Identifying Superconductors with Machine Learning

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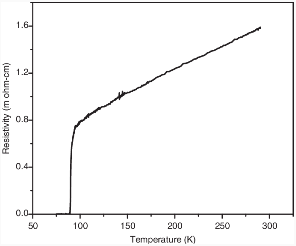
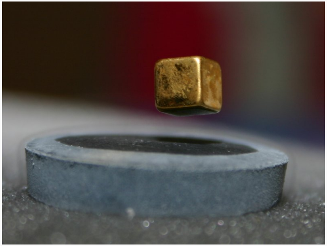
Background

Superconductors

- Superconductors are materials that exhibit two key properties at low temperatures:
  1. The resistivity ρ drops to 0Ω (Current flows without resistance).
  2. Magnetic fields are expelled in the material. (Meissner Effect)

Example: $YBa_2Cu_3O_{7-\delta}$ [VBRS14]





- A superconductor's critical temperature (T_c) is the highest temperature at which it exhibits these two properties.

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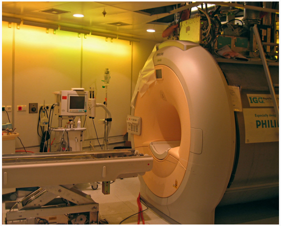
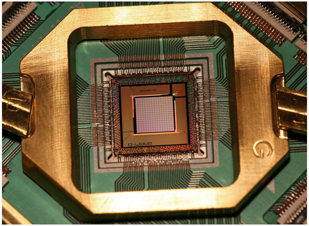
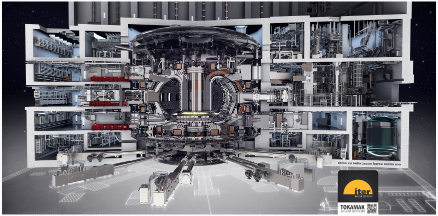
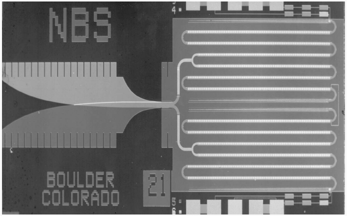
Superconductors

Industrial Applications of Superconductors









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Superconductors

- Superconductivity occurs due to anomalous quantum mechanical pairing of electrons [Coo60].
- Pairing allows for condensation of conducting electrons into a single energy state at the Fermi level, E_F.

$$\underbrace{|\uparrow\rangle + |\downarrow\rangle}_{\text{Spin-1/2 electrons}} \longrightarrow \underbrace{|\uparrow\downarrow\rangle}_{\text{Spin-0 Cooper pair}} \quad \text{[s and d-wave states]}$$

$$\underbrace{|\uparrow\rangle + |\uparrow\rangle}_{\text{Spin-1/2 electrons}} \longrightarrow \underbrace{|\uparrow\uparrow\rangle}_{\text{Spin-1 Cooper pair}} \quad \text{[p and f-wave states]}$$

- Pairing in conventional (i.e. BCS) superconductors is mediated by phonons [BCS57] (s-wave).
- Pairing in unconventional superconductors remains a deep mystery [ZLI+21] (s,p,d,f-waves).

Prediction of T_c

- Prediction of T_c via *ab initio* methods is only possible for BCS superconductors.

McMillan Equation [McM68]

$$T_c = \frac{\vartheta}{1.45} \exp\left(-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right)$$

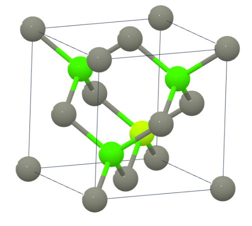
(ϑ: characteristic phonon frequency, μ^*: Coulomb pseudopotential, λ: electron-phonon coupling)

- In doped and alloyed superconductors, defects break the fundamental symmetries of the material lattice.
- In these materials, λ is prohibitively expensive to compute.

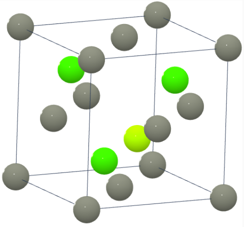
Alternative Methods for Predicting T_c

- There has been great interest in exploring machine learning of T_c. (e.g. see: [SOK+18][KKN+21][XQH+22])
- Very few of these approaches directly incorporate atomic structure (e.g. [CG22]).
- Crystalline structures are naturally interpreted as periodic graphs:

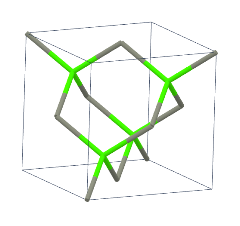
ZnSe (graph)



Atoms (nodes)



Bonds (edges)



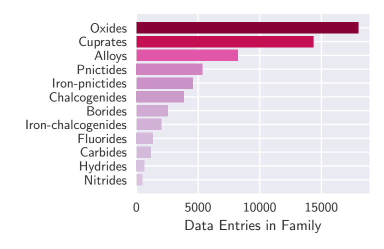
- In this work, we applied graph neural networks to identify superconductors and predict T_c from raw atomic structure.

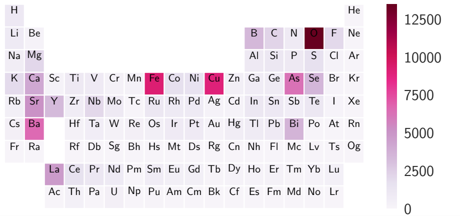
Methods

Data Sources

- We combined two large experimental measurement datasets (*Supercon v1* and *v2*).

Dataset Distribution

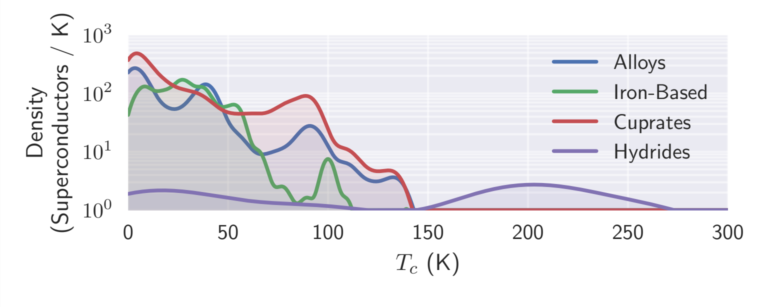




- These datasets had T_c measurements and superconductor chemical formulas, but no atomic structure.

Data Sources

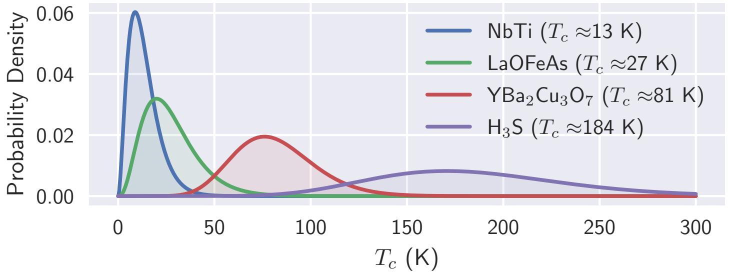
Distribution of T_c measurements



Data Sources

- For each superconducting material, multiple measurements were reported due to differences in experimental conditions (applied pressure, substrate, monocrystalline vs. polycrystalline, etc.)

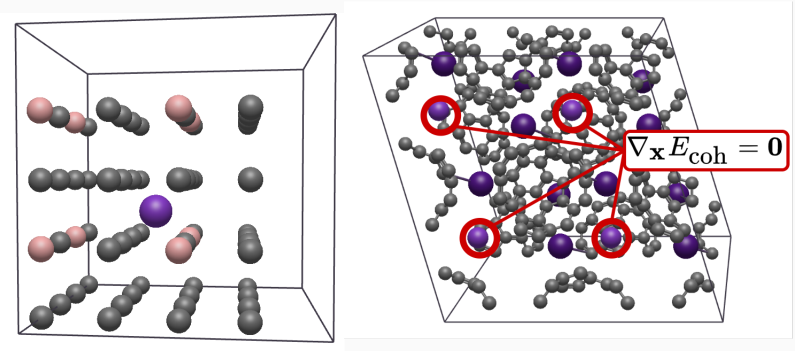
Empirical Fits of T_c distributions



Data Sources

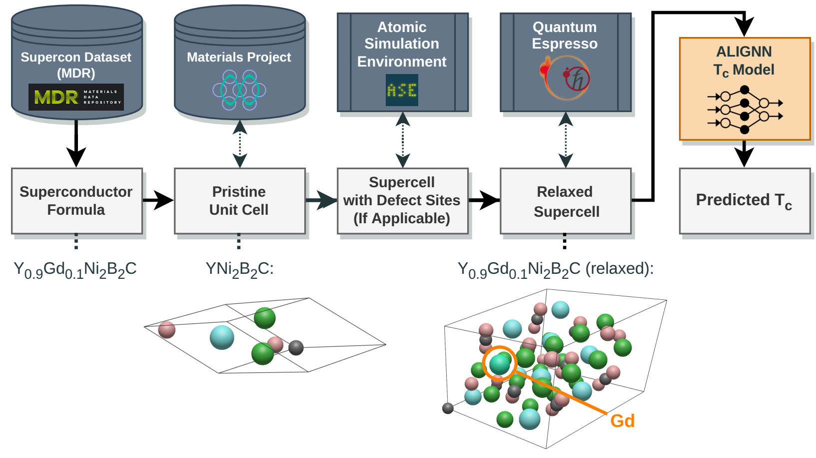
- A significant challenge was handling the placement of defects (vacancies, substitutions, interstitials, etc.)

Examples of defect placement: SC lattice (left), KCs_3C_{60} (right).



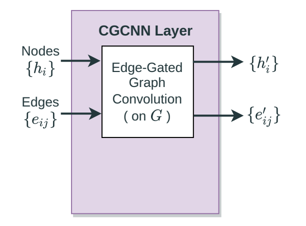
Generating Atomic Structures

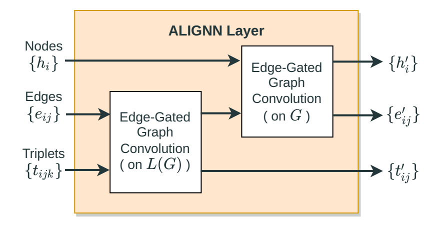
Data Generation Pipeline

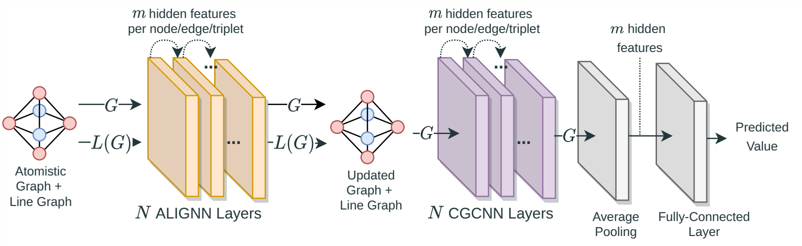


CGCNN and ALIGNN Model

CGCNN and ALIGNN Model Architecture [XG18][CD21]





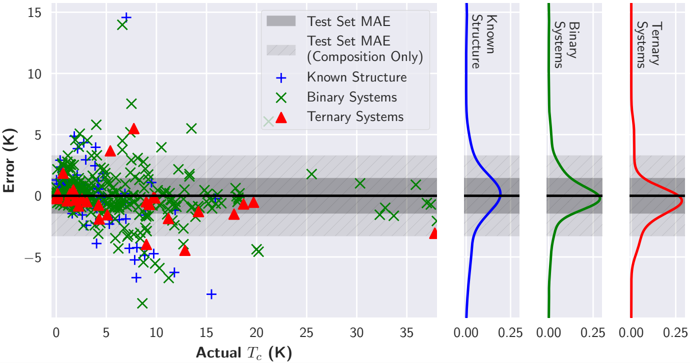


Results

Model Evaluation

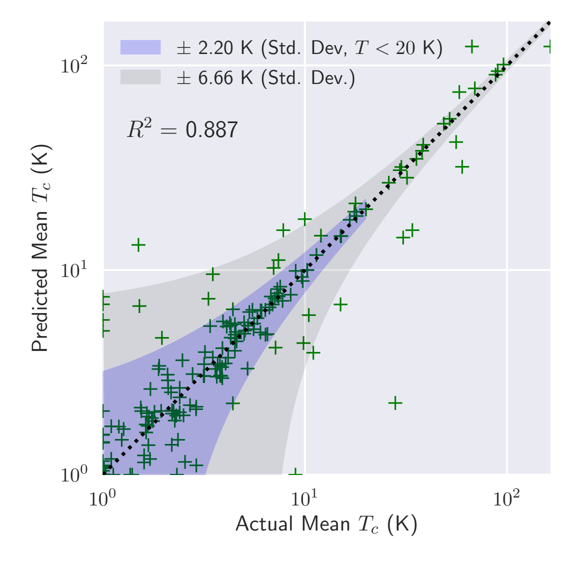
Predicting T_c (Conventional Doped and Alloyed Superconductors)

Test Set Performance:		
Model	Mean Abs. Err. (K)	MAD/MAE
ALIGNN	**1.43 K**	**3.28**
CGCNN	1.52 K	3.10
Avg. Pooling (Composition Only)	3.28 K	1.43



Model Evaluation

Predicting T_c (All Superconductors)

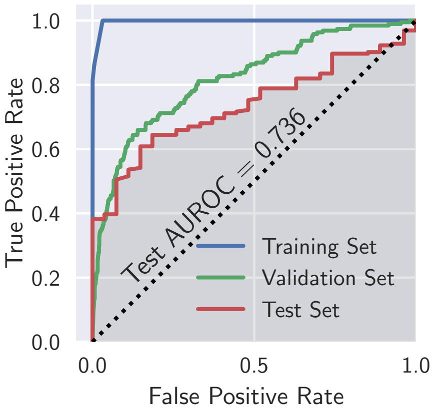


Model Evaluation

Classifying Superconductors (Confusion Matrix and ROC Curve)

		Predicted Superconductor	
		Yes	**No**
Contained in Dataset	**Yes**	**Total: 102** $TaSe_3$, AlCu, W_2C, Nb_3, RhGe, Ce, $TlNiSe_2$, $SrIr_2$	**Total: 92** $LaPd_2Al_3$, Ru_2Zr, In_3Sn, La_3Sn, $PdZr_2$
	No	**Total: 95** $YbLuB_{24}$, Ti_3Ir*, $CePb_3$*, $SrAu_5$, $SrGe_3$*	**Total: 917** Sc_3Nb, Yb_5Sn_3, $Ba(SmSe_2)_2$, $YAsO_4$, Th_2Zn

*** Materials that are actual superconductors, but were not contained in the dataset.**



Conclusion

Conclusion & Future Work

Summary

- We trained a structure-based graph neural network model (ALIGNN) to predict the T_c with a standard deviation error of 6.66 K ($2.20K$ for low-T_c).
- The model can serve as an alternative to *ab-initio* methods for predicting T_c in BCS superconductors.
- We also trained a classification model to identify new superconductors. After screening materials in the Materials Project database, we found roughly 600 candidate superconductors.

Future Work

- Incorporating more data, verifying the correctness of structures.
- Exploring other models that may generalize better outside of the training data.

Questions

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Database of Candidate Superconductors

https://cburdine.github.io/files/superconductors.html

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