Deep Learning Model for Finding New Superconductors

Tomohiko Konno*
National Institute of Information and Communications Technology
Tokyo Japan
tomohiko@nict.go.jp

Hodaka Kurokawa†
The University of Tokyo
Tokyo, Japan
scottie0018@gmail.com

Fuyuki Nabeshima
The University of Tokyo

Yuki Sakishita
The University of Tokyo

Ryo Ogawa
The University of Tokyo

Iwao Hosako
National Institute of Information and Communications Technology

Atsutaka Maeda
The University of Tokyo

Abstract

It is very difficult for both theories and computational methods to predict the superconducting transition temperatures (T_c) of superconductors for strongly correlated systems, in which high-temperature superconductivity emerges. Exploration of new superconductors still relies on the experience and intuition of experts, and is largely a process of experimental trial and error. In one study, only 3% of the candidate materials showed superconductivity [1]. Here we report an interdisciplinary attempt for finding new superconductors based on deep learning. We represented the periodic table in a way that allows a deep learning model to learn it. Although we used only the chemical composition of materials as information, we obtained an R^2 value of 0.92 for predicting T_c for materials in a database of superconductors. We obtained three remarkable results. The deep learning method can predict superconductivity for a material with a precision of 62%, which shows the usefulness of the model; it found the recently discovered superconductor $CaBi_2$, which is not in the superconductor database; and it found Fe-based high-temperature superconductors (discovered in 2008) from the training data before 2008. These results open the way for the discovery of new high-temperature superconductor families.

1 Introduction

Extensive research has been conducted on superconductors with a high superconducting transition temperature, T_c, because of their many promising applications, such as low-loss power cables, powerful electromagnets, and fast digital circuits. However, finding new superconductors is very difficult. In one study, it was reported [1] that only 3% of candidate materials showed superconductivity. Theoretical approaches have been proposed for predicting new superconductors. According to Bardeen-Cooper-Schrieffer (BCS) theory [2], which explains phonon-mediated superconductivity in many materials, high T_c is expected for compounds made of light elements. T_c values of over 200 K have been reported for sulfur hydride [3] and lanthanum hydride [4]. However, very high pressures

*Corresponding author
†Second corresponding author

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(over 150 GPa) are required. Superconductivity with rather high T_c has been observed for cuprates [5] and iron-based materials [6] at ambient pressure, where unconventional superconductivity beyond the BCS framework is realized. However, the strong electron correlations in these materials make it very difficult to conduct first-principles calculations [7–10] to calculate their electronic structures and predict T_c values. Therefore, new approaches for finding superconductors are needed. Materials informatics, which applies the principles of informatics to materials science, has attracted much interest [12, 11]. Among machine learning methods, deep learning has achieved great progress. To predict the material properties of materials using the conventional methods in materials informatics, researchers must design the input features of the materials; this is called feature engineering. It is very difficult for a human to design the appropriate features. A deep learning method can design and optimize features, giving it higher representation capabilities and potential compared to those of conventional methods.

2 Results and Methods

Reading Periodic Table Here, we report a deep learning model for the exploration of new superconductors. Using deep learning to discover new superconductor families from known ones is analogous to using one to recognize dogs from training data containing only cats. This form of learning, called zero-shot learning, is very difficult. However, the properties of elements, which can be learned by deep learning, can be applied to materials. Our strategy is to suitably represent these properties, use this representation as training data, and have the deep learning model learn these properties. We made the deep learning model learn how to read the periodic table as human experts do. Although humans cannot recall tens of thousands of data points, computers can. For this purpose, we represented the periodic table in a way that allows a deep learning model to learn it.This method, named reading periodic table, is our first contribution to deep learning. We considered inorganic crystal superconductors because the number of known organic superconductors is small. We used only the composition of materials because the applied superconductor database does not have sufficient spatial information.

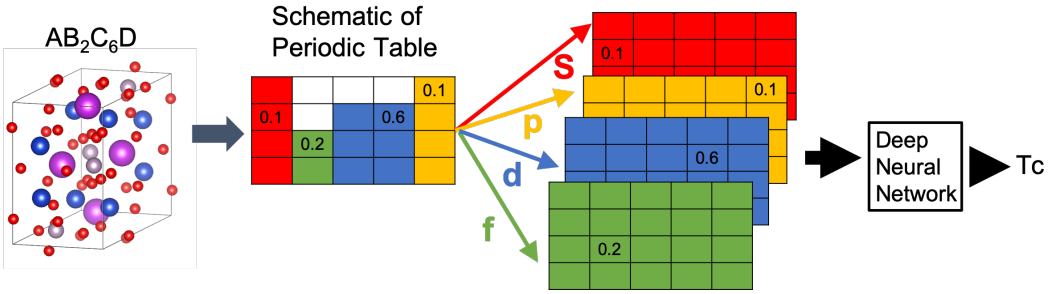

Figure 1: Proposed method named reading period table. The representation of a material by the method. The composition ratios of the material [13] are entered into the two-dimensional periodic table. We then divide the original table into four tables corresponding to s-, p-, d-, and f-blocks, which show the orbital characteristics of the valence electrons, to allow the deep learning model to learn the valence orbital blocks. The dimensions of the representation are $4 \times 32 \times 7$. The neural network learns the rules from the periodic table by convolutional layers.

We used the deep learning model to predict the critical temperatures, T_c, of superconductors in the SuperCon dataset [14], which has the T_c values of about 13,000 superconductors. We refer to the model trained with only SuperCon as the preliminary model. The train-test split was 0.05. The R^2 value is 0.92, which is higher than that previously reported (0.88) for a random forest regression model [15], where materials were restricted to those with $T_c > 10$ K (half of all materials). In contrast, our preliminary model does not have any restrictions regarding T_c. The random forest regression model requires many appropriate input features of the materials (e.g., atomic mass, band gap, atomic configuration, melting temperature) to be manually designed. Here, even without such feature engineering, we achieved much better results.

The problem in using data of superconductors only and the method named garbage-in to overcome it We used the preliminary model trained with SuperCon to predict the T_c values of 48,000

inorganic materials in the Crystallography Open Database (COD) to find new superconductors for experiments. However, for about 17,000 of the materials, the predicted T_c was > 10 K, which is unreasonable. The failure to find new superconductors by this preliminary model seems to originate from the fact that the training data (SuperCon) included only 60 non-superconductors; the preliminary model was thus unable to learn non-superconductors. Data on non-superconductors are needed to differentiate superconductors from non-superconductors. However, no such dataset is available. Hence, we created synthetic data on non-superconductors, supposing that the T_c values of the inorganic materials in COD that are not in SuperCon are 0 K under the assumption that most of these materials do not become superconductors with finite T_c. We used the synthetic data and SuperCon as the training data. We refer to this data generation method as garbage-in, which is our second contribution to deep learning. As demonstrated by the above results for the preliminary model, scores of tests using only superconductor data, SuperCon, are not good for evaluating models. Usually, density functional theory is applied for evaluation in materials informatics; however, density functional theory cannot be used to evaluate models, because it is very difficult to calculate T_c for strongly correlated systems. A database of non-superconductors is thus necessary.

The prediction of superconductivity We applied a list of materials reported by Ref. [1] to evaluate the models. The list has about 400 materials found since 2010; importantly, it includes 330 non-superconductors. To temporally separate the materials on the list from the training data, we used only the data added to SuperCon or COD before 2010 as training data. To compare the capability of a model with expert predictions, we evaluated whether the model could predict superconductivity for the given materials. Randomly selecting a material from the list with T_c > 0 K yields a precision of 32%. This is considered the baseline because all the materials on the list were expected to be superconductors before the experiments. The model predicted T_c, and whether the T_c value will be higher than 0 K resulted in a precision of 62%, an accuracy of 76%, a recall of 67%, and a f1 score of 63%. The precision is about two times higher than the baseline (32%) and 10 sigma away from it. The AUC was 0.78. Another interesting threshold is 10 K because only a limited number of superconductors have a T_c of > 10 K. The deep learning method predicted materials with this T_c with a precision of 75%, which is about seven times higher than the baseline random precision (10%). The accuracy, recall, and f1 score were 95%, 76%, and 75%, respectively. The AUC was 0.94. In contrast, the preliminary model, trained with SuperCon only, predicted that all the materials would be superconductors, even though the training data were up to the year 2018 (i.e., not temporally separated). We also performed random forest binary classification with garbage-in and deep learning binary classification, which classify whether the T_c is beyond 0 K and 10 K. The AUC were 0.78 and 0.96 respectively. The results, summarized in Table 1, demonstrate that our deep learning model has good capability to predict superconductivity and outperformed random forest. When it comes to materials search, recall is very important. Recall and f1 score were much better in our deep learning method than random forest.

	Precision	Recall	f1 score
Baseline (0 K)	0.32	–	–
Our DL model Reg (0 K)	0.62	0.67	0.63
Our DL model Cls (0 K)	0.72	0.50	0.59
Random Forest Cls (0 K)	0.71	0.27	0.39
Baseline (10 K)	0.10	–	–
Our DL model Reg (10 K)	0.75	0.76	0.75
Our DL model Cls (10 K)	0.76	0.77	0.77
Random Forest Cls (10 K)	0.88	0.26	0.40

Table 1: Scores for predictions of superconductivity for materials reported by Ref. [1]. Reg and Cls are abbreviations for regression and classification respectively.

The discovery of superconductor $CaBi_2$ Next, we used the model to predict the T_c values of the materials in COD. The number of materials predicted to be superconductors was different every time we trained the models from scratch, which is expected with deep learning. We made a search target list for the experiment. After we removed cuprates and Fe-based superconductors (FeSCs) from the list, we obtained 900 materials predicted to be superconductors with $T_c > 0$ K, 250 materials with $T_c > 4$ K, and 70 materials with $T_c > 10$ K, which is more reasonable compared to the results

obtained using the preliminary model. These materials are candidates for new superconductors. Although the prediction results on materials reported by Hosono et al. show that the model is useful, experiments (currently under way) are required to validate the method. The list included $CaBi_2$, which was recently found to be a superconductor [16] and is not listed in SuperCon. We had not known it was a superconductor beforehand. It can be concluded that the deep learning model found an actual superconductor.

The discovery of Fe-based superconductors (FeSC) To test the capability of our deep learning model of finding new types of superconductor, we investigated whether we could find high-T_c FeSCs by using the model trained with data before 2008, the year FeSCs were discovered. We removed two materials, LaFePO and LaFePFO, from the training data because their discovery in 2006 led to the discovery of high-T_c FeSCs. We used the 1,399 FeSCs known as of 2018 in SuperCon as the test data. A total of about 130 training and test runs were used. Although the models were made stochastically, we found some FeSCs that were predicted to have finite T_c. A histogram of the number of predicted FeSCs with $T_c > 0$ K is shown in Fig. 2. We obtained the same results for high-T_c cuprates. (see Supplementary Information). When we used shallow 10-layer networks that had as good R^2, precision, etc., as the current large model, FeSCs were not found. This is not strange, because most iron compounds show magnetism, which is incompatible with superconductivity, and there are few superconductors including iron except for FeSCs. Indeed, few researchers had anticipated that FeSCs could have high Tc values. It is recognized that larger models have better generalization performances. The fact that the larger model found FeSCs can be explained by a larger model having an improved search capability for new superconductors. These results suggest that FeSCs and cuprate superconductors might have been found by our deep learning model.

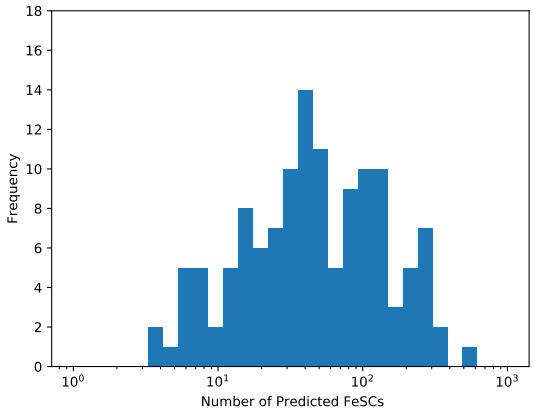

Figure 2: Histogram of the number of predicted FeSCs with $T_c > 0$ K (log scale).

3 Concluding discussion and the summary of contribution

If we had searched for FeSCs following the prediction, we would have discovered FeSCs. However, the predicted T_c of the FeSCs was rather low in our attempt to *discover* FeSCs. FeSCs might thus have been a low-priority target depending on how the model prediction was used. This problem will be considered in future research. We will incorporate crystal structure information to enhance the capability of the model of finding new high-T_c superconductor families. Nevertheless, the present model is still useful as an auxiliary tool. Furthermore, the present method could be applied to other problems where crystal structure is difficult to obtain. Even though our method does not require feature engineering, unlike conventional methods in materials informatics, it achieved much better results. Our deep learning method may replace existing methods, just as other deep learning methods have done in computer vision, natural language processing, and reinforcement learning. Deep learning requires failure data (e.g., non-superconductors) for accurate prediction. As many datasets in materials search are random train-test split, we must prepare temporal separate train-test dataset for the progress in the field. Because our method does not use specific properties of superconductors and uses only chemical formulas, the method can be applied to other problems with, in particular, inorganic materials. We are almost ready for the paper on the application to other problems. We

demonstrated the usefulness of our method and deep learning. Our results open the way to the discovery of new high-T_c superconductor families.

The contribution in methods: (1) The learning representation method named Reading Periodic Table that makes deep learning learn to read periodic table and learn the laws of elements in order to find novel type of materials unseen in the data set; (2) The method, named Garbage-in, that synthesizes necessary failure data; (3) The model evaluation method to use the list of materials reported by Ref. [1] as the test and use the training data reported before the list was begun to be made; (4) The first deep learning model for superconductors.

The results: (1) The prediction of superconductivity with much higher precision than human experts, high recall, and high f1 scores; (2) The discovery of superconductor $CaBi_2$, which was not in the superconductor dataset; (3) The discovery of Fe-based superconductors by the training data only before the actual reported year.

arXiv paper: The paper is found from the link.

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A Scatter plot of predicted and true (SuperCon) T_{c}

The scatter plot of the prediction only using the data of superconductors (SuperCon) is illustrated in Fig. 3. It is not the averaged predicted T_{c}, but one instance.

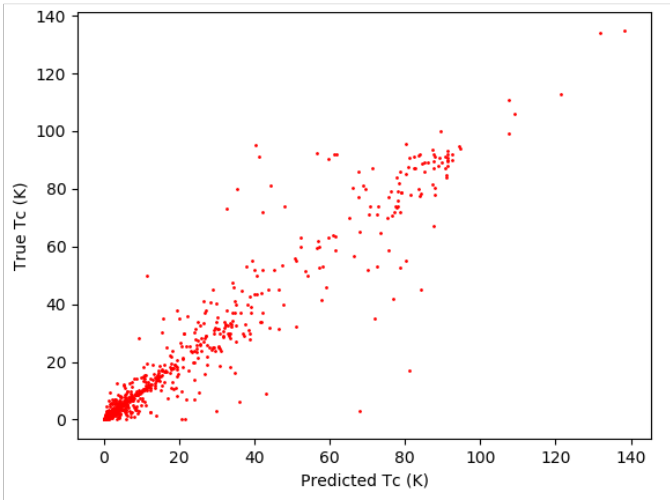


Figure 3: Scatter plot of predicted and true (SuperCon) T_{c} values.

B methods

B.1 The method named reading periodic table: representation of periodic table

B.1.1 Representation of elements as one-hot vectors

Any one of the 118 elements of the periodic table can be represented by a one-hot vector. For example, He can be represented by a 118-dimensional vector $(0, 1, 0, \cdots, 0)$ and H can be represented by $(1, 0, \cdots, 0)$. The fictional compound H_2He_3 would be represented by $(2, 3, 0, \cdots, 0)$ or $(2/5, 3/5, 0, \cdots, 0)$. There are two problems associated with representing materials by one-hot vectors. First, neural networks do not learn about elements and their combinations that do not appear in the training data. Second, one-hot vector representations do not reflect the properties of the elements, especially when data are scarce. Elements are treated as quite different entities in one-hot representations, even though the properties of the elements are known from quantum mechanics.

B.1.2 Learning of periodic table

To overcome these problems, we introduce a method that enables the deep learning model to learn the periodic table. The information on elements is reflected by the data representation, which the deep learning model uses to learn the properties. The properties of the elements and their similarities are reflected in the periodic table.The composition ratios of materials are entered into the periodic table and we then divide the periodic table into four tables corresponding to the s-, p-, d-, and f-blocks because differences in the valence orbitals are important. The dimensions of the representation are $4 \times 32 \times 7$. The deep learning model learns the periodic table using its convolutional layers. With knowledge of the periodic table and element properties, the deep learning model can predict unknown materials from known ones.

B.2 Garbage-in: a method for creating synthetic data on non-superconductors

We have a database of superconductors. However, to explore new superconductors we also need a database of non-superconductors, which does not exist. Hence, we created synthetic data. Under the

assumption that most of the inorganic materials in COD do not become superconductors with finite T_c, we input the inorganic materials in COD, with $T_c = 0$, to the deep learning model as training data along with SuperCon. The method is illustrated in Fig. 4. The overall scheme of training is illustrated in fig. 5.

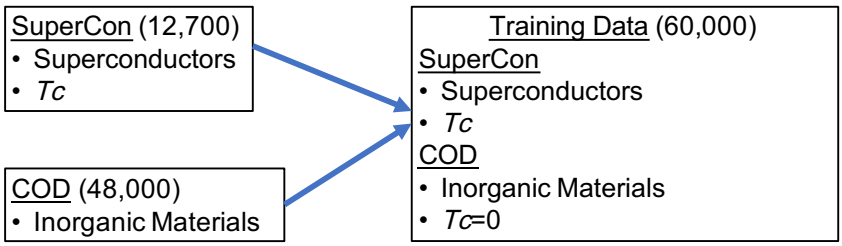


Figure 4: Synthetic data generation method named garbage-in.

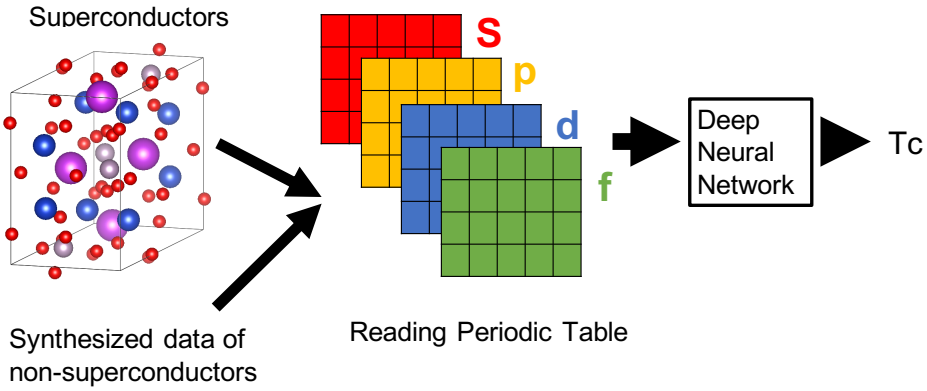


Figure 5: Overall scheme. The data of superconductors from SuperCon and the data of non-superconductors synthesized by garbage-in are transformed into the representation by reading periodic table in order for neural networks to learn the rules, then the deep neural network is trained to output T_c

B.3 List of candidate materials

We used the 48,000 inorganic materials in COD, 1,000 of which were used as test data. The remaining 47,000 materials and 12,000 materials in SuperCon were used as training data. Then, we obtained predicted T_c values of the 1,000 materials in the test data. We repeated the procedure 48 times with different test data. This produced a candidate materials list. If we generate materials by generative models, which output chemical composition virtually, we do not yet know how to synthesize the generated materials. COD is thus used because it is a list of previously synthesized materials.

B.4 Data availability

SuperCon [14], COD [17–19], and the materials reported by Ref. [1] are openly available and free to use. The materials reported by Hosono et al. have undetermined variables, such as x in $H_{2-x}O_{1+x}$. We investigated related papers and input the values for such variables. We then made a list of materials for the evaluation of models. This list will be openly available for the community.

B.5 Code availability

We are planning to open the code after some experiments on the candidate materials are completed. The code will be available on reasonable request.

B.6 Data handling

B.6.1 Definitions of conventional, cuprate, and Fe-based superconductors

Cuprate superconductors are defined as materials that contain Cu, O, and more than one other element. The exceptions are Cu, La, and O. FeSCs are defined as materials that contain Fe and either As, S, Se, or P. All other superconductors are considered to be conventional.

B.6.2 Removal of problematic data

We removed materials whose composition ends with variables such as "+x". About 7,000 materials were removed from SuperCon. If we know the accurate compositions of these materials and include them in the data, this should improve the deep learning model. We input appropriate values for variables such as "x" for the materials reported by Hosono et al. after reviewing the original studies, because there were only about 300 materials left after temporal separation.

B.6.3 Treatment of materials with same composition but different T_{c} values in SuperCon

SuperCon contains materials with the same composition but different T_{c} values. We decided to use the median value of T_{c}.

B.6.4 Treatment of materials without T_{c} values in SuperCon

Of the 17,000 remaining materials, about 4,000 did not have T_{c} values. We considered setting $T_{\mathrm{c}} = 0$ for these materials or just excluding them. A comparison of the regression results of the preliminary models with SuperCon indicated that excluding the materials without T_{c} values was better, so this was done.

B.6.5 Treatment of COD data

We use only the inorganic materials in COD. We remove duplicates, data with compositions difficult for machines to read, and overlap with SuperCon and the materials reported by Hosono et al. After this process, about 48,000 materials remained.

B.6.6 Overlap among SuperCon, COD, and materials reported by Hosono et al.

The overlap with SuperCon was removed from COD and the materials reported by Hosono et al.

B.6.7 Temporal separation of materials

Since the materials reported by Hosono et al. were collected starting from 2010, we used data from before 2010 as the training data. Using data from before 2008 as the training data and using the materials reported by Hosono et al. to check the reliability of the models also resulted in temporal separation.

B.7 Neural networks

A smooth L1 loss function was used. The optimizer was Adam [20]. For the prediction of T_{c} values for the materials in SuperCon by the preliminary model, the learning rate was 2×10^{-6}, the batch size was 32, the number of epochs was 6,000, T_{c} was in the linear scale, and the number of layers was 64. It took about 50 hours for training (see Supplementary Information). For the prediction of T_{c} values for the materials in SuperCon by the model with garbage-in, the number of epochs was set to 1,000. It took about 45 hours for training because the training dataset was five times larger than the preliminary model. For the prediction of superconductivity for the materials reported by Hosono et al., the learning rate was 10^{-4}, the batch size was 32, the number of epochs was 200, T_{c} was in the linear scale, and the number of layers was 64. For the prediction of FeSCs, the learning rate was 10^{-4}, the batch size was 32, the number of epochs was 200, T_{c} was in the linear scale, and the number of layers was 64. For making the candidate material list for the experiment and the discovery of $CaBi_2$ from the list, the learning rate was 10^{-4}, the batch size was 32, the number of epochs was 500, T_{c} was in the log scale after the addition of 0.1 to T_{c}, and the number of layers was 9. The

network was different because these predictions were done at the start of our research. We also found the superconductor $CaBi_2$ using the 64-layer network.

B.8 Random Forest

Random forest analysis were performed by using weighted average, weighted variance, maximum, minimum, range, mode, median, and mean absolute difference of the 32 features of elements in compositions. (See supplementary information.) The features were obtained from Magpie [21]. The results were the averages over 10 models. Random forest analysis using only the data of superconductors, without garbage-in, met the same problem as our deep learning model. It predicted about 60% of the materials were to be superconductors. We performed the classification if the T_c is beyond 0 K or not for materials reported by Hosono et al, because it is almost impossible for random forest regression to estimate $T_c = 0$, because random forest is an ensemble estimation. If even one tree estimates $T_c > 0$, then random forest regression estimates $T_c > 0$. The classification between 10 K was also done.

B.9 Training and test data used for main results

Main result	Training data	Test data
Prediction of superconductors from materials reported by Ref. [1]	SuperCon and COD before 2010	Materials reported by Hosono et al.
Superconductor $CaBi_2$ found in candidate material list	SuperCon and COD in 2018	COD in 2018
FeSCs found from training data before discovery year	SuperCon and COD before 2008	FeSCs in SuperCon in 2018

Table 2: Summary of main results.

The training data and test data used for the main results are summarized in Table 2.

C Supplementary information

C.1 Other hyper parameters

We obtained an R^2 value of 0.93 for the prediction of T_c for the materials in SuperCon by the best preliminary model with the same train-test split (0.15) as that used in a previous study [15], because in the previous study, only the R^2 value of the best model (to our understanding), 0.88, was reported, which is less than our R^2 value of 0.93. For a train-test split of 0.05, the median of R^2 was 0.92 for 56 models, which is presented in the main text. For the prediction of T_c values for the materials in SuperCon by the model with garbage-in and a train-test split of 0.05, the median of R^2 was 0.85 for 55 models. For the prediction of superconductivity for the materials reported by Ref. [1], the reported scores are the median values for 29 models.

C.2 Prediction of superconductivity in FeSCs by deep learning model

The number of predicted FeSCs varied with the model because models trained with the same training data can become different depending on their initial weights and the input order of the training data. The models were stochastically constructed. However, once a model is constructed, the output is deterministic unless stochastic layers are used. Of note, we always found some high-T_c FeSCs that were predicted to have a finite T_c.

C.2.1 Check of models based on materials reported by Hosono et al.

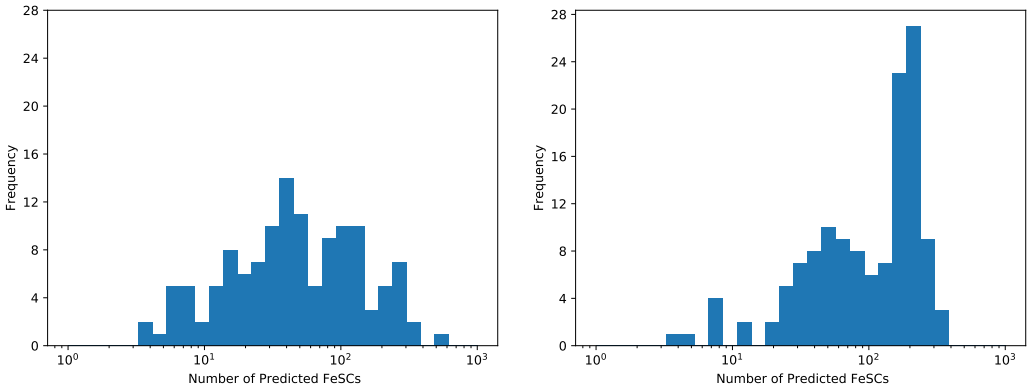
A model that predicts superconductivity for all materials or makes random predictions will have a precision that is equal to the baseline random precision. The validity of the models was checked using the materials reported by Hosono et al., which can be used to reject the model. We used the models to predict whether the materials on the list had a superconducting transition temperature of above 0 K, and checked whether the precision was higher than the baseline random precision. The mean precision was 0.5 for about 130 training and test runs and the baseline random precision was 0.32. The precision was about two times higher than the baseline. We also checked whether each model satisfied the condition that the precision be sufficiently higher than the baseline.

C.2.2 Predictions using various combinations of training data

To confirm the reliability of a model, we checked whether the model learned the feature of superconductivity by checking the effect of training data on the number of predicted FeSCs. We compared the predictions of five models trained using different data based on SuperCon and COD. The training data were as follows: (i) data before 2008 without LaFePFO and LaFePO; (ii) data before 2008 with LaFePFO and LaFePO; (iii) only conventional superconductors as of 2018; (iv) only cuprates as of 2018; and (v) both conventional superconductors and cuprates as of 2018. These models predicted the T_c values of the FeSCs in SuperCon. In total, about 130 training and test runs were used for (i) and (ii) and about 170 training and test runs were used for (iii), (iv), and (v).

Figure 6 shows the results for (i) and (ii). As shown, the number of predicted FeSCs in Fig. 6b is higher than that in Fig. 6a. The average number of FeSCs predicted to have finite T_c increased from 80 to 129. The median increased from 44 to 130. We checked the validity of the models using the materials reported by Hosono et al. When evaluating model (i), we removed materials containing Fe from the list. This was not done when evaluating model (ii). The baseline random precision and model precision were 0.32 and 0.5, respectively, for model (i), and 0.32 and 0.5, respectively, for model (ii). The model precision was sufficiently higher than the baseline, indicating that the models were valid.

These results show that these two materials had a large impact on the predictions. It is surprising, in view of deep learning, that 2 out of 60,000 training data points had such a significant influence on the model. However, this influence is reasonable because human experts can infer many FeSCs if they know that LaFePFO and LaFePO are superconductors. The results for (iii) and (v) are shown in Fig. 7. Model (iv) (trained with only cuprates) could not predict any FeSCs. As shown in the results of (iii) and (v), the average number of the FeSCs predicted to have finite T_c increased from 46 to 123 when cuprates were included in the training data. The median increased from 15 to 80. The model learned the feature of cuprates, and the number of predicted FeSCs was increased by the addition of cuprates. We checked the models using the materials reported by Hosono et al. We removed

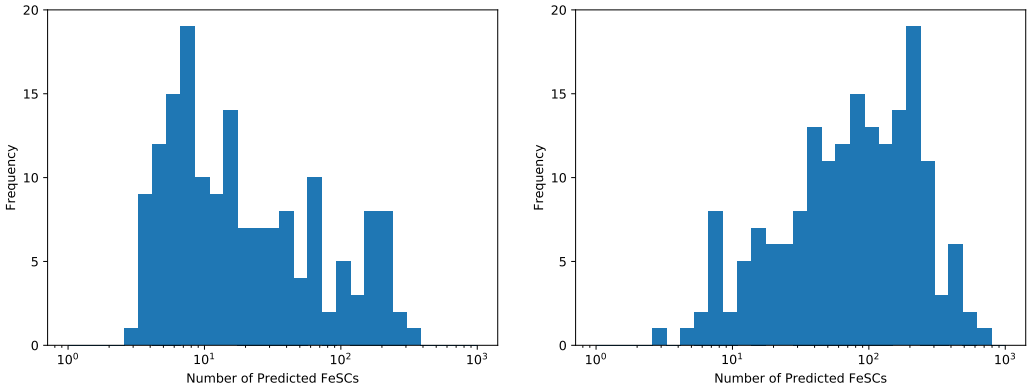


(a) Without LaFePFO and LaFePO. (b) With LaFePFO and LaFePO.

Figure 6: Comparison of histograms of predicted FeSCs by model trained with data before 2008 with and without LaFePFO and LaFePO (log scale).

materials containing Fe from the materials on the list. The baseline random precision was 0.2. The mean precision values were 0.41 and 0.35, respectively, for models (iii) and (v), indicating that the models were valid since they are three times higher than the baseline value.

The above results show that the addition of training data increased the number of FeSCs with finite T_c. We conclude that the model learned the feature of superconductivity. This confirms the reliability of the model, which was also confirmed by checking the precision of the prediction of superconductivities from the materials reported by Hosono et al.



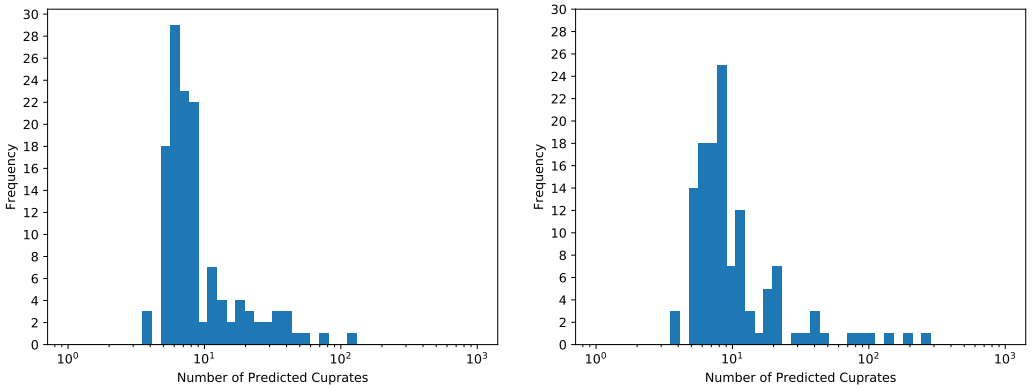
(a) Trained with conventional superconductors. (b) Trained with conventional and cuprate superconductors.

Figure 7: Histograms of predicted FeSCs (log scale).

C.3 Prediction of superconductivity in cuprates

It was checked whether the deep learning model could predict cuprates when trained with data that did not include cuprates. We trained models with the following data combinations: (i) only conventional superconductors; (ii) only FeSCs; and (iii) both conventional superconductors and FeSCs. The data were as of 2018. We repeated the training and test approximately 130 times. The results for models (i) and (iii) are shown in Fig. 8. Model (ii) (trained with only FeSCs) could not predict any cuprates with finite T_c, which is consistent with the prediction of FeSCs from cuprates. The average numbers of cuprates predicted to have finite T_c were 12 and 17 for models (i) and (iii), respectively. The

median values were 7 and 9, respectively. In contrast to the prediction of FeSCs, the mean and median values were almost unchanged by the addition of cuprates to the training data. In SuperCon, the number of FeSCs is less than a quarter of the number of cuprates, which might have led to the difference between the predictions of FeSCs and cuprates. The models were checked using the materials reported by Hosono et al. The baseline random precision was 0.20. The mean precision values were 0.41 and 0.52 for models (i) and (iii), respectively. The precision values are sufficiently higher than the baseline random precision. Although care should be taken when interpreting the results (i.e., deep learning predicted cuprates as candidate superconductors), the results show the possibility of exploring superconductors using deep learning.



(a) Trained with conventional superconductors.

(b) Trained with conventional and Fe-based superconductors.

Figure 8: Histograms of predicted cuprate superconductors (log scale).

C.4 The Features used in Random Forest

The 32 basic features of elements used for random forest classification are as follows.

> AtomicWeight, Column, DipolePolarizability, FirstIonizationEnergy, GSbandgap, GSenergy-pa, GSestBCClatcnt, GSestFCClatcnt, GSmagmom, GSvolume-pa, ICSDVolume, IsAlkali, IsDBlock, IsFBlock, IsMetal, IsMetalloid, IsNonmetal, MendeleevNumber, NdUnfilled, NdValence, NfUnfilled, NfValence, NpUnfilled, NpValence, NsUnfilled, NsValence, Number, NUnfilled, NValance, Polarizability, Row, FirstIonizationEnergies.

We used the weighted average, weighted variance, maximum, minimum, range, mode, median, and mean absolute difference of the basic features. Thus, in total, we used 256 features.