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Mining data from hemodynamic simulations via multilayer perceptron neural network

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Abstract

Arterial geometry variability is present both within and across individuals. A multilayer perceptron neural network was proposed for mining data generated from computer simulations. The proposed approach was applied to analyze the influence of geometric parameters on maximal wall shear stress (MWSS) in the human carotid artery bifurcation. A parametric model was used for generating a set of observational data that contains the maximum wall shear stress values for a range of probable arterial geometries. The data set was mined via a multilayer perceptron making it possible to predict values of the maximum wall shear stress for new geometries that were not in the training data set.

Introduction

After heart disease and cancer, the third most common cause of death is stroke. Probably the most frequent stroke is of the embolic type with a heart disease as the source. The carotid bifurcation stenosis is also a significant cause of stroke, producing the infarction in the carotid region by embolization or thrombosis at the site of narrowing. The thrombosis development and embolization is conditioned by the local hemodynamics which can be investigated experimentally and/or by computer modeling.

Increase of stoke risk is induced by many factors: age, systolic and diastolic hypertension, diabetes, cigarette smoking, etc. Changes of the geometrical vessel dimensions in the region of the carotid artery bifurcation certainly affect the blood flow and may lead to stenosis process (Schulz et al. 2001). It has been shown that the vessel diameter at the carotid artery bifurcation changes considerably with age (Kojić et al. 2008). There are many CFD simulations which assume that arterial geometry is precisely defined (Perktold et al. 1986, Perktold et al. 1987, Perktold et al. 1991). There is also a geometric uncertainty for each patient so that there is a need for prediction tool in clinics which can be run in real time. This problem is particularly challenging because it is difficult to characterize the observed geometric variability using a small number of variables. A statistical assessment hence becomes beneficial to gain an insight into the relationship between flow patterns and geometric attributes. The basic idea could be to construct probabilistic models for the input uncertainties which will replace classical CFD calculations and to give output of interest very quickly.

Simulations of pulsatile flow in human carotid artery have been performed in Perktold papers (Perktold et al. 1986, Perktold et al. 1987, Perktold et al. 1991). Wall shear stress (WSS) has been identified to play a major role in the progression and complication of atherosclerosis (Glagov et al. 1988).

One of the standard approaches for statistical analysis is the Monte Carlo simulation technique where the computer model is run repeatedly for randomly generated values of the inputs, and subsequently, the resulting data is postprocessed to estimate the output statistics (Rubinstein 1981). However, due to the CPU requirement of a large sample-size, this approach becomes computationally prohibitive, particularly when high-fidelity models are used.

Kolachalama used Bayesian Gaussian process emulator to access the relationship between geometric parameters and Maximal Wall Shear Stress (MWSS) and to obtain geometries having maximum and minimum values of the output MWSS (Kolachalama et al. 2007).

In the present work, we proposed the multilayer perceptron neural network to study the relationship between geometric factors and hemodynamic metrics MWSS. The structure of multilayer perceptron is described in (Ranković 2008, Shepherd 1997). The present approach can be viewed as a computer-based data mining strategy which extracts useful information and synthesizes interesting relationships from data sets generated by running computer simulations on selected cases. The human carotid artery bifurcation was chosen for analysis since it is a common site for arterial disease to occur (Bharadvaj et al. 1982). Large changes in the magnitude of maximum wall shear stress (MWSS) can play a role in the embolic mechanism by which carotid lesions can induce stroke (Lorthois et al. 2000). Hence, it is important to understand the correlation between the geometric variability and MWSS in the human carotid artery. Set of candidate geometries were randomly created for steady state three dimensional flow analysis. The generated data were then used to construct a multilayer perceptron neural network which approximated the MWSS as a function of geometric variables.

Finite element model of the carotid artery bifurcation

Here, we describe the basic concept of generation of the carotid artery bifurcation finite element (FE) models, with appropriate boundary conditions. A 3D finite element model with 3D fluid finite elements (8-node isoparametric elements with velocity calculation at all nodes and pressure calculated at the element level) is generated for the carotid artery geometry as described below. The CFD post-processing results gives an insight into the local hemodynamics, as well as the blood mechanical action on the vessel walls, such as distributions of pressure and shear stress on the wall surfaces.

A simplified carotid artery bifurcation geometry is shown in Fig. 1. The geometric parameters are used for the generation of the blood vessel internal surfaces, which are the boundaries for the blood flow domain. With the use of these geometric parameters, a 3D finite element model for the blood flow domain is generated. Such FE model is shown in Fig. 2. It is assumed that the bifurcation has the symmetry plane, hence the FE model is generated for the half of the entire domain. The calculation is performed for this half, but the results can be seen for the entire domain.

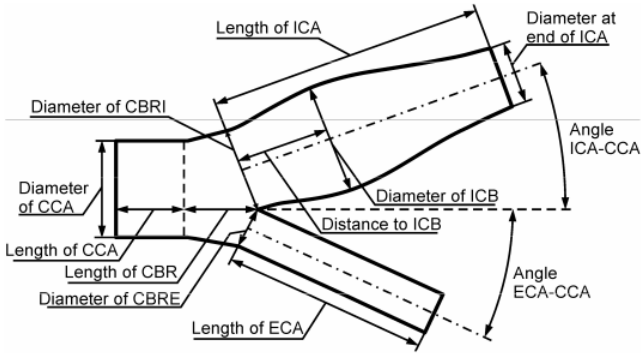

Fig. 1. Geometrical data for the carotid artery model. The abbrevations here are: CCA – common carotid artery, CBR – carotid bifurcation region, CBRE – carotid bifurcation region external, ECA- external carotid artery, CBRI- carotid bifurcation region internal, ICA- internal carotid artery, ICB- internal carotid bulbus

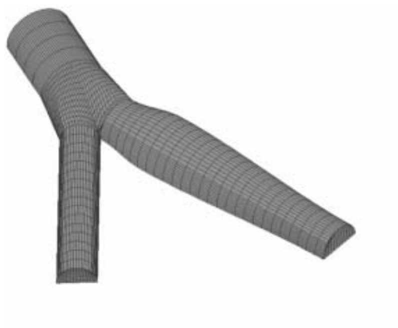

Fig. 2. A FE model of the carotid artery bifurcation generated using the parameters shown in Fig. 1.

Steady state simulation for the 300 geometries were undertaken and MWSS for each geometry was extracted for constructing multilayer perceptron. A parabolic inflow velocity profile was applied at the common artery entering cross-section. Velocity of the central point at the common artery entering cross-section is V_{av}=93.8 mm/s.

All velocity components at the fixed walls are set to be zero. Also, the velocity components at the plane of symmetry in the direction normal to the plane, are set to zero. The principal assumptions in the present study were to consider the flow as steady, blood as a Newtonian fluid and the walls to be rigid. After obtaining a converged solution, the magnitude of MWSS was extracted for each geometry in order to create the training data for multilayer perceptron neural network.

Multilayer perceptron and backpropagation algorithm

Multilayer perceptron is feed-forward neural network usually trained with backpropagation algorithm. This neural network consists of one input layer, one output layer and one or more hidden layers of neurons. Figure 3 shows multilayer perceptron with *m* layers.

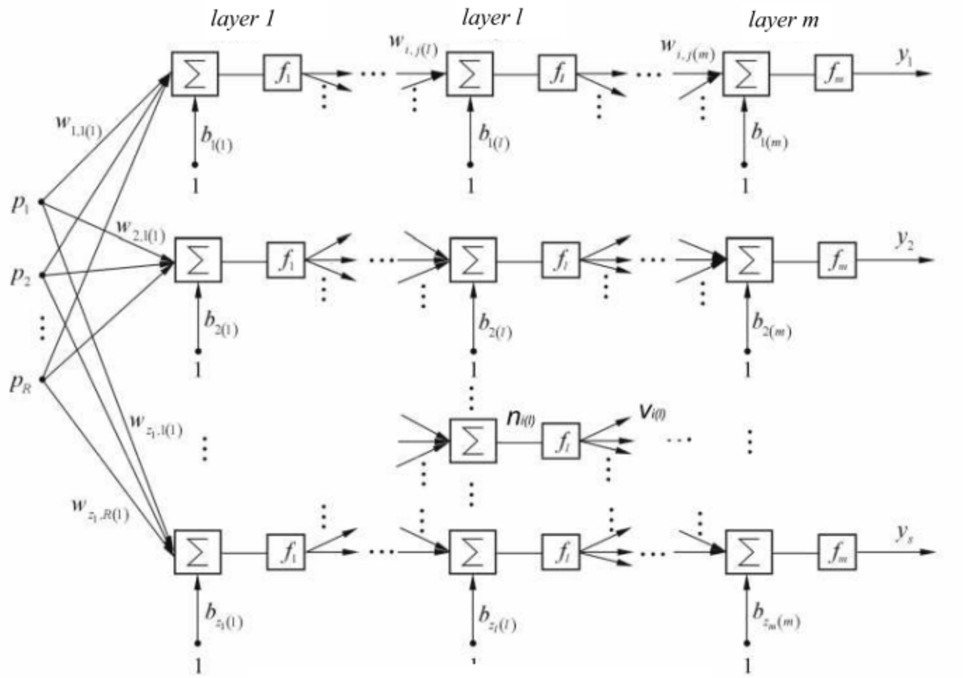

Fig. 3. Multilayer perceptron with m layers of neurons

$p_1, p_2, \ldots, p_R$ – input signals

m – number of layers

z_l – number of neurons in l-th layer

$w_{i,j(l)}$ – weight between i-th neuron in l-th layer and j-th neuron in l-1-th layer.

$b_{i(l)}$ – bias of i-th neuron in l-th layer

$v_{i(l)}$ – output of i-th neuron in l-th layer

f_l – activation function of neurons in l-th layer

Backpropagation algorithm requires existing training points defined by their input vectors and vectors of targets.

$q_1, q_2, \ldots, q_N$ – N training points

$p_1^{(1)}, p_2^{(1)}, \ldots, p_R^{(1)}$ – inputs of training point q_1

$p_1^{(N)}, p_2^{(N)}, \ldots, p_R^{(N)}$ – inputs of training point q_N

$t_1^{(1)}, t_2^{(1)}, \ldots, t_s^{(1)}$ – targets of training point q_1

$t_1^{(N)}, t_2^{(N)}, \ldots, t_s^{(N)}$ – targets of training point q_N

First step of backpropagation algorithm is initialization of starting values for weights and biases $w_{i,j(l)}(1)$ i $b_{i(l)}(1)$. These values are chosen randomly within an interval.

After defining the learning rate and criterion for learning stop, one of the training points is being placed on neural network input. Then, the outputs of all neurons are calculated. Output of i-th neuron in l-th layer for k-th training point is:

$$v_{i(l)}^{(k)} = f_l\left(n_{i(l)}^{(k)}\right) \tag{1}$$

$$n_{i(l)}^{(k)} = \sum_{j=1}^{z_{l-1}} w_{i,j(l)} v_{j(l-1)}^{(k)} + b_{i(l)} \tag{2}$$

Output of i-th neuron in m-th layer is at the same time i-th output of neural network:

$$v_{i(m)}^{(k)} = y_i^{(k)} = f_m\left(n_{i(m)}^{(k)}\right) \tag{3}$$

$$n_{i(m)}^{(k)} = \sum_{j=1}^{z_{m-1}} w_{i,j(m)} v_{j(m-1)}^{(k)} + b_{i(m)} \tag{4}$$

Equations (1)-(4) evaluate outputs from all neurons. Now, adaptation of neural network parameters (weights and biases) can start. Criteria function, which describes how much real outputs disagree with targets, is defined:

$$E^{(k)} = \frac{1}{2}\sum_{i=1}^{s} e_i^{(k)2} = \frac{1}{2}\sum_{i=1}^{s}\left(t_i^{(k)} - y_i^{(k)}\right)^2 = \frac{1}{2}\sum_{i=1}^{s}\left(t_i^{(k)} - v_{i(m)}^{(k)}\right)^2 \tag{5}$$

The objective of adapting parameters is to make real outputs as close as possible to targets. Adaptation of weights between neurons in m-1-th layer (last hidden layer) and neurons in m-th layer (output layer) is performing iteratively:

$$w_{i,j(m)}(t+1) = w_{i,j(m)}(t) + \Delta w_{i,j(m)}(t+1) \tag{6}$$

$$\Delta w_{i,j(m)}(t+1) = -\eta\frac{\partial E^{(k)}}{\partial w_{i,j(m)}} + \alpha\Delta w_{i,j(m)}(t) \tag{7}$$

where α is positive number – momentum constant, which defines influence of previous modification on a new one. Usually it takes value 0.9. Equation (8) represents adaptation of biases of neurons in output layer.

$$b_{i(m)}(t+1) = b_{i(m)}(t) - \eta\frac{\partial E^{(k)}}{\partial b_{i(m)}} \tag{8}$$

Adaptation of neural network parameters in other layers is performing according to the equations (9), (10) and (11).

$$w_{i,j(l)}(t+1) = w_{i,j(l)}(t) + \Delta w_{i,j(l)}(t+1) \tag{9}$$

$$\Delta w_{i,j(l)}(t+1) = -\eta\frac{\partial E^{(k)}}{\partial w_{i,j(l)}} + \alpha\Delta w_{i,j(l)}(t) \tag{10}$$

$$b_{i(l)}(t+1) = b_{i(l)}(t) - \eta\frac{\partial E^{(k)}}{\partial b_{i(l)}} \tag{11}$$

Adaptation of neural network parameters is performed for all training points. After all training points are presented to neural network epoch is done and criterion for learning stop is checked. If it is satisfied learning stops, otherwise new epoch starts.

Data set for training and testing neural network

To demonstrate the applicability of multilayer perceptron for assesing the relationships between a wide range of geometric parameters and MWSS, geometric parameters shown in Figure 1 are used as input variables for neural network (12 input variables total). The perturbation of each parameter was taken as 30% of the corresponding mean value given in Table 1. To obtain reasonable data set, 300 geometries were generated. 280 geometries were generated for training neural network, and 20 geometries were generated for testing neural network. The values of geometric parameters for all geometries used for training and testing neural network are shown in the form of a scatter plots in Figure 5.

Description	Mean value
Diameter of CCA	6,2
Length of CCA	7,44
Length of CBR	7,316
Diameter of CBRI	4,9
Diameter of CBRE	3,658
Angle ICA-CCA	25
Angle ECA-CCA	25
Length of ICA	26,04
Length of ECA	18,6
Distance to ICB	5,39
Diameter of ICB	6,5
Diameter at end of ICA	4,34

Table 1. Dimensions of human carotid artery bifurcation

All geometries were created by entering corresponding parameters values in FEM software. For each geometry the value of MWSS is extracted. Density of the blood is ρ=1.05 [g/cm^3], dynamic viscosity is μ=0.0367 [P] and it is assumed that blood is a Newtonian fluid. The values of MWSS extracted for all the geometries that were used as training and testing data for the multilayer perceptron are shown in the form of a scatter plot in Figure 4.

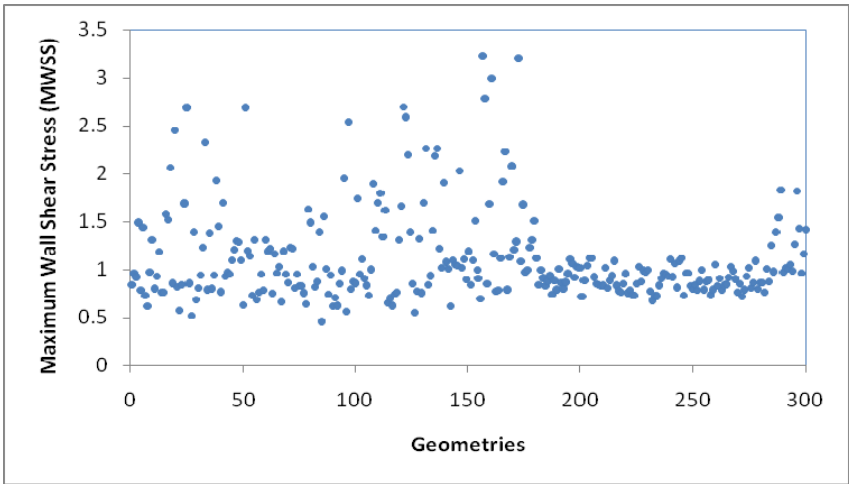

Fig. 4. Scatter plot of the MWSS vs geometry cases considered (Units of MWSS in Pa)

As can be seen from the Figure 4, there is a significant change in the magnitude of MWSS for the cases considered for this study. This suggests that variations in geometry have a significant impact on the value of MWSS.

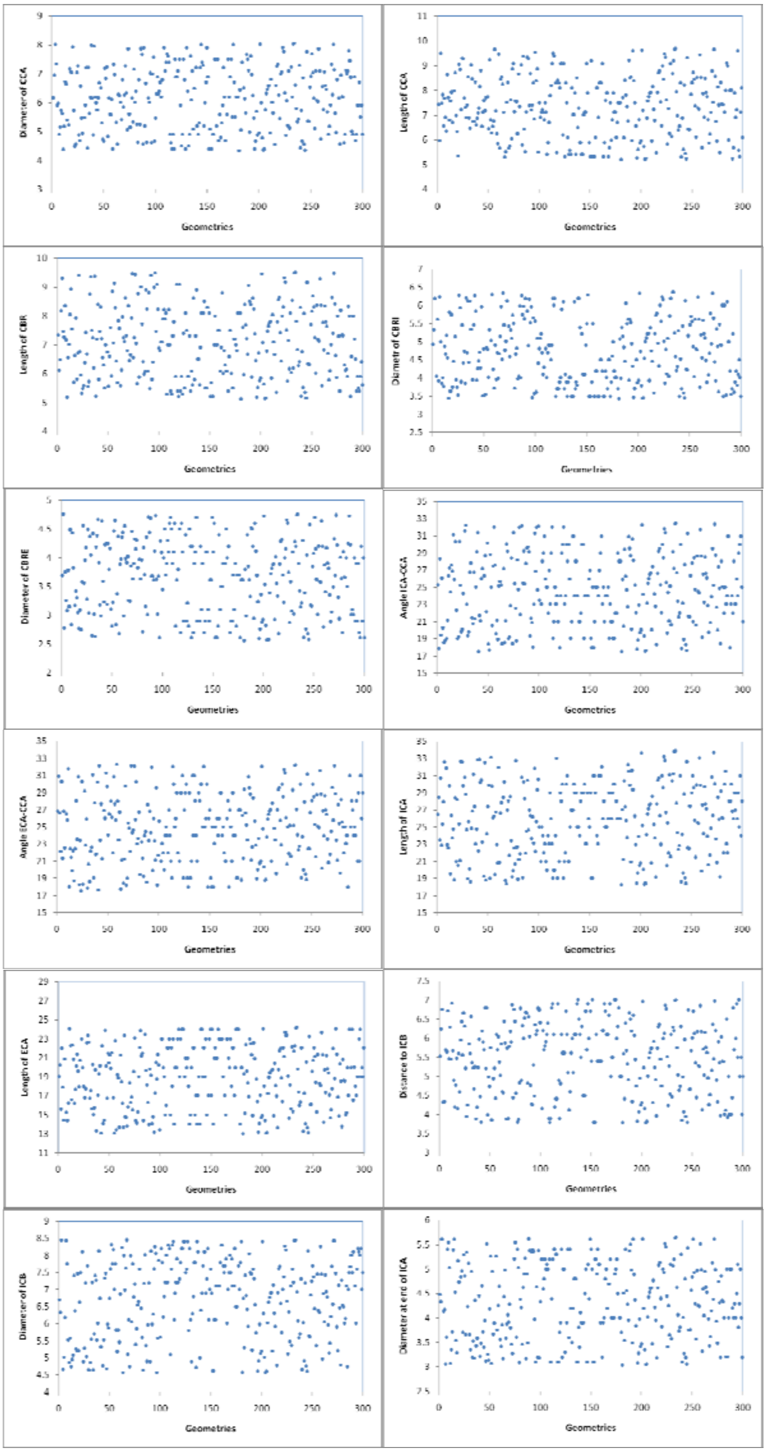

Fig. 5. Values of geometric parameters for 300 geometries.

Neural network details

In the present work we used multilayer perceptron neural network and we trained it using backpropagation algorithm. For creating and training neural network we used Neural Network Toolbox 4.0 developed for MATLAB 6.0.

Multilayer perceptron with 5 neurons in hidden layer gave the best results. Numbers of neurons in input and output layers are defined by the problem we are solving, hence neural network has 12 neurons in input layer and 1 neuron in output layer (figure 6). This structure of neural network can be shortly written as 12-5-1.

Activation functions of neurons in hidden layer are unipolar sigmoid (which gave better results than bipolar sigmoid functions), while the activation function of neuron in output layer is linear.

In order to improve learning success and learning rate, we used moment method. Momentum constant was define as 0.95 while learning rate was 0.01.

Two criteria for learning stop were defined: mean square error and maximum number of epochs. Mean square error was defined as MS=0,01, while the maximum number of epochs was 19000. Learning stops when first of the two criteria is satisfied. In our case learning stopped after 19000 epochs of learning.

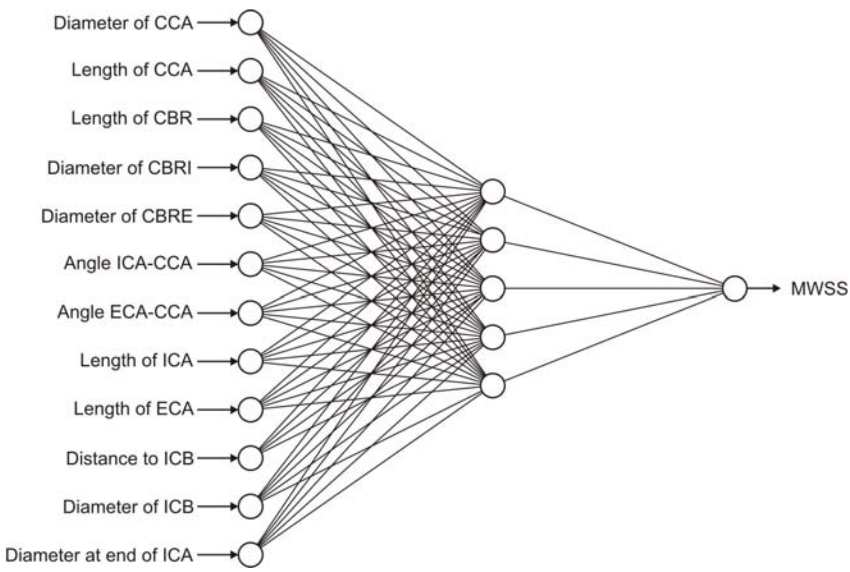

Fig. 6. Structure of used neural network

Results of prediction

After learning of multilayer perceptron is done, testing points (20 geometries) are brought on neural network inputs. Neural network outputs MWSS' are compared with calculated values of MWSS:

$$\Delta MWSS = \left| MWSS' - MWSS \right| \quad (12)$$

The differences between calculated and predicted values of MWSS are shown in table 2.

		Computed values of Maximum Wall Shear Stress (MWSS)	Predicted values of Maximum Wall Shear Stress (MWSS')	ΔMWSS	ΔMWSS / MWSS,%
testing points	1	0.864	0.886	0.022	2.581 %
	2	0.763	0.709	0.054	7.064 %
	3	1.010	1.279	0.269	26.673 %
	4	0.875	0.868	0.007	0.800 %
	5	1.250	1.400	0.150	11.984 %
	6	0.970	1.050	0.080	8.278 %
	7	1.380	1.634	0.254	18.370 %
	8	1.540	1.656	0.116	7.500 %
	9	1.830	1.758	0.072	3.918 %
	10	0.972	0.923	0.049	5.041 %
	11	1.020	1.037	0.017	1.637 %
	12	1.010	1.006	0.004	0.436 %
	13	1.050	0.961	0.089	8.495 %
	14	0.987	0.882	0.105	10.659 %
	15	1.260	1.393	0.133	10.516 %
	16	1.820	1.847	0.027	1.456 %
	17	1.430	1.462	0.032	2.224 %
	18	0.960	0.999	0.039	4.063 %
	19	1.160	1.260	0.100	8.655 %
	20	1.420	1.462	0.042	2.972 %
			Min.	0.004	0.436 %
			Max.	0.269	26.673 %

Table 2. Results of predicting MWSS using neural network

Figure 7 shows calculated and predicted values of MWSS for 20 testing points. Thus, point 3 is predicted with error 27%, while other points have errors smaller than 20%.

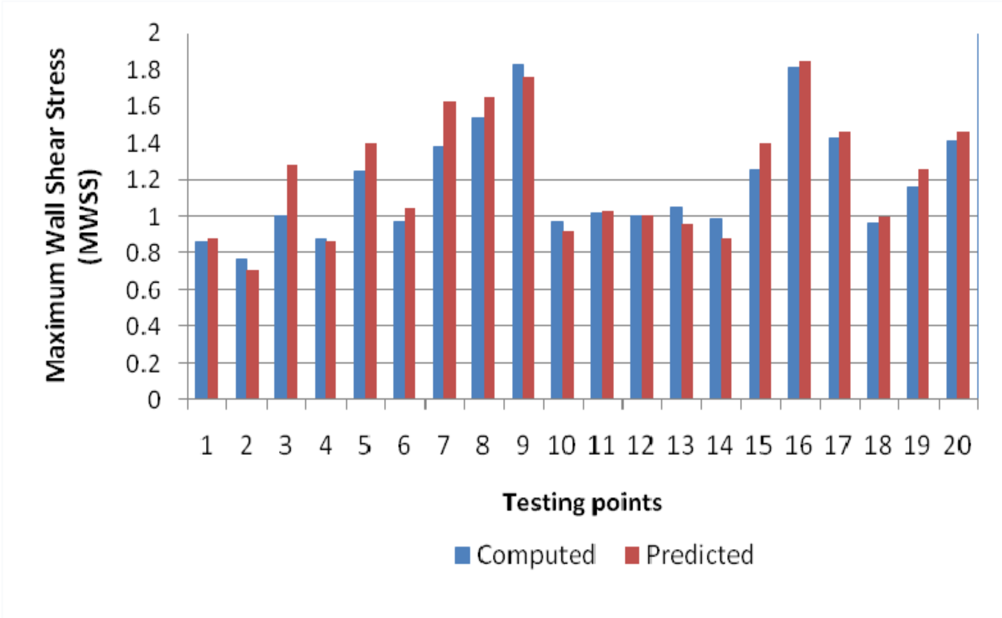

Fig. 7. Calculated and predicted values of MWSS for 20 testing points.

Discussion and Conclusion

This work presented a neural network approach for data mining. The methodology was applied on a hemodynamic problem in which the geometric parameters affecting maximal wall shear stress (MWSS) in the human carotid bifurcation were analyzed. The results obtained from computer simulations were used as training data to construct a multilayer perceptron neural network. After neural network was constructed, it was tested on a 20 new geometries that were not in the training data set. The results have shown reasonable small errors, which indicates that the multilayer perceptron is capable of predicting MWSS for different geometries of carotid artery bifurcation. This can be used to aid the assessment of stroke risk for a given patient's geometry in real time.

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