Modeling Grain Size Using Grain Orientation in Polycrystalline Materials

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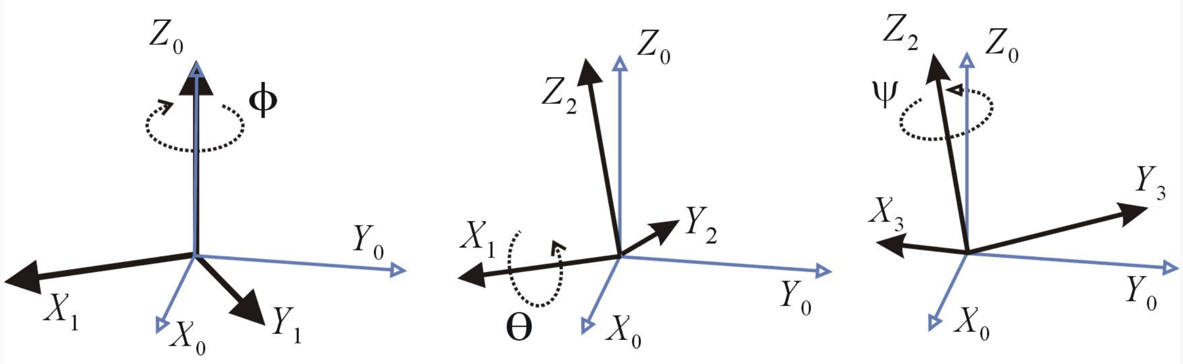
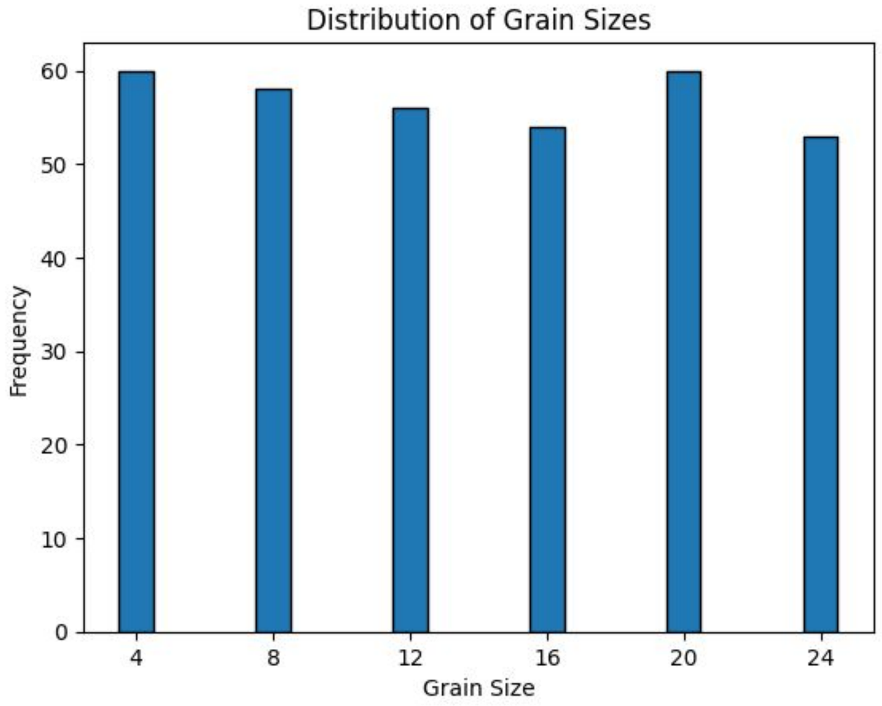
Euler Angles and Grain Orientation

- 3 successive rotations (3-1-3) that transform a reference coordinate system to align with the grains micro axes
- Explain how a grain is oriented relative to material macro axes
- Describe non-uniform properties like directional strength and deformation behavior
- Question: Does the distribution of grain orientations correlate with grain size?

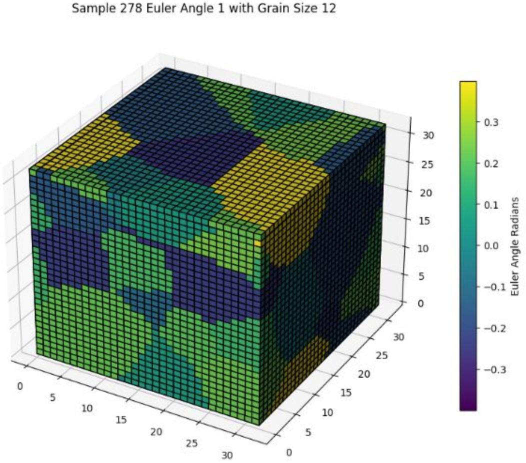


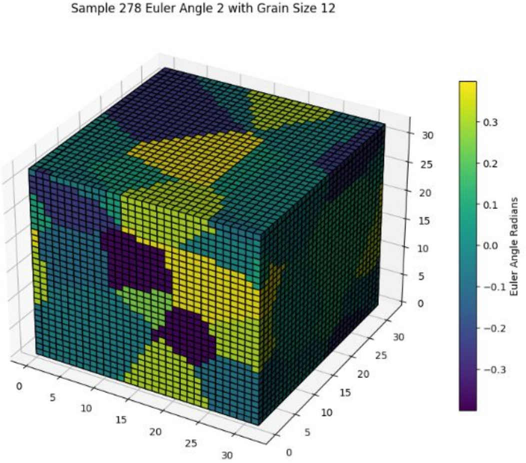
Data Extraction and Preparation

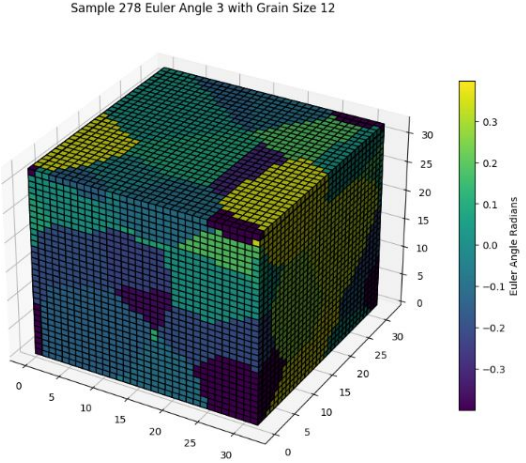
- Dataset is synthetically created using NEPER at ORNL.
- Consists of 341 complete sample folders containing: .grn2 (grain ID), .ori (Euler angles) and grain size files.
- Reshaped 2D 1024 x 32 grain ID data into 3D 32 x 32 x 32 voxel arrays storing grain IDs.
- Included the 3 Euler angle rotations for each voxel forming 4D 32 x 32 x 32 x 3 arrays.



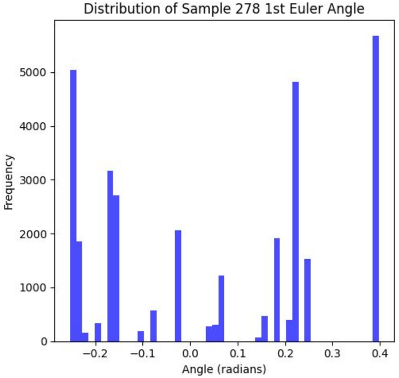
Data Exploration

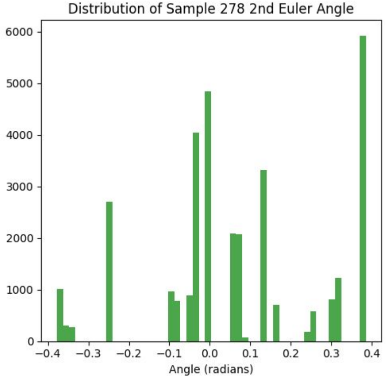


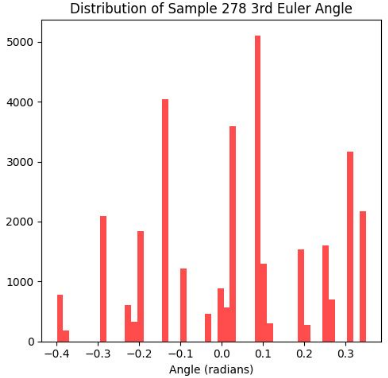




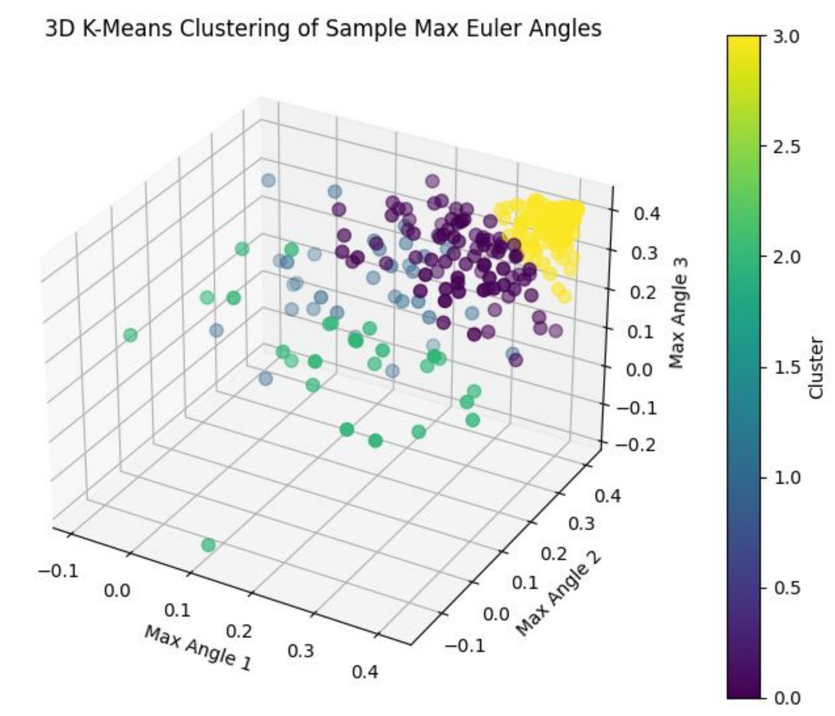
- Randomly selected Sample # 278
- Colorbar is Euler angles range -.3, .3 (radians) or -17, 17 (degrees)
- Grain size for this sample = 12

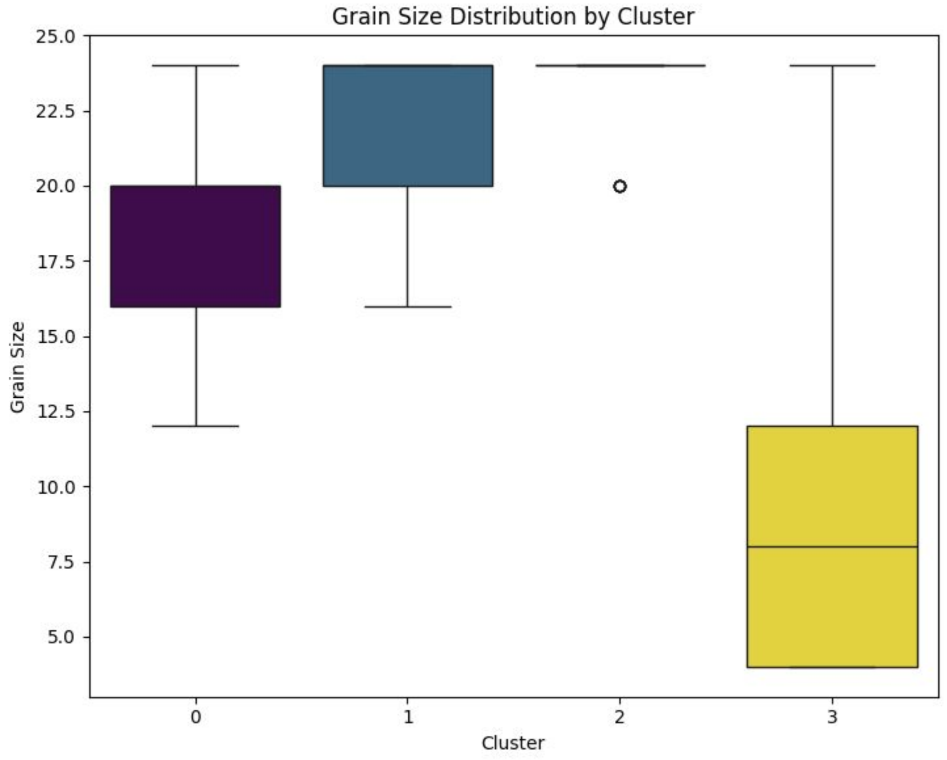




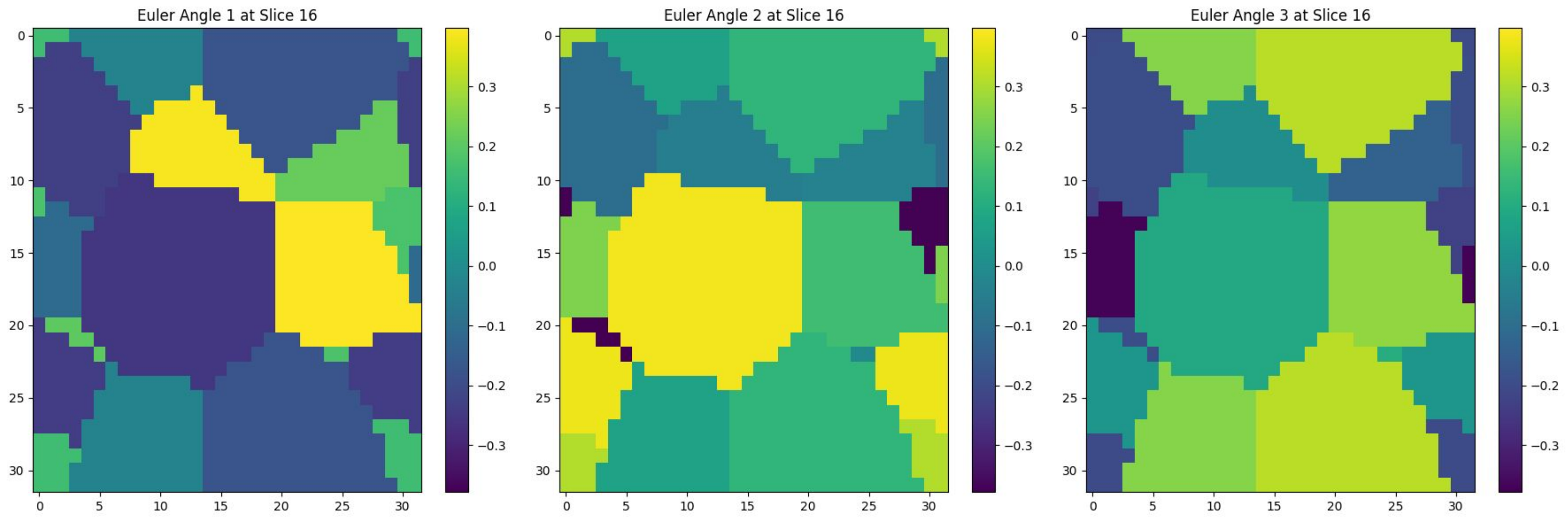


Unsupervised Learning - K-Means Clustering





Two-Point Correlation Statistics



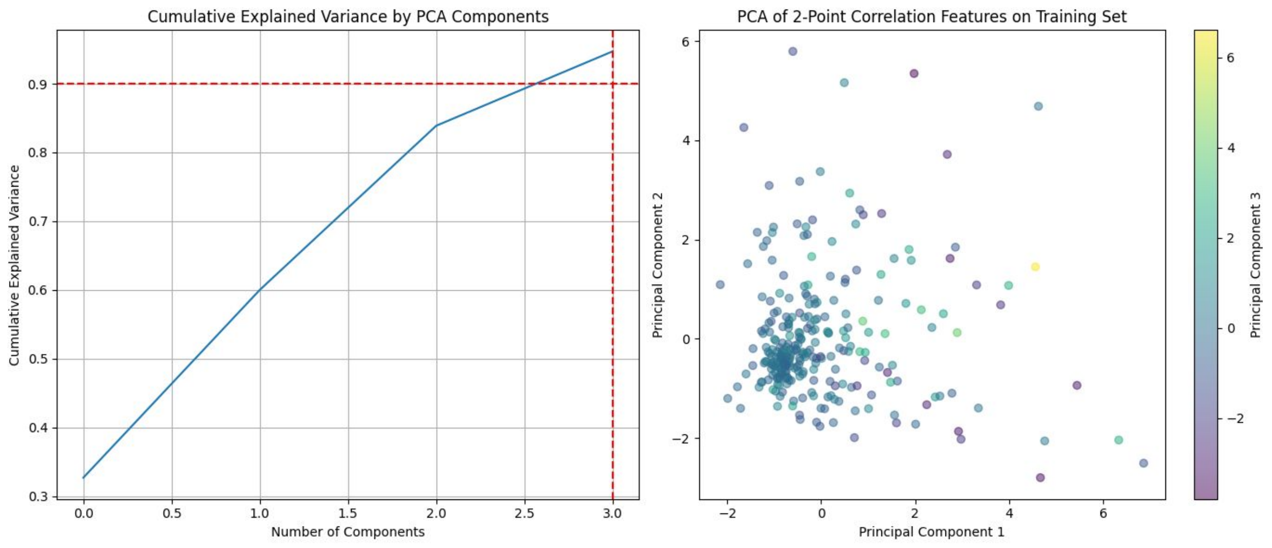
- Take 2D center slice (#16) from 3D sample, define the distance between pairs to calculate statistics for lag_n = 4, 8, 16
- Iterate through each voxel in the slice, compute correlation between original voxel and another voxel that is at the specified lag distance away and within the plane of the slice
- Calculate the correlations of all voxel pairs at lag_n by computing the product of the pair's Euler angles then take the average of those products for all pairs for each lag_n and
- Repeat process for each Euler angle orientation

Why?

- Flattening the 341 sample's data from 32x32x32x3 to 1D yields 98,304 features, need another way to describe data
- Describes how the orientation of grains vary spatially for each angle orientation within the distance of 4, 8 and 16 voxels

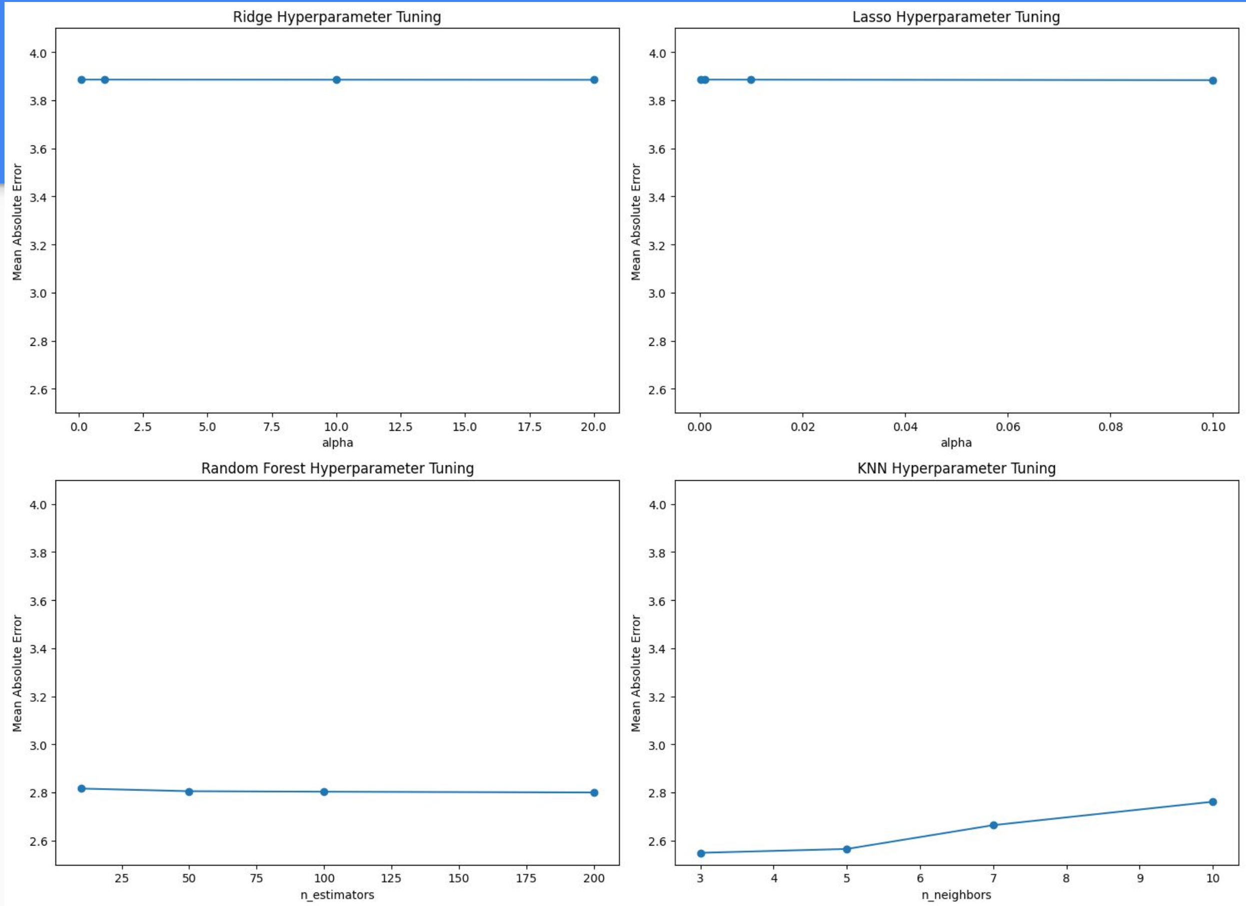
Principal Component Analysis (PCA)

Total number of principal components: 4
Explained variance by each component: [0.32677825 0.27318454 0.23887114 0.10820887]



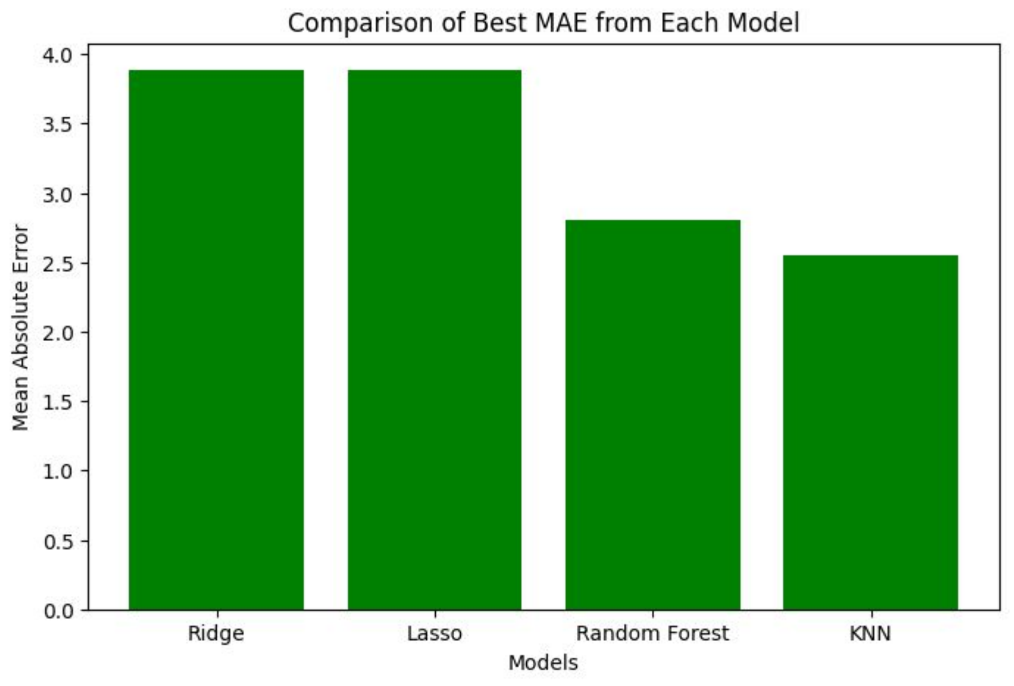
Regression Models and Hyperparameter Tuning

- Ridge - alpha: large increases coef. shrinkage
- Lasso - alpha: large increases coef. shrinkage to 0
- Random Forest - n_estimators: # of trees, more trees more complexity
- KNN - n_neighbors: smaller is more flexible

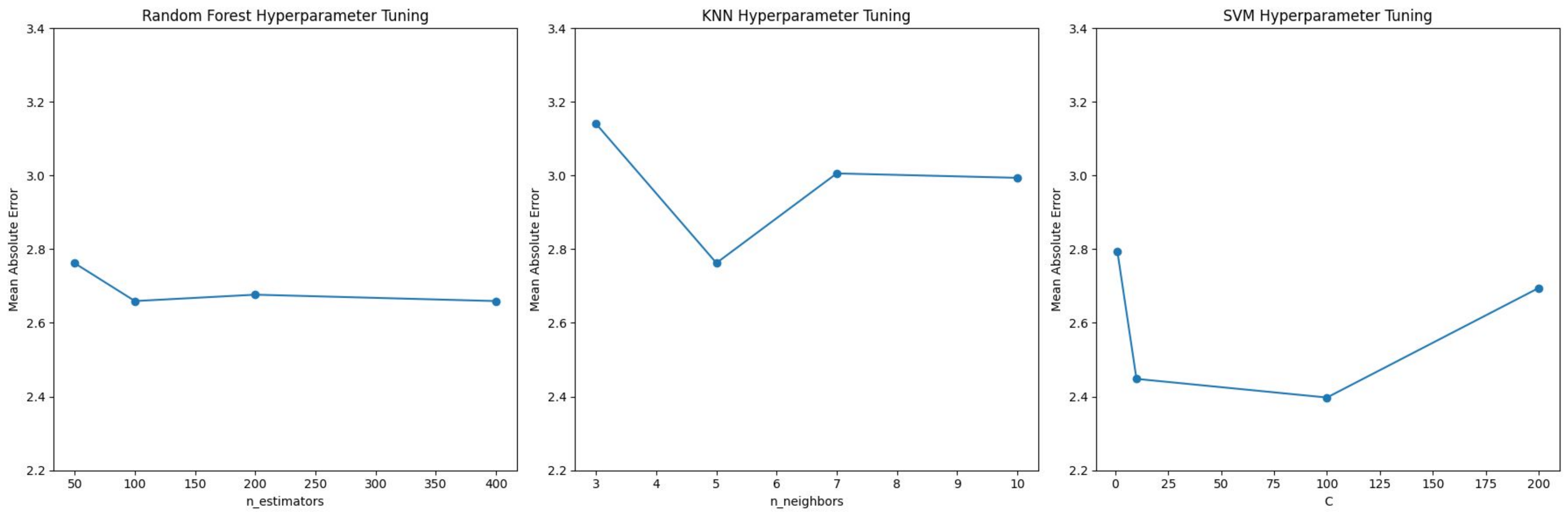


Regression Model Performance

- Model = Ridge,
  Min MAE = 3.88,
  alpha = 20
- Model = Lasso,
  Min MAE 3.88,
  alpha = 0.1
- Model = Random Forest,
  Min MAE = 2.8,
  n_estimators = 200
- Model = KNN,
  Min MAE = 2.55,
  n_neighbors = 3

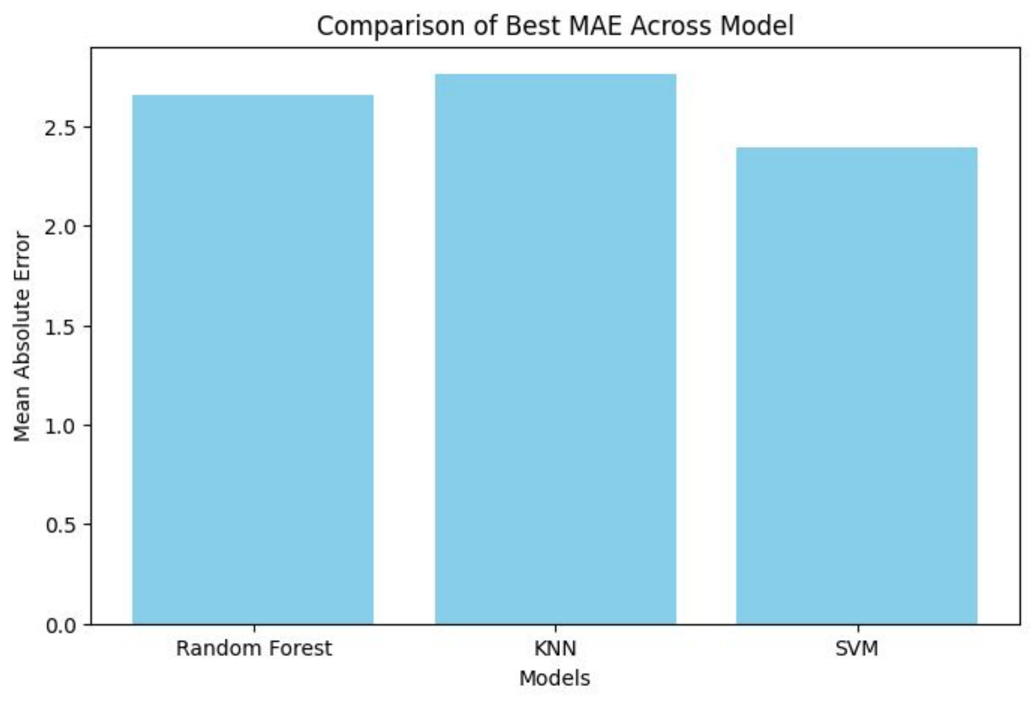


Classification Model and Hyperparameter Tuning



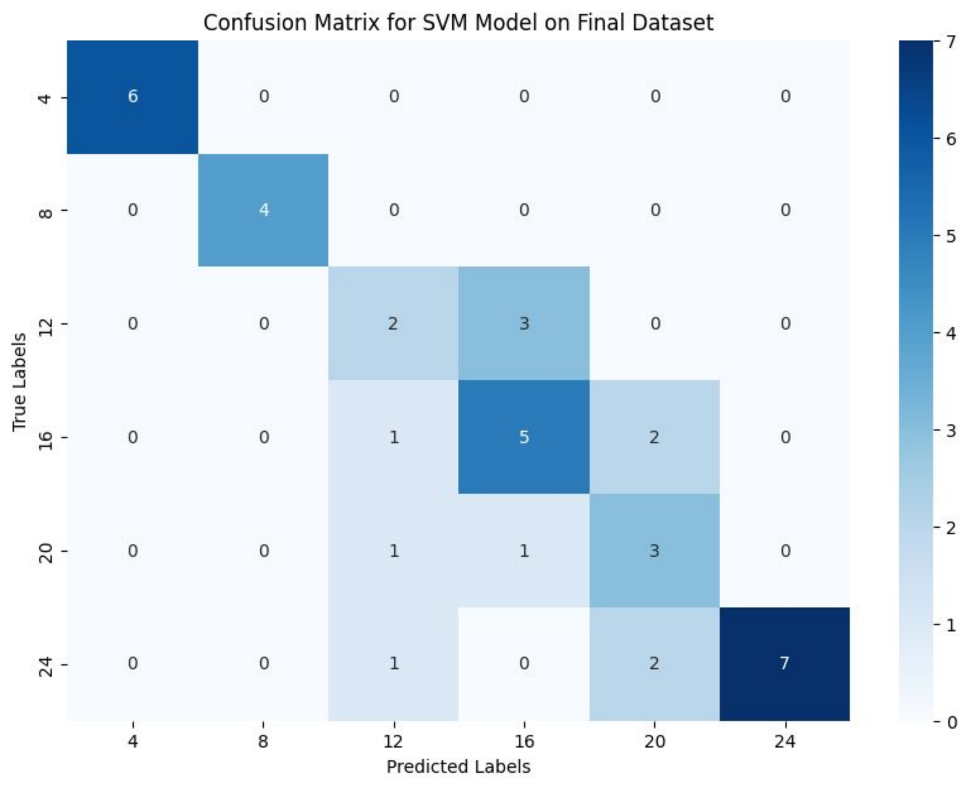
Classification Model Performance

- Model = Random Forest,
  Min MAE = 2.66,
  n_estimators = 400
- Model = KNN,
  Min MAE = 2.76,
  n_neighbors = 5
- Model = SVM,
  Min MAE = 2.4,
  C = 100
- Higher C reg. to lower bias



Mean Absolute Error and Final Results

- Why MAE? 1/n ∑ |yi - yi^|
- Uses units of target, ordinal labels, classification and regression models
- MAE Test Data: 1.47
- Accuracy Test Data: .71
- Perfect at grain sizes 4, 8, okay at 24, bad at 12, 16, 20



Q & A

- Project notebook: Click here
- References:
  - A Comparative Study of the Efficacy of Local/Global and Parametric/ Nonparametric Machine Learning Methods for Establishing Structure–Property Linkages in High-Contrast 3D Elastic Composites Patxi Fernandez-Zelaia, Yuksel C. Yabansu & Surya R. Kalidindi https://par.nsf.gov/servlets/purl/10147978
  - Microstructure informatics using higher-order statistics and efficient data-mining protocols https://link.springer.com/article/10.1007/s11837-011-0057-7