

Project 1: Microstructure Stiffness Analysis

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Introduction

Microstructure Stiffness:

- 15 Independent Variables
- 1 Dependent Variable (Stiffness Magnitude)

Approaches:

- Normalized Regression
- Artificial Neural Network

Methodology: Normalized Regression

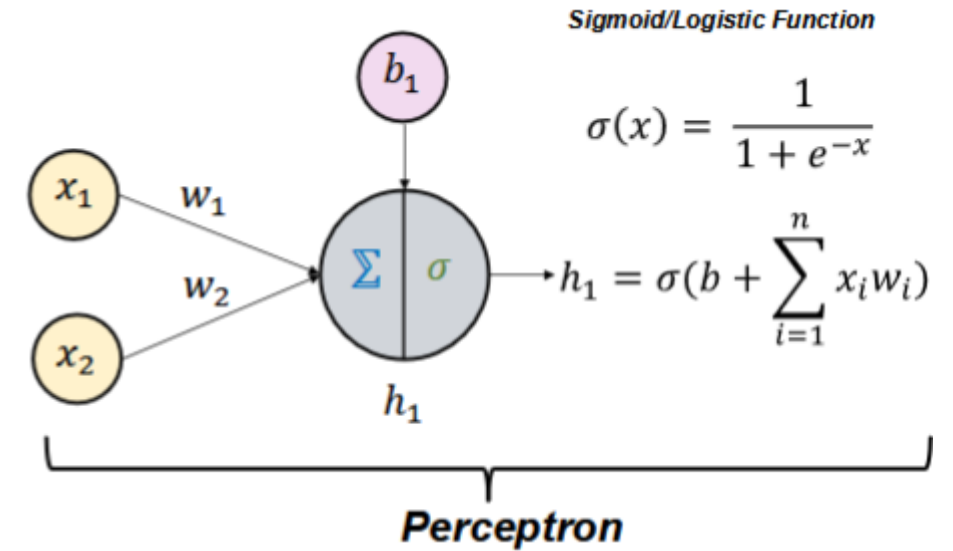
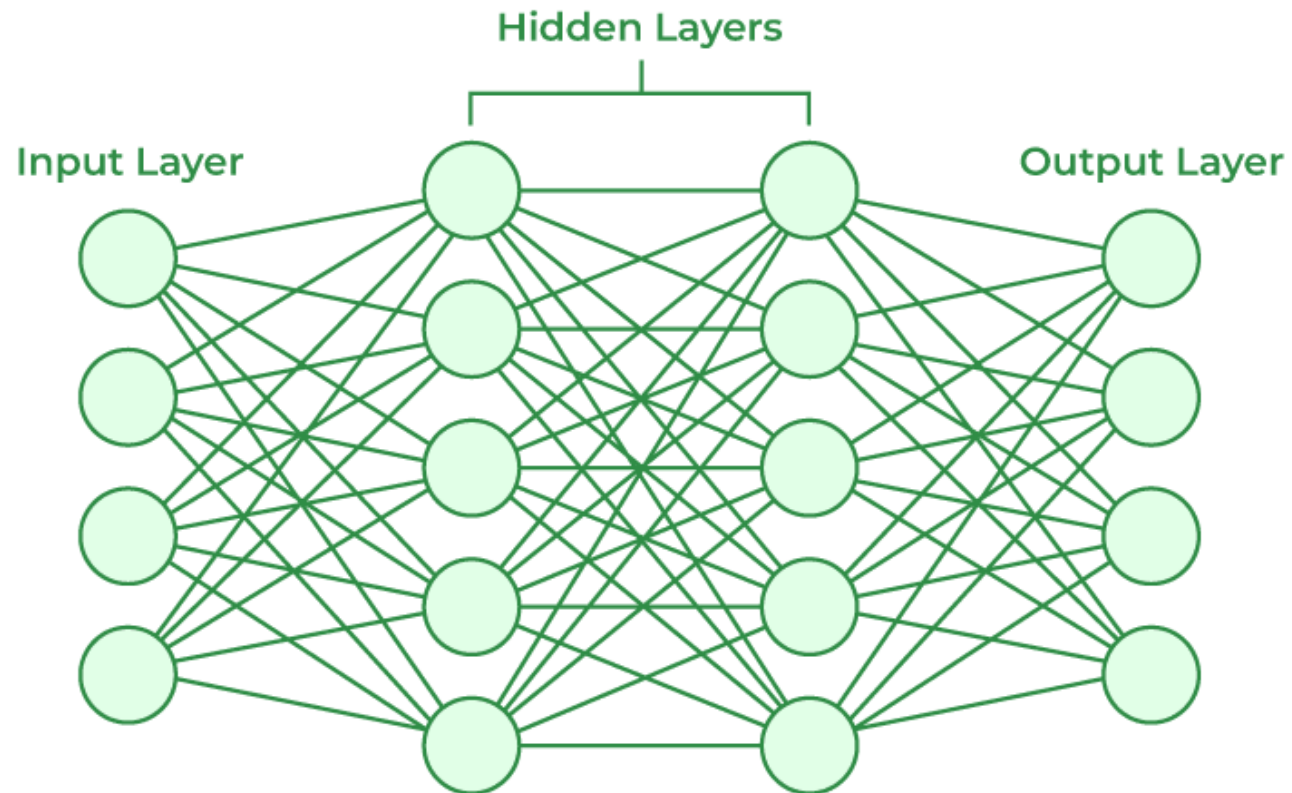
Ridge regression

$$\mathbf{w}_R = \operatorname{argmin}_{\mathbf{w} \in \mathbb{R}^D} (\|\mathbf{y} - \mathbf{X}^T \mathbf{w}\|_2^2 + \lambda \|\mathbf{w}\|_2^2)$$

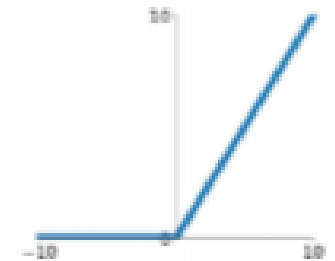
LASSO regression

$$\mathbf{w}_L = \operatorname{argmin}_{\mathbf{w} \in \mathbb{R}^D} (\|\mathbf{y} - \mathbf{X}^T \mathbf{w}\|_2^2 + \lambda \|\mathbf{w}\|_1)$$

Methodology: ANN

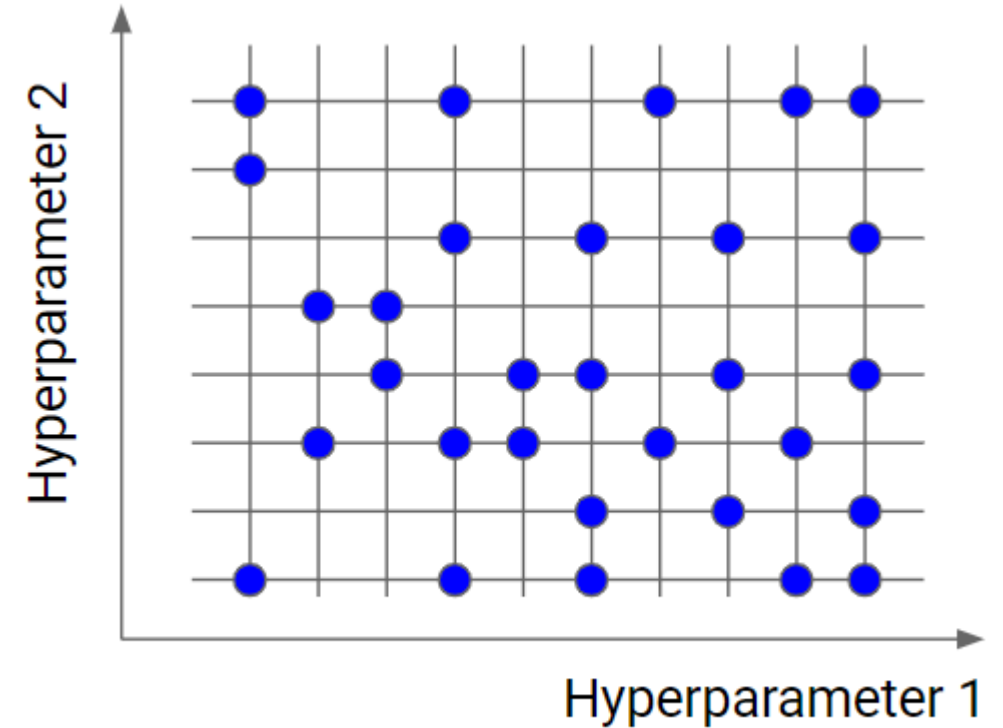


ReLU
 $\max(0, x)$



Methodology: Grid Search

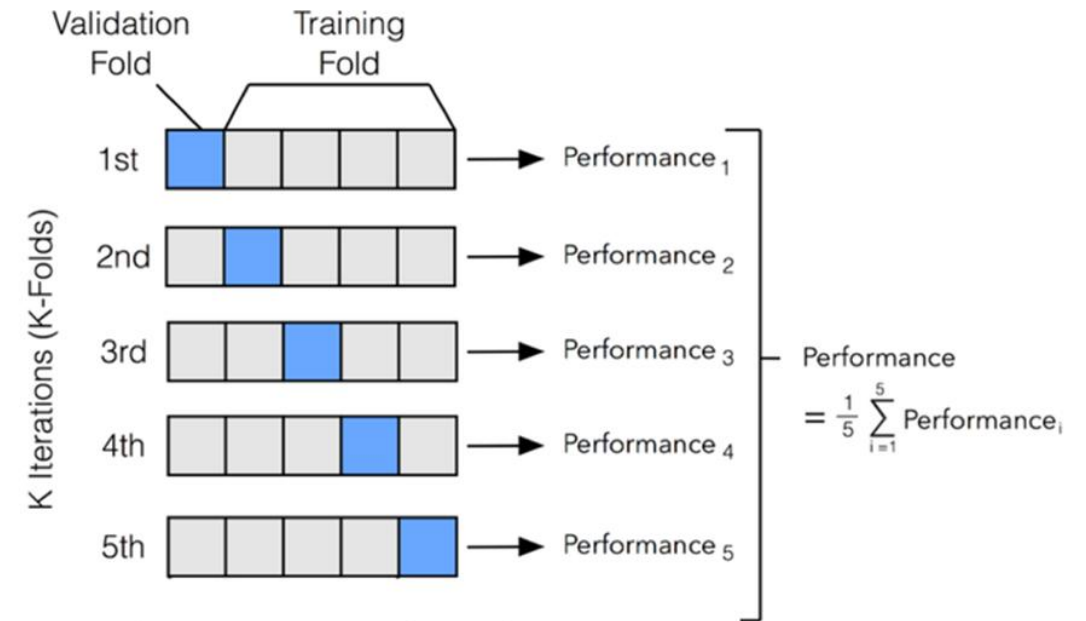
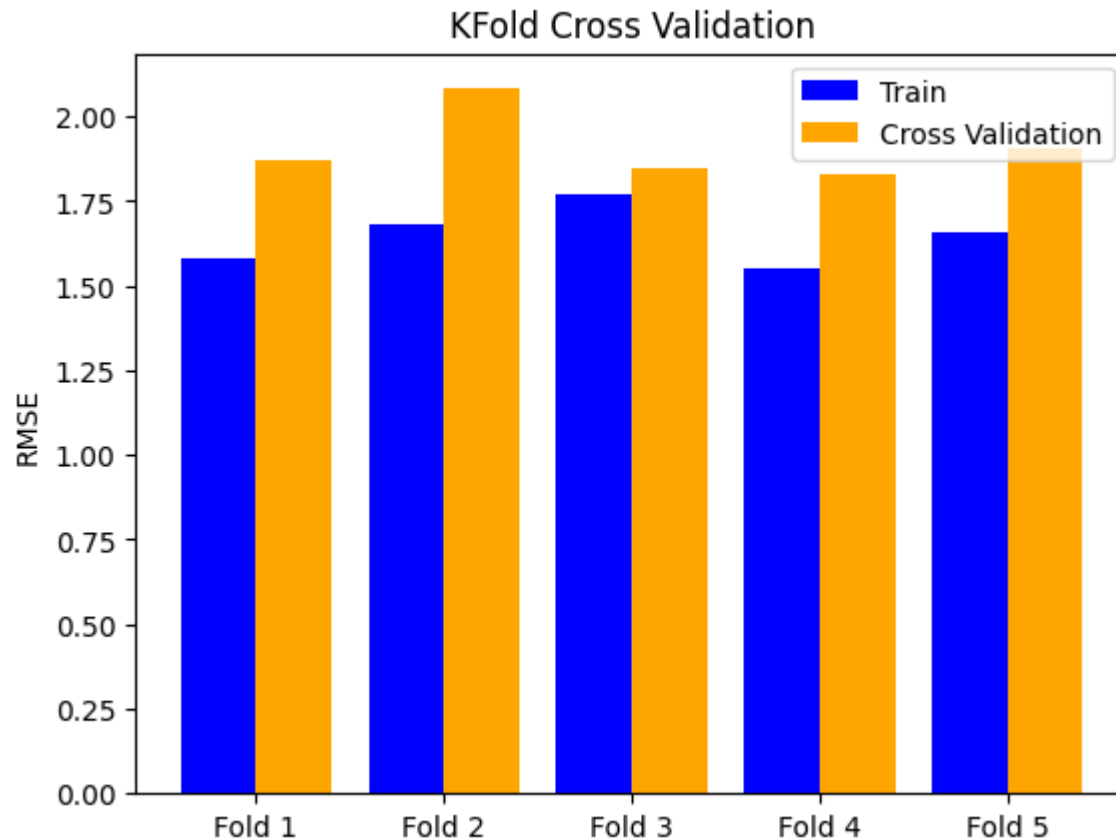
- A grid search was used for tuning hyperparameters and determining the best combination for the training dataset
- This allowed us to test several combinations of parameters at once



```
param_grid = {  
    'hidden_layer_sizes': [(100,50),(55,55),(25),(50,25,13),(50),(15),(30,30),(30,30,30)],  
    'alpha': [0.0001,0.001,0.005,0.01,0.05,0.1],  
    'learning_rate_init': [0.1, 0.01, 0.001],  
    'activation': ['relu','tanh']  
}
```

Methodology: KFold Cross Validation

- All models were tested using a KFold Cross Validation to determine if there was overfitting prior to predicting test data

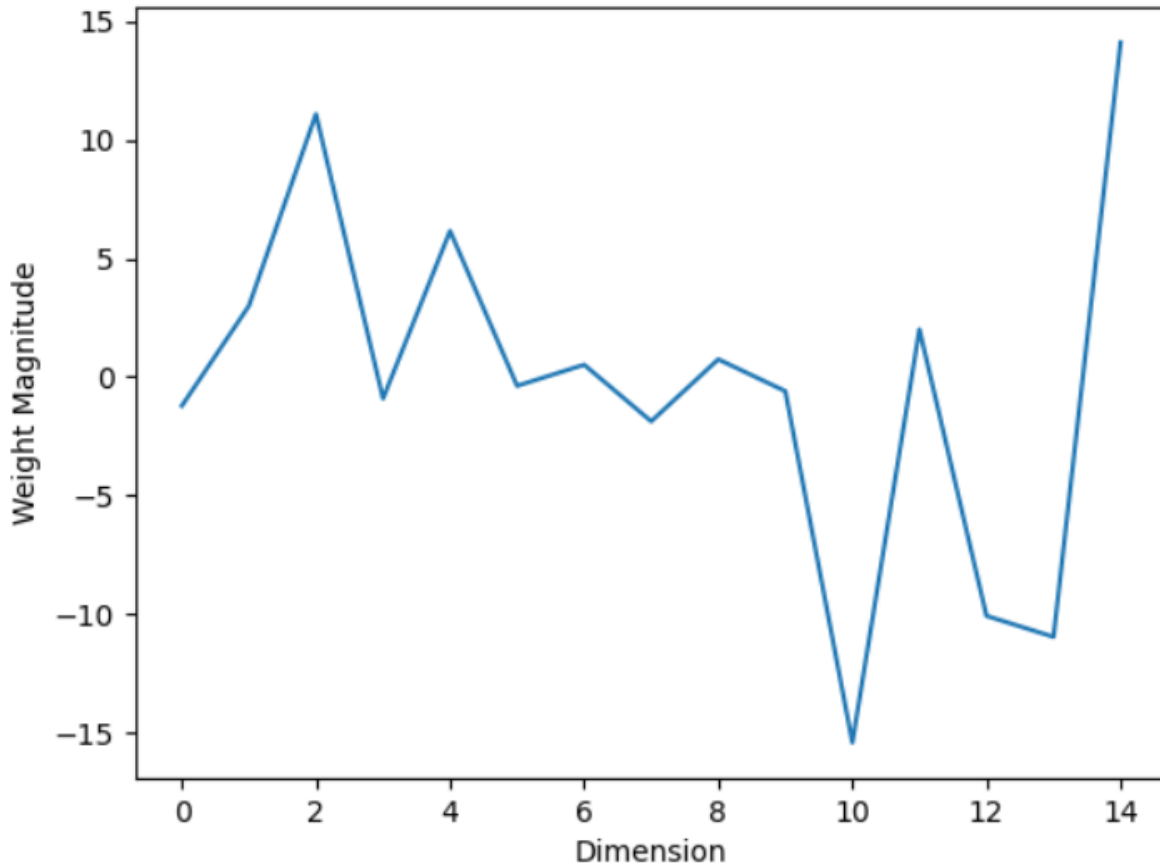


Ridge & Lasso Linear Regression

Alpha = 1.0

Loss (RMSE) = 8.032

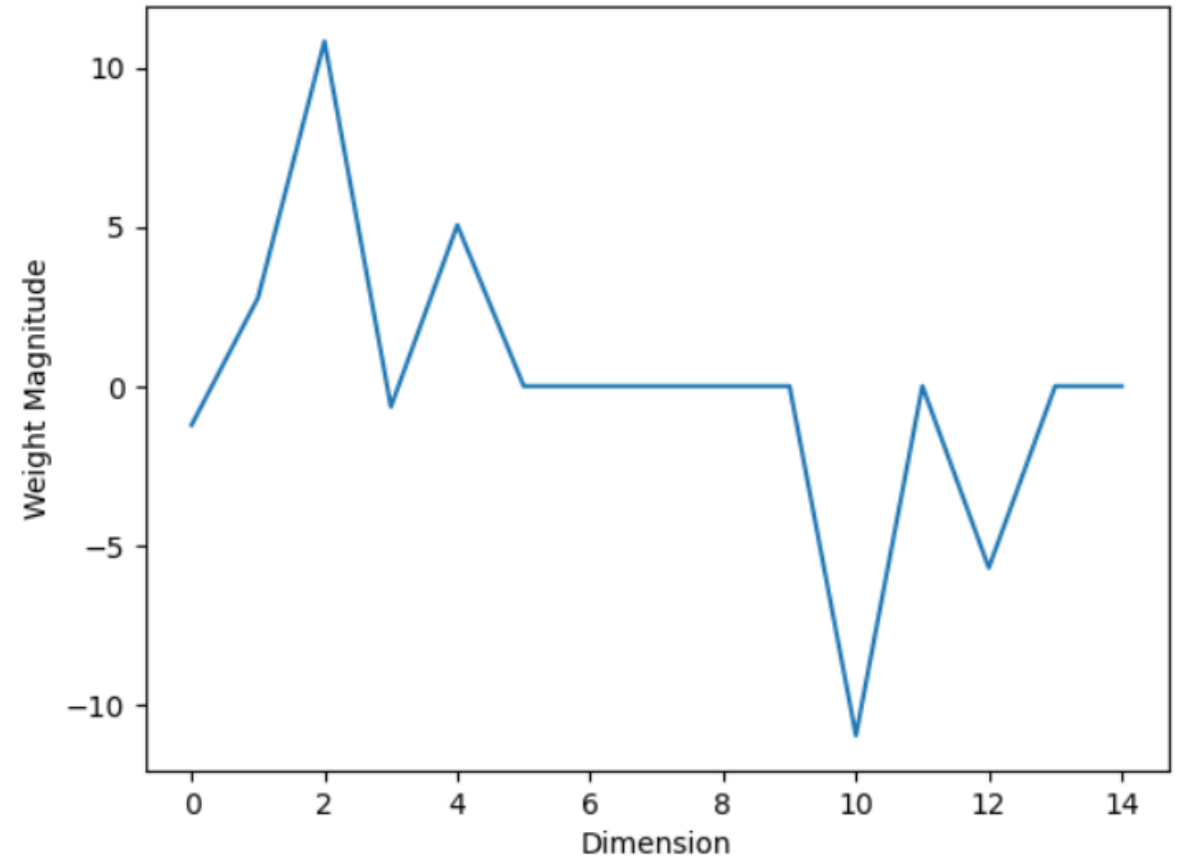
Linear Ridge Regression Coefficients



Alpha = .25

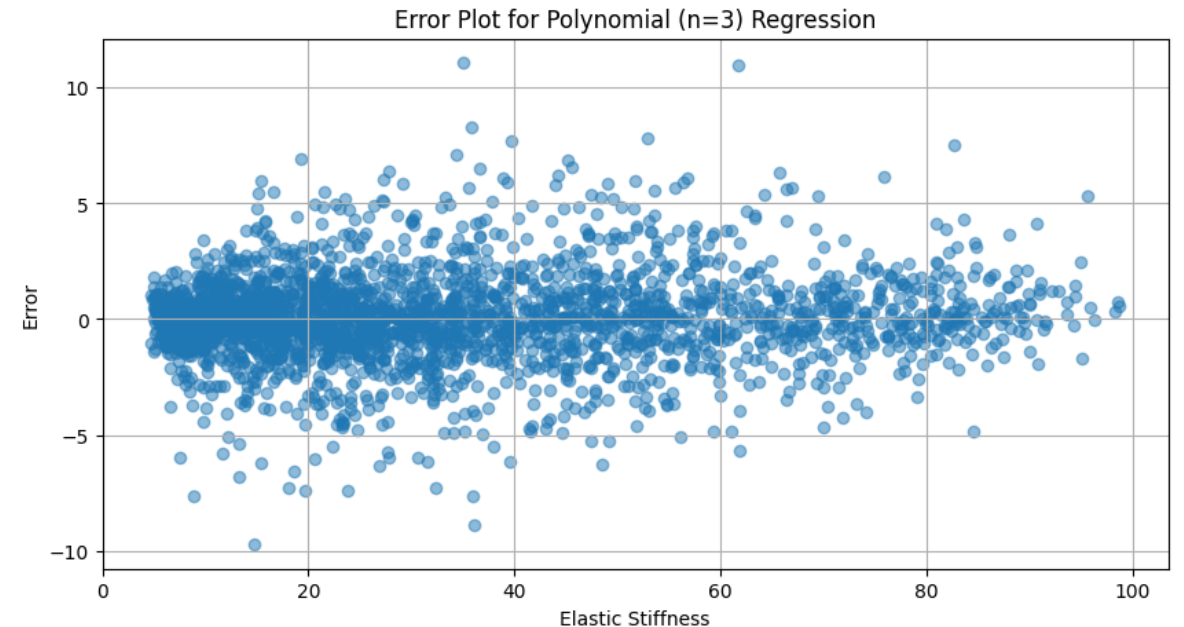
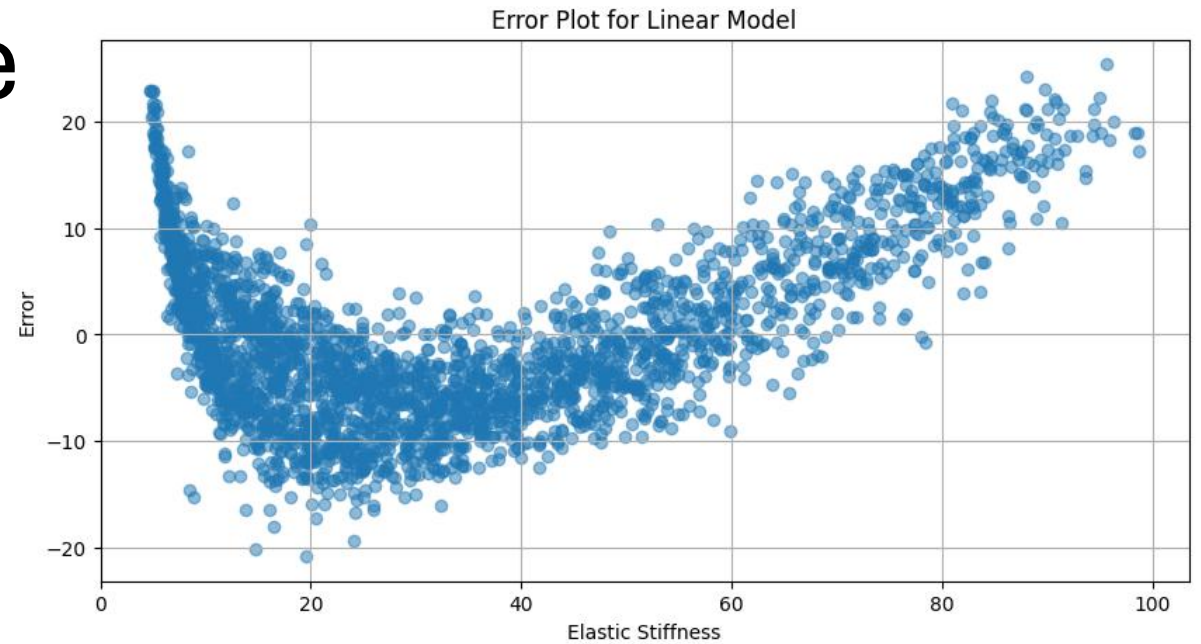
Loss (RMSE) = 8.524

Linear Lasso Regression Coefficients



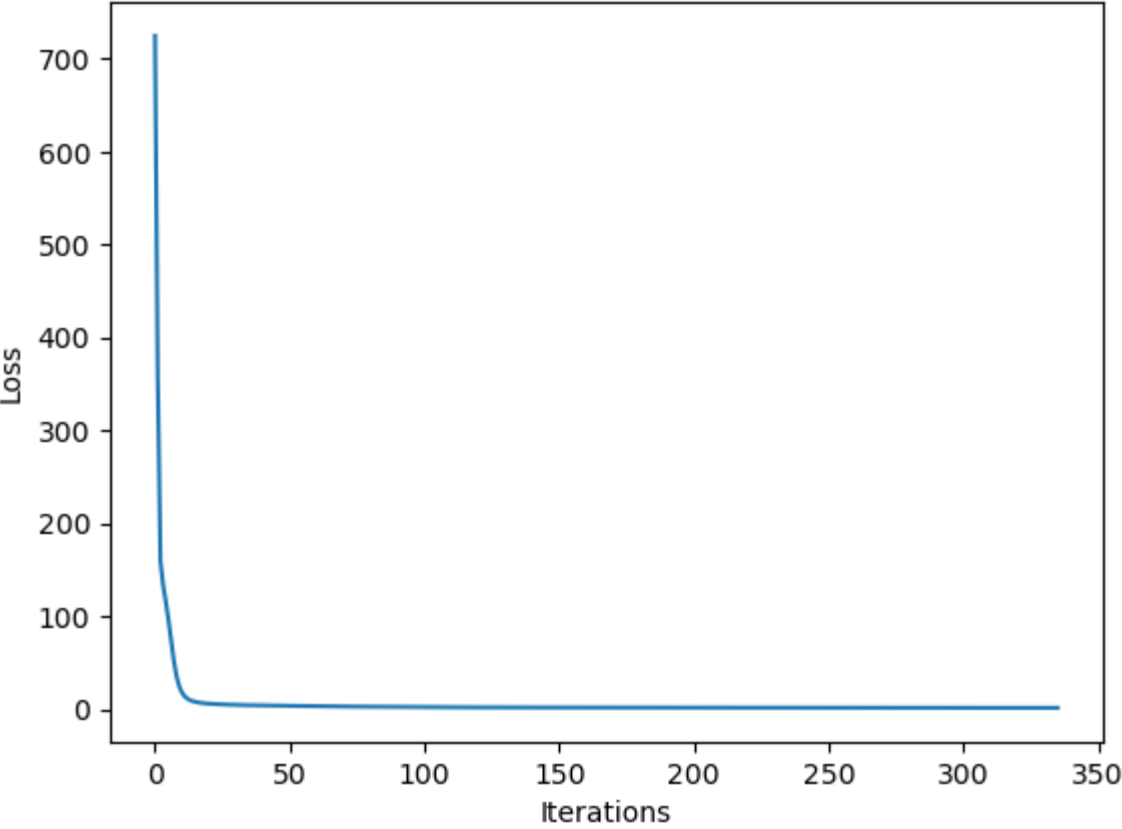
Polynomial Multivariate Regression

- The linear model error plot indicated a possible polynomial relationship, so we decided to attempt a multivariate polynomial regression
- A 3rd degree regression resulted in a RMSE of 1.94 as well as no indications of overfitting



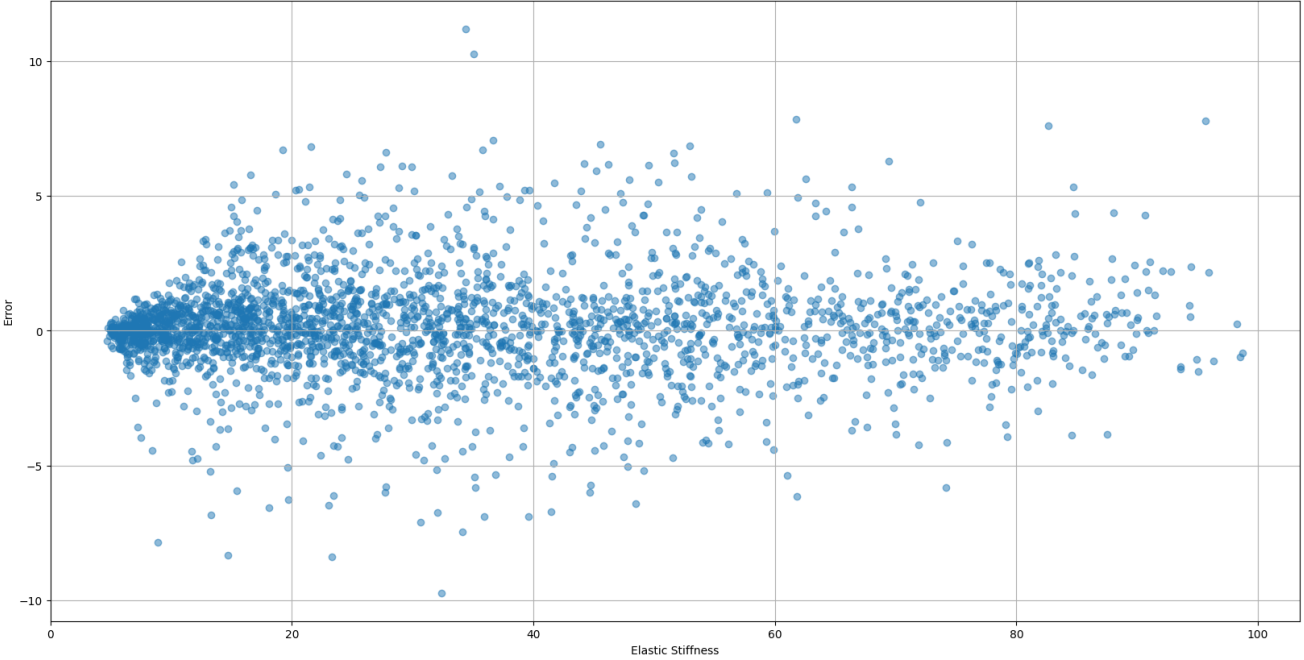
Results: ANN

Loss Curve



Parameter	Configuration
Hidden Layer Geometry	(55, 55)
Regularization (alpha)	.0001
Learning Rate	'constant', 0.001
Activation Function	ReLu
Solver	adam
K-fold Cross Validation	5 Fold
Loss (RMSE)	1.893

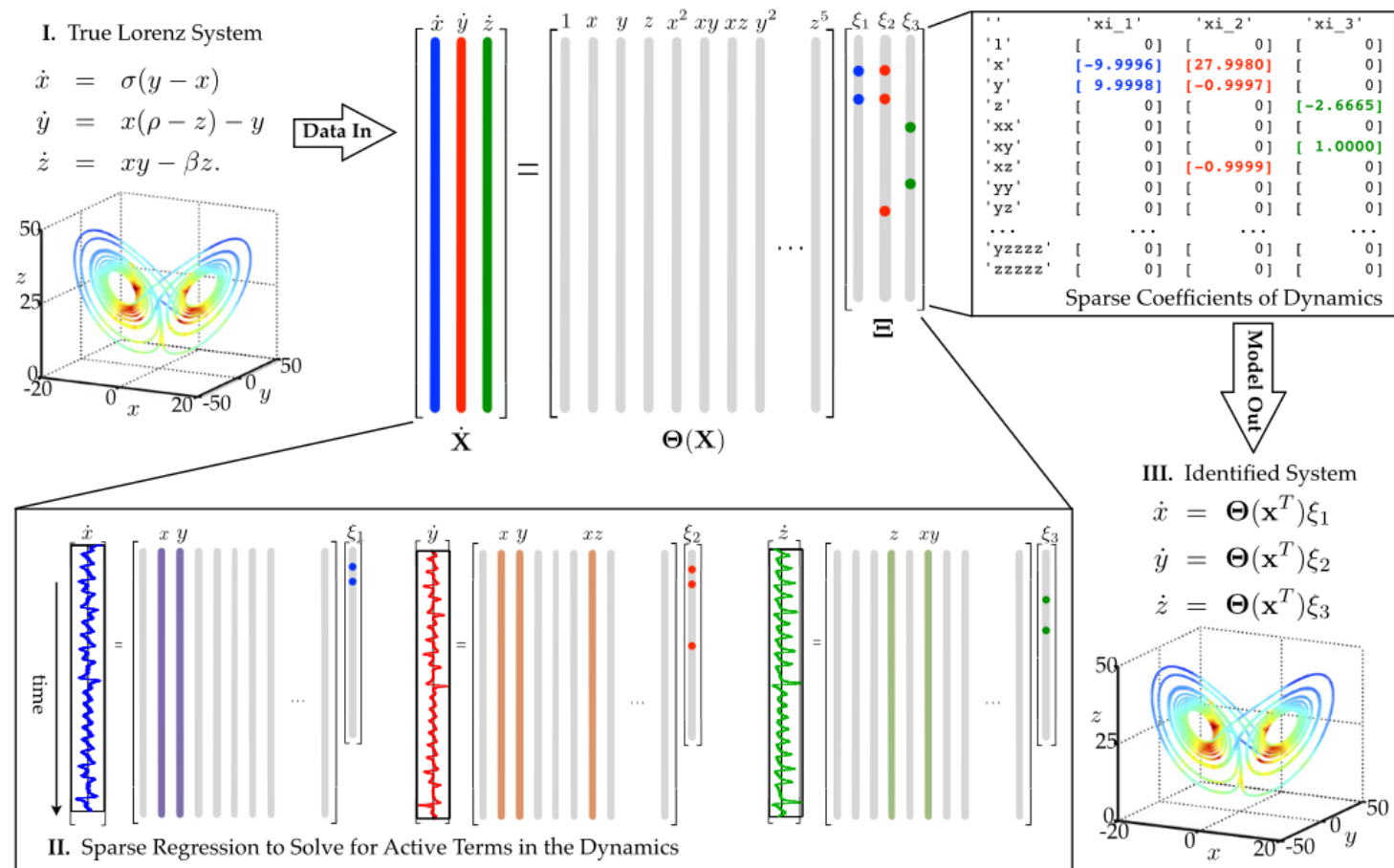
Error Plot for Chosen Model



Summary

- ANN with 2 hidden layers with 55 neurons is the chosen model with a RMSE of 1.893 (activation: relu, solver: adam, alpha: 0.001, learning rate: 0.001)
 - 76.6% decrease in RMSE from a normal linear regression
 - 2.4% decrease over the multivariate polynomial regression
- Utilizing a grid search made tuning of hyperparameters a semi-automated process and allowed us to test several combinations
- Lasso Regression suggests that PC 6,7,8,9,12,14,15 are all insignificant determiners of elastic stiffness

Future Work (Symbolic Regression)



S.L. Brunton, J.L. Proctor, & J.N. Kutz, Discovering governing equations from data by sparse identification of nonlinear dynamical systems, Proc. Natl. Acad. Sci. U.S.A. 113 (15) 3932-3937, <https://doi.org/10.1073/pnas.1517384113> (2016).