EECE5644 HW3

CONTENT

Question 1

For this problem many multilayer perceptron (MLP) were used to approximate class label posteriors. Minimum average cross-entropy loss was used to train the MLP and the trained models were then used to approximate a MAP classification rule to achieve minimum probability of error on a validation dataset.
For this exercise a 3-dimensional real-values random vector x was generated from 4 classes with uniform priors and Gaussian class conditional pdfs. The distributions used are shown below.

$$P(L = \mathrm{l}) = 0.25, \text{for } \mathrm{l} = [0,1,2,3]$$

$$m_0 = \begin{bmatrix} 2.6 \\ 2.6 \\ 0 \end{bmatrix} \mathrm{c}_0 = \begin{bmatrix} 1.0630 & 0.0587 & 0.0184 \\ 0.0587 & 1.0608 & 0.0280 \\ 0.0184 & 0.0280 & 1.0377 \end{bmatrix}$$

$$m_1 = \begin{bmatrix} 2.6 \\ 0 \\ 0 \end{bmatrix} \mathrm{c}_1 = \begin{bmatrix} 1.0747 & 0.0271 & 0.0733 \\ 0.0271 & 1.0175 & 0.0371 \\ 0.0733 & 0.0371 & 1.0968 \end{bmatrix}$$

$$m_2 = \begin{bmatrix} 0 \\ 2.6 \\ 0 \end{bmatrix} \mathrm{c}_2 = \begin{bmatrix} 1.0436 & 0.0522 & 0.0423 \\ 0.0522 & 1.0886 & 0.0794 \\ 0.0423 & 0.0794 & 1.0742 \end{bmatrix}$$

$$m_3 = \begin{bmatrix} 0 \\ 0 \\ 2.6 \end{bmatrix} \mathrm{c}_3 = \begin{bmatrix} 1.0262 & 0.0114 & 0.0120 \\ 0.0114 & 1.0176 & 0.0080 \\ 0.0120 & 0.0080 & 1.0314 \end{bmatrix}$$

A 2-layer MLP with one hidden and one output later was specified and implemented. The output layer was a “softmax” function as is the default for the Matlab “patternnet” function that was used for implementation. In the problem a smooth-ramp style activation function was specified and it could be implemented by change the activation function like net.layers{1}.transferFcn='logsig'. However there is not a built-in function of that type for “patternnet” in Matlab. Due to the challenges inherent in implementing it in the Matlab environment is too difficult(need to define it by myself), the default “tansig” function was used after asking the professor's permission.
For training datasets with 100, 200, 500, 1000, 2000, and 5000 samples were generated and for validation a test dataset with 100,000 samples was generated. Plots of the generated data are shown in Figure 1 and Figure 2.

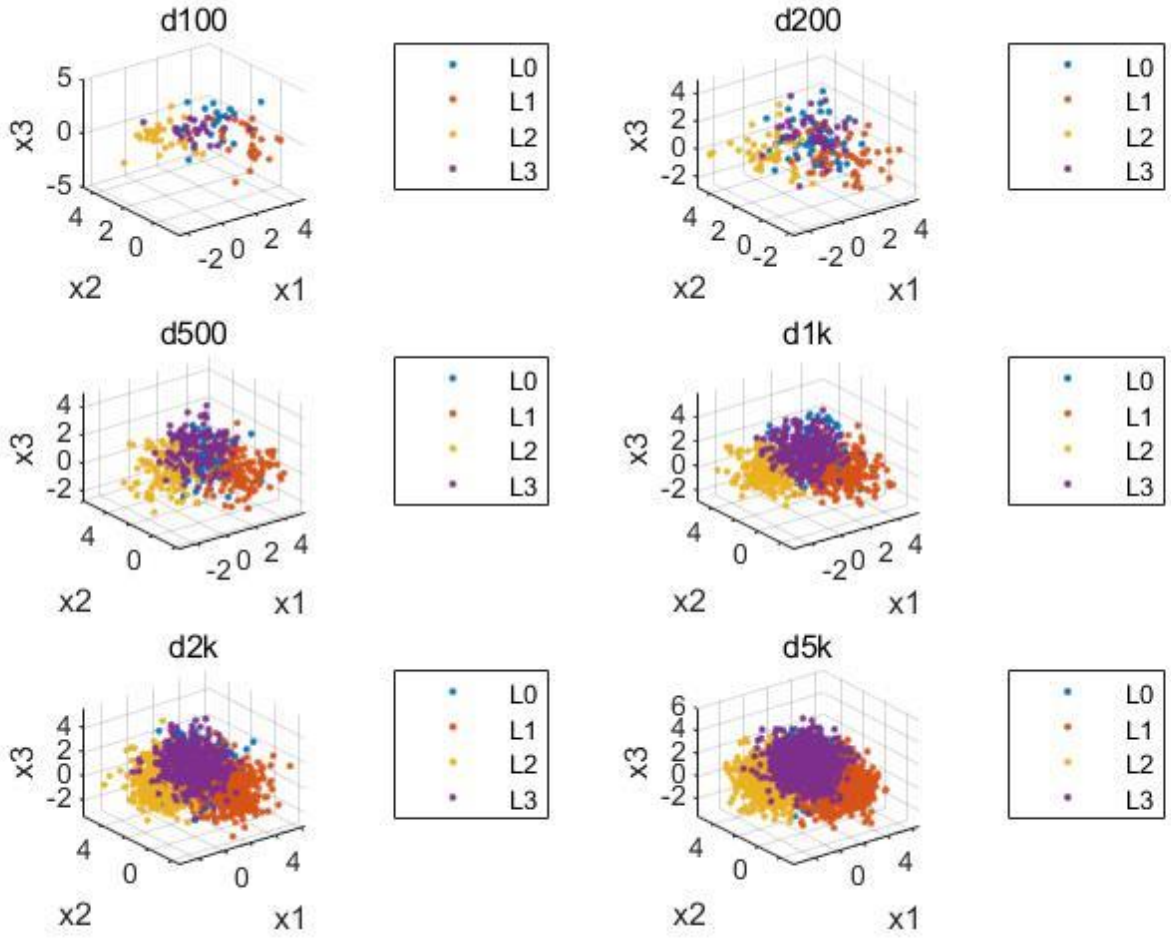


Figure 1: Training Datasets

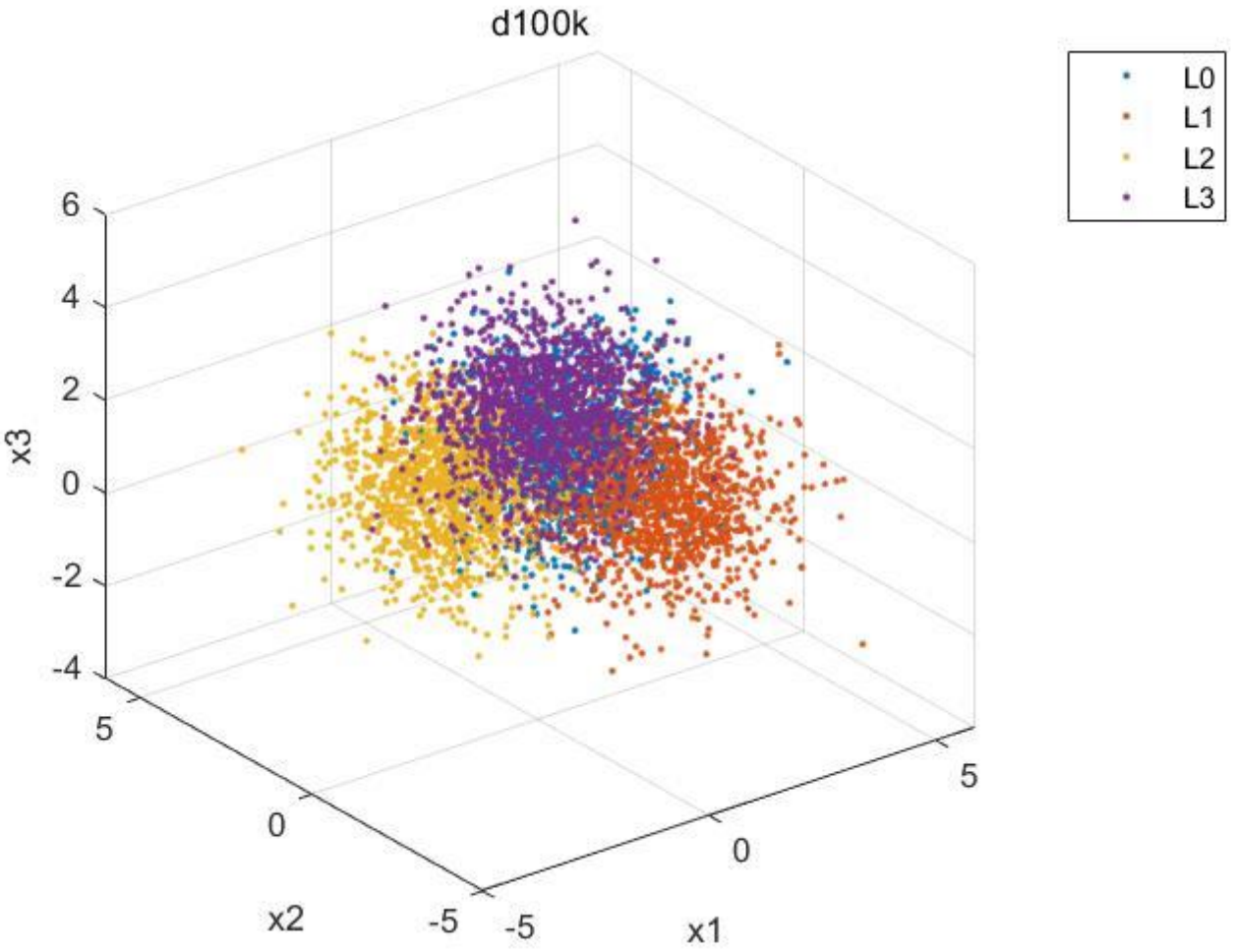


Figure 2: Validation Dataset

For each training dataset 10-fold cross validation was performed to determine the optimal amount of perceptron for the MLP model. The optimal number was the one that resulted in the minimum probability of error across the cross validation runs. Once the number of perceptron was selected a final model was then trained on the entire training dataset. Finally, this trained model was evaluated using the test dataset and the probability of error was calculated as the metric of model performance.

Figure 3 shows the results of this procedure. As can be seen in the plot, the overall probability of error is well correlated with the size of the training dataset. As the size of the dataset increases the probability of error decreases and approaches the optimal probability of error as estimated using the true pdf of the underlying data. This demonstrates that as the quantity of training data increases the model estimate is able to be improved resulting in more accurate classifications.

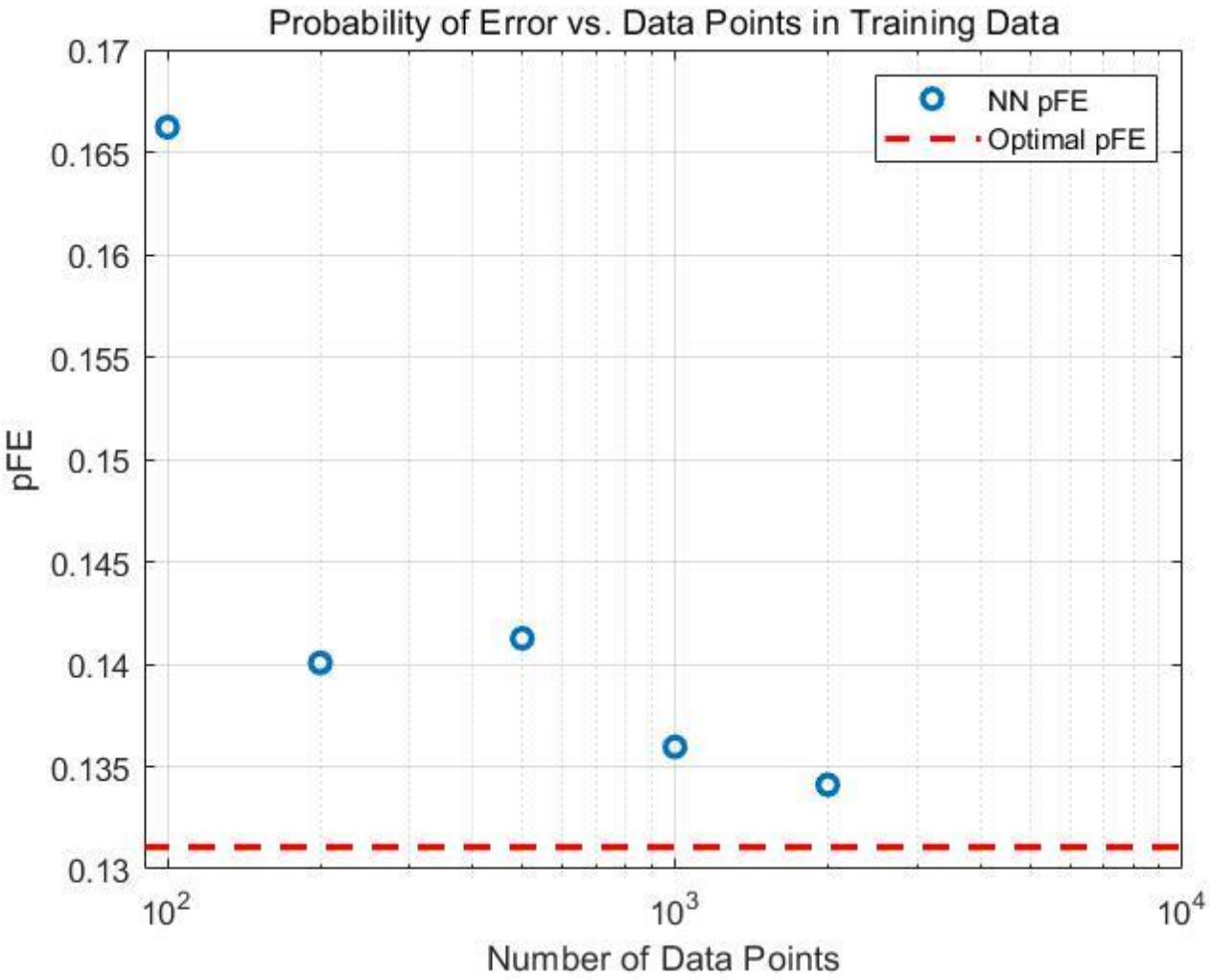


Figure 3: Probability of Error vs. Number of Data Points

Figure 4 shows a plot of the optimal amount of perceptron versus the number of data points in a dataset. Except for the data point for the 1000-point training set the optimal amount of perceptron appears to increase as the size of the training dataset increases. This was expected since as the size of the dataset increases the complexity of the model can also increase in a meaningful way. More data means more features than can be modelled and therefore model complexity increases.

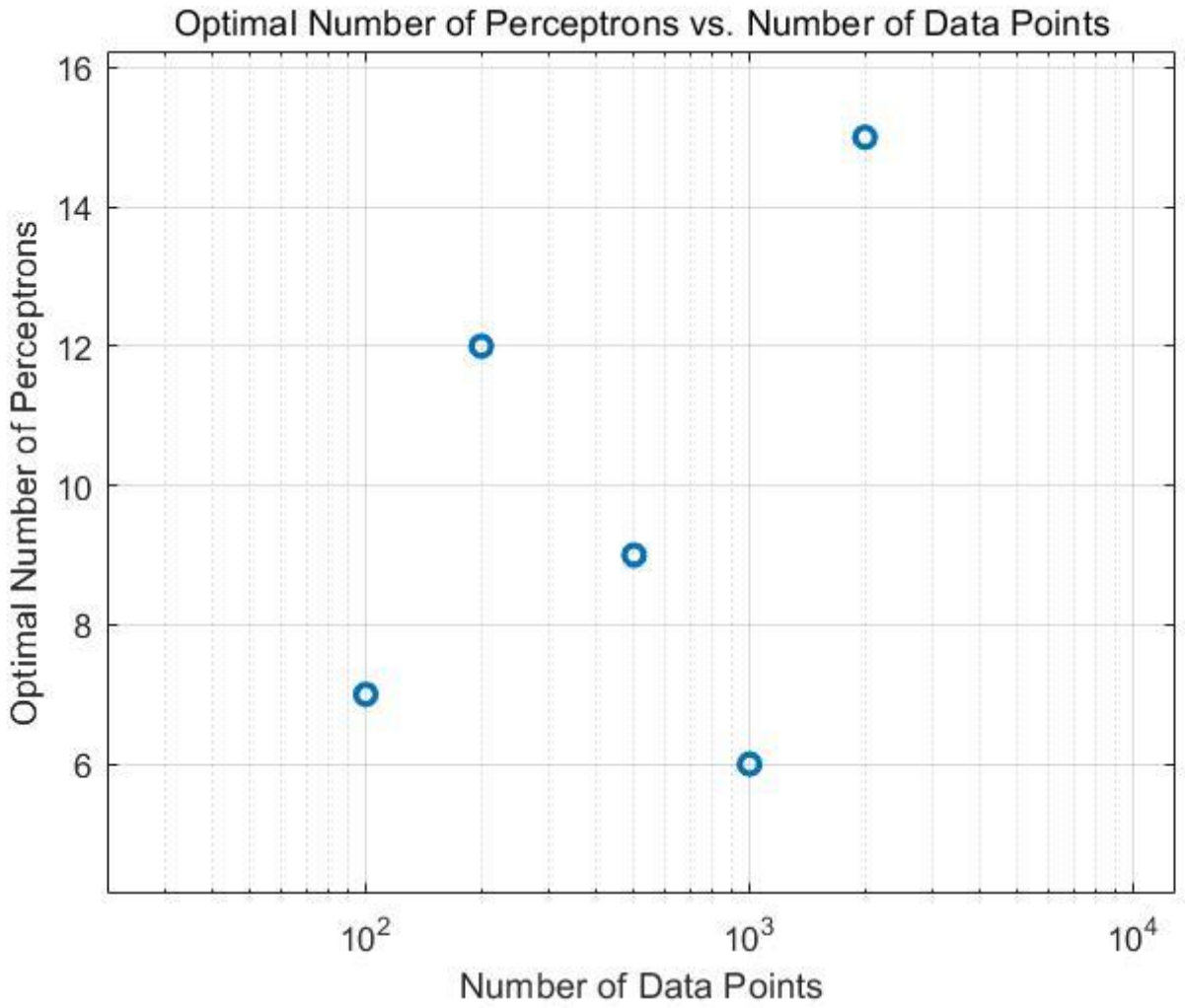


Figure 4: Optimal Amount of Perceptron for a Given Dataset Size

Table 1 shows the optimal and the neutron network minimum probability of error with different datasets.

Table 1: optimal and NN Probability of Error

	Optimal P_e	NN P_e
100	13.00%	16.62%
200	12.00%	14.01%
500	12.00%	14.13%
1000	11.90%	13.60%
2000	12.55%	13.41%
5000	12.94%	13.21%
10000	13.11%	-

Figure 5 below shows a plot of the cross-validation results for all training datasets. In the plot the probability of error is shown as a function of the amount of perceptron. The probability of error starts very large for a single perceptron and then rapidly decreases as the number of perceptron increases. A minimum is identified at 10 and the probability error slowly increases as the number of perceptron is increased. While the optimal number of perceptron varied between training datasets the overall relationship between the probability of error and the number of perceptron generally followed this pattern.

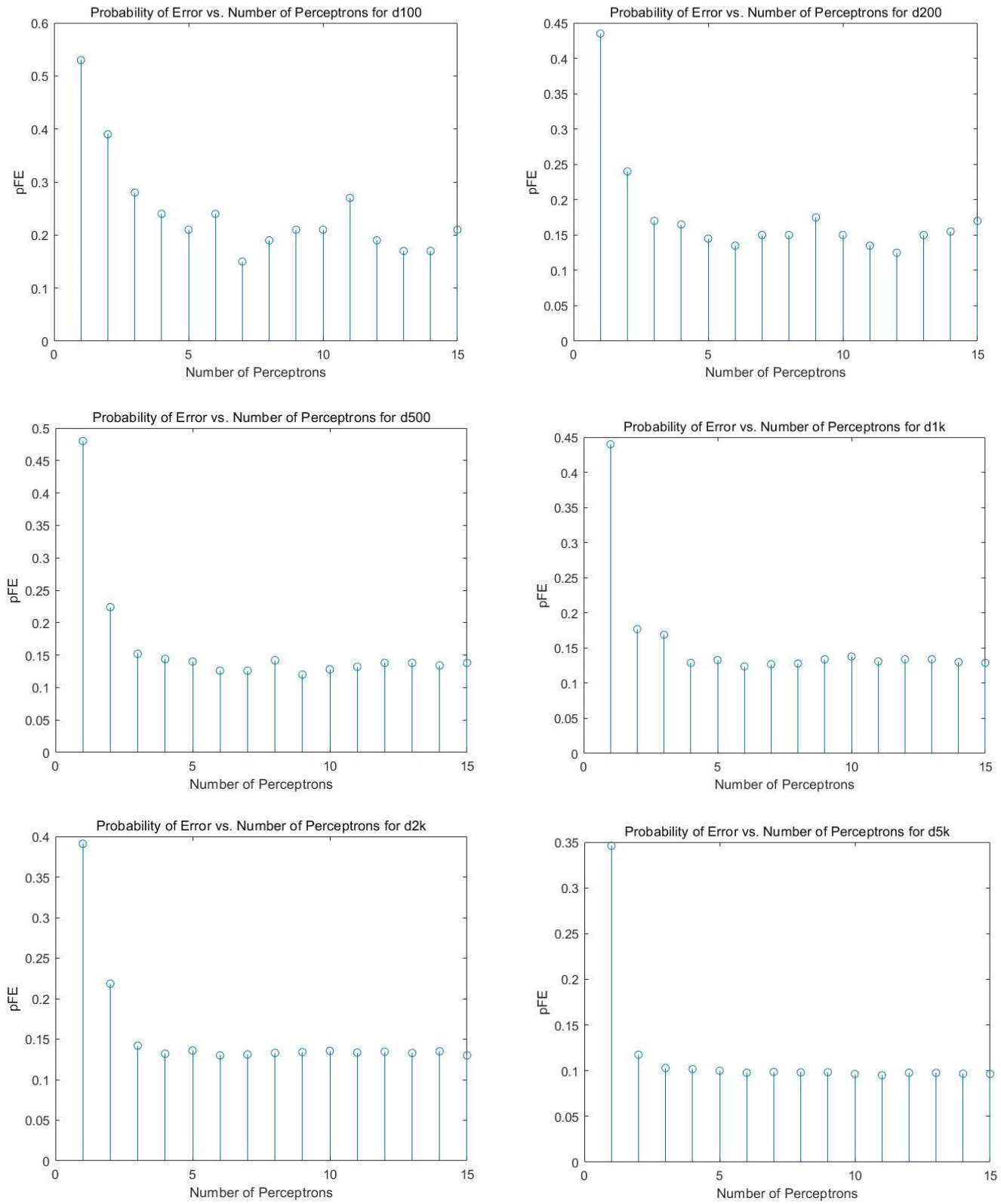


Figure 5: Probability of Error vs. Amount of Perceptron for training datasets

Figure 6 and figure 7 show the X vectors with the correct and incorrect classification for training datasets and validate dataset.

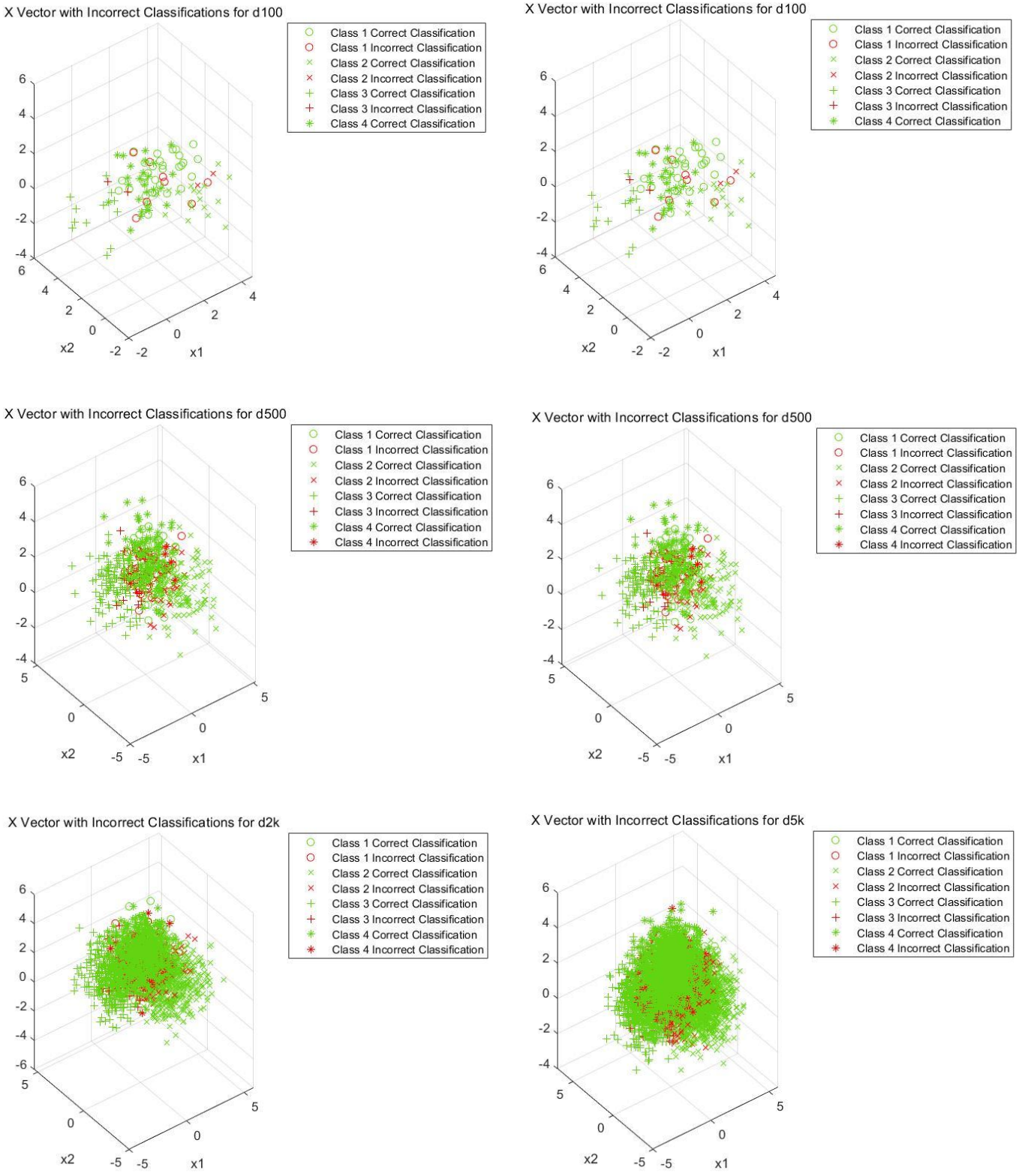


Figure 6: X vector with Classifications for training datasets

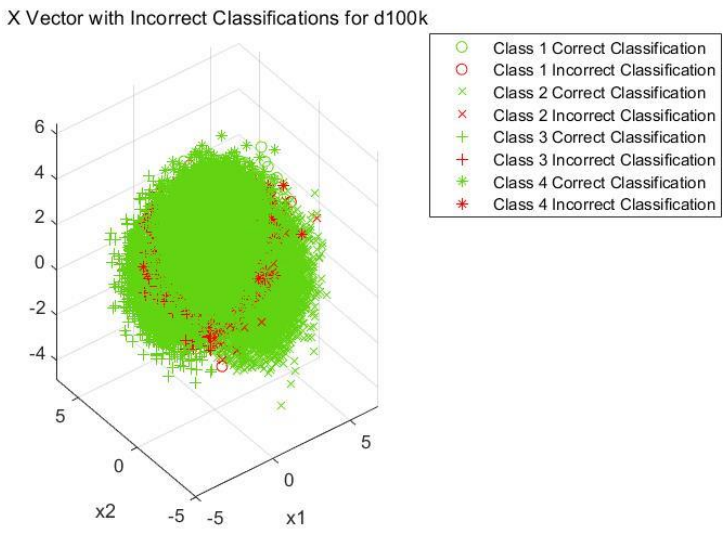


Figure 6: X vector with Classifications for validate dataset

Question 2

1. Class conditional PDFs and mixture coe_cients:

$$\mu_1 = \begin{bmatrix} 10 \\ -10 \end{bmatrix} \sigma_1^2 = \begin{bmatrix} 15 & 1 \\ 1 & 15 \end{bmatrix} \mathrm{P}_1 = 0.2$$

$$\mu_2 = \begin{bmatrix} -10 \\ 10 \end{bmatrix} \sigma_2^2 = \begin{bmatrix} 17 & 3 \\ 3 & 17 \end{bmatrix} P_2 = 0.3$$

$$\mu_3 = \begin{bmatrix} -10 \\ -10 \end{bmatrix} \sigma_3^2 = \begin{bmatrix} 19 & 5 \\ 5 & 19 \end{bmatrix} P_3 = 0.23$$

$$\mu_4 = \begin{bmatrix} 10 \\ 10 \end{bmatrix} \sigma_4^2 = \begin{bmatrix} 21 & 7 \\ 7 & 21 \end{bmatrix} P_4 = 0.27$$

2. Data with 10, 100, 1000 and 10k samples are generated using the GMM model described above. Figure 7 below shows the realization of the models with different samples.

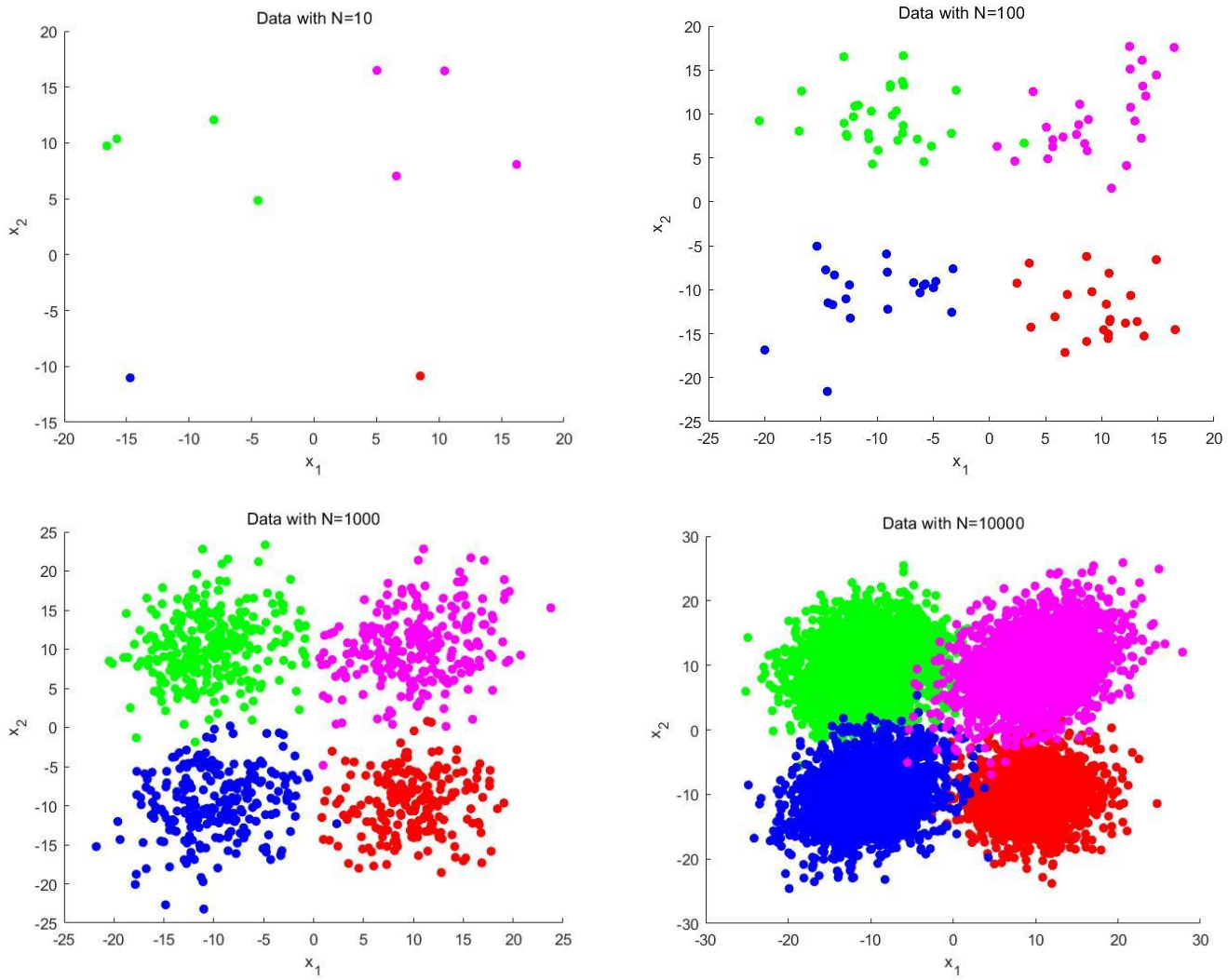
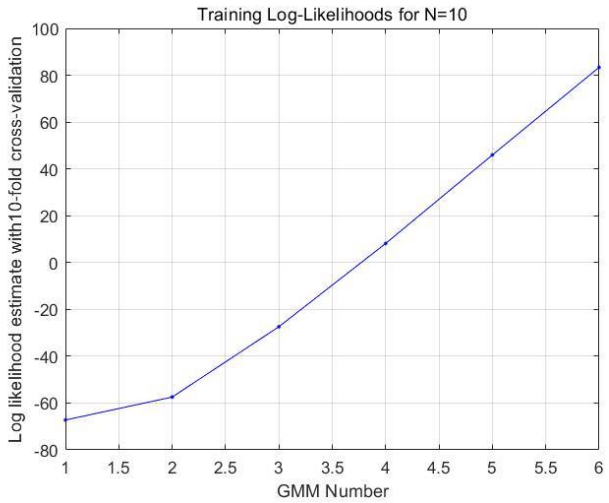
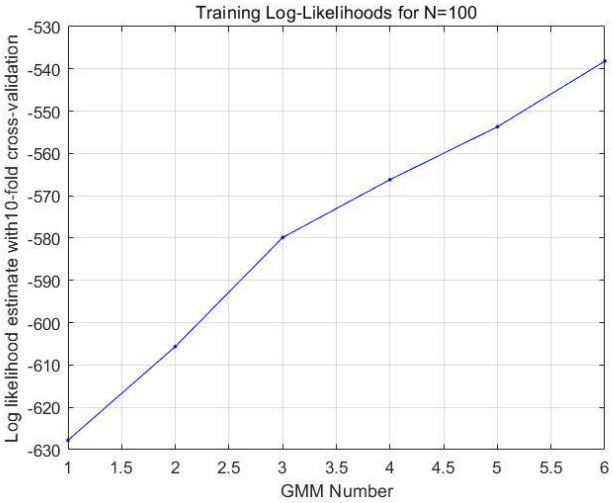
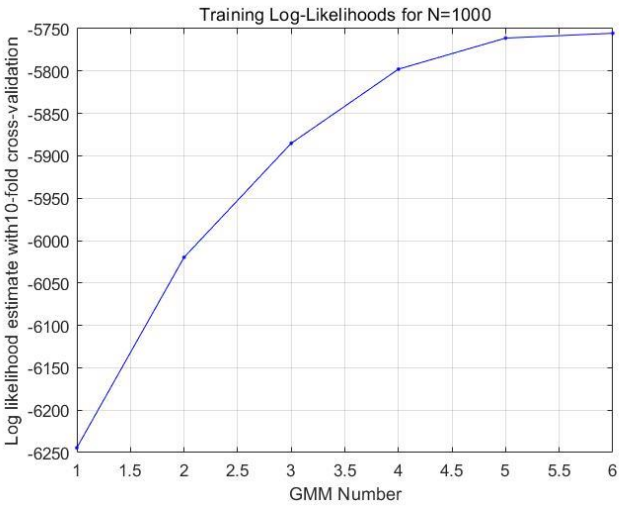


Figure 7: Data visualization

3. With number of samples=1000 or 10k, log likelihood and BICs indicate number of components=4 is a good model for this data. What's more, when n components=4, the score quickly falls and plateaus when Components=1,2,3,5,6. Considering Occam's razor, number of components=4 is obviously the best option.







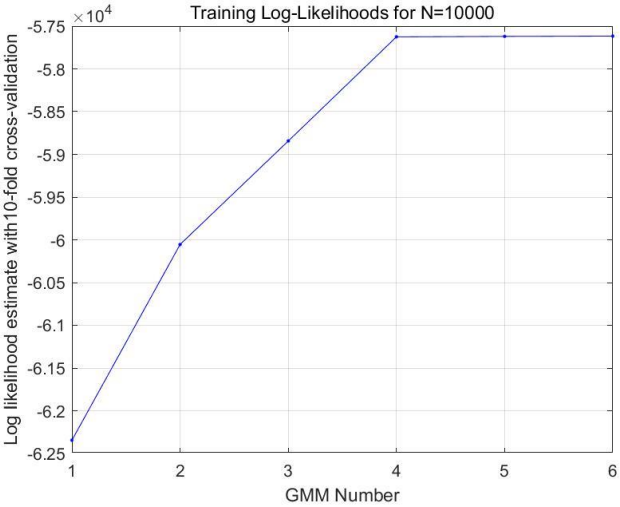
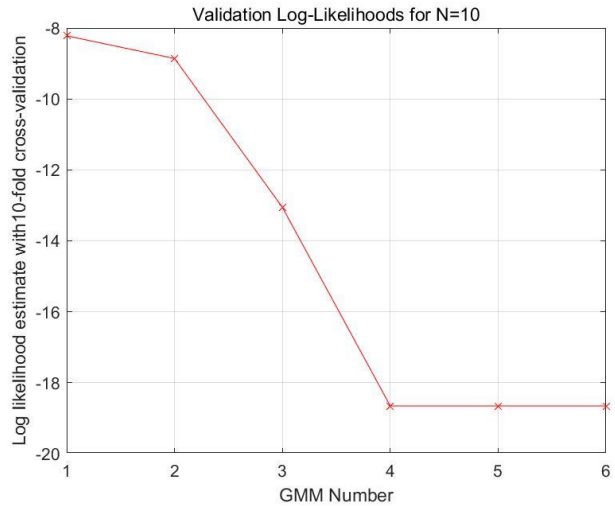
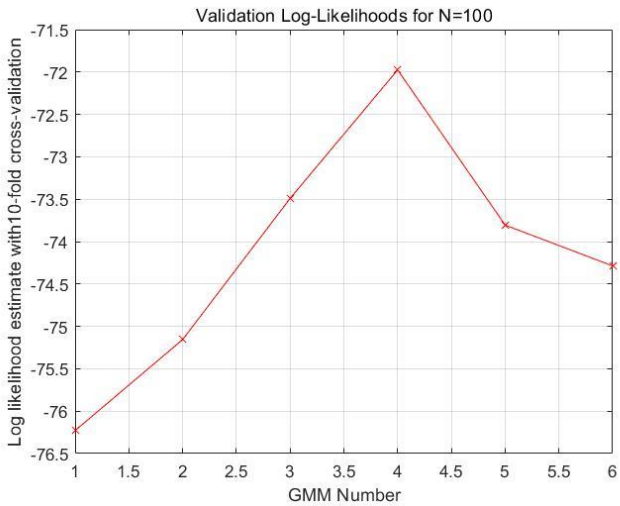
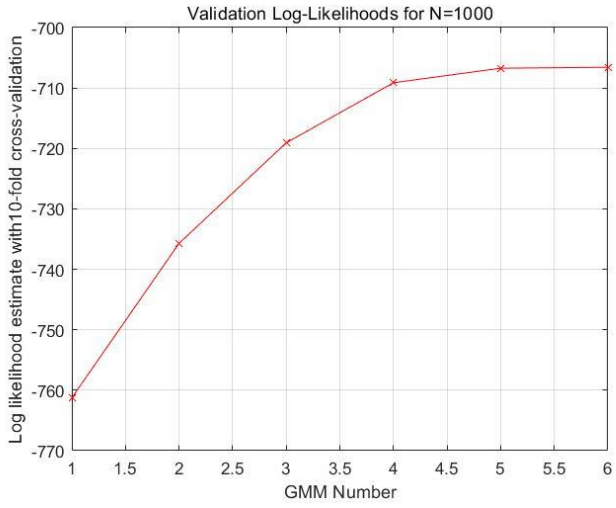


Figure 8: Training log_likelihoods for all datasets







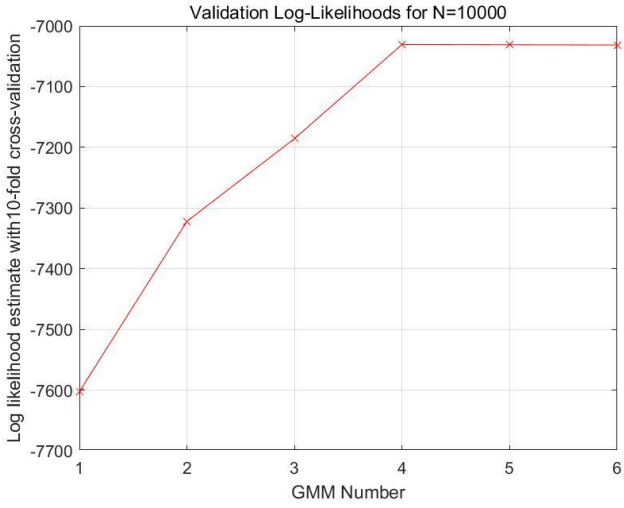
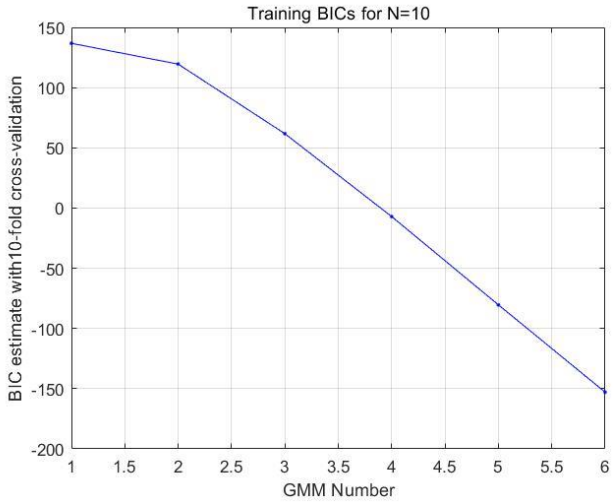
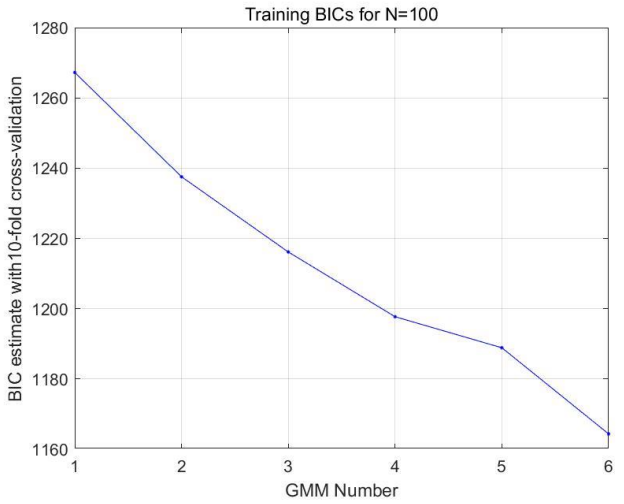
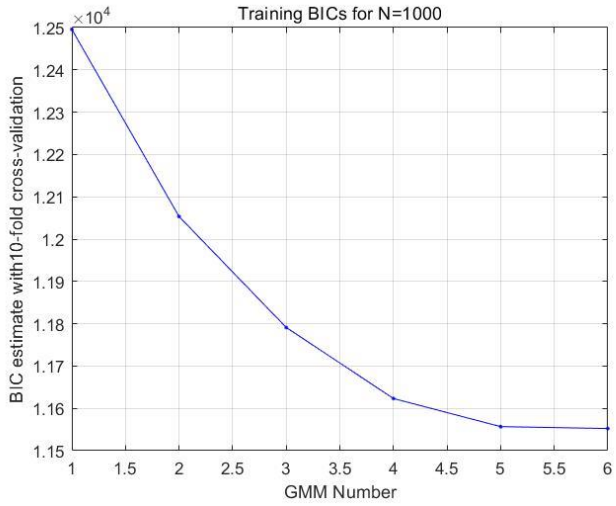


Figure 9: Validation log_likelihoods for all datasets







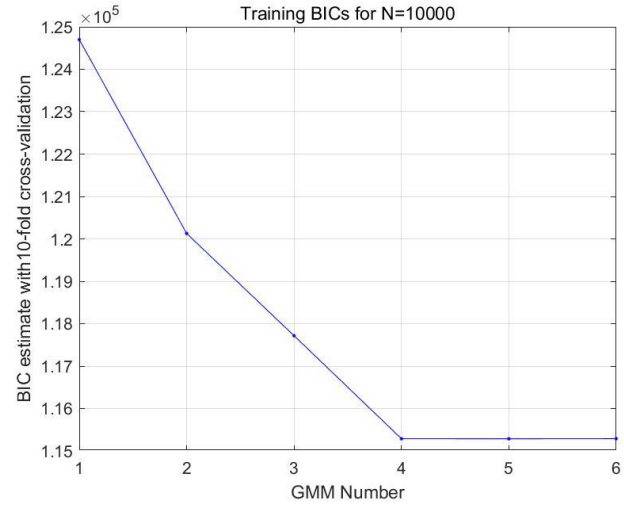


Figure 10: Training BICs for all datasets

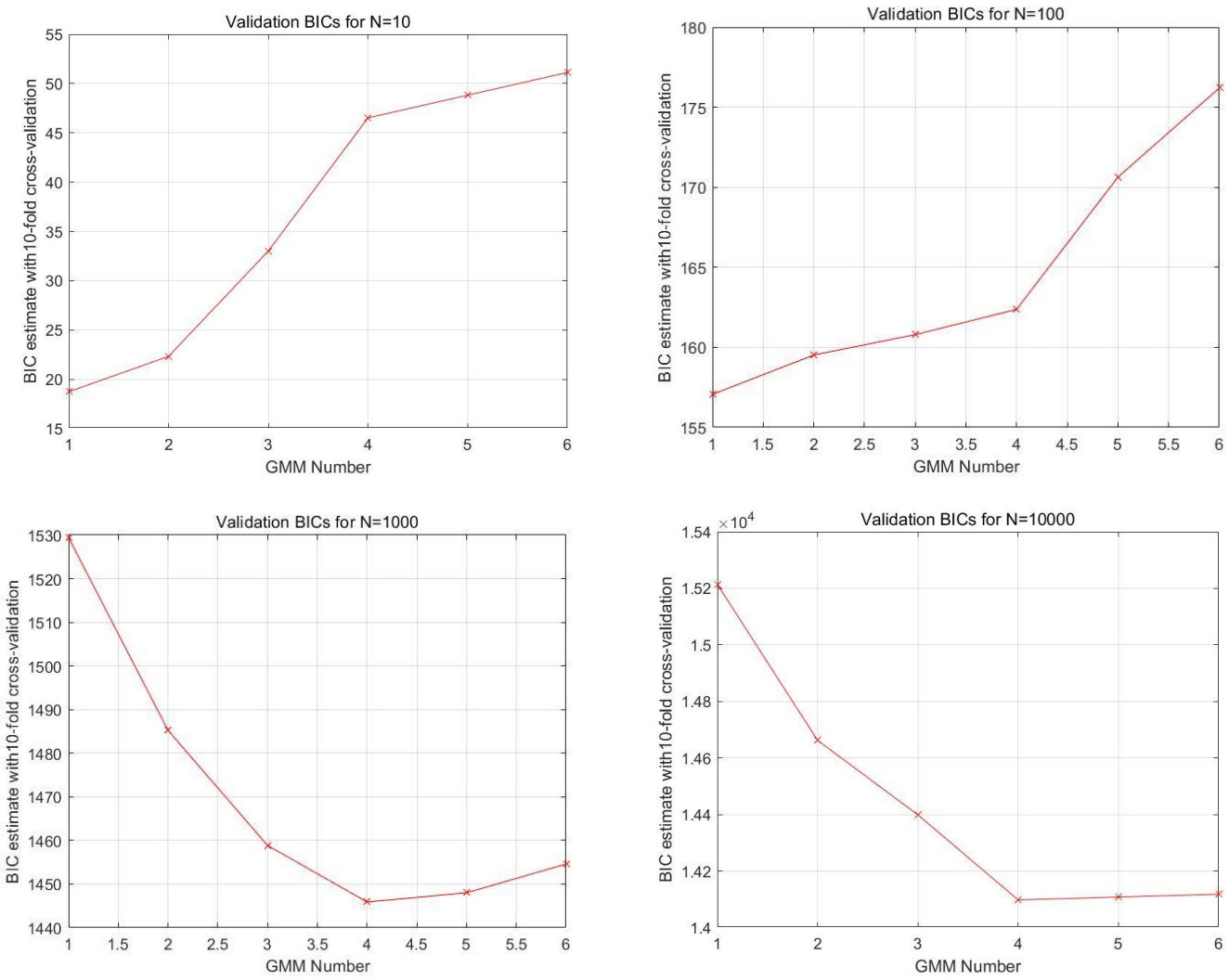


Figure 11: Validation BICs for all datasets

4. I am not able to get the algorithm converging in all cases, despite adding Gaussian noise to the training set, re-initializing mu values multiple times throughout, or adjusting the original distribution itself. Therefore, the algorithm has be limited for each combination of parameters. This does not provide a solution for the convergence issue, but there still some data to show the performance of the algorithm.
   Though we expect that the model order of 4 gets selected higher number of times as data increases, it does not seem to be happening in this case. possible reason could be that since we are using bootstrapping, the training sets thus generated might not have covered data such that it can capture the variation. Or secondly, the results could also depend on the size of training and validations sets generated. In order to check if the correct model order is selected for more data or if it also depends on the size of training and validation set, the following table is plotted.
   Figure 12 below shows the results of running the algorithm for the first experiment and keeping track of when each component number was selected as the winner for the tenth and twentieth experiment(figure13 and figure 14) and the result after all 30 experiments(figure15).

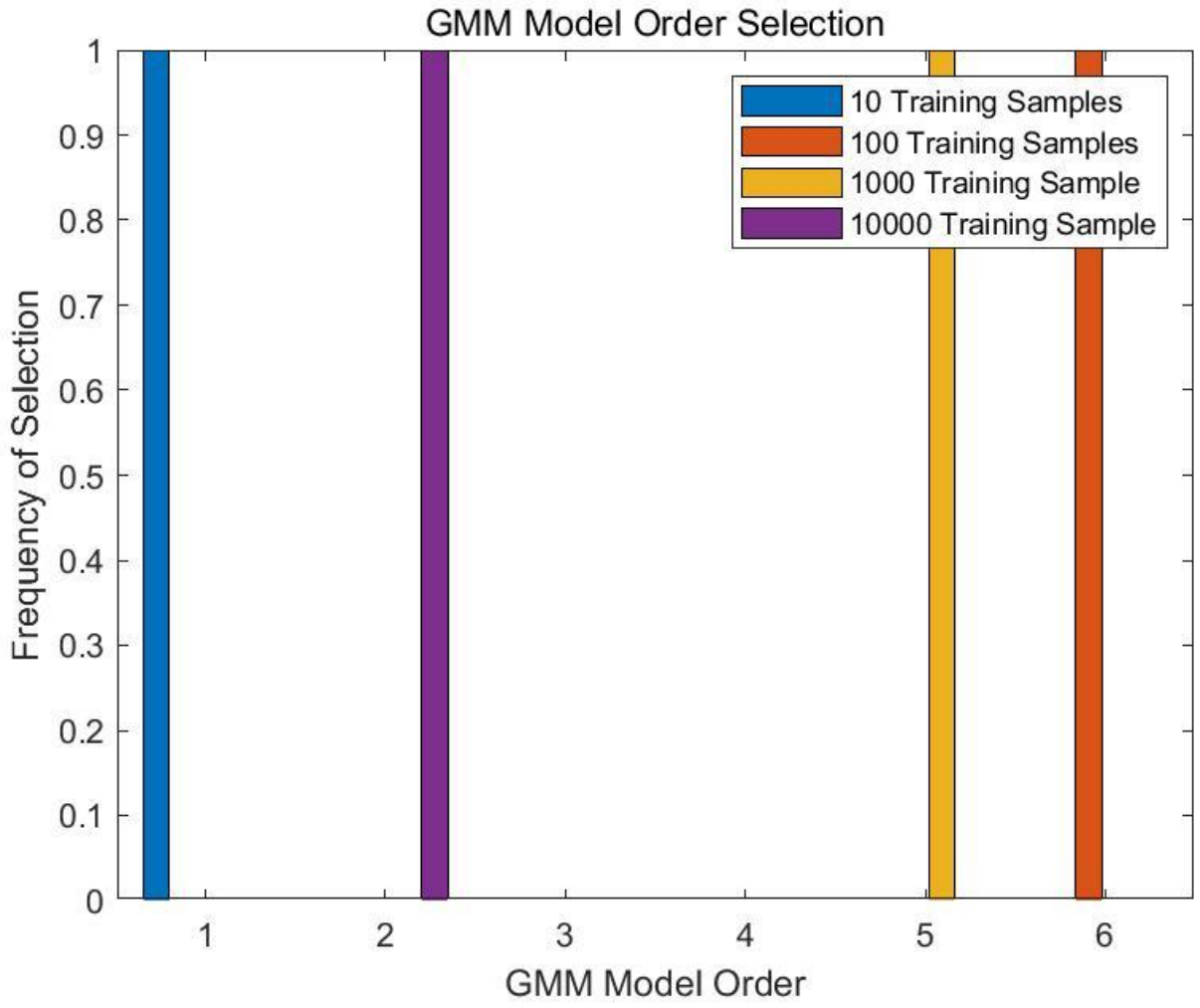


Figure 12: GMM Component Selection for 1st experiment

As shown in the figure12, when only 10 data points were used to form the training data set, most of the iterations ended with lower-valued component numbers being selected (2 component GMMs). This makes sense since the 10 points would be very spread out and it would be difficult to form as many as 6 groups based on just those 10 points. With 100 and 1000 sample data sets, however, the distribution was normal-shaped, with the center (winner in most iterations) being a 4-component GMM. This shows that with more points at disposal to form the training set, the algorithm can pick the correct component number more often.

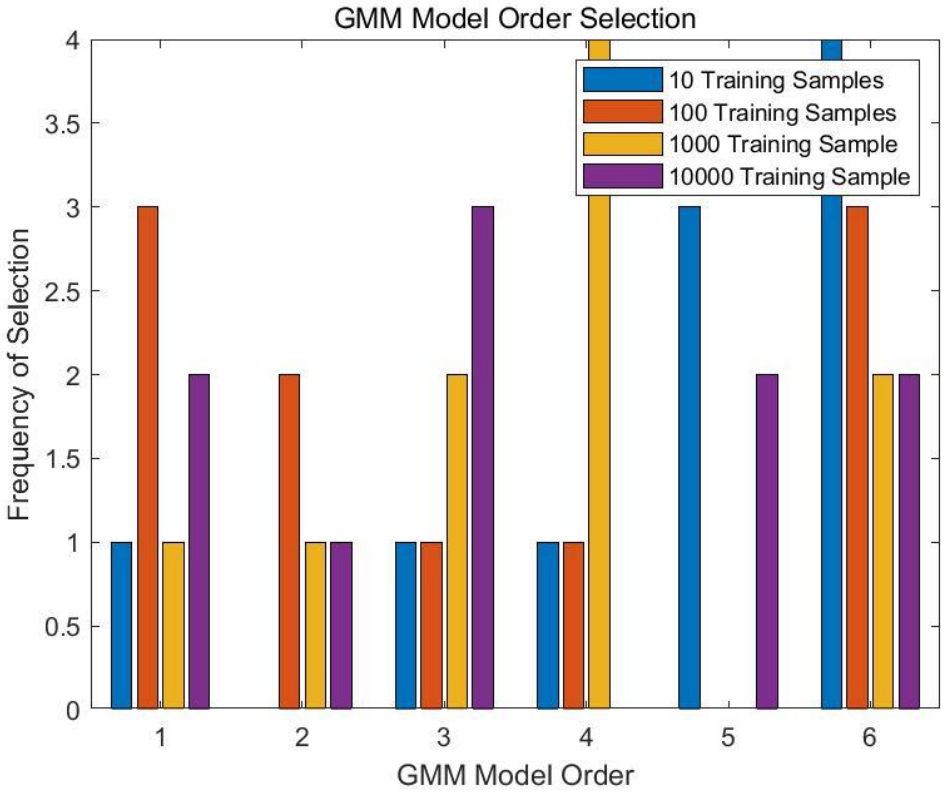


Figure 13: GMM Component Selection for 10th experiment

Table 2: Rate of order selection for 10th experiment

	1	2	3	4	5	6
10	10.00%	0.00%	10.00%	10.00%	30.00%	40.00%
100	30.00%	20.00%	10.00%	10.00%	0.00%	30.00%
1000	10.00%	10.00%	20.00%	40.00%	0.00%	20.00%
10k	20.00%	10.00%	30.00%	0.00%	20.00%	20.00%

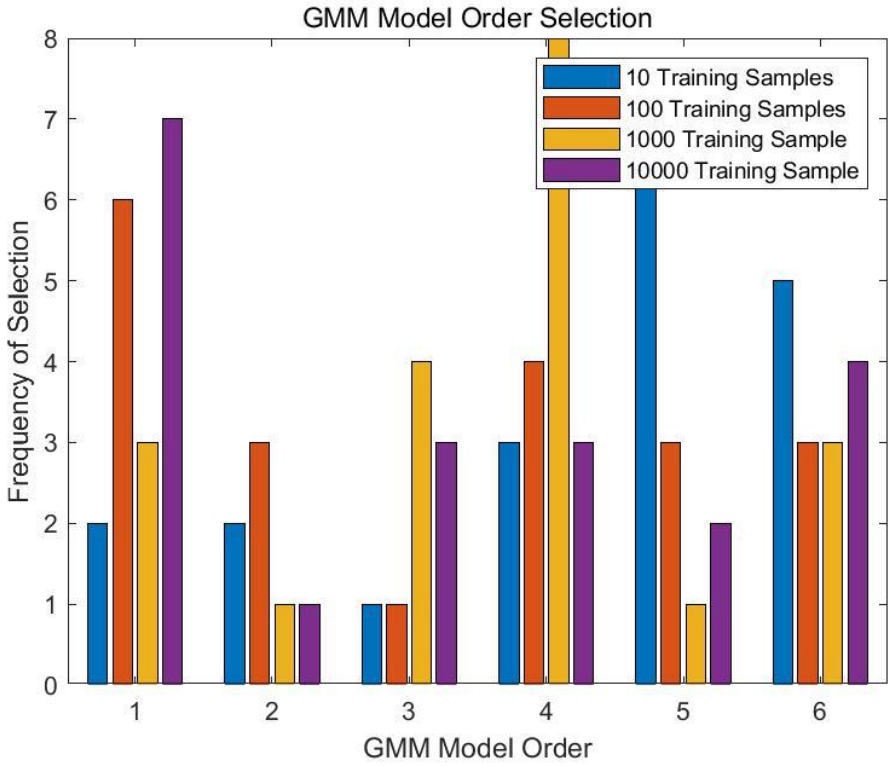


Figure 14: GMM Component Selection for 20th experiment

Table 2: Rate of order selection for 20th experiment

	1	2	3	4	5	6
10	10.00%	10.00%	5.00%	15.00%	35.00%	25.00%
100	30.00%	15.00%	5.00%	20.00%	15.00%	15.00%
1000	15.00%	5.00%	20.00%	40.00%	5.00%	15.00%
10k	35.00%	5.00%	15.00%	15.00%	10.00%	20.00%

From the above figures and tables it can be noticed that though there is not necessarily a pattern with increase in size of training/validations sets, there is a clear pattern with an increase in size of actual data from which we generate training/validation sets. This is as we expected - as the data increases, the estimation gets better and the frequency of correct model order selection increases.

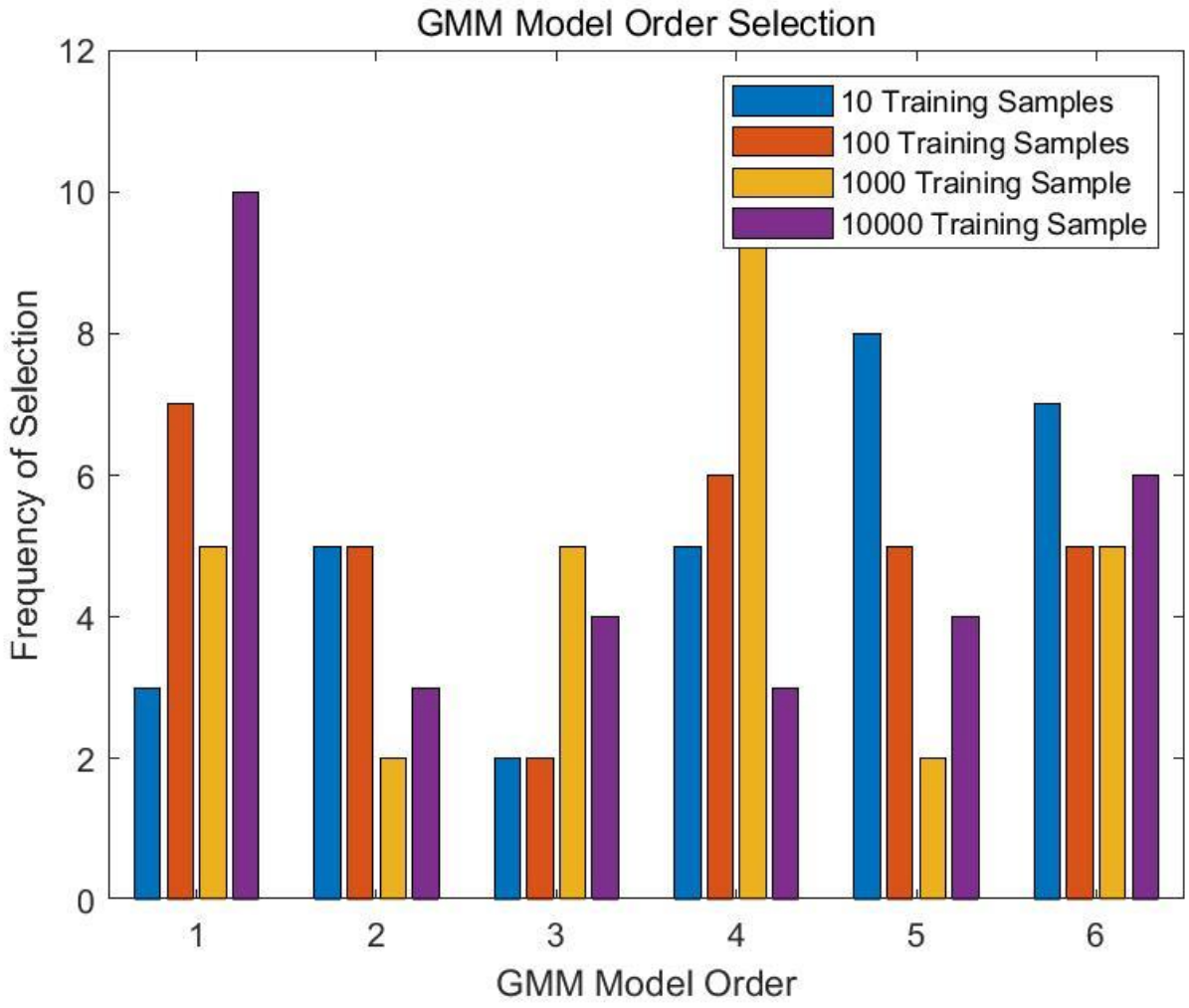


Figure 15: GMM Component Selection after 30 experiments

Table 2: Rate of order selection

	1	2	3	4	5	6
10	10.00%	16.67%	6.67%	16.67%	26.67%	23.33%
100	23.33%	16.67%	6.67%	20.00%	16.67%	16.67%
1000	16.67%	6.67%	16.67%	36.67%	6.67%	16.67%
10k	33.33%	10.00%	13.33%	10.00%	13.33%	20.00%

For the built-in MATLAB function, for each iteration of the EM algorithm, two things had to be provided the training set, and the number of components. The function then fits a Gaussian mixture with the selected number of components to the training data using the EM algorithm and reports back on the α, μ and Σ values for the distributions. When using the built-in function, to ensure the parameters are not constrained in any way, covariance did not be selected to be diagonal or shared between the distributions (covariance remained independent and full for each component within a GMM). I also chose to add a small regularization term (1^{-10}) to ensure that all covariance matrices are positive-definite as the algorithm is being executed.

Figure 15 upon summarizes the results of running the EM algorithm for 30 experiments. Table 2 shows the rate of order selection. As can be observed, when 10 data points were used to form the

full dataset, the algorithm seemed to favor the higher components GMM. When 100 data points were used to form the full dataset, the algorithm seemed to even out. when 1000 and 10k data points were used to form the full dataset, the algorithm seemed to favor the higher components GMM too, especially for 4-components. This may due to the original 4 components of the true GMM has more close prior value and the center of the mixture model is less overlap. Since MATLAB does not make their function files public, it’s different to look through what makes MATLAB'S implementation and the EM algorithm and the one we discussed in class different. However, the non-built-in function from the previous part seems to have a better performance with the same problem better since it was able to pick the true component number more times.

\

Appendix code for Question 1

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%EECE5644 Fall 2021
% Wang Yinan 001530926 | HW3
%%=========================Question 1=========================%%
% Code help and example from Prof.Deniz
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
clear all;close all;clc;

%%=========================Setup=========================%%
dimensions=3; %Dimension of data
numLabels=4;
Lx={'L0','L1','L2','L3'};
% For min-Perror design, use 0-1 loss
lossMatrix = ones(numLabels,numLabels)-eye(numLabels);
muScale=2.6;
SigmaScale=0.2;
%Define data
D.d100.N=100;
D.d200.N=200;
D.d500.N=500;
D.d1k.N=1e3;
D.d2k.N=2e3;
D.d5k.N=5e3;
D.d100k.N=100e3;
dTypes=fieldnames(D);
%Define Statistics
p=ones(1,numLabels)/numLabels; %Prior
%Label data stats
mu.L0=muScale*[1 1 0]';
RandSig=SigmaScale*rand(dimensions,dimensions);
Sigma.L0(:,:,1)=RandSig*RandSig'+eye(dimensions);
mu.L1=muScale*[1 0 0]';
RandSig=SigmaScale*rand(dimensions,dimensions);
Sigma.L1(:,:,1)=RandSig*RandSig'+eye(dimensions);
mu.L2=muScale*[0 1 0]';
RandSig=SigmaScale*rand(dimensions,dimensions);
Sigma.L2(:,:,1)=RandSig*RandSig'+eye(dimensions);
mu.L3=muScale*[0 0 1]';
RandSig=SigmaScale*rand(dimensions,dimensions);
Sigma.L3(:,:,1)=RandSig*RandSig'+eye(dimensions);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%Generate Data
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
for ind=1:length(dTypes)
    D.(dTypes{ind}).x=zeros(dimensions,D.(dTypes{ind}).N); %Initialize Data
        [D.(dTypes{ind}).x,D.(dTypes{ind}).labels,...
        D.(dTypes{ind}).N_l,D.(dTypes{ind}).p_hat]=...
```

```
        genData(D.(dTypes{ind}).N,p,mu,Sigma,Lx,dimensions);
end
%Plot Training Data
figure;
for ind=1:length(dTypes)-1
    subplot(3,2,ind);
    plotData(D.(dTypes{ind}).x,D.(dTypes{ind}).labels,Lx);
    title([dTypes{ind}]);
    legend 'show';
end

%Plot Validation Data
figure;
plotData(D.(dTypes{ind}).x,D.(dTypes{ind}).labels,Lx);
legend 'show';
title([dTypes{end}]);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%Determine Theoretically Optimal Classifier
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
for ind=1:length(dTypes)
    [D.(dTypes{ind}).opt.PFE, D.(dTypes{ind}).opt.decisions]=...
        optClass(lossMatrix,D.(dTypes{ind}).x,mu,Sigma,...
        p,D.(dTypes{ind}).labels,Lx,dTypes{ind});
    opPFE(ind)=D.(dTypes{ind}).opt.PFE;
    fprintf('Optimal pFE, N=%1.0f: Error=%1.2f%%\n',...
        D.(dTypes{ind}).N,100*D.(dTypes{ind}).opt.PFE);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%Train and Validate Data
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
numPerc=15; %Max number of perceptrons to attempt to train
k=10; %number of folds for kfold validation
for ind=1:length(dTypes)-1
    %kfold validation is in this function
    [D.(dTypes{ind}).net,D.(dTypes{ind}).minPFE,...
        D.(dTypes{ind}).optM,valData.(dTypes{ind}).stats]=...
        kfoldMLP_NN(numPerc,k,D.(dTypes{ind}).x,...
        D.(dTypes{ind}).labels,numLabels);
    %Produce validation data from test dataset
    valData.(dTypes{ind}).yVal=D.(dTypes{ind}).net(D.d100k.x);
    [~,valData.(dTypes{ind}).decisions]=max(valData.(dTypes{ind}).yVal);
    valData.(dTypes{ind}).decisions=valData.(dTypes{ind}).decisions-1;
    %Probability of Error is wrong decisions/num data points
    valData.(dTypes{ind}).pFE=...
        sum(valData.(dTypes{ind}).decisions~=D.d100k.labels)/D.d100k.N;
    outpFE(ind,1)=D.(dTypes{ind}).N;
    outpFE(ind,2)=valData.(dTypes{ind}).pFE;
    outpFE(ind,3)=D.(dTypes{ind}).optM;
```

```
    fprintf('NN pFE, N=%1.0f: Error=%1.2f%%\n',...
        D.(dTypes{ind}).N,100*valData.(dTypes{ind}).pFE);
end

%This code was used to plot the results from the data generated in the main
%function
%Extract cross validation results from structure
for ind=1:length(dTypes)-1
    [~,select]=min(valData.(dTypes{ind}).stats.mPFE);
    M(ind)=(valData.(dTypes{ind}).stats.M(select));
    N(ind)=D.(dTypes{ind}).N;
end
%Plot number of perceptrons vs. pFE for the cross validation runs
for ind=1:length(dTypes)-1
    figure;
    stem(valData.(dTypes{ind}).stats.M,valData.(dTypes{ind}).stats.mPFE);
    xlabel('Number of Perceptrons');
    ylabel('pFE');
    title(['Probability of Error vs. Number of Perceptrons for ' dTypes{ind}]);
end
%Number of perceptrons vs. size of training dataset
figure,semilogx(N(1:end-1),M(1:end-1),'o','LineWidth',2)
grid on;
xlabel('Number of Data Points')
ylabel('Optimal Number of Perceptrons')
ylim([0 10]);
xlim([50 10^4]);
title('Optimal Number of Perceptrons vs. Number of Data Points');
%Prob. of Error vs. size of training data set
figure,semilogx(outpFE(1:end-1,1),outpFE(1:end-1,2),'o','LineWidth',2)
xlim([90 10^4]);
hold all;semilogx(xlim,[opPFE(end) opPFE(end)],'r--','LineWidth',2)
legend('NN pFE','Optimal pFE')
grid on
xlabel('Number of Data Points')
ylabel('pFE')
title('Probability of Error vs. Data Points in Training Data');
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [x,labels,N_l,p_hat]= genData(N,p,mu,Sigma,Lx,d)
%Generates data and labels for random variable x from multiple gaussian
%distributions
numD = length(Lx);
cum_p = [0,cumsum(p)];
u = rand(1,N);
x = zeros(d,N);
labels = zeros(1,N);
for ind=1:numD
    pts = find(cum_p(ind)<u & u<=cum_p(ind+1));
    N_l(ind)=length(pts);
```

```
    x(:,pts) = mvnrnd(mu.(Lx{ind}),Sigma.(Lx{ind}),N_l(ind))';
    labels(pts)=ind-1;
    p_hat(ind)=N_l(ind)/N;
end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function plotData(x,labels,Lx)
%Plots data
for ind=1:length(Lx)
    pindex=labels==ind-1;
    plot3(x(1,pindex),x(2,pindex),x(3,pindex),'.','DisplayName',Lx{ind});
    hold all;
end
grid on;
xlabel('x1');
ylabel('x2');
zlabel('x3');
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function g = evalGaussian(x,mu,Sigma)
% Evaluates the Gaussian pdf N(mu,Sigma) at each coumn of X
[n,N] = size(x);
invSigma = inv(Sigma);
C = (2*pi)^(-n/2) * det(invSigma)^(1/2);
E = -0.5*sum((x-repmat(mu,1,N)).*(invSigma*(x-repmat(mu,1,N))),1);
g = C*exp(E);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [minPFE,decisions]=optClass(lossMatrix,x,mu,Sigma,p,labels,Lx,dTypesind)
% Determine optimal probability of error
symbols='ox+*v';
numLabels=length(Lx);
N=length(x);
for ind = 1:numLabels
    pxgivenl(ind,:) =...
        evalGaussian(x,mu.(Lx{ind}),Sigma.(Lx{ind})); % Evaluate p(x|L=l)
end
px = p*pxgivenl; % Total probability theorem
classPosteriors = pxgivenl.*repmat(p',1,N)./repmat(px,numLabels,1); % P(L=l|x)
% Expected Risk for each label (rows) for each sample (columns)
expectedRisks =lossMatrix*classPosteriors;
% Minimum expected risk decision with 0-1 loss is the same as MAP
[~,decisions] = min(expectedRisks,[],1);
decisions=decisions-1; %Adjust to account for L0 label
fDecision_ind=(decisions~=labels);%Incorrect classificiation vector
minPFE=sum(fDecision_ind)/N;
%Plot Decisions with Incorrect Results
figure;
for ind=1:numLabels
```

```
    class_ind=decisions==ind-1;
    plot3(x(1,class_ind & ~fDecision_ind),...
        x(2,class_ind & ~fDecision_ind),...
        x(3,class_ind & ~fDecision_ind),...
        symbols(ind),'Color',[0.39 0.83 0.07],'DisplayName',...
        ['Class ' num2str(ind) ' Correct Classification']);
    hold on;
    plot3(x(1,class_ind & fDecision_ind),...
        x(2,class_ind & fDecision_ind),...
        x(3,class_ind & fDecision_ind),...
        ['r' symbols(ind)],'DisplayName',...
        ['Class ' num2str(ind) ' Incorrect Classification']);
    hold on;
end
xlabel('x1');
ylabel('x2');
grid on;
title(['X Vector with Incorrect Classifications for ' dTypesind]);
legend 'show';
if 0
%Plot Decisions with Incorrect Decisions
    figure;
    for ind2=1:numLabels
        subplot(3,2,ind2);
        for ind=1:numLabels
            class_ind=decisions==ind-1;
            plot3(x(1,class_ind),x(2,class_ind),x(3,class_ind),...
            '.','DisplayName',['Class ' num2str(ind)]);
            hold on;
        end
        plot3(x(1,fDecision_ind & labels==ind2),...
        x(2,fDecision_ind & labels==ind2),...
        x(3,fDecision_ind & labels==ind2),...
        'kx','DisplayName','Incorrectly Classified','LineWidth',2);
        ylabel('x2');
        grid on;
        title(['X Vector with Incorrect Decisions for Class ' num2str(ind2) ...
            'for ' dTypesind]);
        if ind2==1
            legend 'show';
        elseif ind2==4
            xlabel('x1');
        end
    end
end

end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%This function performs the cross validation and model selection
```

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [outputNet,outputPFE, optM, stats]=kfoldMLP_NN(numPerc,k,x,labels,numLabels)
%Assumes data is evenly divisible by partition choice which it should be
N=length(x);
numValIters=10;
%Create output matrices from labels
y=zeros(numLabels,length(x));
for ind=1:numLabels
    y(ind,:)=(labels==ind-1);
end
%Setup cross validation on training data
partSize=N/k;
partInd=[1:partSize:N length(x)];
%Perform cross validation to select number of perceptrons
for M=1:numPerc
    for ind=1:k
        index.val=partInd(ind):partInd(ind+1);
        index.train=setdiff(1:N,index.val);
        %Create object with M perceptrons in hidden layer
        net=patternnet(M);
        % net.layers{1}.transferFcn = 'softplus';%didn't work
        %Train using training data
        net=train(net,x(:,index.train),y(:,index.train));
        %Validate with remaining data
        yVal=net(x(:,index.val));
        [~,labelVal]=max(yVal);
        labelVal=labelVal-1;
        pFE(ind)=sum(labelVal~=labels(index.val))/partSize;
    end
    %Determine average probability of error for a number of perceptrons
    avgPFE(M)=mean(pFE);
    stats.M=1:M;
    stats.mPFE=avgPFE;
end
%Determine optimal number of perceptrons
[~,optM]=min(avgPFE);
%Train one final time on all the data
for ind=1:numValIters
    netName(ind)={['net' num2str(ind)]};
    finalnet.(netName{ind})=patternnet(optM);
    % finalnet.layers{1}.transferFcn = 'softplus';%Set to RELU
    finalnet.(netName{ind})=train(net,x,y);
    yVal=finalnet.(netName{ind})(x);
    [~,labelVal]=max(yVal);
    labelVal=labelVal-1;
    pFEFinal(ind)=sum(labelVal~=labels)/length(x);
end
[minPFE,outInd]=min(pFEFinal);
stats.finalPFE=pFEFinal;
```

```
outputPFE=minPFE;
outputNet=finalnet.(netName{outInd});
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

Appendix code for Question 2

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%EECE5644 Fall 2021
% Wang Yinan 001530926 | HW3
%%=========================Question 2=========================%%
% Code help and example from Prof.Deniz
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
clear all;close all;clc;

% variance
n=2;
alpha_true=[0.20,0.30,0.23,0.27];
% mu_true=[10 -10 -10 10;-10 10 -10 10];
mu_true(:,1) = [10;-10];
mu_true(:,2) = [-10;10];
mu_true(:,3) = [-10;-10];
mu_true(:,4) = [10;10];
Sigma_true(:,:,1) = [15 1;1 15];
Sigma_true(:,:,2) = [17 3;3 17];
Sigma_true(:,:,3) = [19 5;5 19];
Sigma_true(:,:,4) = [21 7;7 21];

% Number of samples
N=[10,100,1000,10000];

% ensure the program is not stuck
countN = 0;

num_GMM_picks = zeros(length(N),6);
num_GMM_cmp = zeros(length(N),6);

% multi experiments
for a=1:30
    for i=1:length(N)
        [x,label]=generate_samples(N(i),mu_true,Sigma_true,alpha_true);
        GMM_pick=cross_val(x);
        num_GMM_picks(i,GMM_pick)=num_GMM_picks(i,GMM_pick)+1;
    end
    if ~isequal(num_GMM_cmp, num_GMM_picks)
        figure,
        bar(num_GMM_picks');
        legend('10 Training Samples','100 Training Samples', ...
            '1000 Training Sample','10000 Training Sample');
        title('GMM Model Order Selection');
        xlabel('GMM Model Order');ylabel('Frequency of Selection');
        saveas(gcf,['./Q2figs/4-',int2str(a),'.jpg']);
        num_GMM_cmp=num_GMM_picks;
    end
```

```
end


for i=1:length(N)
    countN = countN+1
    % Create appropriate number of data points from each distribution
    [x,label]=generate_samples(N(i),mu_true,Sigma_true,alpha_true);

    % plot
    figure(i);
    scatter(x(1,label==1),x(2,label==1),'r','filled');
    hold on
    scatter(x(1,label==2),x(2,label==2),'g','filled');
    hold on
    scatter(x(1,label==3),x(2,label==3),'b','filled');
    hold on
    scatter(x(1,label==4),x(2,label==4),'m','filled');
    title(strcat('Data with N=',num2str(N(i))));
    xlabel('x_1'),ylabel('x_2')
    saveas(gcf,['./Q2figs/',int2str(i),'.jpg']);

    GMM_pick=cross_val(x);
    num_GMM_picks(i,GMM_pick)=num_GMM_picks(i,GMM_pick)+1;

    %Tolerance for EM stopping criterion
    delta = 1e-4;
    %Regularization parameter for covariance estimates
    regWeight = 1e-10;
    %K-Fold Cross Validation
    K = 10;

    %To determine dimensionality of samples and number of GMM components
    [d,MM] = size(mu_true);

    %Divide the data set into 10 approximately-equal-sized partitions
    dummy = ceil(linspace(0,N(i),K+1));
    for k = 1:K
        indPartitionLimits(k,:) = [dummy(k)+1,dummy(k+1)];
    end
    %Allocate space
    loglikelihoodtrain = zeros(K,6); loglikelihoodvalidate = zeros(K,6);
    Averagelltrain = zeros(1,6); Averagellvalidate = zeros(1,6);

    countM = 0;
    %Try all 6 mixture options
    for M = 1:6

        countM = countM+1
        countk = 0;
```

```
%10-fold cross validation
for k = 1:K
    countk = countk+1
    indValidate = [indPartitionLimits(k,1):indPartitionLimits(k,2)];
    %Using folk k as validation set
    x1Validate = x(1,indValidate);
    x2Validate = x(2,indValidate);
    if k == 1
        indTrain = [indPartitionLimits(k,2)+1:N(i)];
    elseif k == K
        indTrain = [1:indPartitionLimits(k,1)-1];
    else
        indTrain = [1:indPartitionLimits(k-1,2),indPartitionLimits(k+1,2):N(i)];
    end

    %Using all other folds as training set
    x1Train = x(1,indTrain);
    x2Train = x(2,indTrain);
    xTrain = [x1Train; x2Train];
    xValidate = [x1Validate; x2Validate];
    Ntrain = length(indTrain); Nvalidate = length(indValidate);

    %Train model parameters (EM)
    %Initialize the GMM to randomly selected samples
    alpha = ones(1,M)/M;
    shuffledIndices = randperm(Ntrain);
    %Pick M random samples as initial mean estimates (this led
    %to good initial estimates (better log likelihoods))
    mu = xTrain(:,shuffledIndices(1:M));
    %Assign each sample to the nearest mean (better initialization)
    [~,assignedCentroidLabels] = min(pdist2(mu',xTrain'),[],1);
    %Use sample covariances of initial assignments as initial covariance estimates
    for m = 1:M
        Sigma(:,:,m) = cov(xTrain(:,find(assignedCentroidLabels==m))') + regWeight*eye(d,d);
    end
    t = 0;

    %Not converged at the beginning
    Converged = 0;

    while ~Converged
        for l = 1:M
            temp(l,:) = repmat(alpha(l),1,Ntrain).*evalGaussian(xTrain,mu(:,l),Sigma(:,:,l));
        end
        plgivenx = temp./sum(temp,1);
        clear temp
        alphaNew = mean(plgivenx,2);
        w = plgivenx./repmat(sum(plgivenx,2),1,Ntrain);
```

```
                muNew = xTrain*w';
                for l = 1:M
                    v = xTrain-repmat(muNew(:,l),1,Ntrain);
                    u = repmat(w(l,:),d,1).*v;
                    %Adding a small regularization term
                    SigmaNew(:,:,l) = u*v' + regWeight*eye(d,d);
                end
                Dalpha = sum(abs(alphaNew-alpha));
                Dmu = sum(sum(abs(muNew-mu)));
                DSigma = sum(sum(abs(abs(SigmaNew-Sigma))));
                %Check if converged
                Converged = ((Dalpha+Dmu+DSigma)<delta);
                alpha = alphaNew; mu = muNew; Sigma = SigmaNew;
                t = t+1;
            end
            %Validation
            loglikelihoodtrain(k,M) = sum(log(evalGMM(xTrain,alpha,mu,Sigma)));
            loglikelihoodvalidate(k,M) = sum(log(evalGMM(xValidate,alpha,mu,Sigma)));

        end

        %Average Performance Variables
        Averagelltrain(1,M) = mean(loglikelihoodtrain(:,M));
        BICtrain(1,M) = -2*Averagelltrain(1,M)+M*log(N(i));
        Averagellvalidate(1,M) = mean(loglikelihoodvalidate(:,M));
        %Sometimes the log likelihoods for N=10 are zero, leading to
        %negative infinity results. I assume that this is instead the
        %lowest log likelihood value instead (so it is possible to graph).
        if isinf(Averagellvalidate(1,M))
            Averagellvalidate(1,M) = (min(Averagellvalidate(find(isfinite(Averagellvalidate)))));
        end
        BICvalidate(1,M) = -2*Averagellvalidate(1,M)+M*log(N(i));
        %Recording values
        TotBICValidate(i,M) = BICvalidate(1,M);
        TotBICTrain(i,M) = BICtrain(1,M);
        TotAvgllValidate(i,M) = Averagellvalidate(1,M);
        TotAvgllTrain(i,M) = Averagelltrain(1,M);
    end
    %Recording Best Outcomes
    [LowestBIC orderB] = min(BICvalidate)
    [Lowestll orderl] = max(Averagellvalidate)

    % training log-likelihood
    figure(i+4), clf,
    plot(Averagelltrain,'.b');
    hold on;
    plot(Averagelltrain,'-b');
    xlabel('GMM Number'); ylabel(strcat('Log likelihood estimate with ',num2str(K),'-fold cross-
validation'));
```

```
    title(strcat('Training Log-Likelihoods for N=',num2str(N(i))));
    grid on
    xticks(1:1:6)
    saveas(gcf,['./Q2figs/',int2str(i+4),'.jpg']);

    % validation log-likelihood
    figure(i+8), clf,
    plot(Averagellvalidate,'rx');
    hold on;
    plot(Averagellvalidate,'r-');
    xlabel('GMM Number'); ylabel(strcat('Log likelihood estimate with ',num2str(K),'-fold cross-
validation'));
    title(strcat('Validation Log-Likelihoods for N=',num2str(N(i))));
    grid on
    xticks(1:1:6)
    saveas(gcf,['./Q2figs/',int2str(i+8),'.jpg']);

    % training BIC
    figure(i+12), clf,
    plot(BICtrain,'.b');
    hold on;
    plot(BICtrain,'-b');
    xlabel('GMM Number'); ylabel(strcat('BIC estimate with ',num2str(K),'-fold cross-validation'));
    title(strcat('Training BICs for N=',num2str(N(i))));
    grid on
    xticks(1:1:6)
    saveas(gcf,['./Q2figs/',int2str(i+12),'.jpg']);

    % validation BIC
    figure(i+16), clf,
    plot(BICvalidate,'rx');
    hold on;
    plot(BICvalidate,'r-');
    xlabel('GMM Number'); ylabel(strcat('BIC estimate with ',num2str(K),'-fold cross-validation'));
    title(strcat('Validation BICs for N=',num2str(N(i))))
    grid on
    xticks(1:1:6)
    saveas(gcf,['./Q2figs/',int2str(i+16),'.jpg']);

    %Saving values
    BICorder(i) = orderB;
    BIClow(i) = LowestBIC;
    lorder(i) = orderl;
    lllow(i) = Lowestll;
end


%%=========================Question 2 Functions=========================%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

```
% Functions credit to Prof.Deniz
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function x = randGMM(N,alpha,mu,Sigma)
d = size(mu,1); % dimensionality of samples
cum_alpha = [0,cumsum(alpha)];
u = rand(1,N); x = zeros(d,N); labels = zeros(1,N);
for m = 1:length(alpha)
    ind = find(cum_alpha(m)<u & u<=cum_alpha(m+1));
    x(:,ind) = randGaussian(length(ind),mu(:,m),Sigma(:,:,m));
end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function x = randGaussian(N,mu,Sigma)
% Generates N samples from a Gaussian pdf with mean mu covariance Sigma
n = length(mu);
z =  randn(n,N);
A = Sigma^(1/2);
x = A*z + repmat(mu,1,N);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function gmm = evalGMM(x,alpha,mu,Sigma)
gmm = zeros(1,size(x,2));
for m = 1:length(alpha) % evaluate the GMM on the grid
    gmm = gmm + alpha(m)*evalGaussian(x,mu(:,m),Sigma(:,:,m));
end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function g = evalGaussian(x,mu,Sigma)
% Evaluates the Gaussian pdf N(mu,Sigma) at each column of X
[n,N] = size(x);
invSigma = inv(Sigma);
C = (2*pi)^(-n/2) * det(invSigma)^(1/2);
E = -0.5*sum((x-repmat(mu,1,N)).*(invSigma*(x-repmat(mu,1,N))),1);
g = C*exp(E);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function best_GMM=cross_val(x)
%PerformsEMalgorithmtoestimateparametersandevalueteperformance
%oneachdatasetBtimes,with1throughMGMMmodelsconsidered
B=10;M=6;%repetitionsperdataset;maxGMMconsidered
perf_array=zeros(B,M);%savespaceforperformanceevaluation
%Testeachdataset10times
for b=1:B
    %Pickrandomdatapointstofilltrainingandvalidationsetand
    %addnoise
    set_size=500;
    train_index=randi([1,length(x)],[1,set_size]);
    train_set=x(:,train_index)+(1e-3)*randn(2,set_size);
    val_index=randi([1,length(x)],[1,set_size]);
```

```
    val_set=x(:,val_index)+(1e-3)*randn(2,set_size);
    for m=1:M
        %Non?Built?In:runEMalgorithtoestimateparameters
        %[alpha,mu,sigma]=EMforGMM(m,trainset,setsize,valset);
        %Built?Infunction:runEMalgorithmtoestimateparameters
        GMModel=fitgmdist(train_set',M,'RegularizationValue',1e-10);
        alpha=GMModel.ComponentProportion;
        mu=(GMModel.mu)';
        sigma=GMModel.Sigma;
        %Calculatelog?likelihoodperformancewithnewparameters
        perf_array(b,m)=sum(log(evalGMM(val_set,alpha,mu,sigma)));
    end
end
% Ca l cul a t e average per formance f o r each M and f i n d be s t f i t
avg_perf=sum(perf_array)/B;
best_GMM=find(avg_perf==max(avg_perf),1);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [x,label]=generate_samples(N,mu_true,Sigma_true,alpha_true)
% Create appropriate number of data points from each distribution
x=zeros(2,N);
label=zeros(1,N);
for j=1:N
    r=rand(1);
    if r <= alpha_true(1)
        label(j)=1;
    elseif (alpha_true(1)<r)&&(r<=sum(alpha_true(1:2)))
        label(j)=2;
    elseif (sum(alpha_true(1:2))<r)&&(r<=sum(alpha_true(1:3)))
        label(j)=3;
    else
        label(j)=4;
    end
end
Nc=[sum(label==1),sum(label==2),sum(label==3),sum(label==4)];
%{
% when the samples' num is small(like 10)
% there could be non-generated class
if ismember(0,Nc)
    % find non-generated class
    a=find(Nc==0);
    % add 1
    Nc(a)=1;
    % which class's num is the max
    b=find(Nc==max(Nc));
    % minus 1 to keep the total nums
    Nc(b)=Nc(b)-1;
    % find the max-class position in label
    c=find(label==b);
```

```
    % change the first position to non-generated class
    label(c(1))=a;
end
%}
% Generate data
x(:,label==1)=randGaussian(Nc(1),mu_true(:,1),Sigma_true(:,:,1));
x(:,label==2)=randGaussian(Nc(2),mu_true(:,2),Sigma_true(:,:,2));
x(:,label==3)=randGaussian(Nc(3),mu_true(:,3),Sigma_true(:,:,3));
x(:,label==4)=randGaussian(Nc(4),mu_true(:,4),Sigma_true(:,:,4));
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```