The application of unsupervised learning to a dataset of AC susceptibility measurements of High-Temperature Superconductors

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***Abstract*— This work gives an insight if clustering technique applied to the dataset consisting of about 1000 measurements of High-Temperature Superconductors (HTS) using the AC susceptibility method, will allow recovering known and unknown relationships between different types of HTS and their superconducting properties, which depend on the type of superconductor and its preparation procedure. The dataset was simplified by using a Convolutional Autoencoder and the Bag of Words (BOW) representation. K-means and DBSCAN (Density-based spatial clustering of applications with noise) algorithms were used for clustering. The obtained results were visualised by the t-SNE algorithm (t-Distributed Stochastic Neighbor Embedding).**

Keywords*— *High-temperature superconductors, AC susceptibility, unsupervised learning, clustering

I. INTRODUCTION

High-temperature superconductors (HTS) are materials which exhibit properties like zero electrical resistance and expulsion of an external magnetic field from the interior of a superconductor [1]. These unique properties are used in the state of the art applications for the medicine (MRI/NMR machines), science (particle accelerators), transportation (Maglev) and electrical industry (electric power transmission, fault current limiters). The greatest drawback of superconductors is that they only function in low temperatures up to 134 K for $HgBa_2Ca_2Cu_3O_9$ at ambient pressure [2]. Scientists are still pursuing the discovery of room-temperature superconductor. The phenomenon of high-temperature superconductivity is still not fully understood.

Machine learning (ML) is the study of computer algorithms that improve automatically through experience [3]. Machine learning algorithms build a mathematical model based on data, order to make predictions or decisions without being explicitly programmed to do so [4]. Unsupervised learning (UL) is a subfield of ML. UL algorithms look for previously undetected patterns in a dataset with no pre-existing labels and with a minimum of human supervision [5]. The great progress has been made in a quest to discover, develop or refine various machine learning algorithms in recent years. Also, new ways of data analysis (Artificial Neural Network autoencoders [6], t-SNE [7]) have been shown. ML application to the analysis of datasets is a state of the art technique and allows to gain new knowledge in various areas of science and engineering.

Our work aims to provide first insights if clustering technique applied to the dataset consisting of about 1000 measurements of HTS using the AC susceptibility method, will allow recovering known relationships (features) between different types of HTS and their superconducting properties, which depend on sample preparation conditions like sintering and annealing temperatures, etc.

II. THEORY AND EXPERIMENTAL DETAILS

The AC magnetic susceptibility can be written as a complex number by the formula $\chi=\chi'+i\chi''$, where χ' is the dispersion and χ'' is the absorption part of the AC susceptibility. The value of the dispersion part corresponds to the diamagnetic nature - a negative magnetization of the HTS sample when an external magnetic field is applied [8]. The values of χ' and χ'' for HTS change with temperature. Above a certain temperature, called the critical temperature T_c, both parts of AC susceptibility are equal to zero. On the other hand, below critical temperature T_c, the χ' part has negative values and the χ'' part is positive or equal to zero. The shapes of χ'(T) and χ''(T) curves strongly depend on superconductor properties, so measuring the temperature dependence of the complex AC susceptibility χ is the most common procedure for characterizing the properties of a superconductor. On Fig. 1 are shown four selected examples of χ(T) for different types of High-Temperature Superconductors.

III. MAIN METHODOLOGICAL ASSUMPTIONS

(1) A single AC susceptibility measurement χ(T) can be treated as a sequence of several hundred data points (sentence), therefore it can be represented as a collection of smaller subsequences (words) (Fig. 2). Data point is a 3D vector consisting of values of sample temperature, χ' and χ''

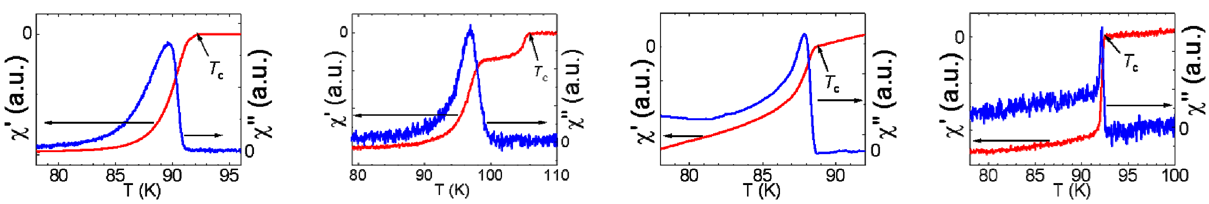

Fig. 1. Examples of χ(T) for selected High-Temperature Superconductors with different superconducting properties.

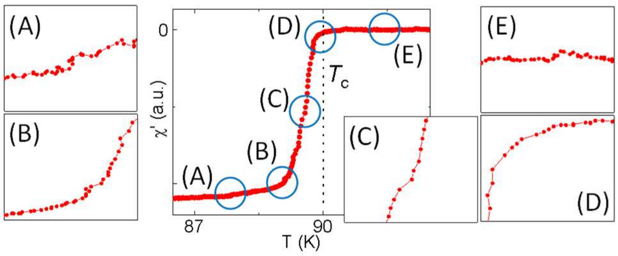

Fig. 2. An idea of Bag Of Words approach in the analysis of χ'(T) measurement. Small figures marked as A, B, C, D and E represent the words with unique features of a sequence shown on middle plot.

parts of AC susceptibility χ. Subsequences are created by a sliding window method. (2) The χ'(T) measurement (sentence) can be represented as a collection of only a few unique subsentences (words). (3) The shape of χ(T) measurement depends on the physical properties (features) of a HTS sample. For any χ(T) measurement word occurrences histogram can be created by using Bag Of Words (BOW) model (Fig. 3). Histogram preserves the most important features of χ'(T) curve. (4) The real part of AC susceptibility χ'(T) curve is sufficient for successful recovery known relationships in χ(T) dataset. (5) All data points are equally spaced in temperature. (6) Variation in data points spacing among different measurements does not influence the features represented in histograms.

IV. The Most Important Details on Computation

All χ'(T) measurements were normalised to [-1,0] range and then were divided into subsequences of the size of about several dozen data points. Values of temperatures were dropped. A data point is a single value of χ'. Resulting subsequences were normalised to [0,1] range. Next, further reduction of dimensionality of subsequences to 9 dimensions (9D) was performed by using an 1D convolutional autoencoder, which task was to learn the most efficient representation for a given subsequence. Then, all subsequences with reduced dimensionality were analysed by K-means and DBSCAN clustering algorithms to find subsequences (words) with unique features (Fig. 2) and create word dictionary. The results of clustering were evaluated by visualisation of the words dataset on 2D plane using the t-SNE algorithm. The most reasonable results were achieved by the k-Means with a number of classes set to 5. In the final step, the autoencoder and word dictionary were used to transform every single measurement in χ'(T) dataset into 5D vector. The vector coordinates correspond to word occurrence in single χ'(T) measurement.

V. Results and Discussion

It is possible to represent the most significant features of a single χ'(T) measurement of HTS sample as 5 numerical values by using Convolutional 1D Autoencoder and Bag Of Words model. The 5D representation of χ'(T) dataset preserves the most important features of measured HTS, because the most distant 5D representations of χ'(T) are for samples, which have the most different superconducting properties i.e. thin layer HTS (very high value of critical current density) and grinded and pressed polycrystalline HTS (current is equal to zero) (Fig.3). However the cluster analysis of 5D χ'(T) dataset by K-Means and DBSCAN did not reveal the existence of clearly distinct classes of χ'(T) measurements. Though a t-SNE visualisation (Fig. 4) shows that some clustering exists and some of the measurements are mainly arranged on some sort of cluster boundary. In our opinion, these results are interesting and more advanced analysis should be tried in future.

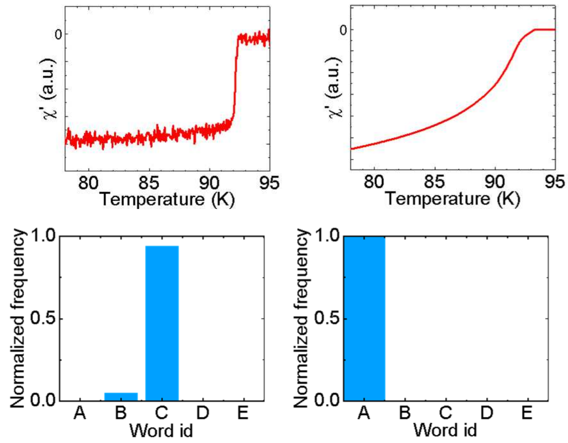

Fig 3. Upper row shows χ'(T) measurements for thin layer HTS (left) and grinded and pressed polycrystalline HTS powder (right). Bottom row shows representations of these measurements in 5D space.

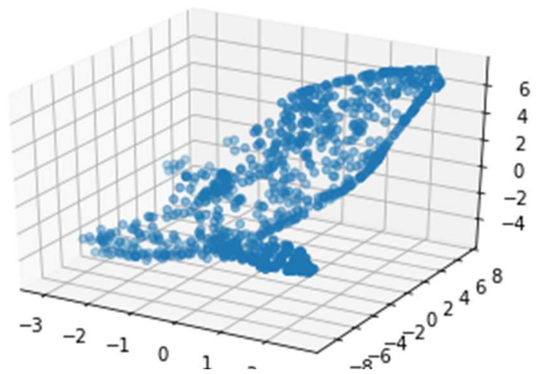

Fig 4. Visualisation of about 1000 measurements of χ'(T) in 3D feature space by t-SNE. Single measurement is 5D vector and is represented as single circle.

Acknowledgment

This work is supported by The National Science Center Poland under Project No. 2018/02/X/ST3/01741.

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