Data Analytics for Designing Fe-9Cr Steels

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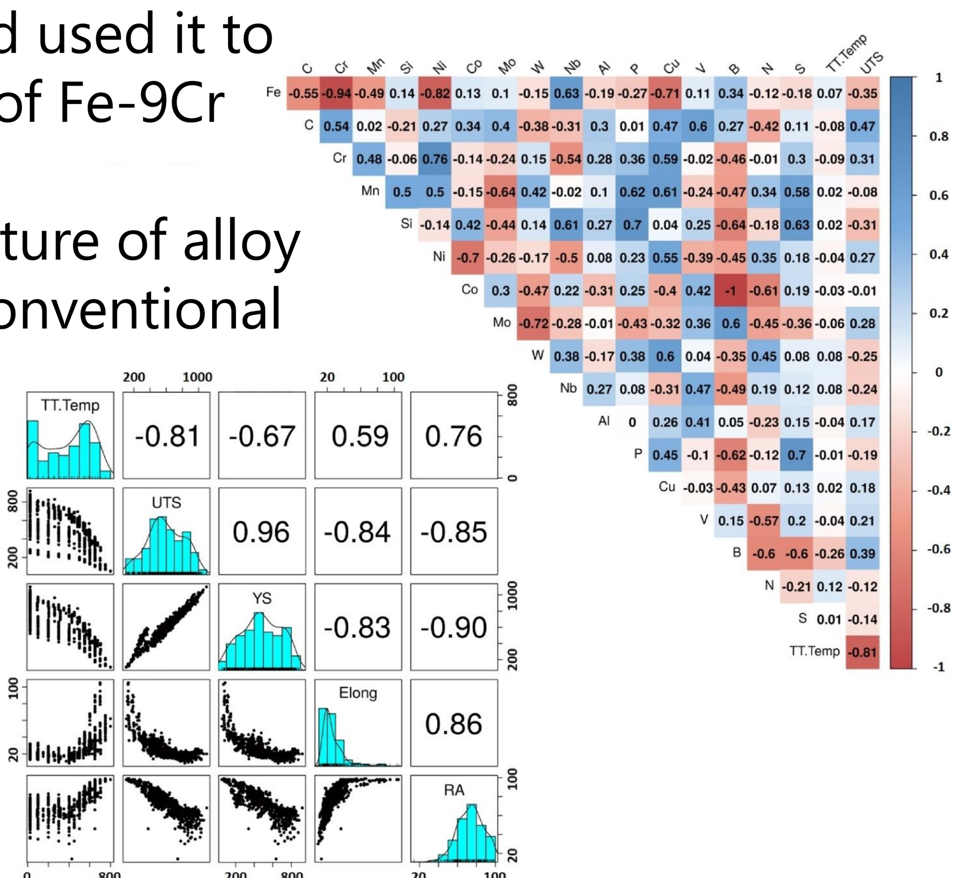
INTRODUCTION and APPROACH

Motivation for this research comes from the desire to shorten the rigorous and time-consuming alloy qualification process. The main consideration for using martensitic-ferritic steels is relatively high microstructural stability at the operating temperature over time, since power plants have a design lifetime of over 30 years. A materials data analytics methodology was developed to evaluate publicly available information on 9% Cr family steel and to handle nonlinear relationships and the sparsity in materials data for this alloy class.[1] Data entries for over 90 unique compositions, processing parameters, and results of tensile mechanical tests used in this study were arranged in 47 columns by 3000 rows.[2]

RESULTS

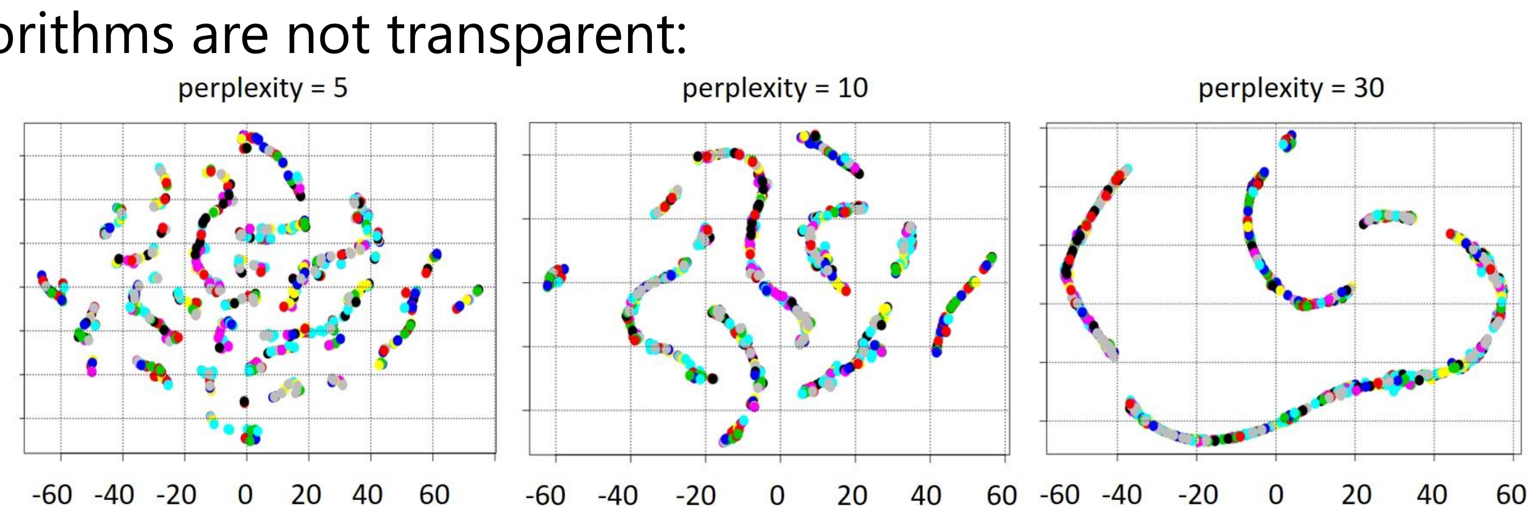
- ✓ NETL developed alloy database and used it to interrogate mechanical properties of Fe-9Cr steels
- ✓ Partitioning revealed the biased nature of alloy datasets, multicollinearity due to conventional design practices.[1]

Exploratory analysis: scatter plots and a heatmap of Pearson correlations

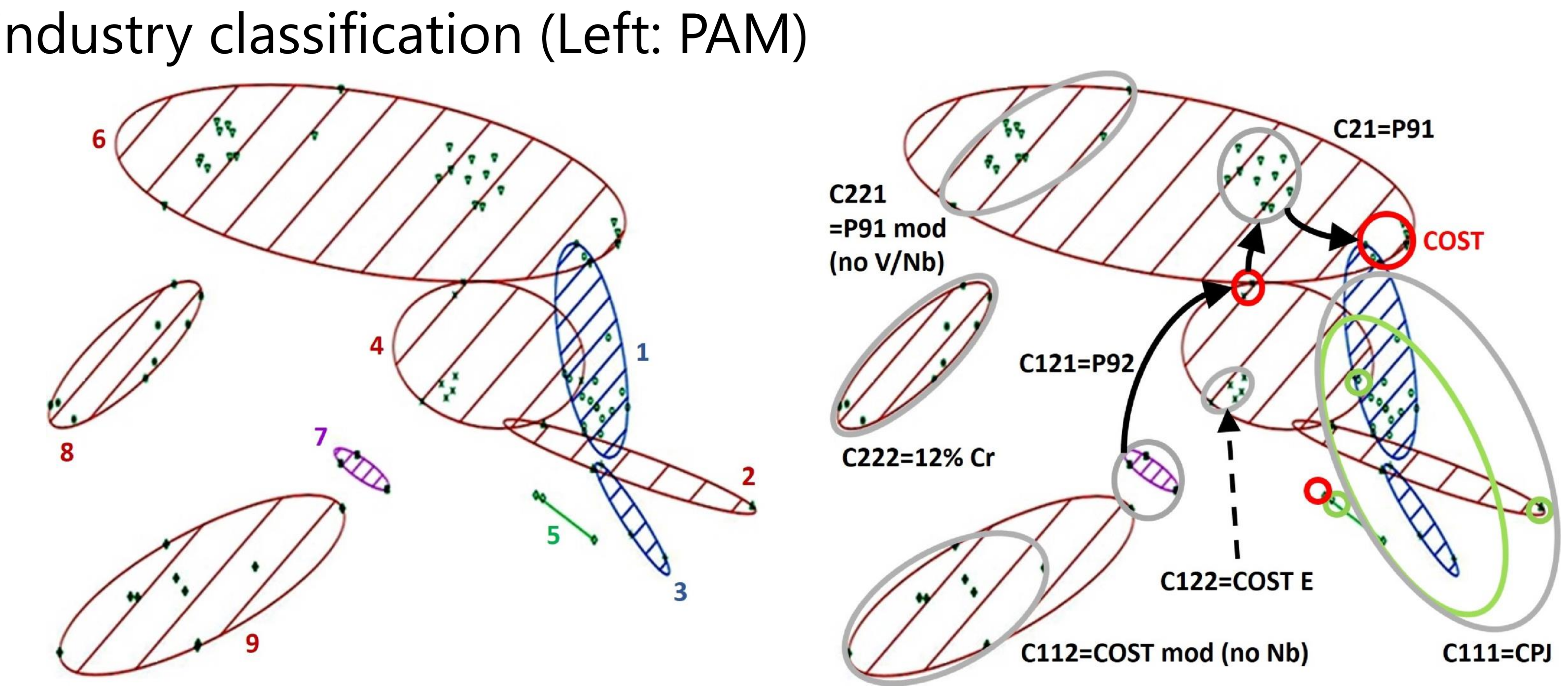


- ✓ Generic algorithms are not transparent:

t-SNE[2]



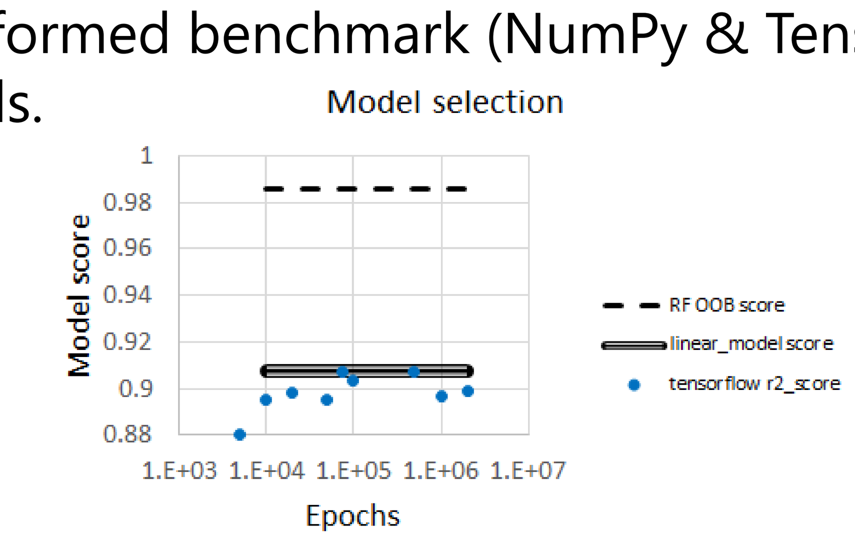
- ✓ New[1] algorithm: clustering for Information Gain (c-IG) without prior dimensionality reduction matched industry classification (Left: PAM)



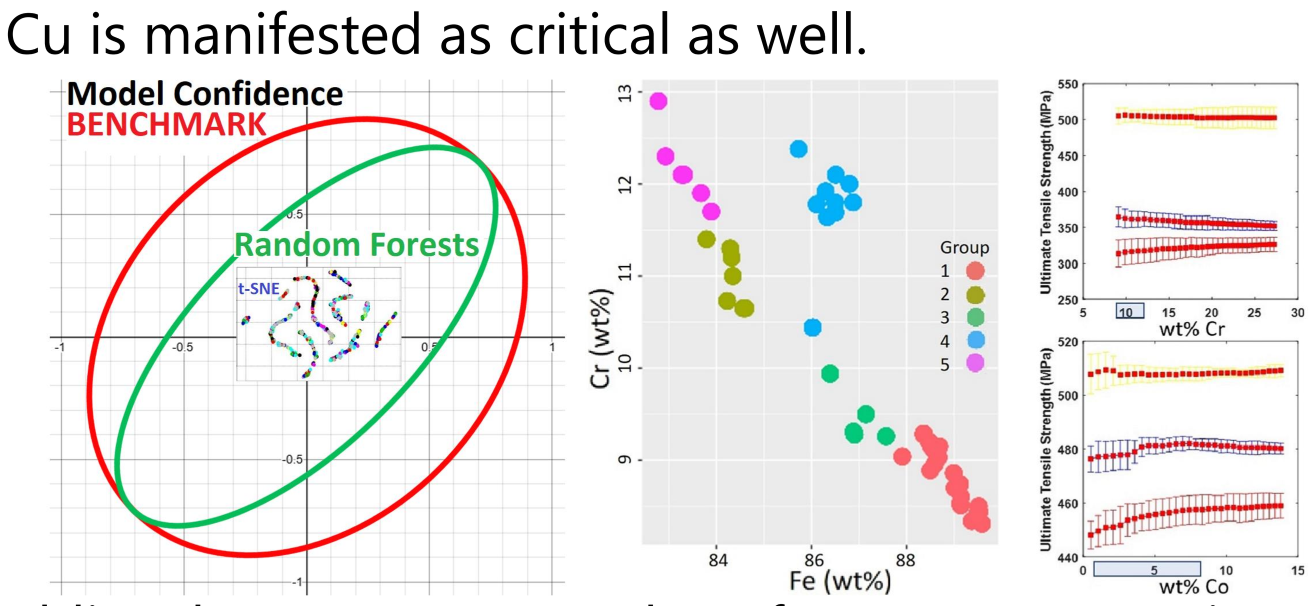
- ✓ New[1] algorithm: Chebyshev metric adopted to modify k-NN using c-IG pre-seeded centroids:

$$\|\boldsymbol{z}\|_p = \left(\sum_{i=1}^{n} |z_i|^p\right)^{1/p}, \text{ for } p \in \mathbf{N} \text{ (natural number, } 1 \le p < \infty)$$

- ✓ Tempering and test temperature effects on the mechanical properties were identified as major contributors (accounting for >80% of the data variation) and modeled first, before searching for minor effects of the composition variations.
- ✓ Ensemble models outperformed benchmark (NumPy & TensorFlow) linear optimization models.



- ✓ Validated ensemble models demonstrated high predictive power; >98% of the tensile strength variation was explained (93% of the design contributors vs 50% for the benchmarks).
- ✓ New alloy designs were explored. C and Mn were identified[1] as global contributors to tensile strength. Among cluster-dependent contributors, Cr, V, N, Si, Ni, and Nb were most consistently identified as major.[3] In ensemble modeling, non-linear behavior associated with Mo, W, Co, and Cu is manifested as critical as well.



- ✓ 29 public releases (papers and conference presentations)

BENEFITS AND FUTURE WORK

The project produced a methodology to guide the DOE-wide effort on materials data analytics for extreme environments. The data-driven models without dimensionality reduction provide a transparent link to the domain knowledge base. The primary data gaps identified as related to missing information on detailed microstructure will be addressed in future work.

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