

PREDICTION OF SUPERCONDUCTING TRANSITION TEMPERATURE USING A MACHINE-LEARNING METHOD

NAPOVED TEMPERATURE PREHODA V SUPERPREVODNOST Z UPORABO METODE STROJNEGA UČENJA

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A high-transition-temperature (high- T_C) superconductor is an important material used in many practical applications like magnetically levitated trains and power transmission. The superconducting transition temperature T_C is determined by the layered crystals, bond lengths, valency properties of the ions and Coulomb coupling between electronic bands in adjacent, spatially separated layers. The optimal T_C can be attained upon doping and applying the pressure for the optimal compounds. There is an algebraic relation for the optimal T_C of the optimal compounds, $T_{CO} = K_B^{-1}\beta/(t\xi)$, where t and ξ are two structural parameters, K_B is Boltzmann's constant, β is a universal constant and T_{CO} is the optimal transition temperature. Nevertheless, the T_C of the non-optimum compounds is smaller than T_{CO} . To predict the T_C for the all compounds, we developed a prediction model based on the machine-learning method called support vector regression (SVR) using structural and electronic parameters to predict T_C . In addition, the principal component analysis (PCA) was applied to reduce dimensions and interdependencies among the parameters, and particle swarm optimization (PSO) was utilized to search for the optimal parameters of SVR for an improved performance of the prediction model. The results showed that the proposed PCA-PSO-SVR model takes advantage of the machine-learning method to directly predict T_C and theoretically provide guidance on measuring T_C .

Keywords: superconducting transition temperature T_C , machine learning, structural and electronic parameters, PCA-PSO-SVR

Visoka temperatura prehoda v superprevodnost (T_C) je pomembna funkcionalna lastnost materiala za mnoge vrste praktične uporabe, kot je naprimer uporaba magnetne levitacije za vlake ali prenos moči. Temperaturo prehoda v superprevodnost T_C določa plastovitost kristala, dolžina medatomskih vezi, valenčne lastnosti ionov in Coulombovo sklapljanje med sosednjimi valenčnimi pasovi prostorsko ločenih plasti. Optimalna T_C se lahko doseže z dopiranjem (dodajanjem, legiranjem) in uporabo tlaka za optimalno kemijsko sestavo. Obstaja algebraična zveza za optimalno T_C optimalne spojine, $T_{CO} = K_B^{-1}\beta/(t\xi)$, kjer sta t in ξ dva strukturna parametra, K_B je Boltzmannova konstanta, β je univerzalna konstanta in T_{CO} je optimalna temperatura prehoda. Vendar je T_C neoptimalne spojine vedno manjša kot T_{CO} . Avtorji tega prispevka so za napoved T_C vseh spojin razvili model na osnovi metode strojnega učenja. Za napoved T_C so uporabili vektorsko regresijo (SVR) z odgovarjajočimi strukturnimi in elektronskimi parametri. Dodatno so uporabili osnovno komponentno analizo (PCA, angl.: Principal Component Analysis), da so lahko zmanjšali soodvisnosti med parametri. Uporabili so še optimizacijo množic delcev (PSO; angl.: Particle Swarm Optimization) za iskanje optimalnih parametrov SVR in izboljšanje lastnosti modela. Raziskave avtorjev tega prispevka so pokazale, da predlagani model PCA-PSO-SVR s pridom izkorišča prednosti metode strojnega učenja za neposredno napoved T_C , in tudi zagotavlja teoretično podlago za merjenje T_C .

Ključne besede: temperatura prehoda v superprevodnost T_C , strojno učenje, strukturni in elektronski parametri, PCA-PSO-SVR

1 INTRODUCTION

As important functional materials, high-transition-temperature (high- T_C) superconductors¹ have some typical physical parameters, such as transition temperature T_C , magnetic susceptibility and critical current density (J_C), which make them very useful in many practical applications like magnetically levitated trains and power transmission.²⁻⁵ Previous researches showed that the high- T_C superconductors are generally characterized by a two-dimensional layered superconducting condensate with unique features that are not traditional superconducting metals.⁶ Their important property, T_C , is determined by their layered crystals, bond lengths, valency properties of the ions, and Coulomb coupling

between electronic bands in adjacent, spatially separated layers.⁷ The optimal T_C can be attained upon doping with other external materials or applying pressure for the optimal high- T_C superconducting compounds.⁸ There is an algebraic relation for the optimal T_C of the optimal compounds:^{7,9}

$$T_{CO} = K_B^{-1}\beta/(t\xi) \quad (1)$$

Here, t is related to the mean spacing between interacting charges in the layers, ξ is the distance between interacting electronic layers, K_B is Boltzmann's constant, β is a universal constant and T_{CO} is the optimal transition temperature.

Formula (1) is a good way to predict the T_{CO} of optimal high- T_C superconducting compounds. However,

non-optimum compounds, in which sample degradation is evident, typically show that T_C is smaller than T_{C0} .⁷ In other words, it is critical to predict T_C of various high- T_C superconducting compounds. In our present work, we developed a prediction model based on a machine-learning method to predict T_C of various high- T_C superconducting compounds using structural and electronic parameters. The results of the prediction model show that the model can predict T_C quickly and accurately.

Recently, in order to accelerate the process of discovery and deployment of new materials, more and more researchers have used machine-learning methods to find new materials, classify them and predict their properties.^{10–13} For high- T_C superconductors and their T_C , researchers developed a computational-intelligence-based model via SVR¹⁴ to estimate the T_C of YBCO superconductors using lattice parameters as the descriptors^{15–17} and manually found the optimal parameters of SVR one by one with the trend charts of the effects of the parameters on the experimental results. It is a very feasible way to estimate the T_C of YBCO superconductors, but the manual parameter optimization may take a lot of time.

In this paper, in order to predict T_C of various high- T_C superconductors, we established a PCA-PSO-SVR model based on a machine-learning method using structural and electronic parameters. These parameters, including ζ (the distance between interacting electronic layers), A (the distance between interacting electronic layers), d (the periodicity), η (the number of type II layers), ν (the number of type I layers), σ (the fractional charge per type I layer) and γ (the factor for calculating σ), related to 31 kinds of high- T_C superconductors that form the dataset from the literature.^{7,9} The dataset has only 31 samples and each sample has only 7 features, which is obviously a small sample set, but the SVR shows many unique advantages of processing small sample sets because of the theory of statistical learning and the minimum principle of structural risk. Hence, we chose the SVR as the regression algorithm of the prediction model. To achieve a higher performance of the model, we adopted automatic optimization with a simple and efficient PSO¹⁸ optimization algorithm instead of the manual optimization used in the previous studies when searching for the optimal SVR parameters. Meanwhile, we found that some parameters are interdependent by analysing the crystal structure and parameters of the high- T_C superconductors, so we used PCA¹⁹ to reduce dimensions and interdependencies in the data pre-processing for a better accuracy of the prediction model. In addition, we also trained the PSO-SVR model and the back-propagation neural network (BPNN)²⁰ with the dataset for comparison. The corresponding experimental results showed that the PCA-PSO-SVR prediction model is more accurate when predicting T_C . Meanwhile, we used additional data to validate the prediction model, and the results were also reasonable. It means that this

prediction model, based on the machine-learning method, can directly predict T_C .

2 ESTABLISHMENT OF THE PREDICTION MODEL

In order to identify the feasibility and validity of the new model, 31 kinds of high- T_C superconductors, including cuprates, ruthenates, ruthenocuprates, iron pnictides and organics, whose T_C values are in a range of [10.5, 145], were selected from the literature⁷ as the dataset. These materials are independent of the locations of two carrier types, of which type I is defined with the BaO-CuO-BaO (or equivalent) layers and type II is defined with the cuprate-plane CuO₂-Y-BuO₂ (or equivalent) layers. The details of the dataset were presented in the Data.docx file. In the process of establishing the prediction model, the structural (Z , A , d , η , ν) and electronic (σ , γ) parameters were scaled to [0,1] with the min-max normalization, and taken as the input vectors, while T_C was the output value for the regression. Given that the parameters are interdependent (e.g., γ is related to σ , and Z is a part of d according to the definition of these two parameters), we used the widely applicable PCA method to reduce the dimensions and interdependencies of the parameters. In the PCA process, first, the covariance matrix of the dataset is calculated, then the eigenvalues of the covariance matrix are calculated, and finally the top d eigenvalue of all the eigenvalues is selected, while the corresponding feature vectors form the solution of the PCA. The selected reduced dimensions are based not only on the contribution rate that can be calculated with Equation (2) but also on the errors of the predicted results of the PCA-PSO-SVR model.

$$C = \frac{\sum_{i=1}^n \lambda_i}{\sum_{j=1}^m \lambda_j} \quad (2)$$

Here, λ_i denotes the i th eigenvalue, n denotes the chosen dimension amount and m denotes the entire dimension amount.

Detailed results of the dimension reduction are discussed in the next section. After reducing the dimensions, the dataset was divided into two parts via the leave-one-out cross-validation (LOOCV)²¹ method. 30 samples were used to train the model and the last one was used to validate the model. Because the dataset was a small sample set and the parameters were nonlinear, we chose SVR as the regression algorithm and a radial basis function (RBF)²² as the kernel function. In the parameter optimization of SVR, the insensitive loss coefficient $\#$ was empirically set as 0.05, and the penalty coefficient C and the width coefficient γ could be optimized with PSO. After searching for the optimal parameters, the corresponding SVR was optimal and the PCA-PSO-SVR prediction model was established as well.

3 RESULTS AND DISCUSSION

During the data pre-processing, we adopted the PCA to process the dataset for reducing the dimensions and interdependencies among the parameters. In order to select the optimal reduced dimensions, the calculated eigenvalues of the covariance matrix of the parameters and the corresponding contribution rates C were sorted and listed in **Tables 1** and **2**. From **Table 2** and **Figure 1**, we can see that with an increase in the reduced dimensions from 1 to 7, the contribution rates also increase. There is a significant improvement from 3 dimensions to 4 dimensions, that is, the contribution rate of 4 dimensions reaches 96.23 % while the contribution rate of 3 dimensions reaches 89.57 %. Meanwhile, when the number of reduced dimensions is more than 4, the contribution rate is close to 100 %, which means that the loss rate is close to 0. Generally speaking, when the contribution rate is over 95 %, the corresponding reduced dimensions of the parameters can represent the original parameters well. In addition, we also made a holistic performance analysis of the impact of the dimensions after adopting the PCA for the proposed model.

Different reduced dimensions from 1 to 7 were used to train and establish the PCA-PSO-SVR prediction model, and every sample of the dataset was used to test each model and obtain the predicted values. Although we do not show those specific predicted values of each sample, we show the mean absolute error (MAE) and root

mean square error (RMSE) of the proposed model, with the dimensionality varying from 1 to 7 in **Figure 2**. When the dimensionality gradually increases to 4, the MAE and RMSE decrease. However, when the dimensionality is bigger than 4, the MAE and RMSE are larger than in the case of the dimensionality being 4. In other words, both MAE and RMSE are minimal when the dimensionality is 4. The reason why 4 dimensions are the best according to the PCA can be explained as follows: when the number of reduced dimensions is smaller than 4, the corresponding contribution rate is lower than 90 %. Therefore, it loses too much information hidden in the original dataset and the result is certainly not accurate. When the number of reduced dimensions is over 4, though the contribution rate is obviously higher than that of 4-dimension, more parameters mean more noise and interference. Thus, 4-dimensional parameters were selected for the regression process based on the comprehensive result analysis of the contribution rate and errors.

In addition to trianing and validating the PCA-PSO-SVR model with the processed dataset, we trained and validated the PSO-SVR and BPNN model with the original dataset. The predicted T_C of each sample obtained with three different models is shown in **Figure 3**; the specific values listed in the Data.docx file and the corresponding absolute errors are also presented. It can be seen that many sample points deviate from the standard line in **Figure 3a**; in other words, the absolute

Table 1: Eigenvalues of the covariance matrix after sorting

Number	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	λ_7
Eigenvalue	0.4257	0.1207	0.0743	0.0462	0.0197	0.0047	0.0017

Table 2: Contribution rates of the dimensions from 1 to 7

Dimension	1	2	3	4	5	6	7
Contribution rate	0.6143	0.7885	0.8957	0.9623	0.9907	0.9976	1.0000

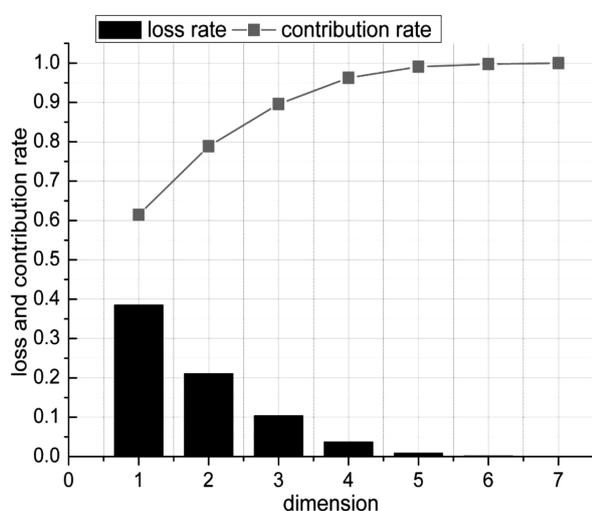


Figure 1: Loss rate and contribution rate of the dimensionality from 1 to 7

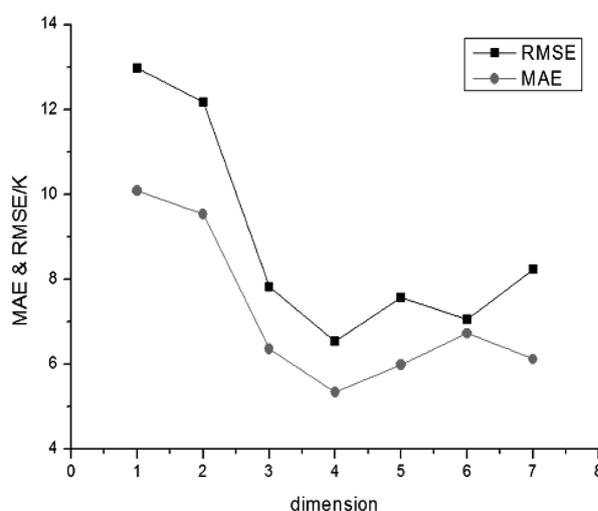


Figure 2: MAE and RMSE of the proposed model with dimensionality from 1 to 7

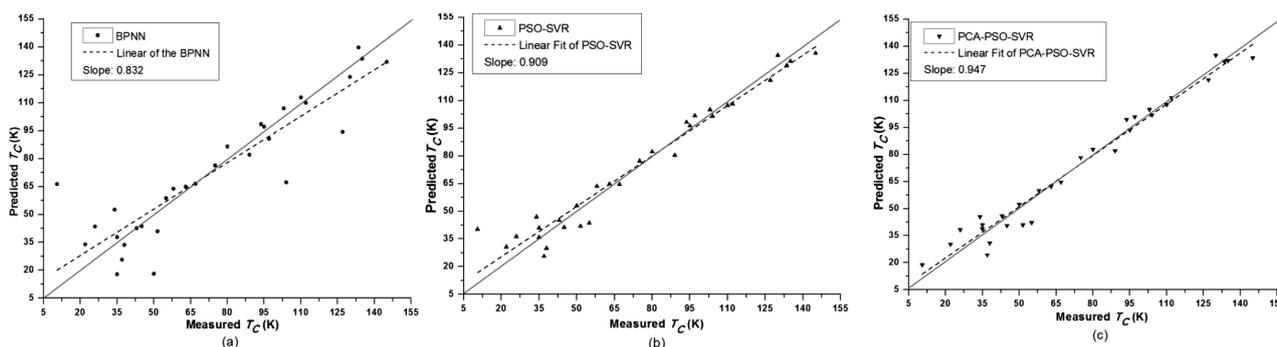


Figure 3: a), b) and c) show the correlation between the measured T_C and T_C predicted by BPNN, PSO-SVR and PCA-PSO-SVR, respectively. 31 kinds of high- T_C superconductors were used with three different methods to predict T_C , represented by circles, up-triangles and down-triangles in every subfigure; the black dashed line represents the corresponding fit line and the red solid line is the standard line. The slope of the fit line was used to determine the performance of the corresponding method, and the three fit-line slopes are 0.832, 0.909 and 0.947, respectively.

Table 3: Comparison of the prediction performance of BPNN, PSO-SVR and PCA-PSO-SVR

methods	MAE/K	MAPE/%	RMSE/K	R
BPNN	10.59	23.46 %	16.44	0.8972
PSO-SVR	6.15	12.56 %	8.23	0.9745
PCA-PSO-SVR	5.34	11.85 %	6.54	0.9843

Table 4: Measured T_C , the T_C predicted with the PCA-PSO-SVR and the corresponding absolute error

No	1	2	3	4	5	6	7
Measured T_C /K	18.0	10.2	6.3	6.9	17.0	16.0	9.5
Predicted T_C /K	22.6697	10.2721	6.7415	6.5941	21.6752	21.1690	9.9879
MAE/K	4.6697	0.0721	0.4415	0.3059	4.6752	5.1690	0.4879

errors of the samples predicted with BPNN are so large that this prediction model is not suitable. Comparing **Figure 3b** with **Figure 3c**, more sample points are presented with the PCA-PSO-SVR model and they are closer to the standard line than the sample points of the PSO-SVR model. Specifically, the accuracy of 19/31 samples obtained with PCA-PSO-SVR is better than that of PSO-SVR; especially for the leftmost sample point, the absolute error dropped from 30 K to 8 K. Based on the singularity of the leftmost sample point, we can say that it is the only organic superconductor that is very different from the others in the dataset and the values of some of its parameters are much bigger than those of the corresponding parameters of the other samples, leading to a big prediction error. Because of the data pre-processing with PCA, the influence of the parameters with large values on the predicted results becomes smaller after projection, so the corresponding absolute error dropped a lot. Meanwhile, we can also see that the fit line of PCA-PSO-SVR is closer to 1 than the other two fit lines, which means that its accuracy is better. The performance of each model can also be analysed statistically as shown with **Table 3**, which includes MAE, the mean absolute percentage error (MAPE), RMSE and the correlation coefficient (R). It can be found that the PCA-PSO-SVR index is the best in all three models, being 5.34 K, 11.85 %, 6.54 k and 0.9843, respectively. Based on the above analysis, the proposed PCA-PSO-SVR model is very suitable to predict the T_C for the dataset.

We added seven $A_x(S)_yTiNCl$ compound high- T_C superconductors,²² which had structural characteristics similar to those of the preceding dataset. By reading and analysing the literature, we extracted the required data, included in the Data.docx file. We used the new data to validate the proposed PCA-PSO-SVR prediction model, and the corresponding predicted values and MAE are included in **Table 4**. Very small MAEs were found for four of the seven samples. Compared with the previous predicted results of the developing prediction model, the current predicted results for all the samples are reasonable. In other words, the PCA-PSO-SVR prediction model exhibited a good accuracy for the above additional data.

4 CONCLUSIONS

In this paper, we provided a PCA-PSO-SVR model for predicting T_C from structural and correlative electronic parameters of high- T_C superconductors. SVR was adopted to deal with the dataset, which was a small sample set, and the PSO algorithm was utilized to search for its optimal parameters to achieve a good performance. The PCA was employed to reduce dimensions and interdependencies between the parameters, and the selected optimal dimensions of the parameters were subsequently utilized in PSO-SVR to train and validate the regression model. In addition, we also trained a PSO-SVR model without the PCA and BPNN, with the

dataset used for comparison. According to the assessment results and comparison, the PCA-PSO-SVR model provided a better accuracy of prediction than the other models for the dataset, and the corresponding MAE was 5.34 k. At last, additional data was used to validate the prediction, and the results were also reasonable. In a word, machine-learning methods can be applied to some domains of materials and the PCA-PSO-SVR ensemble method may be used to predict the T_C of new high- T_C superconductors.

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