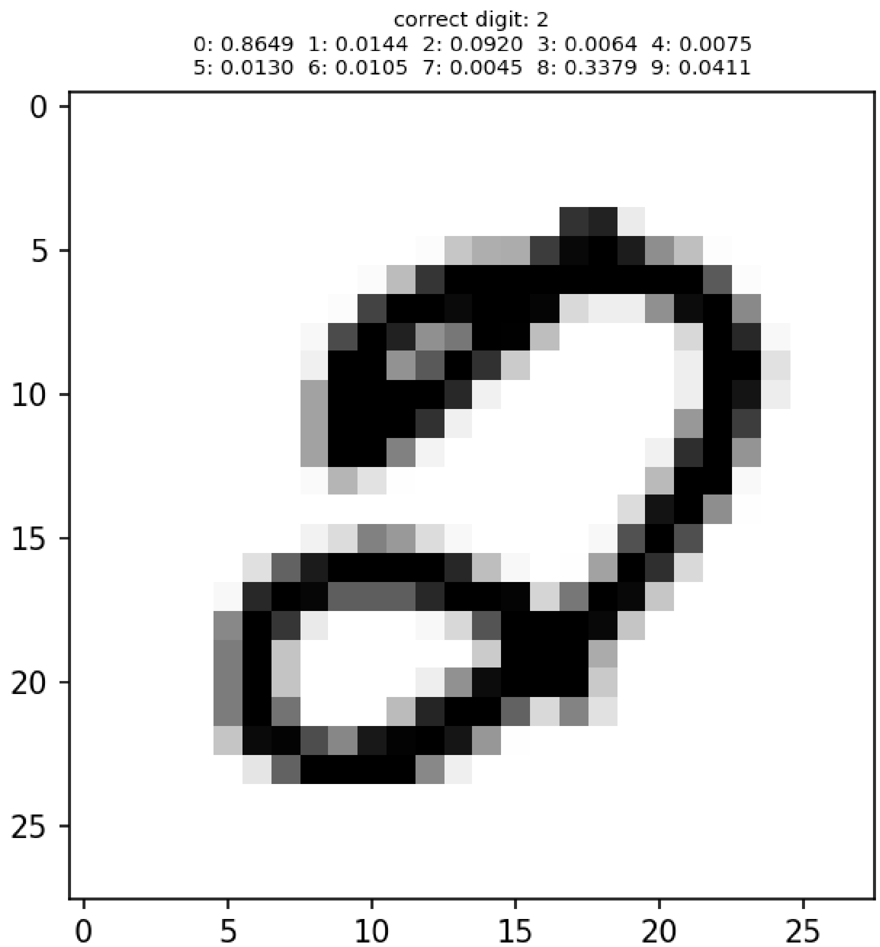
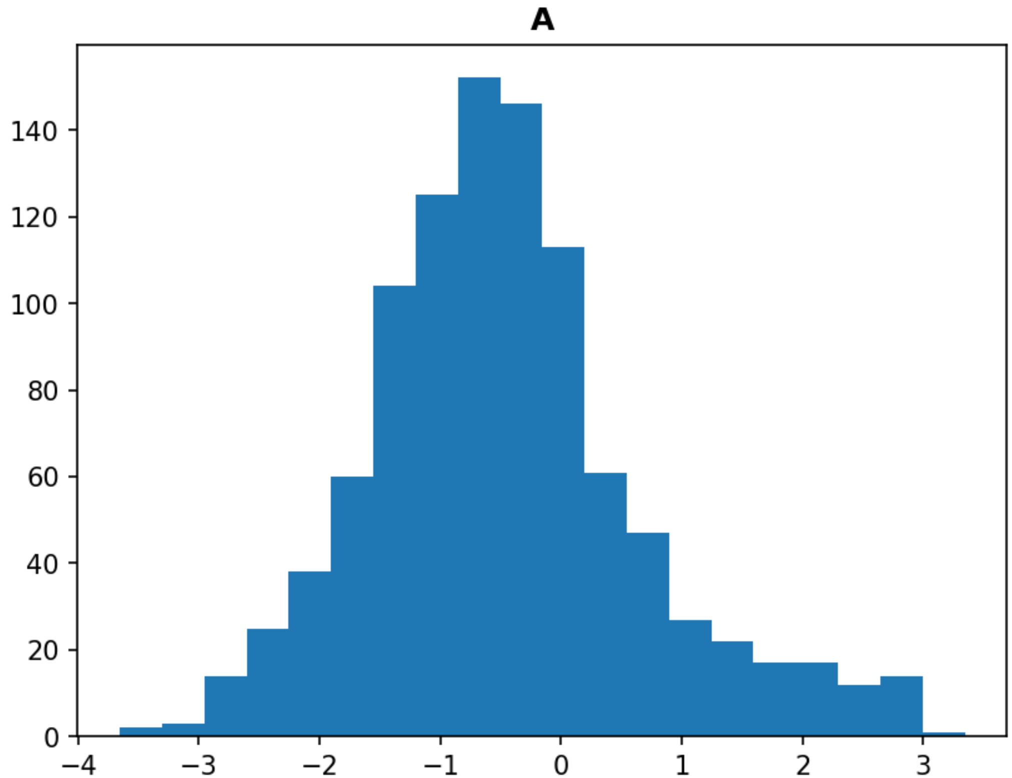
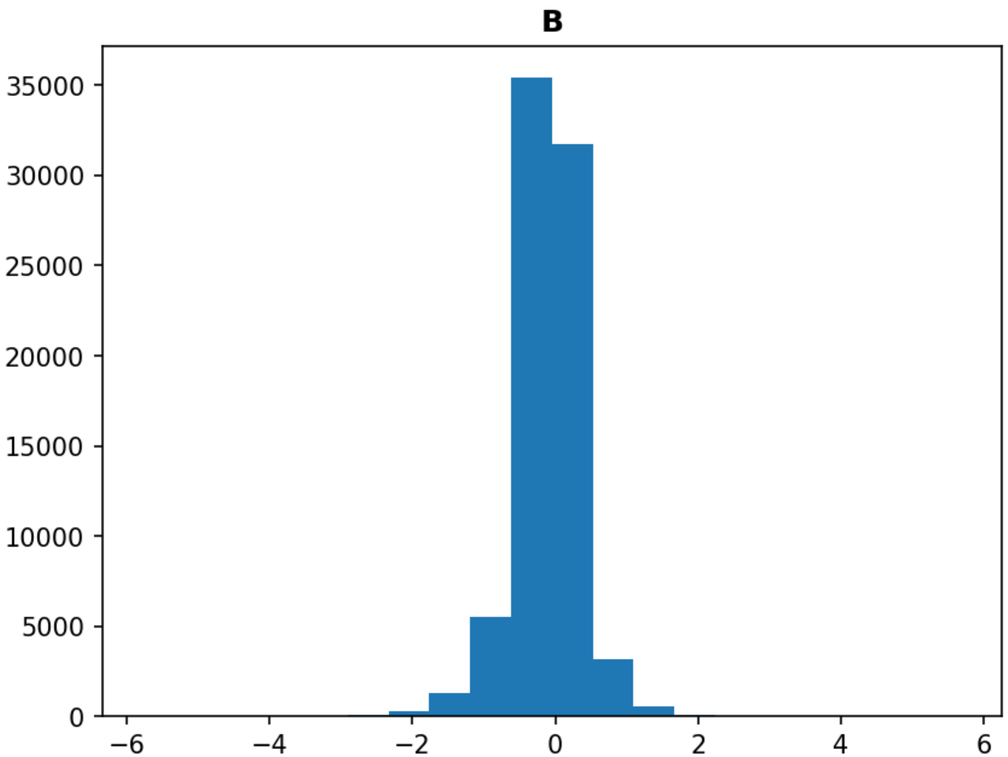


Image Classification Weights

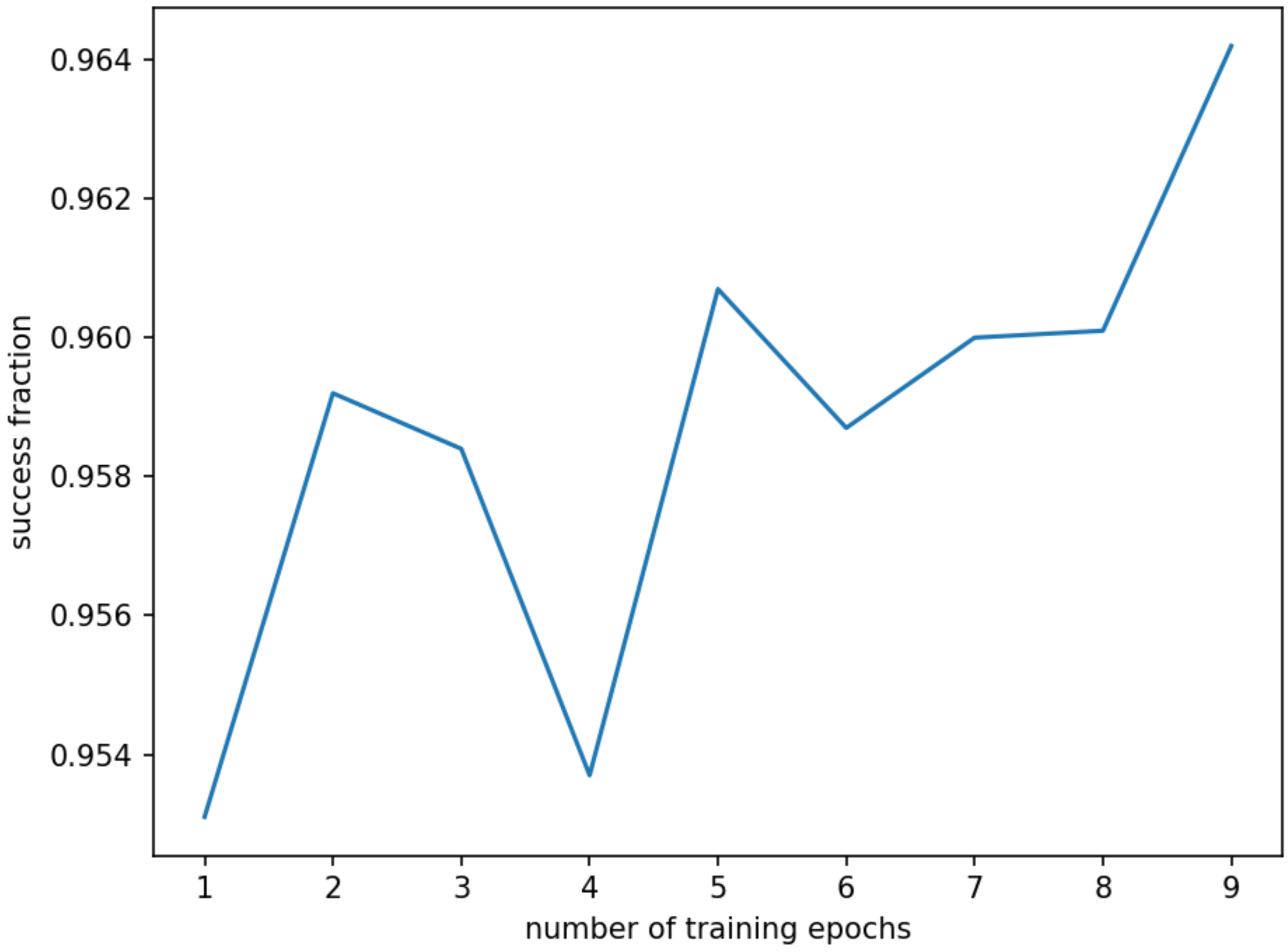
- Weights (matrix elements of **A** and **B**) seem symmetric about 0
  - Interestingly, with more training, the width of the distribution seems to grow





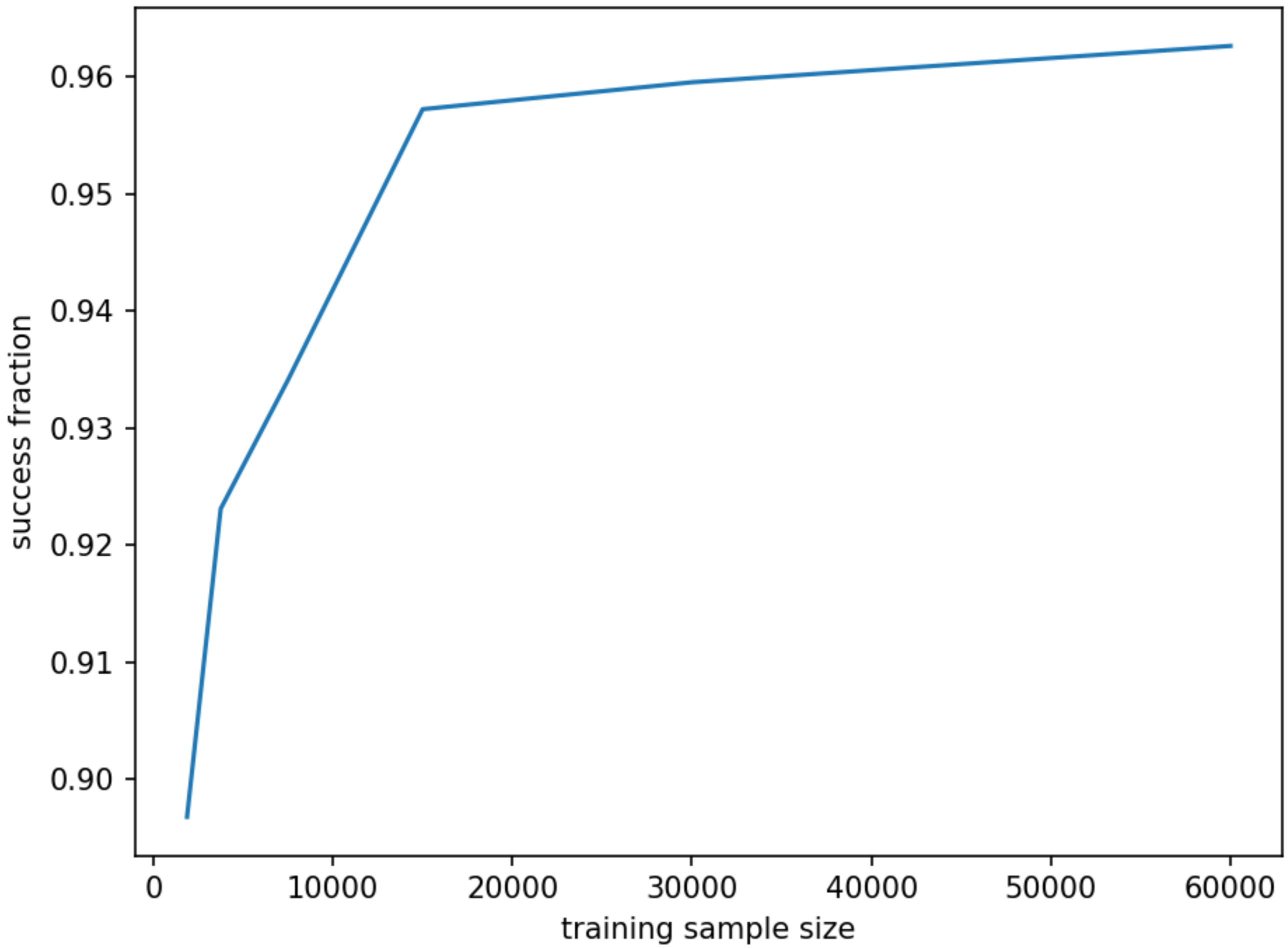
Effect of Number of Epochs

- When we use the full training set (60000 images) the number of epochs (passes through the training data) doesn't seem to matter much



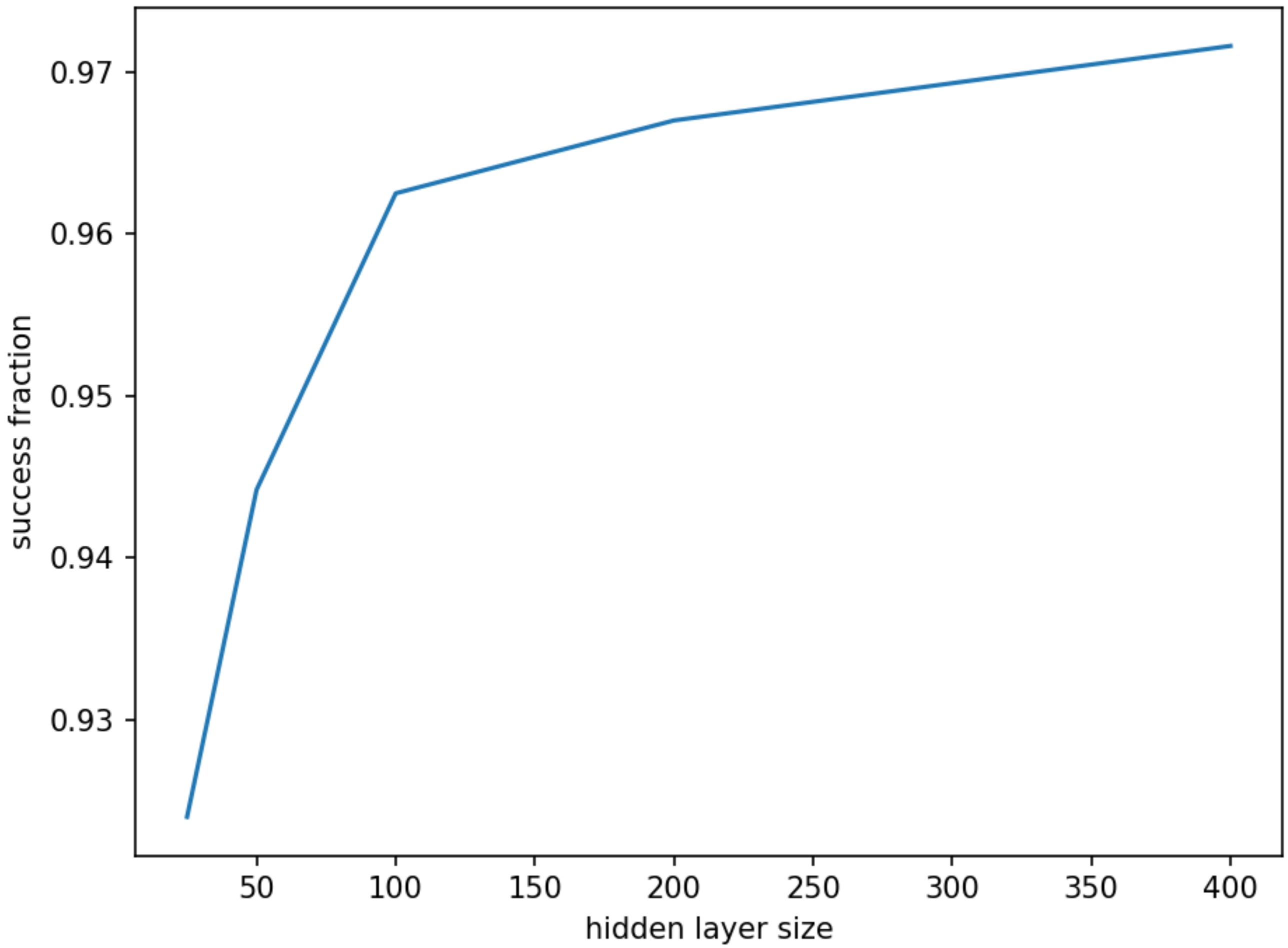
Effect of Training Set Size

- No surprise: the larger the training set, the better we do



Effect of Hidden Layer Size

- Also not unexpected: the larger the hidden layer the better we do



Effect of Learning Rate

- A smaller learning rate seems to do better