# EECE 5644 Fall 2021

# Homework3

Lingyu Yang
002953563

# Question1

In this exercise, to train many MLP to approximate the class label posteriors, using maximum likelihood parameter estimation with minimum average cross-entropy lose 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 ( minimize expected loss with 0-1 loss assignments to correct-incorrect decisions).

**Data Distribution:**

```
dimensions=3;
numLabels=4;
Lx={'L0','L1','L2','L3'};
lossMatrix = ones(numLabels,numLabels)-eye(numLabels);
muScale=2.5;
SigmaScale=0.2;
```

**MLP Structure:** Use a 2-layerMLP (one hidden layer of perceptrons) that has P perceptrons in the first (hidden) layer with smooth-ramp style activation functions. At the output layer use a softmax function (tansig) 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:** For the training dataset, 100, 200, 500, 1000, 2000 and 5000 samples were generated and for validation, a test dataset of 100,000 samples was generated. Figures 1 and 2 show the generated data plots.

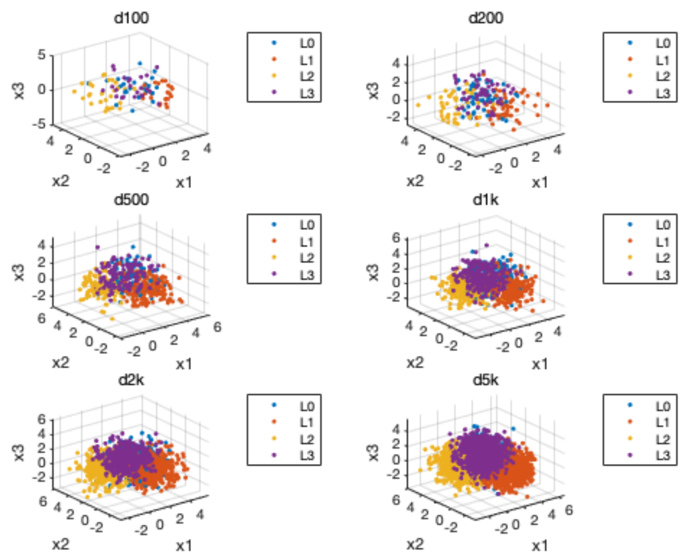



*Figure1. Training Dataset*

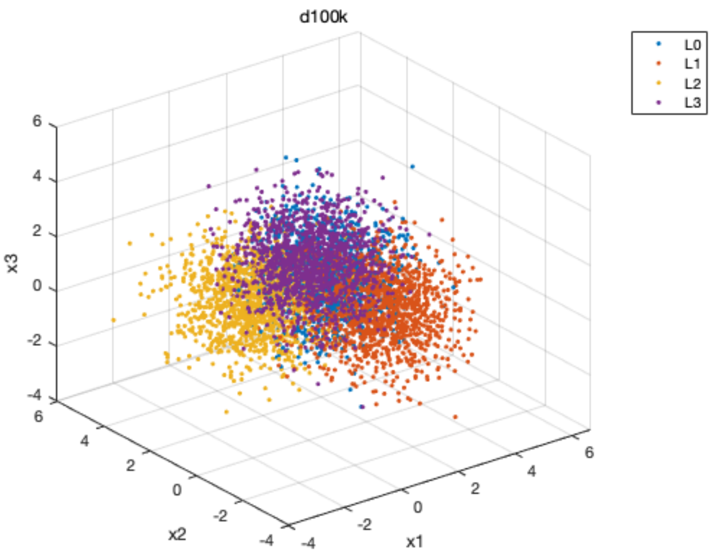



*Figure2. Validation Dataset*

A 10-fold cross-validation is performed on each training dataset to determine the optimal number of perceptrons for the MLP model.

The optimal number is the number that produces the lowest probability of error in the cross-validation run. Once the number of perceptrons is selected, a final model is trained on the entire training dataset. Finally, this training model is evaluated using a test dataset and the error probability is calculated as a measure of model performance.

Figure 3 shows the results of this procedure.

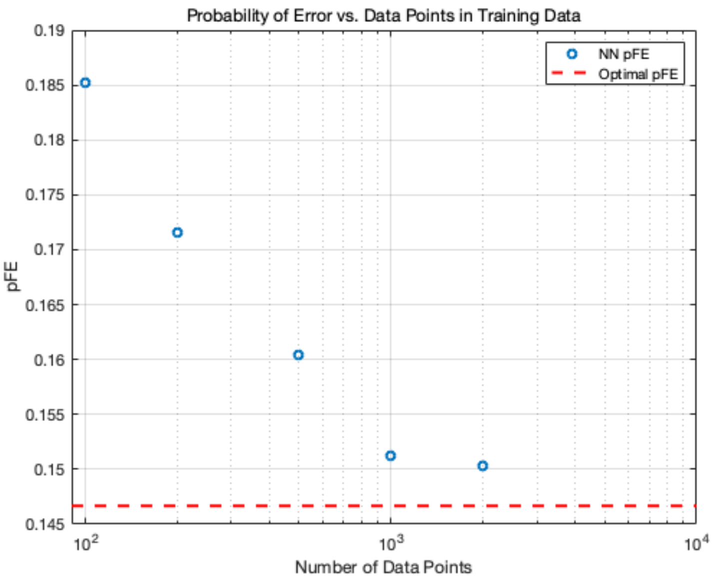



*Figure3. Probability of Error vs. Number of Data Points in Training Data*

As can be seen in Figure 3, the overall error probability correlates well with the size of the training dataset. As the size of the dataset increases, the error probability decreases and approaches the best error probability estimated using the true pdf of the underlying data. This suggests that as the training data size increases, the model estimation can be improved, resulting in more accurate classification.

Figure 4 shows a plot of the number of optimal perceptrons versus the number of data points in the dataset.

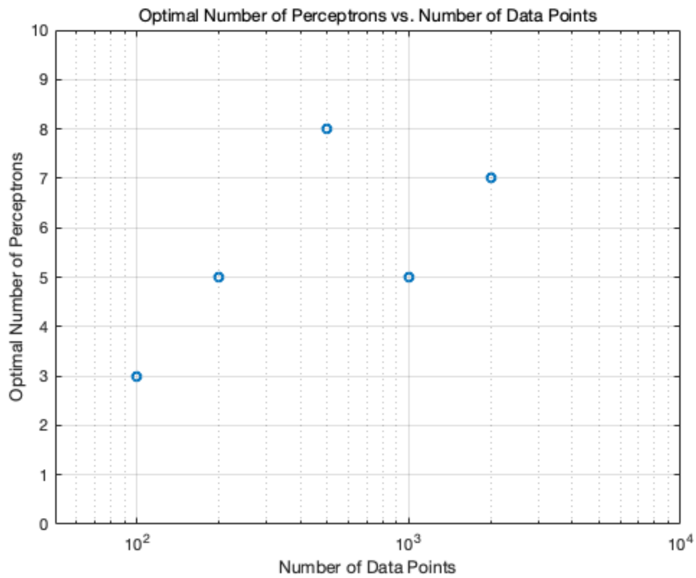



*Figure4. Optimal Number of Perceptrons vs. Number of Data Points*

The number of optimal perceptrons appears to increase with the training dataset, (except for the 1000 data points in the training set, and I do not know why there is such a difference at 1000 samples.). This is expected because as the size of the data set increases, the complexity of the model increases in a meaningful way. More data means that there are more features to be modeled, and therefore the complexity of the model increases.

Figure 5 below shows a plot of the cross-validation results for the training dataset.

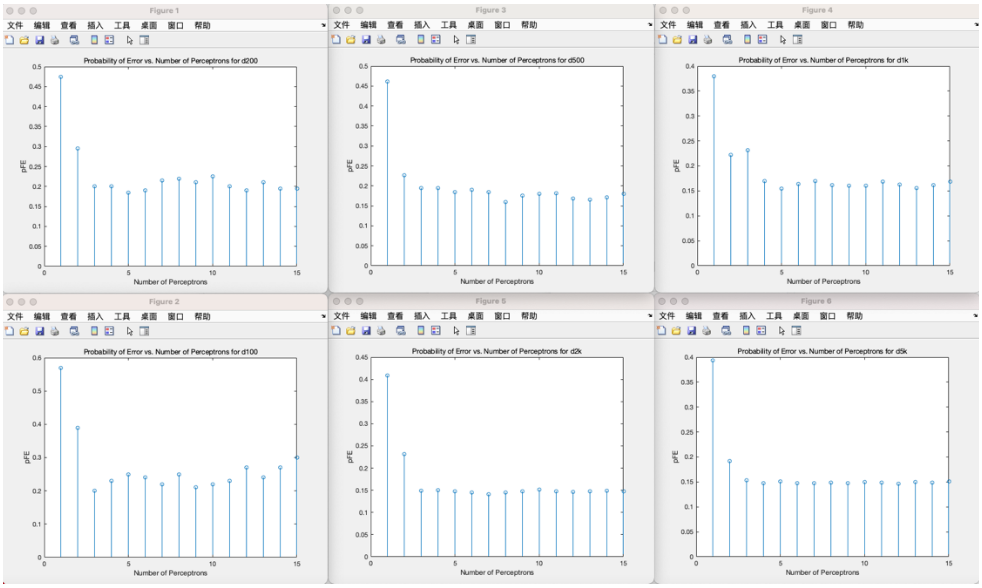


*Figure 5. Probability of Error vs. Number of Perceptrons for all sample training dataset*

The trends are roughly the same, and we use 200 samples as an example(figure6.).

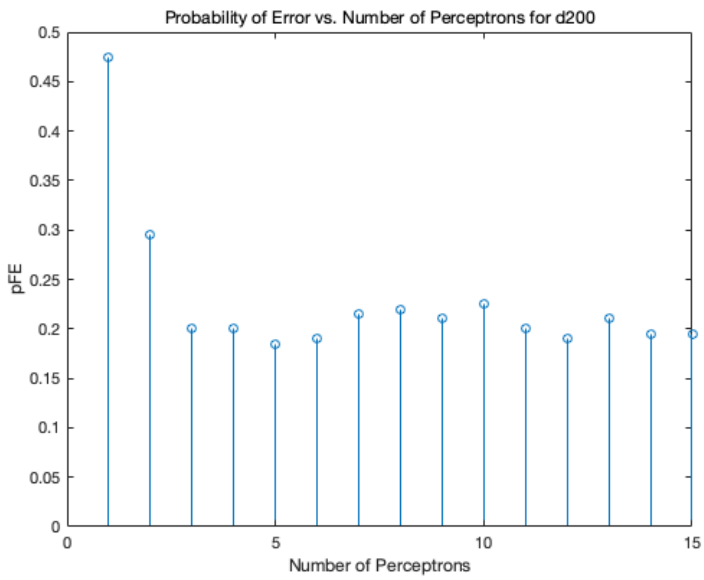


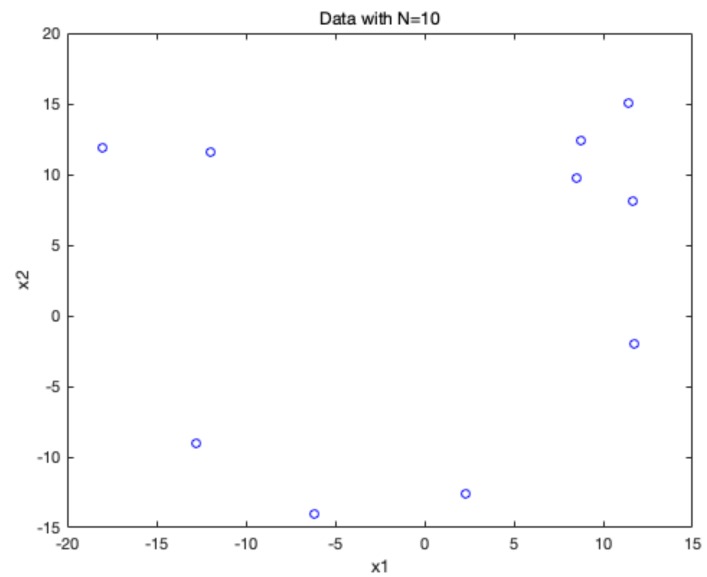

*Figure6. Probability of Error vs. Number of Perceptrons for 200 samples training dataset*

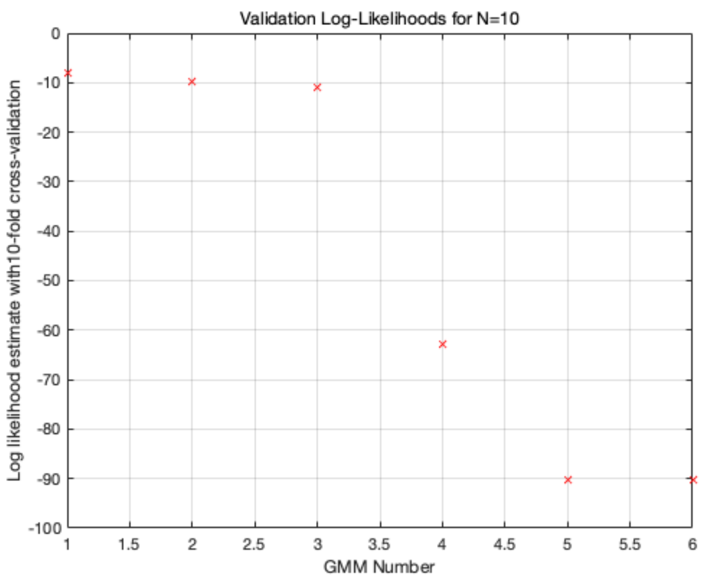
In this figure, the error probability is shown as a function of the number of perceptrons. The error probability for a single perceptron starts very large and then decreases rapidly as the number of perceptrons increases. The minimum value is determined to be about 10, and the probability error slowly increases as the number of perceptrons increases. Although the optimal number of perceptrons varies between training data sets, the overall relationship between error probability and the number of perceptrons usually follows this pattern.

# Question2

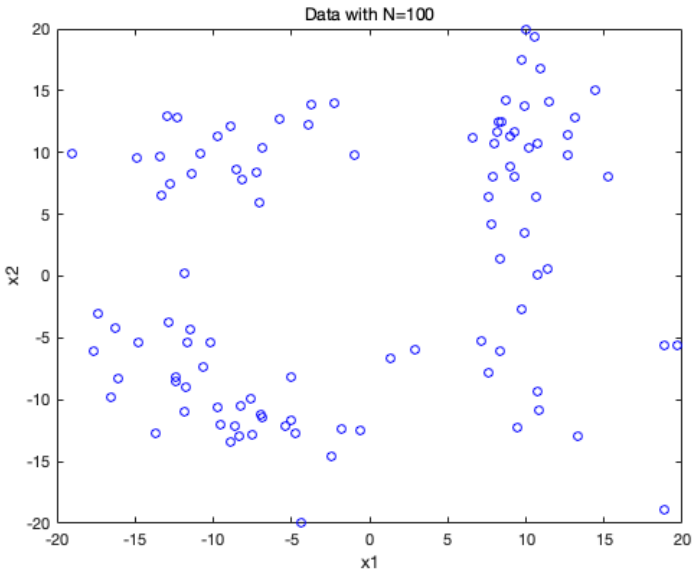
In this problem, we need to perform the following model order selection exercise using a 10-fold cross-validation procedure.
Select a Gaussian Mixture Model as the true probability density function for 2-dimensional real-valued data synthesis. This GMM will have 4 components with different mean vectors, 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.

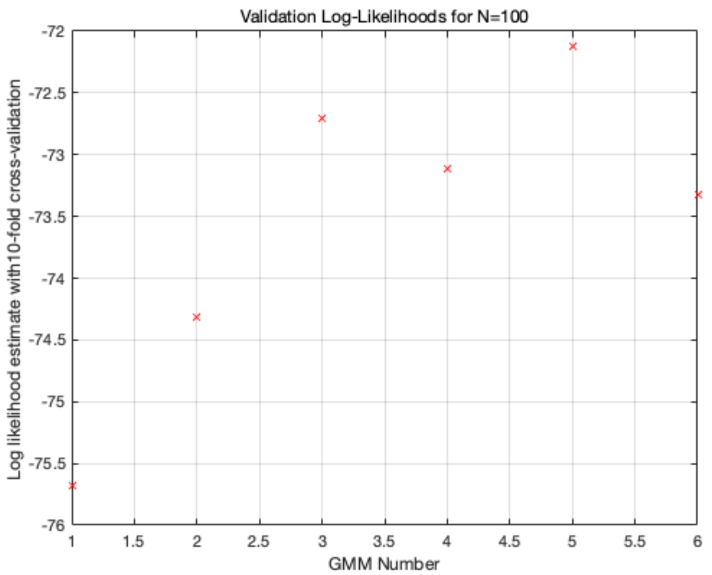
**For 10 simples:**



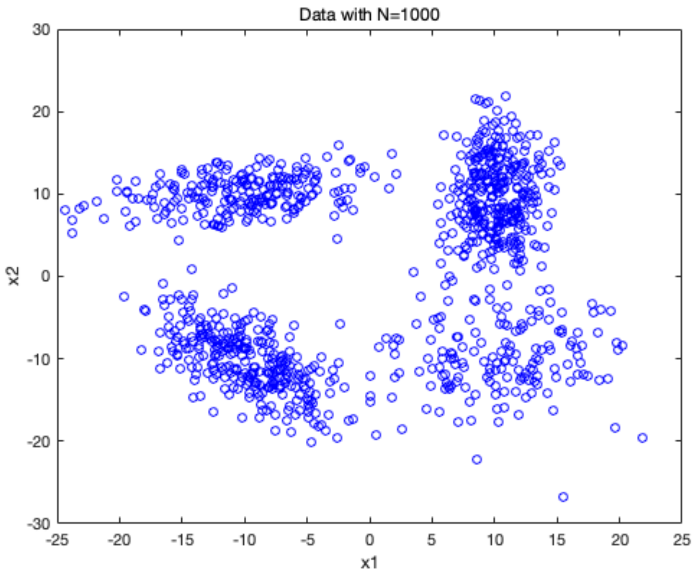



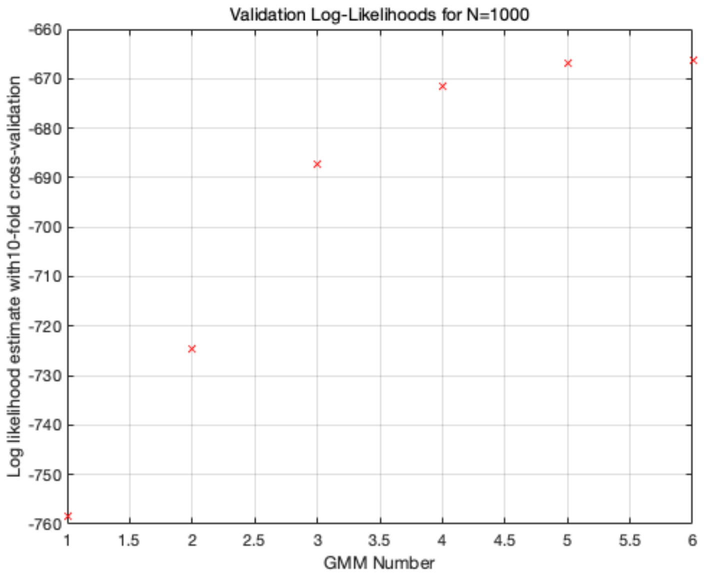
**For 100simples:**



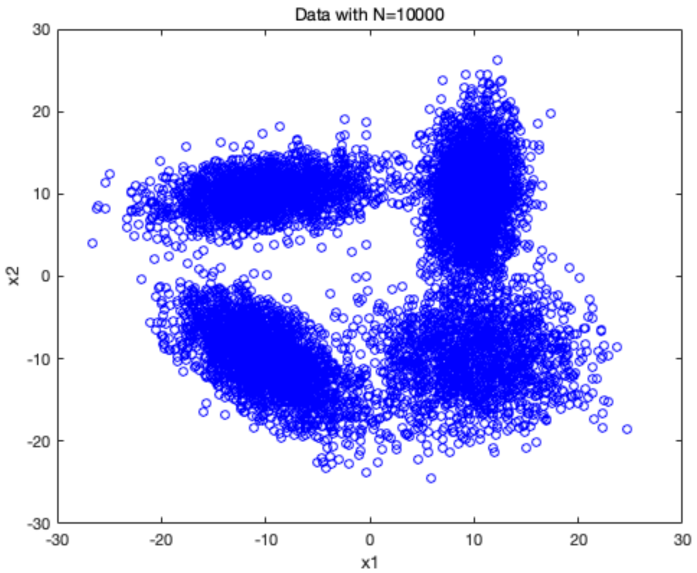



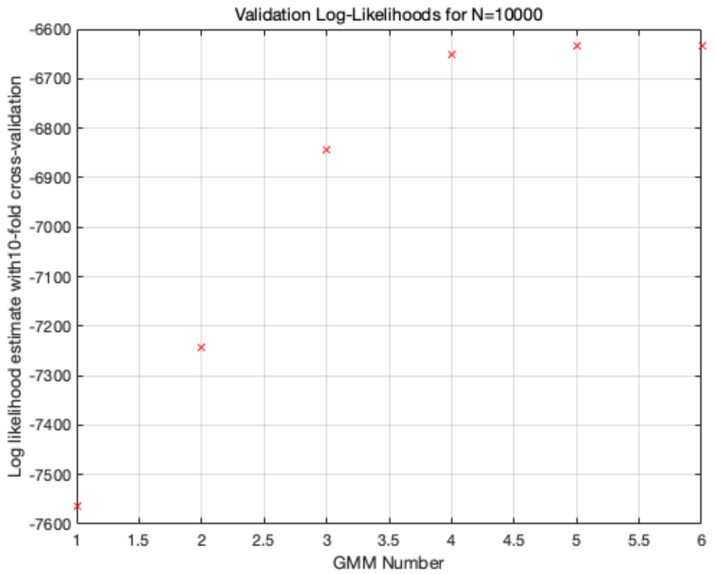
**For 1000simples:**



**For 10000simples:**




**Conclusion:**

1. When the amount of data in our training dataset is too small (e.g., N=10/100) and the EM algorithm results show 1, we have the best model and the algorithm considers it as a decentralized reeling model. Even as the order increases, the likelihood of the effective sample is getting smaller, even to zero. When the samples are large enough (N=1000/10000), the EM algorithm shows that we have the maximum likelihood of the data when the order is equal to around 4, 5, 6.

2. we can see that the model order selection tends to prefer order equal to 4 as the preferred GMM order for the dataset. This is due to the higher value given to the higher order, even though it may be the same as the other orders.

3. When the order is equal to 4 and as the amount of data increases, we can get more accurate results for the validation data.

# Appendix A: Functions used in 1 and 2

```
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 [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 [minPFE,decisions]=optClass(lossMatrix,x,mu,Sigma,p,labels,Lx)
% 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');
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)]);
if ind2==1
legend 'show';
elseif ind2==4
xlabel('x1');
```

```
end
end
end
end

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 B:

## Q1:

```
clear all;
close all;
%Switches to bypass parts 1 and 2 for debugging
dimensions=3;
numLabels=4;
Lx={'L0','L1','L2','L3'};
lossMatrix = ones(numLabels,numLabels)-eye(numLabels);
muScale=2.5;
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);
legend 'show';
title([dTypes{ind}]);
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);
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

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');
```

Q2:

```
%Counting variables to ensure the program is not stuck
countN = 0;

%All four sample sizes
for i = 1:4

    countN = countN+1

    %Tolerance for EM stopping criterion
    delta = 1e-4;
    %Regularization parameter for covariance estimates
    regWeight = 1e-10;
    %K-Fold Cross Validation
    K = 10;
    %Number of samples
    N = [10,100,1000,10000];

    %Generate samples from a 4-component GMM
    alpha_true = [0.17,0.22,0.28,0.33];
    mu_true = [10 -10 -10 10;-10 10 -10 10];
    Sigma_true(:,:,1) = [25 1;1 20];
    Sigma_true(:,:,2) = [27 4;4 5];
    Sigma_true(:,:,3) = [15 -9;-9 15];
    Sigma_true(:,:,4) = [4 1;1 22];
    x = randGMM(N(i),alpha_true,mu_true,Sigma_true);
```

```
    %Plotting data
    figure(i), clf,
    plot(x(1,:),x(2,:),'ob')
    xlabel('x1'); ylabel('x2');
    title(strcat('Data with N=',num2str(N(i))));

    %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)

figure(i+4), clf,
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

figure(i+8), clf,
```

```
plot(Averagellvalidate,'rx');
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

figure(i+12), clf,
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

figure(i+16), clf,
plot(BICvalidate,'rx');
xlabel('GMM Number'); ylabel(strcat('BIC estimate with ',num2str(K),'-fold cross-validation'));
title(strcat('Validation BICs for N=',num2str(N(i))))
grid on

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

end
```