ScGAN: A Generative Adversarial Network To Predict Hypothetical Superconductors

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Superconductors are materials that exhibit zero resistance and expel magnetic fields once cooled below a certain critical temperature, allowing for their application in various technologies such as quantum computers and efficient transmission lines. Of particular interest are High Temperature Superconductors (HTSs), superconductors with a high critical temperature, which lack both an explanation for their mechanisms and a systematic way to search for them, despite having been first discovered over three decades ago. This project proposes ScGAN, a Generative Adversarial Network (GAN) to efficiently predict new superconductors. ScGAN was trained on compounds in the Open Quantum Materials Database and then transfer learned onto four different datasets of superconductors: all of the SuperCon database and three subsets of it chosen by superconducting class. Once trained, 30,000 samples were generated using the version trained on all of SuperCon, and approximately 70.42% of them were determined to be superconducting—a 23-fold increase in discovery rate compared to manual search methods. Furthermore, 99.69% of the samples were novel, demonstrating that ScGAN was able to find new superconductors, including several promising HTS candidates. The other versions of ScGAN also displayed high superconductivity and novelty percentages and predicted superconductors that were similar to their training data, indicating that ScGAN learned the different features of the different classes of superconductors. This project shows a novel, efficient way to search for superconductors, which may be used to find suitable superconductors that can be utilized in technological applications or provide insight into the unsolved problem of high temperature superconductivity.

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