# ChE 492

## UNDERSTANDING SUPERCAPACITOR CHARGE/DISCHARGE RATES USING MICROSTRUCTURE IMAGE PROCESSING

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# Outlines

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- Statement of Purpose
- Supercapacitors
- Machine Learning Models

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- Normalization
- Dummy Coding

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- Parameter Tuning and Model Training
- Regression Models
- Conclusion
- Future Thoughts

# 1- INTRODUCTION

- Statement of Purpose
- Supercapacitors
- Machine Learning Models

# Statement of Purpose

## Problem

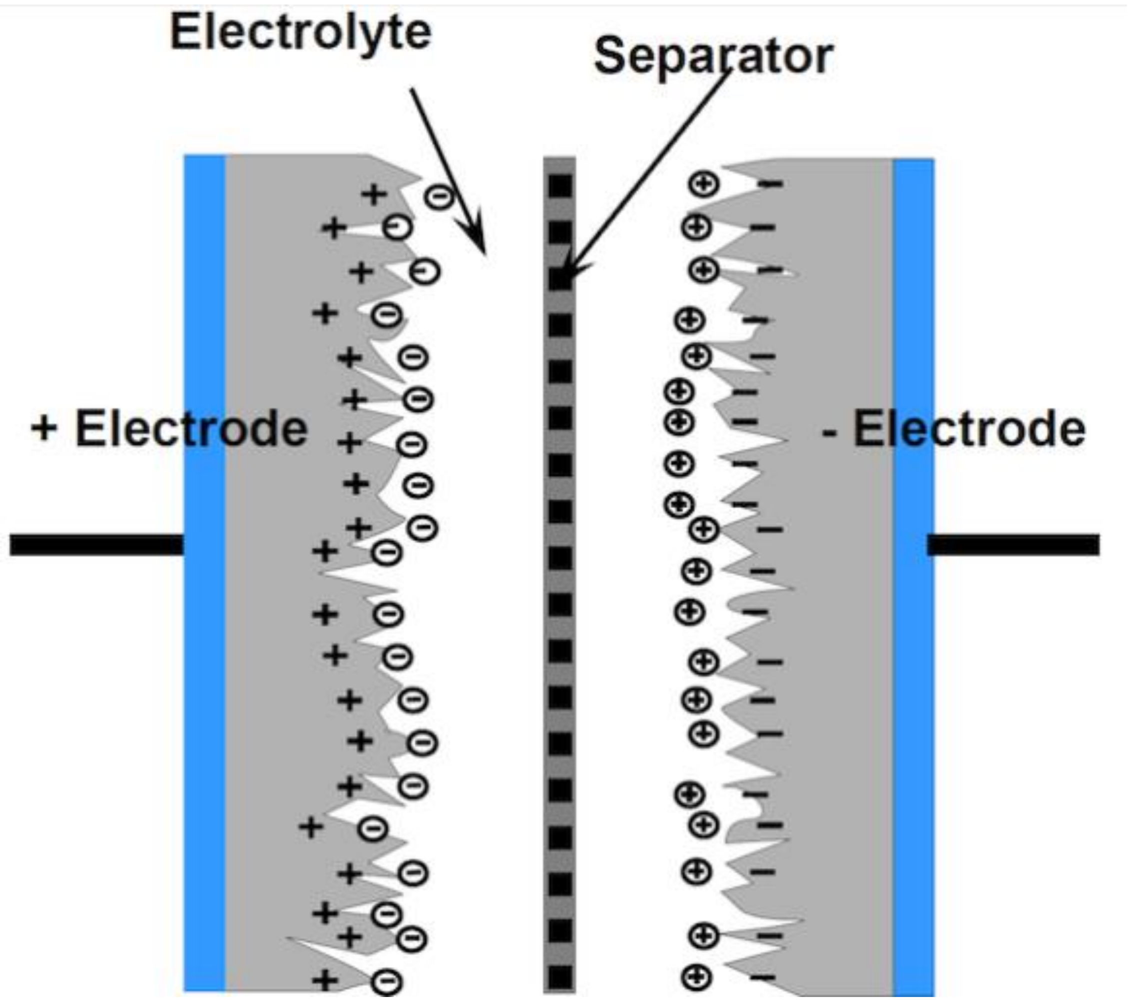
Performance parameters of supercapacitors are highly dependent on material properties of supercapacitors. Therefore, **material selection** process is very important step during supercapacitor design. However, since material selection process is handled by using **trial and error experiments in real life**, material selection is very **time and money consuming process** for researchers.

## Purpose

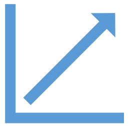
The project aims to design **machine learning algorithm** which is able to predict energy densities of supercapacitors by using input data that is enriched from the results came from **image processing techniques**.

# Supercapacitors

- Energy Storage Devices
- Potential Difference
- New technology compared to other energy storage devices
- Great number of charge/discharge rates
- Long-life span
- Solving problems where batteries insufficient



# Machine Learning Models



Linear Regression

Ridge Regression

Lasso Regression

Regression Tree

Artificial Neural Network

# 2- PRE-PROCESSING

- Data Introduction
- Image Processing
- Filtering Data
- Normalization
- Dummy Coding

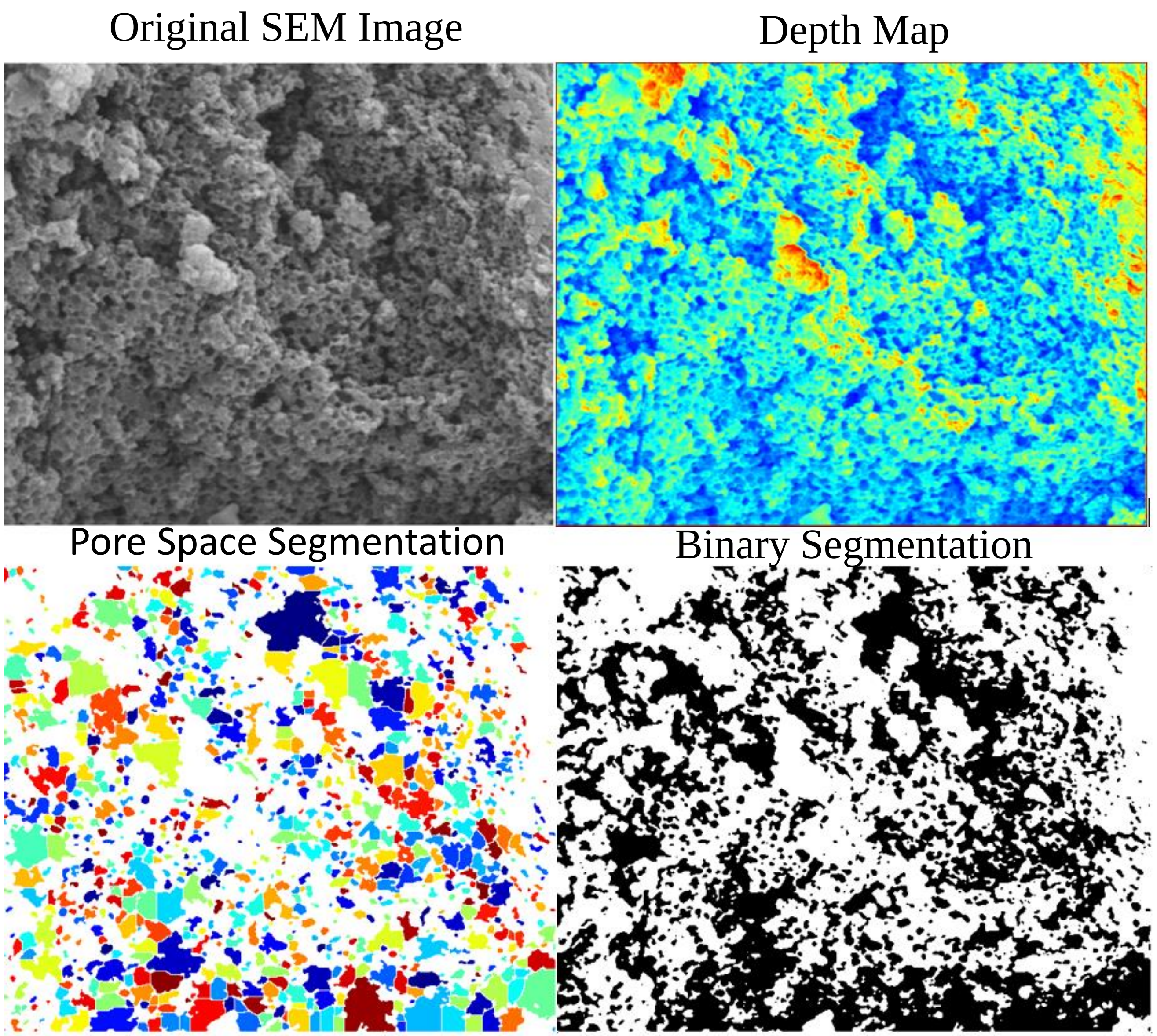
# Data Introduction

- 22 Features
- 1 Response Variable
- 2189 Observations

| | Real Name |
|---|---|
| Features | Electrode Material Group |
| | Heat Treatment Temperature |
| | Specific Surface Area |
| | D- Raman Peak and G- Raman Peak Ratio |
| | Nitrogen Concentration |
| | Oxygen Concentration |
| | Phosphor Concentration |
| | Boron Concentration |
| | Porosity |
| | Pore Volume |
| | Preparation Method for Electrode |
| | Electrolyte Type |
| | Electrolyte Concentration |
| | Normalized Scan Rate |
| | Absolute Potential Window |
| | Separator |
| | Current collector |
| | Salt Anion Volume |
| | Salt Cation Volume |
| | Solvent Dipole Moment |
| | Solvent Volume |
| | Binder Concentration |
| Response Variable | Energy Density |

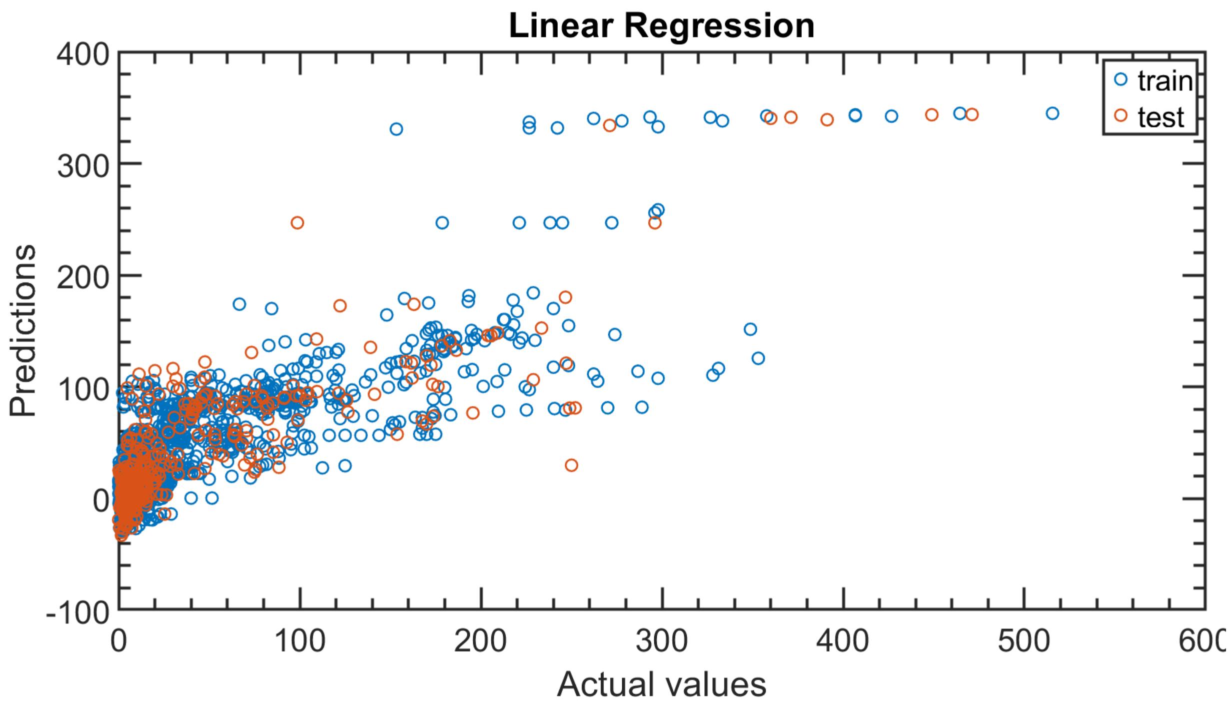
# Image Processing: SEM

- Depth Map: 3D visualization
- Pore Space Segmentation: Average Pore Size
- Binary Segmentation: Porosity
- Data Collection: 107 Articles
- Result: 84 of the 628 missing observations filled and dataset is enriched

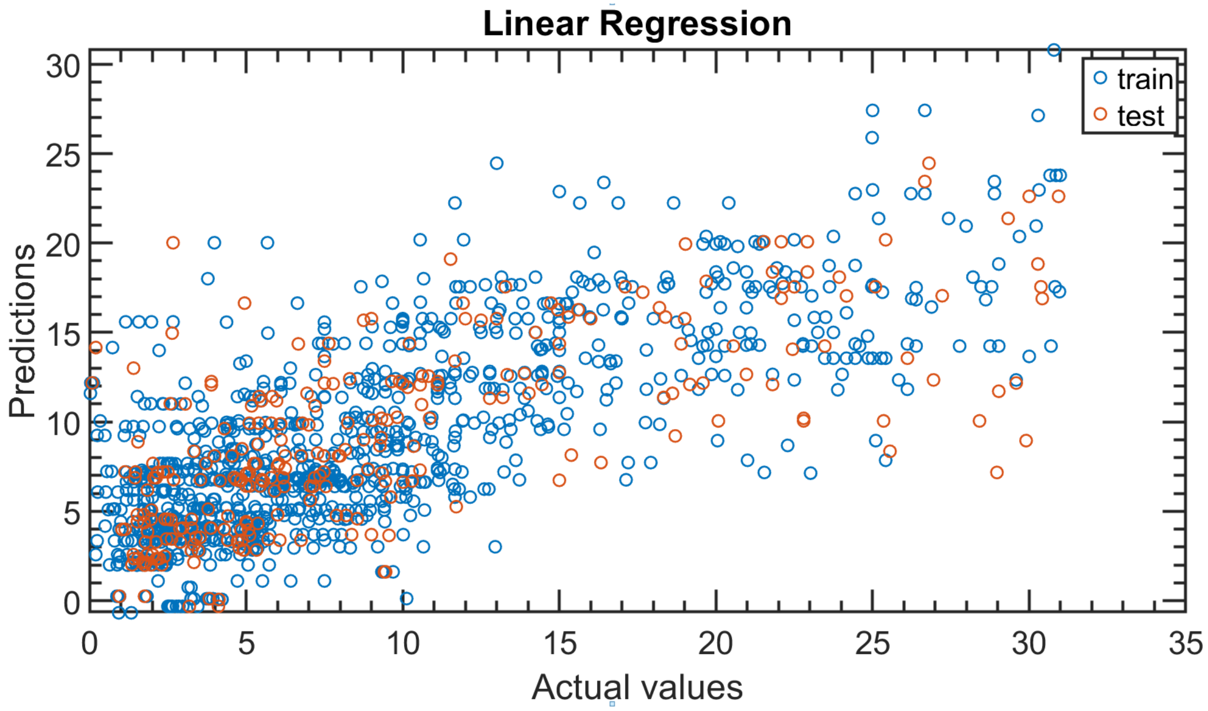


# Filtering Data

Not Filtered

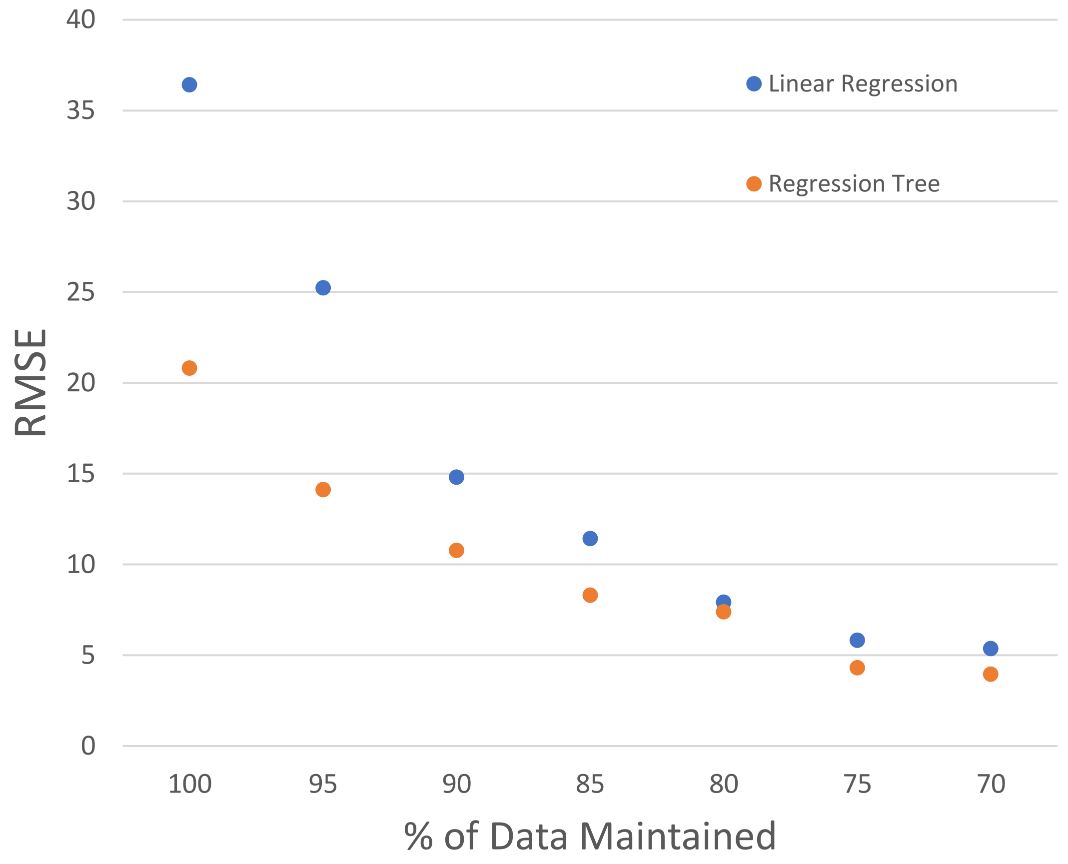



30 % of the Data Eliminated



# Filtering Data

| Percentage of the Data Maintained | Linear Regression Test RMSE | Regression Tree Test RMSE | Threshold Value |
|---|---|---|---|
| 100 | 36.42 | 20.82 | Not Exist |
| 95 | 25.23 | 14.13 | 178 |
| 90 | 14.81 | 10.77 | 107 |
| 85 | 11.42 | 8.31 | 80 |
| 80 | 7.92 | 7.39 | 58 |
| 75 | 5.83 | 4.32 | 42 |
| 70 | 5.37 | 3.96 | 31 |



# Normalization & Dummy Coding

**Min-Max Normalization**

- Numerical columns are bounded between 0 and 1

$$X' = \frac{X - X_{min}}{X_{max} - X_{min}}$$

**Dummy Coding**

- 4 Categories = 4 New Columns

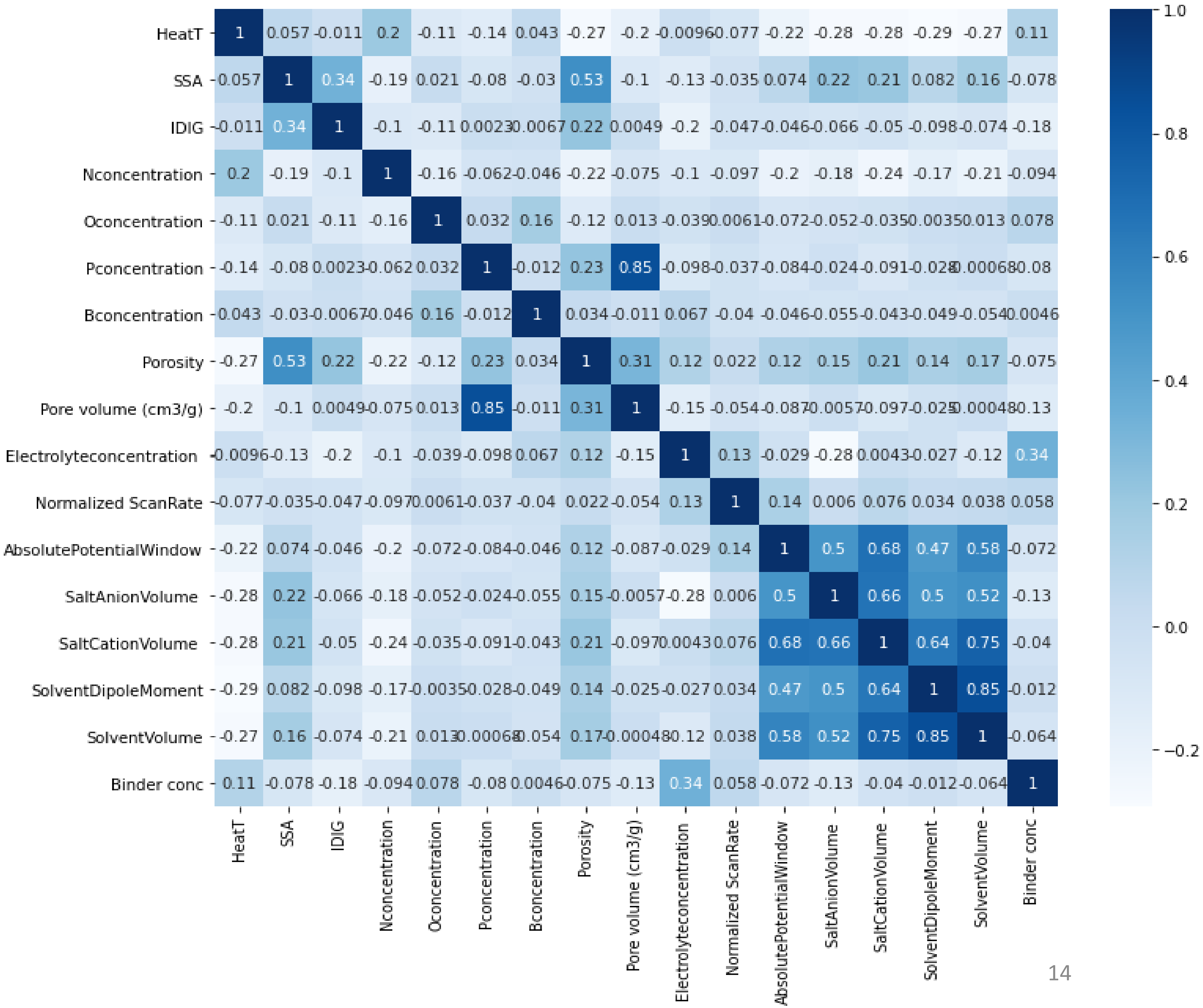
| Categorical Feature | Column For A | Column For B | Column For C | Column For D |
|---|---|---|---|---|
| **A** | 1 | 0 | 0 | 0 |
| **A** | 1 | 0 | 0 | 0 |
| **D** | 0 | 0 | 0 | 1 |
| **B** | 0 | 1 | 0 | 0 |
| **C** | 0 | 0 | 1 | 0 |
| **A** | 1 | 0 | 0 | 0 |
| **D** | 0 | 0 | 0 | 1 |

# 3- Feature Selection

- Correlation Matrix and Heat Map
- F-Test
- Trial and Error Method

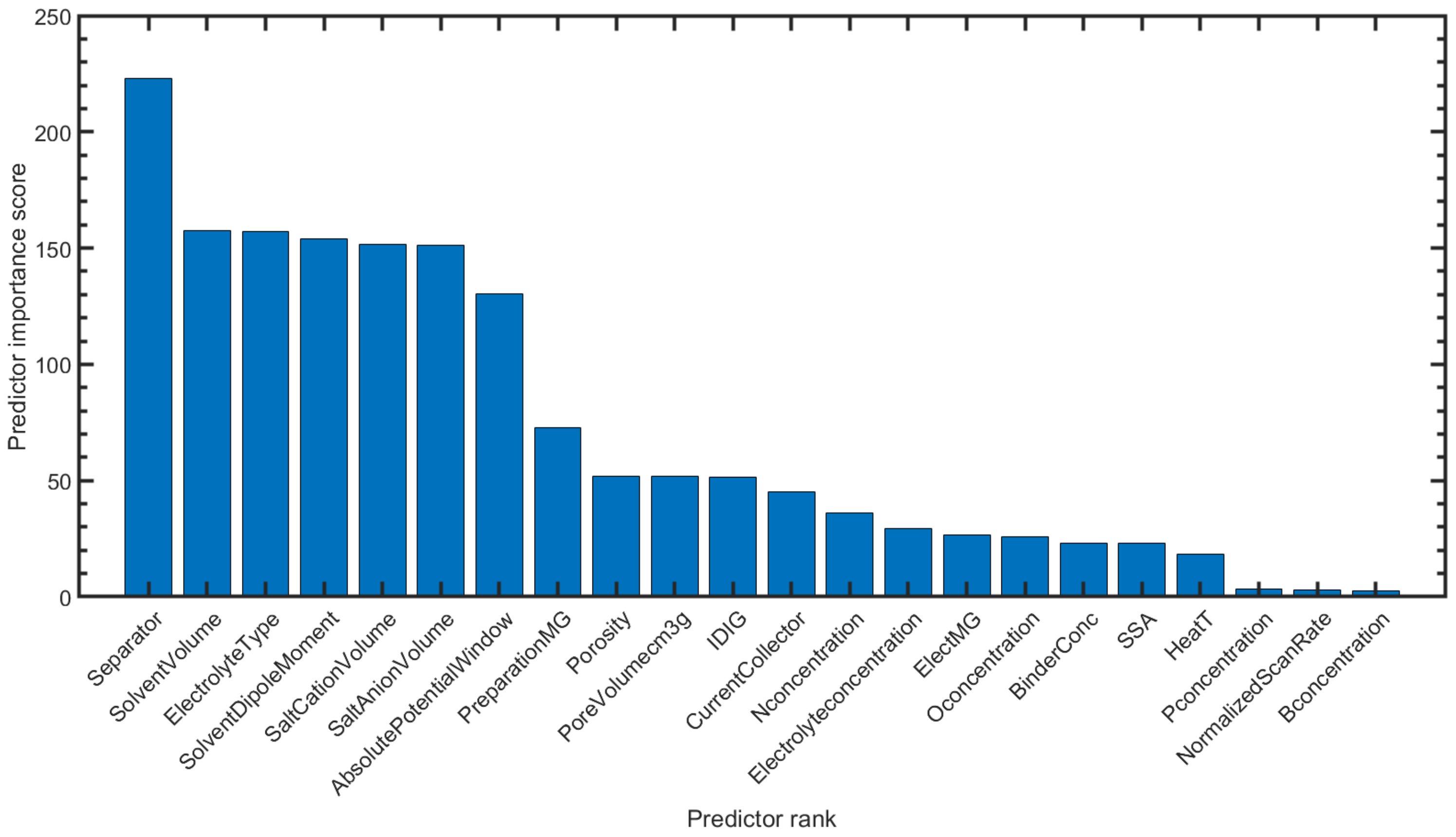
## Correlation Matrix & Heat Map

- Pore volume & P concentration 0.85
- Solvent cation volume & absolute potential window= 0.68
- Solvent cation volume & salt anion volume= 0.66
- Solvent cation volume & solvent dipole moment = 0.64
- Solvent cation volume & solvent volume= 0.75
- Solvent volume & solvent cation volume= 0.85



# F-Test

- MATLAB function: frftest()
- Filter type feature selection method
- Suitable for regression problems
- Suitable for both categorical and numerical data
- The last three features eliminated



# Trial & Error Method

$$\Delta RMSE = \frac{RMSE_i - RMSE_{all}}{RMSE_{all}} \times 100$$

| Features | Root Mean Squared Error | | | | |
|---|---|---|---|---|---|
| | Linear Regression | Lasso Regression | Ridge Regression | Regression Tree | Neural Network |
| **All Features** | 5.0253 | 4.8308 | 5.0233 | 3.9170 | 3.6983 |
| **-Heat T** | 5.0214 | 4.8351 | 5.0219 | 3.6739 | 4.2678 |
| **-SSA** | 5.1657 | 5.0062 | 5.1663 | 4.0361 | 4.1242 |
| **-IDIG** | 5.0802 | 4.9325 | 5.0801 | 3.9275 | 4.1200 |
| **-N Concentration** | 5.0643 | 4.9115 | 5.0647 | 3.7589 | 4.4974 |
| **-O Concentration** | 5.0183 | 4.8312 | 5.0281 | 3.6636 | 4.1665 |
| **-Porosity** | 5.0032 | 4.8229 | 5.0074 | 3.7748 | 3.9573 |
| **-Pore Volume** | 4.9974 | 4.8405 | 5.0197 | 3.6411 | 4.0805 |
| **-Electrolyte Concentration** | 5.0988 | 4.8962 | 5.0978 | 3.7907 | 4.2861 |
| **-Absolute Potential Window** | 5.2498 | 5.0273 | 5.2524 | 3.9560 | 4.0126 |
| **-Salt Anion Volume** | 5.0004 | 4.8413 | 5.0020 | 3.8218 | 4.1896 |
| **-Salt Cation Volume** | 5.0190 | 4.8963 | 5.0199 | 3.7958 | 4.2326 |
| **-Solvent Dipole Moment** | 5.0674 | 4.8789 | 5.0698 | 3.7208 | 3.8870 |
| **-Solvent Volume** | 5.1866 | 4.8907 | 5.0739 | 4.0393 | 4.1894 |
| **-Binder Concentration** | 5.0323 | 4.8538 | 5.0318 | 3.6654 | 3.7445 |
| **-Elect MG** | 5.0637 | 4.8854 | 5.0626 | 3.7469 | 4.5221 |
| **-Preparation MG** | 5.2444 | 5.1532 | 5.2442 | 3.7080 | 4.2128 |
| **-Electrolyte Type** | 5.0315 | 4.8425 | 5.0306 | 3.8413 | 4.1675 |
| **-Separator** | 5.2076 | 5.0415 | 5.2102 | 3.8505 | 5.3960 |
| **-Current Collector** | 5.0444 | 4.9015 | 5.0443 | 3.7158 | 6.1616 |

| Features | Percentage Differences between RMSE values | | | | |
|---|---|---|---|---|---|
| | Linear Regression | Lasso Regression | Ridge Regression | Regression Tree | Neural Network |
| **Heat T** | -0.08 | 0.09 | -0.03 | -6.21 | 15.40 |
| **SSA** | 2.79 | 3.63 | 2.85 | 3.04 | 11.52 |
| **IDIG** | 1.09 | 2.11 | 1.13 | 0.27 | 11.40 |
| **N Concentration** | 0.78 | 1.67 | 0.82 | -4.04 | 21.61 |
| **O Concentration** | -0.14 | 0.01 | 0.10 | -6.47 | 12.66 |
| **Porosity** | -0.44 | -0.16 | -0.32 | -3.63 | 7.00 |
| **Pore Volume** | -0.56 | 0.20 | -0.07 | -7.04 | 10.33 |
| **Electrolyte Concentration** | 1.46 | 1.35 | 1.48 | -3.22 | 15.89 |
| **Absolute Potential Window** | 4.47 | 4.07 | 4.56 | 1.00 | 8.50 |
| **Salt Anion Volume** | -0.50 | 0.22 | -0.42 | -2.43 | 13.28 |
| **Salt Cation Volume** | -0.13 | 1.36 | -0.07 | -3.09 | 14.45 |
| **Solvent Dipole Moment** | 0.84 | 1.00 | 0.93 | -5.01 | 5.10 |
| **Solvent Volume** | 3.21 | 1.24 | 1.01 | 3.12 | 13.28 |
| **Binder Concentration** | 0.14 | 0.48 | 0.17 | -6.42 | 1.25 |
| **Elect MG** | 0.76 | 1.13 | 0.78 | -4.34 | 22.27 |
| **Preparation MG** | 4.36 | 6.67 | 4.40 | -5.34 | 13.91 |
| **Electrolyte Type** | 0.12 | 0.24 | 0.15 | -1.93 | 12.69 |
| **Separator** | 3.63 | 4.36 | 3.72 | -1.70 | 45.90 |
| **Current Collector** | 0.38 | 1.46 | 0.42 | -5.14 | 66.60 |

# 4-RESULTS

- Parameter Tuning and Model Training
- Models
- Conclusion
- Future Thoughts

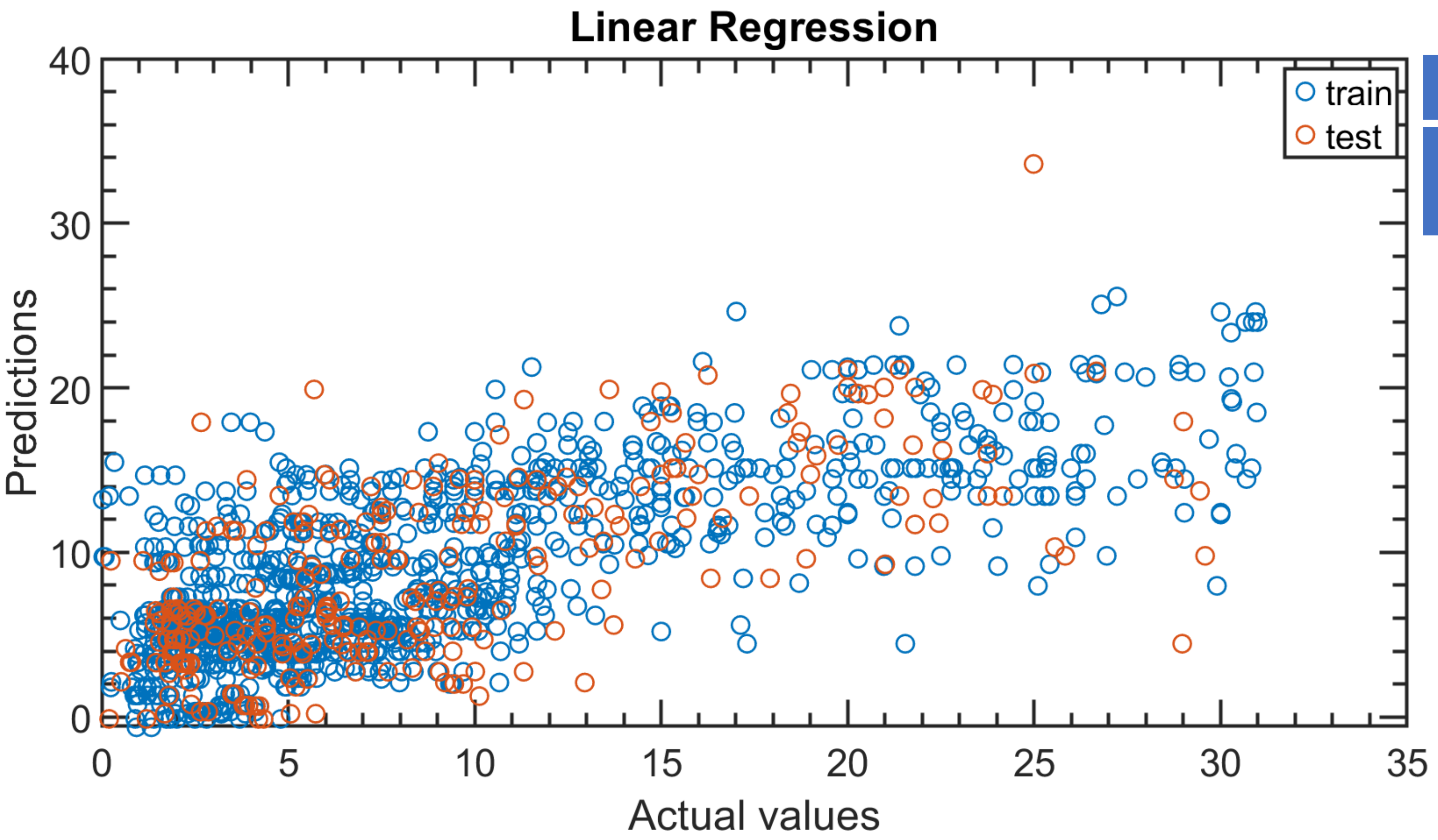
# Parameter Tuning and Model Training

- 3 Parameter Tuned
- 5-Fold Cross Validation
- Training, Validation and Test Sets

| Models | Parameter Tuning | Tuned Variable | Tuned Values |
|---|---|---|---|
| **Linear Regression** | No | - | - |
| **Ridge Regression** | Yes | λ | 4.9 |
| **Lasso Regression** | Yes | α | 1 |
| **Regression Tree** | No | - | - |
| **ANN** | Yes | Hidden Layer Size | 25 |

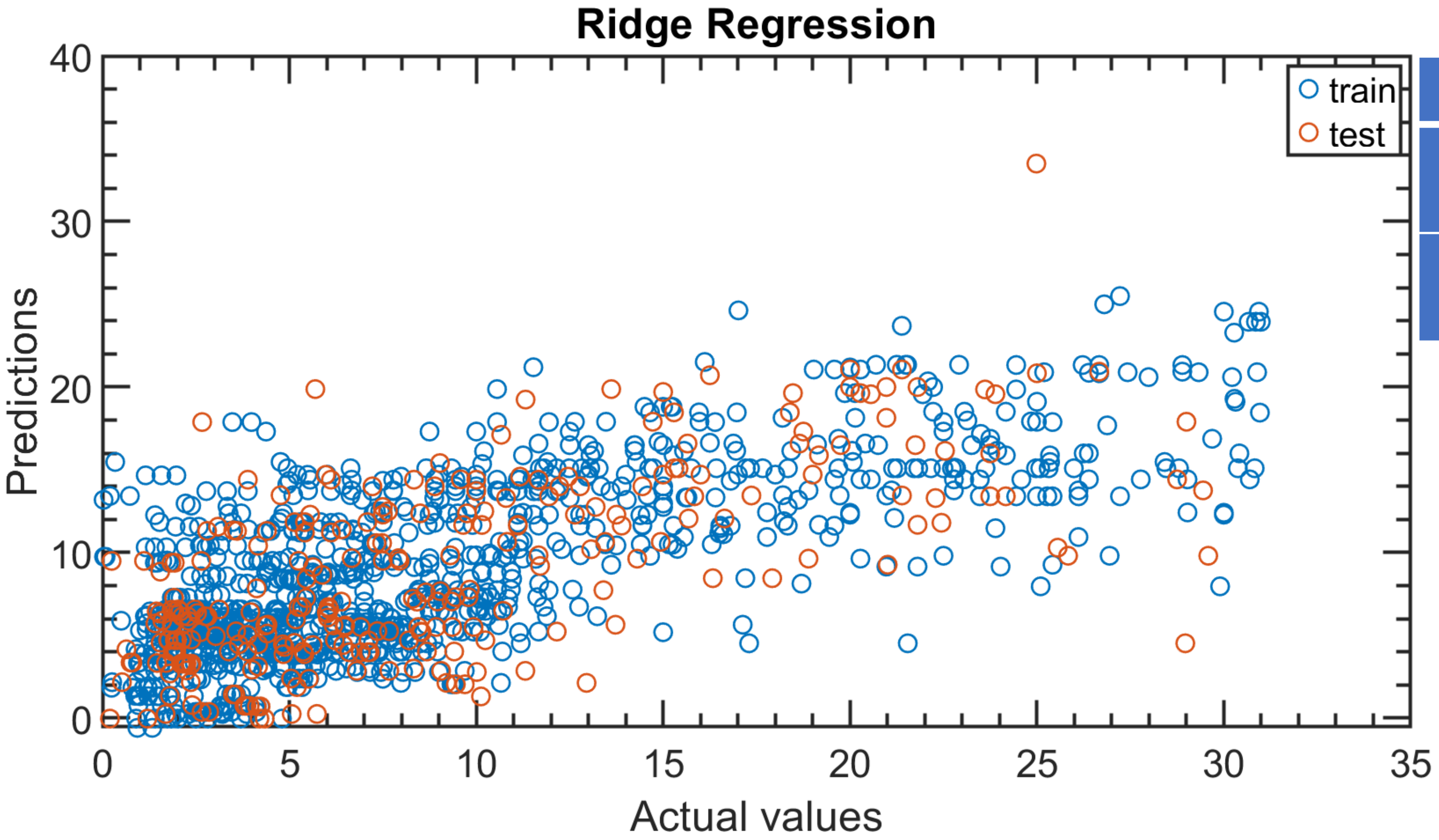
| Data Name | Percentage of the Data | Used Area | Cross Validation |
|---|---|---|---|
| **Full Data** | 100 | - | - |
| **Training Data** | 72 | Used for training models | Yes |
| **Testing Data** | 18 | Testing for the final model | Yes |
| **Validation Data** | 10 | Testing the created model for parameter tuning | No |

# Regression Models: Linear Regression



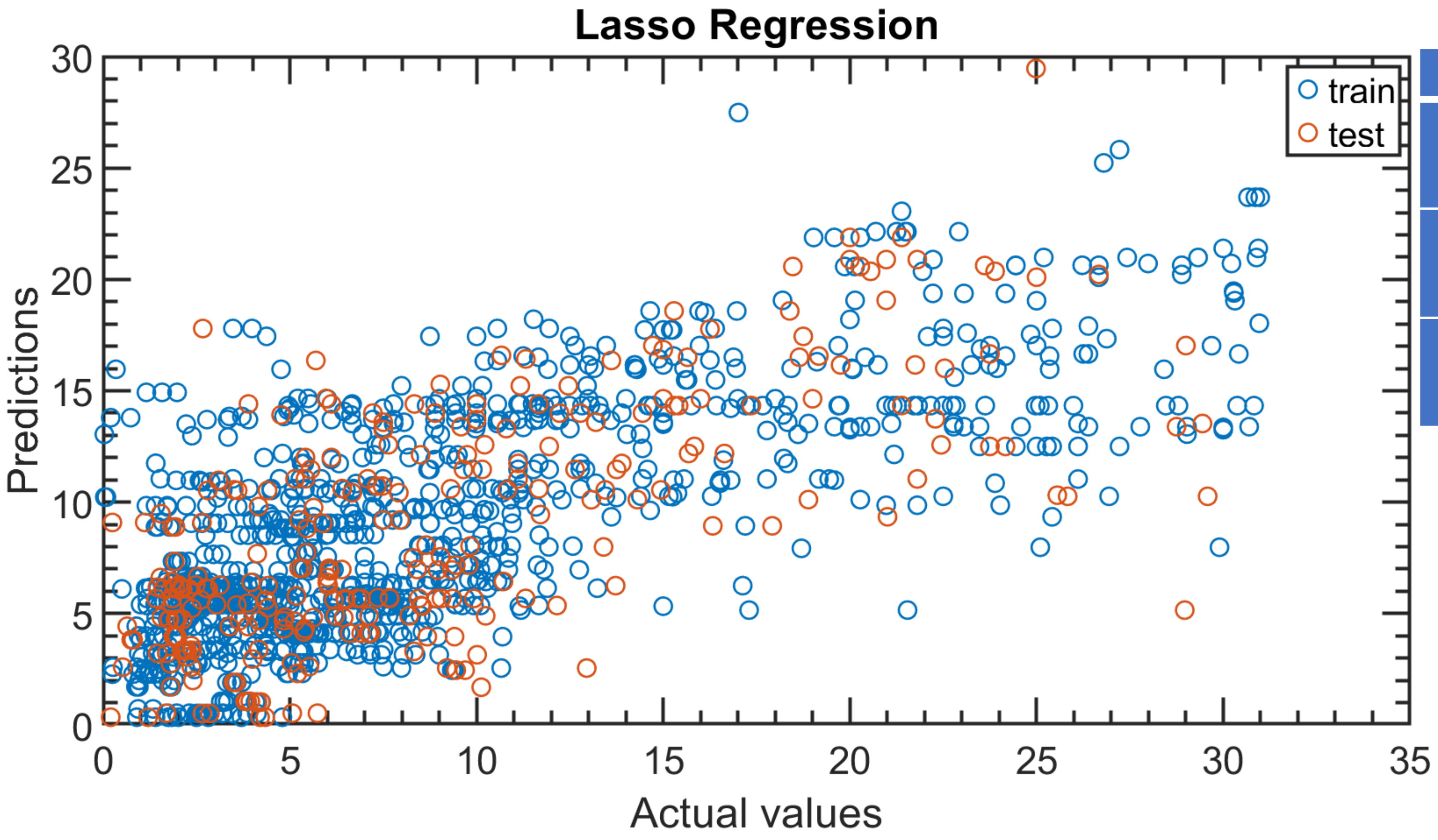

| Model Type | Test RMSE | $R^2$ |
|---|---|---|
| Linear Regression | 5.2343 | 0.2838 |

# Ridge Regression



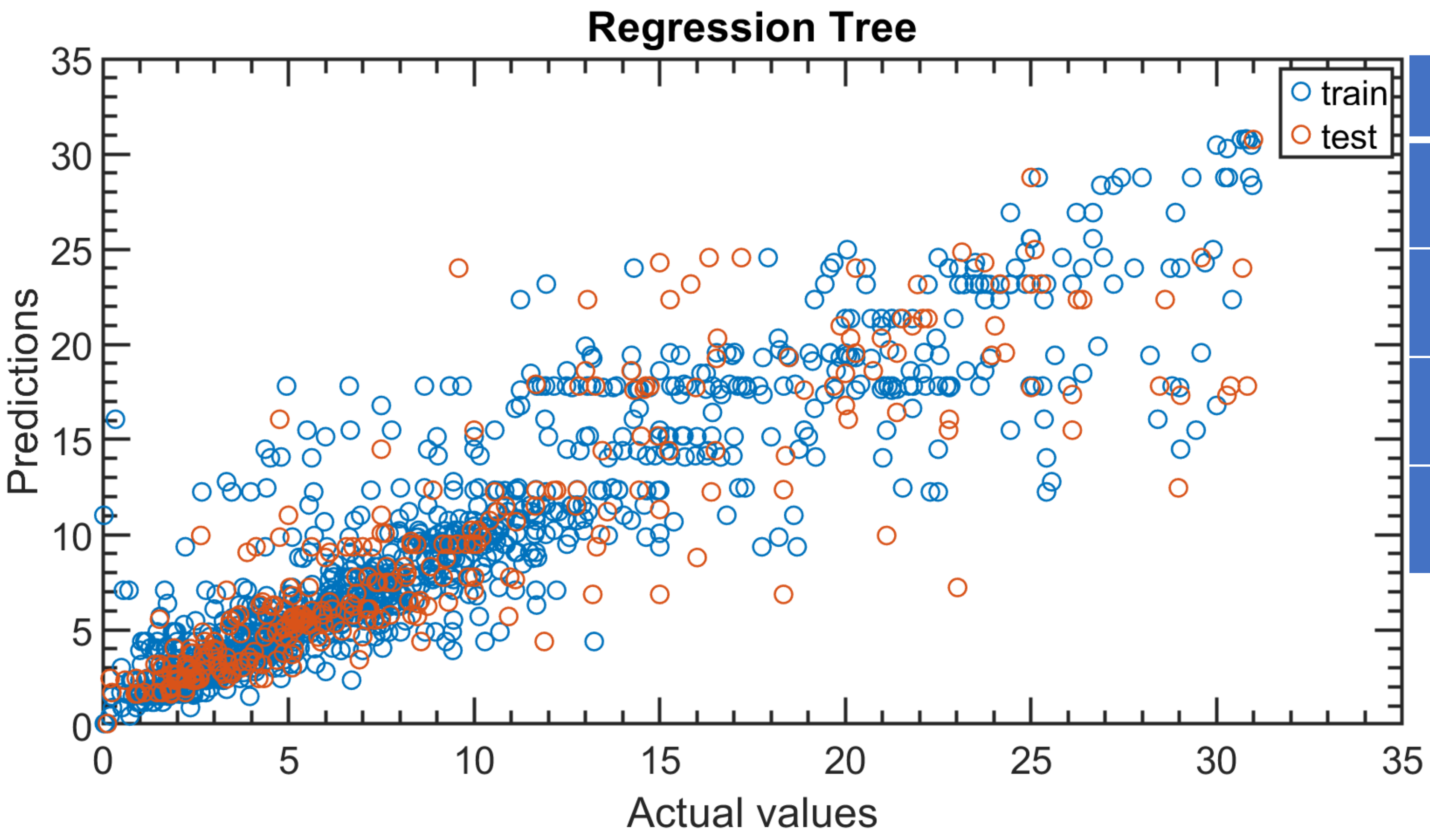

| Model Type | Test RMSE | $R^2$ |
|---|---|---|
| **Linear Regression** | 5.2343 | 0.2838 |
| **Ridge Regression** | 5.2335 | 0.2839 |

# Lasso Regression



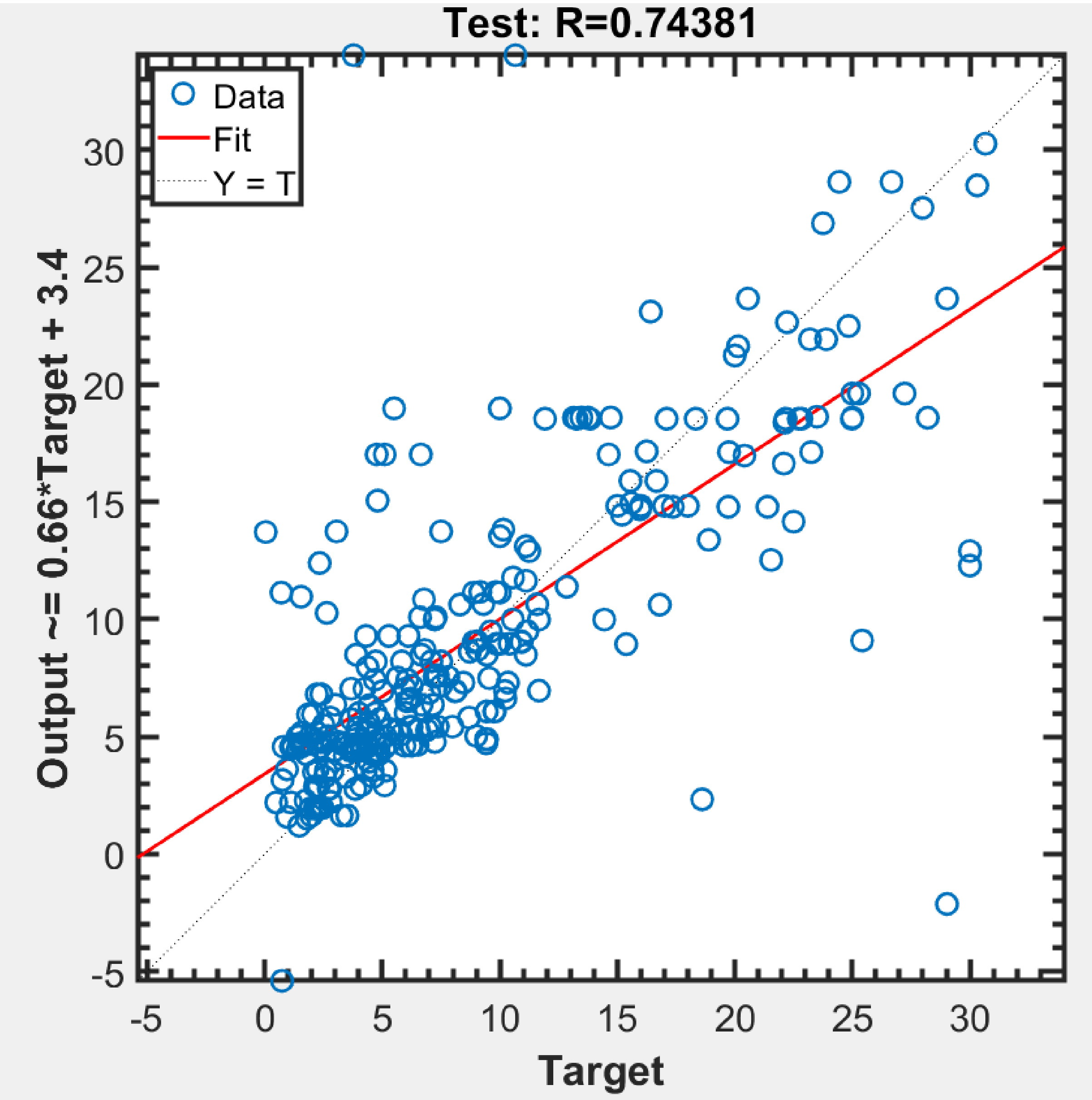

| Model Type | Test RMSE | $R^2$ |
|---|---|---|
| **Linear Regression** | 5.2343 | 0.2838 |
| **Ridge Regression** | 5.2335 | 0.2839 |
| **Lasso Regression** | 5.1288 | 0.2989 |

# Regression Tree

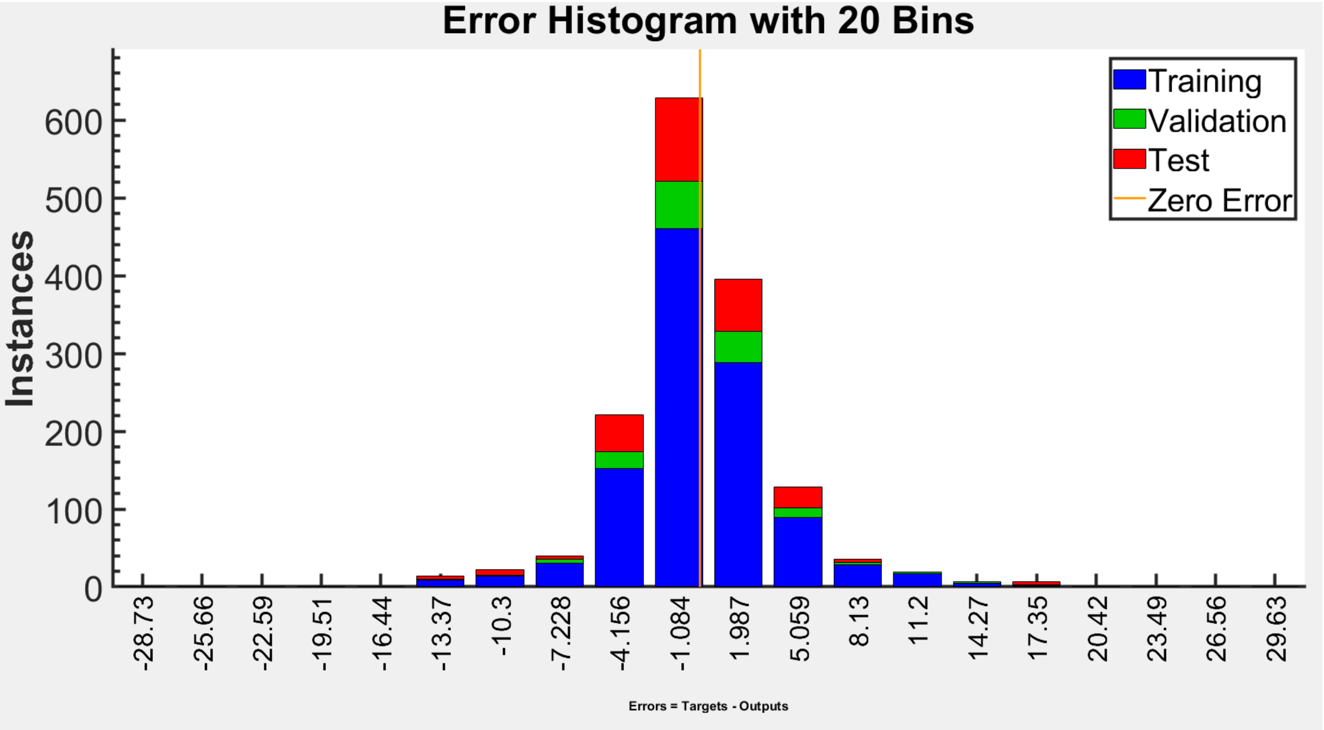



| Model Type | Test RMSE | $R^2$ |
|---|---|---|
| Linear Regression | 5.2343 | 0.2838 |
| Ridge Regression | 5.2335 | 0.2839 |
| Lasso Regression | 5.1288 | 0.2989 |
| Regression Tree | 3.7315 | 0.9567 |

# Artificial Neural Network




| Model Type | Test RMSE | $R^2$ |
|---|---|---|
| **Linear Regression** | 5.2343 | 0.2838 |
| **Ridge Regression** | 5.2335 | 0.2839 |
| **Lasso Regression** | 5.1288 | 0.2989 |
| **Regression Tree** | 3.7315 | 0.9567 |
| **ANN** | 5.010 | 0.7438 |



# Conclusion

- The data set is enriched with the porosity and pore volume values come from SEM image processing results.
- 5 different machine learning models are trained which give accurate predictions.

# Future Thoughts

1

There are also two different response variables that are power density and capacitance. The data for them is available. These two response variables can be used to train new models.

2

Model can be tested with new datasets to ensure model has low variability for different datasets.

# Thank you for the listening

# References


Breiman, L., Friedman, J., Stone, C. J. & Olshen, R., 1984. *Classification and Regression Trees.* s.l.:CRC Press.

Conway, B. E., 1999. *Electrochemical Supercapacitors: Scientific Fundamentals and Technological Applications.* New York: Springer Science+Business Media.

Deringer, V. . L., 2020. Modelling and understanding battery materials with machine-learning-driven atomistic simulations. *JPhys Energy,* Volume 2.

Gu, W. & Yushin, G., 2013. Review of nanostructured carbon materials for electrochemical capacitor applications: advantages and limitations of activated carbon,

carbide-derived carbon, zeolite-templated carbon, carbon aerogels, carbon nanotubes, onion-like carbon, and graphene. *WIREs Energy and Environment.*

Hoerl, A. E. & Kennard, R. W., 1970. Ridge Regression: Biased Estimation for Nonorthogonal Problems. *Technometrics,* Volume 12, pp. 55-67.

IBM , C. E., 2020. *Neural Networks.* [Online]
Available at: https://www.ibm.com/cloud/learn/neural-networks
[Accessed 06 07 2021].

Miller, J. R. & Simon, P., 2008. Electrochemical capacitors for energy management. *Science,* Volume 321, p. 651–652.

Montgomery, D. C. & Runger, G. C., 2014. *Applied Statistics and Probability for Engineers.* 6th ed. s.l.:John Wiley & Sons Singapore Pte. Ltd.

Moody, J., 2019. *towards data science.* [Online]
Available at: https://towardsdatascience.com/what-does-rmse-really-mean-806b65f2e48e
[Accessed 5 july 2021].

Naik, K., 2020. *Complete-Feature-Selection.* [Online]
Available at: https://github.com/krishnaik06/Complete-Feature-Selection
[Accessed 2021].

Nascimento, C. A. O., Giudici, R. & Guardani, R., 2000. Neural network based approach for optimization of industrial chemical processes.

*Computers & Chemical Engineering,* Volume 24, pp. 2303-2314.

Patro, R., 2021. *towards data science.* [Online]
Available at: https://towardsdatascience.com/cross-validation-k-fold-vs-monte-carlo-e54df2fc179b
[Accessed 04 July 2021].

Rabbani , A. & Salehi, S., 2017. Dynamic modeling of the formation damage and mud cake deposition using filtration theories coupled with SEM image processing.

*Journal of Natural Gas Science and Engineering,* Volume 42, pp. 157-168.

Salanne, M., Rotenberg, B., Naoi, K. & et al., 2016. *Efficient storage mechanisms for building better supercapacitors.* s.l.:Nat Energy.

Serway, R. A. & Jewett, J. W., 2013. *Physics for Scientists and Engineers with Modern Phsics.* 9th ed. s.l.:Cengage Learning.

Simon , P. & Gogotsi , Y., 2008. Materials for electrochemical capacitors. *Nature Materials,* Volume 7, pp. 845-854.

Tibshirani, R., 1996. Regression Shrinkage and Selection via the Lasso. *J. R. Statist. Soc. B ,* Volume 58, pp. 267-288.

Wei, J. et al., 2019. Machine Learning in Material Science. *Info Mat,* I(3).