CS461 Homework 2

Due: Oct. 20 11:59 pm

1. Suppose someone asked you to identify a linear model used to generate the noise-free data below ($y = w_0 \cdot 1 + w_1 x_1 + w_2 x_2 + w_3 x_3$). You plan to use MMSE regression to estimate the original model.

data num	(x_1, x_2, x_3)	y
d_1	(4, 1, 1)	16
d_2	(7, 0, 2)	23
d_3	(10, 1, 3)	36
d_4	(13, 0, 4)	43

1.1 Please write a data-matrix $\Phi(4 \times 4)$.

sol)

$$\Phi = \begin{bmatrix} 1 & 4 & 1 & 1 \\ 1 & 7 & 0 & 2 \\ 1 & 10 & 1 & 3 \\ 1 & 13 & 0 & 4 \end{bmatrix}$$

1.2 When the normal equation is shown as below, will it give you an exact solution or MMSE approximated solution?

$$\Phi^t \Phi \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ w_3 \end{bmatrix} = \Phi^t \begin{bmatrix} 16 \\ 23 \\ 36 \\ 43 \end{bmatrix}$$

sol) This gives an exact solution. Data points are noise-free so the vector $[16, 23, 36, 43]^t$ lies on the column space of matrix Φ.

1.3 In the normal equation $\Phi^t\Phi$ is invertible? If not, how would you solve it? Please solve the equation and find $\vec{w}$.

sol) $\Phi^t\Phi$ is not invertible, so pseudo-inverse needs to be used. The pseudo-inverse solution is $\vec{w} = [0, 3, 3, 1]^t$, i.e $y = 3x_1 + 3x_2 + x_3$

$$w = (\Phi^t\Phi)^\dagger \Phi^t \begin{bmatrix} 16 \\ 23 \\ 36 \\ 43 \end{bmatrix}$$

1.4 The person showed you the original model as $y = 1 + 2 \cdot x_1 + 3 \cdot x_2 + 4 \cdot x_3$. Is it the same as yours? If not, why this happened?

Sol) Since $\Phi^t\Phi$ is not invertible; there exist infinitely many solutions for $\vec{w}$.

1.5. The person suggested that, with four additional data points, you could obtain the same result as the original model. Please add the four data points below to your normal equation and compute the new $\vec{w}$. Do you have a different answer from the previous one? What is the chance to obtain the original model using the regression method?

data num	(x_1, x_2, x_3)	y
d_5	(16, 1, 5)	56.04
d_6	(19, 0, 6)	62.77
d_7	(22, 1, 7)	76.04
d_8	(25, 0, 8)	82.96

sol) The new solution is slightly different from the previous solution and it is not close to the original model: $y = 1+2\cdot x_1+3\cdot x_2+4\cdot x_3$. $\Phi^t\Phi$ remains non-invertible even with the additional data points, leading to infinitely many solutions. The chance (probability) to obtain the original model is 0 for $\frac{1}{\infty}$.

1.6. Carefully examine your data matrix from 1.1. If you could delete a column to ensure a unique solution, which column would you remove?

sol) $C_1 + 3 \cdot C_4 = C_2$, so removing any one of the columns C_1, C_2, C_4 will make the matrix have a unique solution.

2. [Lagrangian Function and KKT Conditions] Suppose you have two data points as below to estimate $y = w_0x_1 + w_1x_2$.

data num	(x_1, x_2)	y
d_1	(1 0)	1
d_2	(0,1)	1

2.1 Please set an MMSE objective function $J(\vec{w})$ with the data. What is the optimal solution (w_0, w_1) that minimizes the function?

sol) $J(w) = (w_0 - 1)^2 + (w_1 - 1)^2$ The optimal solution for the objective function is $w^* = (1, 1)$.

2.2 We have only two data points, so the constrained optimization problem for regularization is formulated below. Please define the Lagrangian function for the problem.

$$\vec{w*} = \arg\min_{\vec{w}} J(\vec{w})$$
$$\text{subject to } ||\vec{w}||^2 \leq C$$

sol) $L(\lambda, \vec{w}) = (w_0 - 1)^2 + (w_1 - 1)^2 + \lambda(w_0^2 + w_1^2 - C)$

2.3 Based on KKT conditions, compute the optimal Lagrangian parameter and $\vec{w*}$ for the different $C = \{0.5, 1, 2, 3\}$. Hint: geometrical contours will help you to find the relation between $w*_0$ and $w*_1$.

sol)

- $\nabla_w L(w*, \lambda*) = \begin{bmatrix} \frac{\partial L(w,\lambda)}{\partial w_0} \\ \frac{\partial L(w,\lambda)}{\partial w_1} \end{bmatrix} = \begin{bmatrix} 2(w_0^* - 1) + 2\lambda^* \cdot w_0^* \\ 2(w_1^* - 1) + 2\lambda^* \cdot w_1^* \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \leftrightarrow \lambda* = \frac{1 - w_0^*}{w_0^*} = \frac{1 - w_1^*}{w_1^*}$
- $\lambda* = 0$ if $w*_0^2 + w*_1^2 < C \quad \leftrightarrow \quad w_0^* = w_1^* = 1$ (from $\lambda* = \frac{1 - w_0^*}{w_0^*} = \frac{1 - w_1^*}{w_1^*}$ and $\lambda* = 0$) and $2 = 1 + 1 < C$
- $\lambda* > 0$ if $w*_0^2 + w*_1^2 = C \quad \leftrightarrow \quad w_0^* = w_1^* = \sqrt{\frac{C}{2}}$ and $\lambda* = \frac{1 - \sqrt{\frac{C}{2}}}{\sqrt{\frac{C}{2}}}$

Based on the KKT condition,

- when $C > 2$, $w_0^* = w_1^* = 1$ and $\lambda* = 0$
- when $C \leq 2$ $w_0^* = w_1^* = \sqrt{\frac{C}{2}}$ and $\lambda* = \frac{1 - \sqrt{\frac{C}{2}}}{\sqrt{\frac{C}{2}}}$
- $C = 0.5$, $w_0^* = w_1^* = 1/2$ and $\lambda* = 1$
- $C = 1$, $w_0^* = w_1^* = \sqrt{1/2}$ and $\lambda* = 2\sqrt{\frac{1}{2}} - 1$
- $C = 2$, $w_0^* = w_1^* = 1$ and $\lambda* = 0$
- $C = 3$, $w_0^* = w_1^* = 1$ and $\lambda* = 0$

3. [Learning Sinusoidal Functions] You will recover a sinusoidal function $f(x)$ from noisy data by using MMSE regression. Data samples and required specifications are given below.

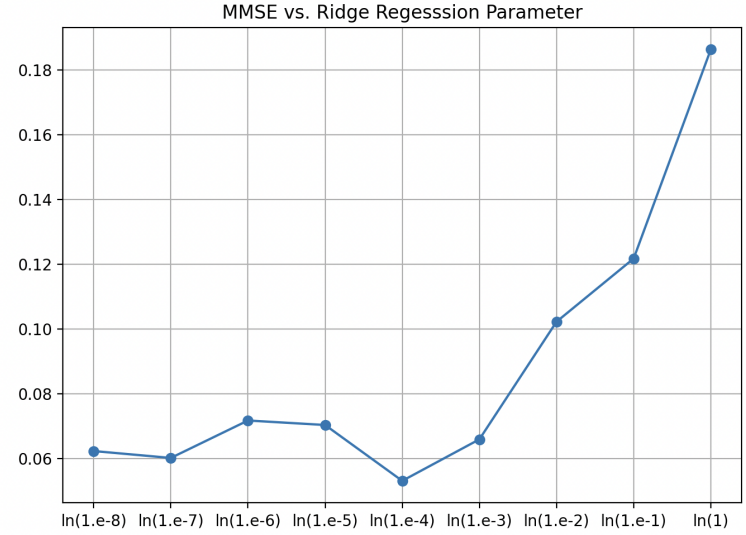
- train and test data files: train.npz, test.npz, and readme.txt
- use ten polynomial basis functions: $1, x, x^2, ..., x^8, x^9$
- use MSE (Mean Square Error) for the performance metric: $\frac{1}{N}\sum_{i=1}^{N}(\vec{w}^t\phi(x_i) - y_i)^2$
- use five-fold cross-validation for the selection of the parameter of ridge regression λ

3.1 Write the code "ols_regression.py" to implement an MMSE regression model (five cross-validation and ordinary MMSE) and report one validation error averaging the five cross-validations.

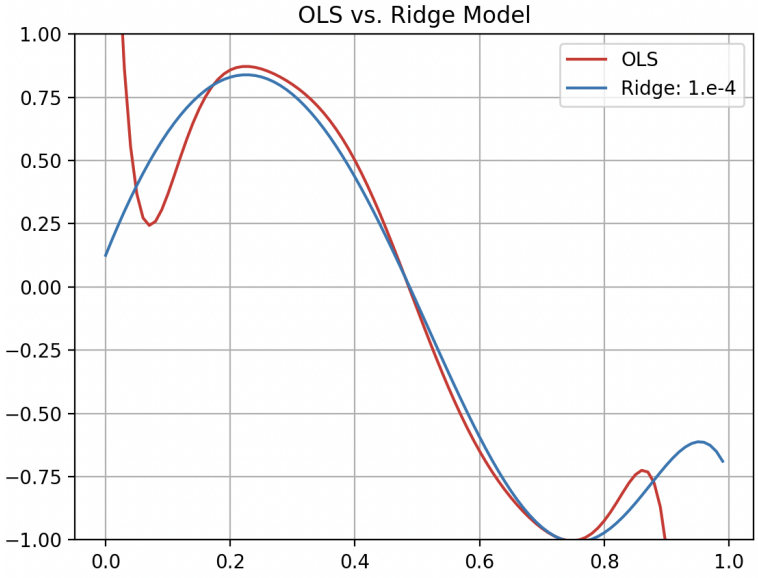
sol) Averaged five cross-validation error ≈ 0.21

3.2 Write the code "ridge_regression.py" to implement a ridge regression model (five cross-validation and ridge MMSE) and plot the averaged validation error for different ridge parameters: $0 \leq \lambda \leq 1$. Hint: possible λs are 1e−8, 1e−7, ..., 0.5, 1 but the spacing is up to your design. Based on the plot, select the $\lambda*$ and save the corresponding models $w(\lambda*)$. Additionally, save the five models for the ordinary MMSE $w(\lambda = 0)$.

sol) Averaged five cross-validation error ≈ 0.05 and $\lambda* = 1.e-4$.



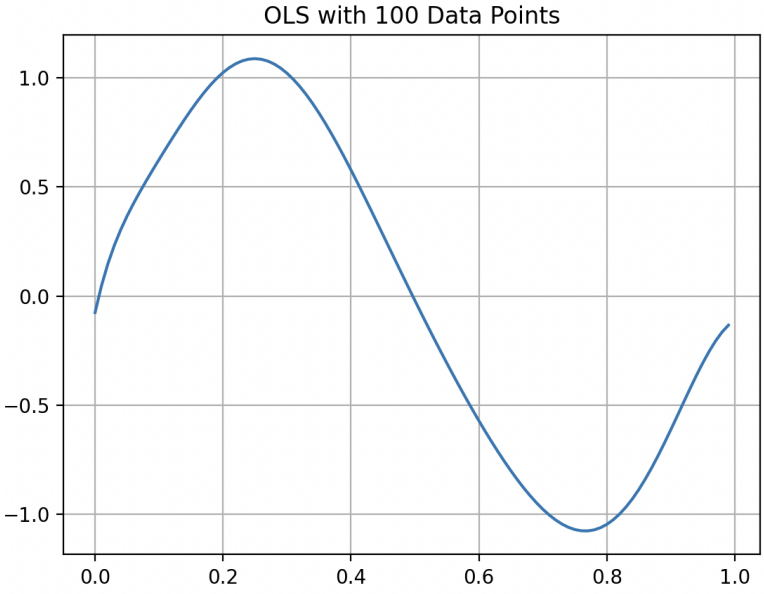
3.3 Plot the two models: $w(\lambda = 0)$ and $w(\lambda*)$ over the range $0 \leq x \leq 1$. The five models can be averaged: w=np.mean(w, axis=0).



3.4 Evaluate the two models with "test.npz" and report the two test MSEs.

- OLS test MSE ≈ 0.27
- Ridge $(1.0e-4)$ test MSE ≈ 0.024

3.5 Write the code "ols_regresssion_largeset.py" to implement a regression model with "train_100.npz" without any regularization and cross validation. Plot the model over the range $0 \leq x \leq 1$.



3.6. Based on your answers in 3.3, 3.4, and 3.5, please provide two possible solutions to control the effective complexity in machine learning.

sol)

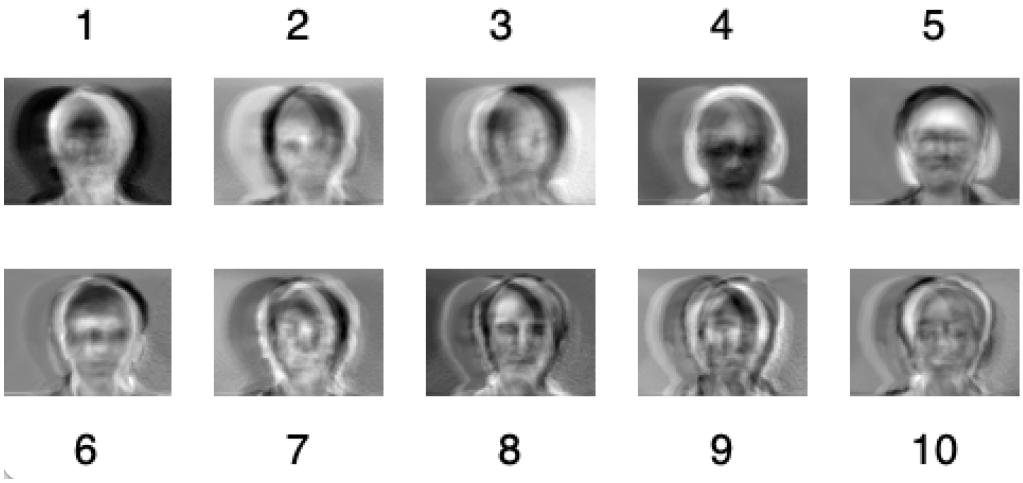
1. Ridge Regression and its parameter selection based on cross-validation
2. Increase of the number of data points

4. [Eigenface] Spectral decomposition is applied to a large set of images to extract the most dominant correlations between images. You will approximate one test facial image by using $\vec{x} \simeq \vec{x'} = \bar{x} + E_M E_M^t (x - \bar{x})$. E_M is the eigenvectors of $COV(X, X)$ that correspond to the M largest eigenvalues where random vector X represents the whole facial data.

4.1 Please compute $COV(X, X)$ and $E[X]$ and spectral decomposition $COV(X, X) = E\Lambda E^t$ by using the gif images in "train" folder. You can use numpy and PIL and no need to submit your computations.

4.2 Approximate the test image in "test" folder for different M values: 2, 10, 100, 1,000, 4,000. Present the five images in your report. Select one representative image for each M.

4.3 Represent the eigenvectors corresponding to the 10 largest eigenvalues in grayscale images. Please include the ten images in your report and explain how the eigenimages capture the various features and aspects of human faces. Hint: you may need this formula for visualization: $\frac{x - min(x)}{max(x) - min(x)} \times 256$.

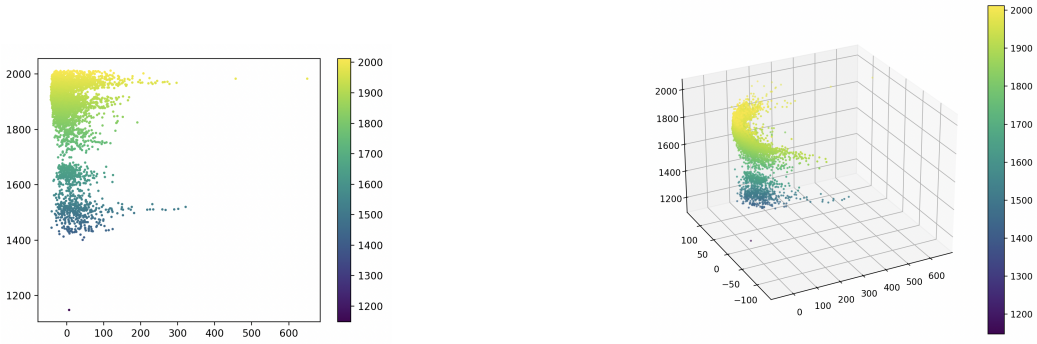


sol)

The top eigenimages show the important patterns to describe human faces. The first three capture global information like the location or overall structure of faces while the subsequent ones represent more detailed local information like eyes, noses, and mouth. We can recognize more subtle expressions and variations from the later images.

5. [Extra 25 Points, Estimation of Year of Made] You will build a predictor of the year of made for art by using the embedding collected from a deep-CNN style classifier (VGG-16). It is a high dimensional embedding as 512-D. After conducting dimensional reduction to 2-D and whitening, a polynomial feature map will be constructed for regression. Data samples and required specifications are given below.

- train and test data files: vgg16_train.npz, vgg16_test.npz, readme.txt
- use any order polynomial basis functions as you want: for example, $1, x_1, x_1^2, x_2, x_1x_2, x_2^2$
- use MSE (Mean Square Error) for the performance metric



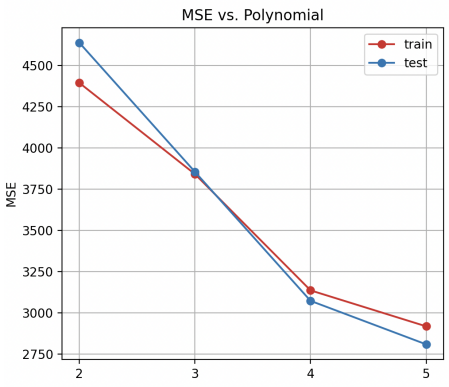
(a) Year over M: 1 PCA

(b) Year over M: 2 PCA

Figure 1: Year Information over PCA Space

5.1 Dimensional Reduction and Whitening: Please use PCA formula $\Lambda^{-1/2}E_M^t(x-\bar{x})$. Scatter plots for the case of M=1 and M=2 are shown above. Please reproduce the plots. Based on the figures, please reason why 2-D projection will be more promising in year prediction than 1-D case.

5.2 Train: Write the code "year_train.py" to implement a 2-D regression model to predict the year of made using vgg16_train.npz. Try any order of polynomial basis as you want and test your models on a validation set. For simplicity, please use a subset of the training set for validation to finalize your model (no cross-validation). Hint: you could increase the order until observing overfitting or performance stagnation.



sol) The polynomials of degree 2 to 5 were attempted.

5.3 Test: Write the code "year_test.py" to evaluate your model on vgg16_test.npz. Report a test MSE score and identify the image where your model shows the most accurate prediction and the image where it shows the least accurate prediction (report image filenames).

sol)

(a) the most accurate image: id 9593: (gt: 1925 vs. prediction 1924.89)

(b) the least accurate image: id 847: (gt: 1455 vs. prediction 1885)

Figure 2: "The Most and Least Accurate Predication Examples"