Clustering Superconductors Using Unsupervised Machine Learning

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Abstract

In this work we used unsupervised machine learning methods in order to find possible clustering structures in superconducting materials data sets. We used the SuperCon database, as well as our own data sets compiled from literature, in order to explore how machine learning algorithms group superconductors. Both conventional clustering methods like k-means, hierarchical or Gaussian mixtures, as well as clustering methods based on artificial neural networks like self-organizing maps, were used. For dimensionality reduction and visualization t-SNE was found to be the best choice. Our results indicate that machine learning techniques can achieve, and in some cases exceed, human level performance. Calculations suggest that the clustering of superconducting materials works best when machine learning techniques are used in concert with human knowledge of superconductors. We also show that in order to resolve fine subcluster structure in the data, clustering of superconducting materials should be done in stages.

Keywords: clustering, high temperature superconductors, unsupervised machine learning

1. Introduction

In recent years a number of artificial intelligence (AI) studies of superconductors have been performed [1, 2, 3, 4, 5, 6, 7], using either machine learning (ML) or deep learning techniques. In some of these studies, the superconducting critical temperature of known superconductors was predicted, i.e. calculated. Most of these studies achieved impressive values of statistical parameters, such as $R^2$ or RMSE. However, none of them have (yet) led to the discovery of new superconducting materials, which should be the ultimate goal of AI studies.

It was recently pointed out [8] that AI models achieved high values of statistical parameters because they used traditional k-fold cross-validation procedures, in particular leave-one-out cross validation which is its special case. These cross validation techniques have been shown to result in unrealistically high values of statistical parameters when applied to highly clustered data sets [8]. Moreover, they have been known to have problems when extrapolating to new classes of materials [1]. As an alternative, an approach called leave-one-cluster-out cross validation was proposed [8], which was supposed to alleviate the problem. The idea is that instead of searching for new superconducting materials, AI is used to search for new classes of superconducting materials. However, the problem is that there is currently no universally accepted classification of superconductors. There have been numerous attempts to classify superconductors based on their crystal structure, physical properties, pairing mechanics, etc. [9, 10] but none of them are universally accepted.

Over the past century, superconductivity has been found in a variety of different systems, such as metals, oxides, alloys, organic materials, heavy fermions,
etc. These systems can have vastly different physical, chemical and all other properties, which makes it difficult for humans to classify. In a recent study Hirsch, Maple and Marcillio [10] made the most comprehensive attempt yet to separate superconductors into different classes, based on the physical mechanism of superconductivity. They identified 32 classes, separated into three big groups: conventional (with 12 classes), potentially unconventional (with 9 classes) and unconventional (with 11 classes). However, some superconductors in this study can be found in several different classes.

In this work we used a ML technique called clustering in order to separate superconductors into classes (or clusters). Our hope is that ML might be able to separate superconductors into physically meaningful groups, which would in turn lead to the discovery of entirely new groups of superconductors. Additionally, ML techniques have been known to both provide additional insights and reveal hidden patterns in other groups of materials not previously known to humans [11].

Our results reveal that data-driven ML techniques can indeed separate superconductors into groups, achieving and in some cases exceeding human level performance. However, there are also limitations, which will need to be addressed in the future. In particular, constructing a more reliable database, which will undoubtedly result in better ML calculations. Clustering results obtained on the test data sets we compiled from literature, confirm this claim. Our calculations indicate that, at least for superconducting materials data, clustering in stages is the best approach.

2. Clustering

Clustering is one of the most common tasks of unsupervised machine learning [12, 13]. The main goal of unsupervised learning algorithms is to find patterns and learn meaningful relationships in data in order to describe its underlying structure. However, in unsupervised machine learning one does not know the correct output; thus the results of calculations cannot be assessed in terms of accuracy or correctness. Instead, clustering is an exploratory technique. One must not assume there is a single "true" clustering. One should rather be interested in exploring different clusterings of the same data set to learn more about it. Using commercially available clustering programs as a "black box" should not be done, as it may lead to erroneous results and conclusions.

Before we attempt to cluster superconductors, there are several issues that need to be addressed, such as the choice of a clustering technique, the number of clusters, the choice of the distance function, dimensionality reduction and visualizations. All these issues are discussed below in separate subsections before clustering results are presented.

2.1. Conventional Clustering Methods

We used several conventional clustering methods [12, 13]: k-means, k-medoids, hierarchical, Gaussian mixtures, DBSCAN, etc. For most of them the number of clusters is an input parameter, which is selected based on the data set. DBSCAN is one of the few that does not require the number of clusters to be specified. Another important factor that affects clustering is the distance function used to calculate similarly/dissimilarity between data points. We have tried several standard distance functions such as Euclidean, cityblock, cosine, Chebychev, etc. In our calculations with superconductors, the cosine distance function has usually produced the best results.

A procedure for selecting the best clustering method was recently proposed in Ref. [14]. It is referred to as Iterative Label Spreading, and it allows one to visually assess the quality of clusters, before any clustering is done. It was shown to be particularly suitable for noisy, high dimensional data typically encountered in materials science.

2.2. Neural Network–Based Clustering Methods

In recent years artificial neural networks, especially deep neural networks, have become widely used in a number of disciplines such as image and speech processing, chemistry, biology, material science, etc [15]. Although neural networks are used primarily for supervised learning tasks [15] such as regression and classification, they can also be used for unsupervised learning, i.e. clustering.

In this work we used a neural network based clustering method known as the Self-Organizing Map (SOM) algorithm. SOMs perform nonlinear transformations of a multidimensional data set into a low-dimensional set that retains the intrinsic topological properties of the original data set. The network is trained to transform a so-called "input space", whose dimension equals the number of predictors, into a low-dimensional output called "map space". The most important parameter of these calculations is the number of nodes, which is equivalent to the number of clusters. In addition, one also needs to carefully choose the topology of the input
layer. Two most commonly used topologies are rectangular and hexagonal. In our calculations with superconducting materials, SOMs have consistently performed better compared to conventional clustering algorithms.

2.3. The Choice of Predictors

One of the most important issues in machine learning calculations is the choice of predictors. Similar to what we did in our previous work [6], we used chemical composition as the only predictor for clustering calculations. We previously showed that the use of a large number of predictors does not necessarily lead to any improvements in ML models. We suggested that the predictors must be carefully selected based on the machine learning task. In calculations with superconductors, one should use those predictors that are known (or at least believed) to be closely related to superconductivity, such as crystal symmetry, electronic band structure, number of valence electrons, etc. The problem is that these predictors are not systematically reported in the existing databases. They should be included in future databases, as they might result in more reliable machine learning calculations.

2.4. The Number of Clusters

As mentioned above, clustering is an exploratory technique, and the "correct" number of clusters does not exist. Most clustering techniques treat the number of clusters as a parameter of calculations, which can be adjusted based on the data set. There are several algorithms one can use in order to estimate the optimal number of clusters. The most commonly used are: Calinski-Harabasz criterion, Davies-Bouldin index, silhouette and dendrogram plots [12]. A dendrogram plot in particular allows one to explore not only cluster, but also sub-cluster structure in the data. Iterative Label Spreading can also be used to estimate the number of clusters [14]. However, in our experience, the best way to estimate the optimal number of clusters is by combining machine learning calculations with human knowledge of superconducting materials. This approach can produce the most physically meaningful clustering.

Another important issue that one must be aware of is outliers in the data set used. In most AI studies of superconductors the SuperCon database [16] was used, which contains a number of wrong entries, either in terms of chemical composition or in terms of superconducting critical temperature \( T_c \). We previously estimated that they might account for up to 20% of the entire database, in particular for the cuprate entries [6]. These wrong entries can have strong effect on AI calculations, as they can create false clusters. Future calculations would benefit from an improved database, as we show here by using our own data sets compiled from literature.

2.5. Dimensionality Reduction and Data Visualization

Similar to what we did in our previous publication [6], we used element-vectors to mathematically represent superconductors based on their chemical composition. In this approach, each superconductor is represented with a 1×96 vector. As is sometimes done in machine learning, this dimension can be reduced to allow more efficient calculations. A variety of different techniques have been developed over the years: PCA (or SVD), random projections, MDS, etc. [17]. However, our calculation with superconductors indicate that the best results are achieved when using a nonlinear dimensionality reduction technique called t-distributed Stochastic Neighbor Embedding (t-SNE) [18].

t-SNE has been used extensively for machine learning calculations in materials science, and our calculations also indicate that it is the best choice for superconductors. It is a non-linear transformation that reduces the number of dimensions down to two or three, none of which have any physical meaning. This not only allows more efficient calculations, but also visualization of high dimensional data in a low dimensional space. Another useful feature of t-SNE is that it allows easy manual backward validation, which we used extensively to investigate interesting data points, as well as outliers.

One must be careful when using t-SNE, however. Due to its stochastic nature, its results can be difficult to interpret [19]. The most important parameter for t-SNE calculations is the so-called perplexity. Perplexity value must be carefully chosen to avoid misinterpretations [19]. In our calculations we performed a number of runs with different values of perplexity in order to eliminate spurious features. Depending on the size of analyzed data set, the values of perplexity we used were between 5 and 500. Fig.1 shows schematically the workflow chart for the whole project.

3. Clustering Test Data Sets

In order to test the feasibility of clustering methods, we first compiled several test sets of superconductors from literature [9,10], each consisting of 25–40 materials. Such a small number of entries allows us to look into each superconductor individually and verify its cluster assignment. In the first set, we included a variety of different superconductors from literature, including elements, cuprates, pnictides, heavy fermions,
transition metal dichalcogenides, Chevrel compounds, etc. In Fig. 2 we display the results of clustering analysis and plot them using t-SNE. The two axes ($Y_1$ and $Y_2$) are the reduced dimensions of the original data set; they do not have any physical meaning. One can readily identify three major clusters, which correspond to cuprates (red circles), pnictides (green circles) and what we previously [6] called “others” (blue circles). The three clusters are well separated from each other, and no data points can be found between them. It is also possible to identify some sub-cluster structures in Fig. 2. However in our experience, it is better to do clustering in steps: once we identify the three main clusters, we cluster each of them separately.

It is interesting to notice that in Fig. 2 oxide superconductors $\text{Sr}_2\text{RuO}_4$, $\text{Ba}_0.6\text{K}_0.4\text{BiO}_3$, $\text{LiTi}_2\text{O}_4$ and the recently discovered [20] nickelate $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$ are clustered with the cuprates. This should not be surprising, as they are chemically much more similar to cuprates (copper-oxides) than to any other group of superconductors shown in Fig. 2.

The second test set includes only cuprates [9, 10, 21] and has 39 materials. Fig. 3 shows the results of clustering, where one can identify eight major cuprate families: BSCCO (red), LSCO (black), YBCO (purple), NCCO (orange), Hg-based (dark yellow), TI-based (blue), Pb-based (green) and infinite layer (magenta). We notice that the hole-doped LSCO family is separated from the electron-doped NCCO family, even though they are chemically and crystallographically very similar and are often assumed to belong to the same family [9]. Similarly, TI-based and Hg-based cuprates are considered to be in the same family, but the algorithm was able to separate. Not surprisingly, they are located close to each other in Fig. 3.

The last test set contains 25 pnictide superconductors [22, 23]. The results of clustering are shown in Fig. 4. One can identify five major pnictide families: 11/111 (green), 122 (magenta), 1111 (red), 245 (blue), and 42622 (black). All five families are well separated, with no data points in between clusters. We notice that there might be some sub-cluster structure within the 11/111 family, which might be resolvable with a larger data set.

4. Clustering SuperCon Database

The results presented in the previous section (Figs. 2, 3 and 4) indicated that clustering methods were capable of distinguishing between different types of superconductors. We then proceeded to cluster the SuperCon database [16]. After removing incorrect, incomplete and multiple entries, we were left with about 16,000 superconducting materials. In order to improve the learning process, we removed entries with eight or more elements. We also note that the number of pnictide entries in the database is much smaller compared with cuprates and others. Our calculations indicate that clustering works better when the number of constituents in each cluster is similar. Therefore, for our calculations we randomly selected between 1,400 and 1,500 superconductors of each type, for a total of approximately...
Figure 3: (Color online). t-SNE plot of the cuprate test set consisting of 39 cuprate superconductors. Machine learning clustering identified eight major cuprate families: BSCCO (red), LSCO (black), YBCO (purple), NCCO (orange), Hg-based (dark yellow), Tl-based (blue), Pb-based (green) and infinite layer (magenta).

Figure 4: (Color online). t-SNE plot of the pnictide test set consisting of 25 pnictide superconductors. Machine Learning clustering was able to identify five major families: 11/111 (green), 122 (magenta), 1111 (red), 245 (blue), and 42622 (black).

Figure 5: (Color online). t-SNE plot of 4,500 randomly selected superconductors from the SuperCon database. Three clusters are clearly seen, and they correspond to cuprate (red), pnictide (green) and other (blue) superconductors.

4,500 entries.

In Fig. 3 we show the results of clustering applied to this data set. Similar to Fig. 2, one can identify three major clusters, which correspond to cuprates, pnictides and others. However, unlike clustering achieved for the test set in Fig. 2, the separation of clusters is not as clear, and there are points between the clusters. This is not surprising considering the size and quality of SuperCon database.

After that, we extracted cuprates from the SuperCon database as superconductors containing both copper and oxygen. The results of clustering are shown in Fig. 6. We can identify seven clusters, which correspond to YBCO (red), LSCO (dark yellow), BSCCO (orange), Hg-based (blue), Tl-based (magenta), NCCO (green) and a cluster (black) that contains a variety of different cuprates, which the program was unable to cluster with any other family. Manual backward validation indicates that this cluster contains mostly cuprates with rare-earth elements like lutetium, dysprosium, erbium, holmium, etc. We also notice that, unlike our test set in Fig. 3, we are not able to identify the Pb-based and infinite layer families in Fig. 6 which we speculate is because of only a small number of their entries existing in the database.

Next, we extracted pnictides from the SuperCon database as entries that have iron and at least one of the following: arsenic, phosphorous, selenium or tel-
lurium. This resulted in a set with only about 1,400 entries. In Fig. 7 we show the result of clustering. The t-SNE plot indicates that there are four well separated clusters: 11111 (red), 122 (black), 1111 (green) and 245 (blue). We notice that the 11111 and 245 clusters are much more compact compared to 122 and 1111 clusters. This might be due to the fact that there are significantly fewer entries of 11111 and 245 superconductors in the SuperCon database. It is also clear that there is some sub-cluster structure in the 122 and 1111 clusters, which might be resolvable with a larger data set. ML clustering was not able to resolve the 42622 family, as there were very few entries of them in the database.

After removing cuprates and pnictides, we were left with approximately 7,000 superconductors, which we refer to as others. This is a very diverse set of materials, and clustering it is not an easy task. As mentioned above, for most clustering algorithms the number of desired clusters is an input parameter. However, for other superconductors we do not a priori know the number of clusters. As a result, we used DBSCAN algorithm which does not require the number of clusters to be prespecified [24].

The results of calculations on other superconductors are shown in Fig. 8. The algorithm separated this data set into 24 clusters. We were able to identify them and they are listed in Table[1]. For each cluster several representative examples are shown. We notice that in each cluster there is predominant element or a group of elements, which is the common thread for that particular cluster. This is not surprising, as the chemical composition was used as the only predictor in these calculations. DBSCAN also identify a number of outliers among other superconductors, shown with open circles in Fig. 8. These points are usually separated from the main clusters. Some outliers are: BaHg, LiHg3, Ni0.3Th0.7, Th0.988U0.012, Cr0.75Ru0.25, Co0.96Mo0.04U6, Co0.98Rh0.02U6, Gd0.001Th0.999, Ag0.7Zn0.3, Ag0.625Al0.375, etc. In our opinion, these materials, and in particular their derivatives, should be explored further as seeds for potentially new classes of superconducting materials.

5. Summary

We have made the first attempt at clustering superconductors using ML methods. It was shown that ML clustering can achieve, and in some cases (cuprates, for example) exceed human level performance. Clustering was done based on chemical composition only. We speculate that when additional physical parameters are included as predictors, even better results might be obtained. In particular, one should consider empirical predictors that are believed [28] to have strong relations
Table 1: Clusters identified in Fig. 8 using DBSCAN. Several examples of superconductors from each cluster are shown in the last column.

| Cluster number | Common thread | Examples |
|----------------|---------------|----------|
| 1              | Zr- and Ti-based | \(\text{Zr}_2\text{Cu}_0.9\text{Cu}_{0.1}, \text{Zr}_{0.8}\text{Mo}_{0.2}, \text{Ir}_{0.1}\text{Ti}_{0.9}, \text{Ti}_{0.576}\text{V}_{0.384}\text{Ru}_{0.04}\) |
| 2              | V-based       | \(\text{PtV}_3, \text{Ga}_{0.3}\text{V}_{0.7}, \text{V}_{3}\text{Si}_{0.6}\text{Sn}_{0.4}\) |
| 3              | Si-based      | \(\text{SrGa}_{0.5}\text{Si}_{1.5}, \text{CaAl}_{0.8}\text{Ga}_{0.2}\text{Si}, \text{Lu}_3\text{Ir}_3\text{Si}_5\) |
| 4              | S-based       | \(\text{Cu}_1.5\text{Mo}_{0.5}\text{S}_6, \text{NbPbS}_3, \text{Ni}_{0.02}\text{TaS}_2\) |
| 5              | In-based      | \(\text{CeIn}_3, \text{ThIn}_{1.5}\text{Sn}_{1.5}, \text{Bi}_{0.343}\text{In}_{0.657}\) |
| 6              | Pd-based      | \(\text{Li}_2\text{Pd}_1\text{B}, \text{As}_{0.5}\text{Ni}_{0.06}\text{Pd}_{0.44}, \text{ZrPd}_2\text{Al}\) |
| 7              | Te-based      | \(\text{IrTe}_3, \text{Pb}_{0.983}\text{Te}_{0.015}\text{Te}, \text{Ir}_{0.95}\text{Pd}_{0.05}\text{Te}_2\) |
| 8              | La-based      | \(\text{Bi}_3\text{La}_4, \text{La}_3\text{Rh}_2\text{Ge}_2, \text{AlGd}_{0.001}\text{La}_2\) |
| 9              | Se-based      | \(\text{TiSe}_2, \text{Sn}_{0.2}\text{WSe}_2, \text{La}_{2.85}\text{Pt}_{0.15}\text{Se}_4\) |
| 10             | C-based       | \(\text{C}_{1.35}\text{La}, \text{Cs}_2\text{RhC}_6, \text{La}_{0.2}\text{Th}_0.4\text{NiC}_2\) |
| 11             | Pt-based      | \(\text{SrPt}_3\text{P}, \text{Pt}_3\text{Th}, \text{PtP}_3\text{B}_3\text{C}\) |
| 12             | Ni-based      | \(\text{GdSmNi}_2, \text{HoNi}_3\text{B}_2\text{C}, \text{MgC}_{1.25}\text{Ni}_3\) |
| 13             | Nb-based      | \(\text{Nb}_4\text{Sb}, \text{AlGeNb}_3, \text{Nb}_4\text{FeSi}\) |
| 14             | Ge-based      | \(\text{ThP}_2\text{Ge}_3, \text{Pd}_{0.8}\text{Eu}_{0.5}\text{Pt}_2\text{Ge}_{12}, \text{CeNiGe}_3\) |
| 15             | B-based       | \(\text{MgB}_2, \text{DyRh}_3\text{Ir}_3\text{B}_4, \text{CaRh}_3\text{B}_2\) |
| 16             | Be-based      | \(\text{LuBe}_{13}, \text{Be}_{0.9}\text{Ni}_{0.1}, \text{MgReBe}_{12}\) |
| 17             | Oxides        | \(\text{Ba}_{0.19}\text{K}_{0.81}\text{BiO}_3, \text{Ag}_{3}\text{Pb}_2\text{O}_6, \text{Bi}_{3}\text{S}_2\text{Se}_{0.09}\text{O}_4\) |
| 18             | Bi-based      | \(\text{Bi}_{1.6}\text{Ti}_{0.4}, \text{Bi}_2\text{Bi}_1, \text{Bi}_{0.523}\text{Pb}_{0.477}\text{Sn}_{0.553}\) |
| 19             | Au-based      | \(\text{Au}_{0.84}\text{In}_{0.16}, \text{AlScAu}_2, \text{Au}_{0.85}\text{Pd}_{0.15}\text{Ga}_2\) |
| 20             | Ir-based      | \(\text{CaIr}_2, \text{SrIr}_2\text{As}_2, \text{Ir}_{0.8}\text{Pt}_{0.2}\) |
| 21             | Sn-based      | \(\text{NbSn}_3, \text{Ca}_{2.25}\text{Sn}_{0.75}\text{RhSn}_3, \text{RhSn}_2\) |
| 22             | Ta-based      | \(\text{Hf}_{0.4}\text{Ta}_{0.6}, \text{Be}_2\text{Ta}_3, \text{Nd}_{0.72}\text{Ta}_3\text{C}_{2.8}\text{S}_2\) |
| 23             | Ru-based      | \(\text{Ce}_{0.85}\text{La}_{0.15}\text{Ru}_2, \text{Ir}_{0.41}\text{Ru}_{0.57}, \text{Cr}_{0.5}\text{Ru}_{0.5}\) |
| 24             | NbN-based     | \(\text{NbC}_{0.5}\text{Ni}_{0.47}, \text{Nb}_2\text{BN}, \text{NbN}_{0.87}\text{O}_{0.13}\) |
with superconductivity, such as crystal symmetry, layered structure, density of states at the Fermi level, the number of valence electrons, etc. We showed that the best results are achieved when superconducting materials are clustered in steps. A similar approach might be useful in other data-driven materials calculations.

We also discussed the limiting factors, i.e. wrong entries in the database. One can hope that with a more reliable database, which will also include more predictors, better clustering results can be achieved. In that regard, the recently initiated SuperMat project [29], which uses text mining and other natural language processing techniques to construct a superconductor database, might turn out to be fruitful.

6. References

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