Machine Learning Modeling of Superconducting Critical Temperature

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Machine Learning for Materials Research Bootcamp
August 2, 2018

Outline

- Short presentation explaining the idea, the data and the ML method
- Three notebooks
  - Quick look at the data
  - Classification models
  - Regression models

V. Stanev, C. Oses, A. Kusne, E. Rodriguez, JP. Paglione, S. Curtarolo, I. Takeuchi,
Machine learning modeling of superconducting critical temperature,
npj Computational Materials 4 (1), 29 (2018)

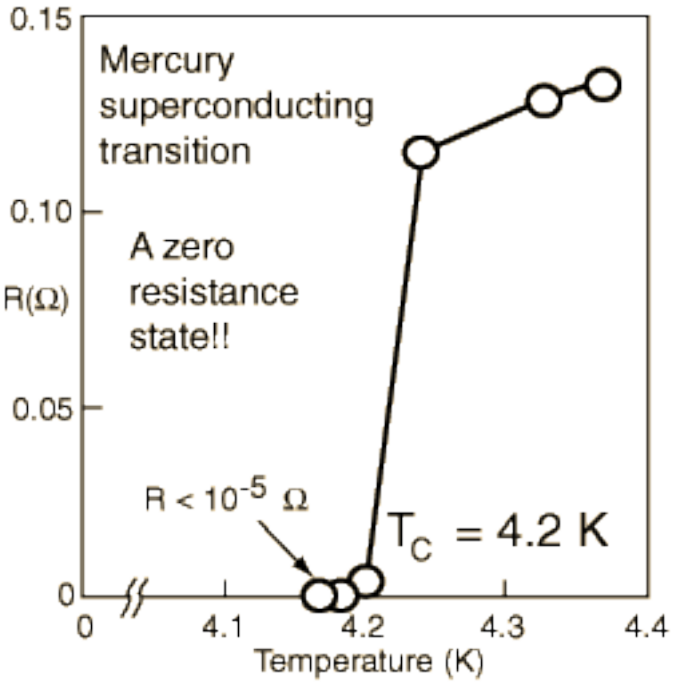
Motivation – what and why

Superconductivity – macroscopic quantum state (below critical temperature T_c)

Apply Machine Learning methods to superconductivity:

1) Better understand superconductivity in known materials – find connection between materials parameters and T_c
2) Search for superconducting materials?

We need data!



Critical temperature data

MatNavi SuperCon database – experimentally measured T_c (http://supercon.nims.go.jp/index_en.html)

~ 22,000 compounds in the database;

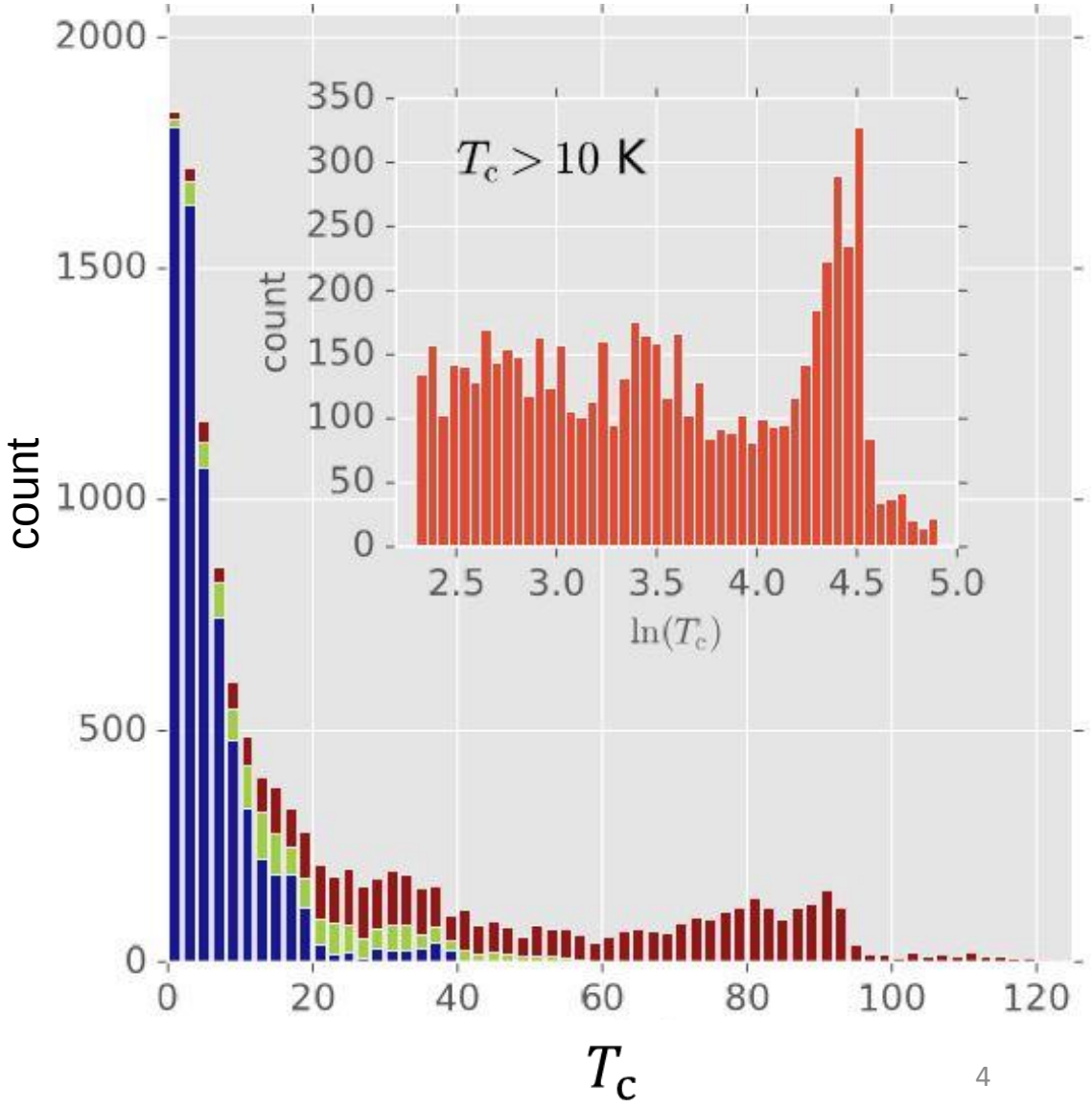
~16,400 after combining/removing the duplicates;

~12,400 with T_c plus about 4000 without T_c (what should we do with them?)

5700 cuprates (35%)

1500 Fe-based (9%)

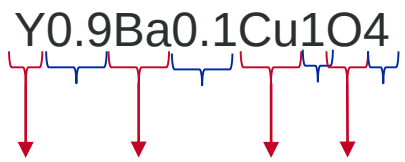
MatNavi
NIMS 物質・材料データベース



Predictors for T_c

We have only composition and T_c. Need some predictors!

Use Magpie to generate elemental features



elemental properties

composite property:
average, range, std, max, min

std(Electronegativity) = standard deviation of elemental electronegativities

A general-purpose machine learning framework for predicting properties of inorganic materials

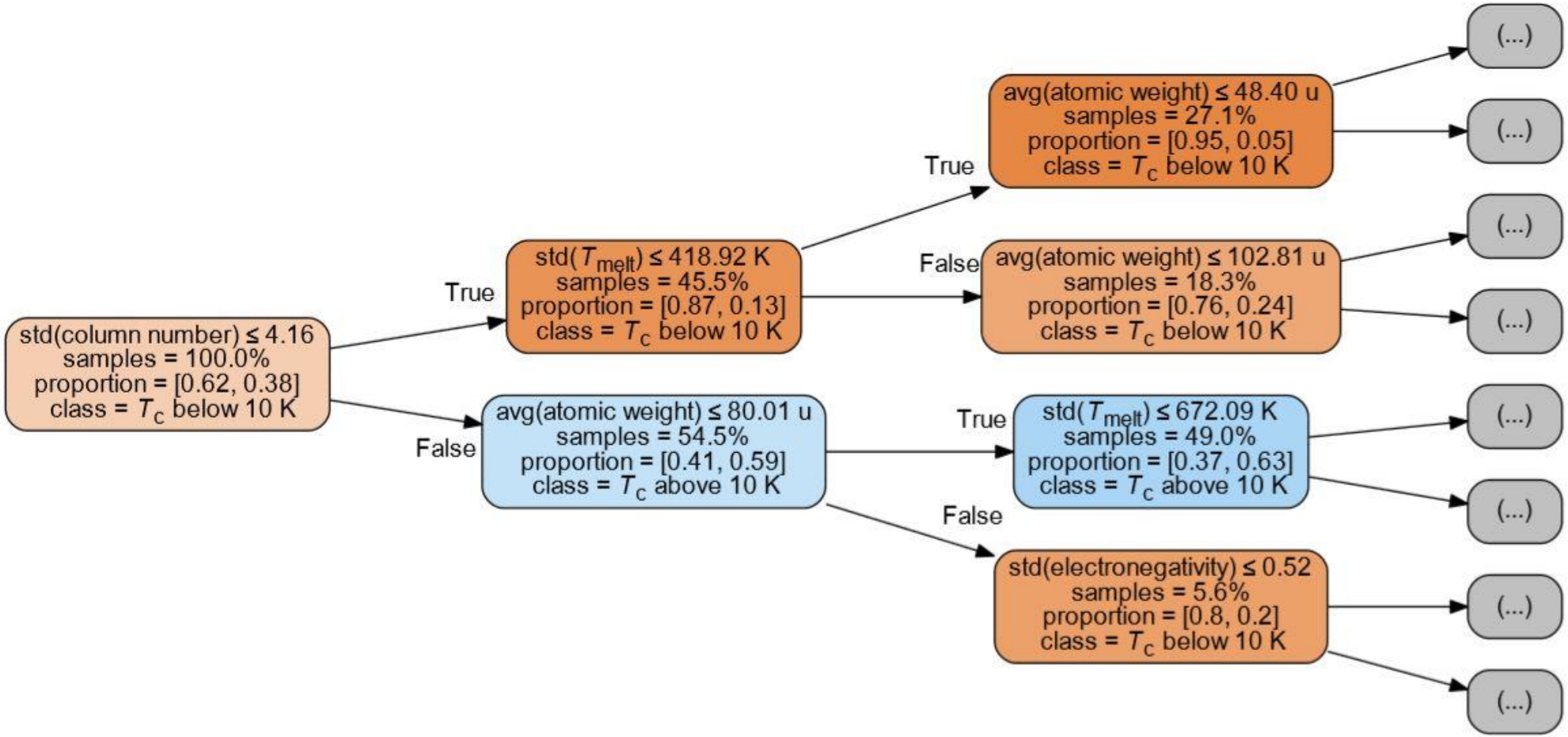
Logan Ward[1], Ankit Agrawal[2], Alok Choudhary[2] and Christopher Wolverton[1]

npj Computational Materials, (2016)

Atomic Number	Mendeleev Number[9]	Atomic Weight	Melting Temperature	Column
Row	Covalent Radius	Electronegativity*	# s Valence Electrons	# p Valence Electrons
# d Valence Electrons	# f Valence Electrons	Total # Valance Electrons	# Unfilled s States†	# Unfilled p States†
# Unfilled d States†	# Unfilled f States†	Total # Unfilled States†	Specific Volume of 0 K Ground State‡	Band Gap Energy of 0 K Ground State‡
Magnetic Moment (per atom) of 0 K ground state‡		Space Group Number of 0 K Ground State‡		

Random forest I

Now we have predictors and target (T_c). Let's create ML model.
Use decision trees – can be used for both regression and classification.



Random forest II

Now we have predictors and target (T_c). Let's create ML model.
Use decision trees – can be used for both regression and classification.

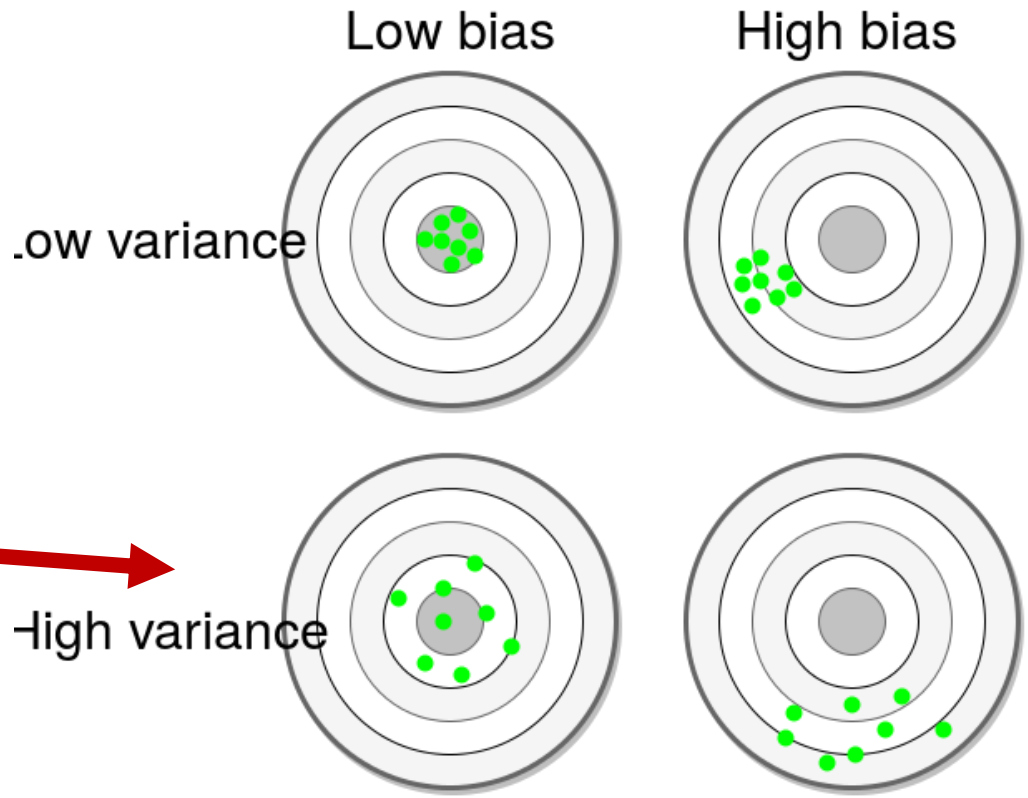
Pros:

- don't require pre-processing of the data
- can learn very non-linear functions
- can be inspected/interpreted

Cons:

- Easy to overfit – tend to be low bias/high variance

Use averaging to reduce the variance!
Bootstrap aggregation (bagging)

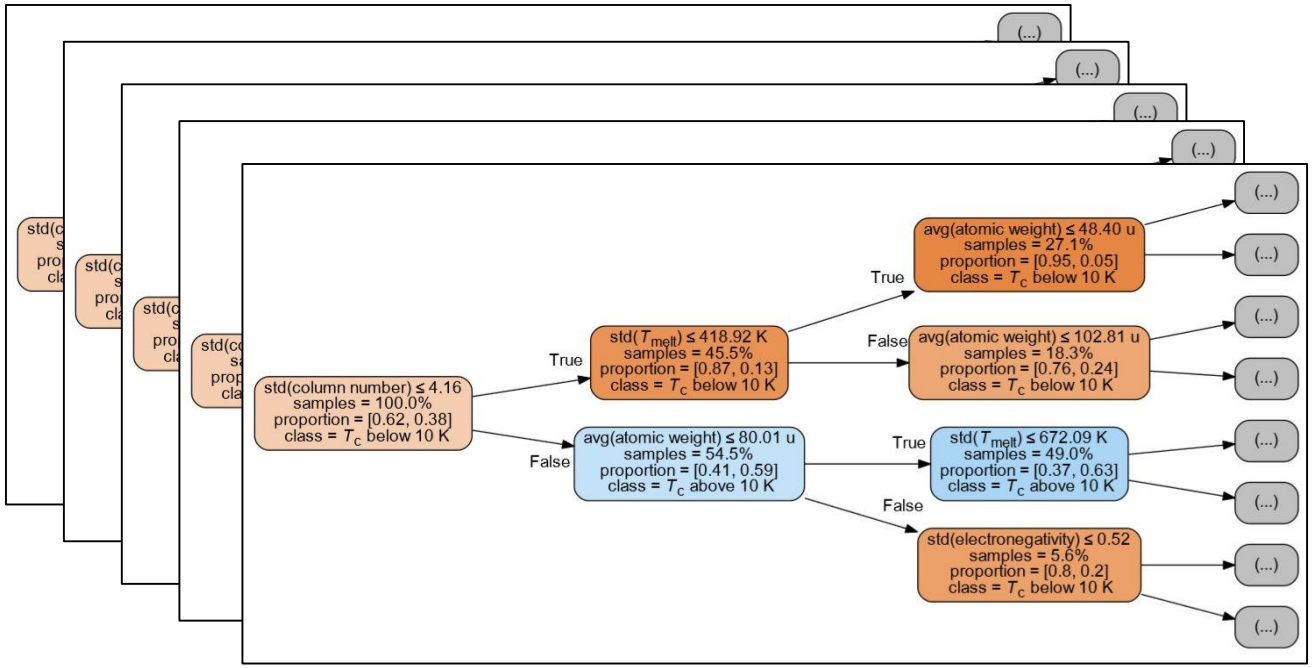


Random forest III

Random forest – combine many individual decision trees.

1. Each tree is grown on a bootstrapped sample of the data
2. At each split only a random subsample of the features is used - reduce correlation between the trees
3. Average the results of all the trees

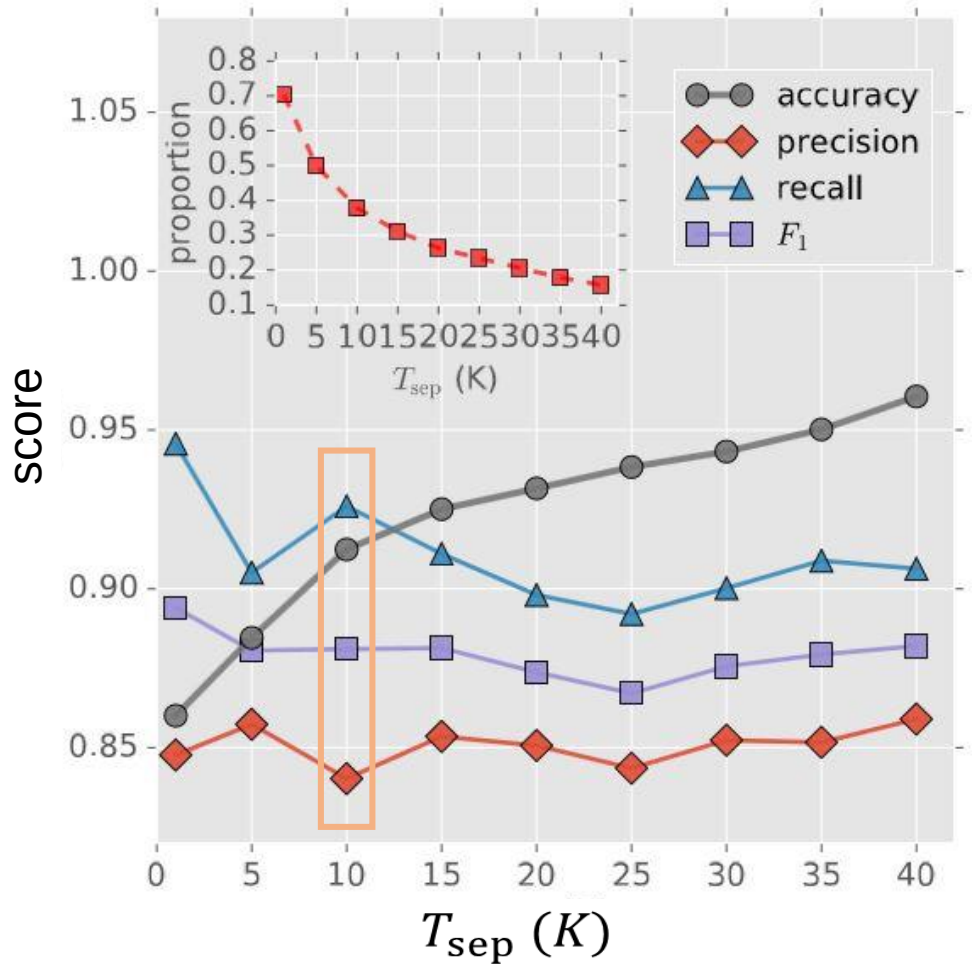
Accurate and easy to use algorithm.
Don’t require too much optimization.
Extra points – feature importance



Classification model for T_c

Separate materials in two classes: above-T_{sep} and below-T_{sep} materials (T_c bigger/smaller than T_{sep}).

Allows us to deal with compounds without T_c. But how to choose T_{sep}?



$$\text{accuracy} \equiv \frac{tp + tn}{tp + tn + fp + fn},$$

$$\text{precision} \equiv \frac{tp}{tp + fp},$$

$$\text{recall} \equiv \frac{tp}{tp + fn},$$

$$F_1 \equiv 2 * \frac{\text{precision} * \text{recall}}{\text{precision} + \text{recall}},$$

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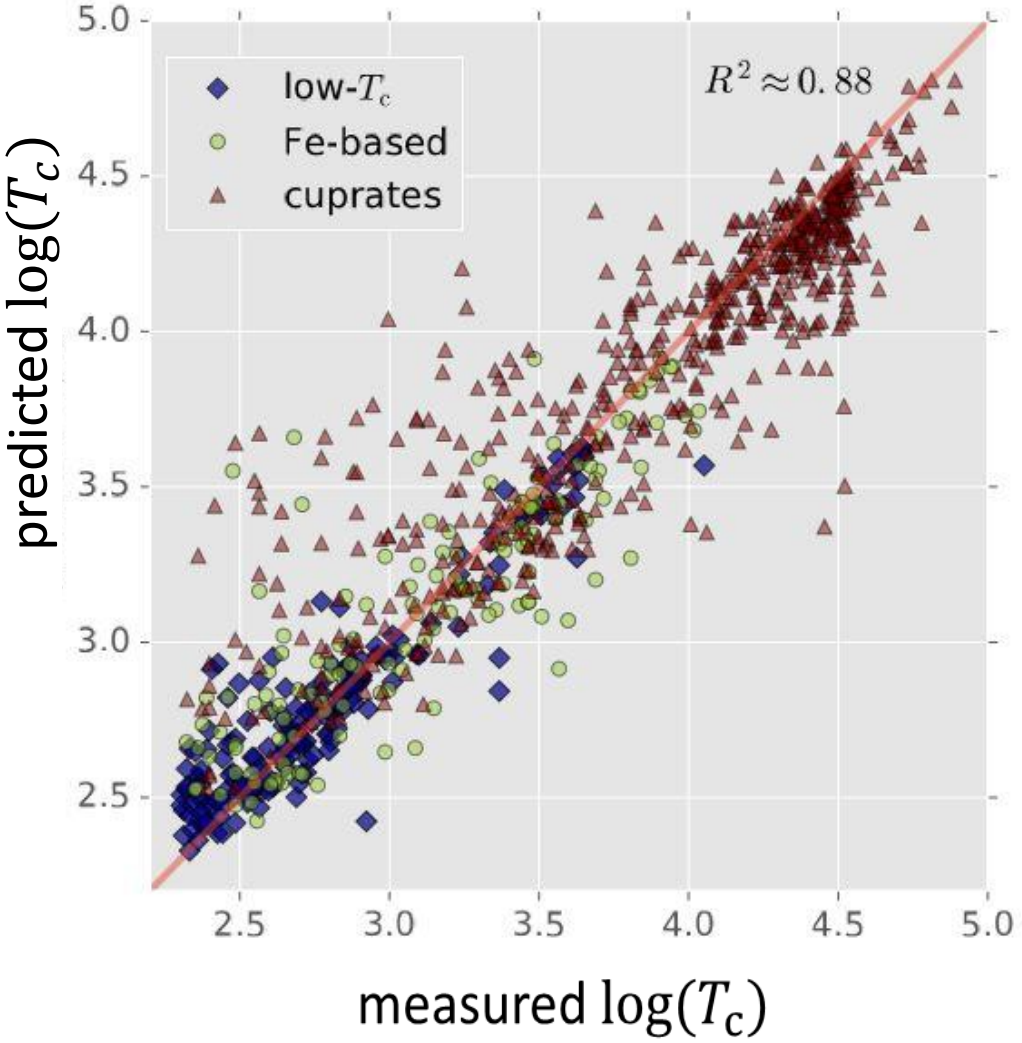
Regression model for T_c

Separat the "T_c > 10 K" materials and fit regression model for T_c



Single model for all families works very well!
But they have different physics…

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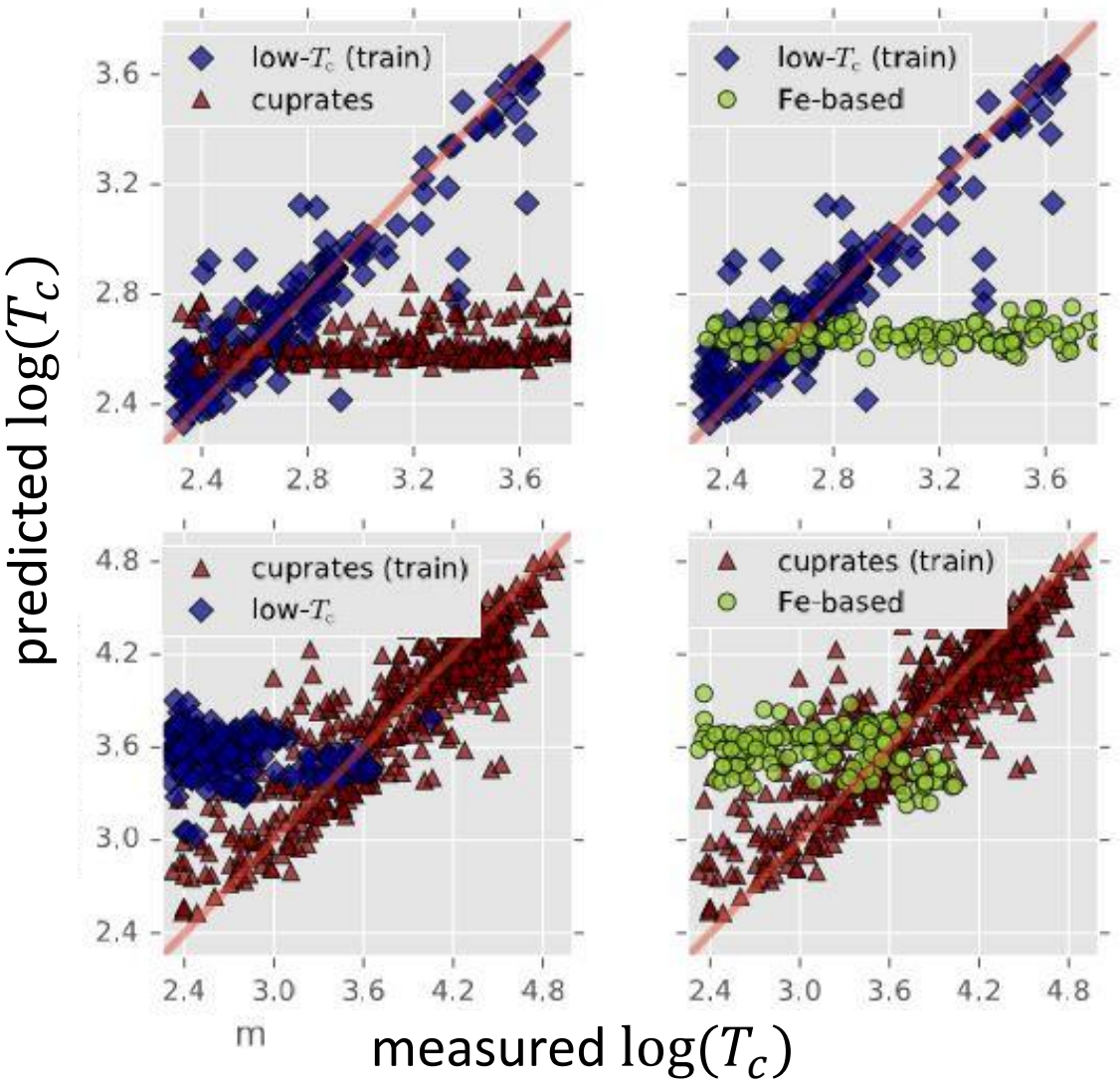
Regression model for T_c II

Separated the "T_c > 10 K" materials and fit regression model for T_c



The model is creating different branches for different groups.

Model trained on a single family - no predictive power for other families.

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Conclusion

- Machine Learning is valuable tool for study of superconductivity
- Use composite descriptors to train classification and regression models

Now let’s try it!