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Machine Learning-Based Prediction of Thermal Behaviour and Shape Memory Response of 4D Printed PLA/bTPU/Lignin Biocomposites Fabricated by Fused Deposition Modelling

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Abstract: This study develops a data-driven framework for predicting the thermal recovery behaviour and shape memory response of biodegradable polymer biocomposites prepared by fused deposition modelling for four-dimensional printing applications. The work addresses the need to reduce trial-and-error experimentation during the design of sustainable thermo-responsive materials. Experimental data from material formulation and thermal recovery testing were used to train and evaluate four regression models: linear regression, support vector regression, random forest, and artificial neural network. Composition, recovery temperature, and recovery time were used as input variables, while recovery angle and shape memory responses were used as target outputs. The artificial neural network achieved the highest coefficient of determination of 0.95 and captured the nonlinear recovery behaviour most consistently. Support vector regression produced the lowest root mean square error of 2.66 and the lowest mean squared error of 7.09, indicating strong numerical accuracy. Random forest showed moderate predictive capability, while linear regression was less effective because of the nonlinear nature of the recovery response. The findings show that artificial neural network modelling provides the most reliable overall prediction for this biocomposite system, while support vector regression is effective for minimizing prediction error. Machine learning can therefore support formulation screening, reduce experimental workload, and guide the development of sustainable shape memory biocomposites for four-dimensional printing applications.

Keywords: Machine learning, 4D printing, shape memory polymer, fused deposition modelling

1. Introduction

The advancement of 4D printing technology has enabled the fabrication of structures capable of programmed shape transformation in response to external stimuli. This capability offers significant potential in biomedical devices, aerospace systems, and soft robotics, where printed components may be designed to change shape, recover programmed geometries, or respond to environmental triggers [1]. Central to this capability is the development of stimuli-responsive polymers, particularly thermo-responsive shape memory polymers, which can recover their original configuration upon thermal activation [2], [3].

Polylactic acid (PLA) is a biodegradable thermoplastic widely used in fused deposition modelling because it provides stiffness, dimensional stability, and printability. However, PLA has limited shape memory performance because of its brittleness and insufficient elastic recovery phase [4]. The incorporation of elastomeric components such as thermoplastic polyurethane can introduce flexibility and improve shape recovery by providing a soft segment capable of elastic deformation and thermal activation. Bio-based thermoplastic polyurethane (bTPU) is particularly attractive because it combines elastomeric behaviour with improved environmental compatibility, and recent work confirms that PLA/TPU-based blends can achieve near-complete shape fixity and recovery ratios exceeding 90% when the elastomeric phase is well dispersed [5], [6].

Lignin is an abundant renewable by-product of the pulping industry and has emerged as a promising sustainable filler because of its aromatic structure and thermal stability [7]. In PLA-based systems, however, lignin application may be restricted by poor compatibility, inadequate dispersion, and weak interfacial adhesion, which can reduce mechanical performance and functional reliability[8]. Surface modification strategies such as acetylation and grafting have been introduced to improve compatibility, yet their influence on the shape memory behaviour of thermally responsive biocomposites remains insufficiently understood [9], [10].

Despite the growing number of studies on PLA-based blends and composites, the combined effects of bTPU and lignin on the shape memory performance of PLA have not been extensively studied, particularly under thermal activation conditions relevant to 4D printing applications. Existing optimization approaches also rely heavily on empirical trial-and-error experimentation, which is time-consuming, resource-intensive, and limited in predictive capabilityc[11]. Data-driven modelling techniques such as artificial neural networks, support vector regression, and random forests offer a practical route for capturing complex relationships between material formulation, processing parameters, and functional performance, and have already demonstrated strong predictive capability for recovery angle and recovery stress in unrelated shape memory systems such as carbon-fibre-reinforced epoxy composites and thermoset [12].

This study integrates material development with machine learning-based prediction to establish a systematic framework for designing sustainable PLA/bTPU/lignin shape memory biocomposites, building on recent perspectives calling for machine learning to bridge molecular design and macroscopic shape memory performance. The proposed approach supports the development of 4D-printable materials with enhanced thermo-responsive performance while reducing experimental workload and improving formulation optimization.

The scope of this manuscript is limited to the development of machine learning models for predicting thermal recovery and shape memory behaviour from experimentally derived formulation and recovery-condition data. The experimental fabrication and testing procedures provide the basis for model training, validation, and interpretation. Accordingly, this study aims to develop and evaluate machine learning models for predicting the effects of formulation variables and processing parameters on the properties of PLA/bTPU/lignin biocomposites fabricated via fused deposition modelling, and to assess the predictive reliability of these models in forecasting the thermal behaviour and shape memory response of PLA/bTPU/lignin biocomposites based on experimental data.

2. Materials and Methods

2.1 Materials

Polylactic acid (PLA; Ingeo 2003D, NatureWorks LLC) was used as the primary biodegradable matrix. PLA is a semi-crystalline thermoplastic with a density of 1.24 g/cm³ and a melt flow index of 6 g/10 min at 210 °C and 2.16 kg. The material has a tensile strength of 53 MPa, tensile modulus of 3.5 GPa, elongation at break of 6.0%, melt temperature of 210 °C, and glass transition temperature of 55 °C.

The bio-based thermoplastic polyurethane (bTPU) employed in this study was LARIPUR 4525EG, supplied by Plastech Technical. The material exhibits a tensile strength of 35 MPa, elongation at break of 600%, and density of approximately 1.1 g/cm³. Its recommended melt processing temperature range is between 190 °C and 210 °C. Alkaline lignin (CAS No. 8068-05-1), supplied in dark brown powder form with a density of 1.3 g/mL at 25 °C, was procured from Sigma-Aldrich, Malaysia.

2.2 4D Shape Recovery Testing

Shape recovery tests were conducted using 4D-printed cantilever specimens according to the protocol reported by Leist et al. [13]. The specimens measured 25.0 mm × 70.0 mm with thicknesses of 1.0 mm, 1.5 mm, and 2.0 mm. Five printed samples were

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evaluated for each composition, and the average shape recovery percentage was calculated from recorded bending angles to determine the one-way shape memory effect.

Each specimen was initially heat-treated in water at 60 °C, 70 °C, or 85 °C for 1, 4, or 7 min. After heating, the specimens were fixed in a temporary deformed shape and cooled to room temperature, after which the deformation angle was recorded. During recovery, the specimens were re-immersed in water under the same temperature and duration conditions to trigger return toward their permanent shape. Recovery angles were measured using a digital protractor.

Shape recovery percentage was calculated as follows:

Shape Recovery (%) = [(recovered angle − deformed angle) / (180° − deformed angle)] × 100.

2.3 Machine Learning Model Development

The machine learning framework was implemented using MATLAB R2025a together with modelling tools associated with Keras and Scikit-Learn. The workflow enabled the development, training, and evaluation of both conventional regression models and deep learning models to examine how formulation variables and processing parameters influence the functional performance of PLA/bTPU/lignin biocomposites [13], [14].

The modelling process began with preparation of the experimental dataset. Input features included the weight percentages of PLA, bTPU, lignin, treated lignin where applicable, recovery temperature, and recovery time. The target variable was recovery angle, while additional shape memory indicators, including shape fixity ratio and shape recovery ratio, were considered for predictive assessment. The dataset was divided into training and testing subsets using an 80:20 split, and input variables were scaled using StandardScaler for SVR and ANN models.

Four regression models were evaluated: linear regression, support vector regression, random forest, and artificial neural network. Linear regression was used as a baseline model, while support vector regression with a radial basis function kernel and random forest with 100 decision trees were used to capture nonlinear relationships. The artificial neural network was developed using a multilayer perceptron architecture with an input layer, two hidden layers containing 64 and 32 neurons with ReLU activation, and a single output neuron. The ANN was trained using the Adam optimizer to minimize mean squared error over 150 epochs.

2.4 Data Preparation, Validation, and Optimization

Prior to model training, the dataset was cleaned, normalized, and encoded where categorical variables were present. Feature selection was performed using Pearson correlation and model-based feature importance to remove redundant or weakly correlated variables. This step reduced dimensionality, minimized overfitting risk, and improved model interpretability.

Model validation was performed using an 80:20 train-test split and five-fold cross-validation on the training data. Hyperparameters were optimized using grid and randomized search strategies with internal cross-validation. For the ANN model, training was evaluated over 100 to 300 epochs, and early stopping was applied to prevent overfitting and unnecessary computation.

Model performance was assessed using the coefficient of determination (R^2), mean squared error (MSE), root mean squared error (RMSE), and mean absolute percentage error (MAPE). Diagnostic visualizations, including residual plots, parity plots, and learning curves, were also used to evaluate model behaviour, error distribution, convergence trends, and prediction reliability [13], [14].

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2.5 Machine Learning Workflow

Table 1 summarizes the complete machine learning workflow, from data preparation and feature selection to model training, validation, and predictive application.

Process Step	**Description**
Data preparation	The dataset was compiled from experimental results, including formulation ratios, printing parameters, and material properties. Data were cleaned, normalized, and encoded before use.
Feature selection	Redundant or low-impact variables were removed using Pearson correlation and feature importance to reduce overfitting.
Model selection	Four models were used: linear regression, support vector regression, random forest, and artificial neural network.
Model training	The ANN was trained using 100–300 epochs, Adam optimizer, and MSE loss function. Early stopping was applied to avoid overfitting.
Validation strategy	An 80:20 train-test split with five-fold cross-validation was used to ensure model reliability and generalizability.
Performance metrics	Model performance was assessed using R^2, MSE, RMSE, and MAPE. Visual diagnostics included residual plots, parity plots, and learning curves.
Predictive application	The best model was used for virtual screening and inverse design to predict optimal inputs for desired shape memory performance.

3. Results and Discussion

3.1 Machine Learning-Based Prediction of Thermal Recovery Behaviour and Shape Memory Response

The integration of machine learning into predictive materials design provides an efficient route for understanding and forecasting shape memory behaviour in 4D printable biocomposites. In this study, four regression models, linear regression (LR), support vector regression (SVR), random forest (RF), and artificial neural network (ANN), were developed to predict the recovery angle and related shape memory response of PLA/bTPU/lignin biocomposites under varying formulation and processing conditions. The models were evaluated using both quantitative statistical metrics and visual comparison between predicted and actual recovery responses.

The machine learning models were designed to predict thermal recovery behaviour and shape memory response parameters, including recovery angle, shape fixity ratio, shape recovery ratio, and recovery time. Because these responses are governed by complex interactions among PLA rigidity, bTPU elasticity, lignin reinforcement, recovery temperature, and exposure time, nonlinear regression models were expected to perform better than linear approaches.

3.2 Training and Validation Scatter Plot Analysis

Predicted-versus-actual scatter plots were used to assess the predictive reliability of each model for both training and validation datasets [14], [15]. From Figure 1, the ANN model showed strong clustering of data points around the parity line, indicating robust generalization and strong agreement between experimental and predicted recovery angles. SVR also demonstrated good alignment with the parity line, although occasional underprediction was observed in the validation dataset, particularly at higher recovery values.

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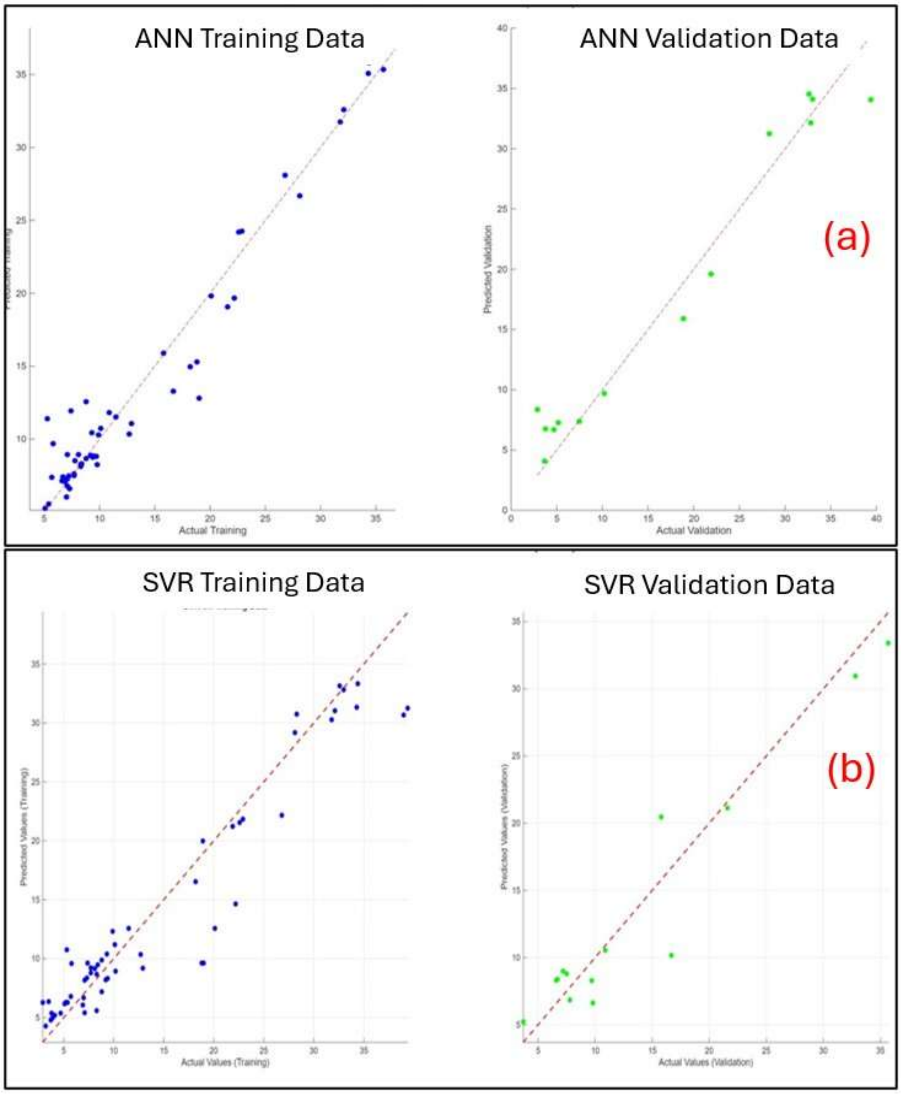
In contrast, RF displayed greater dispersion, especially in the validation data, suggesting moderate predictive consistency. LR showed the largest deviations from the parity line and was less effective in representing the nonlinear nature of recovery behaviour in the biocomposite system. These observations confirm that graphical validation is useful for identifying bias, assessing model fit, and detecting limitations in model generalization.



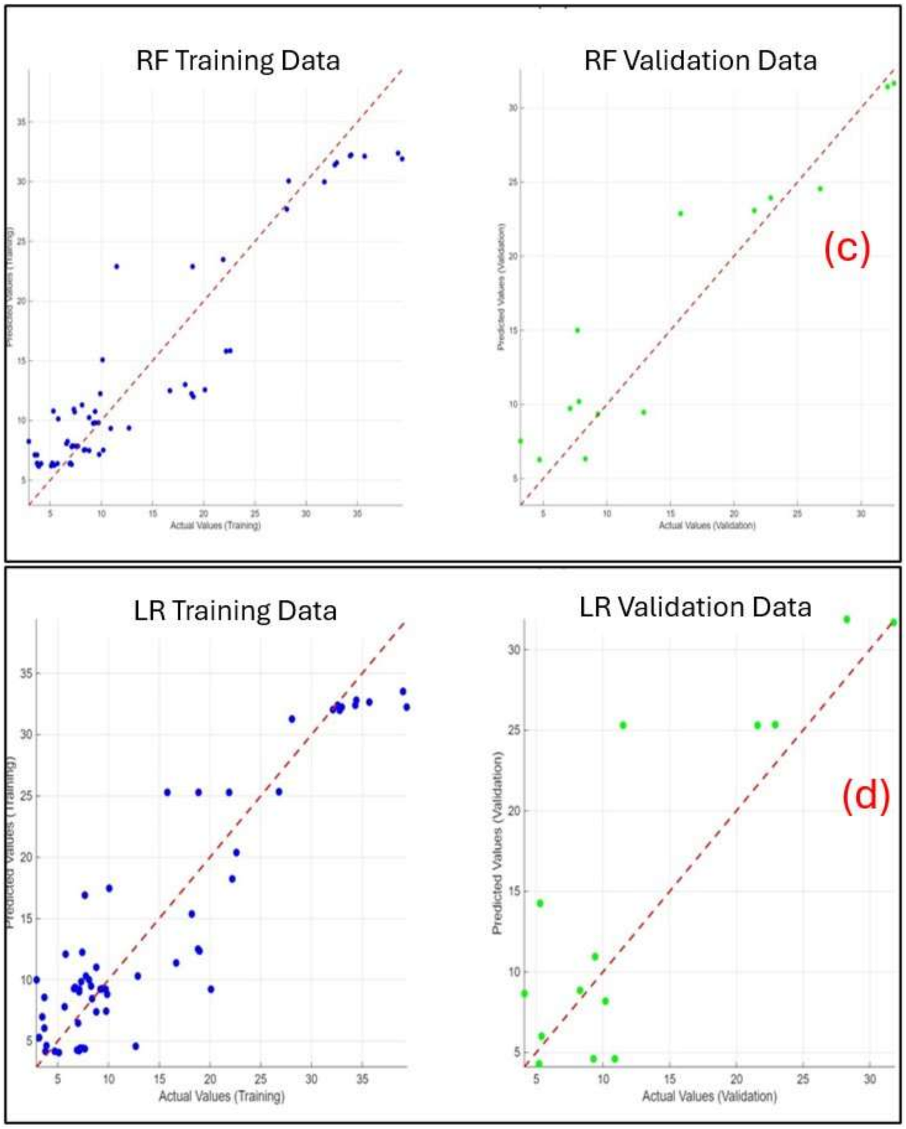


Figure 1. Predicted versus actual values for (a) ANN, (b) SVR, (c) RF, and (d) LR models for shape recovery ratio (Rr) prediction. Both datasets demonstrate strong predictive alignment with minimal deviation from the parity line.

The recovery angle represents the angular displacement between the deformed and recovered configurations; a lower final recovery angle indicates more complete recovery. Based on the predicted and experimental values, model performance was further quantified using R^2, MSE, RMSE, and MAPE. The combined graphical and statistical evaluation showed that ANN captured the nonlinear recovery trend most effectively, while SVR provided strong numerical accuracy but showed minor underprediction in selected recovery zones.

3.3 Predictive Accuracy of Machine Learning Models (strengthened comparative framing)

The ANN model demonstrated the strongest overall predictive capability, achieving an R^2 value of 0.95, MSE of 8.86, RMSE of 2.98, and MAPE of 28.46%. This trend is consistent with recent comparative ML studies on shape memory systems, where kernel-based and neural approaches consistently outperform tree ensembles for small, smooth experimental datasets typical of shape-memory recovery testing. Although SVR produced slightly lower error values, with an MSE of 7.09 and RMSE of 2.66, ANN provided smoother and more realistic predictive curves across the full recovery-angle range, a pattern also reported for carbon-fibre-reinforced shape memory epoxy composites, where SVR achieved the highest accuracy with controlled generalization ($R^2 = 0.944$) while random forest exhibited comparatively limited effectiveness ($R^2 = 0.842$). This qualitative agreement is important because shape memory behaviour is highly sensitive to small variations in formulation, thermal activation, and processing parameters, consistent with the broader literature on machine-learning-guided shape memory polymer design [16], [17].

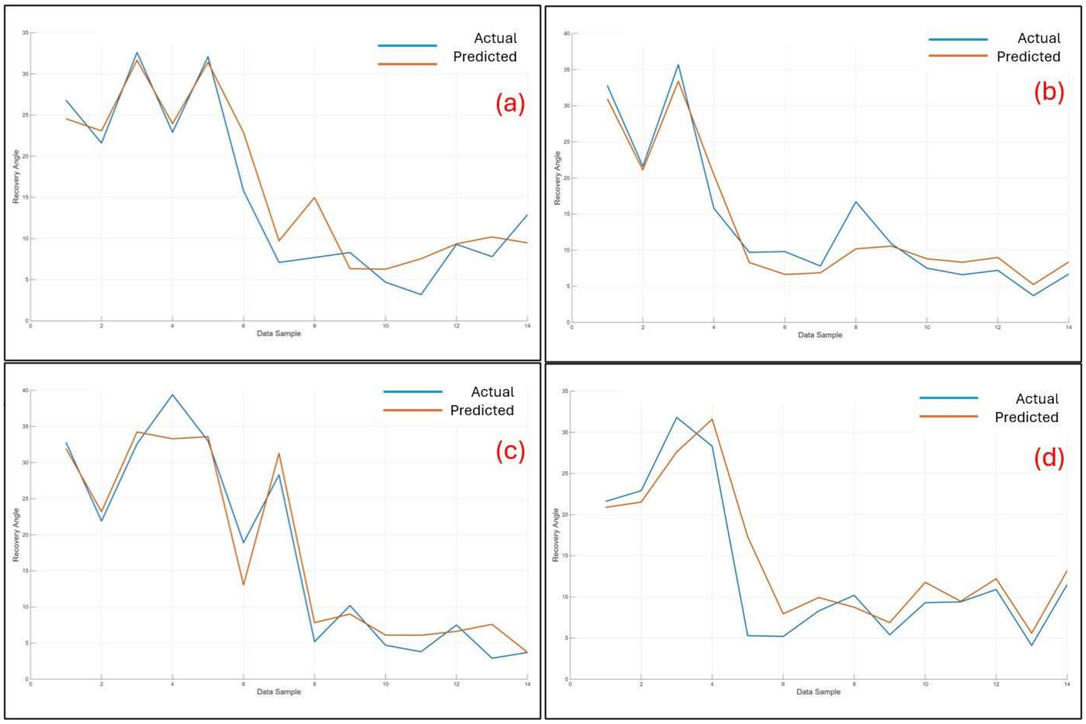


Figure 2. Measured versus predicted recovery angles for PLA/bTPU-L biocomposites using four machine learning models: (a) artificial neural network (ANN), (b) linear regression (LR), (c) random forest (RF), and (d) support vector regression (SVR).

LR served as a baseline model and achieved an R^2 value of 0.87, MSE of 13.82, RMSE of 3.72, and MAPE of 22.63%. Despite this reasonable R^2 value, LR failed to capture nonlinear dependencies and tended to smooth out important peaks and troughs in the experimental response. This limitation reflects the inability of a purely linear model to represent the multifactorial interactions among composition, thermal transitions, and shape recovery mechanisms, echoing prior findings that deep learning and kernel-based models substantially outperform linear approaches for thermomechanical shape memory prediction [18].

RF achieved an R^2 value of 0.87, MSE of 11.61, RMSE of 3.41, and MAPE of 32.30%. The ensemble structure of RF provided some ability to capture local fluctuations in recovery behaviour, particularly in mid-range values. However, its predictions were less consistent across the dataset, indicating that further tuning or hybridization may be required for highly dynamic shape memory systems, consistent with reports that tree-based ensembles are less suitable than kernel or gradient-based methods for small, smooth datasets in shape memory recovery prediction.

SVR achieved an R^2 value of 0.92, MSE of 7.09, RMSE of 2.66, and MAPE of 19.99%, making it the best model in terms of error magnitude. Its radial basis function kernel enabled effective modelling of nonlinear relationships, especially at lower recovery angles. However, SVR slightly underpredicted sharp recovery peaks at higher values, suggesting lower adaptability than ANN when multiple nonlinear transitions are present [19], [20].

The comparative test-set performance of the four regression models is summarized in Table 2.

Table 2. Performance metrics of machine learning models on the test dataset.

Machine Learning Model	R^2	MSE	RMSE	MAPE
Linear Regression (LR)	0.87	13.82	3.72	22.63%
Support Vector Regression (SVR)	0.92	7.09	2.66	19.99%
Random Forest (RF)	0.87	11.61	3.41	32.30%
Artificial Neural Network (ANN)	0.95	8.86	2.98	28.46%

3.4 Structure–Property and Shape Memory Interpretation

The experimental and predictive findings indicate that the structure–property relationship of PLA/bTPU/lignin biocomposites is governed by the combined effects of PLA stiffness, bTPU elasticity, and lignin reinforcement. The incorporation of bTPU reduces the brittleness of PLA and improves flexibility, thereby supporting enhanced shape recovery behaviour, consistent with observations that PLA/TPU-based blends with well-dispersed elastomeric phases can achieve shape recovery ratios exceeding 90% at low activation temperatures –, . Lignin contributes stiffness and thermal resistance, but excessive lignin loading may reduce tensile strength and functional consistency because of agglomeration and weaker interfacial adhesion; this is corroborated by studies on high-lignin-content PLA blends processed via fused deposition modelling, which report tensile strength losses after repeated extrusion cycles when compatibility is not adequately addressed [21].

Thermomechanical and thermal responses further suggest that the bTPU phase acts as a soft segment that facilitates thermal activation, while lignin improves thermal stability through its aromatic structure [5], [6], [22]. Morphological considerations also indicate that phase distribution and interfacial bonding strongly influence mechanical integrity and shape memory performance, and acetylation-based surface modification has been shown to markedly improve the interfacial morphology and compatibility of lignin within PLA matrices, supporting its relevance for future formulation refinement in this system [21], [23]. Increased lignin content may also increase hydrophilicity and water absorption, which can affect dimensional stability under environmental exposure [24].

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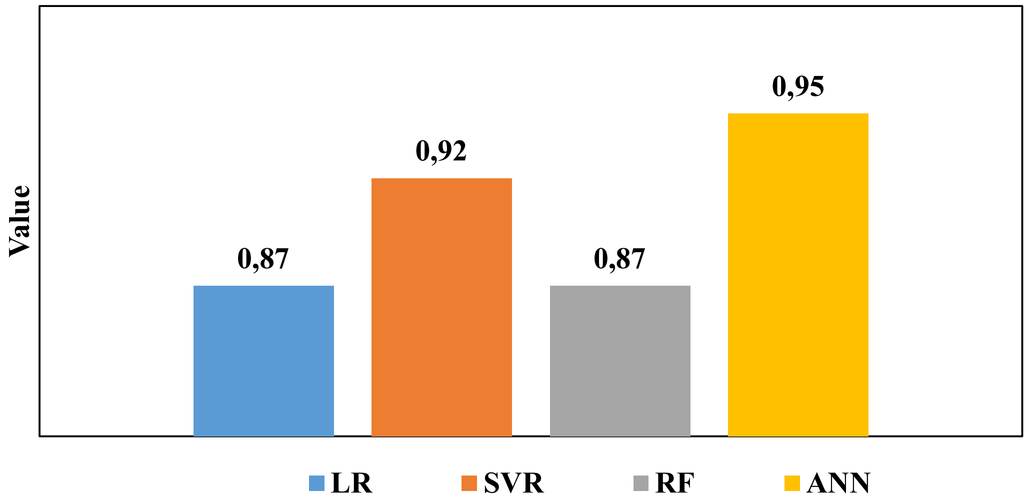

Figure 3. Coefficient of determination (R^2) for all machine learning models. The ANN demonstrated the highest predictive accuracy, followed by SVR, while RF and LR showed comparatively lower performance.

Overall, the PLA/bTPU/lignin biocomposites exhibited improved thermal responsiveness compared with neat PLA, with the interaction between the rigid PLA phase, elastic bTPU phase, and reinforcing lignin phase controlling shape fixation and recovery under thermal stimuli, in agreement with the authors' own prior characterization of this material system. The machine learning results support the use of ANN-based prediction as a data-driven tool for optimizing such formulations and reducing dependence on extensive trial-and-error experimentation, consistent with the growing consensus that machine learning frameworks can accelerate the discovery and optimization of shape memory polymers across chemistries [25].

4. Conclusion

This study demonstrated the feasibility of integrating experimental investigation and machine learning modelling to evaluate PLA/bTPU/lignin biocomposites for 4D printing applications. The incorporation of bTPU improved flexibility and thermal recovery behaviour, while lignin contributed reinforcement and thermal stability. However, lignin dispersion and interfacial adhesion remained critical factors influencing mechanical and functional reliability.

Among the machine learning models evaluated, ANN achieved the highest R^2 value of 0.95 and provided the most consistent representation of nonlinear shape recovery behaviour. SVR achieved the lowest error magnitude, with an RMSE of 2.66 and MSE of 7.09, but showed some underprediction at higher recovery values. RF offered moderate predictive performance and may be useful for feature interpretation, while LR was limited by its inability to capture nonlinear material behaviour.

The findings confirm that ANN-based prediction can support the design and optimization of thermo-responsive PLA/bTPU/lignin biocomposites by capturing complex interactions among formulation variables, processing parameters, and recovery response. This data-driven framework can reduce experimental workload, accelerate formulation screening, and support the development of sustainable high-performance materials for 4D printing applications.

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Conflict of Interest

The authors declare no conflict of interest.

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