△ Access

Retrain

< Back to all views

Intro to Citrination Data View

Data Summary Model Report

Models

Learn more about Model Reports and Machine Learning in our Citrination Knowledge Base.

Property Fatigue strength

Property Fatigue strength



Model Settings

Table representation of the machine learning algorithm and hyperparameters from the most recent machine learning training session. The Lolo estimator is Citrine's open source machine-learning library.

Algorithm: Ensemble of non-linear estimators		
Number of estimators	145	
Minimum samples per leaf	1	
Maximum tree depth	30	
Uses jackknife method of uncertainty estimation	true	
Leaf model	Mean	

Number of cross-validation folds: 3

Important Features

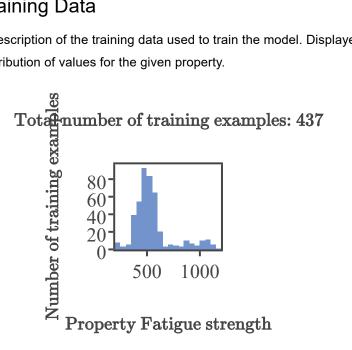
A list of features used to train the model ranked by importance scores. Importance scores sum to 1 and are representative of a given feature's contribution to the model's performance. Learn about the features that are used as inputs to machine learning models on the Citrination Platform.

Property Fatigue strength	
Property Normalizing temperature	70%
mean of Packing density for formula	4%
mean of Non-dimensional band gap for formula	4%
mean of Elemental melting temperature for formula	4%
mean of DFT energy density for formula	3%
mean of Elemental work function for formula	2%
mean of Elemental atomic volume for formula	2%
mean of Elemental electron density for formula	2%
mean of Shear Modulus Melting Temp Product for formula	1%
mean of Trouton's Ratio for formula	1%
mean of Liquid ratio for formula	1%
mean of Elemental crystal structure (space group) for formula	1%
mean of Number of unfilled s valence electrons for formula	1%
mean of Elastic Poisson Ratio for formula	1%
mean of Zunger Pseudopotential radius ratio for formula	1%
mean of Non-dimensional liquid range for formula	1%
mean of Number of p valence electrons for formula	1%
mean of Modulii sum for formula	0%
mean of DFT volume ratio for formula	0%
mean of Non-dimensional work function for formula	0%

Property Fatigue strength		
mean of Number of s valence electrons for formula	0%	
mean of Radius of s orbitals for formula	0%	
mean of Miracle Ratio for formula	0%	
mean of Interatomic distance for formula	0%	
mean of Ratio of Electron Affinity to Electronegativity for formula	0%	
mean of Elemental bulk modulus for formula	0%	
mean of Liquid range for formula	0%	
mean of Number of unfilled p valence electrons for formula	0%	
mean of Total number of valence electrons for formula	0%	
mean of Conduction ionization energy for formula	0%	
Maximum atomic fraction for formula	0%	
Property Through hardening time	0%	
Maximum radius difference for formula	0%	
Property Through hardening temperature	0%	

Training Data

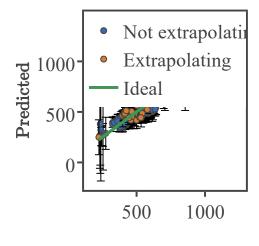
A description of the training data used to train the model. Displayed below are the number of training examples and a distribution of values for the given property.



Performance

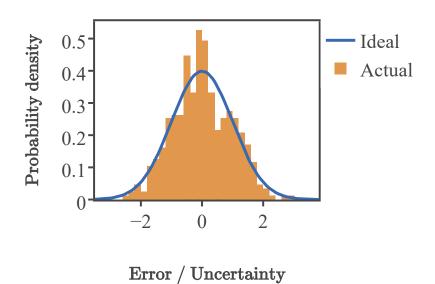
Error Metric	Value
Non-dimensional model error (NDME) (0.0 for a perfect model)	0.291
Standard error in the estimate of NDME (0.0 for a perfect estimate)	0.0177
Root mean squared error (RMSE) (0.0 for a perfect model)	54.2
Standard Error in the estimate of RMSE (0.0 for a perfect estimate)	3.30
Uncertainty calibration: fraction of actual values within the prediction error bars (0.68 is perfectly calibrated)	0.680
Uncertainty calibration: root mean square of standardized errors (RMSSE) (1.0 is perfectly calibrated)	0.950

Property Fatigue strength



Actual

Distribution of Standard Residuals



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