MACHINE LEARNING FOR TUNEABLE BAND-GAPS

A brief presentation to report the details of the summer research project for design credit

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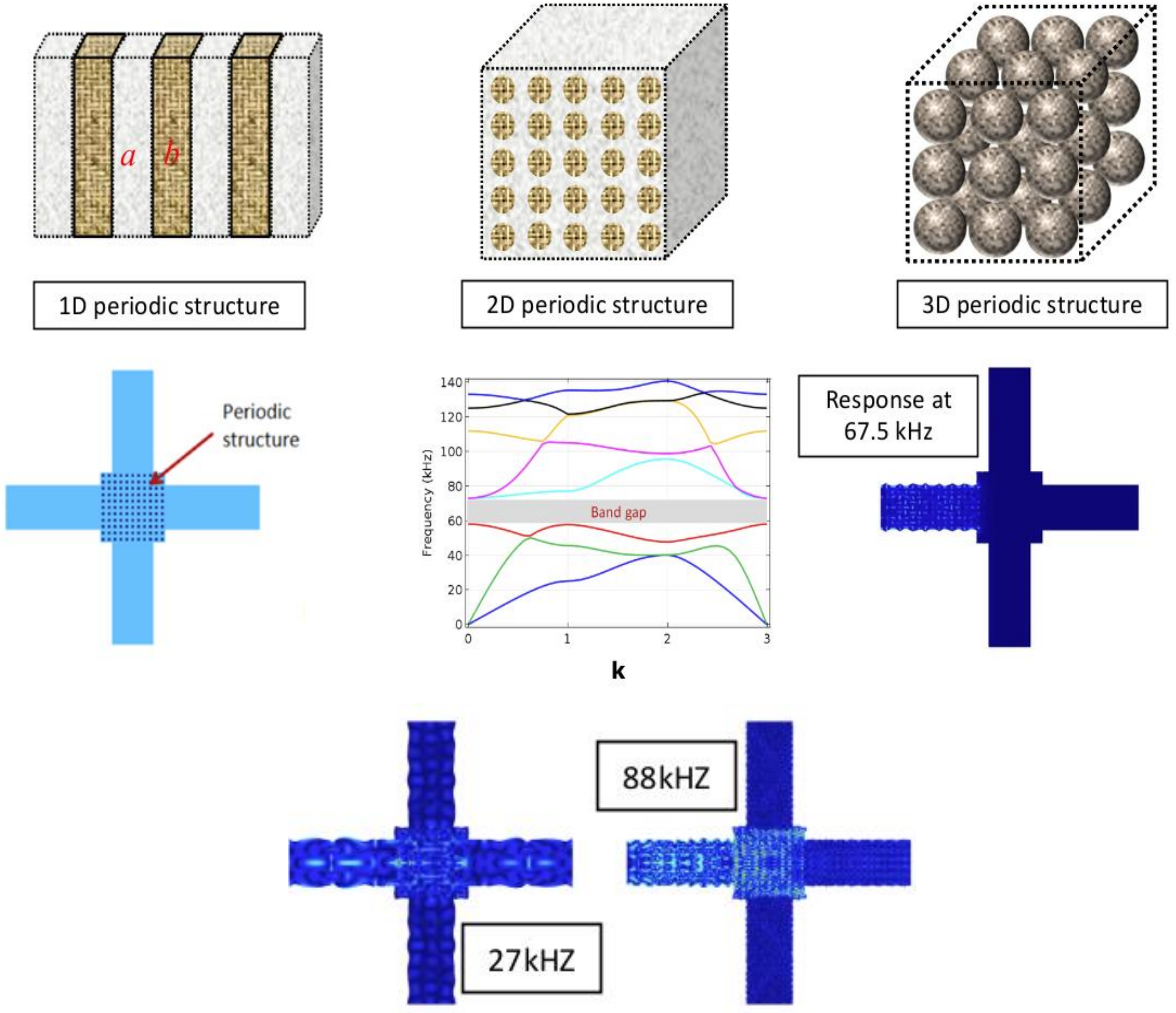
PHONONIC STRUCTURES AND BAND GAPS

A brief overview of phononic structures and their band gaps

PHONONIC STRUCTURES

A phonic crystal is an artificially manufactured structure, or material, with periodic constitutive or geometric properties that are designed to influence the characteristics of mechanical wave propagation.

When engineering these crystals, it is possible to isolate vibration within a certain frequency range. Vibration within this selected frequency range, referred to as the **band gap**, is attenuated by a mechanism of wave interferences within the periodic system.



Phononic crystals and band gaps

Courtesy: https://www.comsol.com/blogs/modeling-phononic-band-gap-materials-and-structures/

SOFT TUNABLE PHONONIC STRUCTURES

- **Hard Material based phononic structures**

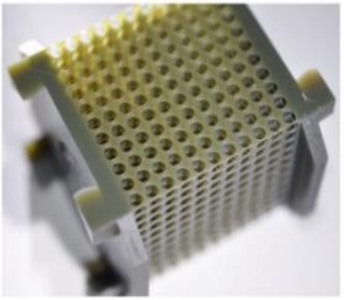
Once the structure is fabricated, it is difficult to substantially shift band gaps during use.

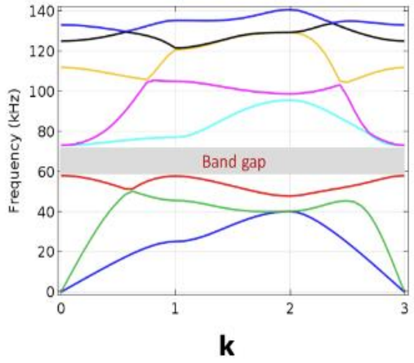
- **Tunable phononic band gap structures**

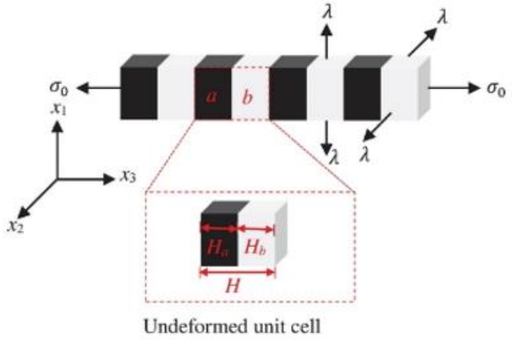
Frequency range can be adapted for wide range of applications

- **Soft active elastomers**

Undergo large deformation or shape change when subjected to external loading, i.e., mechanical, electrical, magnetic fields.

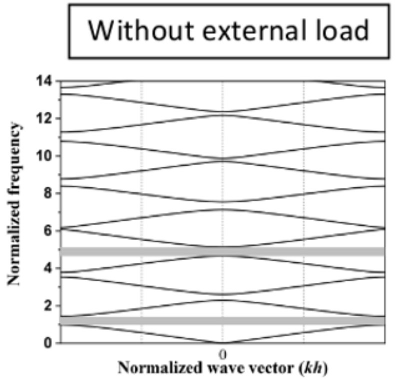


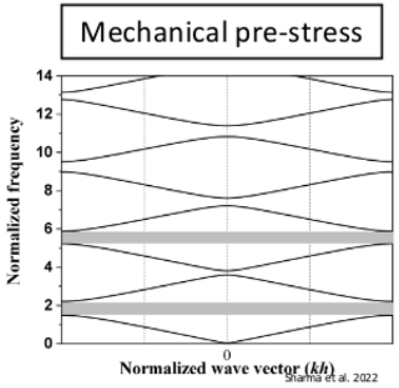




Applications:

- Vibration isolation technology
- Noise suppression
- Frequency filters

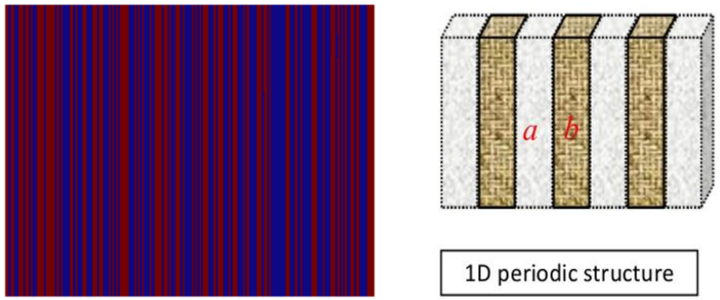




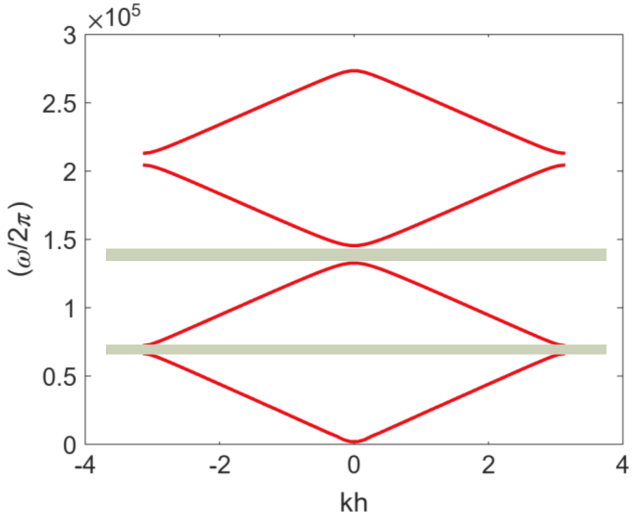
AIM OF THE PROJECT

The project is aimed to create a ML model that can be utilised to obtain the values of the first two tuneable band-gaps that are present in a 1-D structured phononic crystal with a composition of two substances using the mechanical and electromagnetic properties of the crystal.

The current method is to compute solutions of complex mathematical functions to ascertain the wavelengths' values primarily using MATLAB. To simplify and increase the efficiency of the process, this machine learning based solution has been proposed.



Structure of the 1-D structure



Wavelengths and bandgaps of the structure above

METHODOLOGY

Process followed for the project

DATA

Data is generated using MATLAB scripts provided by our project supervisor, Dr. Sharma through the implementation of his research paper [*Topology optimization of soft compressible phononic laminates for widening the mechanically tunable band gaps, ISSN 0263-8223, https://doi.org/10.1016/j.compstruct.2022.115389*].

The following are taken as features/input variables:

Property of unit cell	Range/Form
Length (L)	0.1 to 10
Applied magnetic flux density (B)	-5 to 5
Shear Contrast Parameter (α)	0.05 to 50
Microstructure	A 1x200 binary vector
Magnetic contrast parameter (β)	0.05 to 50
Local measure of volume change parameter(J)	2 to 1000

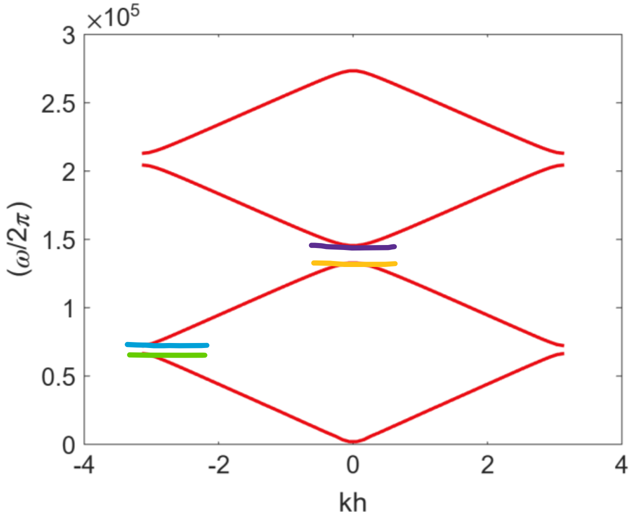
The target/output variables are:

ω_{max1}

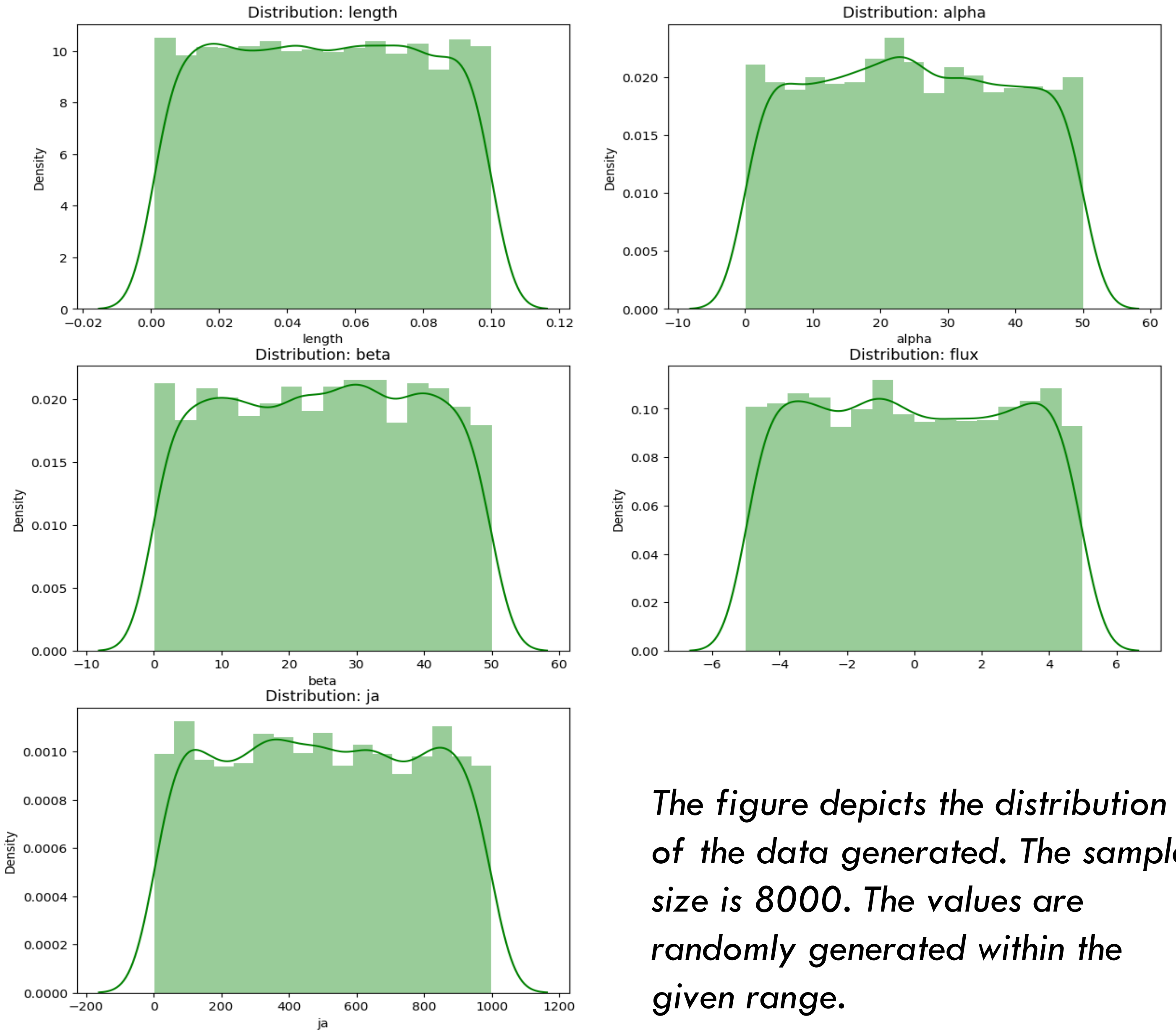
ω_{min2}

ω_{max2}

ω_{min3}



Target Variables in Data



The figure depicts the distribution of the data generated. The sample size is 8000. The values are randomly generated within the given range.

DATA MANIPULATION

Data

Processing

- Original
- Normalisation
- Standardisation

PCA

- PCA is applied over all the datasets

Train-Test-Split

- 4:1 ratio split over all datasets normalise, standardised, original, pca before and after

DATA MANIPULATION

Original Data

Data1

The data is kept as it is **without any feature engineering.**

Data1_Normalised

The data is Normalised

Data1_Normalised_PCA

- The data is processed using PCA

Data1_Standardised

The data is Standardised

Data1_Standardised_PCA

- The data is processed further using PCA

Data2

The Microstructure feature is originally a 200 column set. It is **reduced to a set of 20 columns each of 10 bits which are converted to decimal values.**

Data2_Normalised

The data is Normalised

Data2_Normalised_PCA

- The data is processed using PCA

Data2_Standardised

The data is Standardised

Data2_Standardised_PCA

- The data is processed further using PCA

Data3

The Data2_Standardised has Microstructure in 20 columns, it is further **reduced to a single column by adding those 20 standardised decimal values.**

Data3_Standardised

- The data is Standardised
- Data3_Standardised_PCA
  - The data is processed further using PCA

FEATURE IMPORTANCE

DATA3

Features	Correlation
Length (L)	-0.375538
Shear Contrast Parameter (α)	-0.167207
Magnetic contrast parameter (β)	0.146558
Applied magnetic flux density (B)	0.111587
Local measure of volume change parameter(J)	0.035253
Microstructure	0.0977

DATA2

Features	Correlation
Length (L)	-0.375538
Shear Contrast Parameter (α)	-0.167207
Magnetic contrast parameter (β)	0.146558
Applied magnetic flux density (B)	0.111587
Local measure of volume change parameter(J)	0.035253
Microstructure	0.0067

DATA1

Features	Correlation
Length (L)	-0.375538
Shear Contrast Parameter (α)	-0.167207
Magnetic contrast parameter (β)	0.146558
Applied magnetic flux density (B)	0.111587
Local measure of volume change parameter(J)	0.035253
Microstructure	0.000050

MODELS TRAINED

We trained **80+** models of different regressors for predicting. We also applied **5-fold cross validation** on the models and used **GridSearchCV for hyperparameter tuning.**

For linear regressor, AdaBoost, gradient boosting, and random forest regressor models, we utilized the scikit-learn library. As for the artificial neural network (ANN) regressor, we employed the Keras library for implementation.

- Linear Regressor: Utilized to establish a linear relationship between dependent and independent variables.
- AdaBoost: Employed to combine weak learners and improve overall prediction accuracy.
- Gradient Boosting: Utilized for ensemble learning, sequentially improving model performance by correcting errors.
- Random Forest Regressor: Utilized to create an ensemble of decision trees, resulting in robust and accurate predictions.
- ANN Regressor: Used to model complex relationships and solve regression problems using artificial neural networks.

Linear Regressor
AdaBoost Regressor
Gradient Boost Regressor
Random Forest Regressor
ANN

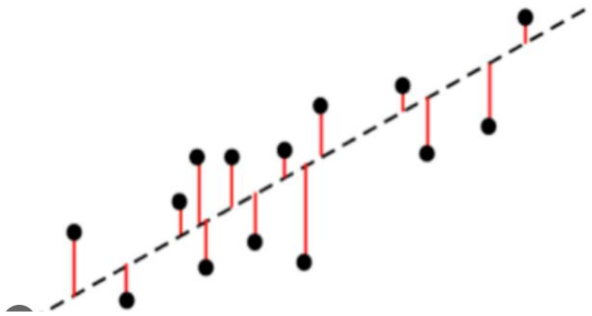
MODEL EVALUATION

The models were evaluated using the R-squared metric for regressors. It was utilised so as to attain robust and easy to understand performance values ranged between -1 to 1 so as to be able to compare the various models trained.

Formula

$$R^2 = 1 - \frac{RSS}{TSS}$$

R^2 = coefficient of determination
RSS = sum of squares of residuals
TSS = total sum of squares



$$\text{RSS} = \Sigma\left(y_i - \widehat{y}_i\right)^2$$

Where: y_i is the actual value and, $\widehat{y}_i$ is the predicted value.

$$\text{TSS} = \Sigma\left(y_i - \overline{y}\right)^2$$

Where: y_i is the actual value and $\overline{y}$ is the mean value of the variable/feature

R-squared score diagram and formula

RESULTS

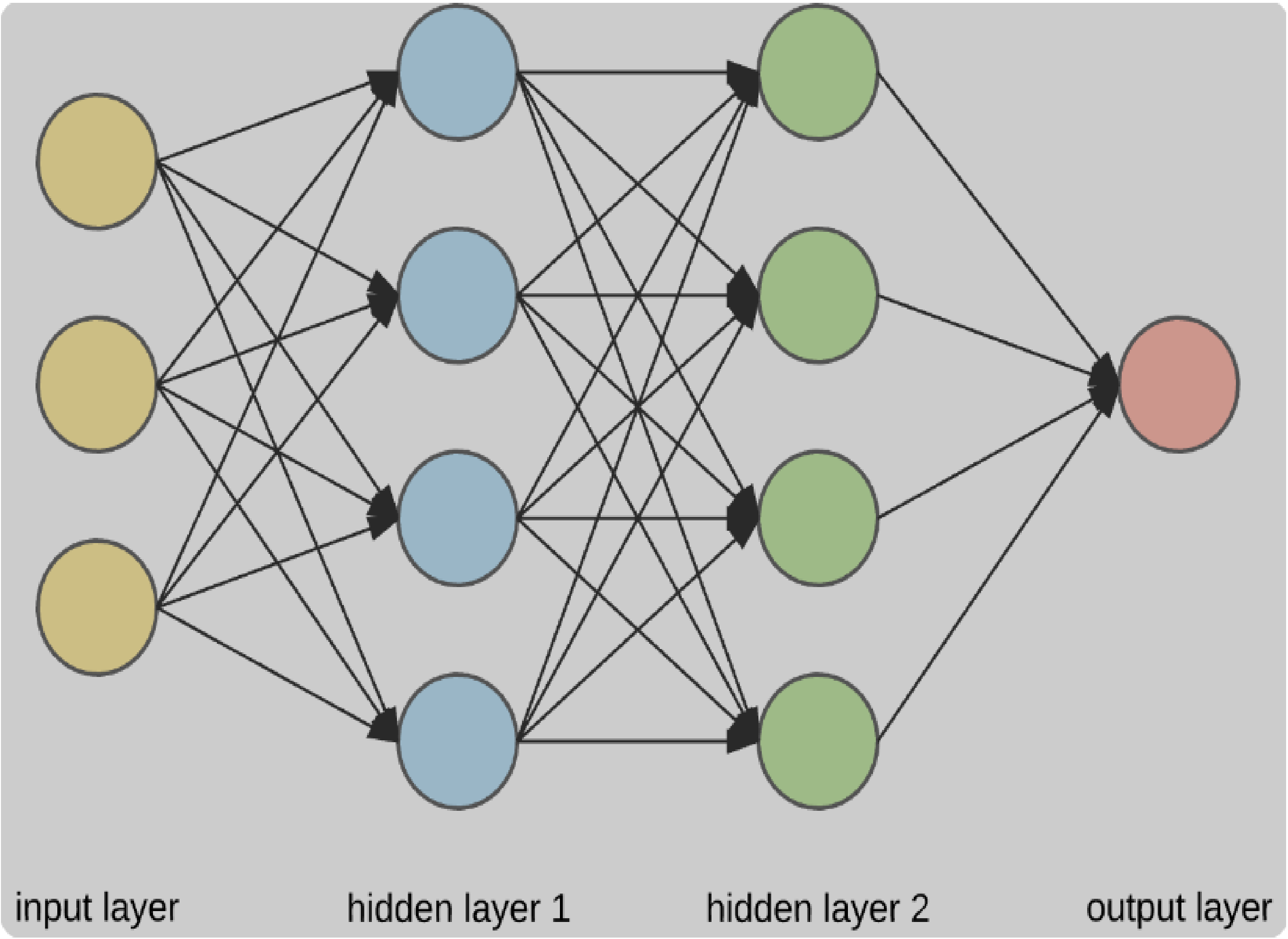
Outcomes of the project

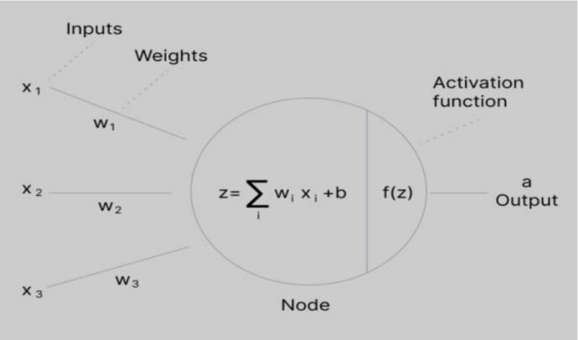
PERFORMANCE OF MODELS

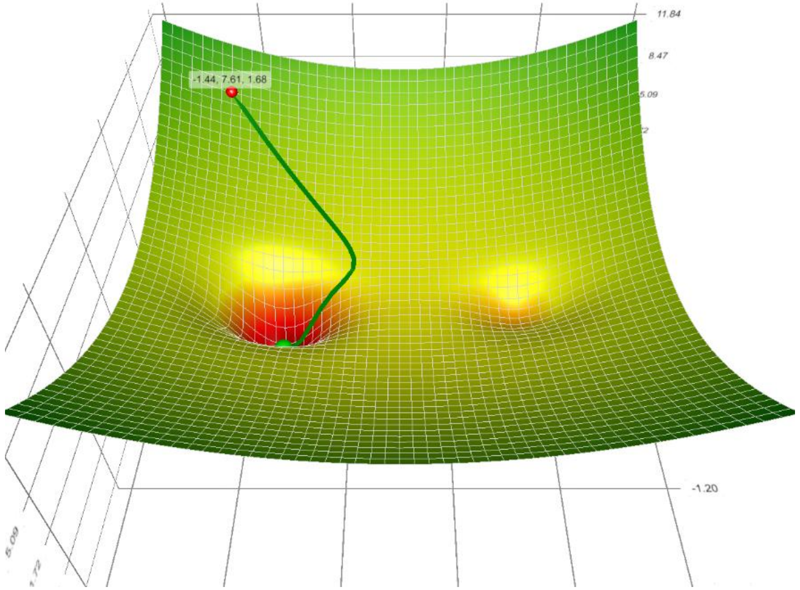
Model type	Best R-2 Score on Testing dataset
Linear Regressor	0.612
AdaBoost Regressor	0.741
Gradient Boost Regressor	0.789
Random Forest Regressor	0.828
Artificial Neural Network	0.934

ANN (ARTIFICIAL NEURAL NETWORK)

The most optimal ML model attained for the task and its configuration







Optimizer

After conducting numerous experiments, we have successfully identified the optimal structure and hyperparameters of the ANN, resulting in the best possible outcome.

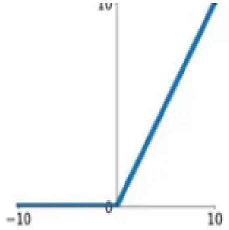
Optimal Configuration for ANN:

- Optimizer: RMSprop , Adam
- Activation Function: "ReLU" , "elu"
- Structure (Hidden Layers with Nodes):

  128, 128, 64, 32

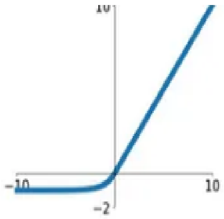
ReLU

$$\max(0, x)$$



ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



- Batch Size: 140 (Using a higher batch size resulted in more robust and faster convergence)(Number of training examples used in each iteration of the training process in a machine learning model)
- Number of Epochs: 2000
- Total Runtime: Training + Testing = 8 minutes
- Loss Function: Mean Absolute Error (This choice prevents harsh penalization for errors, considering the high range of results)
- R2 Score (Testing): 0.92 to 0.94 (Demonstrating a strong correlation between predicted and actual values).
- R2 Score (Training) : 0.98 to 0.99 (The training score is notably high because the results are generated by a mathematical function. Therefore, there is no need to be concerned about its performance during training)

With this optimized configuration, the artificial neural network achieves impressive results, showcasing faster convergence and improved accuracy compared to other setups.

CONTRIBUTION

Anshu Raj	❑ Data Preprocessing ▪ Feature Reduction (Binary addition) ▪ Standardisation and Normalisation ❑ Training Models ▪ Artificial Neural Network ❑ Hyperparameter Tuning
Yash Shrivastava	❑ Data Generation using MATLAB ❑ Data Preprocessing ▪ Feature Importance (Correlation, Feature Permutation, RFR importance) ▪ Feature Reduction (PCA and others) ▪ Standardisation and Normalisation ❑ Training Models ▪ Linear Regressor ▪ Gradient Boosting Regressor ▪ AdaBoost Regressor ▪ Random Forest Regressor