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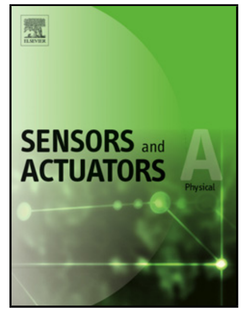

4D Printing Soft Robots Guided by Machine Learning and Finite Element Models

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4D Printing Soft Robots Guided by Machine Learning and Finite Element Models

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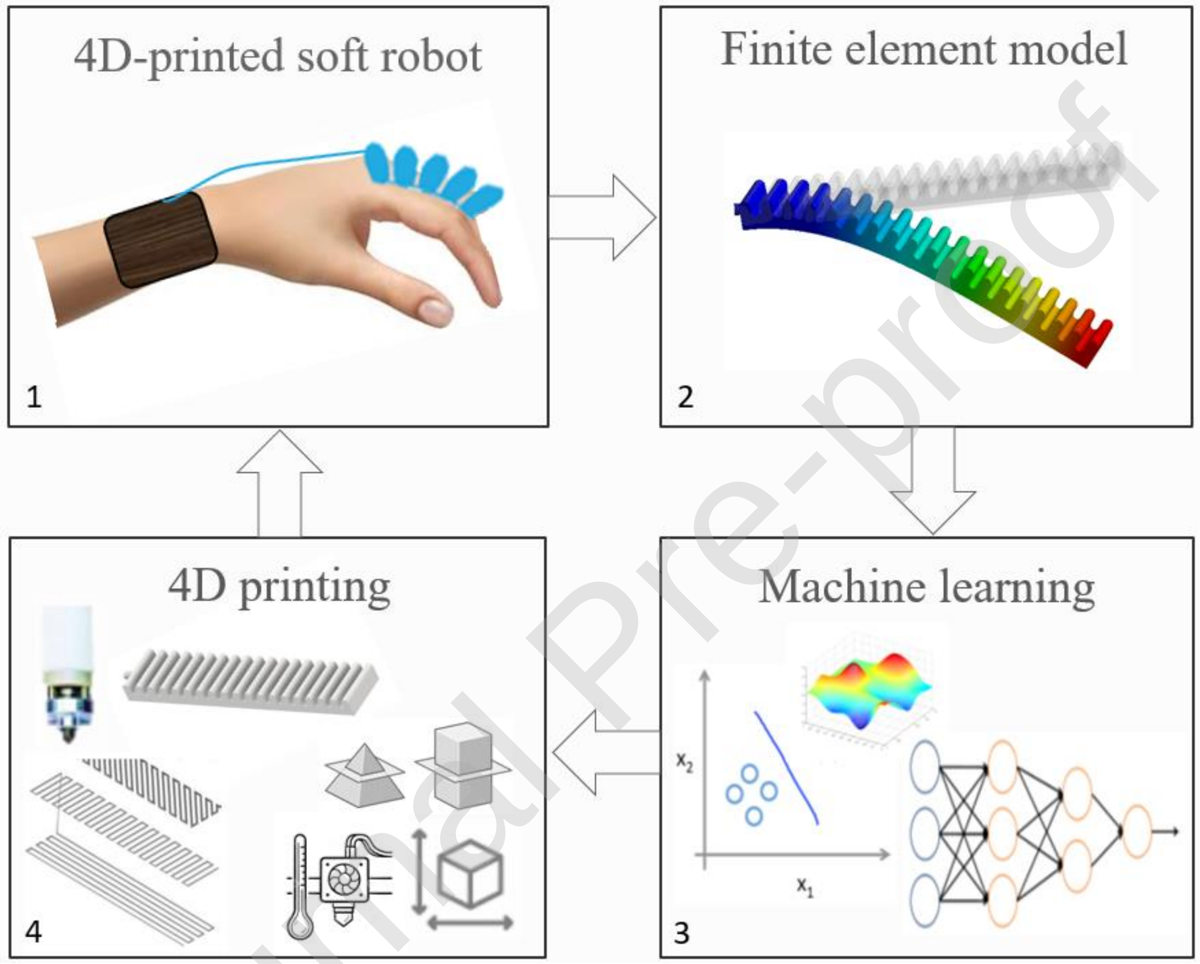
Graphical Abstract



Highlights

- A machine learning approach is introduced to estimate 4D-printed soft robots bending behaviour.
- A finite element model is developed to reflect the nonlinear behaviour of the pneumatic soft actuators.
- The 4D-printed soft actuators geometrical requirements are obtained via machine learning to realize the bending required for specific tasks.
- The experimental tests validate the efficacy of the presented machine learning model for 4D printing soft robots.

Abstract
This paper presents a method for four-dimensional (4D) printing of soft pneumatic actuator robot (SPA)s, using nonlinear machine learning (ML) and finite element model (FEM). A FEM is developed to accurately simulate experimental actuation to obtain training data for the ML modeling. More than a thousand data training samples from the hyperelastic material FEM model generated to use as training data for the ML model, which was developed to predict the geometrical requirements of the 4D-printed SPA to realize the bending required for specific tasks. The ML model accurately predicted FEM and experimental data and proved to be a viable solution for 4D printing of soft robots and dynamic structures. This work helps to understand how to develop geometrical soft robots' designs for nonlinear 4D printing problems using ML and FEM.
Keywords: 4D printing; Machine learning; finite element modeling; soft robotics; soft pneumatic actuators

Introduction

Robotics has been synonymous with high precision and rigidity. However, in recent years the new technology of soft robotics has emerged adding flexibility and adaptability that was not previously possible with rigid robots [1]. The advancements of three-dimensional (3D) printing manifested in soft robotics as four-dimensional (4D) printing where the fourth dimension refers to the time-dependent response of the printed mechanism to variable stimuli, such as heat, electricity, magnetism, and pneumatic pressure.

The 4D-printed soft pneumatic actuator (SPA) focused in this study consists of finger-like structures with bellows, which inflate when pressurized causing it to extend and bend. Compared to the rigid counterparts, it is low cost, lightweight, easy to manufacture, adaptable, flexible, and deformable [1, 2]. Moreover, the softness and flexibility minimize the impact on human skin or other delicate objects and surfaces. These types of soft robot actuators were utilized in the design of a soft surgical manipulator in a closed-loop system [1]. The potential for this technology also lies in its use for the rehabilitation of a wrist and finger exoskeleton to assist the movement of joints [3]. 3D/4D printing is being studied due to its capability to produce soft robots and actuators with complex inner structures [3, 4]. Ninjaflex material proved to be a good choice as it could be 3D printed without air bubbles and has hyperelastic properties that provide flexibility and sensitivity to applied stress [2, 5].

One of the current challenges in the 4D printing of soft robots and actuators is the modeling and prediction of their motion particularly due to the nonlinearity of the material [6-8]. A linear analytical model often fails to accurately predict the actuation behavior of the 4D printed actuators whereas numerical simulations incorporated with nonlinear material principles improve accuracy [9]. However, using the advantage of machine learning (ML) techniques trained via numerical results [10] could help save time and effort during the design [11].

A pure data-driven modeling approach [9, 10] enables the prediction of actuation behavior under different operating conditions without precise material models. A combination of the accuracy of FEM modeling [12] and the time efficiency of ML to formulate a neural network algorithm was introduced [11]. The FEM was employed for training the data and the artificial neural network (ANN) to create the model, a method that will be utilized in this study to predict the deflection angle in response to a varying input air pressure. The nonlinear model was solved in ANSYS using Ogden constitutive model due to its accuracy, based on the uniaxial tensile test data [2, 13, 14]. Convergence of a nonlinear model is more difficult to achieve than linear models, due to material behavior approximation, large deformations, and creep [14]. This could be resolved by increasing the mesh size and therefore the stiffness of the geometrical model [15].

Methodology

Fabrication

In this study, a 3D printing technique [3] is employed to fabricate a bellows-type SPA. This approach enables customization of the 4D-printed SPA without postprocessing. An elastomeric filament NinjaFlex (NinjaTek, PA) was used to fabricate the actuators by a Flashforge FDM 3D printer with a 0.4 mm nozzle diameter and 0.1 mm layer resolution. An open-source 3D printing program, Cura, was used to input printing parameters. The CAD files are imported to Cura software and the actuator's layers were extruded sideways in a bottom-up layout. The parameters used for printing the SPAs in different sizes and geometries (Fig.1) are provided in Table S1. Note that the geometry of the actuator consists of a 2D shape seen from the side view, which is extruded to create width with a constant cross-section. It is also observed that the channel running between the bellows has the same wall thickness as the bellows, except for the thicker bottom layer of the actuator.

Analytical model

The analytical method outlined by [16] estimates the bending angle for a given pressure input and dimensions. The derivation of this method stems from the idea that a difference between the center of pressure in an actuator and the centroid of the cross-section of the actuator causes it to bend toward the bottom of the cross-section. The pressure applied causes a tensile force to produce a bending moment that causes the deflection. It must be noted that this method uses a constant modulus of elasticity, as a generalization, however in reality this value would not remain constant and therefore we introduce a margin for error in the results. In the method introduced in [16], an effective modulus is calculated using experimental results from stress-strain data.

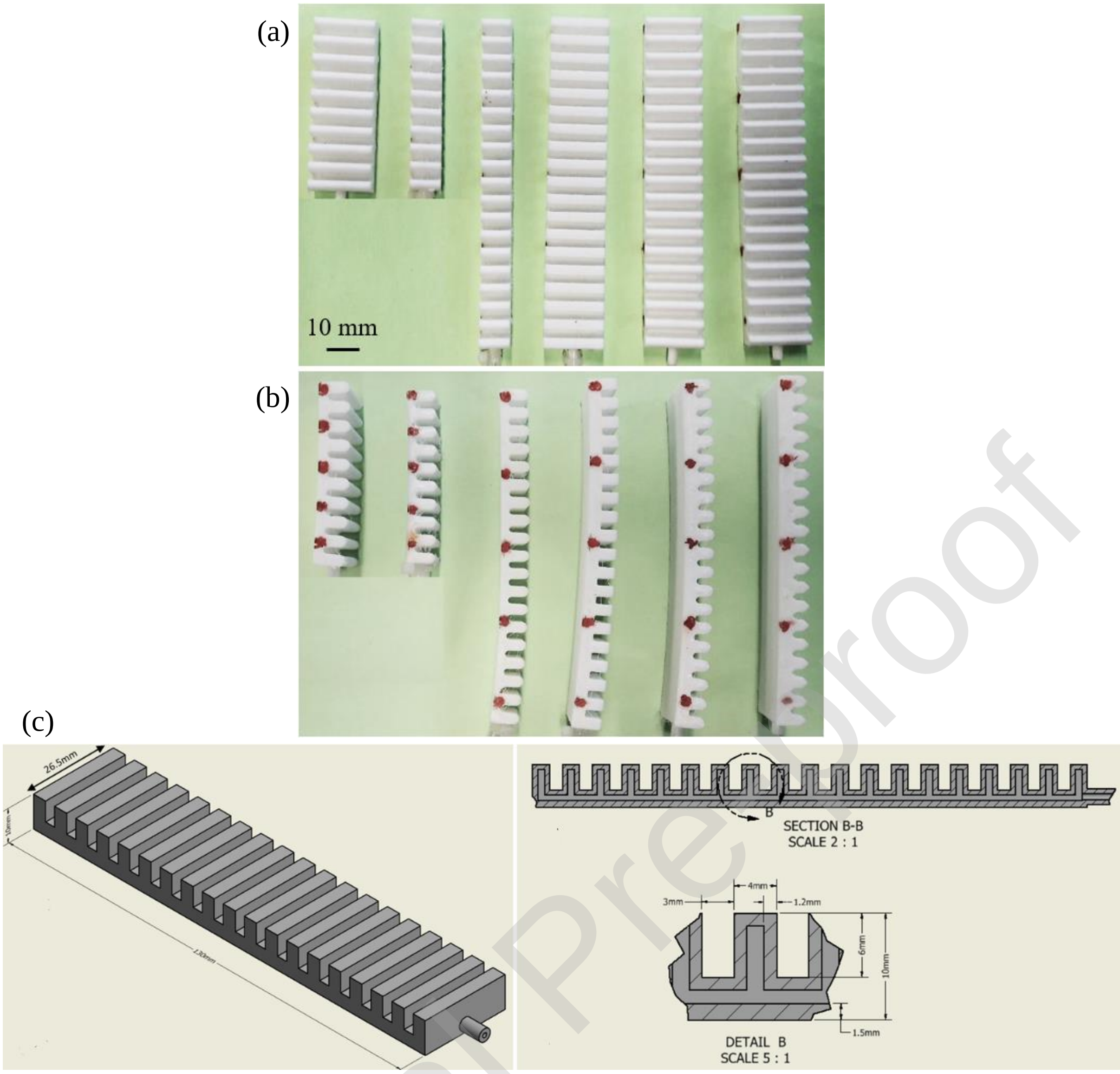
(a)
(b)
(c)


Fig. 1. The geometry of the 4D-printed soft actuators from (a) top; (b) side views; and (c) detailed dimensions.

The analytical expression derived for the steady-state bending angle of the actuator [16] is used to calculate the bending angle of the actuator as:

$$\theta(P) = \frac{L_i A^2 e}{A_w E^2 I} P^2 + \frac{L_i A e}{EI} P = CP^2 + DP \tag{1}$$

where the center of pressure, P, is taken to be at the centroid of the cross-section of the air chamber, e is the distance from the centroid of the actuator cross-section to the center of pressure, L_i is initial length, A is the area of the cross-section of the chamber, and A_w is the area of the cross-section of the actuator. An assumed constant cross-sectional shape is used as the actuator is designed as a shape that is extruded along its length [16]. The bending angle was calculated using the method outlined in [16] and compared to the experimental results. It is observed that the results of the analytical approach did not closely match experimental results, and therefore not feasible for modeling actuation behavior of hyperelastic materials, hence, a more complex model is required.

Finite element modeling using hyperplastic material constitutive laws

The 4D printing performance in terms of the bending angle of SPAs of three different shapes and sizes was simulated using ANSYS. The bellow shapes analyzed in this project, as shown in Fig. 2, were rectangular, circular, and triangular. The actuators were modeled to reflect the 4D-printed SPAs experimental results of the bending angle in response to varying input air pressures. The behavior of hyperelastic materials, could not be accurately modeled using a linear method due to their nonlinear elasticity, exhibiting strains of up to 800% [17]. A nonlinear material model could be developed by fitting a curve to a stress-strain data set using a suitable hyperelastic material constitutive model and then extracting the coefficients that are unique to that material.

The strain energy density function in Mooney-Rivlin and Yeoh models is formed by strain invariants, whereas the Ogden model uses principal stretch ratios to represent the strain energy density function of the hyperelastic material [17]. There are several models with their pros and cons, including Mooney-Rivlin, Ogden, Yeoh, Neo-Hookean, Arruda-Boyce, and Blatz-Ko [2, 18].

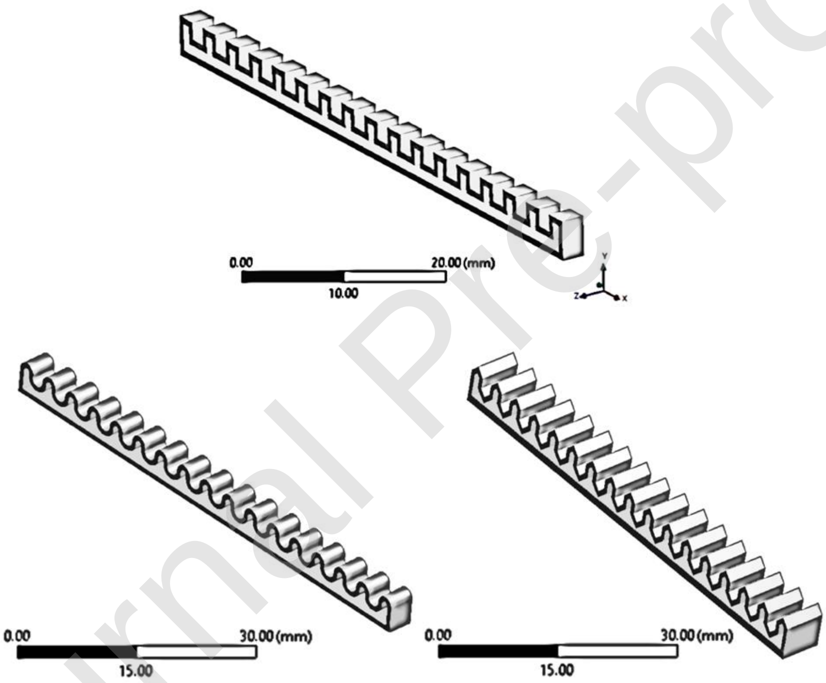


Fig. 2. Cross-sections of the rectangular, circular, and triangular shapes of actuators.

In this study, it was found that the Ogden 3-parameter model [3] was the closest fitting model. The general form of the Ogden model for incompressibility is given by (2) [2], where μ_i and α_i are material constants, and λ_1, λ_2 and λ_3 are stretch ratios.

$$W(\lambda_1, \lambda_2) = \sum_{i=1}^{N} \frac{\mu_i}{\alpha_i}\left[\lambda_1^{\alpha_i} + \lambda_2^{\alpha_i} + \lambda_1^{-\alpha_i}\lambda_2^{-\alpha_i} - 3\right] \qquad (2)$$

Table S2 gives the hyperelastic model material coefficients.

A quadratic tetrahedral mesh was used for the models, and the settings were enabled to capture the curvature of the geometry for the circular actuator. In the meshing setup, the material was set to nonlinear, the actuator fixed at one end, large deformations, and weak springs turned on to account for the comparatively large strains.

The simulation of the actuators using ANSYS validated the experimental results as shown in Fig. 3 with the corresponding images of the SPA under input pressure from 0 to 130 KPa. Also, Fig. 4 shows the comparison of bending angle simulation results of various-shaped actuators in which the rectangular-shaped actuator exhibits the highest bending angles, followed by circular and triangular. We can speculate that this is due to the larger surface area at the top of the bellows where the air pressure is applied, causing greater inflation of the bellows and therefore more bending.

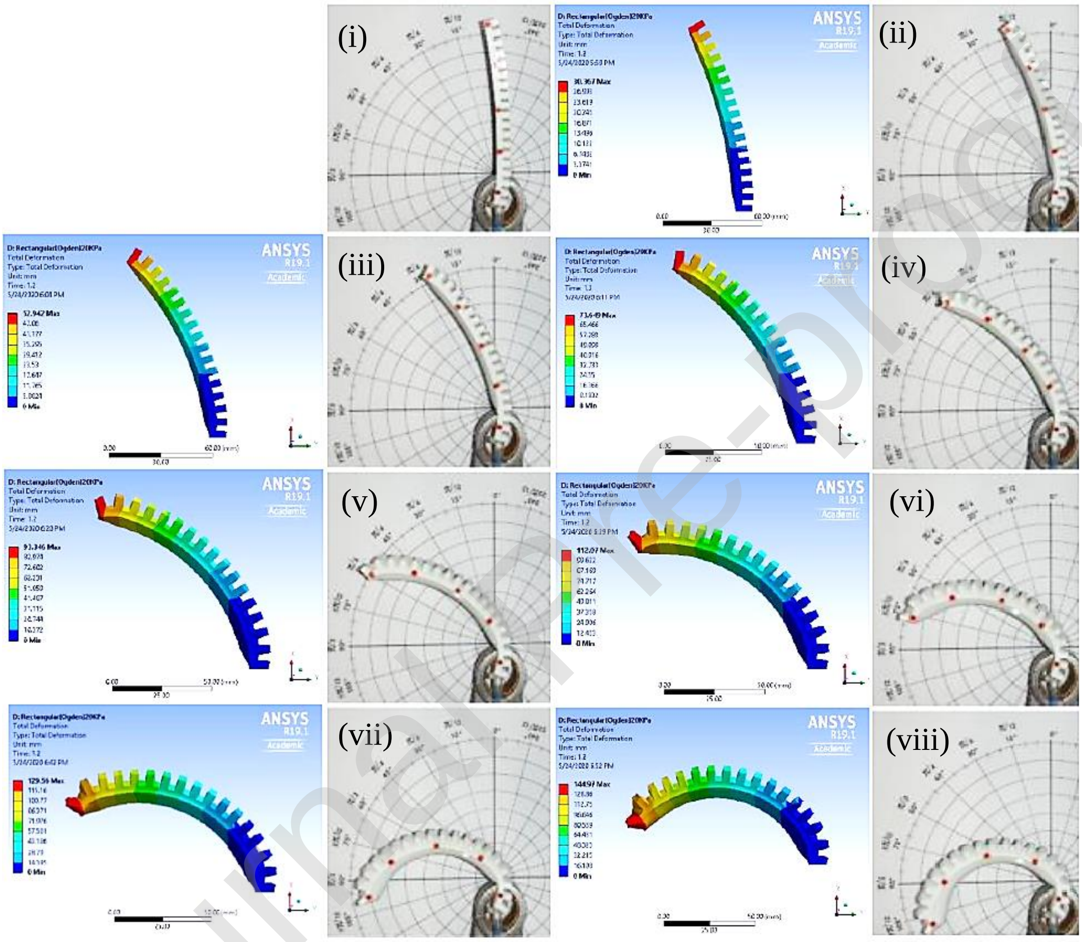


Fig. 3. Bending angles comparisons of FEM simulations and experimental results for rectangular-shaped SPA with input pressure applied from 0 to 130 KPa.

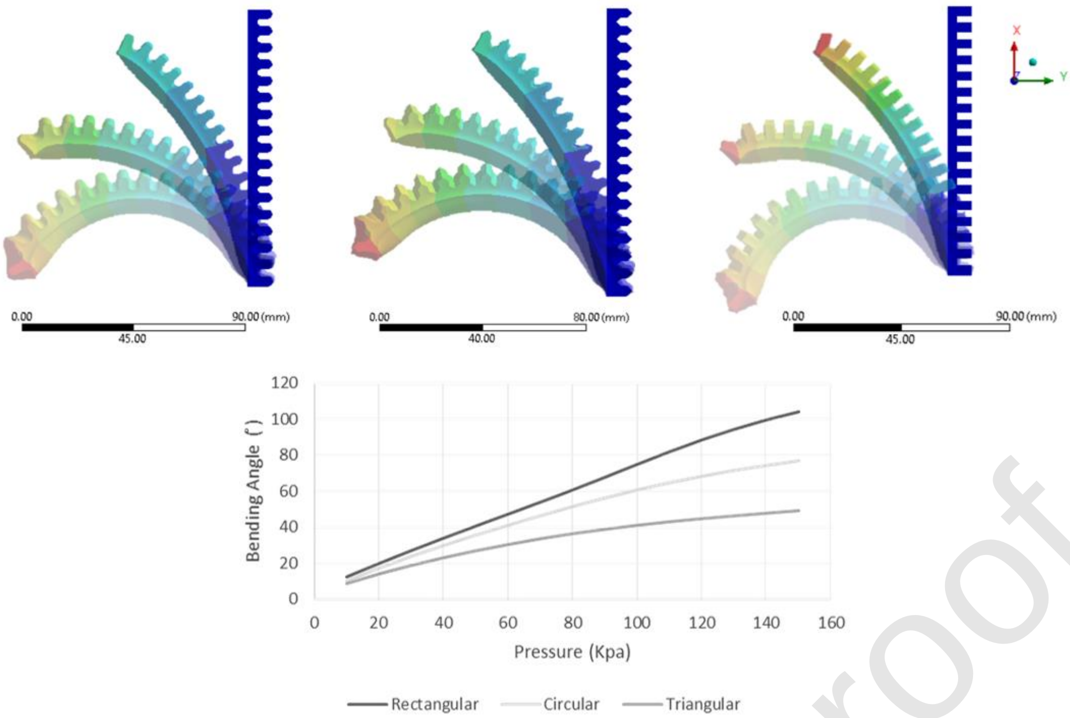


Fig. 4. FEM results comparing the bending sequence simulations of circular, triangular, and rectangular 4D-printed SPAs from left to right, respectively (top), and bending angle comparisons versus input pressure (bottom).

Training data acquisition from FEM

In the process of dimensioning the geometry of the 4D-printed actuators, parameters were set to the dimensions associated with the width, height, and bellow thickness. The range of values used as the input parameters are outlined in Table 1.

Table 1. Variables and their value ranges for FEM simulations

Variable	Minimum	Maximum	Interval
Height (mm)	8	10	1
Width (mm)	10	50	5
Bottom Wall Thickness (mm)	1.2	2	0.2
Air Pressure (KPa)	10	150	10

Initial analysis of the data

An analysis of variance (ANOVA) is needed in this study to disprove the null hypothesis, in which all groups are compatible meaning that the spread of each of their means about the total mean are small enough to assume they all have the same mean [19]. In disproving the null hypothesis, the variability between the groups should be demonstrated [20]. In an earlier study [21] the structural optimization of a SPA was analyzed for four variables and achieved a global ANOVA with a 95% confidence level that the bottom layer thickness had the highest influence on the bending angle. A global ANOVA was conducted here to determine the influence of each variable on the bending angle. In Fig. S1, the p-value is zero for all variables which disprove the null hypothesis. In comparing the F-values for the different variables, we can see that the

input pressure, with an F-value of *1438.72*, has the strongest influence on the bending angle as expected. The second-largest influence was the height with an F-value of *985.1*3, attributed to the increased surface area of the bellow to air pressure, causing greater inflation. This is followed by the width with an F-value of *744.54* and then the shape factor with an F-value of *580.56*. The bottom wall thickness, with an F-value of *23.49*, has a relatively small impact on the bending angle, probably due to the range of values limited by the printing requirements.
The correlations between the input variables and the bending angle are plotted in Fig. 5 and Fig. 6 where Fig. 5 gives the correlations between height, width, and bending angle, and Fig. 6 gives the correlations between bottom wall thickness, pressure, and bending angle. The height and pressure show positive correlations with the bending angle. The width shows a positive correlation with the bending angle until a certain point for the circular and triangular actuators, after which shows a downwards trend. The bottom layer thickness appears to have little influence on the bending angle, showing a negative correlation.

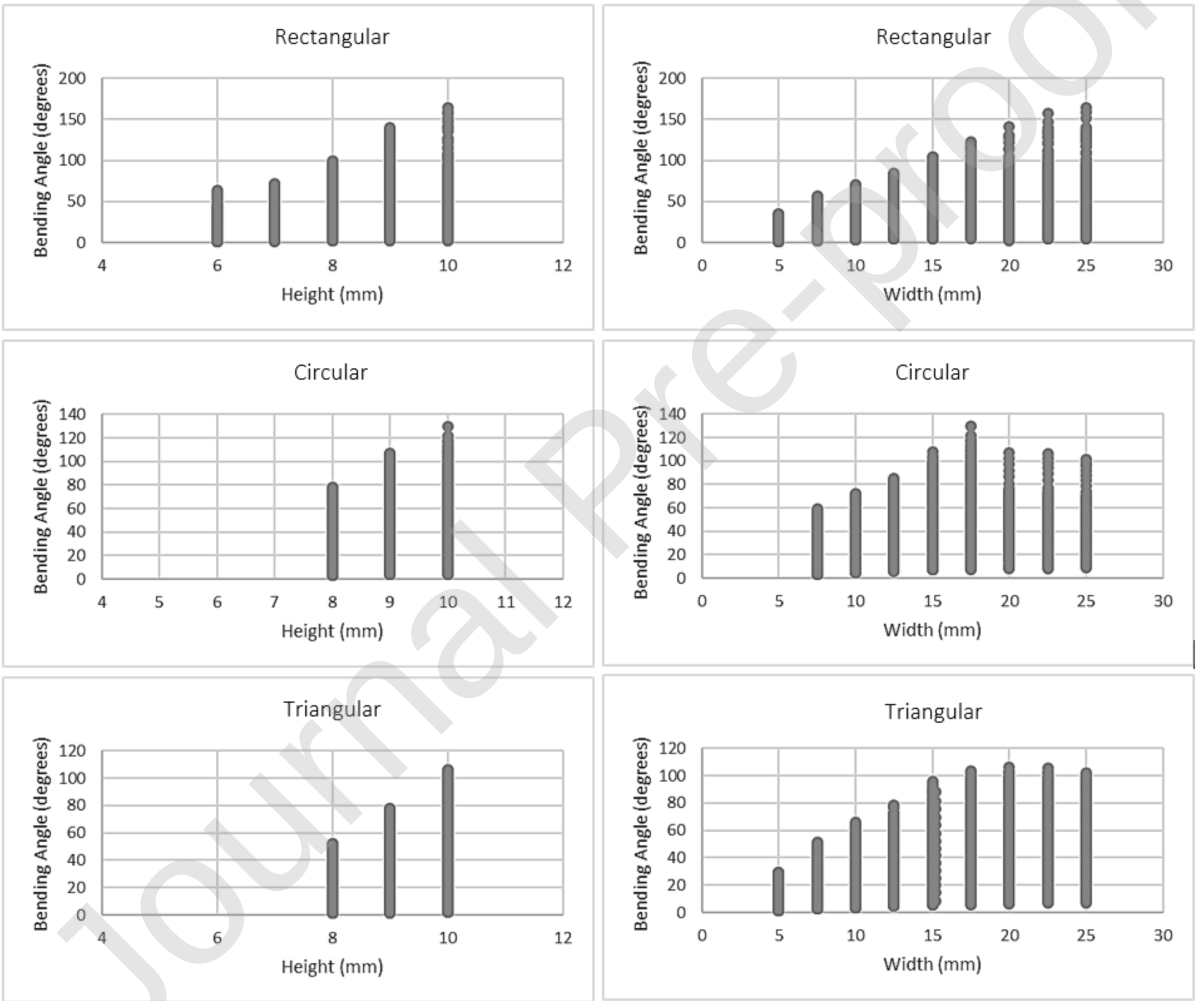


Fig. 5. Correlations between height and bending angle (left column) and between the width and bending angle (right column) for the rectangular, circular, and triangular actuators, from top to bottom respectively.

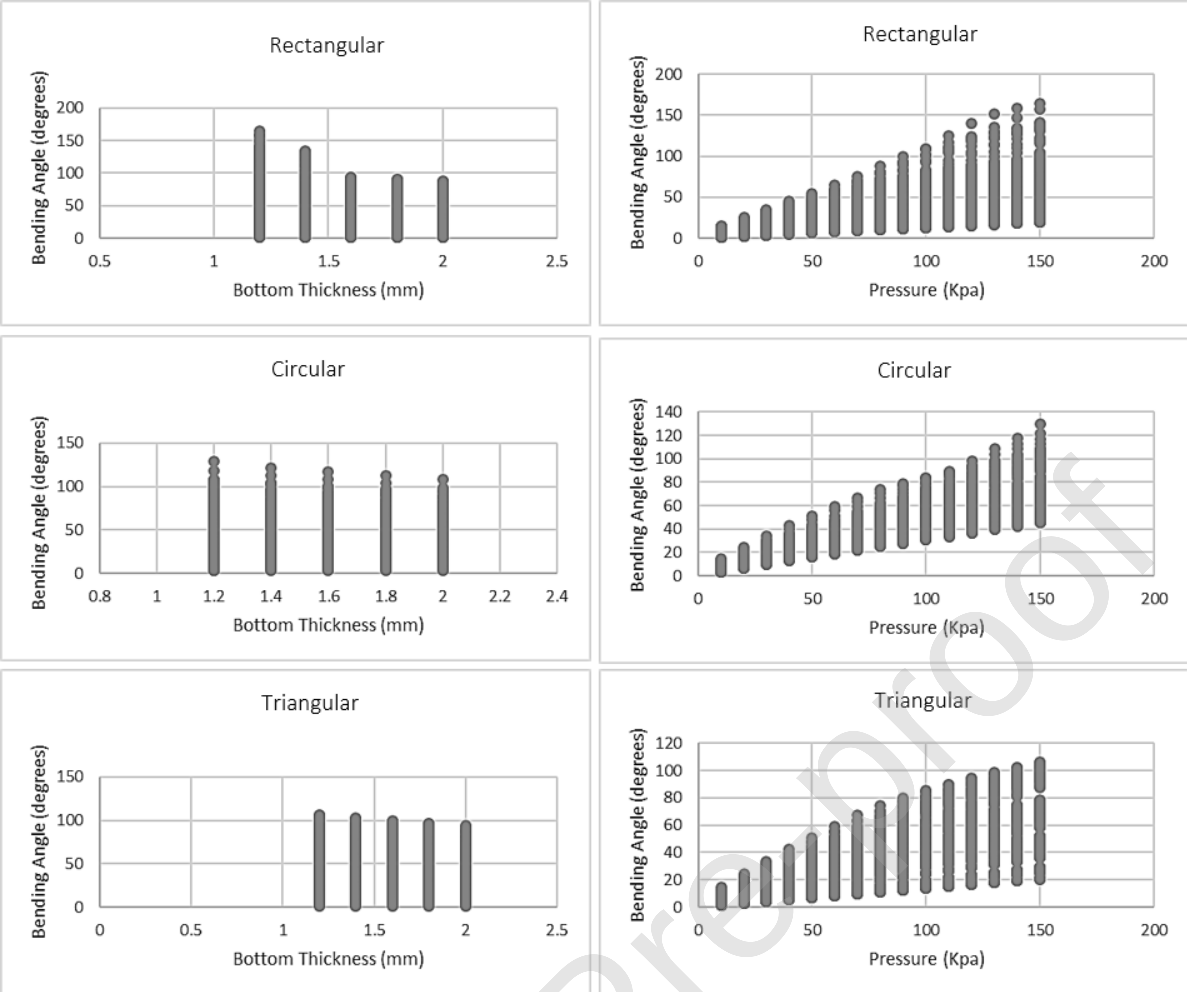


Fig. 6. Correlations between bottom wall thickness and bending angle (left) and between pressure and bending angle (right) for the rectangular, circular, and triangular actuators, from top to bottom respectively.

Linear regression

Linear regression is a method to create predictions based on historical data and consists of a dependent variable and one or more independent variables. This study uses four independent variables; height, width, bottom wall thickness, and air pressure, and therefore a multiple linear regression is used. The general equation for multiple linear regression is given by (3), where Y is the dependent variable, β is a vector of regression coefficients, X is the independent variables, and the ϵ value is the error [10]:

$$Y = \beta_0 + \beta_1 X_1 + \cdots \beta_k X_k + \epsilon \quad (3)$$

To evaluate the models, the R-squared and mean squared error (MSE) are used. R-squared, or the coefficient of multiple determination, is a measure of how close the data is fitted to the regression line. The multiple linear regression models for each 4D-printed actuator shape are modeled using the regression tool on MATLAB, where the inputs and outputs are imported to the workspace as a numerical array with the various categories as the columns. The linear model is then trained, and the regression coefficients and residual plots are provided. The residual plots in Fig. 7 show high bending angle residuals for the input pressure true response obtained from linear regression models for specific shape models of different actuator shapes.

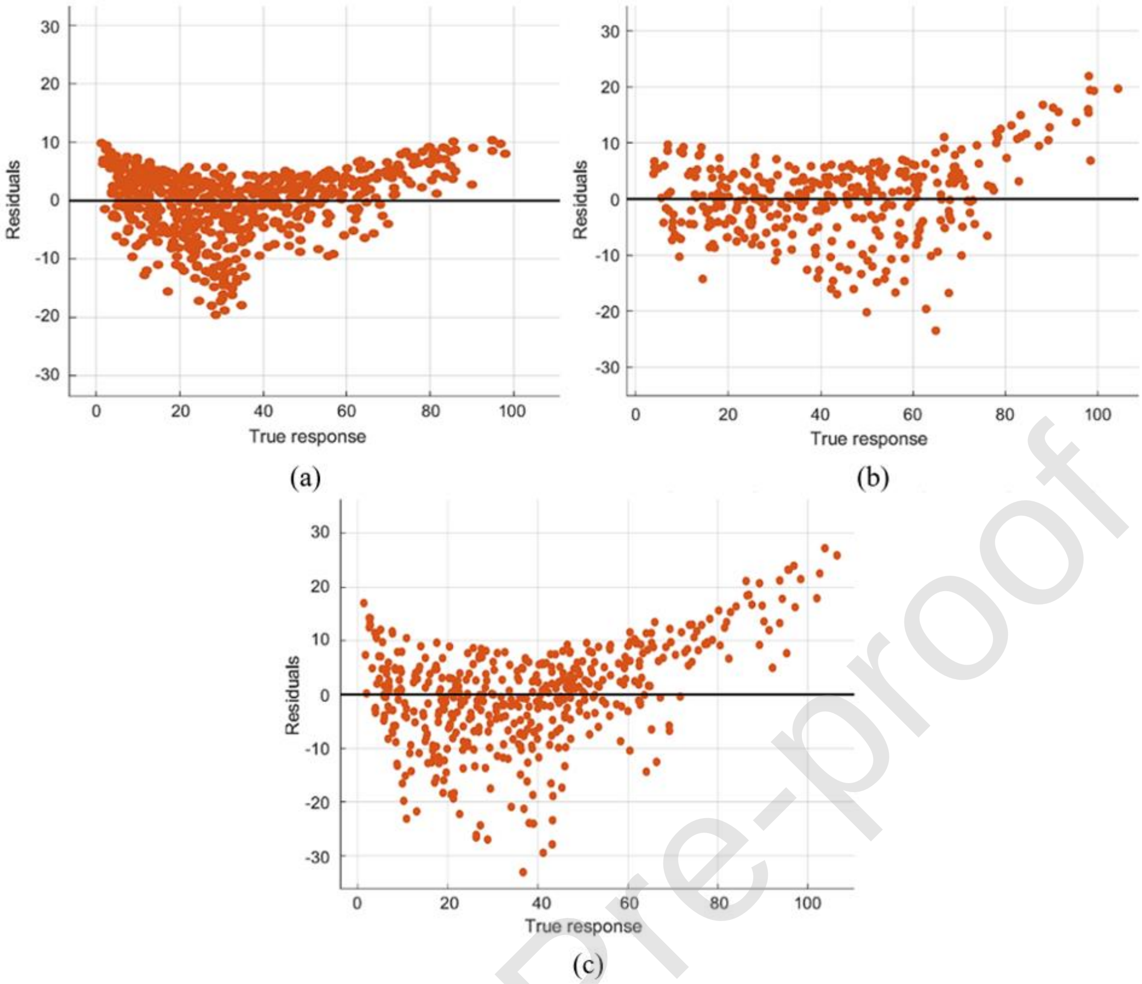


Fig. 7. Residual plots for (a) rectangular (b) circular (c) triangular linear regression models.

Table 2 gives the regression coefficients for the linear regression models, where X_1, X_2, X_3 and X_4 are the height, width, bottom wall thickness, and air pressure respectively. Table 3 gives the regression coefficients for the linear regression model that encompasses all actuator shapes, where X_1, X_2, X_3, X_4, X_5 and X_6 are the rectangular variable, the circular variable, the height, width, bottom wall thickness, and air pressure, respectively. The linear regression models of the differently shaped actuators, as well as the model incorporating all shapes, show large residual error between the simulation results and the predicted values. High MSE values, as shown in Table 4, indicate that a linear representation of the data is not a good fit, which can be expected due to the nonlinear deformation of the material.

Table 2. *Regression* coefficients for the linear regression model for the three individual actuator shapes.

	$\boldsymbol{\beta_0}$	$\boldsymbol{X_1}$	$\boldsymbol{X_2}$	$\boldsymbol{X_3}$	$\boldsymbol{X_4}$
Rectangular	-75.108	8.205	1.576	-3.284	0.396
Circular	-63.348	6.002	1.580	-5.040	0.484
Triangular	-93.247	8.942	1.557	-2.991	0.383

Table 3. Regression coefficients for the linear regression model that encompasses all shapes.

	$\boldsymbol{\beta_0}$	$\boldsymbol{X_1}$	$\boldsymbol{X_2}$	$\boldsymbol{X_3}$	$\boldsymbol{X_4}$	$\boldsymbol{X_5}$	$\boldsymbol{X_6}$
All Shapes	-86.491	12.064	8.925	8.004	1.586	-3.708	0.4126

Table 4. MSE values for the linear regression models.

Shapes	MSE	R-Squared
Rectangular	148.4003	0.74
Circular	54.586	0.90
Triangular	88.973	0.84
All Shapes	108.4	0.81

Machine learning modeling using artificial neural network

The ML method in this project is constructed on the supervised learning ANN [11], which is based on labeled training data consisting of input values and the corresponding desired outputs, known as target data, to solve complex differential equations while taking into consideration nonlinearities that would be otherwise ignored [11]. The MSE loss function measures the error of the model and is used for regression problems [22]. The general formula for this is given by (3) [15].

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \widetilde{y_i})^2 \left(Y - f(X)\right) \tag{4}$$

Where y_i, $\widetilde{y_i}$, and n are the network output, target data, and the number of training data, respectively. To optimize the algorithm, the MSE must be minimized using a gradient-based method while updating the weights and biases [23]. Backpropagation is the term used to describe the refining of the weights and biases of the network to optimize the model [24].

In this study, the actuator variables and the bending configuration serve as input and target data, respectively. The FE-Model is simulated several times with randomly generated actuation profiles to acquire training results, which are divided into three sets: training, validation, and test set. The data is normalized in the first process of training. This gives the data a mean close to zero and places it within a specified range, which speeds up the training [25]. This is a default process when using MATLAB to train a neural network.

The parameters shown in Table S3 are adopted from a study on the closed-loop control system of a SPA [11]. The bending curvature and angle were taken as outputs and the model was deemed a good model with small output errors. The Levenberg-Marquardt solution method is also used in regression analysis and ANN for modeling a soft finger with an embedded flex sensor [11, 16]. ANN was noted to better capture the nonlinearity of the material compared to the linear regression model.

In this study, Matlab Machine Learning was used to determine the most suitable machine learning model for predicting the bending angle of a 4D-printed soft pneumatic actuator, where the multilayer ANN has opted which use Euclidean distances between the inputs and weights of a neuron, multiplied by the bias [23]. It uses the Gaussian activation function which makes the neurons more locally sensitive [23]. Similar to the feedforward neural network, it consists of an input layer, hidden layer/s, and output, uses backpropagation to train, however typically has a faster learning speed and used for function approximation problems [23]. The ANN is trained using the Neural Network Toolbox on MATLAB. The inputs and outputs are imported, and an initial neural network is created and imported to the workspace.

The Bayesian Regularization method was found to be the training algorithm that produced the most accurate results for these neural networks. The networks of this type are created for the rectangular, circular, and triangular-shaped actuators, as well as all shapes combined. The model using all actuator shapes incorporates the three shapes using two Boolean variables. The ANN model for the circular actuator was found to be the most accurate model, whereas the model using all shapes produced the least accurate results. Yet, the neural network model due it its ability to encompass all three actuator shapes were used in further refinement of the model. The optimal number of layers and neurons is determined through an optimization loop [26] to determine the configuration that results in the lowest error and best fit were ended to 2 layers each 10 neurons configurations. An analysis was performed on the influence of the activation function used at each layer on the accuracy of the output of the model. The tan-sigmoid activation function was found to produce the lowest MSE for the model as shown in Fig. 8.

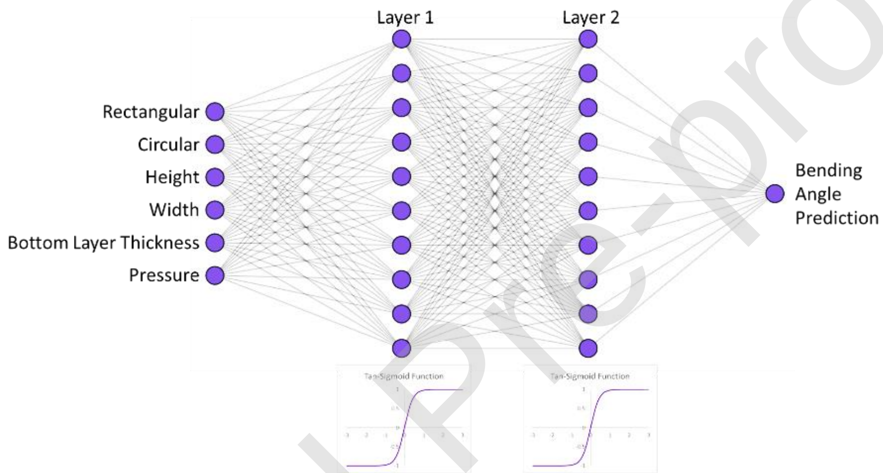


Fig. 8. Optimized ANN configuration for predicting the 4D-printed SPA bending angle.

As seen in Fig. 9, the neural network model is a near-perfect fit to the FEM simulation data, which means that the accuracy of the machine learning model is directly dependent on the accuracy of the FEM model. Fig. 9 shows the FEM model superimposed onto the actuator used in the experiment for air pressure of *120 KPa*. It also shows the neural network and linear regression outputs.

The FEM simulations were conducted for only the rectangular actuator. The neural network was trained using the method obtained from the optimization of the ML model and compared to the experimental and FEM results in Fig. 10. The FEM results and ANN more accurately reflect the experimental results using this model; however, it is evident that there is some error at lower air pressures. We observe that the training MSE value is better, probably due to the smaller number of data causing a better overall fit.

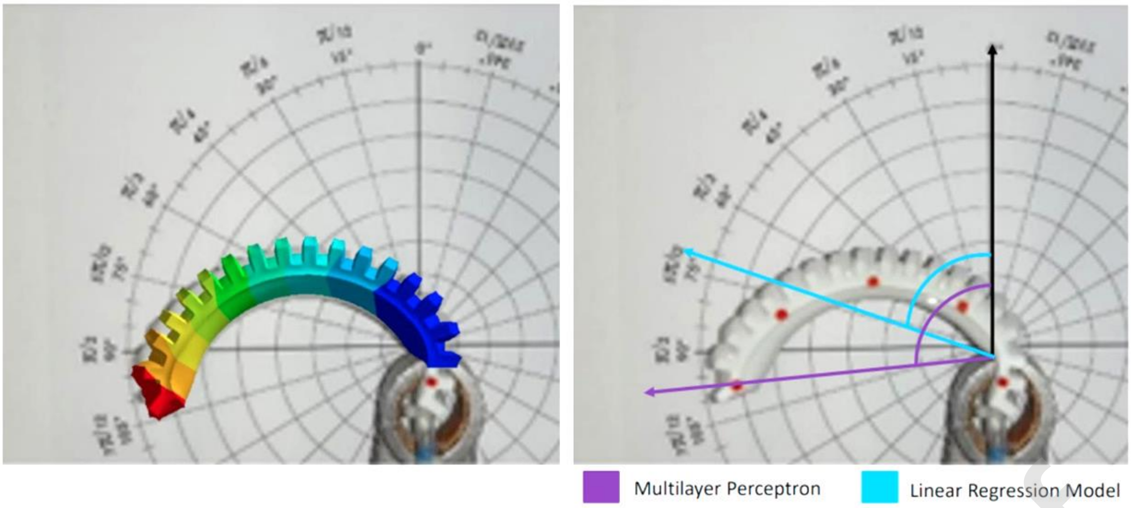


Fig. 9. Superimposed FEM model and neural network prediction on experiment for a rectangular actuator.

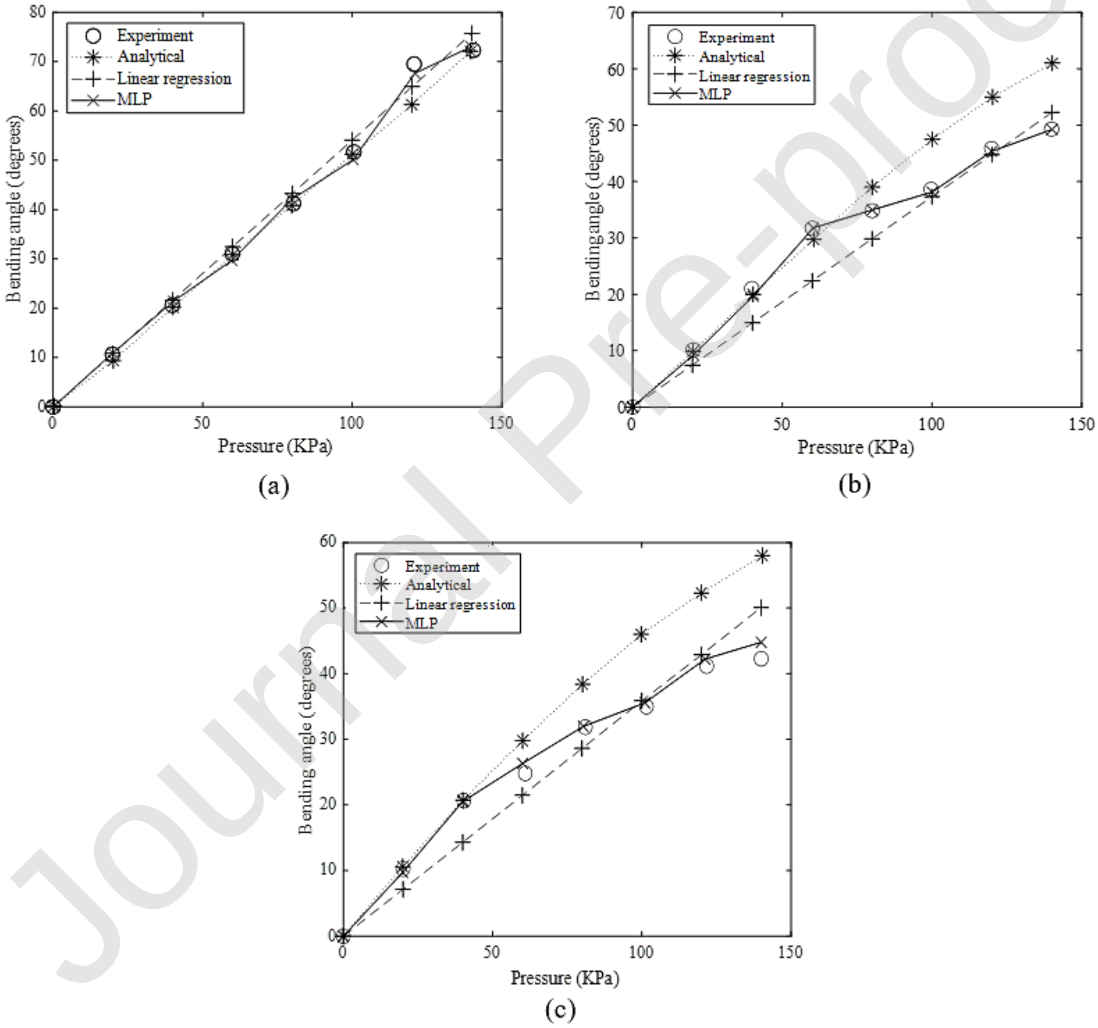


Fig. 10. Model comparison for the rectangular, circular, and triangular actuators from top to bottom respectively.

4D-printed soft actuator shape classification using machine learning

The study so far achieved the bending angle prediction of 4D-printed SPA using ML, however, the capability of ML to predict the geometrical features of the 4D-printed constructs to obtain a required bending angle, for a set of design constraints should be tested. Therefore, a classification model was trained using the bending prediction developed earlier that can determine the 4D-printed SPA shape that would produce the required bending angle given the geometry and input pressure. It was trained using the classifier wizard on MATLAB, which enables importing input and output data and training and optimizing a classification model. To begin with, all classification training methods were tested for the dataset containing all actuator shapes, with the best model being the Medium Gaussian support vector machines (SVM) method. This model had an original accuracy of *82.8%*, and as shown in Fig. 11 the model had a low score in distinguishing the circular shape from the others. An accuracy of *94.3%* was then achieved with the optimization of the hyperparameters of the SVM optimizable classification model. This indicates that the actuator shape for the given input parameters can be predicted with a high level of accuracy for design purposes (see Fig. 11). Classification models were then created to compare two shapes (Fig. 12). The circular versus triangular accuracy diagram model achieves *100%* accuracy meaning that there is little to no error when distinguishing between the circular and triangular shapes. The circular versus rectangular accuracy diagram model achieves *91.8%* accuracy, having the lowest confidence level out of the three models comparing two shapes. The triangular versus rectangular accuracy diagram model achieves *98.9%* accuracy. In the end, experimental tests of the 4D-printed SPAs based on the ML classification model were carried out to demonstrate the successful grasp of objects with different bending and geometry specifications (Fig. 13, Video S1 and S2).

Fig. 11. Classification model accuracy diagrams of three shapes; (left) before and, (right) after optimization.

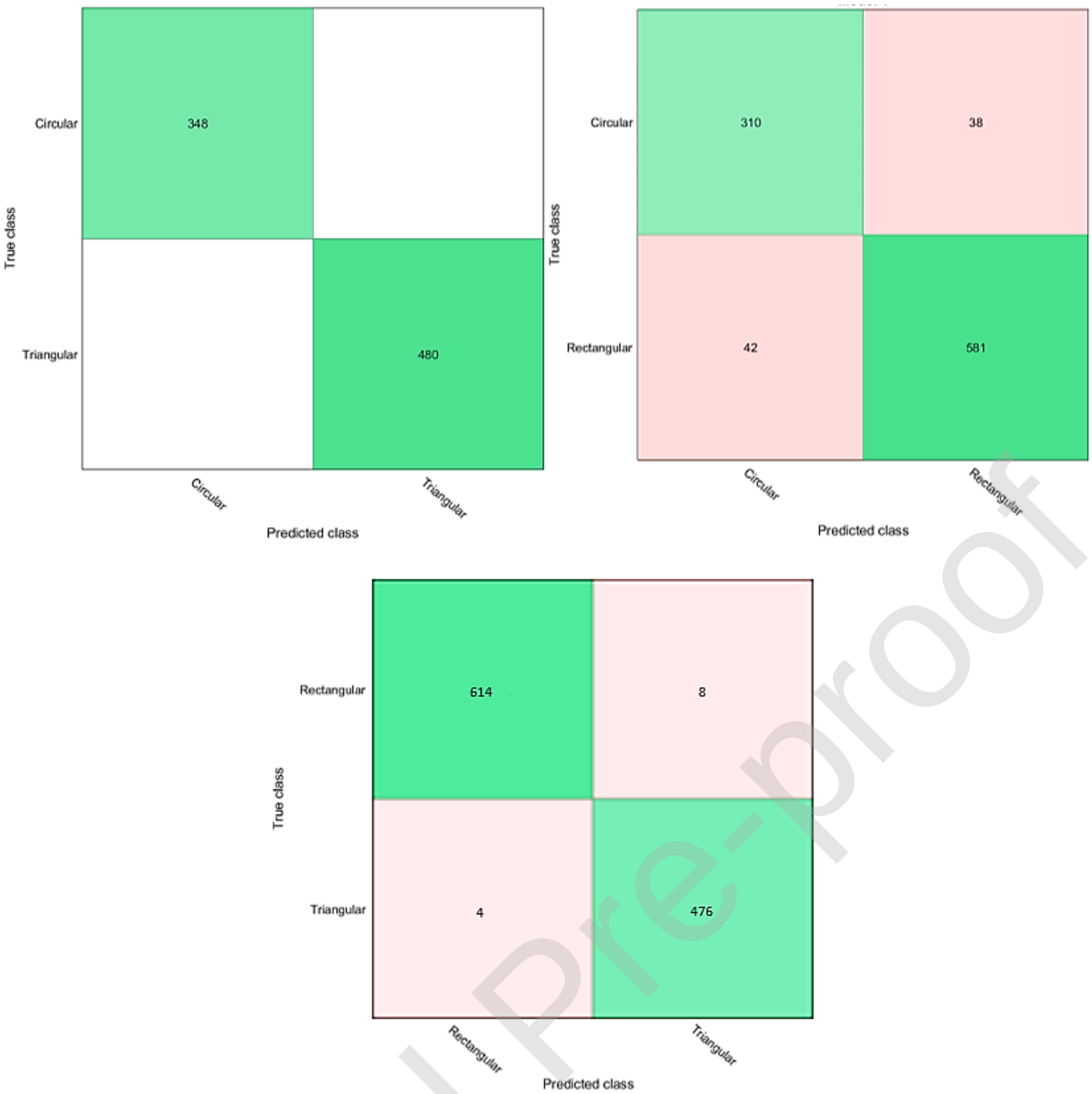


Fig. 12. Classification model accuracy diagrams of two shapes.

Fig. 13. Experimental tests of the 4D-printed SPAs based on the ML Classification model to grasp objects with different bending and geometry specifications.

Discussions

The comparison of the different models used to predict the bending angle of the 4D-printed SPAs indicates that the ML successfully predicted the experimental results trained by FEM simulation data. The ineffectiveness of the analytical model stemmed from the utilization of a linear stress-strain relationship. This assumption failed to take into consideration the non-linear behavior of the hyperelastic material. It also assumed isotropy which is not the case due to the additive manufacturing method. This validated the need for a model that could cover the complexities and nonlinearities of the material and geometry in 4D printing. The linear regression model also lacked accuracy as the rigidity of this model is unsuited to the complexity of the problem and does not allow for the variation of influence of each variable as the bending angle increases. The hyperelastic model with Ogden 3-parameter material coefficients found the most suitable constitutive model in ANSYS to fit the experimental data, validating the effectiveness of using FEM to simulate real actuation resulting in an accurate ML model to accurately predict the bending angle of 4D-printed SPA.

Having achieved a reliable ML model to predict the bending angle of actuators the study continued to estimate the geometrical specifications required to develop 4D-printed SPAs based on the input variables. The classification model for predicting shape is useful for design purposes and enables the user to achieve their desired motion in 4D printing if, for example, there are geometrical requirements or limitations. The results from the ANOVA analysis enabled the identification of the variables that will maximize actuation which can ultimately lead to efficiency in energy requirements and cost of the actuator. The classification model was developed by optimizing the hyperparameters to create a model with 94.3% accuracy of distinguishing between the three actuator shapes and the results were experimentally validated on grasping different size objects.

This approach of ML-based modeling could be tailored to the other types of 4D printing studies where the new design parameters could be defined first and after validating the experimental results in FEM all the simulation data could be used to create a new ML model. Future work may be conducted to analyze the blocking force. This work may be used to develop control systems utilizing this technology and design, or for design purposes of closed-loop 4D-printed soft robots and actuators with specific functional and geometrical requirements. External loads are not taken into account in this study. In real-world 4D printing problems, the impacts of these variables must be considered.

Conclusion

The outcome of this work is a machine learning (ML) and Finite element (FE) driven model that can accurately estimate the 4D-printed soft pneumatic actuator (SPA)s requirements to achieve a specific bending angle. It followed the development and simulation of a finite element model (FEM) which accurately reflects experimental results given a suitable nonlinear hyperelastic model. The study proves that a ML model is more suited to a nonlinear problem than a linear analytical or regression model. Models for predicting bending angle, pressure, and shape were successfully developed, and the results of an analysis of variance (ANOVA) indicated the level of influence of each variable on bending angle where the height was found to have the highest influence on bending angle, with bottom wall thickness having negligible influence. The rectangular-shaped actuator exhibited the highest bending angles for a given geometry, followed by circular and triangular. The variables used were the bellow shape, height, width, bottom layer thickness, and air pressure. Using this data, a ML learning model was developed and optimized to predict the bending angle given a certain set of inputs. The classification model was developed by optimizing the hyperparameters to create a model with 94.3% accuracy of distinguishing between the three actuator shapes. The importance of this work lies in the accurate modeling of nonlinear materials and complex geometries in 4D printing. The ML model accurately predicted experimentally validated FEM data and proved to be a viable solution for modeling such 4D-printed structure given an accurate FEM model.

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Author declaration

Conflict of Interest

No conflict of interest exists.

Funding

Funding was received for this work.

Intellectual Property

We confirm that we have given due consideration to the protection of intellectual property associated with this work and that there are no impediments to publication, including the timing of publication, with respect to intellectual property. In so doing we confirm that we have followed the regulations of our institutions concerning intellectual property.

Research Ethics

We further confirm that any aspect of the work covered in this manuscript that has involved human patients has been conducted with the ethical approval of all relevant bodies and that such approvals are acknowledged within the manuscript.

IRB approval was obtained (required for studies and series of 3 or more cases)

Written consent to publish potentially identifying information, such as details or the case and photographs, was obtained from the patient(s) or their legal guardian(s).

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The authorship be based on the following four criteria:

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All listed authors meet the criteria. We attest that all authors contributed significantly to the creation of this manuscript.

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