Intelligent Systems Lab

Michele Baldassini

Department of Information Engineering – University of Pisa

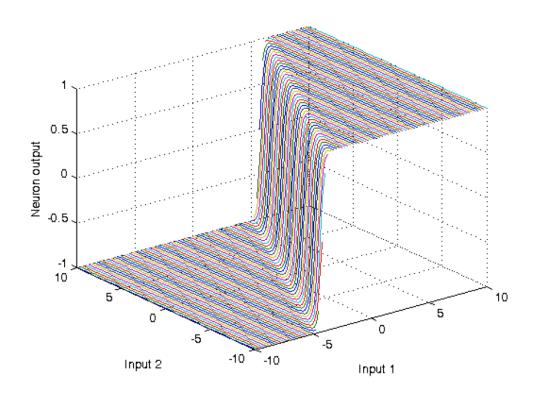


michele.baldassini@unifi.it

Simple Neuron

Calculate the output of a simple neuron

```
Define neuron parameters
 close all, clear all, clc, format compact % Neuron weights
 w = [4 -2]
% Neuron bias
  b = -3
  % Activation function
 func = 'tansig'
 % func = 'purelin'
% func = 'hardlim'
 % func = 'logsig'
       Define input vector
 p = [2 3]
       Calculate neuron output
 activation_potential = p*w'+b
neuron_output = feval(func, activation_potential)
Plot neuron output over the range of inputs [p1, p2] = meshgrid(-10:.25:10); z = feval(func, [p1(:) p2(:)]*w'+b); z = reshape(z, length(p1), length(p2)); plot3(p1, p2, z) grid on
 xlabel('Input 1')
  ylabel('Input 2')
 zlabel('Neuron output')
```



Custom Neural Networks

Create Custom Neural Networks

```
Define one sample: inputs and outputs
close all, clear all, clc, format compact
inputs = [1:6]' % input vector (6-dimensional pattern)
outputs = [12]' % corresponding target output vector
  Define and custom network
% create network
net = network( ...
                  % numInputs, number of inputs,
1, ...
                  % numLayers, number of layers
2, ...
[1; 0], ...
                  % biasConnect, numLayers-by-1 Boolean vector,
                  % inputConnect, numLayers-by-numInputs Boolean matrix,
[1; 0], ...
                  % layerConnect, numLayers-by-numLayers Boolean matrix
[0 0; 1 0], ...
[0 1] ...
                  % outputConnect, 1-by-numLayers Boolean vector
% View network structure
view(net);
```

Train Custom Neural Networks

```
Define topology and transfer function
% number of hidden layer neurons
net.layers{1}.size = 5;
% hidden layer transfer function
net.layers{1}.transferFcn = 'logsig';
view(net);
    Define topology and transfer function
net = configure(net,inputs,outputs);
view(net);

    Train net and calculate neuron output

% initial network response without training initial_output = net(inputs)
% network training net.trainFcn = 'trainIm';
net.performFcn = 'mse';
net = train(net,inputs,outputs);
% network response after training
final output = net(inputs)
initial output =
final output =
    1.0000
```

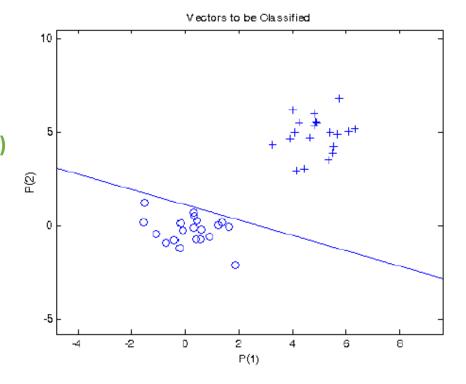
2.0000

Perceptron

Classification of linearly separable data with a perceptron

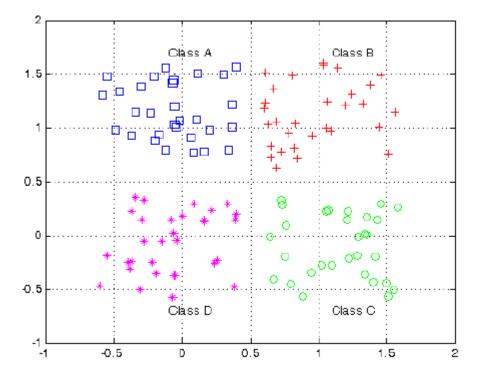
```
Define input and output data
close all, clear all, clc, format compact
% number of samples of each class
N = 20:
% define inputs and outputs
offset = 5:
                                         % offset for second class
x = [randn(2,N) randn(2,N)+offset];
                                         % inputs
y = [zeros(1,N) ones(1,N)];
                                         % outputs
% Plot input samples with PLOTPV (Plot perceptron input/target vectors)
figure(1)
plotpv(x,y);
   Create and train perceptron
net = perceptron;
net = train(net,x,y);
view(net);
   Plot decision boundary
figure(1)
```

plotpc(net.IW{1},net.b{1});



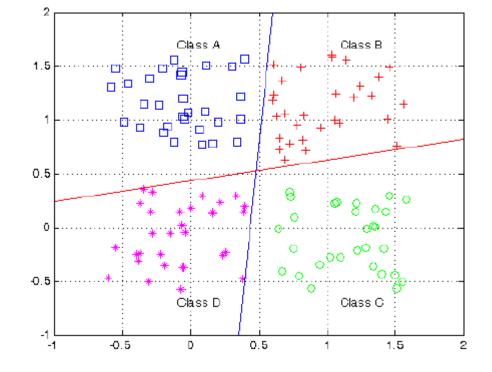
Classification of a 4-class problem with a perceptron (1/2)

```
Define data
close all, clear all, clc, format compact
% number of samples of each class
K = 30;
% define classes
                       % offset of classes
 a = .6:
A = [rand(1,K)-q; rand(1,K)+q];
B = [rand(1,K)+q; rand(1,K)+q];
C = [rand(1,K)+q; rand(1,K)-q];
D = [rand(1,K)-q; rand(1,K)-q];
plot(A(1,:),A(2,:),'bs')
hold on
grid on
 plot(D(1,:),D(2,:), m*')
text(.5-q,.5+2*q,'Class A')
text(.5+q,.5+2*q,'Class B')
text(.5+q,.5-2*q,'Class C')
text(.5-q,.5-2*q,'Class D')
% define output coding for classes
a = [0 1]';
b = [1 1]';
c = [1 \ 0]';
d = [0 \ 0]';
       Prepare inputs & outputs for perceptron training
% define inputs (combine samples from all four classes)
P = [A B C D];
% define targets
T = [repmat(a,1,length(A)) repmat(b,1,length(B)) ...
repmat(c,1,length(C)) repmat(d,1,length(D))];
%plotpv(P,T);
```



Classification of a 4-class problem with a perceptron (2/2)

Create and train a perceptron net = perceptron; E = 1: net.adaptParam.passes = 1; linehandle = plotpc(net.IW{1},net.b{1}); n = 0: while (sse(E) & n<1000) $n = \dot{n} + 1$: [net,Y,E] = adapt(net,P,T);linehandle = plotpc(net.IW{1},net.b{1},linehandle); drawnow; % show perceptron structure view(net); ADAPT returns a new network object that performs as a better classifier, the network output, and the error. This loop allows the network to adapt for xx passes, plots the classification line and continues until the error is zero. How to use trained perceptron % For example, classify an input vector of [0.7; 1.2] p = [0.7; 1.2] y = net(p) % compare response with output coding (a,b,c,d) 0.7000 1.2000



Exercises Part 1

1. Train a perceptron to perform classification with the following inputs and outputs:

```
X = [-0.5 - 0.5 + 0.3 - 0.1; -0.5 + 0.5 - 0.5 + 1.0];
T = [1   1   0   0];
Test with:
X = [0.7; 1.2];
```

2. Train a perceptron to perform classification with the following inputs and outputs:

```
X = [-0.5 - 0.5 + 0.3 - 0.1 - 40; -0.5 + 0.5 - 0.5 + 1.0 50];
T = [1 1 0 0 1];
Test with:
x = [0.7; 1.2];
```

Multilayer Perceptron

Generate feedforward neural network

net = feedforwardnet(hiddenSizes,trainFcn)

- returns a feedforward neural network with a hidden layer size of hiddenSizes and training function, specified by trainFcn
- Feedforward networks consist of a series of layers. The first layer has a connection from the network input. Each subsequent layer has a connection from the previous layer. The final layer produces the network's output.
- You can use feedforward networks for any kind of input to output mapping. A feedforward network with one hidden layer and enough neurons in the hidden layers can fit any finite inputoutput mapping problem.
- Specialized versions of the feedforward network include fitting and pattern recognition networks
- A variation on the feedforward network is the cascade forward network, which has additional connections from the input to every layer, and from each layer to all following layers

Train and Test

Train the network net using the training data.

```
net = train(net, x, t);
```

View the trained network.

view(net)

Estimate the targets using the trained network.

y = net(x);

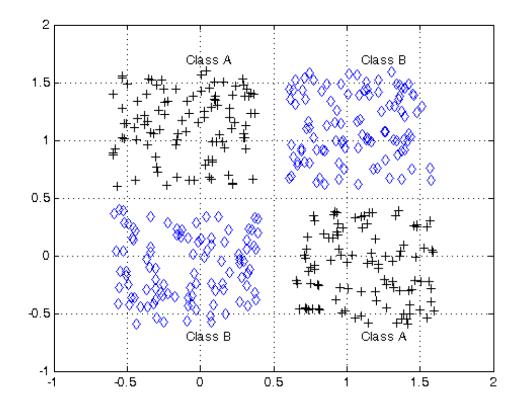
 Assess the performance of the trained network. The default performance function is mean squared error.

perf = perform(net, y, t);

Solving XOR problem with a multilayer perceptron (1/4)

Define 4 clusters of input data

```
close all, clear all, clc, format compact % number of samples of each class
 K = 100;
 % define classes
                        % offset of classes
A = [rand(1,K)-q; rand(1,K)+q];
B = [rand(1,K)+q; rand(1,K)+q];
C = [rand(1,K)+q; rand(1,K)-q];
D = [rand(1,K)-q; rand(1,K)-q];
% plot classes
 plot(A(1,:),A(2,:), 'k+')
 hold on
grid on
text(.5-q,.5+2*q,'Class A')
text(.5+q,.5+2*q,'Class B')
text(.5+q,.5-2*q,'Class A')
text(.5-q,.5-2*q,'Class B')
```



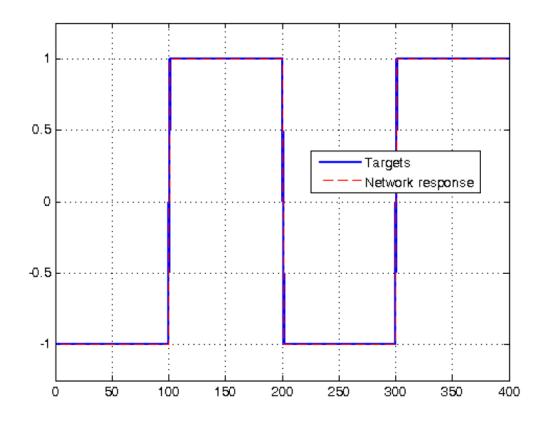
Solving XOR problem with a multilayer perceptron (2/4)

```
Define output coding for XOR problem
% encode clusters a and c as one class, and b and d as another class
a = -1:
            %alb
c = -1:
            % -----
            % d | c
b = 1;
d = 1:
   Prepare inputs & outputs for network training
% define inputs (combine samples from all four classes)
P = [A B C D];
% define targets
T = [repmat(a,1,length(A)) repmat(b,1,length(B)) ...
repmat(c,1,length(C)) repmat(d,1,length(D)) ];
% view inputs | outputs
%[P'T']
   Create and train a multilayer perceptron
% create a neural network
net = feedforwardnet([5 3]);
% train net
net.divideParam.trainRatio = 1:
                                      % training set [%]
net.divideParam.valRatio = 0;
                                      % validation set [%]
net.divideParam.testRatio = 0:
                                      % test set [%]
% train a neural network
[net,tr,Y,E] = train(net,P,T);
% show network
view(net)
```

Solving XOR problem with a multilayer perceptron (3/4)

Plot targets and network response to see how good the network learns the data

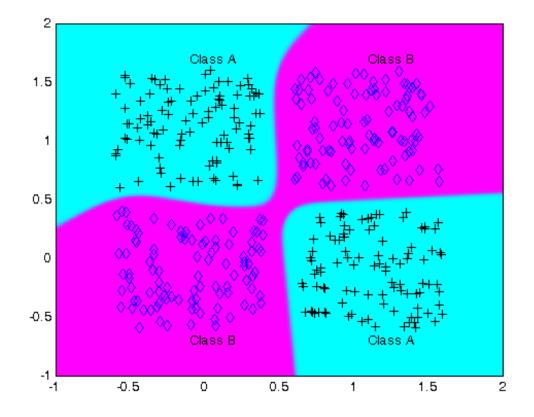
```
figure(2)
plot(T','linewidth',2)
hold on
plot(Y','r--')
grid on
legend('Targets','Network response','location','best')
ylim([-1.25 1.25])
```



Solving XOR problem with a multilayer perceptron (4/4)

Plot classification result for the complete input space

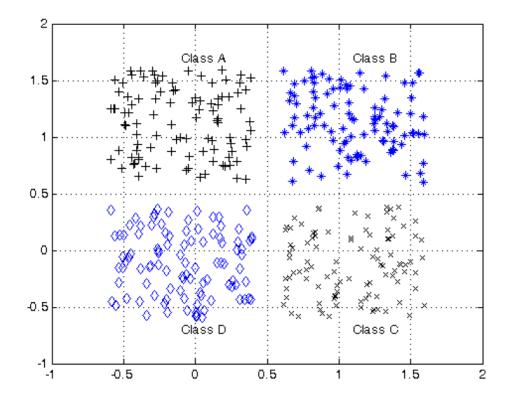
```
generate a grid
span = -1:.005:2;
[P1,P2] = meshgrid(span,span);
pp = [P1(:) P2(:)]';
% simulate neural network on a grid
aa = net(pp);
% translate output into [-1,1]
%aa = -1 + 2*(aa>0);
% plot classification regions
figure(1)
mesh(P1,P2,reshape(aa,length(span),length(span))-5);
colormap cool
```



Classification of a 4-class problem with a multilayer perceptron (1/4)

Define 4 clusters of input data

```
close all, clear all, clc, format compact % number of samples of each class
 K = 100;
 % define classes
                       % offset of classes
A = [rand(1,K)-q; rand(1,K)+q];
B = [rand(1,K)+q; rand(1,K)+q];
C = [rand(1,K)+q; rand(1,K)-q];
D = [rand(1,K)-q; rand(1,K)-q];
plot(A(1,:),A(2,:), 'k+')
 hold on
grid on
text(.5-q,.5+2*q,'Class A')
text(.5+q,.5+2*q,'Class B'
text(.5+q,.5-2*q,'Class C')
text(.5-q,.5-2*q,'Class D')
```



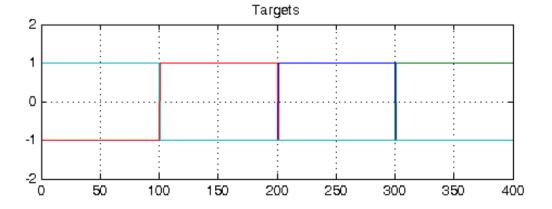
Classification of a 4-class problem with a multilayer perceptron (2/4)

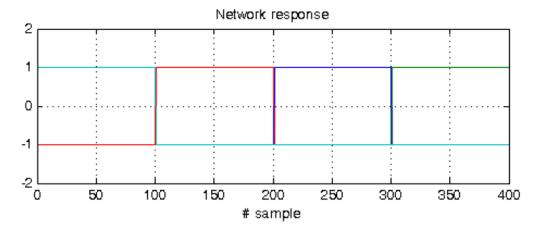
```
Define output coding for all 4 clusters
% coding (+1/-1) of 4 separate classes
a = [-1 -1 -1 +1]';
b = [-1 - 1 + 1 - 1]';
d = [-1 + 1 - 1 - 1]'
c = [+1 -1 -1 -1] ';
   Prepare inputs & outputs for network training
% define inputs (combine samples from all four classes)
P = [A B C D];
% define targets
T = [repmat(a,1,length(A)) repmat(b,1,length(B)) ... repmat(c,1,length(C)) repmat(d,1,length(D)) ];
   Create and train a multilayer perceptron
% create a neural network
net = feedforwardnet([4 3]);
% train net
net.divideParam.trainRatio = 1;
                                     % training set [%]
net.divideParam.valRatio = 0;
                                     % validation set [%]
net.divideParam.testRatio = 0;
                                     % test set [%]
% train a neural network
[net,tr,Y,E] = train(net,P,T);
% show network
view(net)
```

Classification of a 4-class problem with a multilayer perceptron (3/4)

Evaluate network performance and plot results

```
% evaluate performance: decoding network response
[m,i] = max(T);
                                 % target class
  m,j] = max(Y); % predicted class
= length(Y); % number of all samples
= 0; % number of missclassified samples
find(i-j), % if there exist missclassified samples
k = length(find(i-j)); % get a number of missclassified samples
[m,i] = max(Y);
N = length(Y);
k = 0;
if find(i-j),
end
fprintf('Correct classified samples: %.1f%% samples\n', 100*(N-k)/N)
% plot network output
figure;
subplot(211)
plot(T')
title('Targets')
ylim([-2 2])
grid on
subplot(212)
plot(Y')
title('Network response') xlabel('# sample')
ylim([-2 2])
grid on
```

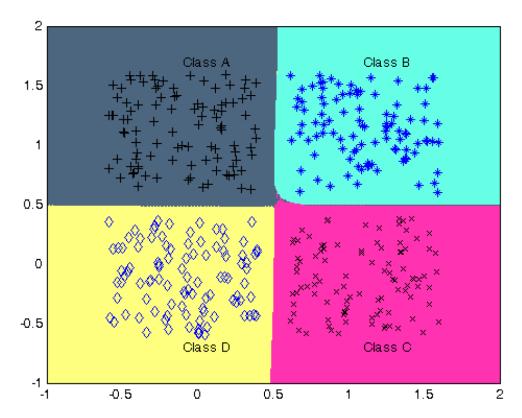




Classification of a 4-class problem with a multilayer perceptron (4/4)

Plot classification result for the complete input space

```
% generate a grid
span = -1:.01:2;
[P1,P2] = meshgrid(span,span);
pp = [P1(:) P2(:)]';
% simualte neural network on a grid
aa = net(pp);
% plot classification regions based on MAX activation
figure(1)
m = mesh(P1,P2,reshape(aa(1,:),length(span),length(span))-5);
set(m, 'facecolor', [1 0.2 .7], 'linestyle', 'none');
hold on
m = mesh(P1,P2,reshape(aa(2,:),length(span),length(span))-5);
set(m,'facecolor',[1 1.0 0.5],'linestyle','none');
m = mesh(P1,P2,reshape(aa(3,:),length(span),length(span))-5);
set(m, 'facecolor', [.4 1.0 0.9], 'linestyle', 'none');
m = mesh(P1,P2,reshape(aa(4,:),length(span),length(span))-5);
set(m, 'facecolor', [.3.40.5], 'linestyle', 'none');
view(2)
```



Exercises Part 2

- 1. Train and test a multilayer perceptron to perform classification of a 5-class problem. Use dataset_mlp.mat (X are inputs, T are targets).
- 2. Plot classification result for the complete input space.

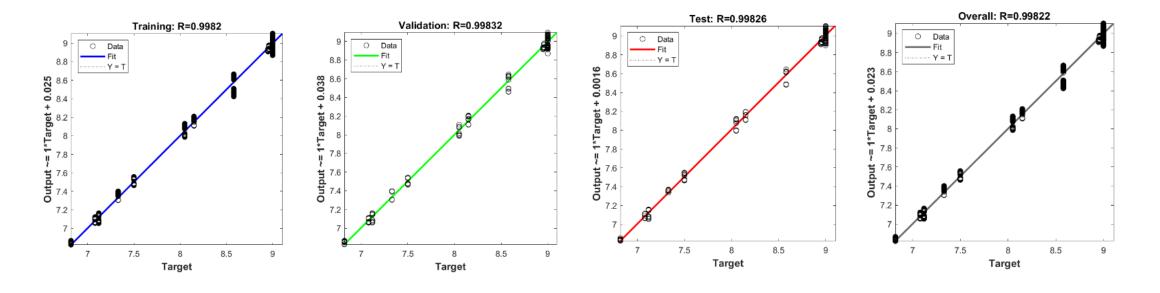
Fitnet

Generate fitting neural network (Fitnet)

```
net = fitnet(hiddenSizes,trainFcn)
x= inputs;
t = targets;
% Create a Fitting Network
hiddenLayerSize = 10;
net = fitnet(hiddenLayerSize);
net = train(net, x, t);
output=net(net, x);
```

Plot linear regression

plotregression(targs1,outs1,'name1',targs2,outs2,'name2',...)



Exercises Part 3

- 1. Train and test a fitting neural network (Fitnet) using dataset_regression.mat.
- 2. Evaluate the performance by plotting the regression and the error histogram.

Patternnet

Generate pattern recognition network (patternnet)

net = patternnet(hiddenSizes, trainFcn, performFcn)

creates an object named *net* of kind network, representing a 2-layer ANN.

- The number of hidden units has to be provided as a single integer number, expressing the size of the hidden layer, or as an integer row vector, whose elements indicate the size of the correspondent hidden layers.
- The second optional parameter selects the training algorithm by a string saved in the *trainFcn* property, which in the default case takes the value 'trainscg' (Scaled Conjugate Gradient Descent methods).
- The third optional parameter selects the performance function by a string saved in the *performFcn* property, which in the default case takes the value 'crossentropy'.

The object has several options, which can be reached by the dot notation *object.property* or explore by clicking on the interactively visualization of the object in the *Matlab Command Window*, which allows to see all the available options for each property too.

The network object is still not fully defined, since some variables will be adapted to fit the data dimension at the calling of the function train.

Dataset

Data for ANNs training (as well as for others available Machine Learning methods) must be provided in matrix form, storing each sample column-wise.

For example, data to define the *XOR* problem can be simply defined via an input matrix *X* and a target matrix *Y* as:

```
X = [0 \ 0 \ 1 \ 1; \ 0 \ 1 \ 0 \ 1];

Y = [0 \ 1 \ 1 \ 0];
```

- For 2-class problem targets can be provided as a row vector of the same length of the number of samples.
- For multi-class problem (and as an alternative for 2-class problem too) targets can be provided in the one-hot encoding form, i.e. as a matrix with as many columns as the number of samples, each one composed by all 0 with only a 1 in the position indicating the class.

ind2vec and **vec2ind** allow indices to be represented either by themselves, or as vectors containing a 1 in the row of the index they represent.

Configuration

Once we have defined data, the network can be fully defined and designed by the command:

net = configure(net , X, Y);

- For each layer, an object of kind *nnetLayer* is created and stored in a cell array under the field *layers* of the *network* object. The number of connections (the weights of the network) for each units corresponds to the layer input dimension.
- The options of each layer can be reached by the dot notation object.layer{numberOfLayer}.property.
- The field initFcn contains the weights initialization methods.
- The activation function is stored in the transferFcn property.
- In the hidden layers the default values is the 'tansig' (Hyperbolic Tangent Sigmoid), whereas the output layers has the 'logsig' (Logistic Sigmoid) or the 'softmax' for 1-dimensional and multi-dimensional target respectively.
- The 'crossentropy' penalty function is set by default in the field performFcn.

Training (1/7)

The function *train* itself makes available many options (as for instance *useParallel* and *useGPU* for heavy computations) directly accessible from its interactive help window. However, it can take as input just the *network* object, the *input* and the *target* matrices.

The optimization starts by dividing data in *Training*, *Validation* and *Test* sets. The splitting ratio can be changed by the options *divideParam*.

In the default setting, data are randomly divided, but if you want for example to decide which data are used for *test*, you can change the way the data are distributed by the option *divideFcn*.

In this case, because of the small size of the dataset, we drop validation and test by setting:

net.divideFcn = ' '

Training (2/7)

In the following code, we set the training function to the classic gradient descent method 'traingd', we deactivate the training interactive GUI by net.trainParam.showWindow (boolean) and activate the printing of the training state in the Command Window by net.trainParam.showCommandLine(boolean). Also the learning rate is part of the trainParam options under the fields Ir.

```
net.trainFcn = 'traingd'
net.trainParam.showWindow = 0
net.trainParam.showCommandLine = 1
net.trainParam.lr = 0.01
```

Training (3/7)

Training starts by the calling: [net, t r] = train(net, X, Y)

this generates a printing, ending in this case with:

Epoch 825/1000, Time 0.426, Performance 0.51544/0, Gradient 0.15234/1e-05, Validation Checks 0/6 Epoch 850/1000, Time 0.439, Performance 0.50987/0, Gradient 0.14626/1e-05, Validation Checks 0/6 Epoch 875/1000, Time 0.452, Performance 0.50472/0, Gradient 0.14073/1e-05, Validation Checks 0/6 Epoch 900/1000, Time 0.467, Performance 0.49994/0, Gradient 0.13569/1e-05, Validation Checks 0/6 Epoch 925/1000, Time 0.48, Performance 0.49549/0, Gradient 0.1311/1e-05, Validation Checks 0/6 Epoch 950/1000, Time 0.493, Performance 0.49133/0, Gradient 0.12693/1e-05, Validation Checks 0/6 Epoch 975/1000, Time 0.506, Performance 0.48742/0, Gradient 0.12313/1e-05, Validation Checks 0/6 Epoch 1000/1000, Time 0.518, Performance 0.48373/0, Gradient 0.11968/1e-05, Validation Checks 0/6 Training with TRAINGD completed: Maximum epoch reached.

Training (4/7)

The training stops after the max number of epochs is reached (which can be set by options *object.trainParam.epochs*).

Each column shows the state of one of the stopping criteria used.

The output variable *tr* stores the training options.

The fields *perf*, *vperf* and *tperf* contain the performance of the network evaluated at each epoch on the *Training*, *Validation* and *Test* sets respectively (the last two are *NaN* in this case), which can be used for example to plot performances.

If we pass data organized in a single matrix, the function will exploit the full batch learning method accumulating gradients overall the training set.

Training (5/7)

To set a mini-batch mode, data have to be manually split in sub-matrix with the same number of column and organized in a *cell-array*. However, let us consider for a moment a general data set composed by N samples in the features space \mathbb{R}^D with a target of dimension C, so that $X \in \mathbb{R}^{D \times N}$ and $Y \in \mathbb{R}^{C \times N}$. All the mini-batches have to be of the same size b, so that it is in general convenient to choose the batch size to be a factor of N.

In this case, we can generate data for the training function organizing the input and target in the correspondent *cell-array*.

Training (6/7)

```
N = size(X, 2);
                                   % number of samples
n_batch = N/ batchsize;
                                   % number of batches
input{n_batch} = [ ];
                                   % input cell –array initialization
target{n_batch} = [ ];
                                   % target cell –array initialization
p = randperm(N);
                                   % generating a random permutated index for data shuffling
X = X(:,p);
                                   % samples permutation
Y = Y(:, p);
                                   % target permutation
for i = 1 : n_batch
  input{i} = X(:, (1 : batchsize) + (i -1) * batchsize);
  target{i} = Y(:, (1 : batchsize) + (i -1) * batchsize);
end
```

Training (7/7)

However, in order to perform a pure Stochastic Gradient Descent optimization, in which the ANNs parameters are updated for each sample, the training function 'train' has to be employed skipping to split data previously. A remark has to be done since this particular function does not support the GPU computing. The network (trained or not) can be easily evaluated on data by passing the input data as argument to a function named as the network object. Performance of the prediction with respect to the targets can be evaluated by the function perform according to the correspondent loss function option *object.performFcn*:

f = net(X);
perform(net, Y, f)

Stopping criteria and Regularization (1/2)

Early stopping is a well known procedure in Machine Learning to avoid overfitting and improve generalization. Different kind of stopping criteria can be used regulated by the network object options in the field *trainParam*. Arbitrarily methods are based on the number of epochs (*epochs*) and the training time (*time*, default *Inf*).

A criterion based on the training set:

- check the loss (object.trainParam.goal, default = 0) or
- the parameters gradients (object.trainParam.min_grad, default = 10-6) to reach a minimum threshold.

Stopping criteria and Regularization (2/2)

A general early stopping method is implemented by checking the error on the validation set and interrupting training when validation error does not improve for a number of consecutive epochs given by max_fail (default=6).

of the network object. The field *regularization* contains the weight (real number in [0, 1]) balancing the contribution of a term trying to minimizing the norm of the network weights versus the satisfaction of the penalty function. However, the network is designed to mainly rely on the validation checks, indeed regularization applies only to few kind of penalties and the default weight is 0.

Drawing separation surfaces (1/3)

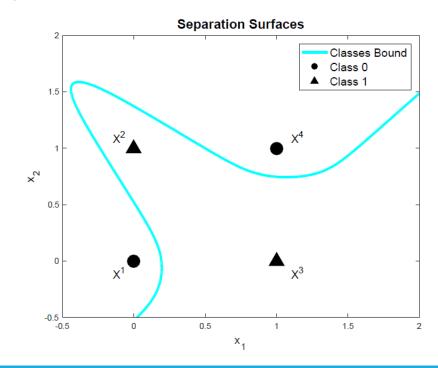
When dealing with low dimensional data (as in the *XOR* case), can be useful to visualize the prediction of the network directly in the input space.

The network predictions will be evaluated on a grid of the input space, generated by the Matlab function *meshgrid*, since the main functions used for the plotting (*contour* or, if you want a color surface *pcolor*) require as input three matrices of the same dimensions expressing, in each correspondent element, the coordinates of a 3-D point (which in our case will be first input dimension, second input dimension and prediction).

Drawing separation surfaces (2/3)

Once we trained the network described until now, the boundary for the 2-classes separation is generated by the following code

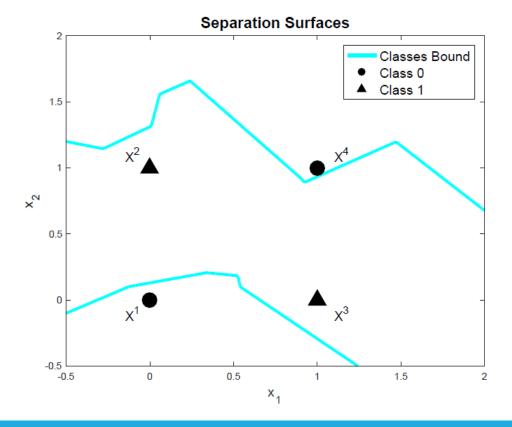
```
% generating input space grid
[xp1, xp2] = meshgrid(-0.5 : 0.01 : 2, -0.5 : 0.01 : 2);
                                                             % network evaluation on the gridding (reshaped to fit network input dimension)
f = net([xp1(:)'; xp2(:)']);
                                                             % reshaping prediction in correspondent matrix form
f = reshape(f, size(xp1, 1), []);
contour(xp1, xp2, f, [.5, .5], 'LineWidth', 3 , 'Color', 'c');
                                                             % drawing separation surfaces
hold on;
scatter(X(1, [1, 4]), X(2, [1, 4]), 200, 'o', 'filled', 'MarkerEdgeColor', 'k', ...
'MarkerFaceColor', 'k', 'LineWidth', 2);
                                                             % drawing data points
scatter(X(1, [2, 3]), X(2, [2, 3]), 200, '^', 'filled', 'MarkerEdgeColor', 'k', ...
'MarkerFaceColor', 'k', 'LineWidth', 2);
                                                             %setting axis bounds
axis([-0.5, 2, -0.5, 2]);
%labeling data points
c={'X^1', 'X^2', 'X^3', 'X^4'};
                                                              %labels
                                                             %labels horizontal translation wrt points
dx = [-.15, -.15, .1, .1];
25dy=[-.1, .1, -.1, 1];
                                                             %labels vertical translation wrt points
text(X(1, :) + dx, X(2, :) + dy, c, 'FontSize', 14); %showing labels as text
%plotlabels
xlabel('x_1', 'FontSize', 14)
ylabel('x_2', 'FontSize', 14)
title('SeparationSurfaces', 'FontSize', 16);
h = legend({'ClassesBound', 'Class0', 'Class1'}, 'Location', 'NorthEast');
set(h, 'FontSize', 14);
```



Drawing separation surfaces (3/3)

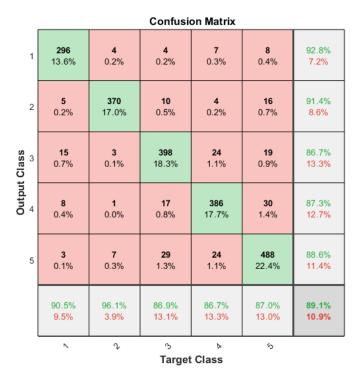
We report the same evaluation after the training of a 4-layers network using 5, 3 and 2 units in the first, second and third hidden layers respectively, each one using the *ReLU* as activation ('poslin' in Matlab). This new network can be defined by:

```
% 3+output layers network initialization
n = patternnet([5, 3, 2]);
% network configuration
net = configure(n, X, Y);
% setting optimization function
net.trainFcn = 'traingd';
% setting data splitting ratios (illustrative)
net.divideParam.trainRatio = 1;
net.divideParam.valRat io = 0:
net.divideParam.testRatio = 0;
net.trainParam.showCommandLine = 1;
net.trainParam.lr = 0.01;
% setting the activation layer-wise
net.layers{1}.transferFcn = 'poslin';
net.layers{2}.transferFcn = 'poslin';
net.layers{3}.transferFcn = 'poslin';
```



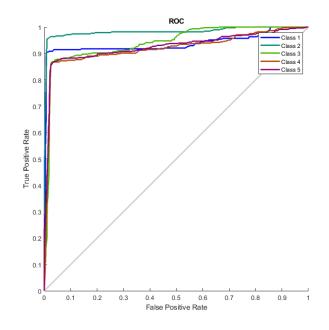
Plot classification confusion matrix

plotconfusion(targets1,outputs1, 'name1',targets2,outputs2, 'name2',...)

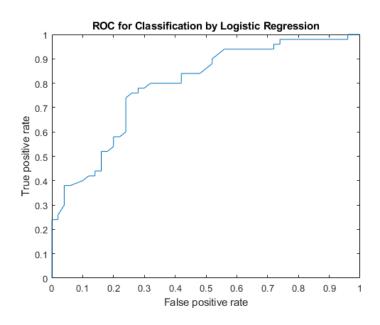


Plot receiver operating characteristic

plotroc(targs1,outs1,'name1',targs2,outs2,'name2',...)



[X,Y,T,AUC] = perfcurve(labels,scores,posclass)



scores: a vector of classifier predictions

labels: true class labels

posclass: positive class label.

Hyperparameters

- Number of neurons
- Number of hidden layers
- Activation functions
- Learning Rate
- Momentum
- Performance function

```
num_neurons = 5 : 1 : 15;
for i = 1 : numel(num_neurons)
    k = num_neurons(i);
    ...
end
```

Exercises Part 4

- 1. Train and test a pattern recognition neural network(Patternnet) using dataset_classification.mat.
- Evaluate the performance by plotting the confusion matrix and ROC.
 Using the command[c,cm]=confusion(testT,testY) compute the overall percentages of correct and incorrect classification

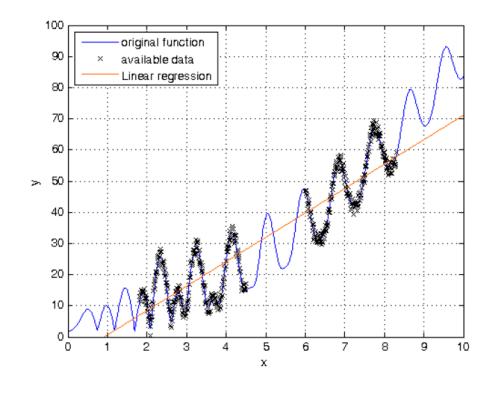
Function approximation with RBFN

Data generator

```
%% Data generator function
function [X,Xtrain,Ytrain,fig] = data_generator()
  % data generator
  X = 0.01:.01:10;
  f = abs(besselj(2,X*7).*asind(X/2) + (X.^1.95)) + 2;
  fig = figure;
  plot(X,f,'b-')
  hold on
  grid on
  % available data points
  Ytrain = f + 5*(rand(1,length(f))-.5);
  Xtrain = X([181:450 601:830]);
  Ytrain = Ytrain([181:450 601:830]);
  plot(Xtrain,Ytrain,'kx')
  xlabel('x')
  ylabel('v')
  ylim([0 100])
  legend('original function', 'available data', 'location', 'northwest')
end
```

Linear Regression

```
close all, clear all, clc, format compact
% generate data
[X,Xtrain,Ytrain,fig] = data_generator();
% no hidden layers
net = feedforwardnet([]);
% one hidden layer with linear transfer functions
% net = feedforwardnet([10]);
% net.layers{1}.transferFcn = 'purelin';
% set early stopping parameters
net.divideParam.trainRatio = 1.0; % training set
                                               % training set [%] % validation set [%]
net.divideParam.valRatio = 0.0;
net.divideParam.testRatio = 0.0;
                                               % test set [%]
% train a neural network
net.trainParam.epochs = 200;
net = train(net,Xtrain,Ytrain):
% view net
view (net)
% simulate a network over complete input range
Y = net(X);
% plot network response
figure(fig)
plot(X,Y,'color',[1 .4 0])
legend('original function', 'available data', 'Linear regression', 'location', 'northwest')
```



Exact RBFN

```
% generate data
[X,Xtrain,Ytrain,fig] = data_generator();
                                                                            original function
                                                                            available data
                                                                            Exact RBFN
% choose a spread constant
spread = .4;
% create a neural network
net = newrbe(Xtrain,Ytrain,spread);
% view net
view (net)
% simulate a network over complete input range
Y = net(X);
% plot network response
figure(fig)
plot(X,Y,'r')
legend('original function','available data','Exact RBFN','location','northwest')
```

RBFN

NEWRB, neurons = 40, MSE = 1.94627

```
Performance is 1.94627, Goal is 0
                                                                                                            10<sup>3</sup>
 % generate data
 [X,Xtrain,Ytrain,fig] = data_generator();
 % choose a spread constant
 spread = .2;
                                                                                                           10<sup>2</sup>
 % choose max number of neurons
 K = 40:
 % performance goal (SSE)
 goal = 0;
% number of neurons to add between displays
 Ki = 5;
 % create a neural network
net = newrb(Xtrain,Ytrain,goal,spread,K,Ki);
                                                                                                           10<sup>1</sup>
 % view net
 view (net)
 % simulate a network over complete input range
 Y = net(X);
% plot network response
                                                                                                           10
                                                                                                                                 10
                                                                                                                                           15
                                                                                                                                                    20
                                                                                                                                                              25
                                                                                                                                                                       30
 figure(fig)
plot(X,Y,'r')
                                                                                                                                                40 Epochs
 legend('original function', 'available data', 'RBFN', 'location', 'northwest')
NEWRB, neurons = 0, MSE = 333.938

NEWRB, neurons = 5, MSE = 47.271

NEWRB, neurons = 10, MSE = 12.3371

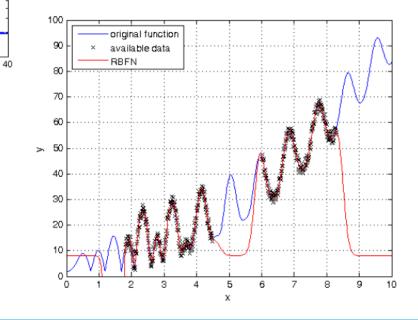
NEWRB, neurons = 15, MSE = 9.26908

NEWRB, neurons = 20, MSE = 4.16992

NEWRB, neurons = 25, MSE = 2.82444

NEWRB, neurons = 30, MSE = 2.43353

NEWRB, neurons = 30, MSE = 2.43353
NEWRB, neurons = 35, MSE = 2.06149
```



Train

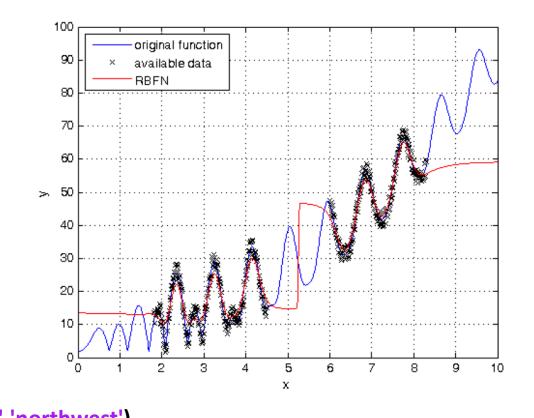
Test

35

-Validation

Generalized Regression Neural Networks (GRNN)

```
% generate data
[X,Xtrain,Ytrain,fig] = data_generator();
% choose a spread constant
spread = .12;
% create a neural network
net = newgrnn(Xtrain,Ytrain,spread);
% view net
view (net)
% simulate a network over complete input range
Y = net(X);
% plot network response
figure(fig)
plot(X,Y,'r')
legend('original function','available data','RBFN','location','northwest')
```

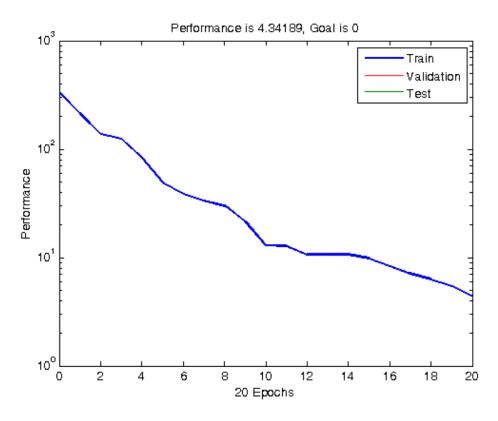


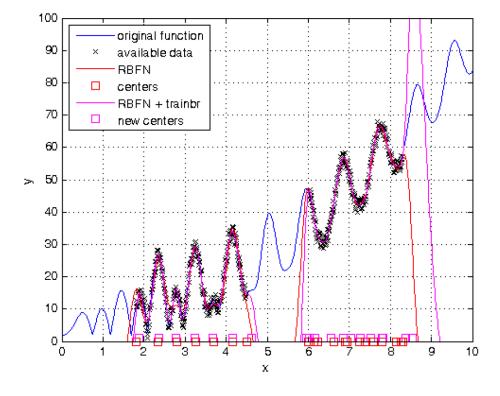
RBFN trained by Bayesian regularization (1/2)

```
generate data
[X,Xtrain,Ytrain,fig] = data generator();
% choose a spread constant spread = .2;
% choose max number of neurons
K = 20;
% performance goal (SSE)
goal = 0;
% number of neurons to add between displays
Ki = 20:
% create a neural network
net = newrb(Xtrain,Ytrain,goal,spread,K,Ki);
% view net
view (net)
% simulate a network over complete input range
Y = net(X);
% plot network response
figure(fig)
plot(X,Y,'r')
% Show RBFN centers
c = net.iw{1};
plot(c,zeros(size(c)),'rs')
legend('original function','available data','RBFN','centers','location','northwest')
% Retrain a RBFN using Bayesian regularization backpropagation
net.trainFcn='trainbr';
net.trainParam.epochs = 100;
% perform Levenberg-Marquardt training with Bayesian regularization
net = train(net,Xtrain,Ytrain);
% simulate a network over complete input range
Y = net(X);
% plot network response
figure(fig)
plot(X,Y, m')
% Show RBFN centers
c = net.iw{1};
plot(c,ones(size(c)),'ms')
legend('original function', 'available data', 'RBFN', 'centers', 'RBFN + trainbr', 'new centers', 'location', 'northwest')
```

RBFN trained by Bayesian regularization (2/2)

NEWRB, neurons = 0, MSE = 334.852NEWRB, neurons = 20, MSE = 4.34189





MLP

% generate data [X,Xtrain,Ytrain,fig] = data_generator();		100 90			iginal t		- 1				:	!	:		
% % create a neural network net = feedforwardnet([12 6]); % set early stopping parameters net.divideParam.trainRatio = 1.0; net.divideParam.valRatio = 0.0; net.divideParam.testRatio = 0.0; % train a neural network net.trainParam.epochs = 200; net = train(net,Xtrain,Ytrain); %	% training set [%] % validation set [%] % test set [%]	80 70 60 >- 50			/ailable	e data						*	Ň	Λ	
		40					 &	À		····/		V			
<pre>% view net view (net) % simulate a network over complete inp Y = net(X); % plot network response figure(fig) plot(X,Y,'color',[1 .4 0]) legend('original function','available data</pre>		20 10) 	1	2	3		4	5 x	<u>V</u>	6	7	8	9	

Exercises Part 5

1. Train and test a Radial Basis Neural Networks (RBFN) with the following inputs and outputs

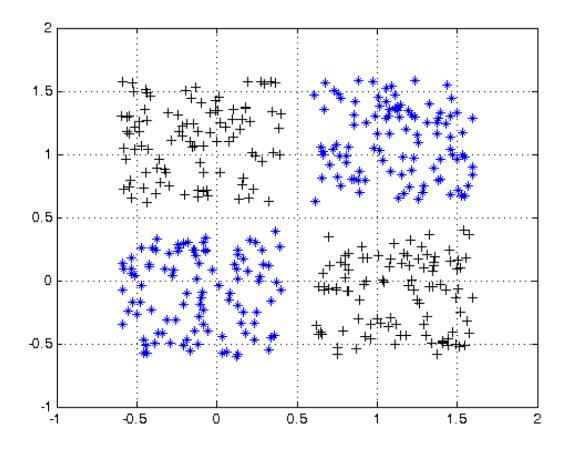
- 2. Repeat the exercise 1 considering the case of underlapping Neurons (eg=0.02 and sc=0.01)
- 3. Repeat the exercise 1 considering the case of overlapping Neurons (eq=0.02 and sc=100)

Radial Basis Function Networks for Classification of XOR problem

Classification of XOR problem with an exact RBFN (1/4)

Create input data

```
close all, clear all, clc, format compact
% number of samples of each class
K = 100;
% define classes
q = .6; % offset of classes
% define 2 groups of input data
A = [rand(1,K)-q rand(1,K)+q;
  rand(1,K)+q rand(1,K)-q];
B = [rand(1,K)+q rand(1,K)-q;
  rand(1,K)+q rand(1,K)-q];
% plot data
plot(A(1,:),A(2,:),'k+',B(1,:),B(2,:),'b*')
grid on
hold on
```



Classification of XOR problem with an exact RBFN (2/4)

```
Define output coding
% coding (+1/-1) for 2-class XOR problem
a = -1:
b = 1;
  Prepare inputs & outputs for network training
% define inputs (combine samples from all four classes)
P = [A B];
% define targets
T = [repmat(a,1,length(A)) repmat(b,1,length(B))];
  Create an exact RBFN
% choose a spread constant
spread = 1;
% create a neural network
net = newrbe(P,T,spread);
% view network
view(net)
```

Classification of XOR problem with an exact RBFN (3/4)

```
Evaluate network performance
% simulate a network on training data
Y = net(P);
% calculate [%] of correct classifications

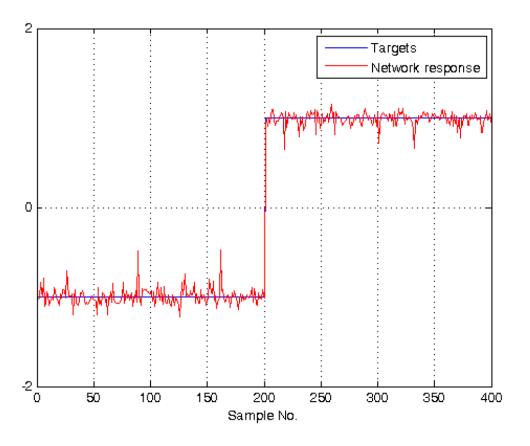
correct = 100 * length(find(T.*Y > 0)) / length(T);

fprintf('\nSpread = %.2f\n',spread)

fprintf('Num of neurons = %d\n',net.layers{1}.size)

fprintf('Correct class = %.2f %%\n',correct)

% plot targets and network response
figure;
plot(T')
hold on
grid on
plot(Y'.'r'
ylim([-2 2])
set(gca,'ytick',[-2 0 2])
legend('Targets','Network response') xlabel('Sample No.')
Spread = 1.00
Num of neurons = 400
Correct class = 100.00 %
```

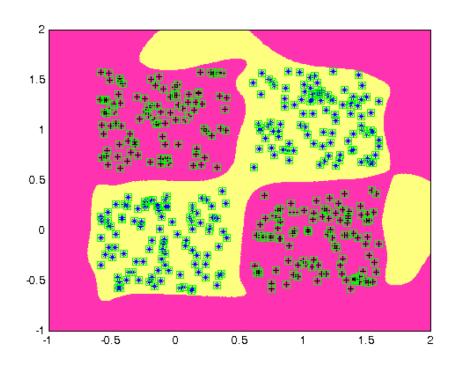


Classification of XOR problem with an exact RBFN (4/4)

Plot classification result

```
% generate a grid
span = -1:.025:2;
[P1,P2] = meshgrid(span,span);
pp = [P1(:) P2(:)]';
% simualte neural network on a grid
aa = sim(net,pp);
% plot classification regions based on MAX activation
figure(1)
ma = mesh(P1,P2,reshape(-aa,length(span),length(span))-5);
mb = mesh(P1,P2,reshape( aa,length(span),length(span))-5);
set(ma,'facecolor',[1 0.2 .7],'linestyle','none');
set(mb,'facecolor',[1 1.0 .5],'linestyle','none');
view(2)
```

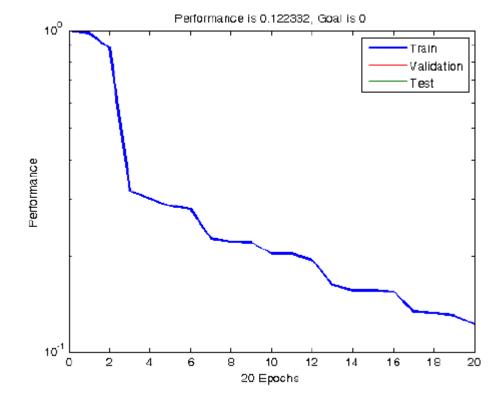
Plot RBFN centers plot(net.iw{1}(:,1),net.iw{1}(:,2),'gs')



Classification of XOR problem with a RBFN (1/3)

Create a RBFN

```
% NEWRB algorithm
% The following steps are repeated until the network's mean squared error
% falls below goal:
% 1. The network is simulated
% 2. The input vector with the greatest error is found % 3. A radbas neuron is added with weights equal to that vector % 4. The purelin layer weights are redesigned to minimize error
% choose a spread constant
spread = 2;
% choose max number of neurons
K = 20:
% performance goal (SSE)
goal = 0;
% number of neurons to add between displays
Ki = 4:
% create a neural network
net = newrb(P,T,goal,spread,K,Ki);
% view network
view(net)
NEWRB, neurons = 0, MSE = 1
NEWRB, neurons = 4, MSE = 0.302296
NEWRB, neurons = 8, MSE = 0.221059
NEWRB, neurons = 12, MSE = 0.193983
NEWRB, neurons = 16, MSE = 0.154859
NEWRB, neurons = 20, MSE = 0.122332
```

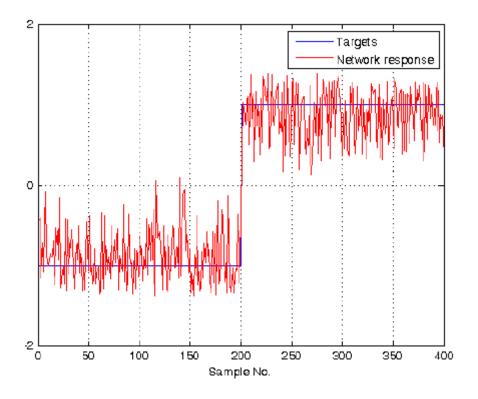


Classification of XOR problem with a RBFN (2/3)

Evaluate network performance

```
% simulate RBFN on training data
Y = net(P);
% calculate [%] of correct classifications
correct = 100 * length(find(T.*Y > 0)) / length(T);
fprintf('\nSpread = %.2f\n',spread)
fprintf('Num of neurons = %d\n',net.layers{1}.size)
fprintf('Correct class = %.2f %%\n',correct)
% plot targets and network response
figure;
plot(T')
hold on
grid on
plot(Y','r')
ylim([-2 2])
set(gca,'ytick',[-2 0 2])
legend('Targets','Network response')
xlabel('Sample No.')

Spread = 2.00
Num of neurons = 20
Correct class = 99.50 %
```



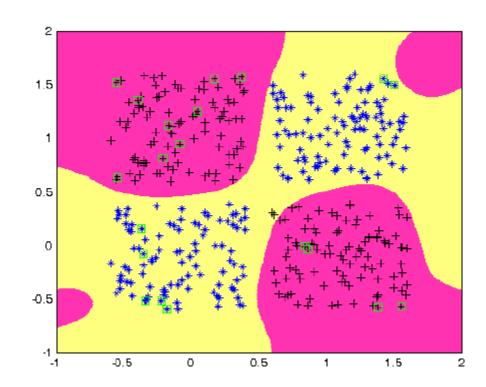
Classification of XOR problem with a RBFN (3/3)

Plot classification result

```
% generate a grid
span = -1:.025:2;
[P1,P2] = meshgrid(span,span);
pp = [P1(:) P2(:)]';
% simualte neural network on a grid
aa = sim(net,pp);
% plot classification regions based on MAX activation
figure(1)
ma = mesh(P1,P2,reshape(-aa,length(span),length(span))-5);
mb = mesh(P1,P2,reshape( aa,length(span),length(span))-5);
set(ma,'facecolor',[1 0.2 .7],'linestyle','none');
set(mb,'facecolor',[1 1.0 .5],'linestyle','none');
view(2)
```

Plot RBFN centers

plot(net.iw{1}(:,1),net.iw{1}(:,2),'gs')



Exercises Part 6

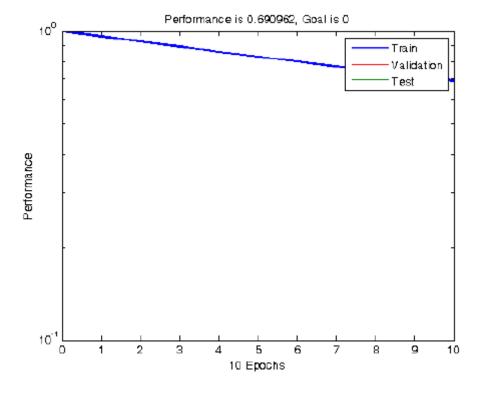
- 1. Train and test a Radial Basis Function Networks to perform classification of a 5-class problem. Use dataset_mlp.mat (X are inputs, T are targets).
- 2. Plot classification result for the complete input space.
- 3. Repeat the exercise 1 considering the case of underlapping Neurons and overlapping Neurons

Bayesian regularization for RBFN

Bayesian regularization for RBFN (1/5)

Create a RBFN

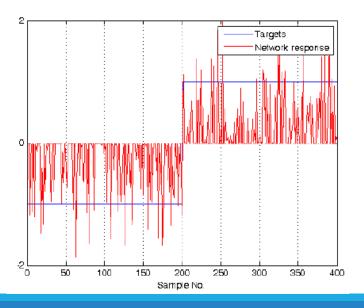
```
% NEWRB algorithm
% The following steps are repeated until the network's mean squared error
% falls below goal:
% 1. The network is simulated
% 2. The input vector with the greatest error is found % 3. A radbas neuron is added with weights equal to that vector % 4. The purelin layer weights are redesigned to minimize error
% choose a spread constant
spread = .1;
% choose max number of neurons
K = 10:
% performance goal (SSE)
goal = 0;
% number of neurons to add between displays
Ki = 2;
% create a neural network
net = newrb(P,T,goal,spread,K,Ki);
% view network
view(net)
NEWRB, neurons = 0, MSE = 1
NEWRB, neurons = 2, MSE = 0.928277
NEWRB, neurons = 4, MSE = 0.855829
NEWRB, neurons = 6, MSE = 0.798564
NEWRB, neurons = 8, MSE = 0.742854
NEWRB, neurons = 10, MSE = 0.690962
```



Bayesian regularization for RBFN (2/5)

```
Evaluate network performance
% check RBFN spread
actual_spread = net.b{1}
% simulate RBFN on training data
 Y = net(P);
% calculate [%] of correct classifications
correct = 100 * length(find(T.*Y > 0)) / length(T);
fprintf('\nSpread = %.2f\n',spread)
fprintf('Num of neurons = %d\n',net.layers{1}.size)
fprintf('Correct class = %.2f %%\n',correct)
% plot targets and network response
% to see how good the network learns the data
figure;
plot(T')
 ylim([-2 2])
 set(gca,'ytick',[-2 0 2])
hold on
grid on
 plot(Y','r')
legend('Targets','Network response') xlabel('Sample No.')
```

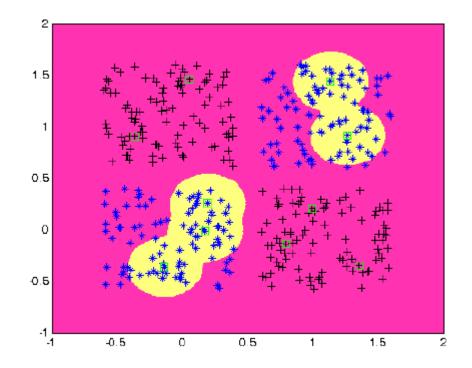
```
actual_spread =
8.3255
8.3255
8.3255
8.3255
8.3255
8.3255
8.3255
8.3255
8.3255
8.3255
8.3255
8.3255
Spread = 0.10
Num of neurons = 10
Correct class = 79.50 %
```



Bayesian regularization for RBFN (3/5)

Plot classification result

```
% generate a grid
span = -1:.025:2;
[P1,P2] = meshgrid(span,span);
pp = [P1(:) P2(:)]';
% simualte neural network on a grid
aa = sim(net,pp);
% plot classification regions based on MAX activation
figure(1)
ma = mesh(P1,P2,reshape(-aa,length(span),length(span))-5);
mb = mesh(P1,P2,reshape(aa,length(span),length(span))-5);
set(ma, 'facecolor', [1 0.2 .7], 'linestyle', 'none');
set(mb, 'facecolor', [1 1.0 .5], 'linestyle', 'none');
view(2)
% plot RBFN centers
plot(net.iw{1}(:,1),net.iw{1}(:,2),'gs')
```



Bayesian regularization for RBFN (4/5)

% plot targets and network response

legend('Targets','Network response')

figure;

hold on grid on plot(Y','r')

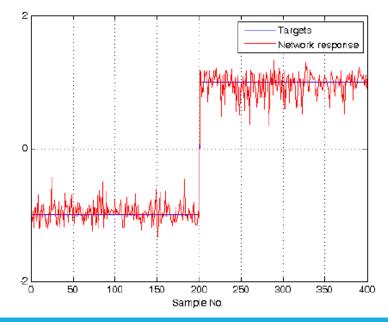
ylim([-2 2])

set(gca,'ytick',[-2 0 2])

xlabel('Sample No.')

```
    Retrain a RBFN using Bayesian regularization backpropagation % define custom training function: Bayesian regularization backpropagation net.trainFcn='trainbr'; % perform Levenberg-Marquardt training with Bayesian regularization net = train(net,P,T);
    Evaluate network performance after Bayesian regularization training % check new RBFN spread spread after training = net.b{1} % simulate RBFN on training data Y = net(P); % calculate [%] of correct classifications correct = 100 * length(find(T.*Y > 0)) / length(T); fprintf('Num of neurons = %d\n',net.layers{1}.size) fprintf('Correct class = %.2f %%\n',correct)
```

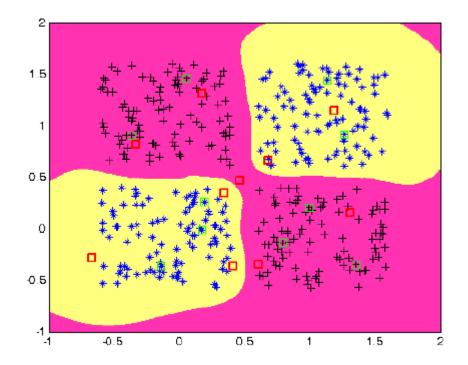
```
spread_after_training =
2.9924
3.0201
0.7809
0.5933
2.6968
2.8934
2.2121
2.9748
2.7584
3.5739
Num of neurons = 10
Correct class = 100.00 %
```



Bayesian regularization for RBFN (5/5)

Plot classification result after Bayesian regularization training

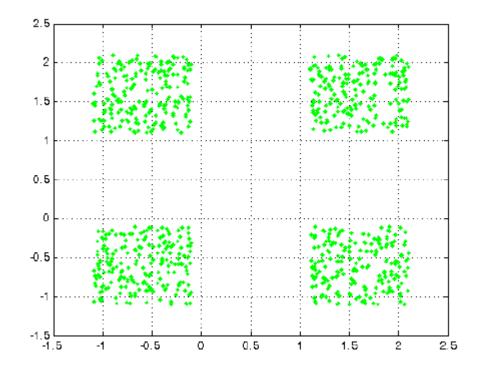
```
% generate a grid
span = -1:.025:2;
[P1,P2] = meshgrid(span,span);
pp = [P1(:) P2(:)]';
% simualte neural network on a grid
aa = sim(net,pp);
% plot classification regions based on MAX activation
figure(1)
ma = mesh(P1,P2,reshape(-aa,length(span),length(span))-5);
mb = mesh(P1,P2,reshape(aa,length(span),length(span))-5);
set(ma, 'facecolor', [1 0.2 .7], 'linestyle', 'none');
set(mb, 'facecolor', [1 1.0 .5], 'linestyle', 'none');
view(2)
% plot modified RBFN centers
plot(net.iw{1}(:,1),net.iw{1}(:,2), 'rs', 'linewidth', 2);
```



1D and 2D Self Organized Map

1D-SOM(1/2)

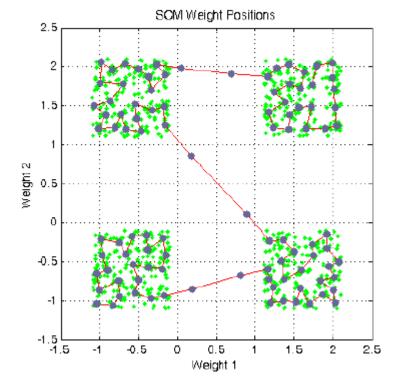
Define 4 clusters of input data close all, clear all, clc, format compact % number of samples of each cluster K = 200; % offset of classes q = 1.1; % define 4 clusters of input data P = [rand(1,K)-q rand(1,K)+q rand(1,K)+q rand(1,K)-q; rand(1,K)+q rand(1,K)-q rand(1,K)-q rand(1,K)-q]; % plot clusters plot(P(1,:),P(2,:),'g.') hold on grid on



1D-SOM(2/2)

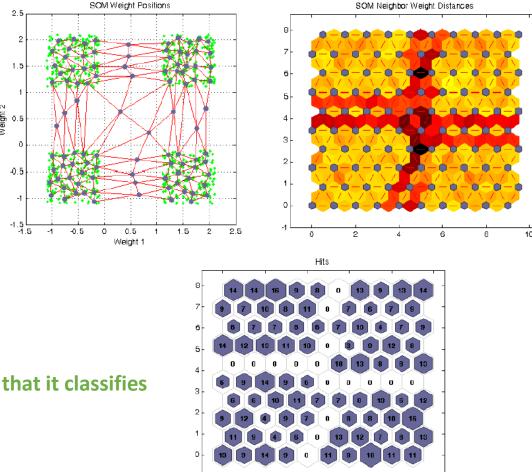
Create and train 1D-SOM

```
% SOM parameters
dimensions = [100];
coverSteps = 100;
initNeighbor = 10;
topologyFcn = 'gridtop';
distanceFcn = 'linkdist';
% define net
net1 = selforgmap(dimensions,coverSteps, ...
  initNeighbor,topologyFcn,distanceFcn);
% train
[net1,Y] = train(net1,P);
  Plot 1D-SOM results
% plot input data and SOM weight positions
plotsompos(net1,P);
grid on
```



2D-SOM

Create and train 2D-SOM % SOM parameters dimensions = [10 10]; coverSteps = 100; initNeighbor = 4; weight 2 topologyFcn = 'hextop'; distanceFcn = 'linkdist'; % define net net12 = selforgmap(dimensions,coverSteps, ...
initNeighbor,topologyFcn,distanceFcn); % train 0.5 [net2,Y] = train(net2,P); Weight 1 Plot 2D-SOM results % plot input data and SOM weight positions plotsompos(net2,P); grid on % plot SOM neighbor distances plotsomnd(net2) % plot for each SOM neuron the number of input vectors that it classifies figure plotsomhits(net2,P)



Exercises Part 7

- 1. Using One-Dimensional Self-organizing Map classify the following points into natural classes.
 angles = 0:0.5*pi/99:0.5*pi;
 X = [sin(angles); cos(angles)];
- 4. Using Two-Dimensional Self-organizing Map classify 1000 two-element vectors in a rectangle. X = rands(2, 1000);

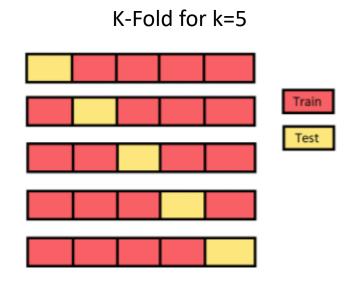
Cross-Validation

Partition data for cross-validation (KFold)

cvpartition defines a random partition on a data set. Use this partition to define training and test sets
for validating a statistical model using cross-validation. Use training to extract the training indices and
test to extract the test indices for cross-validation. Use repartition to define a new random partition of
the same type as a given cvpartition object.

c = cvpartition(n,'KFold',k)
c = cvpartition(group, 'KFold',k,'Stratify',stratifyOption)

- When you specify group as the first input argument, cvpartition discards rows of observations corresponding to missing values in group.
- If you specify 'Stratify', false, then cvpartition ignores the class information in group and creates a nonstratified random partition.
 Otherwise, the function implements stratification by default.



Partition data for cross-validation (Holdout)

In the non-exhaustive method, we don't compute for all possible combinations of the original data. This is the simplest method of all. In Holdout validation, the data is randomly partitioned into train and test set.

Most of the times it is 70/30 or 80/20 split.

We train our model in the training set, and it'll be tested in the test set to see how well the model is performing for unknown events.

```
c = cvpartition(n,'Holdout',p)
c = cvpartition(group,'Holdout',p,'Stratify',stratifyOption)

idxTrain = training(c);
dataTrain = data(idxTrain, :);
idxTest = test(c);
dataTest = data(idxTest, :);
```

Holdout Validation- 70% train and 30% test



Partition data for cross-validation (Leaveout)

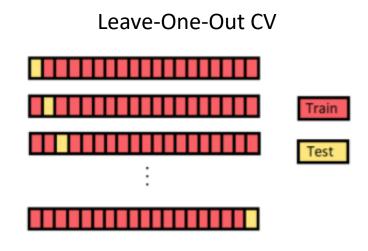
• Leave-one-out is a special case of KFold in which the number of folds equals the number of observations.

In LOO, one observation is taken out of the training set as a validation set. We will train the model without this validation set and later test whether it correctly classify the observation.

c = cvpartition(n,'Leaveout')

c = cvpartition(n,'Resubstitution')

c that does not partition the data.
 Both the training set and the test set contain all of the original n observations.



Exercises Part 8

- 1. Train and test a pattern recognition neural network(Patternnet) using $dataset_classification.mat$ performing k-Fold cross validation with k = 10.
- 2. Evaluate the performance by plotting the confusion matrix and ROC. Get the best network in terms of performance.