# ISTA 421/521 – Homework 2

Due: Tuesday, September 30, 10pm 12 points total Undergraduate / 16 points total Graduate

STUDENT NAME

Undergraduate / Graduate

# Instructions

In this assignment you are required to write 3 scripts in python. They will be submitted as 3 separate files, although you are free to copy chunks of code from one script to the next as desired. The names for the script files are specified in problems 1, 5 and 8, below.

Included in the homework 2 release are two sample scripts (fitpoly\_incomplete.py and cv\_demo\_incomplete.py) and two data files (womens100.csv, and synthdata2014.csv). The sample scripts are provided for your convenience — you may use any part of the code in those scripts for your submissions. Note that neither will run just as provided: you must fill in the calculation of w. The data files are provided in .csv (comma separated values) format. The script fitpoly\_incomplete.py shows how to load the files.

All problems except problem 1 require that you provide some "written" answer (in some cases also figures), so you will also submit a .pdf of your written answers. (You can use IATEX or any other system (including handwritten; plots, of course, must be program-generated) as long as the final version is in PDF.)

The final submission will include (minimally) the three scripts and a PDF version of your written part of the assignment. You are required to create either a .zip or tarball (.tar.gz / .tgz) archive of all of the files for your submission and submit the archive to the d2l dropbox by the date/time deadline above.

NOTE: Problems 6 and 7 are required for Graduate students only; Undergraduates may complete them for extra credit equal to the point value.

(FCMA refers to the course text: Rogers and Girolami (2012), A First Course in Machine Learning. For general notes on using LATEX to typeset math, see: http://en.wikibooks.org/wiki/LaTeX/Mathematics)

# 1. [2 points] Adapted from Exercise 1.2 of FCMA p.35:

Write a Python script that can find the parameters  $\mathbf{w}$  for an arbitrary dataset of  $x_n, t_n$  pairs. You will use this script to answer problem 2, which only requires fitting a simple line to the data (i.e., you only need to fit parameters  $w_0$  and  $w_1$ ); however, in problems 5 and 8 you will need to fit higher-order polynomial models (e.g.,  $t = w_0 + w_1 x + w_2 x^2 + ...$ ), so it is recommended that your script is generalized to handle higher-order polynomials. The script fitpoly\_incomplete.py is provided to help get you started. fitpoly\_incomplete.py provides helper functions to read data, plot data, and plot the model (once you've determined the weight vector  $\mathbf{w}$ ), but the function for computing linear least-squares fit, fitpoly (starting on line 36), is incomplete – you need to fill this in – it takes as input the data vector  $\mathbf{x}$ , the target values vector  $\mathbf{t}$ , and the scalar model\_order, which is an integer representing the polynomial order of the model; fitpoly is intended to return the  $\mathbf{w}$  (column) vector (e.g., as a numpy matrix such as the following:

The above isn't literally the code you'd use, but shows how you can create and transpose matrices, with row and column vectors simply being limiting cases of matrices with one row or 3 rows with 1 value each, respectively). You will want to look at the numpy package, including the linear algebra package numpy.linalg, for linear algebra operators. Also, you don't have to use fitpoly\_incomplete.py; you can write your own script from scratch. Whichever you choose, your script must have the ability to plot the data with the fitted model.

Just to state the obvious: the objective of this exercise is for you to implement the linear least squares fit solution (i.e., the normal equations) – in their general matrix form. **DO NOT** use existing least squares solvers, such as numpy.linalg.lstsq, or scikit learn's sklearn.linear\_model.LogisticRegression; however, it is certainly fine to use these to help *verify* your implementation's output.

You will submit your script as a stand-alone file called fitpoly.py.

## Solution:

2. [1 point] Adapted from Exercise 1.6 of FCMA p.35:

Table 1.3 (p.13) of FCMA lists the women's 100m gold medal Olympic results – this data is provided in the file womens100.csv in the data folder. Using your script from problem 1, find the 1st-order polynomial model (i.e., a line with parameters  $w_0$  and  $w_1$ ) that minimizes the squared loss of this data. Report the model here as a linear equation and also include a figure that plots your model with the data.

#### **Solution:**

3. [1 point] Adapted from Exercise 1.7 of FCMA p.35:

Using the model obtained in the previous exercise, predict the women's winning time at the 2012 and 2016 Olympic games; report the values here. What is the squared error of your model's prediction for Shelly-Ann Fraser-Price's gold medal time of 10.75 seconds in the 2012 Olympics women's 100m race?

#### Solution:

4. [1 point] Adapted from Exercise 1.9 of FCMA p.36:

Use your python script from problem 1 to load the data stored in the file synthdata2014.csv (in the data folder). Fit a 3rd order polynomial function  $-f(x; \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + w_3 x^3$  – to this data (if you extended the fitpoly\_incomplete.py script, then model\_order= 3). Present and describe the parameters you obtain fitting to this data. Also, plot the data and your linear-fit model and include the plot in your answer.

#### **Solution:**

5. [3 points] Write a script that implements K-fold cross-validation to choose the polynomial order (between orders 0 and 7) with the best predictive error for the synthdata2014.csv. The provided script cv\_demo\_incomplete.py implements the synthetic data experiment described in Ch 1 (pp.31-32) of the book; you are welcome to use and adapt any part of this code you like; keep in mind that this script won't successfully execute until you add the general (matrix form) normal equation calculation on line 81. Note also that in the synthetic data experiment in cv\_demo\_incomplete.py, 1000 test data points are generated in addition to the 100 data points used for 10-fold cross-validation; for problem 5, you won't have this independent test set, only the data from synthdata.csv on which to perform K-fold cross-validation.

Run your script with 10-fold cross-validation and Leave-One-Out-CV (LOOCV). Which model order do the two cross-validation methods predict as the best order for predictive accuracy? Do the two different cross-validation runs agree?

Report the best-fit model parameters for the best model order according to 10-fold CV, and plot this model with the data. Include a plot of the CV-loss and training loss for the 8 different (0..7) polynomial model orders for both the 10-fold cross-validation and for LOOCV.

You will submit your script as a stand-alone file called cv.py

### Solution:

# 6. [2 points - Required only for Graduates] Exercise 1.10 from FCMA p.36

Derive the optimal least squares parameter value,  $\hat{\mathbf{w}}$ , for the total training loss:

$$\mathcal{L} = \sum_{n=1}^{N} \left( t_n - \mathbf{w}^{\top} \mathbf{x}_n \right)^2$$

How does the expression compare with that derived from the average (mean) loss? (Hint: Express this loss in the **full** matrix form and derive the normal equation.)

#### **Solution:**

# 7. [2 points – Required only for Graduates] Exercise 1.11 from FCMA p.36

The following expression is known as the weighted average loss:

$$\mathcal{L} = \frac{1}{N} \sum_{n=1}^{N} \alpha_n \left( t_n - \mathbf{w}^{\top} \mathbf{x}_n \right)^2$$

where the influence of each data point is controlled by its associated parameter. Assuming that each  $\alpha_n$  is fixed, derive the optimal least squares parameter value  $\hat{\mathbf{w}}$ . (Hint: When expressing in the full matrix form, the *alpha*'s become a matrix...)

### Solution:

# 8. [4 points] Variant of Exercise 1.12 from FCMA p.36

Write a new Python script that uses K-fold cross-validation to find the value of  $\lambda$  that gives the (approximate) best predictive performance on the synthetic data (synthdata.csv) using regularized least squares with a 7th order polynomial model. Report here the lambda you identified, the best fit linear model using that lambda (as a linear equation) and include a plot of the MSE loss as a function of  $\lambda$  that shows the loss curve with a minimum, and a plot of the best-fit model with the data.

You will submit the script as a stand-alone file called regularize.py.

#### Solution: