Annotation and Classification of Graphs of Property Values Reported in Material Science Literature

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RESEARCH

Annotation and Classification of Graphs of Property Values Reported in Material Science Literature

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Abstract

Building a system for extracting information from the scientific literature is an important research topic in the field of inorganic materials science. However, conventional extracting systems have a limitation in that they do not extract characteristic values from non-textual components, such as charts, diagrams, and tables, which provide key information in many scientific documents. Although there have been several studies on identifying the characteristic values of graphs in the literature, there is no general method that classifies graphs according to the property conditions of the values in the field of materials science. Therefore, in this study, we focus on the graphs that are figures representing graphically numerical data, such as a bar graph and line graph, as the first step towards developing a framework for extracting material property information from such non-contextual components. We propose deep-learning-based classification models for identifying the types of graph properties, such as temperature and time, by combining graph images, text in graphs, and captions in neural networks. To train and evaluate the models, we construct a material graph dataset with different types of material properties from a large collection of data from journals in the field of materials science. By using cloud sourcing, we annotated 16,668 images in about 3 days. Our experimental results demonstrate that the best model can achieve high performance with a micro-averaged F-score of 0.961.

Keywords: Annotation; Figure classification; Materials Informatics; Multimodal information; Information Extraction

¹Introduction

²Given the emergence of data science and machine learning in materials science,²
³increased importance is placed on obtaining data. Data in materials science are³
⁴particularly heterogeneous due to the significant wide range of classes of materials⁴
⁵and the variety of material properties. In recent studies, several extraction tools⁵
⁶have been applied, based on natural language processing from literature [1, 2, 3].⁶
⁷However, these data may appear in several ways in literature, such as tables and fig-⁷
⁸ures, which are often ignored in natural language processing, although they contain⁸
⁹a significant amount of data on experimental measurements of materials proper-⁹
¹⁰ties. In this study, we focus particularly on graphs, which are figures representing¹⁰
¹¹graphically numerical data, such as a bar graph and line graph, because they are of-¹¹
¹²ten employed to show the evidence supporting the main claims in materials science¹²
¹³literature and thus often include the most important information in the literature.¹³
¹⁴Several methods have recently been reported to automatically consume and codify¹⁴
¹⁵information in figures of scientific literature across domains, such as image classi-¹⁵
¹⁶fication and optical character recognition [4, 5], based on techniques adapted from¹⁶
¹⁷the field of computer vision. These methods have immense potential to obtain data¹⁷
¹⁸necessary for data-driven materials research based on the literature. Furthermore,¹⁸
¹⁹there have been several studies on identifying the characteristic values from fig-¹⁹
²⁰ures and tables in literature using machine-learning-based approaches; for example,²⁰
²¹parsing result figures [6], extracting the values from tables [7], classifying the fig-²¹
²²ures of biomedical articles on five predefined figure types [8], and quantifying data²²
²³from microscopy images [9]. However, in the field of materials science, there is no²³
²⁴reported general method for identifying the characteristic values of graphs.²⁴

²⁵In this study, as the first step towards automatic information extraction from²⁵
²⁶graphs, we focus on automatically extracting and classifying graphs in the materials²⁶
²⁷science literature. To achieve this, we construct a dataset that classifies graphs²⁷
²⁸according to types of conditions. We define new conditions for graph classification²⁸
²⁹based on the examination of actual graphs reported in the “Journal of Material²⁹
³⁰Chemistry A (2015-2019)”^[1] in this paper (see Figures 3 and 4). We annotated the³⁰
³¹types based on the images and captions. Furthermore, we propose deep-learning-³¹
³²based classification models that utilize multimodal information of graphs, consisting³²

³³^[1]<https://www.rsc.org/journals-books-databases/about-journals/journal-of-materials-chemistry-a/>³³

of graph images, text in graphs, and captions. A representative process for the¹
classification of graphs is shown in Fig. 1. We first prepare baseline models for²
each modal information, which are popularly employed as baselines for natural³
language processing and image processing. We then consider two models to combine⁴
the unimodal information: one integrates the feature representations of unimodal⁵
models, while the other aggregates the prediction results of unimodal models. The⁶
best multimodal model classified graphs with a micro-F1 score of 96.1% using the⁷
proposed dataset, which represents a better performance than unimodal models.⁸

The primary contributions of this study can be summarized as follows:

- We construct a dataset classifying graphs reported in the materials science literature using pre-defined conditions.
- The experimental results show that the constructed dataset can be used to train a deep-learning-based model, which classifies graphs according to their characteristic conditions with a micro-F1 score of 96.1%. This demonstrates that the dataset is useful for training the deep-learning-based model.
- We show that using the multimodal information of graphs can improve the classification performance.

Methods

Constructing graph dataset

Our dataset is a set of triples of graph images, captions, and labels, obtained based on property conditions. The overview of the construction of the property value graph dataset from published papers is shown in Fig. 2. The dataset is constructed by extracting graph images from a large collection of published journal papers in the field of materials science. Then, we label the images leveraging crowdsourcing, enabling the creation of large datasets in short periods. In the following sections, we explain the construction in detail.

Label definition

To classify the images according to their corresponding conditions, we define the types of graphs using the following conditions. Examples of each type and graph are shown in Figures 3 and 4.

- ¹ *Temperature:* The temperature condition is a parameter for heat treatment, which¹
² is a process of heating and cooling a material to improve its properties (see²
³ Figure 3(a)).³
- ⁴ *Time:* The time condition is a parameter for the time course of each process and⁴
⁵ measurement in materials synthesis (see Figure 3(b)).⁵
- ⁶ *Angle:* The angle condition is a parameter for analyzing the X-ray diffraction⁶
⁷ patterns to determine the state and physical properties of materials (see Figure⁷
⁸ 3(c)).⁸
- ⁹ *Wavelength:* The wavelength condition is a parameter often used to analyze the⁹
¹⁰ components of materials (see Figure 3(d)) by various methods, such as ab-¹⁰
¹¹ sorption spectroscopy.¹¹
- ¹² *Capacity:* The capacity condition is a parameter related to battery performance.¹²
¹³ To represent the performance, charge and discharge curves are often drawn¹³
¹⁴ (Figure 3(f)).¹⁴
- ¹⁵ *Pressure:* The pressure condition is a parameter related to the absorption and¹⁵
¹⁶ desorption operations on the surfaces of materials. For example, it is shown¹⁶
¹⁷ on the horizontal axes of adsorption–desorption isotherms (see Figure 3(g)).¹⁷
- ¹⁸ *Ohm:* The ohm condition is a parameter related to the performance of materials as¹⁸
¹⁹ counter electrodes. To analyze it, Nyquist plots are drawn many times (Figure¹⁹
²⁰ 3(g)).²⁰
- ²¹ *Voltage:* The voltage condition is a parameter that reveals the electrochemical²¹
²² reaction mechanism of materials. For this purpose, discharge and charge curves²²
²³ are drawn (Figure 3(h)).²³
- ²⁴ *Energy:* The energy condition is used in several methods for the analysis of the²⁴
²⁵ compositions of materials, such as X-ray spectroscopy and X-ray Absorption²⁵
²⁶ Near Edge Structure (Figure 3(i)).²⁶
- ²⁷ *Raman shift:* The Raman shift condition is a parameter used in Raman spec-²⁷
²⁸ troscopy, which measures Raman intensity to evaluate the physical properties²⁸
²⁹ of materials (Figure 3(j)).²⁹
- ³⁰ *Cycle:* The cycle condition is a parameter used for the evaluation of the material³⁰
³¹ durability against various indices (Figure 4(k)).³¹
- ³² *Other:* Graphs of measurement conditions other than the 11 listed above (Figure³²
³³ 4(l)).³³

1 Additionally, we define a label “*Not target*” in classifying the figures reported in¹
 2 the paper, which indicates figures that are not graphs. Such figures include pho-²
 3 tographs, images of compounds, and diagrams with multiple figures, as shown in³
 4 Fig. 4. 4

5 *Collecting paper data* 6

7 The journal named “Journal of Material Chemistry A (2015-2019)”^[2] from the⁷
 8 Royal Society of Chemistry (RSC), which mainly publishes papers dealing with the⁸
 9 synthesis of materials for batteries was selected as the target. The papers provided⁹
 10 by RSC are in the XML format and contain figures, tables, and schemes. The¹⁰
 11 statistics of the target article data are listed in Table 1. 11

12 Table 1: Statistics of the target article data 12

13	Papers	14,071	13
14	Figures	91,019	14
15	Tables	12,082	15
16	Schemes	4,180	16

17 As shown in Fig. 5, a figure extracted from the paper may contain a single graph¹⁷
 18 or multiple graphs, referred to as “one-graph figure” or “multiple-graph figure,”¹⁸
 19 respectively. 19

20 *Splitting one-graph and multiple-graph figures* 20

21 We aim to construct a dataset containing only one-graph figures to avoid any dif-²¹
 22 ficulties in splitting multiple-graph figures. Thus, the selection was completed as²²
 23 follows. 23

24 First, one-graph and multiple-graph figures were extracted using different meth-²⁴
 25 ods. One-graph figures were extracted using the Compound Figure Separator (CFS)²⁵
 26 proposed by Tsutsui et al. [10]. The figures that were classified as 0 or 1 figure by²⁶
 27 CFS were chosen as one-graph figures. We extracted 8,634 one-graph figures from²⁷
 28 91,019 figures obtained from 14,071 papers, as shown in Table 1. Multiple-graph²⁸
 29 figures were extracted by applying regular expressions to the figure captions. This²⁹
 30 rule judges whether a caption contains “(a-z)” or “(A-Z)” and extracts the cor-³⁰
 31 responding figures as multiple-graph figures. For example, if we apply the rule to³¹
 32 the caption “(a) X-ray diffraction patterns of samples; SEM images of (b) carbon³²
 33 33

^[2]<https://www.rsc.org/journals-books-databases/about-journals/journal-of-materials-chemistry-a/>

spheres, (c and d) MnO_2 , and (e and f) MnO_2/C composite” (Figure 1 of [11]), the figure is extracted as a multiple-graph figure because it contains four instances of “(a-z)” or “(A-Z)” in the caption. As a result, 64,361 multiple-graph figures were extracted.

Next, we designed a binary classification model for one-graph and multiple-graph figures using Lobe^[3], which is a machine learning tool for easily training the custom image classifier. We randomly sampled 1,000 one-graph images and 1,000 multiple-graph images to train the classifier. We applied the trained classifier using Lobe to the 91,091 images from 14,071 papers and extracted 16,668 one-graph figures.

Annotation details

Annotation was performed using crowdsourcing to reduce the time required. We employed annotators via the Amazon Mechanical Turk^[4] to label the extracted graph images. To ensure the quality of the dataset, a maximum of nine annotators were used to annotate one figure. The annotation process took about three days, and 732 annotators participated in this task.

Label integration

Our dataset contains up to nine labels per figure, but there are cases with variations in labels due to the complexity of the figure, misunderstandings, etc. Therefore, we implemented majority voting, which is a typical quality management method for crowdsourcing. Majority voting is implemented by selecting the label with the highest number of occurrences among the annotated labels. In addition, we set a threshold on the agreement rate in the majority vote and extracted only annotation data with agreement rates above the threshold. To determine the threshold, 100 figures were annotated by two annotators. The agreement between the two annotators was 83%. Considering that the number of annotators is more than two, we set the threshold to 80% Table 2 shows the size of the dataset after label integration.

Evaluation of the dataset

First, we randomly sampled 100 figures in the dataset and annotated them using an annotator. We evaluated the annotations by comparing them with the labels of

^[3]<https://www.lobe.ai/>

^[4]<https://www.mturk.com/>

Table 2: Dataset statistics

label	instances
Temperature	792
Time	966
Angle	717
Wavelength	1,035
Capacity	55
Pressure	246
Ohm	192
Voltage	369
Energy	241
Raman shift	172
Cycle	269
Other	193
Not target	1,805
all	7,052

the dataset. The results show that the accuracy of the labels in the dataset was 99%^[5], indicating that the labeling is accurate.

Classification with unimodal information

We utilize three types of information: graph images, graph text extracted using Textract^[6], and captions for classification. In this section, we discuss classification using each of the three types of information. We prepared different classification models for each type of information (unimodal information). In the following sections, we describe graph image classification, graph text classification, and caption classification in order.

Graph image classification

For image-based classification, we use two models, viz. ResNet[12] and EfficientNet[13], which have been reported to perform well in image-based tasks and can easily employ transfer learning. We trained these models by fine-tuning them on the constructed dataset.

^[5]Please note that the 100 figures sampled here are different from those in the last section. The figures in the last section are noisy. They include difficult cases that cause disagreement among annotators in crowd sourcing

^[6]<https://aws.amazon.com/textract/>

¹ ResNet is a model that can learn deep layered models by introducing residual¹
²connections. In our experiment, the images were resized to 224×224 pixels, and²
³we employed ResNet50. 3

⁴ EfficientNet is a model that achieves high performance with fewer parameters⁴
⁵than conventional models through model scaling. EfficientNet-B0 was used in our⁵
⁶experiments for the same reason as ResNet. 6

⁷ Here, we describe the flow of prediction using these two models. 7

⁸ First, we create a feature vector $\hat{\mathbf{x}}$ from the input image tensor $\mathbf{x}$ using these two⁸
⁹models. Since each input image is an RGB image resized to 224×224 pixels, the⁹
¹⁰dimensions of the input image tensor $\mathbf{x}$ are $(224, 224, 3)$. 10
¹¹ 11

$$\hat{\mathbf{x}} = Model(\mathbf{x}) \quad (1)$$

¹² Please note that the dimensions of the feature vector $\hat{\mathbf{x}}$ are different for these two¹²
¹³models. 13
¹⁴ 14

¹⁵ The feature vector $\hat{\mathbf{x}}$ is then passed to a single-layer fully connected (FC) network,¹⁵
¹⁶and finally, the probability $\mathbf{p}$ of each label is calculated by applying a softmax¹⁶
¹⁷function for prediction. 17
¹⁸ 18

$$\mathbf{o} = FC(\hat{\mathbf{x}}) \quad (2)$$

$$\mathbf{p}(\mathbf{y} | \mathbf{x}; \boldsymbol{\theta}) = softmax(\mathbf{o}) \quad (3)$$

¹⁹ Here, $\boldsymbol{\theta}$ represents the parameters of the model, and $\mathbf{y}$ represents a set of candidate¹⁹
²⁰labels for prediction. We choose the label with the highest probability $\mathbf{p}$ for the input²⁰
²¹sentence representation $\mathbf{x}$ as the prediction result. 21
²² 22

²³Graph text classification 23

²⁴ In this section, we explain the flow of prediction using text extracted by Textract²⁴
²⁵from the graph images. 25

²⁶ Since Textract extracts text word by word without any contextual information,²⁶
²⁷the feature vector of the text $\mathbf{t}$ is represented by a bag-of-words (BoW) or a term²⁷
²⁸frequency-inverse document frequency (TF-IDF). 28
²⁹ 29

The probability $\mathbf{p}$ of each label is predicted by passing the feature vector $\mathbf{t}$ through a two-layer fully connected network and applying a softmax function to the output.

3

$$\hat{\mathbf{t}} = FC_1(\mathbf{t}) \quad (4)$$

$$\mathbf{o} = FC_2(ReLU(\hat{\mathbf{t}})) \quad (5)$$

$$\mathbf{p}(\mathbf{y} | \mathbf{x}; \boldsymbol{\theta}) = softmax(\mathbf{o}) \quad (6)$$

7

Here, $ReLU$ is the nonlinear activation function

9

Caption classification

Two models are used for classification with caption texts: a convolutional neural

network (CNN) as a baseline, and a CNN with Mat-Word2Vec [14] (Mat-CNN),

which is domain-specific word embedding for materials science.

The CNN creates feature representations of sentences from randomly initialized

word representations and predicts the labels based on the representations. In the

following paragraphs, we explain the prediction process.

First, we obtain the representation of an input sentence $\mathbf{s}$ using random word

representations.

19

$$\mathbf{s} = [\mathbf{w}_0^T, \mathbf{w}_1^T, \dots, \mathbf{w}_{N-1}^T] \quad (7)$$

where $\mathbf{s}$ is the list of 100-dimensional vector representations $\mathbf{w}$ of words, and N is

the maximum sentence length.

Next, we generate a feature vector of the sentence $\hat{\mathbf{s}}$ using the CNN from the word

representations $\mathbf{s}$.

$$\hat{\mathbf{s}} = CNN(\mathbf{s}) \quad (8)$$

Finally, as shown in Eqs. (2) and (3), the feature vector $\mathbf{s}$ is passed through a

single-layer FC neural network, and the probability $\mathbf{p}$ of each label is calculated by

applying a softmax function to the output. We choose the label with the highest

probability $\mathbf{p}$ for the input sentence representation $\mathbf{s}$ as the prediction result.

For Mat-CNN, we initialize the word representation $\mathbf{w}$ of Materials Science Word

Embeddings, acquired by Kim et al. from literature using Word2Vec [14]. We pre-

dicted the relation in the same manner as for the CNN described above.

¹Classification with two types of multimodal information

²We consider the prediction based on any two out of the following three types of
³information: graph image, graph text, and captions.

⁴The feature representation vectors of two types of information are combined to
⁵produce the final feature representation vector $\mathbf{h}_1$. For instance, to create a feature
⁶representation vector from an image and its caption, we combine their representa-
⁷tions, as shown in Eqs. (1) and (8): $\mathbf{h}_1 = [\mathbf{x}; \hat{\mathbf{s}}]$.

⁸Finally, we pass the feature vector $\mathbf{h}_1$ through a single-layer FC neural network,
⁹according to Eqs. (2) and (3), and apply a softmax function to the output to predict
¹⁰the probability $\mathbf{p}$ of each label.

¹³Classification with multimodal information

¹⁴We adopt two approaches to combine the three types of information: one involves
¹⁵combining features similar to the case of two multimodal models, and the other
¹⁶involves ensembling each type of model.

¹⁷The method for combining the features is the same as that for using two types
¹⁸of information. Using Eqs. (1), (4) and (8), the feature vector for prediction is
¹⁹represented as $\mathbf{h}_1 = [\mathbf{x}; \hat{\mathbf{t}}; \hat{\mathbf{s}}]$. We refer to this method as the **Concat** method.

²⁰In the second method, predictions are made by multiple models trained separately
²¹on each type of information, and the final prediction label is determined by their
²²majority vote. We refer to this method as the **Ensemble** method.

²⁵Implementation Details

²⁶We used a g4dn.4xlarge instance of Amazon Elastic Compute Cloud (Amazon
²⁷EC2)^[7] as the computing environment. The g4dn.4xlarge instance contains Second-
²⁸Generation Intel Xeon Scalable (Cascade Lake) processors and an NVIDIA T4 Ten-
²⁹sor Core GPU. We used the machine learning library PyTorch^[8] to implement the
³⁰model described above.

³²^[7]<https://aws.amazon.com/ec2/?ec2-whats-new.sort-by=item.additionalFields.postDateTime&>

³³[ec2-whats-new.sort-order=desc](https://pytorch.org/)

^[8]<https://pytorch.org/>

Table 3: Search range for hyper-parameters

Optimizer	Adam[17], Momentum SGD [18]
Learning rate	$1e^{-4} - 1e^{-2}$
Weight decay	$1e^{-10} - 1e^{-3}$
Batch size	[16, 32]
Dropout rate	0.0 – 0.5
Convolution filter size	[3, 5, 7]
Number of filters	[50, 100, 200]

Results and discussion

In this section, we evaluate the performance of the trained graph classifier using the constructed dataset.

Experimental setup

In this section, we explain the evaluation method and the setting of various hyper-parameters for evaluation.

Evaluation method

We employed the holdout method to evaluate the classification performance and the F-score was used as an evaluation index. The dataset was divided into training, development, and test datasets in a ratio of 6:2:2, such that the labels were distributed close to each other.

Setting various hyperparameters

The hyper-parameters during training were determined by choosing them from the parameters presented in Table 3. We aimed at producing the highest micro-averaged F-scores on the development dataset. Tuning was performed by pruning the branches with the Successive Halving [15] algorithm, implemented in a hyper-parameter optimization framework Optuna[16]. During tuning, early stopping was performed at 20 epochs.

Graph image classification

We trained and evaluated EfficientNet and ResNet for graph image classification; the results are listed in Table 4. EfficientNet showed the higher performance between the two models for all labels, while the labels of “Not target” and “Voltage” are low. This suggested that it is difficult to extract the features of “Not target”

Table 4: Classification using graph images

	EfficientNet	ResNet
Temperature	0.911	0.888
Time	0.924	0.867
Angle	0.958	0.975
Wavelength	0.966	0.959
Capacity	0.400	0.556
Pressure	0.759	0.637
Ohm	0.933	0.933
Voltage	0.859	0.797
Energy	0.760	0.779
Raman shift	0.857	0.800
Cycle	0.829	0.863
Other	0.286	0.143
Not target	0.949	0.975
Macro	0.799	0.782
Micro	0.900	0.892

and “Voltage” from the images, and the images of “Not target” are considered to contain other diagrams (e.g., microscopic images, flowcharts, and other diagrams with diverse variations), which may increase the difficulty of classification. The images of “Voltage” were also considered more difficult to classify than the other images because they are similar to some images of “Energy”. The micro-averaged and macro-averaged F-scores for each label did not differ significantly among the models. However, the F-score for each label varied, indicating that each model was accurate for different labels.

In addition, to check the tendency of misclassification in the graph images, we employ the confusion matrix of EfficientNet, which shows the highest classification performance (Figure 6). The vertical axis shows the correct labels and the horizontal axis shows the labels predicted by the model. Figure 6 shows that there were many errors in “Other” classification. In particular, there are many cases where “Other” is mistakenly predicted as “Capacity” or “Cycle” and “Time” is mistakenly predicted as “Other”. “Other” contains various graphs that do not belong to the labels defined according to the material properties. Therefore, We consider that graphs that are similar in general shape with “Capacity”, “Cycle”, and “Time” are also included in “Other”, which may have caused the error. Such error cases suggest that it is very difficult to classify information related to the context of the graph, such as properties, based on the general shape of the graph using images.

Table 5: Graph text classification

	BoW	TF-IDF
Temperature	0.948	0.922
Time	0.948	0.923
Angle	0.940	0.935
Wavelength	0.990	0.945
Capacity	0.800	0.737
Pressure	0.980	0.948
Ohm	0.829	0.817
Voltage	0.855	0.748
Energy	0.882	0.857
Raman shift	0.985	0.970
Cycle	0.826	0.826
Other	0.543	0.475
Not target	0.940	0.893
Macro	0.882	0.846
Micro	0.928	0.894

Graph text classification

The text extracted by Textract was classified by creating a feature representation using BoW and TF-IDF; the results are listed in Table 5. For all the labels, BoW produced higher F-scores than TF-IDF.

Similar to image classification, we show the confusion matrix of BoW, which has the highest classification performance, in Figure 7. There were many errors in the “Other” class. Particularly, there were many cases where “Other” was misclassified as “Angle” or “Not target”. Many of the images of “Angle” have intensity on the vertical axes. On the other hand, the images of “Other” occasionally have the intensity as that in the vertical axis. Therefore, we consider that the BoW of the “Other” sometimes resembles that of the “Angle”, causing misclassification between them. We believe that “Other” is mistaken as “Not target” because it is difficult to create features for both. In addition, there are many cases where “Voltage” was misclassified as “Not target”. The images of “Voltage” occasionally have some text in images of figures. We consider that the model misclassified “Voltage” as “Not target” because there are many images containing little or no text in “Not target”, such as microscopic images and flowcharts.

Caption classification

We trained and evaluated CNN and Mat-CNN using only the figure captions; the results are shown in Table 6, with Mat-CNN showing the best performance. For all

Table 6: Classification using captions

	CNN	Mat-CNN
Temperature	0.792	0.816
Time	0.707	0.769
Angle	0.944	0.955
Wavelength	0.899	0.901
Capacity	0.167	0.167
Pressure	0.800	0.839
Ohm	0.961	0.950
Voltage	0.738	0.803
Energy	0.744	0.763
Raman shift	0.853	0.811
Cycle	0.660	0.726
Other	0.000	0.207
Not target	0.870	0.928
Macro	0.703	0.741
Micro	0.817	0.851

the labels except “*Ohm*” and “*Raman shift*”, Mat-CNN showed a higher F-score than CNN, indicating that the word representations pre-trained from literature are useful for figure classification.

We show the confusion matrix of Mat-CNN in Figure 8. Several errors were observed for “*Time*”. Particularly, there were many cases in which time was misclassified as “*Cycle*”, “*Not target*”, “*Other*”, or “*Voltage*”. In several cases, the model also predicted “*Time*” erroneously. In particular, there were cases in which “*Cycle*”, “*Not target*”, “*Other*”, or “*Voltage*” were misclassified as “*Time*”. The distribution of labels that are easily mispredicted as “*Time*” and those that are easily mispredicted by “*Time*” are similar, suggesting that the contextual feature representation of “*Time*”’s captions is similar to that of misclassified labels.

Classification with two multimodal information

When considering two types of information, we used the model that showed the best performance for individual training. Specifically, the EfficientNet, BoW, and Mat-CNN models were used for the image of the figure, the text extracted by Textextract from the images, and the captions, respectively.

The results are shown in Table 7. Image+Text and Text+Caption showed similar overall performances, but Text+Caption showed slightly higher micro-averaged and macro-averaged F-scores for each label. Furthermore, the F-score of Caption+Image was much lower than those of Image+Text and Text+Caption, indicating that the

Table 7: Classification with two types of multimodal information

	Image+Text	Text+Caption	Caption+Image
Temperature	0.959	0.968	0.891
Time	0.941	0.944	0.828
Angle	0.953	0.986	0.989
Wavelength	0.990	0.990	0.936
Capacity	0.737	0.800	0.533
Pressure	0.990	0.980	0.830
Ohm	0.909	0.987	0.947
Voltage	0.901	0.901	0.855
Energy	0.894	0.939	0.865
Raman shift	0.985	0.985	0.831
Cycle	0.900	0.863	0.775
Other	0.541	0.590	0.130
Not target	0.985	0.967	0.989
Macro	0.899	0.915	0.800
Micro	0.949	0.954	0.901

text extracted from the images is useful for graph classification. The F-score for each label varied, indicating that the best label depended on how the information was combined.

Classification model with all multimodal information

Prediction was performed using all three types of information: the images of the figures, the text extracted by Textract from the images, and the captions. Similar to the classification with two multimodal information, we used the model that showed the best performance for individual training.

The results are shown in Table 8. The F-scores of the Concat method were higher than those for the classification with one or two types of multimodal information, indicating that both types of information are useful for figure classification. The Concat method showed higher performance in terms of both micro-averaged and macro-averaged F-scores for each label than the ensemble method, indicating that learning by creating a representation that integrates the three types of information is more accurate than that by using the three pieces of information individually.

Conclusions

In this paper, we proposed an approach to classify graphs according to their property conditions. We constructed a manually annotated dataset for classification using property conditions and evaluated the same. We also proposed and evaluated deep-

Table 8: Classification with all multimodal information

	Concat	Ensemble
Temperature	0.962	0.952
Time	0.959	0.929
Angle	0.997	0.990
Wavelength	0.993	0.988
Capacity	0.700	0.625
Pressure	0.970	0.879
Ohm	0.974	1.000
Voltage	0.940	0.944
Energy	0.918	0.957
Raman shift	0.985	0.971
Cycle	0.907	0.916
Other	0.603	0.415
Not target	0.981	0.969
Macro	0.914	0.887
Micro	0.961	0.950

learning-based classification models in both unimodal and multimodal settings. To the best of our knowledge, this is the first study to classify graphs according to their property conditions using multimodal information with deep learning models.

The results showed that the models label the graphs and classify property conditions, with micro-averaged F-score as high as 0.961. Furthermore, we showed that the simultaneous use of the graph images, the text in the graphs, and the captions can improve the classification performance.

In future, we will improve these classification models. We consider several ways to improve the performance of these models. First, we will investigate the method to achieve more effective use of multimodal information. Second, we will consider incorporating the in-text citations of figures in the manuscript. Third, we will construct a model that can handle multiple-graph figures. We will also consider the automatic extraction of information from graphs and other non-textual components.

Abbreviations

- RSC:** Royal Society of Chemistry
CFS: Compound Figure Separator
FC: fully connected
BoW: bag-of-words
TF-IDF: term frequency-inverse document frequency
CNN: convolutional neural network
Mat-CNN: convolutional neural network with Mat-Word2Vec

¹ Declarations	1
² Acknowledgements	2
Not applicable.	
³	3
⁴ Funding	4
Not applicable.	
⁵	5
⁶ Availability of data and materials	6
The paper data of RSC in an XML format that we used to build the dataset is not free. Therefore, we released the	
⁷ script to reproduce our dataset from the paper data that can be purchased from the RSC at	7
⁸ https://github.com/NaokiIinuma/property-values-graphs_dataset .	8
⁹ Competing interests	9
The authors declare that they have no competing interests.	
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¹¹ Consent for publication	11
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¹²	12
¹³ Authors' contributions	13
All authors contributed to the production of the manuscript. KF, JO and MM supervised all steps of the work. NI	
¹⁴ built the system and carried out the experiments. All authors read and approved the final manuscript.	14
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Figures

abstract.pdf

Figure 1: Example of classification process of graphs

dataflow.pdf

Figure 2: Overview of dataset construction

fig-sample1.pdf

Figure 3: Examples graph images 1

(a)[19], (b)[20], (c)[21], (d)[20], (e)[22], (f)[23], (g)[24], (h)[25], (i)[26], (j)[21],
(k)[27], (l)[28]

fig-sample2.pdf

Figure 4: Example graph images 2

(a)[20], (b)[29], (c)[30]

one-multi.pdf

Figure 5: Sample of “one-graph figure” and “multiple-graph figure”

(a)[31], (b)[32]

Figures

Figure 1

Example of classification process of graphs

Figure 2

Overview of dataset construction

Figure 3

Examples graph images 1 (a)[19], (b)[20], (c)[21], (d)[20], (e)[22], (f)[23], (g)[24], (h)[25], (i)[26], (j)[21], (k) [27], (l)[28]

Figure 4

Example graph images 2 (a)[20], (b)[29], (c)[30]

Figure 5

Sample of "one-graph figure" and "multiple-graph figure" (a)[31], (b)[32]

Figure 6

Confusion matrix of gold labels (vertical axis) vs. EfficientNet predictions (horizontal axis)

Figure 7

Confusion matrix of gold labels (vertical axis) vs. BoW predictions (horizontal axis)

Figure 8

Confusion matrix of gold labels (vertical axis) vs. Mat-CNN predictions (horizontal axis)