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.

However...

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

Method: Generative Adversarial Network

- 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 QMOD (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.

Data Analysis & Results

<table>
<thead>
<tr>
<th>GAN Version</th>
<th>Novel %</th>
<th>Superconducting %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Entirety of SuperCon</td>
<td>99.66%</td>
<td>70.42%</td>
</tr>
<tr>
<td>Cuprates</td>
<td>99.74%</td>
<td>71.98%</td>
</tr>
<tr>
<td>Pnictides</td>
<td>99.32%</td>
<td>67.29%</td>
</tr>
<tr>
<td>Others</td>
<td>98.89%</td>
<td>64.39%</td>
</tr>
</tbody>
</table>

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.

Conclusion

Successes

1. Created the first-ever GAN to predict superconductors $\rightarrow$ best method of obtaining candidates for superconductivity in existence.
2. Exceeded the benchmarks of the manual search.

<table>
<thead>
<tr>
<th>Manual Search</th>
<th>My GAN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Success Rate</td>
<td>3% $\rightarrow$ 70.42%</td>
</tr>
<tr>
<td>Max $T_c$</td>
<td>58 K $\rightarrow$ 133 K</td>
</tr>
</tbody>
</table>

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

Applications

- Discover new High Temperature Superconductors $\rightarrow$ for use in applications
- For 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.

Unless otherwise noted, all images were created by the STS finalist.