Introduction to MLP; Single Layer Networks

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Machine Learning Practical — MLP Lecture 1
23 September 2015
http://www.inf.ed.ac.uk/teaching/courses/mlp/

MLP – Course Details

- People
  - Lecturer: Steve Renals
  - TA: Pawel Swietojanski
  - Demonstrator: Matt Graham
  - Marker: Vladimir Nikishkin
- Format
  - Assessed by coursework only
  - 1 lecture/week
  - 1 lab/week (but multiple sessions)
- Requirements
  - **Programming Ability** (we will use python/numpy)
  - **Mathematical Confidence**
  - **Knowledge of Machine Learning** (e.g. Inf2B, IAML)

Do not do MLP if you do not meet the requirements

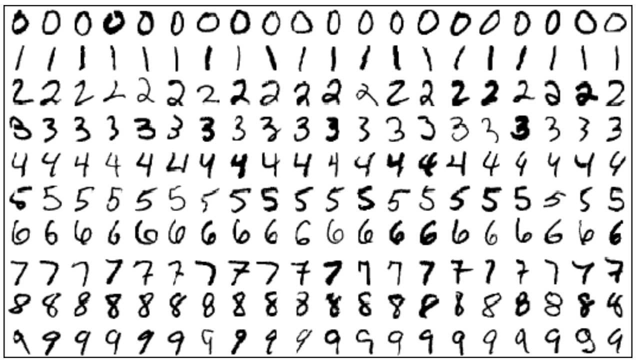
MLP – Course Content

- Main focus: implementing deep neural networks
- Main task: handwritten digit recognition (MNIST)
- Approach: implement DNN training and experimental setups within a provided framework
- What will you implement?
  - Single layer networks
  - Multi-layer (deep) networks
  - Convolutional networks
  - (Recurrent networks?)

Practicals and Coursework

- Practical work will be carried out using Python / Numpy / iPython notebook
- We'll provide a basic framework (which you will help to write) introduced through the labs
- Two pieces of assessed coursework:
  1. Implementing and testing of a basic deep neural network on the MNIST handwritten digit classification task (*due 22 October 2015, worth 30%*)
  2. Implementing and testing a convolutional network on MNIST, plus further experiments (*due 14 January 2016, worth 70%*)

MNIST Handwritten Digits



Practical Questions

- *Must I work within the provided framework?* – **Yes**
- *Can I look at other deep neural network software (e.g Theano, Torch, ...)?* – **Yes, if you want to**
- *Can I copy other software?* **No**
- *Can I discuss my practical work with other students?* – **Yes**
- *Can we work together?* – **No**

Good Scholarly Practice. Please remember the University requirement as regards all assessed work. Details about this can be found at:
http://www.ed.ac.uk/schools-departments/academic-services/students/undergraduate/discipline/academic-misconduct
and at:
http://web.inf.ed.ac.uk/infweb/admin/policies/academic-misconduct

Reading List

- Michael Nielsen, *Neural Networks and Deep Learning* 2015. http://neuralnetworksanddeeplearning.com
- Yoshua Bengio, Ian Goodfellow and Aaron Courville, *Deep Learning*, 2015. http://www.iro.umontreal.ca/~bengioy/dlbook
- Christopher M Bishop, *Neural Networks for Pattern Recognition*, 1995, Clarendon Press.

Single Layer Networks – Overview

- Learn a system which maps an input vector **x** to a an output vector **y**
- **Runtime:** compute the output **y** for each input **x**
- **Training:** The aim is to optimise the parameters of the system such that the correct **y** is computed for each **x**
- **Generalisation:** We are most interested in the output accuracy of the system for unseen test data
- **Single Layer Network:** Use a single layer of computation (linear) to map between input and output

Single Layer Networks

Input vector $\mathbf{x} = (x_1, x_1, \ldots, x_d)^T$

Output vector $\mathbf{y} = (y_1, \ldots, y_K)^T$

Weight matrix $\mathbf{W}$: w_{ki} is the weight from input x_i to output y_k

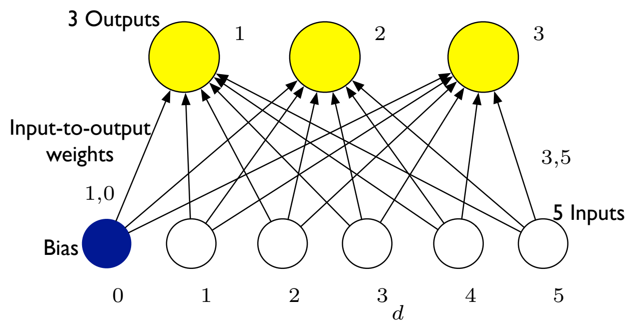
Bias w_{k0} is the bias for output k

$$y_k = \sum_{i=1}^{d} w_{ki} x_i + w_{k0}$$

If we define $x_0 = 1$ we can simplify the above to

$$y_k = \sum_{i=0}^{d} w_{ki} x_i \quad ; \quad \mathbf{y} = \mathbf{Wx}$$

Single Layer Networks



$$\mathbf{y} = \mathbf{Wx} \qquad k = \sum_{i=0}^{d} \quad ki \quad i$$

Training Single Layer Networks

Training set N input/output pairs $\{(\mathbf{x}^n, \mathbf{t}^n) : 1 \leq n \leq N\}$

Target vector $\mathbf{t}^n = (t_1^n, \ldots, t_K^n)^T$ – the target output for input $\mathbf{x}^n$

Training problem Set the values of the weight matrix $\mathbf{W}$ such that each input $\mathbf{x}^n$ is mapped to its target $\mathbf{t}^n$

Error function We define the training problem in terms of an error function E defined in terms of the network outputs $\mathbf{y}^n$ and the targets $\mathbf{t}^n$. Training corresponds to minimizing the error function E

Notes

1. This is a *supervised* learning setup - there is a target output for each input.
2. We can also write the network output vector as $\mathbf{y}^n(\mathbf{x}^n; \mathbf{W})$ to explicitly show the dependence on the weight matrix and the input vector.

Error function

- Error function should measure how far an output vector is from its target
- Take the (squared) Euclidean distance – *squared error function*:

$$E = \frac{1}{2} \sum_{n=1}^{N} ||\mathbf{y}^n - \mathbf{t}^n||^2 = \sum_{n=1}^{N} E^n$$

$$E^n = \frac{1}{2} ||\mathbf{y}^n - \mathbf{t}^n||^2$$

E is the total error summed over the training set
E^n is the error for the nth training example

- Can write E^n in terms of components:

$$E^n = \frac{1}{2} \sum_{k=1}^{K} (y_k^n - t_k^n)^2$$

- Training process: set $\mathbf{W}$ to minimise E given the training set

Weight space and gradients

- **Weight space:** A $K \times d$ dimension space – each possible weight matrix corresponds to a point in weight space. $E(\mathbf{W})$ is the value of the error at a specific point in weight space (given the training data).
- **Gradient** of $E(\mathbf{W})$ given $\mathbf{W}$ is $\nabla_{\mathbf{W}} E$, the vector of partial derivatives of E with respect to the elements of $\mathbf{W}$:

$$\nabla_{\mathbf{W}} E = \left(\frac{\partial E}{\partial w_{10}}, \ldots, \frac{\partial E}{\partial w_{ki}}, \ldots, \frac{\partial E}{\partial w_{Kd}} \right)^T .$$

- **Gradient Descent Training:** adjust the weight matrix by moving a small direction down the gradient, which is the direction along which E decreases most rapidly.
  - update each weight w_{ki} by adding a factor $-\eta \cdot \partial E / \partial w_{ki}$
  - η is a small constant called the *step size* or *learning rate*.

Gradient Descent Procedure

1. Initialise the weight matrix with small random weights and load the training data
2. For each epoch
   1. Initialise weight changes Δw_{ki} to zero
   2. For each training example n:
      1. Compute the error E^n
      2. Compute the gradients $\partial E^n / \partial w_{ki}$ for all k, i
      3. Update the total gradient by a small amount in the direction of $\nabla_{\mathbf{W}} E$):
      $$\Delta w_{ki} \leftarrow \Delta w_{ki} + \frac{\partial E^n}{\partial w_{ki}} \quad \forall k, i$$
   3. Update weights: $w_{ki} \leftarrow w_{ki} - \eta \Delta w_{ki} \quad \forall k, i$

Terminate either after a fixed number of epochs, or when the error stops decreasing by more than a threshold.
(An epoch is a complete pass through the training data)

Applying gradient descent to a single-layer network

- Need to differentiate the error function with respect to each weight:

$$E^n = \frac{1}{2} \sum_{k=1}^{K} (y_k^n - t_k^n)^2 = \frac{1}{2} \sum_{k=1}^{K} \left(\sum_{i=0}^{d} w_{ki} x_i^n - t_k^n \right)^2$$

$$\frac{\partial E^n}{\partial w_{rs}} = (y_r^n - t_r^n) x_s^n = \delta_r^n x_s^n \quad ; \quad \delta_r^n = y_r^n - t_r^n$$

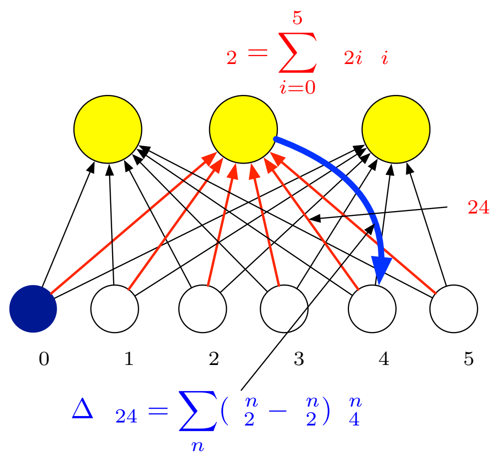
$$\frac{\partial E}{\partial w_{rs}} = \sum_{n=1}^{N} \frac{\partial E^n}{\partial w_{rs}} = \sum_{n=1}^{N} \delta_r^n x_s^n$$

- So the weight update is

$$w_{rs} \leftarrow w_{rs} - \eta \sum_{n=1}^{N} \delta_r^n x_s^n$$

This is sometimes called the *delta rule.*

Applying gradient descent to a single-layer network


$2 = \sum_{i=0}^{5} \; 2i \; i$
24
0
1
2
3
4
5
$\Delta \; 24 = \sum_n (\; {}^n_2 - \; {}^n_2) \; {}^n_4$

Gradient Descent Pseudocode

```
1: procedure GRADIENTDESCENTTRAINING($\mathbf{X}, \mathbf{T}, \mathbf{W}$)
2:     initialize $\mathbf{W}$ to small random numbers
3:     while not converged do
4:         for all $k, i$: $\Delta w_{ki} \leftarrow 0$
5:         for $n \leftarrow 1, N$ do
6:             for $k \leftarrow 1, K$ do
7:                 $y_k^n \leftarrow \sum_{i=0}^{d} w_{ki} x_i^n$
8:                 $\delta_k^n \leftarrow y_k^n - t_k^n$
9:                 for $i \leftarrow 1, d$ do
10:                    $\Delta w_{ki} \leftarrow \Delta w_{ki} + \delta_k^n \cdot x_i^n$
11:                end for
12:            end for
13:        end for
14:        for all $k, i$: $w_{ki} \leftarrow w_{ki} - \eta \cdot \Delta w_{ki}$
15:    end while
16: end procedure
```

Exact solution?

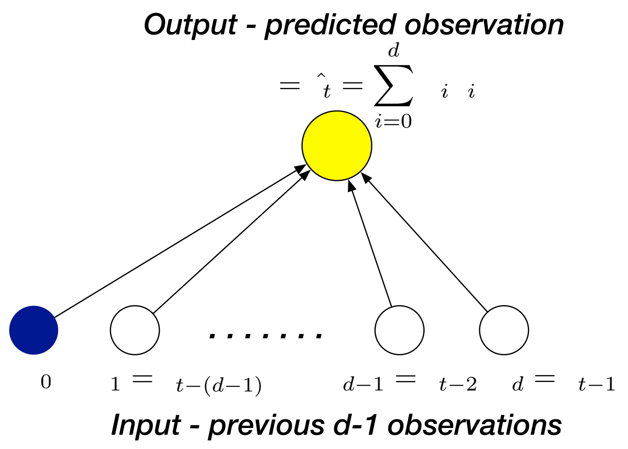
A single layer network is a set of linear equations... Can we not solve for the weights diectly given a training set? Why use gradient descent?

This is indeed possible for single-layer systems (consider linear regression!). But direct solutions are not possible for (more interesting) systems with nonlinearities and multiple layers, covered in the rest of the course. So we just look at iterative optimisation schemes.

Example: Rainfall Prediction

```
Daily Southern Scotland precipitation (mm). Values may change after QC.
Alexander & Jones (2001, Atmospheric Science Letters).
Format=Year, Month, 1-31 daily precipitation values.
 1931    1   1.40    2.10    2.50    0.10    0.00    0.00    0.90    6.20    1.90    4.90    7.30    0.80    0.30   2
 1931    2   0.90    0.60    0.40    1.10    6.69    3.00    7.59    7.79    7.99    9.59   24.17    1.90    0.20   4
 1931    3   0.00    1.30    0.00    0.00    0.00    0.50    0.40    0.60    1.00    0.00    0.10    7.30    6.20   0
 1931    4   3.99    3.49    0.00    2.70    0.00    0.00    1.80    1.80    0.00    0.20    3.39    2.40    1.40   1
 1931    5   1.70    0.00    0.70    0.00    5.62    0.70   13.14    0.80   11.13   11.23    0.60    1.70   10.83   8
 1931    6   1.40   16.40    3.70    0.10    5.80   12.90    4.30    4.50   10.40   13.20    0.30    0.10    9.30  29
 1931    7   9.49    1.70    8.69    4.10    2.50   13.29    2.70    5.60    3.10    1.30    7.59    3.90    2.30   7
 1931    8   0.20    0.00    0.00    0.00    0.00    0.60    2.00    0.60    6.60    0.60    0.90    1.20    0.50   4
 1931    9   9.86    4.33    1.01    0.10    0.30    1.01    0.80    1.31    0.00    0.30    4.23    0.00    1.01   1
 1931   10  23.18    5.30    4.20    6.89    4.10   11.29   10.09    5.80   11.99    1.80    2.00    5.10    0.30   0
 1931   11   6.60   20.40   24.80    3.30    3.30    2.60    5.20    4.20    8.00   13.60    3.50    0.90    8.50  15
 1931   12   3.20   21.60   16.00    5.80    8.40    0.70    6.90    4.80    2.80    1.10    1.10    0.90    2.50   3
 1932    1  12.71   41.12   22.51    7.20   12.41    5.70    1.70    1.80   24.41    3.80    0.80   13.71    4.30  17
 1932    2   0.00    0.22    0.00    0.54    0.33    0.11    0.00    0.00    0.22    0.11    0.22    0.00    0.00   0
 1932    3   0.10    0.00    0.00    1.60    8.30    4.10   10.00    1.10    0.00    0.00    0.00    0.60    0.50   0
 1932    4   7.41    4.61    1.10    0.10    9.41    8.61    2.10   13.62   17.63    4.71    0.70    0.30   10.02   3
 1932    5   0.10    0.20    0.00    0.10    0.70    0.10    0.80    1.00    0.30    0.00   10.51   17.42    4.11   1
 1932    6   0.00    0.00    0.00    0.20    0.00    0.00    0.60    0.20    0.50    0.00    0.00    0.10    0.00   0
 1932    7   2.41    7.62   13.94    7.42    1.30    1.30    1.80    3.81    2.61    4.01    1.00    4.81    9.93   0
 1932    8   0.00    1.70    0.30    1.00    2.70    4.61    3.40    2.60    0.50    1.30    9.61    1.80    3.81   0
 1932    9  19.37    7.39    9.69    2.70    3.50    3.79   16.68    5.29    4.69   16.88    3.50    1.00   14.08   2
 1932   10   4.40    0.50    0.10    1.80    6.40    8.20   14.69   18.39    4.30    2.80    0.10   16.19    2.20   0
 1932   11  11.37    8.08    5.79    0.00    0.00    0.00    0.00    0.20    0.00    0.00    0.10    0.30    0.00   0
 1932   12  20.23   19.93    3.81    2.40    0.00    0.00    0.00    0.10    0.40    0.40    0.10    0.70    2.30  13
 1933    1   3.40   28.50    2.80   18.80    5.30    4.50   14.60    8.80    0.60    3.50    0.00    3.10    0.50  19
 1933    2   6.10    2.60   14.80   33.10    8.00    9.00    3.10    4.70    7.00    0.10    0.10    0.90    0.10   0
 1933    3   2.59    5.29    3.99    5.99    7.19    7.09    0.30   29.54    5.19    0.00    0.00    0.00    1.10   3
 1933    4   0.40   14.98    3.20    0.50    0.00    0.00    0.00   11.98    1.70    0.10    4.69    0.20    0.00   0
 1933    5   0.00    0.00    4.71    9.92    2.21   13.73    3.81    5.71    1.80    0.10    0.80    0.20    0.00   0
```

Single Layer Network for Rainfall Prediction


Output - predicted observation
$= \hat{}_t = \sum_{i=0}^{d} \; _i \; _i$
0
$1 =$ $t-(d-1)$
. . . .
$d-1 =$ $t-2$
$d =$ $t-1$
Input - previous d-1 observations

Summary

- Single layer network architecture
- Training sets, error functions, and weight space
- Gradient descent training
- Example – Rainfall prediction
- **Lab 1 - Mon/Tue/Wed next week**: Setup, training data
  Signup using the doodle link on the course webpage!
- **Next lecture:**
  - Stochastic gradient descent and minibatches
  - Classification
  - Introduction to multi-layered networks