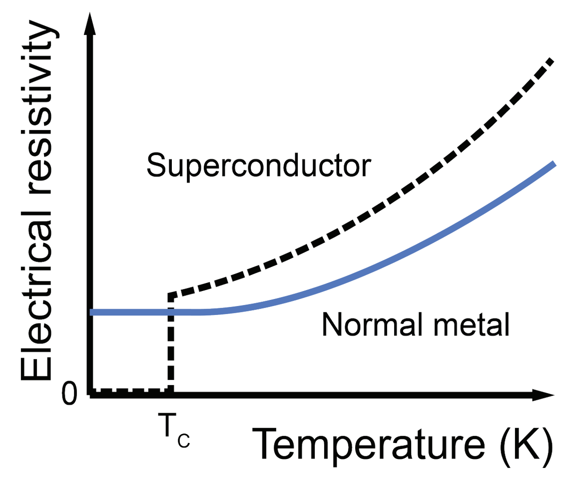
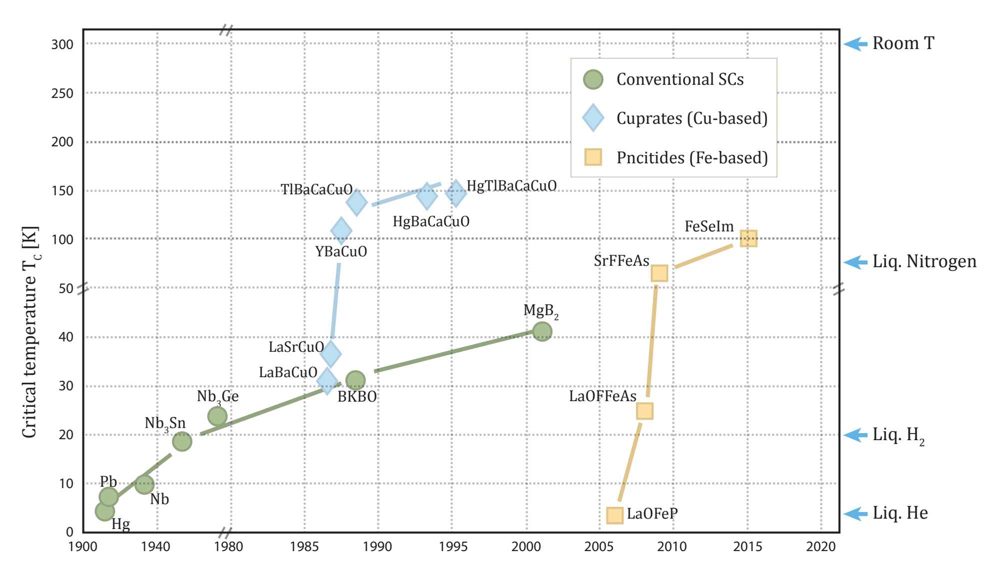
ScGAN: A Generative Adversarial Network to Predict Hypothetical Superconductors

The Search for Superconductors

- Superconductors are materials that **perfectly** conduct electricity once they are cooled below a **critical temperature** T_c
- Used in several important applications: Quantum Computers, Maglev trains, particle accelerators, etc.
- Because low temperatures are hard to maintain, High Temperature Superconductors (HTSs) are desired



Resistivity and Temperature relation. Adapted from Bussman-Holder and Keller, 2019.



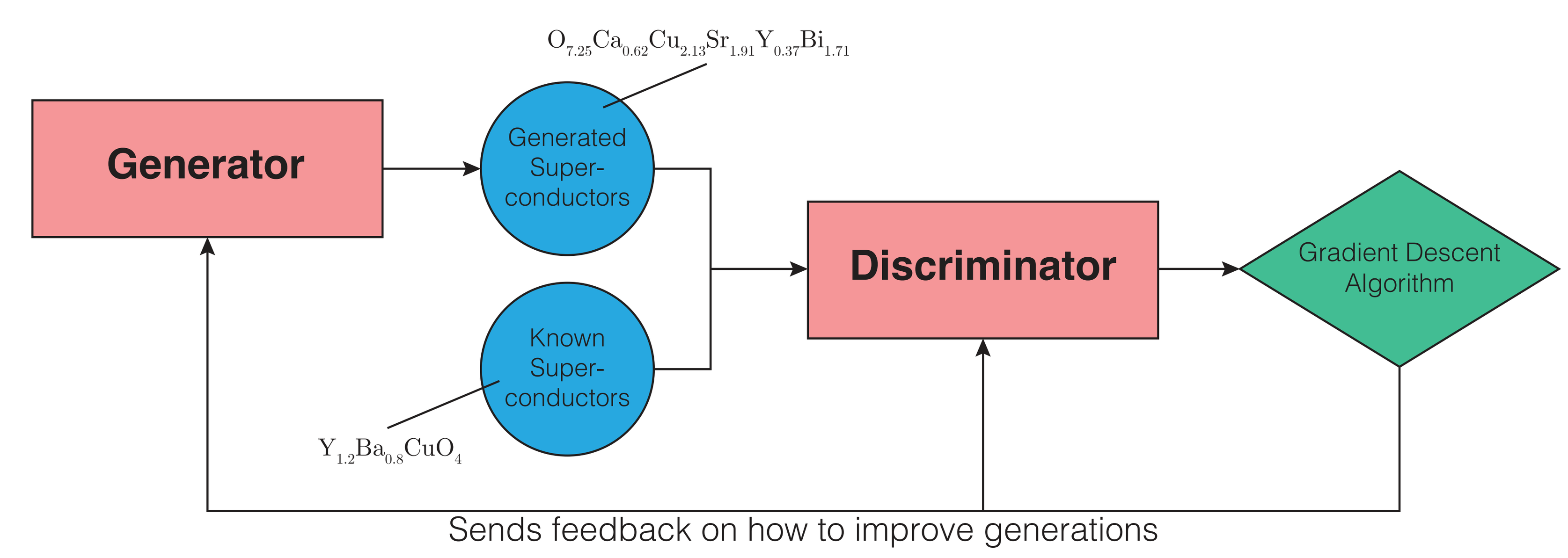
The history of major superconductors' critical temperatures at ambient pressure. Adapted from Ray, 2020.

However...

- Manual searches for HTSs are very **inefficient** (success rates of ≈3%) – essentially just guess and check
- Current computational methods **only classify** –> can only check databases of known compounds for superconductors, which restricts possibilities

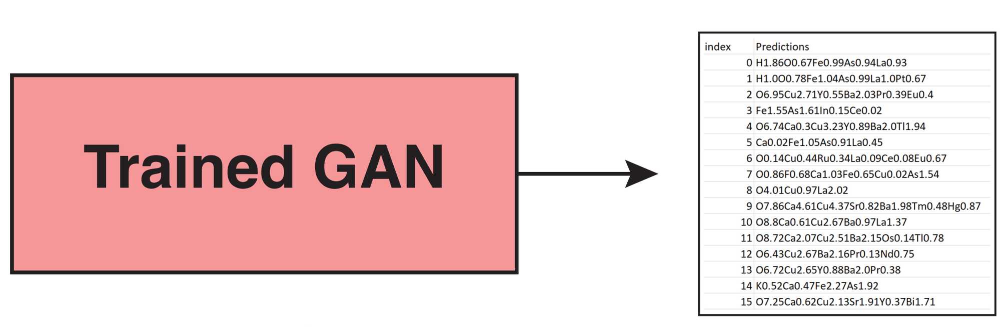
Idea: create a computational model that *directly* outputs a list of new superconductors.

Method: Generative Adversarial Network

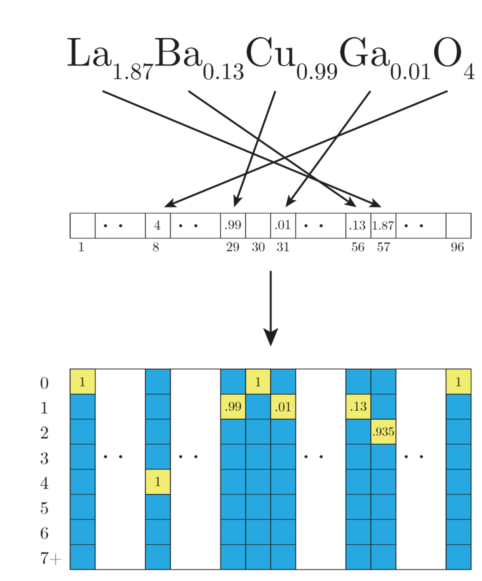


GAN training feedback loop

- Generative Adversarial Network (GAN): machine learning architecture that generates things that resemble the training data. The main idea is to leverage this for superconductors.
- GAN trained on OQMD (general compounds) and transfer learned onto SuperCon (superconductors)
- Also transfer learned onto subsets of SuperCon: cuprates (Cu-based), pnictides (Fe-based), and anything else that remained to see if it could learn features of these different classes



A trained GAN generating a list of candidates.

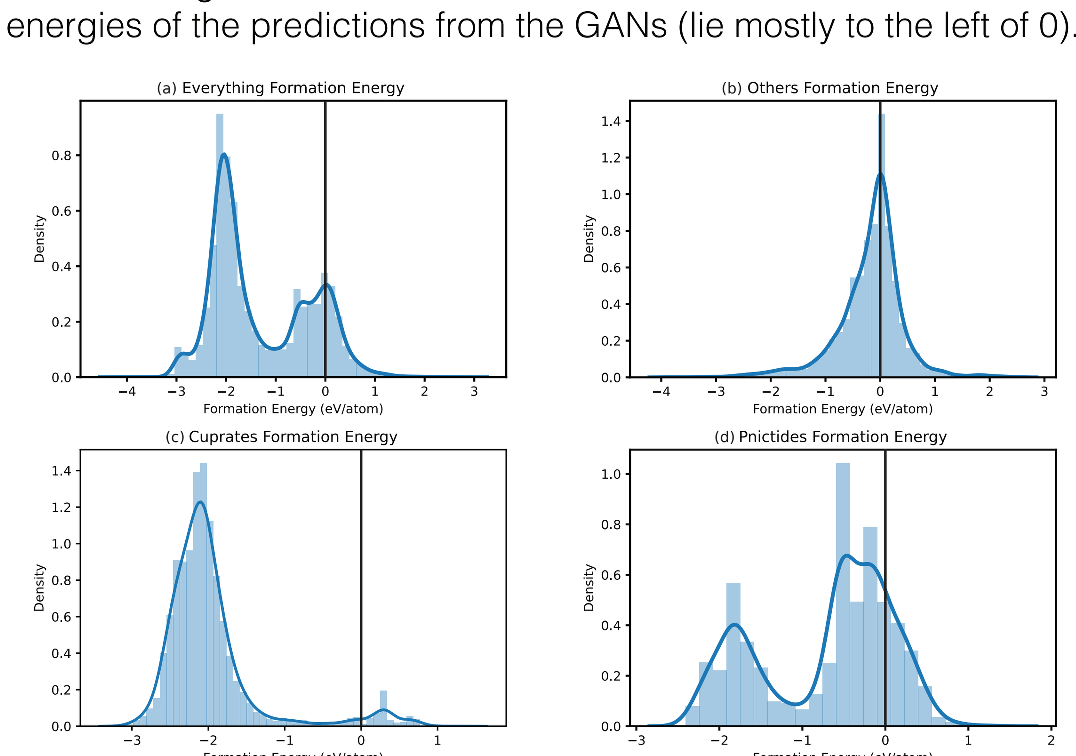


Data encoding for a superconductor. The matrix is what's fed into the GAN.

Data Analysis & Results

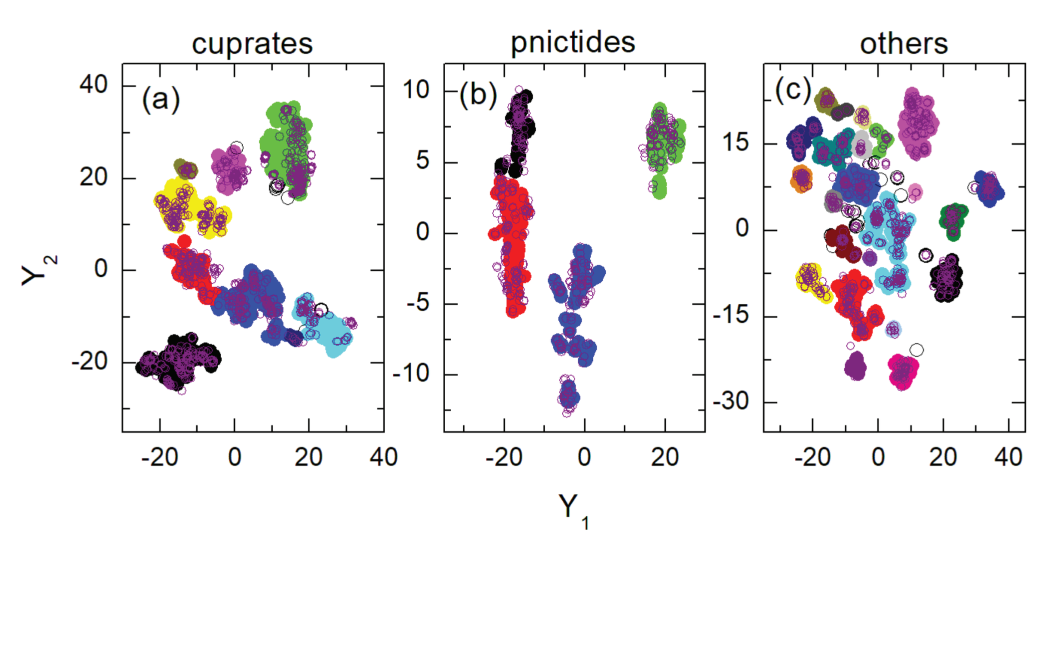
GAN Version	Novel %	Superconducting %
Entirety of SuperCon	99.69%	70.42%
Cuprate	99.74%	71.95%
Pnictides	99.32%	67.89%
Others	98.89%	64.39%

Above: Novelty percentages and superconducting percentages for the candidate lists generated from the GANs. Below: distributions of formation energies of the predictions from the GANs (lie mostly to the left of 0).



- GAN was able to generate predictions **matching** its training data as seen to the right
- Clustering results to the right; GAN was able to generate superconductors from **all** the different major families
  - However, it was unable to generate any novel families

Training Data	Cuprate %	Pnictide %	Other %
Cuprate	92.76%	0.06%	7.18%
Pnictides	0.02%	99.84%	0.14%
Others	0.14%	0.6%	99.26%



Conclusion

Successes

1. Created the **first-ever GAN** to predict superconductors –> **best method** of obtaining candidates for superconductivity in existence
2. **Exceeded** the benchmarks of the manual search:

	Manual Search		My GAN
Success Rate	3%	×23.5 →	70.42%
Max T_c	58 K	+75 K →	133 K

3. The GAN was also able to **learn the features** of the important classes of superconductors: cuprates, pnictides, and others

Compound	Predicted T_c	Class
$PrCaBiSr_2Cu_2O_{7.46}$	104.6 K	Cuprates
$YTiSr_2Cu_{2.74}O_{6.76}$	91.7 K	Cuprates
$TeYSr_2Cu_2O_{7.75}$	89.8 K	Cuprates
$C_{2.52}Ni_{0.92}Y_{0.71}Th_{1.0}$	85.3 K	Others
$Si_{0.62}V_{0.91}Zr_{0.83}$	84.7 K	Others
$Al_{2.34}Te_{0.64}Ir_{1.07}$	84.7 K	Others
$TlCaASr_2Cu_2O_{7.82}$	73.9 K	Cuprates
$YCaBa_2ZnCu_{2.36}O_{7.54}$	71.5 K	Cuprates
$HgCsSrCa_2Cu_{2.56}O_{8.66}$	69.8 K	Cuprates
$Be_{0.16}Si_{1.09}V_{2.67}Y_{1.72}$	62.4 K	Others
$Cu_{1.13}Nb_{3.0}Sb_{0.72}Ir_{1.05}$	59.4 K	Others
$GdCaRuSr_{1.83}Cu_2O_{8.71}$	40.8 K	Cuprates
$Ga_{0.62}Nb_{2.88}Sn_{0.65}Te_{0.79}$	40.8 K	Others
$B_{1.73}C_{1.03}Ni_{1.12}Y_{0.66}Pt_{0.64}$	40.8 K	Others
RuTeSeFe	35.6 K	Pnictides
$TeSSeFe_{1.05}$	31.0 K	Pnictides
$CeCoAs_{2.15}Fe_{1.39}$	23.3 K	Pnictides
$CeThPAsFe_{1.59}$	12.2 K	Pnictides
$GaPrCa_{2.58}As_{12.44}Fe_{6.34}$	11.9 K	Pnictides
NdOAsFe	4.5 K	Pnictides

Selected list of potential superconductor candidates

Applications

- Discover new High Temperature Superconductors
  - –> for use in applications
  - –> to find more examples to help build a theory for HTSs
  - –> to find the "Holy Grail" Room Temperature Superconductor
- Augment Data for future computational work with superconductors

Future Work

- Physically **test** the **candidates** for superconductivity since the tests in this project were computational
- Account for **charge** and **crystal structure** in compound encoding (though it may be difficult due to the lack of such data)
- Employ **active transfer learning** to search specifically for High T_c
- Try different architectures like Conditional GANs