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Optimization of silk yarn hierarchical structure by genetic algorithm to design scaffolds

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A genetic algorithm model has been developed to determine the optimal parameters of mechanical aspects of a silk wire-rope scaffold with the highest predictive accuracy and generalized ability simultaneously. The study pioneered on employing a genetic algorithm (GA) to optimize the parameters of scaffold in tendon and ligament tissue engineering. Experimental results show that the GA model performs the best predictive accuracy to imply mechanical behavior with native values successfully.

Keywords: Artificial neural network, Genetic algorithm, Mechanical properties, Scaffolds, Silk, Tissue engineering

1 Introduction

Scaffolds in tissue engineering provide an initial support and framework for attaching, proliferating and differentiating different cell lines as an extracellular matrix (ECM)[1]. An ideal scaffold, that provides biological signals along with a combination of suitable mechanical behavior, is required for making the successful engineered tissues like tendon and ligament in tissue engineering field[2]. Proper mechanical support is an essential consideration for scaffolds construction. Therefore, various methods have been developed to progress the mechanical performance of scaffolds[3]. Due to suitable mechanical properties, fibre-based scaffolds have been widely used to simulate tendon and ligament tissues[4]. These tissues have special mechanical properties like viscoelastic and non-linear behavior that are similar to fibre-base structurs[5, 6]. On the other hand, textile structures for example woven, knitted, braided or twisted types made of fibres have the most mechanical similarity with tendon and ligament tissues, so they can be the best choice to design and fabricate their scaffold[7].

Silk is one of the famous materials for providing an excellent combination of high strength (up to 4.8 GPa), remarkable toughness, elasticity (up to 35%) and environmental stability. For the first time Altman and Kaplan explored the potential of native silk fibroin fibres as 3 dimensional scaffolds for tissue engineering of the anterior cruciate ligament (ACL). Mechanical properties of human ACL are comparable to textile structure as reported in a study as a twisted structure[8]. Because of the importance of simulation mechanical properties, recently researchers have attempted to develop the relation between structural and mechanical properties of a scaffold by various methods like mathematical or statistical method precisely.

This study has been made to develop a new method to estimate mechanical properties of silk wire-rope scaffold used in tendon and ligament tissue engineering by artificial neural network method. A genetic algorithm model is developed for the automation and optimization of designing a scaffold for the first time.

One of the most powerful information processing systems which mimic the function of the human brain and biological neural networks is artificial neural network (ANN). This technique is useful when there are a large number of effective parameters in the special process without requiring a prior knowledge of the relationships of process factors[9]. Artificial neural networks are compositions of simple processing elements, called artificial neurons[10]. Among different types of ANN, multi-layer perception (MLP) neural networks with back propagation (BP) training procedure for modeling a problem is one of the most commonly used models[11, 12]. From the scientific point of view, to know the effect of some production parameters in various applications

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like tissue engineering and prediction of the scaffold properties, neural network models are the best way to predict and simulate structures[13].

Besides, genetic algorithms (GAs) have been widely and successfully applied to different optimization processes[14]. GAs are well appropriate for the concurrent manipulation of models with changing solutions and structures, since they can search non-linear resolution spaces without requiring gradient information and prior knowledge about model features[15]. According to the environmental adaptation degree of chromosomes, the fitness value is taken as the bases of ranking chromosomes, in order to know which chromosome would survive in the next generation. As a matter of fact, these methods are powerful tools for finding the target optimal formula for optimization problems. By the self-adaptation function and threshold, the system itself has the ability to evolve through optimum solution for the problem[16].

To optimize effective parameters in this study for fabricating a silk wire-rope scaffold, GA was applied to optimize effective parameters which lead to optimum mechanical properties because of its intuitiveness, ease of implementation and its ability to effectively solve highly nonlinear and mixed integer optimization problems[17]. In the proposed GA model, the effective parameters of silk wire-rope scaffold in tendon and ligament tissue engineering are dynamically optimized by implementing the GA evolutionary process and then performing the prediction task using these optimal values. The optimal values of parameters are searched by GAs with a randomly generated initial populations consisting of chromosomes. The values of the two parameters, namely the number of filament and the number of twist in each layer of wire-rope yarn, are directly coded in the chromosomes with real-valued data. The single best chromosome in each generation is the survives of the succeeding generation. Predicting mechanical properties of scaffold has been a major research issue in tissue engineering. Therefore, the genetic algorithm model has been applied to the problem in preparing scaffolds by tissue engineering to verify its accuracy and generalization ability, considering that it is more accurate than the traditional multivariate statistical models and neural network technique.

2 Materials and Methods

According to Wang *et. al.*[8], silk hierarchical structure scaffolds which are similar to the arrangement of collagen fibres in tendon and ligament tissue, were designed. To design an effective model, values of parameters in wire-rope scaffold have to be chosen carefully in advance[18]. These parameters include the number of filament in each layer (parameters P1-P4 for first, second, third and fourth layer respectively), which determines the strength at the break and the number of twist in each layer (parameters P5-P8 for first, second, third and fourth layer respectively), which defines elongation-at-break in a wire-rope scaffold. The number of filament and the number of twist vary from 2 to 5 filaments and 20 to 80 twist/meter in each layer. Scaffolds were identified by the type of structure, by the number of filament and by the number of twist in different layers. For example, if the number of filament in each layer (from first to forth layer) is 2, 5, 5, 3 (labeled 2-5-5-3) and if the number of twist in each layer (from first to fourth layer) is 40, 20, 60, 40 (labeled 40-20-60-40). Figure 1 shows wire-rope scaffold structure schematically.

2.1 Sample Preparation and Experimental Design

The data used in the ANN and GA model were collected from 40 silk wire-rope scaffold samples according to Taguchi orthogonal matrix. A single silk yarn with 200 den yarn count, 11.1N ultimate tensile strength (UTS) and 22.5% elongation-at-break was measured after degumming process. Removal of sericin layer for silk medical application is necessary. Hence, degumming bath of Na_2CO_3 solution at 95–98°C for 30 min and repeating the process for another 60 min in a fresh degumming solution has been done[19].

Forty different scaffolds were characterized by mechanical properties analyzing 30 samples in each group immediately after setting final twisting. Setting the final structure was essential because of ban of

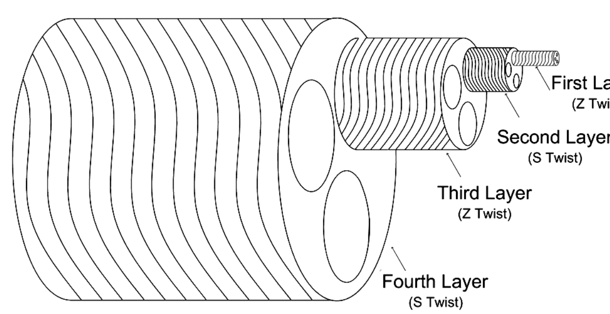

Fig. 1—Wire-rope scaffold design for tendon and ligament tissue engineering

snarling in twisted yarns in the oven at 100°C for 30 min(ref. 20).

The mechanical properties such as UTS, elongation-at-break and stiffness of each sample were measured using a Zwick mechanical testing system. The length of specimens was chosen 32 mm because of the average length of native ACL tissue. Then samples were stretched to failure at a crosshead speed of 50 mm/min. The defined structures and the result of mechanical properties of each sample are shown in Table 1.

2.2 Modeling and Methodology

In this work, the mechanical properties of applicable wire-rope scaffold in tendon and ligament tissue engineering from its structure were predicted by MLP ANN as fitness function of GA to optimize the variable parameters of wire-rope scaffold structure.

First, to model MLP ANN was trained with effective parameters of wire-rope scaffold structure by the error back propagation algorithm to prepare prediction model. In Table 2 input and output parameters in ANN have defined. This whole soft component was implemented using MATLAB R2009a.

2.2.1 Neural Network Model for Predicting Features of ACL

The feed-forward back-propagation neural network was applied to the experimental sample, including 8 input neurons in the input layer, one hidden layer of eight neurons and one output layer of three neurons. Training algorithm function based on the Levenberg-Marquardt optimization theory was chosen to faster convergence of ANN and the over fitting error preserve. First, the effective parameters on the wire-rope scaffold were determined among all possible parameters and then used in ANN input layer (Table 3). After that, predicting the mechanical properties by ANN was studied. The threshold function was set to the 'tangent sigmoid function' and the 'pure line function' for hidden layer and output layers, respectively. The number of epochs was set to 29 and the learning rate was set to 0.01 in each epoch. Table 3 presents the parameter settings in ANN.

2.2.2 Optimized Structure using GA

GA has some parameters that can control algorithm. Also, the parameters must be determined before GA execution, however there is no clear order to determine them. The stopping criteria of GA should be specified by several criteria like exceeded maximum number of generations, no feasible point found, exceeded time limit and terminated optimization by the output or plot function. In this study, stopping condition of GA (defined as the generation) reaches to the specified value with a minimum acceptable fitness values for the best individual in the last generation.

Table 1—Defined structures and the result of mechanical properties of silk wire-rope yarn samples

Sample code	Number of filament (P1 - P4)	Number of twist (P5- P8)	UTS N	Elongation %	Stiffness N/mm
S1	2-2-2-2	20-20-20-20	162	22.9	22.11
S2	2-2-3-3	40-40-40-40	359	29.5	38.03
S3	2-2-4-4	60-60-60-60	622	37.9	51.29
S4	2-2-5-5	80-80-80-80	903	54.7	51.59
S5	2-3-2-2	40-40-60-60	246	36.5	21.06
S6	2-3-3-3	20-20-80-80	600	46.1	40.67
S7	2-3-4-4	80-80-20-20	1130	36.3	97.28
S8	2-3-5-5	60-60-40-40	1790	49.7	112.55
S9	2-4-2-3	60-80-20-40	619	38.2	50.64
S10	2-4-3-2	80-60-40-20	534	32.1	51.99
S11	2-4-4-5	20-40-60-80	1680	66.4	79.07
S12	2-4-5-4	40-20-80-60	1340	54.1	77.4
S13	2-5-2-3	80-60-60-80	627	49.4	39.66
S14	2-5-3-2	60-80-80-60	519	35	46.34
S15	2-5-4-5	40-20-20-40	1460	45.3	100.72
S16	2-5-5-4	20-40-40-20	1620	32.1	157.71
S17	3-2-2-5	20-80-40-60	441	33.4	41.26
S18	3-2-3-4	40-60-20-80	509	47.4	33.56
S19	3-2-4-3	60-40-80-20	398	21.9	56.79
S20	3-2-5-2	80-20-60-40	450	26.7	52.67
S21	3-3-2-5	40-60-80-20	541	30.6	55.25
S22	3-3-3-5	40-60-80-20	1120	41.5	84.34
S23	3-3-4-3	80-20-40-60	903	48.5	58.18
S24	3-3-5-2	60-40-20-80	615	51.2	37.54
S25	3-4-2-4	60-20-40-80	869	56.6	47.98
S26	3-4-3-5	80-40-20-60	1380	55.9	77.15
S27	3-4-4-2	20-60-80-40	833	40.9	63.65
S28	3-4-5-3	40-80-60-20	1820	45.1	126.11
S29	3-5-2-4	80-40-80-40	1140	47.2	75.48
S30	3-5-3-5	60-20-60-20	2060	46.7	137.85
S31	3-5-4-2	40-60-40-80	1190	60.7	61.26
S32	3-5-5-3	20-80-20-60	2470	54.1	142.68
S33	3-5-5-3	20-20-20-20	2392	22.6	330.75
S34	2-5-5-4	40-40-40-40	1641	29.1	176.22
S35	3-5-5-3	40-40-40-40	2385	29.7	250.95
S36	2-5-5-4	20-20-20-20	1652	28.9	178.63
S37	3-5-3-5	20-40-40-20	1957	35.1	174.38
S38	3-4-3-5	40-40-40-40	1449	31.0	146.19
S39	3-5-3-5	40-20-20-40	2163	31.7	213.03
S40	3-4-3-5	20-20-20-20	1311	25.2	162.64

To find the optimized structure of GA, each chromosome was coded with 8 genes. The first to fourth genes were the number of filament in each layer of wire-rope scaffold and the fifth to eighth genes were the number of twist in each layer. Whole genes were coded between-1 to 1. After that, introducing the fitness function was the most important. The fitness function in present work is defined according to following equations:

$$e_{\mathrm{UTS}} = \left| \frac{UTS_{prediction} - UTS_{target}}{UTS_{target}} \right| \quad \ldots (1)$$

$$e_{\mathrm{elogation}} = \left| \frac{elongation_{predicton} - elongation_{target}}{elongation_{target}} \right| \quad \ldots (2)$$

$$\text{Fitness function} = \frac{e_{UTS} + e_{elongation}}{2} \quad \ldots (3)$$

Table 2—Input and output parameters of the neural network model

Variables	Coding	Unit
Inputs		
Number of filament in first layer	P1	-
Number of filament in second layer	P2	-
Number of filament in third layer	P3	-
Number of filament in fourth layer	P4	-
Number of twist in first layer	P5	TPM
Number of twist in second layer	P6	TPM
Number of twist in third layer	P7	TPM
Number of twist in fourth layer	P8	TPM
Outputs		
Ultimate tensile strength	UTS	N
Elongation at break	-	N/mm
Stiffness	-	%

Table 3—The parameter settings in ANN

Parameters of ANN	Value
Network type	Back propagation
Training function	Levenberg Marquardt
Adaptive learning function	LEARNGDM
Performance function	MSEREG
Number of layers	3
Neuron in hidden layer	8
Transfer function of hidden layer	Tangent sigmoid
Transfer function of output layer	Pure line
Epochs	29
Learning rate	0.01

where UTS_{target} = 2160, 1503 and 658 for ACL young, middle and old age; and $elongation_{target}$ = 33, 25 and 13 for ACL young, middle and old age[21].

If the fitness function is lower, its chromosome creates better topology and has greater chances to survive, and GA is searching the highest fitness function or best topology. Figure 2 shows the structure of GA model[22].

The proposed model was developed and implemented in the MATLAB 10 environment. Because of the stochastic algorithm, GA was run many times for each reported case. The utilized system has these characteristics: processor (CPU)–32-bit operating system Core(TM) i3 2.13GHz, RAM– 2.00 G.

3 Results and Discussion

In the present study, the ANN has been applied to design a model for predicting the mechanical properties of wire-rope hierarchical scaffold in applications of tendon and ligament tissue

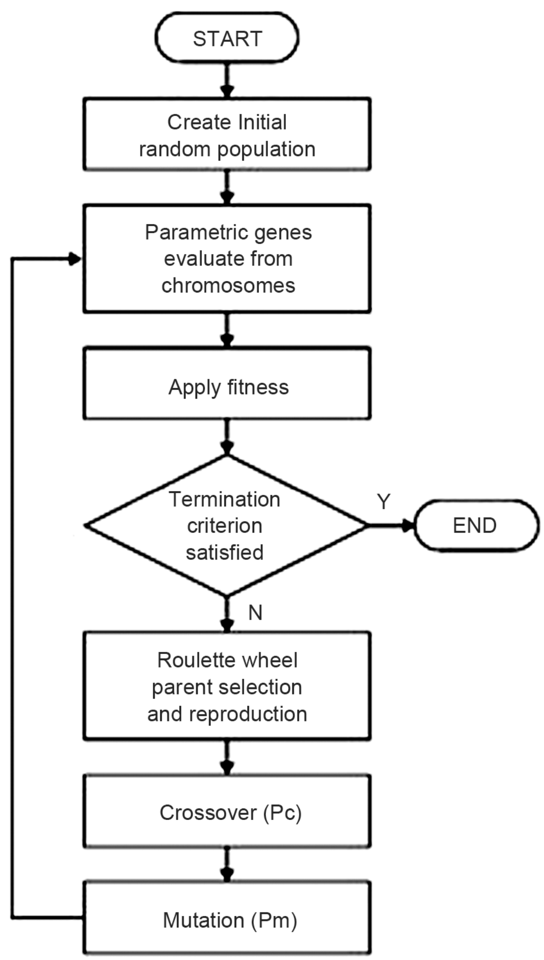

Fig. 2—GA structure[22]

engineering. After that, GA was utilized to optimize the input values in model including the number of filament and the number of twist to receive the best structure.

First of all, the initial population size is optimized. With a large population size, the genetic algorithm searches the solution space more thoroughly, thereby reducing the chance that the algorithm will return a local minimum that is not a global minimum. However, a large population size also causes the algorithm to run more slowly.

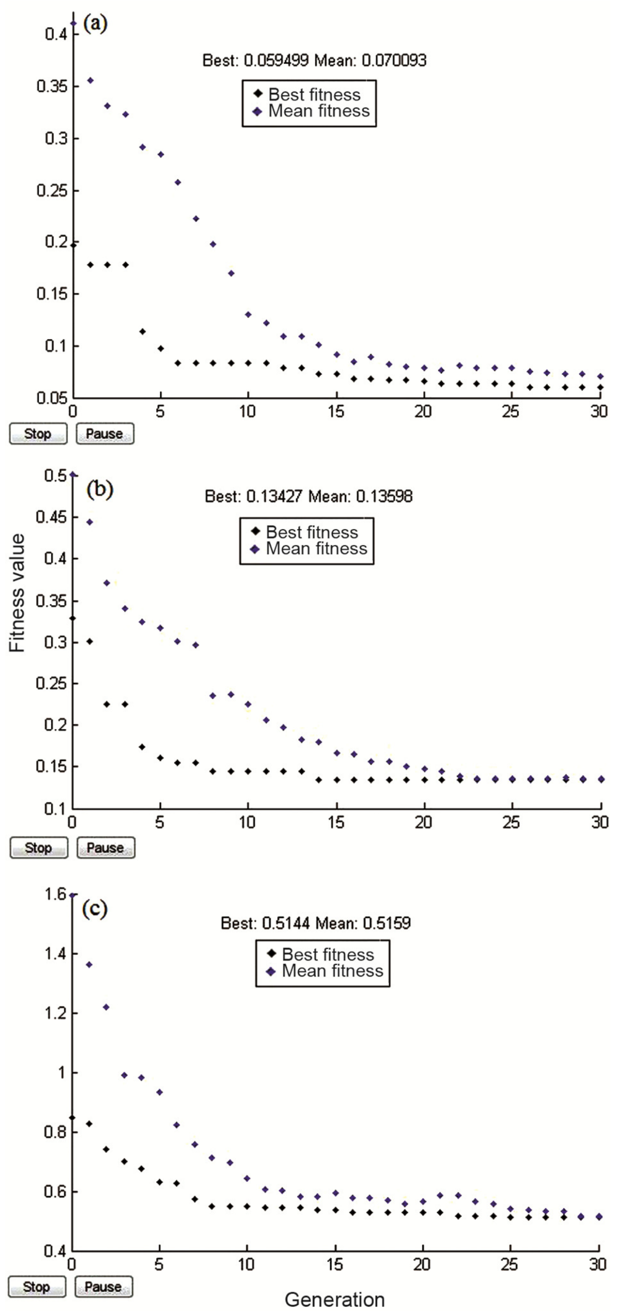

Fig. 3—Fitness value *vs*. generation in GA optimization for (a) young age group, (b) middle age group and (c) old age group

When best and mean fitness function values are closing each other, it means all solutions are becoming similar to each other and there is one solution. Usually, the best fitness value improves after several generations and then it is approximately constant. In generation 30, convergence happens between mean and best values and the mean value is close to the best value, so optimum population size can define 30.

The number of generations is next parameter. It was considered to have 30 generation for young, middle and old age group. Because of considering the time execution and convergence between mean and best values, these values can be selected for the optimum number of generation. Like population size, for large values of generation number, growth of the execution time is remarkable.

In addition to population size and generation number, other GA parameters, after much number of trials, have been set (Table 4).

Figure 3 shows the fitness function values in each generation for young, middle and old age group of people. In all figures for young, middle and old age, mean and the best values are very close and parameters setting in genetic algorithm model according to Table 4 are acceptable.

After finding and running the best GA program, the optimization of input values for young, middle and old age including the number of filament and twist in each layer of wire-rope scaffold and final outputs including UTS, elongation at break and stiffness were predicted according to Table 5. The result shows that the best structure for young, middle and old people is

Table 4—The parameter settings in GA

Parameter of GA	Value
Population type	Double vector
Population size	30
Creation function	Uniform
Display	Iter
Fitness scaling function	Rank
Selection function	Stochastic uniform
Crossover fraction	0.9
Mutation function	Gaussian
Migration direction	Forward
Migration fraction	0.9
Stopping criteria and generation	30 generations (maximum)

Table 5—Optimized result of inputs and outputs parameters for ACL scaffold in young, middle and old age group of people

Optimized parameter	Young age	Middle age	Old age
Inputs			
Number of filament in first layer	2	2	2
Number of filament in second layer	5	5	4
Number of filament in third layer	4	4	3
Number of filament in fourth layer	5	4	4
Number of twist in first layer	57	67	23
Number of twist in second layer	36	44	37
Number of twist in third layer	46	64	18
Number of twist in fourth layer	31	17	25
Outputs			
UTS (N)	1940.2	1463.7	660.19
Elongation at break, %	34.3	31.7	27.2
Stiffness, N/mm	286.1	259.3	153.27

Table 6—The prediction error of testing samples using GA model

Output parameter	Age group	Experimental value	Predicted value	Prediction error, %
UTS N	Young age	1730	1940.2	10.8
	Middle age	1620	1463.7	10.7
	Old age	750	660.19	13.65
Elongation at break, %	Young age	38.3	34.3	11.66
	Middle age	35.1	31.7	10.72
	Old age	30.5	27.2	12.13
Stiffness N/mm	Young age	141.16	286.1	50.66
	Middle age	144.23	259.3	44.38
	Old age	76.84	153.27	49.76

2-5-4-5, 2-5-4-4 and 2-4-3-4 for the number of filament in each layers of wire-rope scaffold, respectively. In addition to the number of filament, the number of twist in each age group is also predicted. By using these values, output parameters (mechanical behavior) are anticipated.

Table 6 presents ability of the best genetic algorithm model to predict the mechanical properties. Also, Table 6 reveals that the prediction error for UTS and elongation-at-break changes from 10.7 to 13.65. For stiffness, the prediction error is much more because of the interaction between UTS and elongation-at-break.

4 Conclusion

Prediction model has been constructed using neural network to predict final mechanical properties of scaffold after extracting and visualizing the main characteristics of the data set. The study of mechanical behavior is based on the desirability approach. GA method is applied to optimize the main characteristics. All these methods have contributed to establish a convenient model that could predict and optimize the global mechanical properties of wire-rope yarn. For example, the best structure of the ACL of young people is 2-5-4-5 and 57-36-46-31 for the number of filament and the number of twist in each layer of wire-rope scaffold, respectively.

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