

Homework 4

Guoxiang Grayson Tong

December 10, 2022

Problem 1:

- (A) Please see the script
- (B) To avoid having negative values inside the square root of \hat{g}_1 , we add a small value of $1e - 12$.
The filters as a function of the eigenvalue of the normalized Laplacian matrix are as:

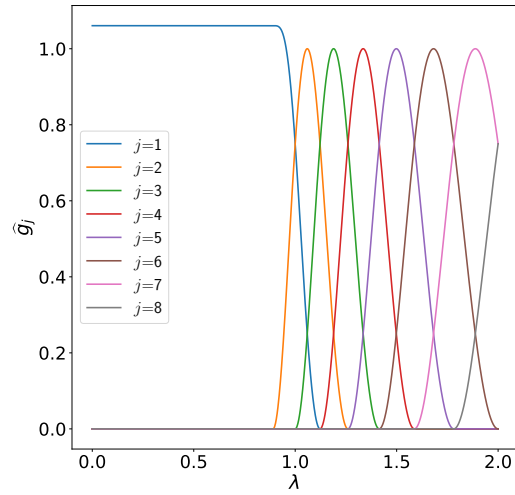


Figure 1: Spectral wavelet filters as functions of eigenvalue λ .

Problem 2:

- (A) Please see the script
- (B) Use the built-in function `pca_lowrank` and randomly pick 10^4 examples from the QM9 dataset.
We are able to do the follow:

$$\hat{\mathbf{F}} \in \mathbb{R}^{10^4 \times 365} \rightarrow \tilde{\mathbf{F}} \in \mathbb{R}^{10^4 \times 2} . \quad (1)$$

The scatter plot as:

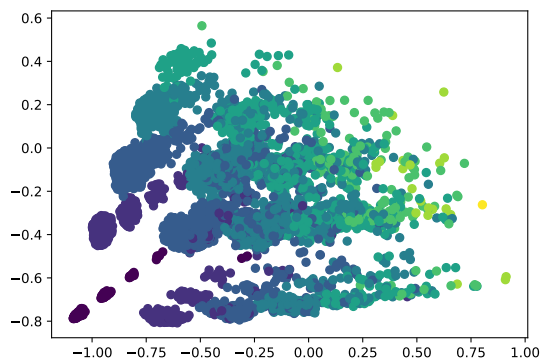


Figure 2: Reduced feature maps colored by the number of hydrogen-bond acceptor atoms.

- (C) We construct a 2-layer fully connected MLP with 10 hidden units, activated by the `ReLU` function. We apply the mini-batch gradient descent method with the `Adam` optimizer to train this MLP model for 500 epoches with a learning rate of 0.01. Besides, the mini-batch size is set as: $n_B = 50$. The loss function as:

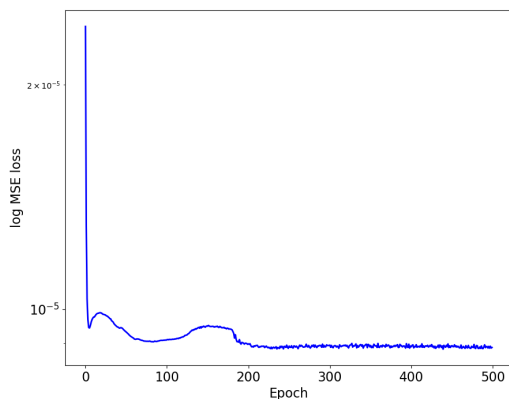


Figure 3: Log MSE training loss.

- (D) The scatter plot as:
-

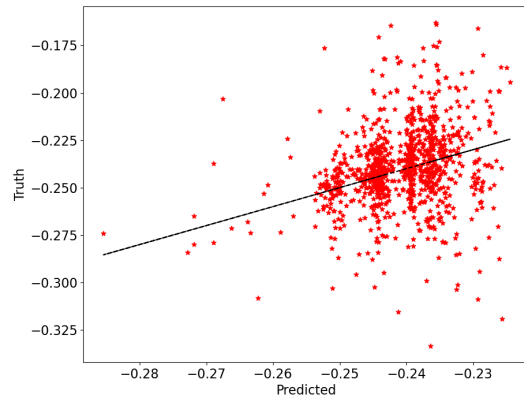


Figure 4: Scatter plot of the correlation between target and prediction.
