Alchemite™ Engine and science update

Dr Gareth Conduit

Acceleration

Model training sped up by 5%

30% faster data processing

Removed two hyperparameters so faster and more robust hyperparameter optimization when training

Usability

Optimization page searches historic formulations

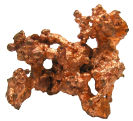
Ability to set the maximum number of ingredients in a composition

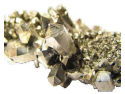
Cr 

Co 

Mo 

W 

Cu 

Nb 

Al 

C 

B 

Ni 

Expose 

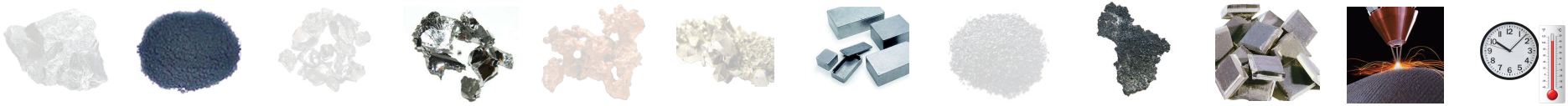
T_{HT} 

Usability

Optimization page searches historic formulations

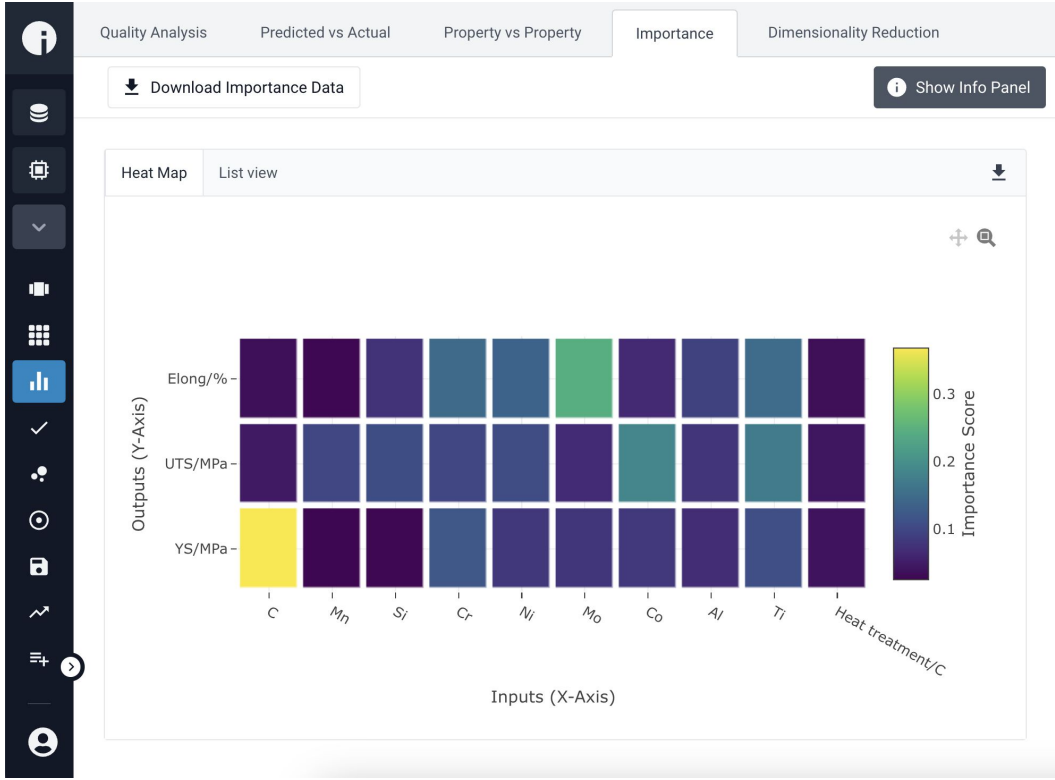
Ability to set the maximum number of ingredients in a composition

	①		②			③		④	⑤		
Cr	Co	Mo	W	Cu	Nb	Al	C	B	Ni	Expose	T_{HT}



Usability

Importance plot explicitly shows impact only of the input variables



Accuracy

Model

Improved selection of input columns

Distributions

Training focuses on uncertainty quality as well as model accuracy

Improved uncertainty estimates when extrapolating

Improved Bayesian probability used in outlier detection

Papers since the previous Focus Group

Design of Materials with Alchemite™
NASA Technical Memorandum, 20220008637

Unveil the unseen: exploit information hidden in noise
Applied Intelligence (2022)

Design of a Ni-based Superalloy for Laser Repair Applications using Probabilistic Neural Network Identification
Data Centric Engineering 3, e30 (2022)

Future plans

Preprocessing

Automated feature engineering including chemical descriptors and unit parsing

Developing tool to better handle time series and images

Optimization

Improve the stability of hyperparameter space

Design for robustness against variations on input variables as well as performance

Analytics

Improved dimensionality reduction including cluster labelling

Questions

What additional machine learning modeling features would you find useful?

What further types of data would you like us to process?

Customers use dimensionality reduction to understand trends, can anyone share particular successes?