Undergraduate Summer Research Project

A Study into the Feasibility of Using Machine Learning to Evaluate the Severity of Coronary Artery Disease.

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Abstract

Coronary heart disease is where atherosclerosis occurs in the coronary arteries. The aim of this project was to investigate the possibility of using Computational Fluid Dynamics (CFD) to train an Artificial Neural Network (ANN) to predict the pressure drop across an idealised stenosis in a coronary artery. A CFD model was created to represent an idealised stenosis and the CFD model creation and analysis were automated to provide data to train an ANN. Initially a Radial Basis Function (RBF) network was trained on the generated data, however this was unsuccessful and so a Multilayer Perceptron (MLP) network was tried instead. The MLP network was more successful than the RBF network, and was able to learn the training data with an average test error of 5% (when using 5-10 hidden units and a weight-decay coefficient of 0.3). There were signs of instability with the MLP network however, which was most likely caused by a lack of training data. Further work would be needed in order to fully automate the data creation - this would enable the significant increase in training data that would almost certainly improve the performance of the MLP network.

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1 Introduction

Coronary Heart Disease

Atherosclerosis is a condition where fatty deposits (such as cholesterol) accumulate inside arteries, this narrows the arteries and consequently impedes the blood flow. Coronary heart disease is where atherosclerosis occurs in the coronary arteries (see Figure 1.1 [1]). Coronary heart disease is the most common cause of myocardial ischemia, which occurs when there is a decreased supply of oxygen to the heart muscle caused by a decrease in blood flow to the heart. Myocardial ischemia can lead to a number of complications including: chest pain, irregular heart rhythm, heart failure and heart attack.

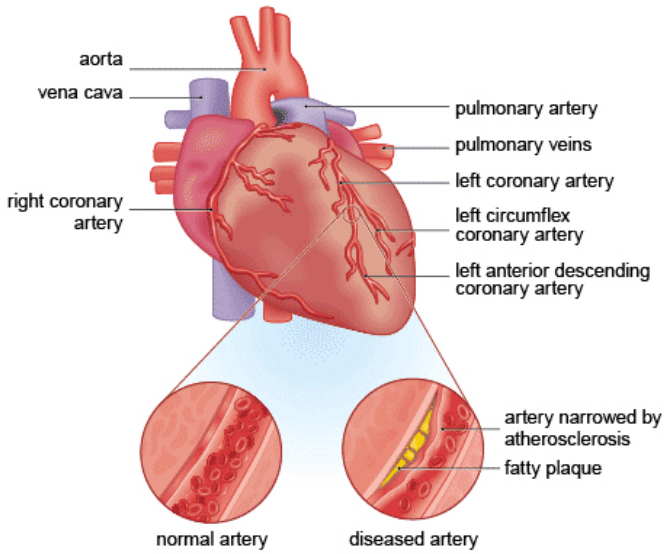

Figure 1.1 – A coronary artery affected by atherosclerosis [1].

Fractional Flow Reserve (FFR)

The fractional flow reserve (FFR) is a dimensionless quantity used to measure the severity of myocardial ischemia in a patient (see Equation 1). In general, if the value of FFR is less than 0.8 then the obstruction is severe enough to cause myocardial ischemia and medical intervention is required.

The FFR is a measure of the pressure drop across the stenosis in the coronary artery and is given as:

$$FFR = \frac{P_b - P_v}{P_a - P_v} \qquad \text{Equation 1}$$

Where: P_b - pressure after lesion (Pa)
P_a - pressure before lesion (Pa)
P_v – central venous pressure (Pa)

However the central venous pressure is close to zero and so is assumed to be negligible [2] hence the equation for the FFR simplifies to:

$$FFR = \frac{P_b}{P_a}$$ Equation 2

Currently the FFR is determined experimentally; a catheter with a transducer pressure sensor at the tip is in inserted into an artery in the groin and then fed to the heart to measure the pressure before and after the stenosis (blockage) in the coronary artery. These pressure measurements need to be taken at maximum blood flow; this is simulated by injecting a drug into the patient (normally adenosine or papaverine). This procedure is unpleasant for the patient and not without risk, hence there is currently research into alternative ways of determining the FFR for a coronary artery.

One non-invasive method of measuring the FFR involves using Computational Fluid Dynamics (CFD). CFD uses a computer to solve the equations that govern fluid flow in order to model the behaviour of fluids. In this process the geometry for the CFD model is taken from an MRI scan, the blood flow through the diseased artery is simulated and the pressure drop is calculated. However, a certain level of skill is required to carry out a CFD analysis and it can be computationally expensive. (This report assumes the reader is familiar with CFD, there are many suitable textbooks which explain the basic principles of CFD; such as: *An introduction to computational fluid dynamics: the finite volume method* by H.K. Versteeg, and W. Malalalsekera [3]).

Machine Learning

Due to the high cost of CFD (in terms of time and money), it is necessary to investigate a quicker and cheaper non-invasive way to measure the FFR. One possible method is to train a machine learning system to predict the FFR value across a stenosis when given a set of input parameters. Machine learning is a branch of computer science which involves training a computer to perform a task (i.e. filter spam emails, predict the weather, recognise handwriting) without being explicitly programmed. One type of machine learning system is an Artificial Neural Network (ANN - see Figure 1.2 [4]). An artificial neural network consists of several layers; an input layer, one or more hidden layers and an output layer. These layers

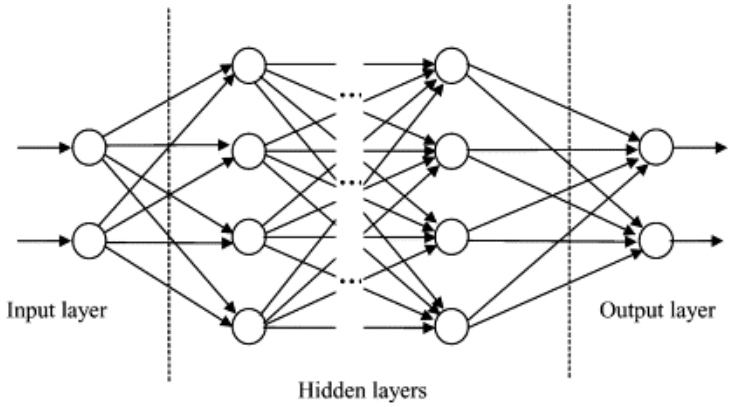

Figure 1.2 – Schematic diagram of a feed-forward artificial neural network.

contain interconnected neurons (or nodes) which 'can be seen as computational units that receive inputs and process them to obtain an output' [5]. The connections between the neurons are weighted and determine how the information passes through the network.

The ANN is trained by providing a set of inputs and outputs to the network (this is called the training data). Then the error between the computed output and the actual output is minimised. Once the network has learned the data then it can be used to predict the outputs for inputs that were not in the original training data. One way of improving the accuracy of the network is to increase the number of neurons (units) in the hidden layer. However, if there are too many hidden units then the network will learn each point individually instead of learning the general trend of the data. This is known as over fitting and is shown in Figure 1.3 [6]. More information on machine learning can be found in *Pattern Recognition and Machine Learning* by Christopher Bishop [7].

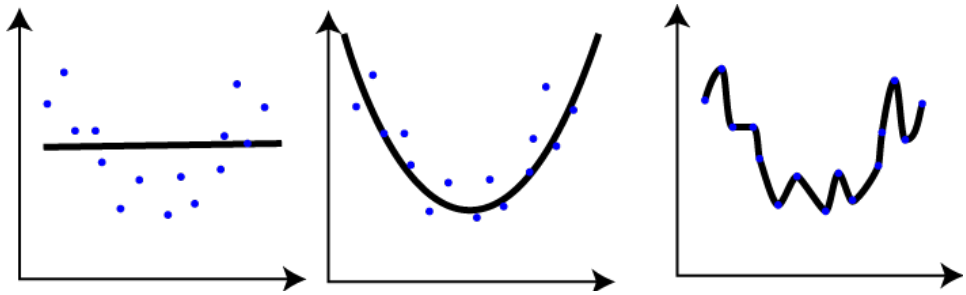

Figure 1.3 – Graphs demonstrating too few hidden units (left image), the correct amount of hidden units (central image) and too many hidden units (right image) [6].

The aim of this project is to investigate the possibility of using CFD to train an Artificial Neural Network to predict the pressure drop across an idealised stenosis in a coronary artery.

2 Methodology

This project involved three main phases. The first phase was to create a CFD model to represent an idealised stenosis. The second phase was to automate the CFD model creation and analysis to provide data to train the ANN. The third phase was to set-up and train an ANN [1].

The CFD Model

Firstly, a CFD model was created to replicate an idealised stenosis. The CFD software used in this project was ANSYS FLUENT [8] (which uses the finite volume method). Several different geometries for the CFD model were tried. The final geometry was chosen by comparing the FFR values given by FLUENT with experimental FFR values. The experimental data consisted of MRI scans and corresponding FFR values for different stenoses. This annonimised data was taken from patients at Derriford Hospital (approved by the Research Ethics Committee). The dimensions for the CFD models were taken from the MRI scans and the FFR value provided by FLUENT was compared with the known FFR value. The FFR value from FLUENT was found by looking at the pressure graph for each stenosis. Figure 2.1 shows where the values for P_a and P_b are taken from the graph and then Equation 2 was used to calculate the FFR.

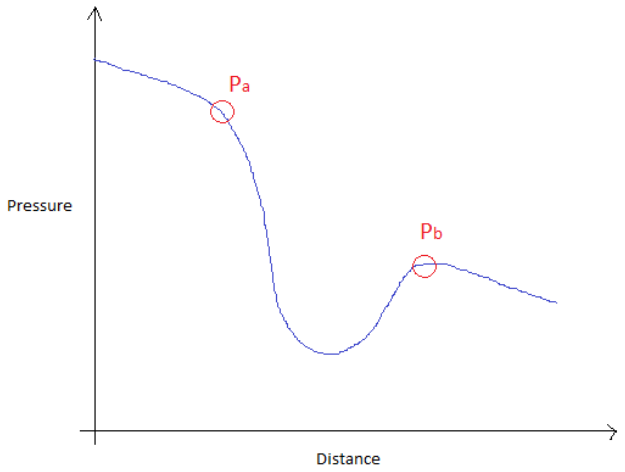

Figure 2.1 –Pressure vs. Distance graph for diseased artery.

The chosen geometry for the CFD model is shown in Figure 2.2. This model has six variable parameters, a fixed inlet and outlet length of 80mm and 100mm respectively, and a fixed outlet diameter of 1.3mm. Figure 2.3 shows the different parameters. D1 is the initial diameter of the artery, D2 is the smallest diameter of the artery (at the point of maximum constriction) and D3 is the recovery diameter. L1 is the length from the onset of the stenosis to the worst point in the stenosis, L2 is the length of maximum constriction of the stenosis and L3 is the length from maximum restriction to the recovery diameter. The inlet length to

[1] Many thanks to Richard Everson for his assistance in the machine learning section of this project.

the stenosis is fixed at 80mm to ensure fully developed flow at the stenosis. The distance was calculated using Equation 3 for entrance length (with a maximum diameter of 5mm and a flow velocity of 0.2 m/s). The outlet length is 100mm to make sure the outlet is at a sufficient distance from the stenosis so it does not affect the pressure drop across the stenosis. The outlet diameter of the model is 1.3mm, this is a typical diameter of the distal tip of the Left Anterior Descending Artery.

Equation 3

$$L_e = D \times 0.06 R_e$$

Where: Le – entrance length (m)
D – diameter (m)
Re – Reynolds number

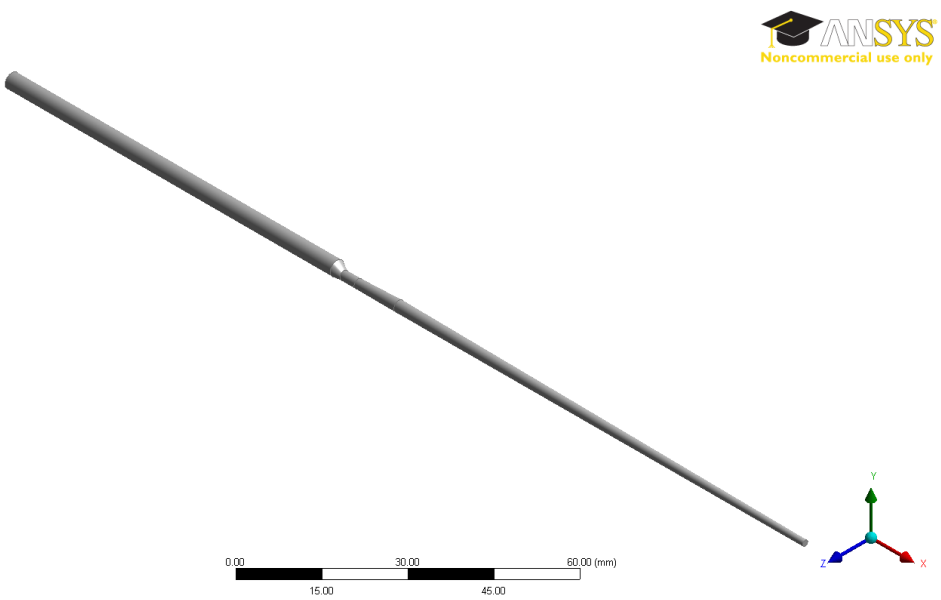

Figure 2.2 – CFD model of artery with idealised stenosis.

Boundary Conditions and Assumptions

For this project the fluid was defined as blood with a density of 1050 kg/m^3 and a viscosity of 0.004 kg/ms. The boundary conditions were defined as velocity at inlet and pressure at outlet, with values of 0.2 m/s and 0 Pa respectively. The walls of the model were rigid with no slip, as the effects of vessel elasticity on the model were assumed to be negligible. The flow was steady state for simplicity, as accurately modelling the pulsatile motion of blood flow would be very difficult and unachievable within the time-frame of this project. It was assumed that no heat transfer was taking place between the vessel walls and the blood flow. The Reynolds number for the flow was much less than the laminar/turbulent boundary value of 2,300 so the flow was set as laminar. A mesh refinement study on the model indicated that a mesh of around 100,000 cells would be sufficient.

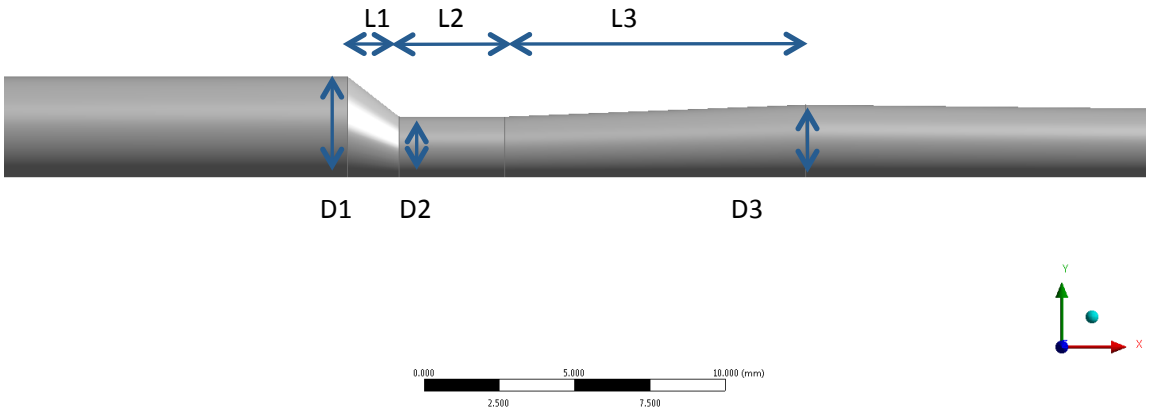

Figure 2.3 – Variable parameters for CFD model of idealised stenosis.

Automating the process

Thirdly, the process of creating the geometry for the model and running the analysis was automated using the parametric analysis function in FLUENT. Figure 2.4 shows the project loaded into ANSYS Workbench, displaying: project schematic, parameter outline and files view. It was decided to use 100 data sets to train the machine learning system. Each data set consisted of the six parameter values (D1, D2, D3, L1, L2, L3) and a corresponding FFR

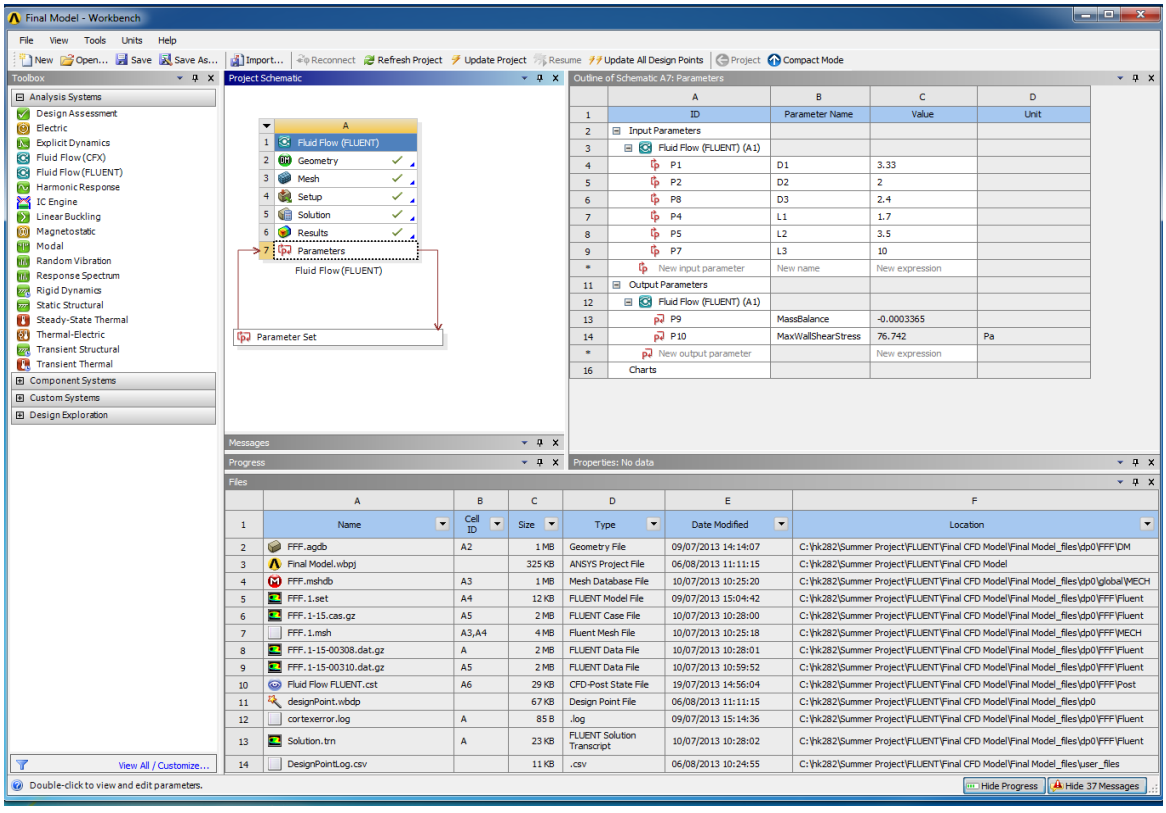

Figure 2.4 - Project loaded into ANSYS Workbench, displaying project schematic, parameter outline and files view.

value. The six variable parameters for the 100 data sets were chosen using the latin hypercube sampling method, this method ensures 'that points are (marginally) spread evenly over the values of each input variable' [9]. The command *lhsdesign* in Matlab [10] was used to automatically generate the parameter values. The range of the parameter values are shown in Table 1 below, these ranges were chosen from assessing the typical sizes of stenoses in the experimental data. Using the parametric analysis function in ANSYS Workbench, 100 different models were created, meshed, and analysed. This formed the data sets for the machine learning. The pressure data for each stenosis model was manually exported as a csv file from ANSYS FLUENT (as a way to automate this part of the process was not found). The csv file was then imported into Matlab where the FFR value was found using a Matlab function written by Richard Everson [11] (see Appendix A).

Table 1 – Range of values for parameters

$2 \leq D1 \leq 5$	$0.3\ D1 \leq D2 \leq 0.9\ D1$	$D2 \leq D3 \leq D1$	$1.5mm \leq L1, L2, L3 \leq 30mm$

Training the ANN

Fourthly, the Netlab [12] toolkit in Matlab was used to select and train two Artificial Neural Networks on the CFD generated data. The two types of ANN were: a Gaussian based Radial Basis Function (RBF) and a Multilayer Perceptron (MLP). These networks were loosely based on the Netlab demonstrations *demrbf1* and *demmlp1*. In order to determine the correct amount of hidden units to use, the number of hidden units was increased incrementally from 1, and the training and test error was recorded. The training error was found using the commands *rbftrain* and *mlptrain* for the RBF network and the MLP network respectively. The test error was found using a technique known as 'leave one out cross validation'. This involves removing one point from the data set and using the remaining points as the training data. The ANN is trained on the *n-1* data points and the point that has been left out is used to test the accuracy of the network. This process is then repeated so that each point in the data is used once as the test data. The training error is the average error over the training data and the test error is the average prediction error over the independent test data. It is important to assess both the training error and the test error, as the training error will automatically decrease with hidden units (due to overfitting) whereas there will be an optimum number of hidden units for the test error (see Figure 2.5).

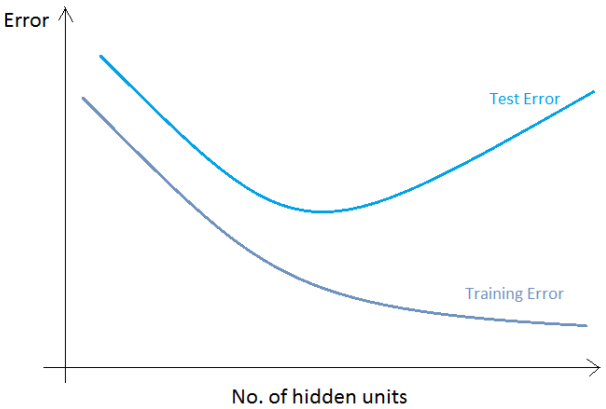

Figure 2.5 – Test error and training error vs. number of hidden units for a typical ANN.

3 Results & Discussion

As mentioned in Methodology, 100 data sets were created to train the ANN. Initially a Gaussian based RBF network was trained on the data from 1 to 11 hidden units (as the training of the network failed when using more than 11 hidden units). Figure 3.1 is a graph of the training error and test error versus the number of hidden units for the RBF. The trend of this graph is very unusual, which together with the failure to run at more than 11 hidden units suggests that there are serious problems with the RBF. Furthermore, the test and training error is around 0.04 - this is the squared error and so corresponds to a percentage error of around 20%.

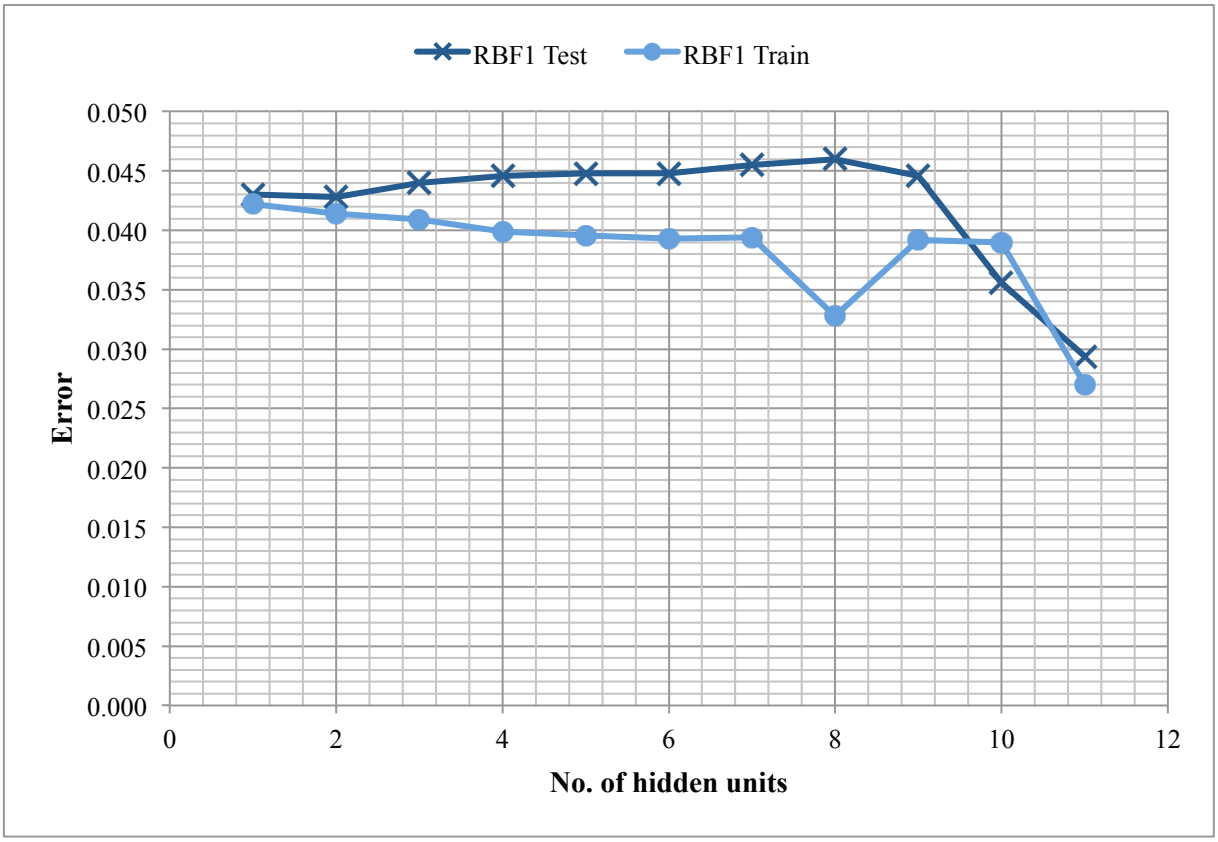

Figure 3.1 – Graph of test error and training error vs. no. of hidden units for RBF1.

To try and alleviate the problems with the RBF, the individual error for each data set was found and five outliers were identified and removed from the data. Next, the 'best error' was found by initialising the network several times, ('because of the dependence of the final network's state on the initial weight configuration, it is common practice to train the same network many times' [13]) and the smallest error was taken. Figure 3.2 shows the initial RBF (RBF1), the RBF with the five outlying data sets removed (RBF2) and with the 'best error' (RBF3). Figure 3.3 shows that while removing the five outlying data sets has reduced the error with the network, neither this nor finding the best error has made any notable improvement to the RBF.

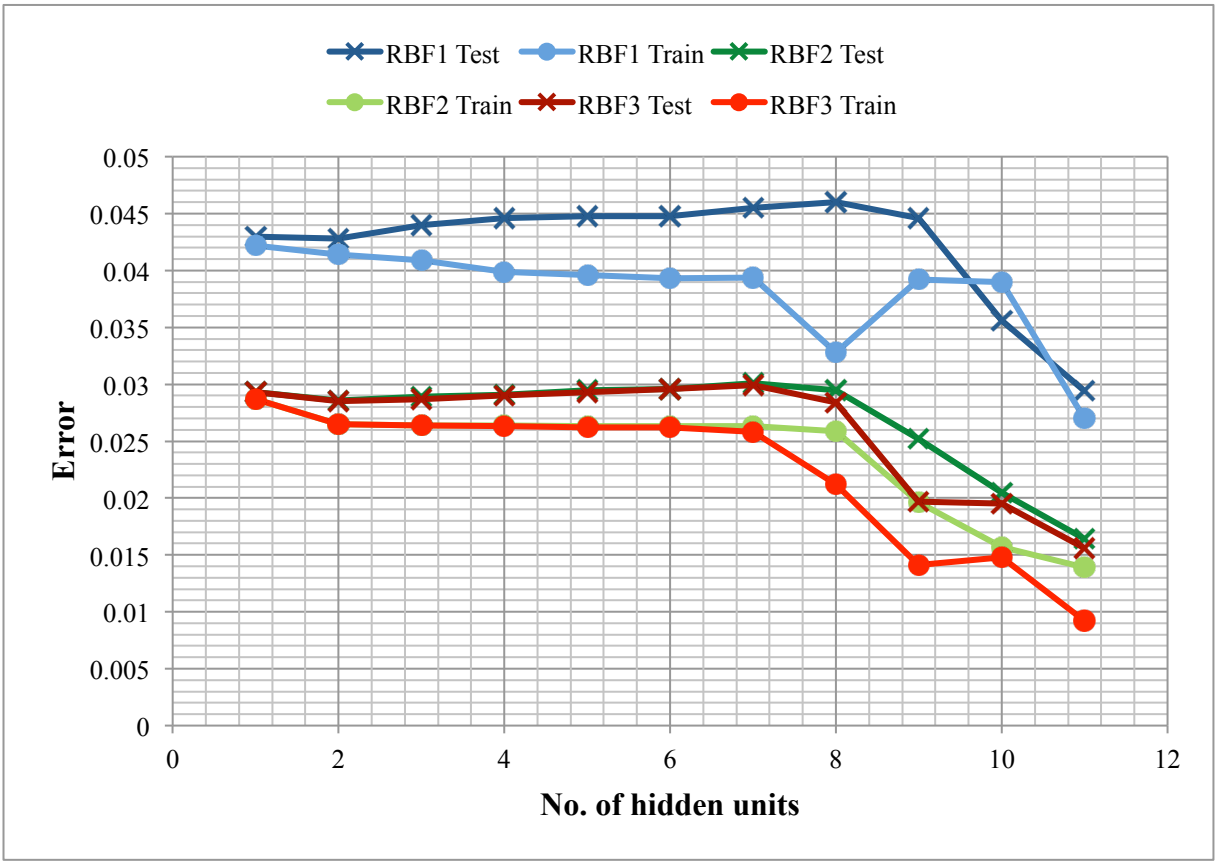

Figure 3.2 – Graph of error vs. no of hidden units for RBF1, RBF2 and RBF3.

As it was evident that there were serious errors with the RBF, an alternative artificial neural network (a Multi-Layer Perceptron) was tried. The MLP was trained on the generated data minus the five outlying data sets. The coefficient of weight decay (α) was fixed at 0.01 and the MLP was trained using 1 to 80 hidden units (see Figure 3.4 for the graph of results). The trend of the training and test error indicates that the MLP had been trained more successfully than the RBF. The test error starts high, quickly decreases and then gradually increases again, with a minimum at around 10 hidden units. This is expected behaviour (see Figure 2.5). The training error decreases and then steadily increases, which is not expected but suggests the network is having difficulty training at high number of hidden units. Although the error for the MLP is better than the RBF, the test error is still quite high at around 0.01 (10%).

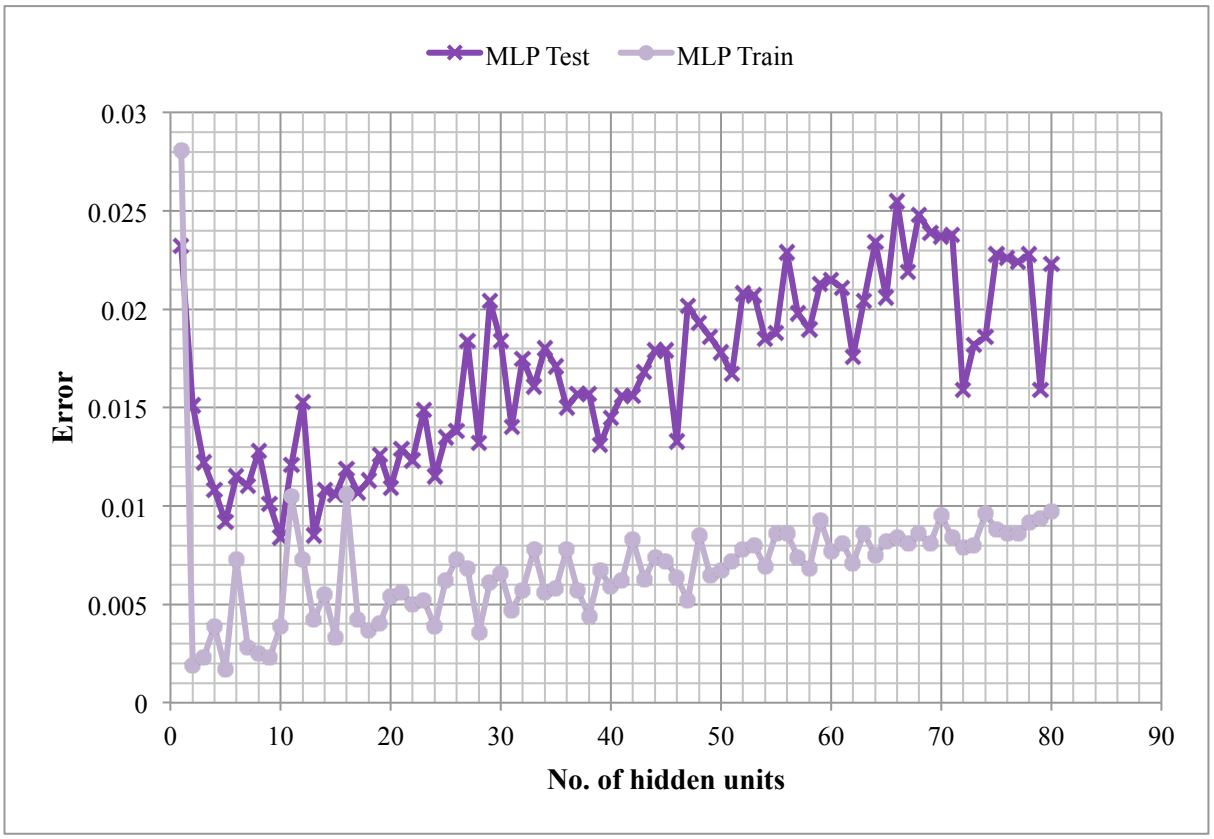

Figure 3.4 – Graph of test error and training error vs. no. of hidden units for MLP.

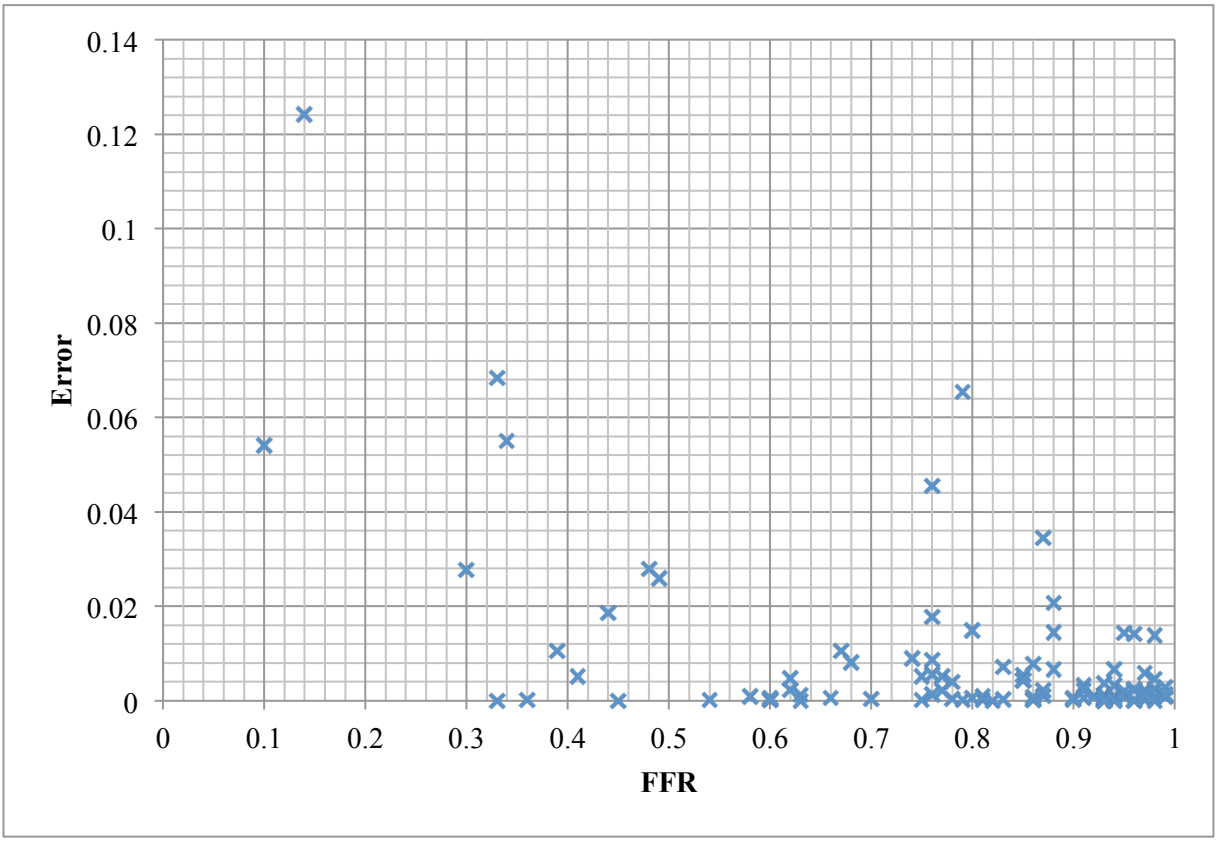

Figure 3.3 – Graph of the test error vs. the FFR value for each individual data set.

To try to reduce the error of the MLP a graph of test error versus FFR was plotted to see if there was any correlation between the error and the FFR value. Figure 3.3 shows that the data sets with the highest error also have very low FFR values. This is most likely because there is a lack of data around the lower FFR values and so the network has difficulty learning these data sets. Figure 3.4 also shows that there are also several data sets with low FFR values. The range of FFR values from the experimental data given by Derriford hospital was 0.67 to 0.98. This is because for the most severe stenoses doctors do not test for the FFR value, they operate immediately. Thus the FFR range of interest is approximately 0.6 – 1. Consequently, it was decided to remove the 15 data sets that had an FFR of less than 0.6 and replace them with data sets that had an FFR of 0.6 or greater and rerun the MLP training. This lowered the error of the MLP (when trained with 10 hidden units and an alpha value of 0.01) from 11% to 7%.

The value of alpha (0.01) was chosen arbitrarily. In order to further improve the MLP the number of hidden units was fixed at 10 and the value of alpha was varied logarithmically from 10^{-5} to 10. Figure 3.5 below is a graph of test error versus alpha for the MLP. From this graph it is apparent that the optimum value for alpha is around 0.3.

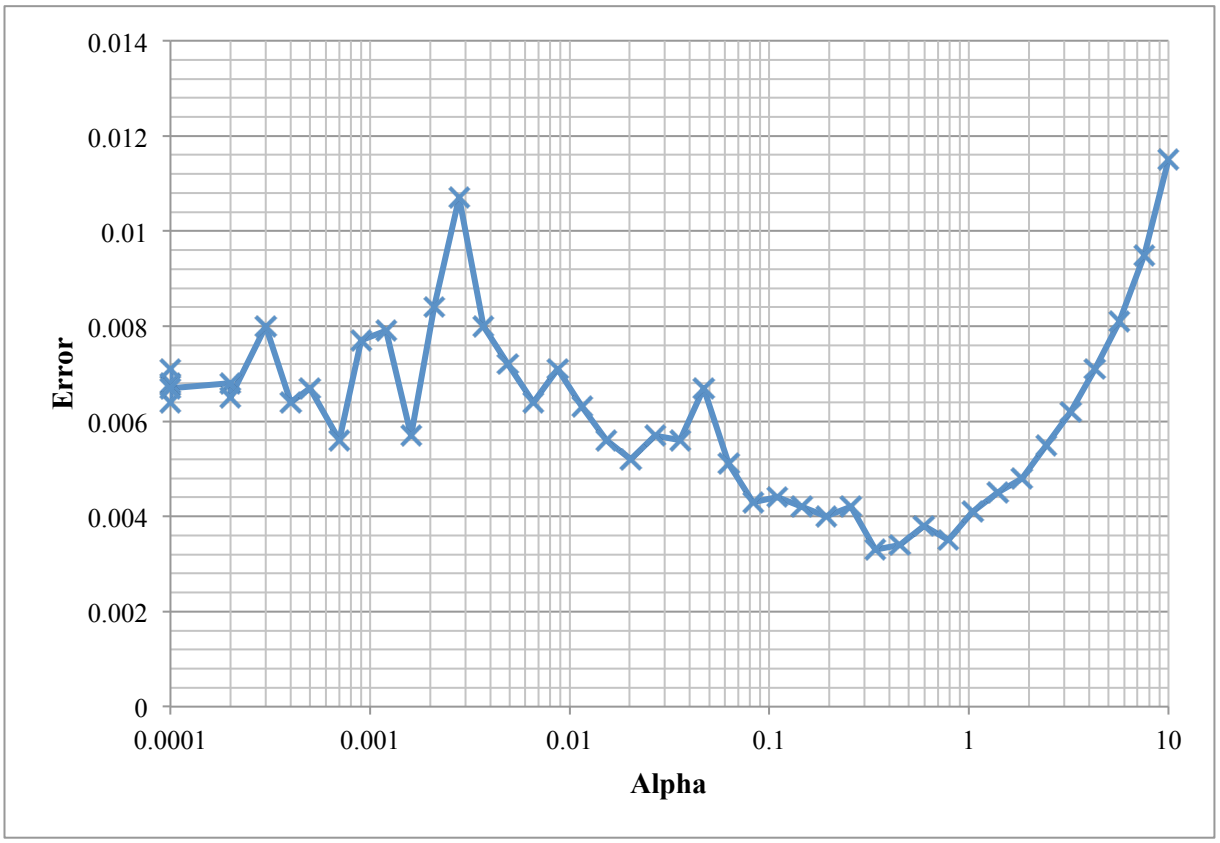

Figure 3.5 – Graph of test error vs. coefficient of weight decay for MLP network.

The MLP was retrained with the improved data (all points with an FFR value between 0.6 and 1), with the optimum alpha value of 0.3 and with the best of four random initialisations (the Matlab code for this can be found in Appendix B). This network was trained with 1 to 25 hidden units; see Figure 3.6 below for the graph of error versus number of hidden units. This graph shows that between 5 and 10 hidden units is the optimum number of hidden units for the MLP. This graph also shows that increasing the value of alpha from 0.01 to 0.3 has caused greater instability within the training error.

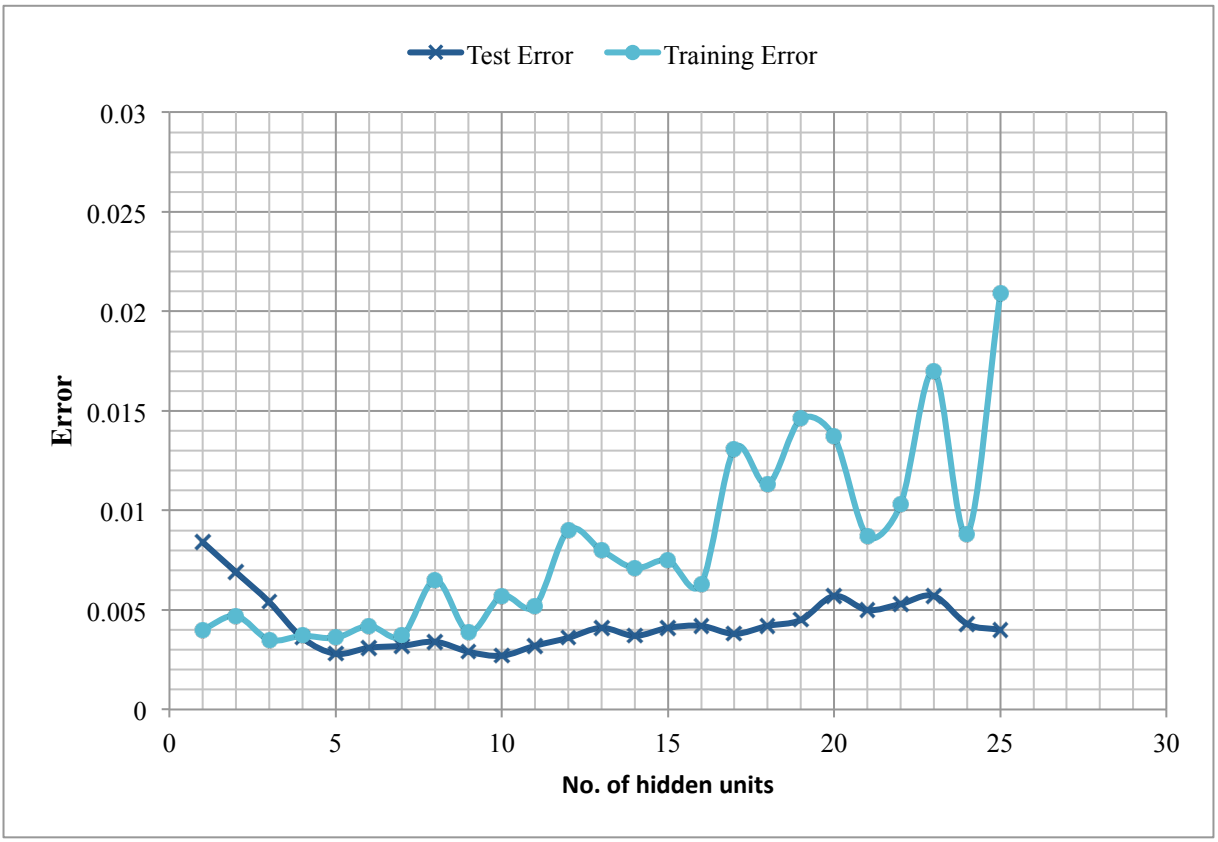

Figure 3.6 – Graph of error vs. number of hidden units for MLP network with alpha = 0.3

Using the results, the MLP network was trained with 5 - 10 hidden units and a coefficient of weight decay of 0.3. This gave an average error of approximately 0.003 or 5 %. Figure 3.6 indicates that there are some issues with the training of the data, in particular at larger number of hidden units. It is also unusual that above four hidden units, the training error is greater than the test error. The instability displayed in the training error of the MLP network demonstrates that the network is having difficulty determining the correct weights to use. Figure 1.2 illustrates that the weights connect all the nodes together in the network (the MLP network used in this project has one hidden layer). The MLP network used in this project has six input nodes and one output node, therefore using ten hidden units results in 70 network weights. The data only contains 100 data sets and this is most probably not enough to determine the network weights at higher number of hidden units. It is therefore most likely that there is not enough data to train the MLP, which is causing the instability within the network.

Another indication that there might not be enough data sets is the failure of the RBF to learn the data. One study by P. Crowder et. al into Radial Basis Functions, found that 'an MLP network appears to outperform an RBF network when there are fewer data points' [14]. The fact that the MLP network has been far more successful in learning the data than the RBF network also indicates that there is not enough training data.

4 Conclusions

In conclusion, this project has used a MLP network (with 5-10 hidden units and an alpha value of 0.3) to predict the FFR value of an idealised stenosis with an average error of 5%. However, this MLP network displayed signs of instability, most likely due to not enough training data. The network was trained on 100 data sets generated from CFD analysis. Although the majority of the process of creating the data sets for the ANN was automated, there were still several steps that had to be done manually. These steps were: exporting the pressure data from ANSYS FLUENT as a csv file, importing the csv file into Matlab, and recording the FFR value. Whilst individually these steps are not particularly laborious, when repeated 100 times it becomes very time-consuming. This was the primary reason why only 100 data sets were created. Further work could be done on this project to fully automate the process of CFD model creation, analysis and FFR calculation. It would be useful to have 1,000 or even 10,000 data sets to train the MLP, which would almost certainly improve its performance

5 References

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6 Appendices

6.1 Appendix A – ffr.m [11]

```
function [FFR] = ffr(filename, doplot)
%  ffr -- find the FFR and ratio of pressure drops
%
%  [FFR] = ffr(filename, doplot)
%
%  filename -- name of the .csv file containing the data as two columns
%  doplot   -- draw a graph of the pressure with the up and downstream
%  points marked.
%
%  The FFR is the pressure at the maximum pressure or turning point
%  downstream of the stenosis.  The upstream pressure is usually at x =
%  0, but is also the pressure just upstream of the abrupt pressure drop.
%

% Copyright (c)  Richard Everson,   University of Exeter, 2013
if nargin < 2, doplot = 1; end

% Read the data
data = importdata(filename, ',');
x = data.data(:,1);
P = data.data(:,2);

% Make sure that x increases with increasing index.
if x(end) < x(1)
  x = x(end:-1:1);
  P = P(end:-1:1);
end
N = length(x);

% Find the gradient using centred differences
g = zeros(N,1);
for j = 2:N-1
  g(j) = (P(j+1)-P(j-1))/(x(j+1)-x(j-1));
end

% Look for the point at which the gradient is zero, starting from the
% downstream end.

found = 0;
for j = N-2:-1:1
  if g(j)*g(j+1) < 0
    t = (0 - g(j))/(g(j+1)-g(j));                % Fraction into the
interval
    % Interpolate the location and pressure
    Pdown = P(j) + t*(P(j+1)-P(j));
    Xdown = x(j) + t*(x(j+1)-x(j));
    found = 1;
    down = j;
    break
  end
end
```

```
if ~found
  % No turning point, so use the point with maximum negative gradient
  % after the step. First find the step.
  disp('Could not find turning point')
end

% Estimate the upstream pressure location by finding the point closest to
% x=0

upstream = find (x >= 0,1,'first');

if ~found
  % Find the downstream point as the point of maximum minimum gradient
  % downstream of the step
  d = find (x >= 0.025,1,'first');
  gg = g;
  gg(g > 0) = NaN;
  gg(1:d) = NaN;
  gg(end) = NaN;                          % Gradient not calculated here
  %plot(x, g, 'b', x, gg, 'r')
  [mx, down] = max(gg);
  Xdown = x(down);
  Pdown = P(down);
end


FFR = Pdown/P(upstream);

if doplot
  plot(x, P, 'b-')
  hold('on')
  plot(Xdown, Pdown, 'ro')
  plot(x(upstream), P(upstream), 'ms')
  title(sprintf('%s    FFR = %g', filename, FFR))
end
```

6.2 Appendix B – MLP_LOOCV_Best_Error.m

```
%   Multilayer perceptron network (2 layer, feed forward) using N data
%   points & LOOCV (Leave One Out Cross Validation).


%   The problem consists of 6 input variables tr_in and one target variable
%   t.


clear all

filename = 'Netlab_100_B.csv';

% import csv file.

data = importdata(filename, ',');

% input data tr_in = [D1 D2 D3 L1 L2 L3], output data t = [FFR].

tr_in = data.data(:,1:6);
t = data.data(:,7);

% Maximum no. of hidden units.
Maxhidden = 25;

% Ecv - Cross Validation (test) Error.
Ecv = zeros(Maxhidden, 1);

% Etr - Training Error.
Etr = zeros(Maxhidden,1);

% N = no. of data sets (rows).
N = size(tr_in, 1);

countIt = 1;

% Maxcount = number of initialisations for each number of hidden units.

Maxcount = 4;
EcvAll = zeros(Maxhidden, Maxcount);
EtrAll = zeros(Maxhidden, Maxcount);

while countIt <=Maxcount          % while loop to run through
                                    initialisations.

for nhidden = [1:Maxhidden]       % for loop to run through hidden units

    SumError = 0;

   for n = 1:N

      % Xtest = input values, Ttest = FFR value >> not included in training
      % data (i.e. row 'n' in tr_in and t).

      Xtest = tr_in(n,:);
```

```
        Ttest = t(n,:);

        % delete row n

        tr_in(n,:) = [];
        t(n,:) = [];

        % Set up network parameters.
        nin = size(tr_in, 2);          % Number of inputs.
        nout = size(t,2);              % Number of outputs.
        alpha = 0.3;                   % Coefficient of weight decay-prior

        % Create and initialize network weight vector.
        net = mlp(nin, nhidden, nout, 'linear', alpha);


        % Set up vector of options for the optimiser.

         options = zeros(1,18);
         options(1) = -1;          % This provides display of error values.
         options(14) = 100;        % Number of training cycles.

        [net, options] = netopt(net, options, tr_in, t, 'scg');

        % Use mlpfwd to predict FFR (Ytest) for set of parameters (Xtest)
        ytest =  mlpfwd(net, Xtest);

        %Test Error, TE

        TE = (Ttest - ytest)^2;

        SumError = SumError + TE;

        % Replace row n that was left out in in matricies tr_in and t.

        tr_in = insertrows(tr_in, Xtest,n-1);
        t = insertrows(t, Ttest,n-1);

    end

    Ecv(nhidden) = SumError/(N-1);
    Etr(nhidden) = (((mlperr(net, tr_in, t))*2)/(N-1));

end

EcvAll(:, countIt) = Ecv

EtrAll(:, countIt) = Etr

countIt = countIt + 1;

end

EcvBest = min(EcvAll,[],2)
EtrBest = min(EtrAll,[],2)

% plot test & training error
```

```
plot(1:Maxhidden, EcvBest, 'bo-')
hold on
plot(1: Maxhidden, EtrBest, 'ro-')
xlabel('Number of hidden units')
ylabel('Error')
legend('Test Error', 'Training Error');
hold off
```