

EECE 5644 Assignment3

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Question 1 (60%)

In this exercise, you will train many multilayer perceptrons (MLP) to approximate the class label posteriors, using maximum likelihood parameter estimation (equivalently, with minimum average cross-entropy loss) to train the MLP. Then, you will use the trained models to approximate a MAP classification rule in an attempt to achieve minimum probability of error (i.e. to minimize expected loss with 0-1 loss assignments to correct-incorrect decisions).

Data Distribution: For $C = 4$ classes with uniform priors, specify Gaussian class-conditional pdfs for a 3-dimensional real-valued random vector x (pick your own mean vectors and covariance matrices for each class). Try to adjust the parameters of the data distribution so that the MAP classifier that uses the true data pdf achieves between 10%–20% probability of error.

MLP Structure: Use a 2-layer MLP (one hidden layer of perceptrons) that has P perceptrons in the first (hidden) layer with smooth-ramp style activation functions (e.g., ISRU, Smooth-ReLU, ELU, etc). At the second/output layer use a softmax function to ensure all outputs are positive and add up to 1. The best number of perceptrons for your custom problem will be selected using cross-validation.

Generate Data: Using your specified data distribution, generate multiple datasets: Training datasets with 100,200,500,1000,2000,5000 samples and a test dataset with 100000 samples. You will use the test dataset only for performance evaluation.

Theoretically Optimal Classifier: Using the knowledge of your true data pdf, construct the minimum-probability-of-error classification rule, apply it on the test dataset, and empirically estimate the probability of error for this theoretically optimal classifier. This provides the aspirational performance level for the MLP classifier.

Model Order Selection: For each of the training sets with different number of samples, perform 10-fold cross-validation, using minimum classification error probability as the objective function, to select the best number of perceptrons (that is justified by

Model Training: For each training set, having identified the best number of perceptrons using cross-validation, using maximum likelihood parameter estimation (minimum cross-entropy loss) train an MLP using each training set with as many perceptrons as you have identified as optimal for that training set. These are your final trained MLP models for class posteriors (possibly each with different number of perceptrons and different weights). Make sure to mitigate the chances of getting stuck at a local optimum by randomly reinitializing each MLP training routine multiple times and getting the highest training-data log-likelihood solution you encounter.

Performance Assessment: Using each trained MLP as a model for class posteriors, and using the MAP decision rule (aiming to minimize the probability of error) classify the samples in the test set and for each trained MLP empirically estimate the probability of error.

Report Process and Results: Describe your process of developing the solution; numerically and visually report the test set empirical probability of error estimates for the theoretically optimal and multiple trained MLP classifiers. For instance show a plot of the empirically

estimated test P(error) for each trained MLP versus number of training samples used in optimizing it (with semilog-x axis), as well as a horizontal line that runs across the plot indicating the empirically estimated test P(error) for the theoretically optimal classifier.

Note: You may use software packages for all aspects of your implementation. Make sure you use tools correctly. Explain in your report how you ensured the software tools do exactly what you need them to do.

Answer:

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.

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

$$m_0 = \begin{bmatrix} 2.6 \\ 2.6 \\ 0 \end{bmatrix} \quad c_0 = \begin{bmatrix} 1.0630 & 0.0587 & 0.0184 \\ 0.0587 & 1.0608 & 0.0280 \\ 0.0184 & 0.0280 & 1.0377 \end{bmatrix}$$

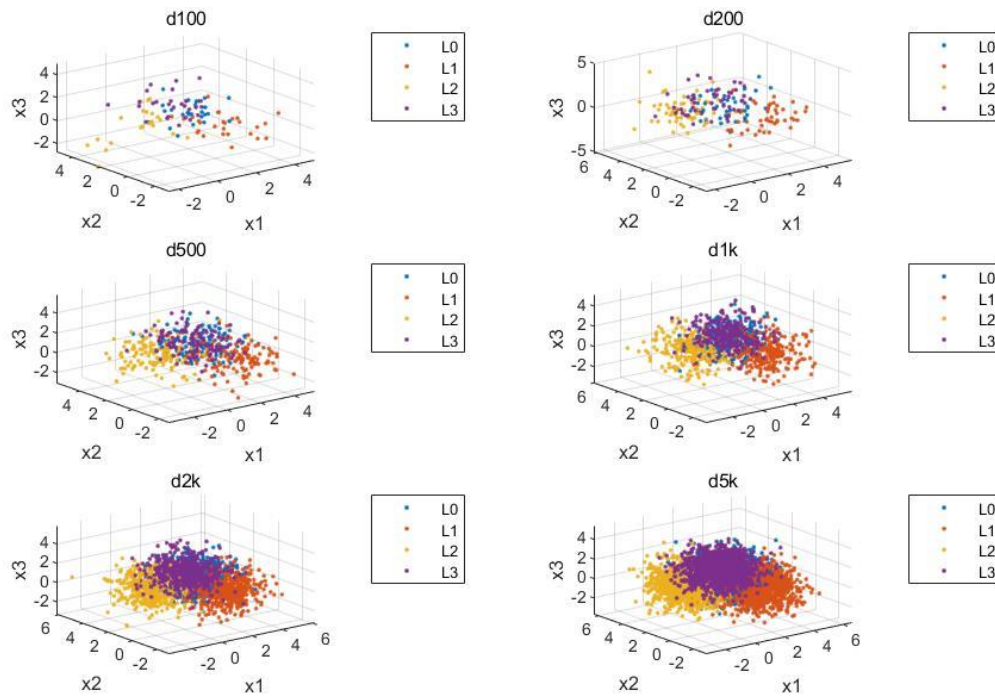
$$m_1 = \begin{bmatrix} 2.6 \\ 0 \\ 0 \end{bmatrix} \quad c_1 = \begin{bmatrix} 1.0747 & 0.0271 & 0.0733 \\ 0.0271 & 1.0175 & 0.0371 \\ 0.0733 & 0.0371 & 1.0968 \end{bmatrix}$$

$$m_2 = \begin{bmatrix} 0 \\ 2.6 \\ 0 \end{bmatrix} \quad c_2 = \begin{bmatrix} 1.0436 & 0.0522 & 0.0423 \\ 0.0522 & 1.0886 & 0.0794 \\ 0.0423 & 0.0794 & 1.0742 \end{bmatrix}$$

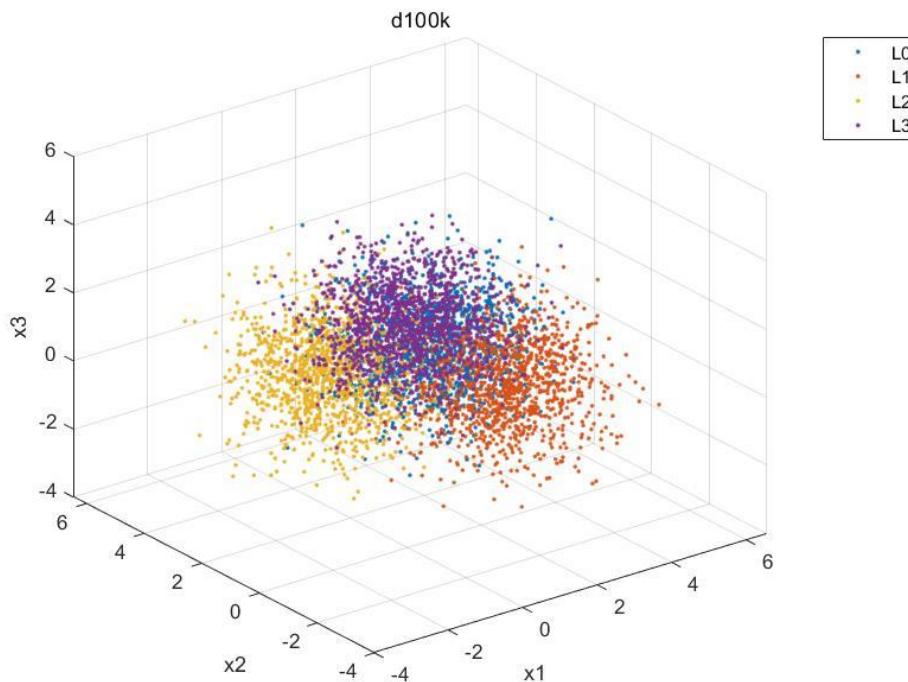
$$m_3 = \begin{bmatrix} 0 \\ 0 \\ 2.6 \end{bmatrix} \quad c_3 = \begin{bmatrix} 1.0262 & 0.0114 & 0.0120 \\ 0.0114 & 1.0176 & 0.0080 \\ 0.0120 & 0.0080 & 1.0314 \end{bmatrix}$$

A 2-layer MLP with one hidden and one output layer 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 my own), 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 training data are shown in the following graph.



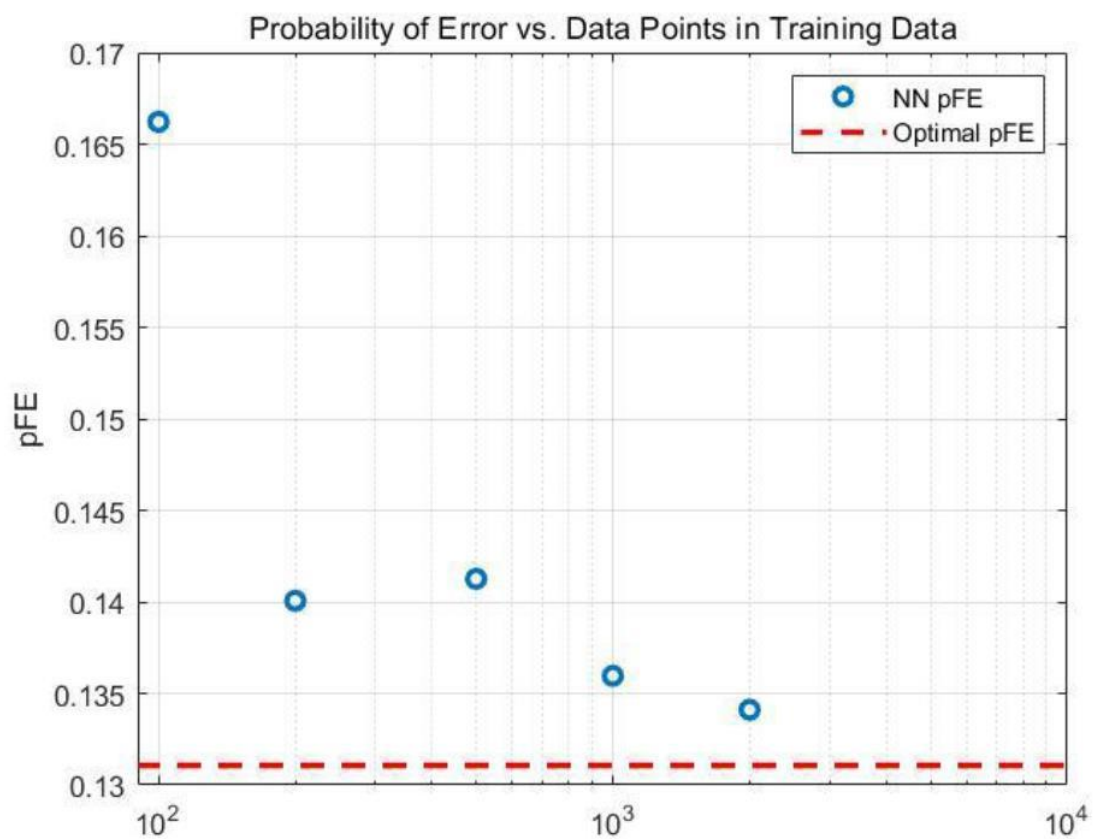
Plots of the generated validation data are shown in the following graph.



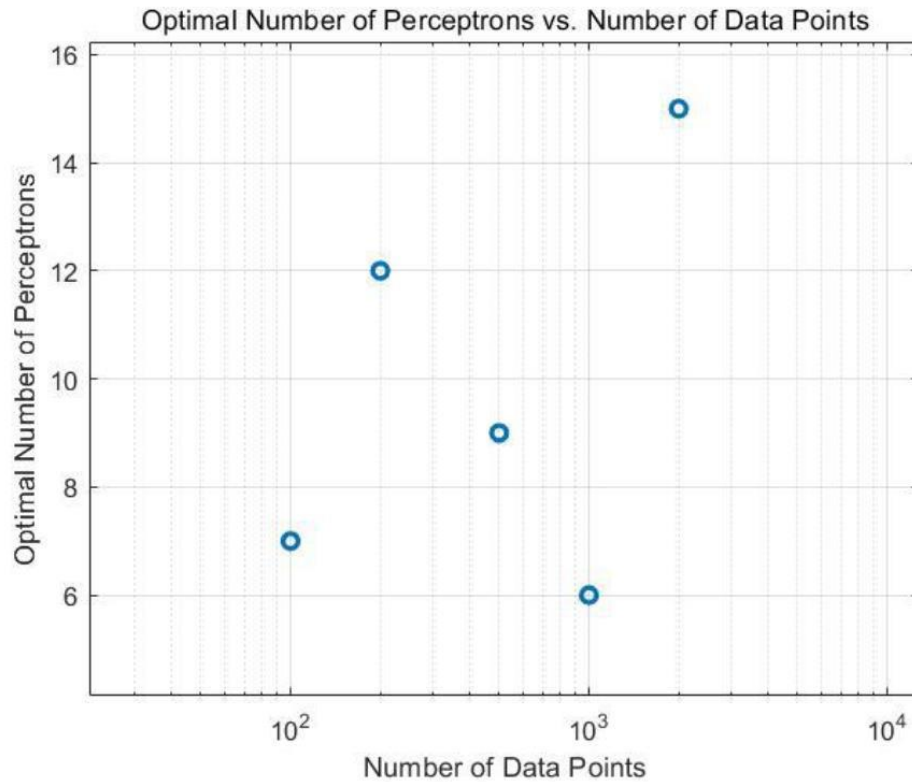
For each training dataset 10-fold cross validation was performed to determine the optimal amount of perceptron for the MLP model. The optimal number was the one that resulted in the minimum probability of error across the cross validation runs. Once the number of perceptron was selected a final model 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.

The next figure 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.



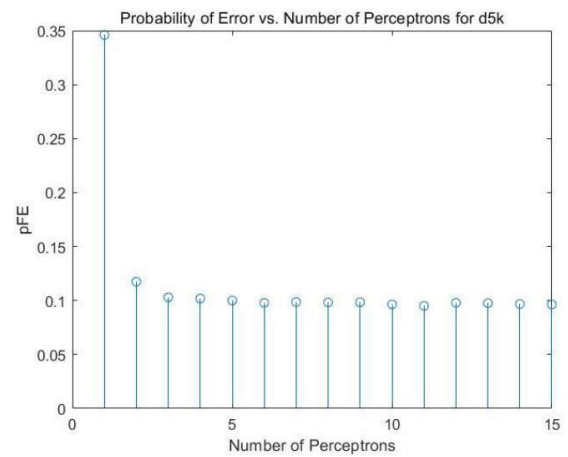
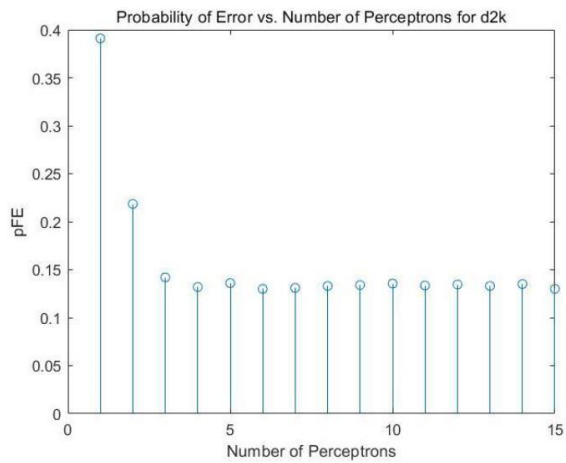
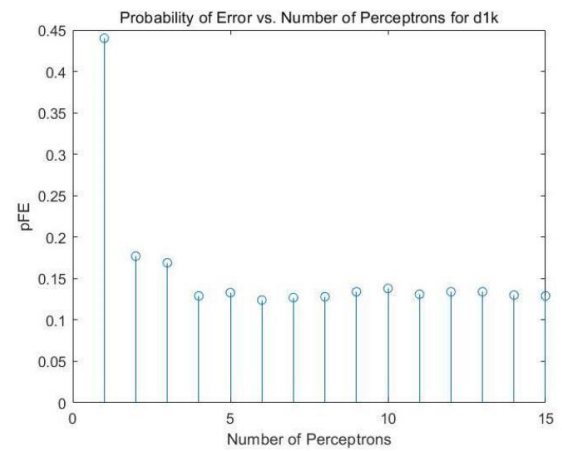
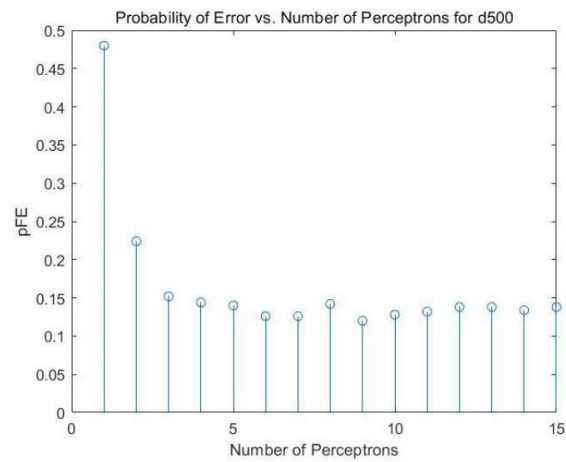
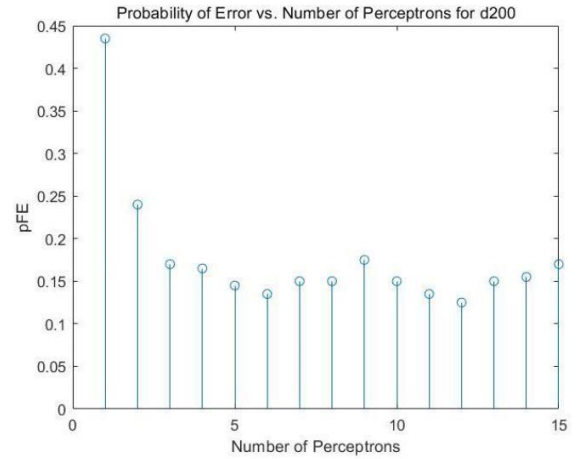
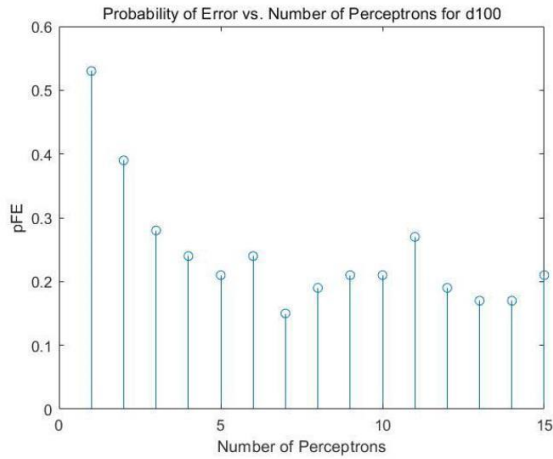
The next plot shows a plot of the optimal amount of perceptron versus the number of data points in a dataset. Except for the data point for the 1000-point training set the optimal amount of perceptron appears to increase as the size of the training dataset increases. This was expected since as the size 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.



The next table shows the optimal and the neuron network minimum probability of error with different datasets.

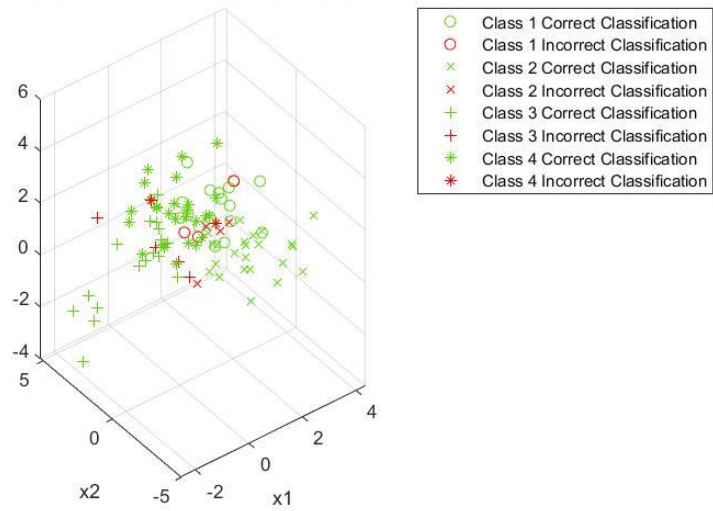
The number of samples	Optimal P_e	NN P_e
100	13.00%	16.62%
200	12.00%	14.01%
500	12.00%	14.13%
1000	11.90%	13.60%
2000	12.55%	13.41%
5000	12.94%	13.21%
10000	13.11%	-

The following plots below show 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.

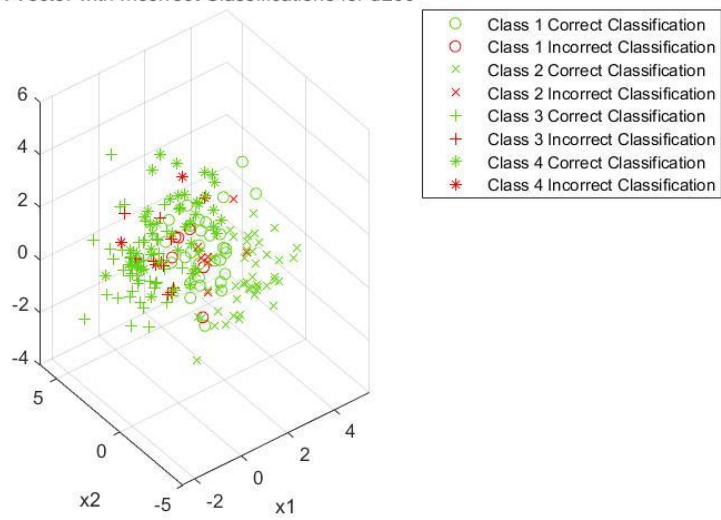


The following graphs show the X vectors with the correct and incorrect classification for training datasets.

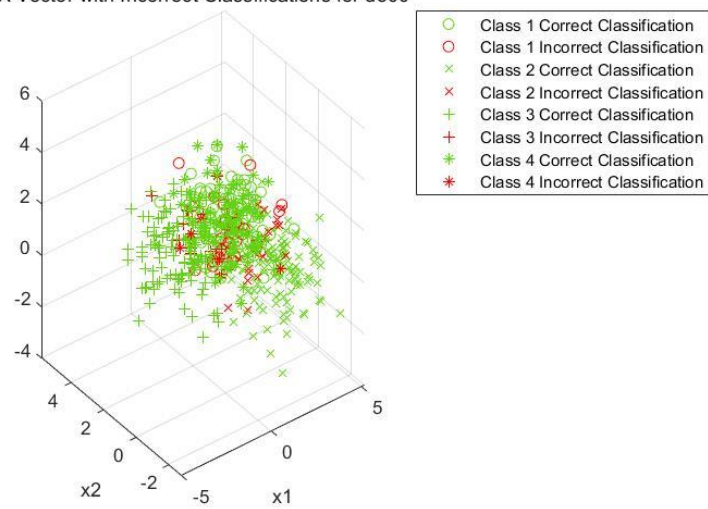
X Vector with Incorrect Classifications for d100



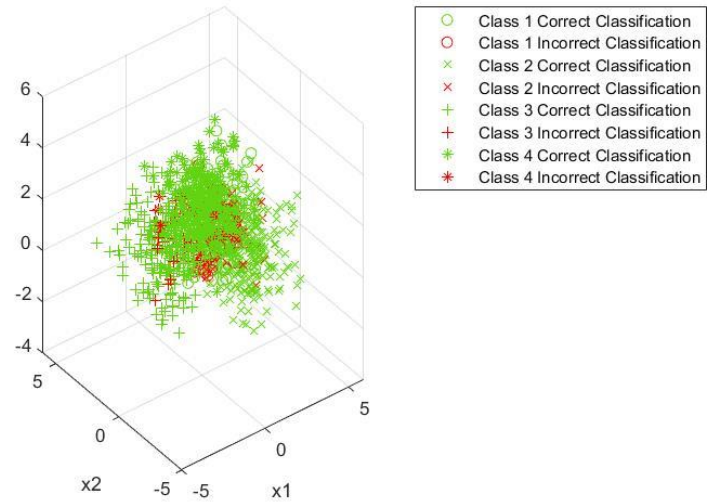
X Vector with Incorrect Classifications for d200



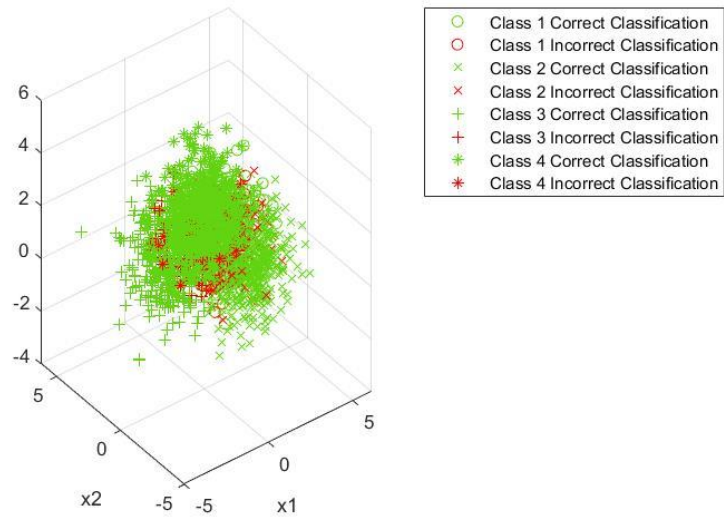
X Vector with Incorrect Classifications for d500



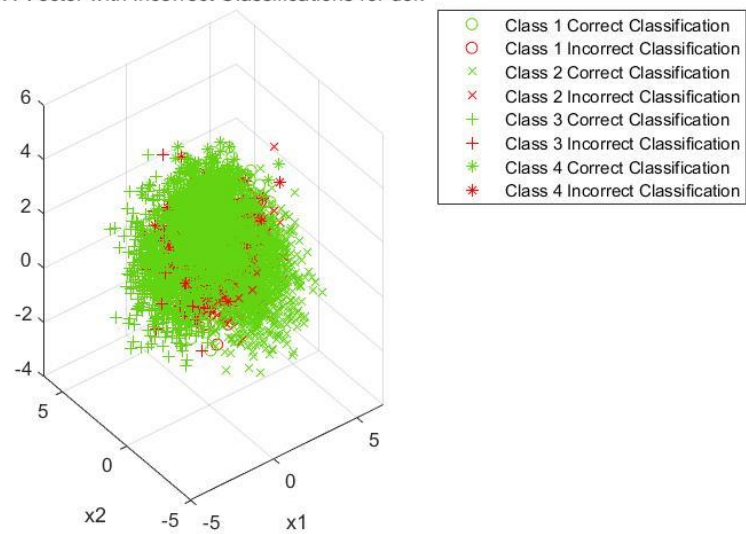
X Vector with Incorrect Classifications for d1k



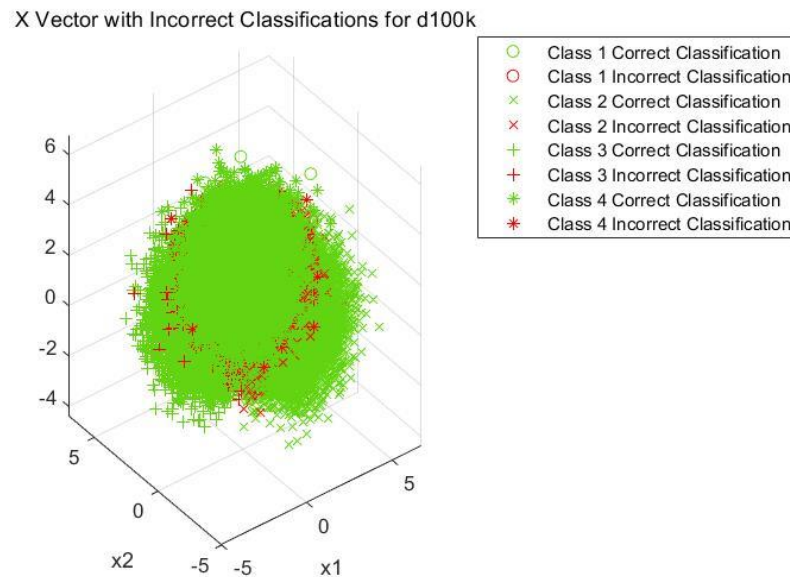
X Vector with Incorrect Classifications for d2k



X Vector with Incorrect Classifications for d5k



The next graph shows the X vectors with the correct and incorrect classification for the validate dataset.



Question 2 (40%)

Conduct the following model order selection exercise using 10-fold cross-validation procedure and report your procedure and results in a comprehensive, convincing, and rigorous fashion:

1. Select a Gaussian Mixture Model as the true probability density function for 2-dimensional real-valued data synthesis. This GMM will have 4 components with different mean vectors, different covariance matrices, and different probability for each Gaussian to be selected as the generator for each sample. Specify the true GMM that generates data.
2. Generate multiple data sets with independent identically distributed samples using this true GMM; these datasets will have respectively 10, 100, 1000, 10000 samples.
3. For each data set, using maximum likelihood parameter estimation principle (e.g. with the EM algorithm), within the framework of K-fold (e.g., 10-fold) cross-validation, evaluate GMMs with different model orders; specifically evaluate candidate GMMs with 1, 2, 3, 4, 5, 6 Gaussian components. Note that both model parameter estimation and validation performance measures to be used is log-likelihood of data.
4. Repeat the experiment multiple times (e.g., at least 30 times) and report your results, indicating the rate at which each of the six GMM orders get selected for each of the datasets you produced. Develop a good way to describe and summarize your experiment results in the form of tables/figures.

Answer:

Class conditional PDFs and mixture coefficients:

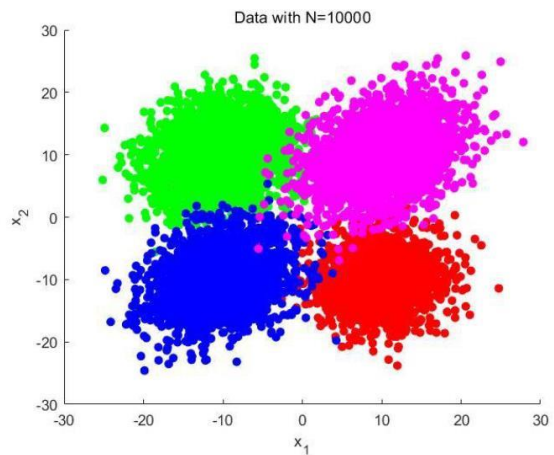
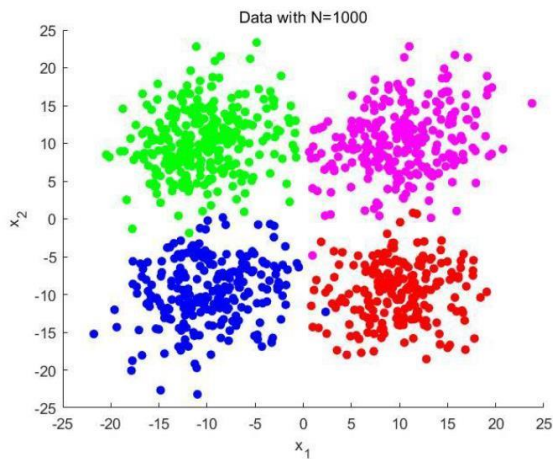
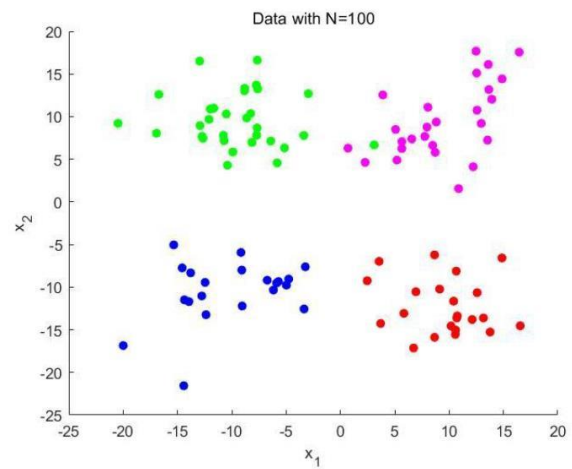
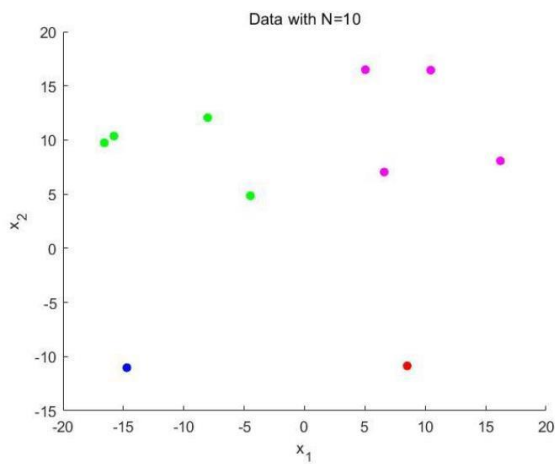
$$\mu_1 = \begin{bmatrix} 10 \\ -10 \end{bmatrix} \sigma_1^2 = \begin{bmatrix} 15 & 1 \\ 1 & 15 \end{bmatrix} P_1 = 0.2$$

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

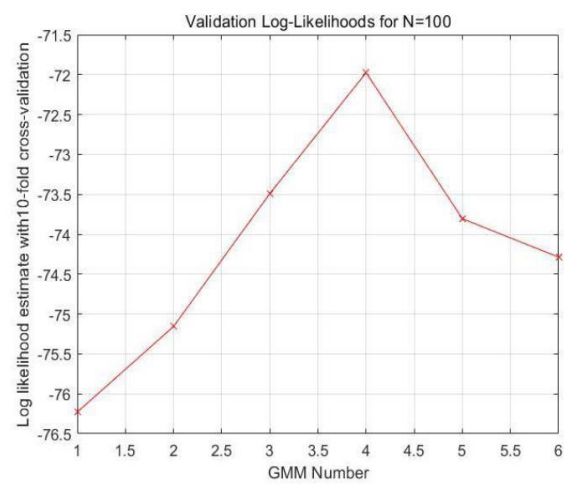
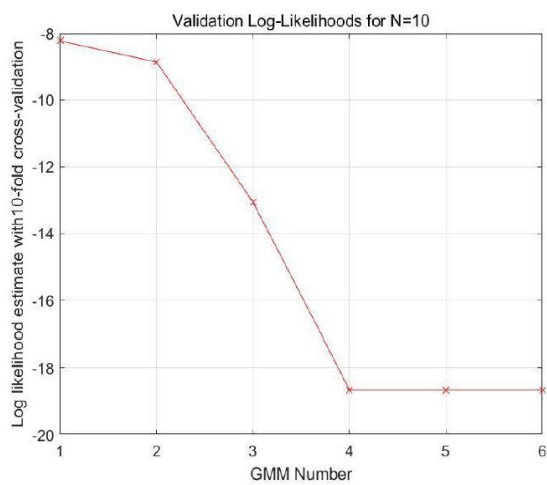
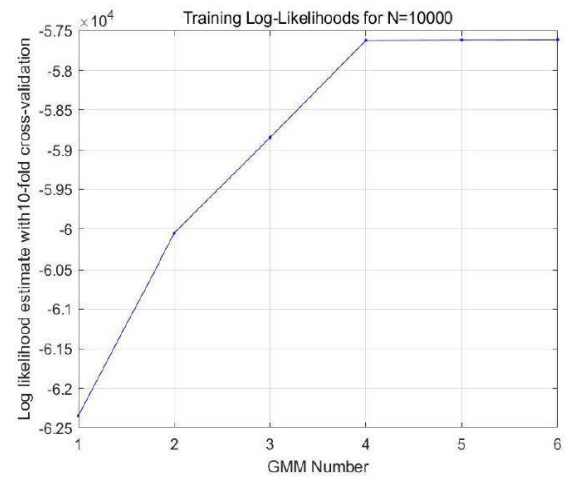
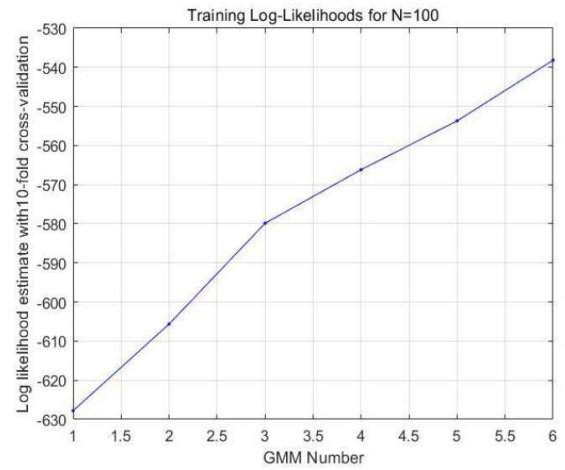
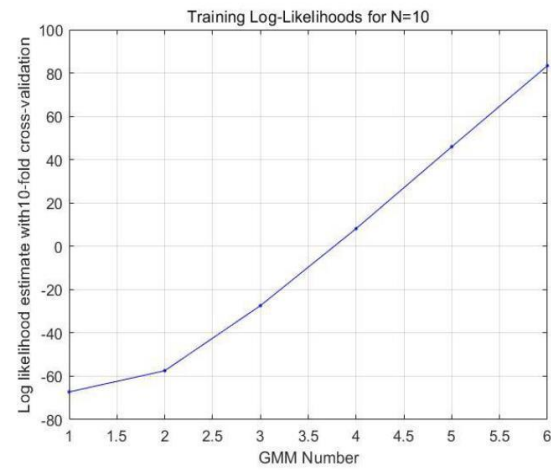
$$\mu_3 = \begin{bmatrix} -10 \\ -10 \end{bmatrix} \sigma_3^2 = \begin{bmatrix} 19 & 5 \\ 5 & 19 \end{bmatrix} P_3 = 0.23$$

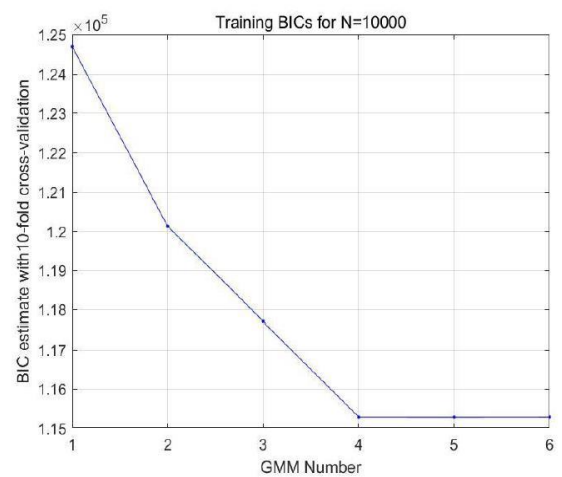
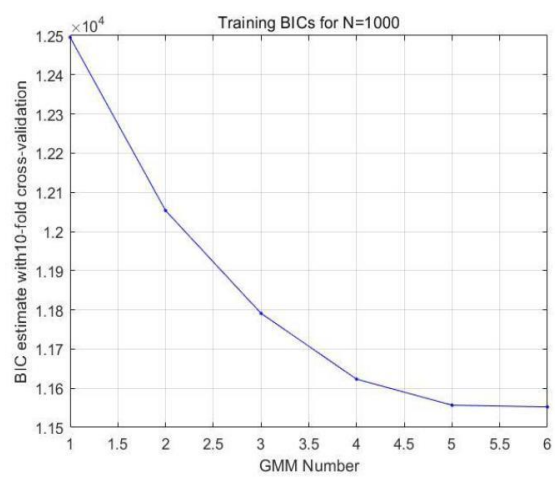
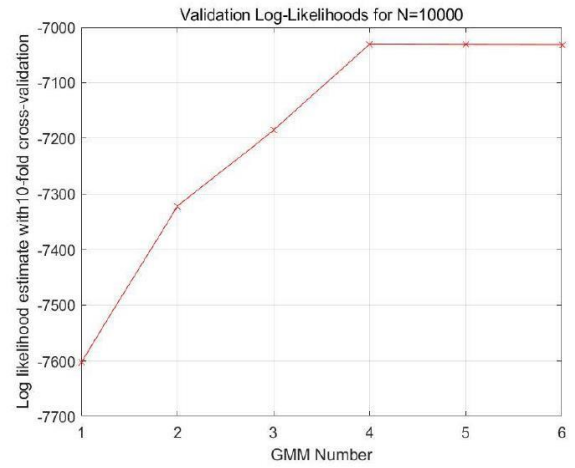
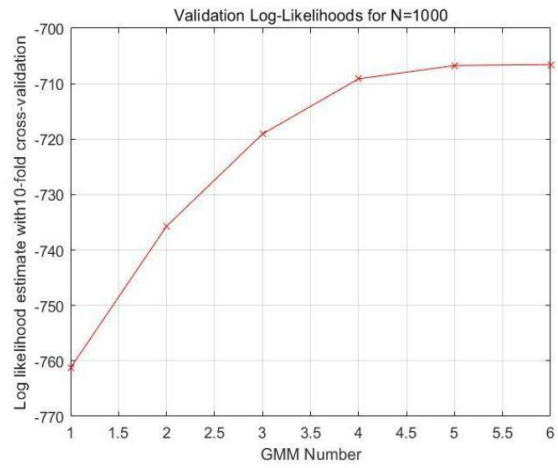
$$\mu_4 = \begin{bmatrix} 10 \\ 10 \end{bmatrix} \sigma_4^2 = \begin{bmatrix} 21 & 7 \\ 7 & 21 \end{bmatrix} P_4 = 0.27$$

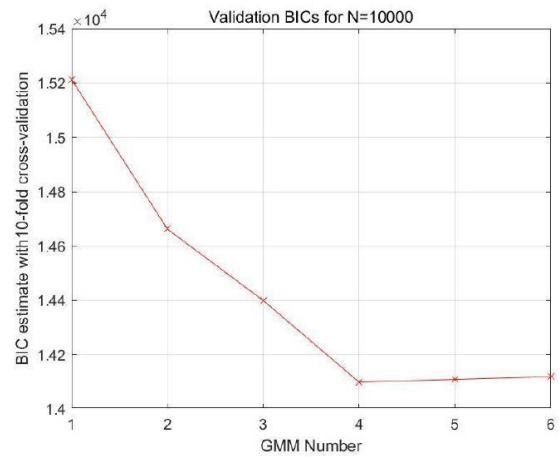
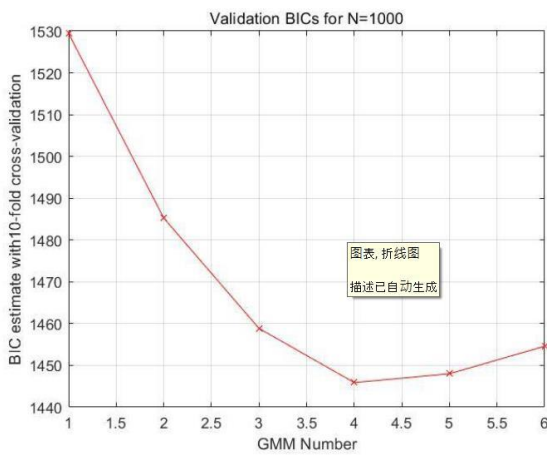
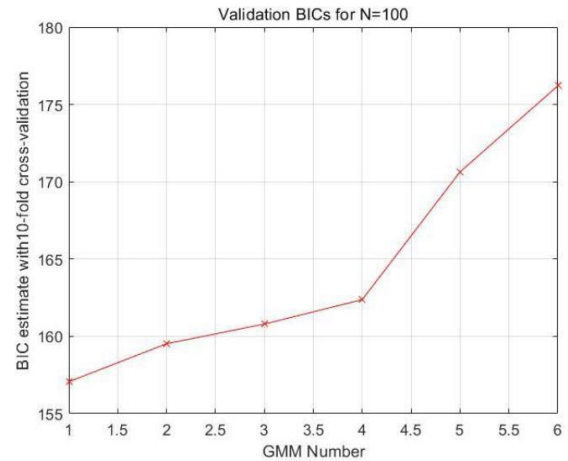
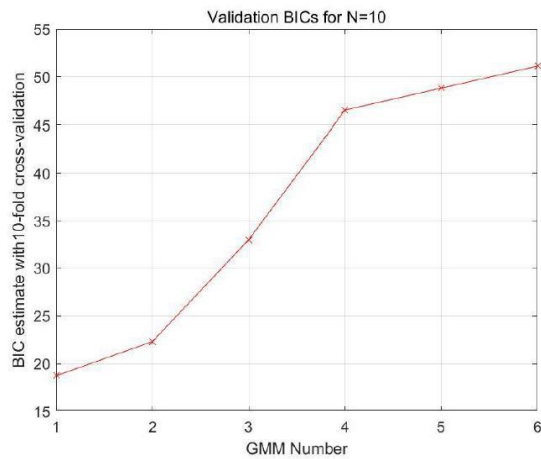
Data with 10, 100, 1000 and 10k samples are generated using the GMM model described above. The figures below show the realization of the models with different samples.



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.







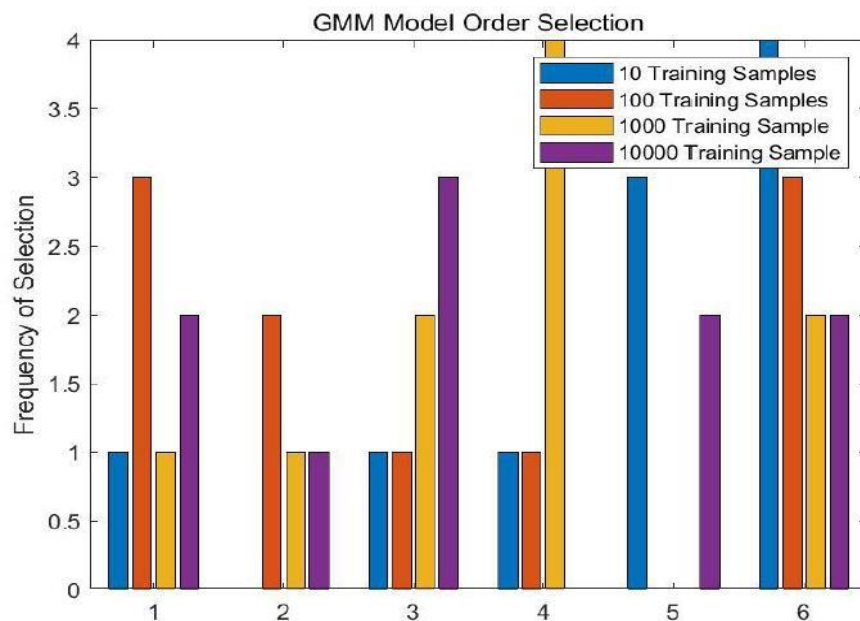
I am not able to get the algorithm converging in all cases, despite adding Gaussian noise to the training set, re-initializing mu values multiple times throughout, or adjusting the original distribution itself. Therefore, the algorithm has been limited for each combination of parameters. This does not provide a solution for the convergence issue, but there is 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. A 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 validation 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. The figure below shows the results of running the algorithm for the first experiment.



As shown in the figure above, 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.

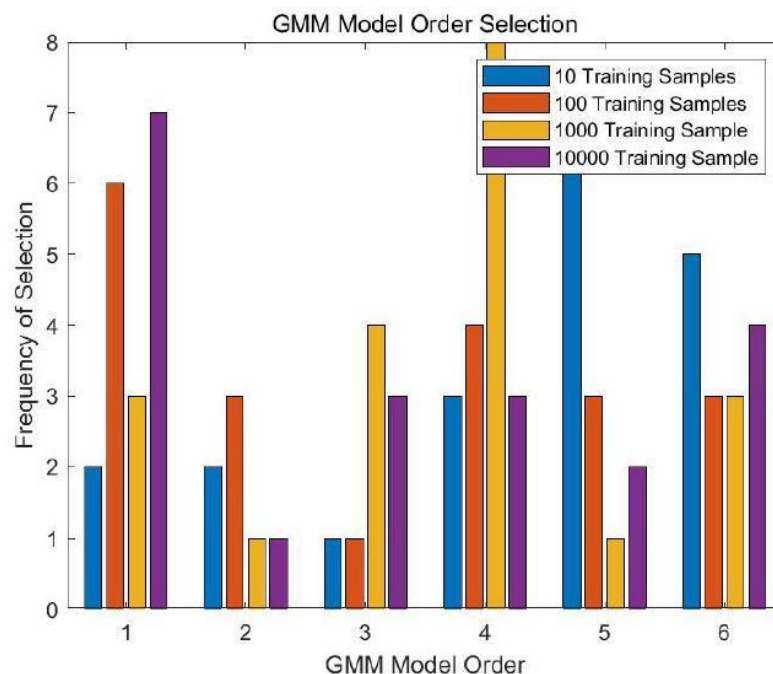
The next graph shows the results when each component number was selected as the winner for the 10th.



The next table shows the 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%

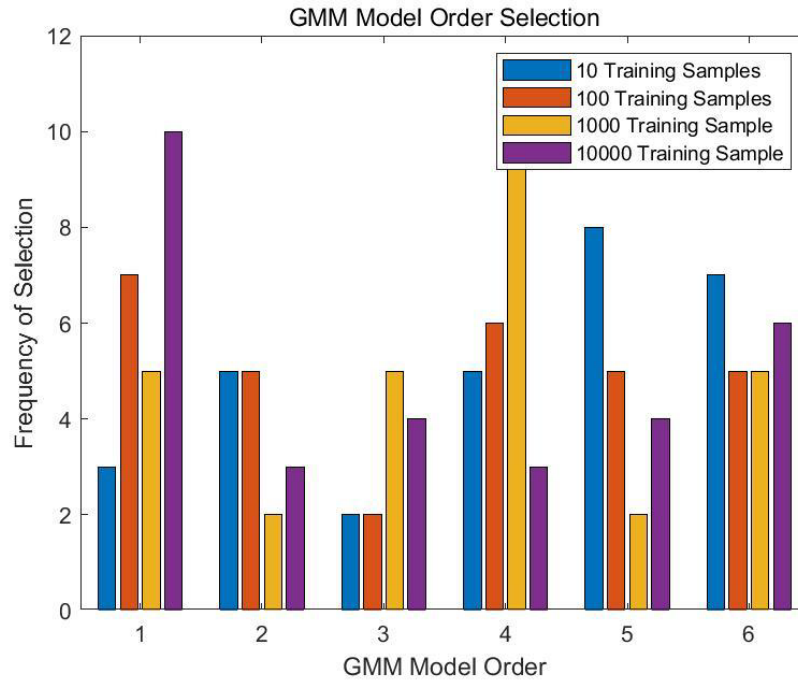
The next graph shows the results when each component number was selected as the winner for the 20th.



The next table shows the 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%

The next graph shows the results when each component number was selected as the winner for the 30th.



The next table shows the rate of order selection for 30th experiment.

	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%

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.

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.

The last figure upon summarizes the results of running the EM algorithm for 30 experiments. The following table 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 be due to the original 4 components of the true GMM has 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.

Codes

Question1 (Matlab)

```
%%=====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]';
```

[illegible]

```

%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')

```

[illegible]


```

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=1)
end
px = p*pxgivenl; % Total probability theorem
classPosteriors = pxgivenl.*repmat(p',1,N)./repmat(px,numLabels,1); % P(L=1|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

```

%%%

Question2 (Matlab)

%%=====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,

```



```

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)
%PerformsEMalgorithmtoestimateparametersandevaluetepformance
%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:runEMalgorithmtoestimateparameters
        %[alpha,mu,sigma]=EMforGMM(m,trainset,ssize,valset);
        %Built-Infunction:runEMalgorithmtoestimateparameters
        GMMModel=fitgmdist(train_set',M,'RegularizationValue',1e-10);
        alpha=GMMModel.ComponentProportion;
    end
end
end

```

```

        mu=(GMMModel.mu)';
        sigma=GMMModel.Sigma;
        %Calculate log-likelihood performance with new parameters
        perf_array(b,m)=sum(log(evalGMM(val_set,alpha,mu,sigma)));
    end
end
% Calculate average performance for each M and find best fit
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
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

[illegible]