Symbolic Integration by Integrating Learning Models with Different Strengths and Weaknesses

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ABSTRACT Integration is indispensable, not only in mathematics, but also in a wide range of other fields. A deep learning method has recently been developed and shown to be capable of integrating mathematical functions that could not previously be integrated on a computer. However, that method treats integration as equivalent to natural language translation and does not reflect mathematical information. In this study, we adjusted the learning model to take mathematical information into account and developed a wide range of learning models that learn the order of numerical operations more robustly. In this way, we achieved a 98.80% correct answer rate with symbolic integration, a higher rate than that of any existing method. We judged the correctness of the integration based on whether the derivative of the primitive function was consistent with the integrand. By building an integrated model based on this strategy, we achieved a 99.79% rate of correct answers with symbolic integration. In summary, we have developed a more accurate method of selecting the correct model than the existing method by judging the result of symbolic integration based on whether the output of the model equals the input formula when the output is differentiated.

INDEX TERMS Deep Learning, Encoder-Decoder, Supervised Learning, Symbolic Integration, Translation Model

I. INTRODUCTION

Integration is required in simulations to predict the behavior of objects in fields such as computer science, aeronautics, mechanical engineering, and systems biology [1]–[4]. Traditionally, numerical integration has been carried out on computers. Various methods of numerical integration have been proposed to approximate small changes of any mathematical function (the integrand) to be integrated. The approximation of small changes, however, always leads to errors. Furthermore, numerical integration requires an initial value of the integrand, i.e., it obtains only particular solutions. A resolution of these problems and limitations is symbolic integration, by which an exact, general solution can be derived. In computerized symbolic integration, the integrand is transformed via a theorem to obtain an integrated function, which is called a primitive function. This symbolic integration process, formulated by Robert Risch in 1970 [5], is known as Risch’s algorithm, and software based on this algorithm, Maxima (http://maxima.sourceforge.net/), has been developed. However, Maxima relies on approximations because Risch’s algorithm involves finding roots, and there is currently no method to derive an analytical expression for a root. Some integrands, therefore, cannot be integrated. Programs have been developed for Mathematica (https://wolfram.com/mathematica/) and Matlab (https://mathworks.com/products/matlab/) as well as by Rubi [6] to perform symbolic integration, but even these programs cannot integrate some functions.

In contrast, deep learning has been widely used in natural language processing to formulate algorithms for language translation [7], [8]. Deep-learning models such as Recurrent Neural Network (RNN) and Transformer have been shown to be Turing-complete and are expected to facilitate learning arbitrary algorithms [9]. Saxton et al. have successfully used Long Short-Term Memory (LSTM), a type of RNN, and the Transformer model to solve a wide range of mathematical
In summary, we proposed a new input format, a subtree method, in which mathematical expressions are input as binary trees with inclusion of mathematical syntactic rules, and we constructed various deep learning models that enable symbolic integration, including this method. We have been able to develop a more accurate method of selecting the correct model than the existing one by using the property that the result of symbolic integration can be judged by the correct answer percentage by ∼1.0% to 99.79%, which exceeded the improvement (0.5%) of the correct answer rate achieved with any single learning model and with the runner-up, Mathematica (98.30%).
A. CREATION OF A DATASET OF INTEGRANDS AND PRIMITIVE FUNCTIONS

To comprehensively generate data for pairs of integrands and primitive functions, we created primitive functions by multiplying up to five elementary functions chosen from \( x, \sin x, \cos x, \tan x, \log(x), \exp(x), \sqrt{x}, \sqrt[3]{x} \), and a function equal to 1 divided by these elementary functions. We then differentiated the created primitive functions using the \( D \) function in Mathematica to obtain the integrand paired with the primitive function. Finally, for the obtained pairs of integrands and primitive functions, we used Mathematica’s \texttt{simplify} function to simplify the functions and remove redundant pairs of integrands and primitive functions. The above procedure created 12,122 nonredundant, independent functions as pairs of integrands and primitive functions. The 12,122 functions were formatted into the description of functions in the model of Lample et al. [11] (string) and the subtree proposed in this study.

The 12,122 functions were divided into strings of tokens, i.e., the smallest units that make sense as mathematical symbols (Supplementary Table 1). We created a string polish dataset in which the functions were expressed as strings in Polish notation and a string IRPP dataset in which the integrand was expressed as a string in reverse Polish notation and the primitive function in Polish notation (Supplementary Fig. 1).

To create the subtree data, we transformed the 12,122 functions into an Abstract Syntax Tree (AST) consisting of binary trees using the \texttt{parseFormula} function of libSBML [18]. We defined a group of three nodes of the AST as a subtree: a parent node, a left child node, and a right child node. The three tokens of the operator or its subject in the order parent node, left child node, and right child node in the subtree were defined as one unit of input to the learning model in the subtree method. We then created a subtree polish dataset consisting of strings obtained by a forward search of the ASTs of the integrands and primitive functions per subtree units. We also created a subtree IRPP dataset consisting of strings obtained by backward and forward searches of the ASTs of the integrands and primitive functions per subtree units, respectively. In this case, if one or both of the left or right child nodes were missing when a node was targeted as the parent node, an “End of Sentence” (EOS) token was added to the missing part of the string (Supplementary Fig. 1).

B. LEARNING MODEL

The LSTM and Transformer models that we constructed took the integrand as input and outputted the corresponding primitive function. The LSTM model consisted of an embedding layer, an LSTM layer, an attention layer, and a fully connected layer; it was identical to the model in a previous study [19], except for the embedding layer and the fully connected layer when the input-output scheme was adopted in a subtree. First, the subtree expressed as a one-hot vector was input to the embedding layer, and then the output was input to the LSTM encoder layer, which finally output the context vector of the subtree. The output context vector and the output from the LSTM decoder layer were then input to the attention layer, which output the element product of these vectors. This output was then input to the fully connected layer, which divided the output into three parts and input them to the softmax function to output the token corresponding to each node of the subtree (Fig. 2).

Four LSTM models were developed: a model with string polish datasets as input and output (LSTM string polish model), a model with a string IRPP dataset (LSTM string IRPP model), a model with a subtree polish dataset (LSTM subtree polish model), and a model with a subtree IRPP dataset (LSTM subtree IRPP model). All hyperparameters in these models were determined by Optuna [20] with a Tree-structured Parzen Estimator (TPE), which uses Bayesian optimization (Supplementary Table 2).

The Transformer model was composed of an embedding layer: a multi-head attention layer composed of parallel, self-attention layers; a block composed of feed-forward layers; and fully connected layers. Except for the embedding layer and the fully connected layer, the rest of the model was the same as the model in a previous study [11]. First, each token that constituted a subtree was expressed as a one-hot vector and was input to the embedding layer. The decoder received the aforementioned input and input it to the multi-head attention layer, and the output from each of these layers was used as input to the subsequent multi-head attention layer. Finally, the output from the last multi-head attention layer was input to the fully connected layers, and this output was split into three parts and input to the softmax function to output the corresponding tokens in the node of the subtree (Supplementary Fig. 2). Four models were developed for the Transformer model and the LSTM model: a model with string polish datasets as input and output (Transformer string polish model), a model with string IRPP datasets (Transformer string IRPP model), a model with...
In (1), the input to the activation function softmax was \( X \) were represented by the following equation:

\[
L = -\frac{1}{m} \sum_{ij} t_{ij} \log y_{ij} \tag{1}
\]

\[
y_{ij} = \frac{\exp(x_{ij})}{\sum_{k=1}^{n} \exp(x_{ik})}
\]

In (1), the input to the activation function softmax was \( X \in \mathbb{R}^{m \times n} \), the output was \( Y \in \mathbb{R}^{m \times n} \), and the training data were \( T \in \mathbb{R}^{m \times n} \). Here, \( m \) is the number of minibatches and \( n \) is the number of dimensions of the hidden state vector.

The training was carried out for 200 epochs for the LSTM model, 600 epochs for the Transformer string model, and 300 epochs for the Transformer subtree model. We adopted the training model that most accurately integrated the validation data. The metric of accuracy was the percentage of correct answers, which was 100 times the number of functions obtained by differentiating the output of the training model with the \( D \) function in Mathematica that agreed with the input function divided by the total number of validated data. This process was carried out until all the training data had been validated. The training model that most accurately integrated the validation data was adopted as the trained model.

The learning model was evaluated by calculating the fraction of correct answers to the test data using the trained model.

### C. Training and Evaluation of the Developed Learning Model

All the models developed in this study were trained using 10-fold cross-validation. The 12,122 functions, which were pairs of integrands and primitive functions, were divided into two groups of 9,697 and 2,425 functions (4:1 ratio). The former was used as the training data, and the latter as the test data. The training data were further split at 9:1. The smaller dataset contained the validation data. The training of each learning model was performed with the training data (except for the validation data) based on the Softmax Cross-Entropy error function represented by the following equation:

\[
L = -\frac{1}{m} \sum_{ij} t_{ij} \log y_{ij} \tag{1}
\]

\[
y_{ij} = \frac{\exp(x_{ij})}{\sum_{k=1}^{n} \exp(x_{ik})}
\]

### D. Evaluation of Existing Symbolic Integration Tools

To verify the superiority of the developed learning model for symbolic integration, we performed symbolic integrations using existing non-learning-based tools such as Mathematica, Maxima, Rubi, and Matlab. We evaluated all the tools by simplifying the integrands for the test data, differentiating the output primitive function with the \( D \) function in Mathematica, assessing the agreement with the input integrands, and calculating the fraction of correct answers. For Mathematica’s symbolic integration, the correct answer rate was calculated with a primitive function obtained by using the \texttt{Integrate} function with the integrand as input, and its derivative was simplified with the \texttt{Simplify} function. For Maxima, the correct answer rate was calculated using the primitive function obtained by using the \texttt{int} function with the integrand as input, and its derivative was simplified with the \texttt{ratsimp} function. For Rubi, the correct answer rate was calculated using the primitive function obtained by using the \texttt{Int} function with the integrand as input, and its derivative was simplified with the \texttt{Simplify} function. For Matlab, the correct answer rate was calculated using the primitive function obtained by using the \texttt{int} function with the integrand as input, and its derivative was simplified with the \texttt{simplify} function. The superiority of the developed learning model was verified by comparing the correct answer rates of the symbolic integration of the test data obtained with the learning model to those obtained with non-learning-based tools.

### E. Analysis of Learning Mechanisms Using LSTM and Transformer Models

We found that the symbolic integration problems that were correctly answered differed among the eight models developed in this study, and especially between the LSTM and Transformer models. These learning models interpreted the given integrand and transformed it into a primitive function based on different learning mechanisms. To better understand the cause of this difference, we analyzed the attention layer in each model to clarify which part of the integrand the symbolic integration focused.

For the LSTM model, we visualized the attention layer, which contained information about which part of a given integrand was targeted when the LSTM model was trained on the string polish and subtree polish datasets. For each input or output unit of the integrand and primitive function to the LSTM model (per token for the string polish dataset and per subtree for the subtree polish dataset), we visualized the weights of the LSTM model that connected them. By visualizing these weights, we could determine which tokens or subtrees of the integrand were targeted when the tokens or subtrees contained in a particular primitive function were output.

For the Transformer model, we visualized the self-attention layer of the encoder from two perspectives: 1)
whether the attention heads within the layer containing the attention head and between the layers related to sequential updating had similar roles, and 2) whether the attention map of the head was uniform from layer to layer.

To clarify whether there was a similar division of roles among the attention heads within the layer containing the attention head and among the layers related to sequential updating, we mapped the attention map of each attention head into a two-dimensional space using multidimensional scaling [21] with Jensen-Shannon (JS) divergence as the dissimilarity. The calculation of self-attention was represented by the following equation as in the Transformer string model (equation 2) in self-attention, we could verify for a given weight, $W_k$, or $W_v$, specific to that layer. The dimensions of $Q$ and $K$ are the numbers of series tokens or subtrees multiplied by $d_k$. The dimension of $V$ is the number of series tokens or subtrees multiplied by $d_v$. The number of dimensions of the value vector. By making a heat map of the weight values, which were the output of the softmax function expressed by (2) in self-attention, we could verify for a given head which token or subtree of the given integrand in self-attention was targeted and how the targets were sequentially updated. In this study as well as in previous studies, we used Multi-head attention [22], a method that computes the value from (2) in multiple parallels to learn more diverse expressions, as follows:

$$\text{MultiHead}(Q, K, V) = \text{concat}(\text{head}_1, \cdots, \text{head}_h)W^O$$  \hspace{1cm} (3)

$$\text{Attention}(Q, K, V) = \text{softmax} \left( \frac{QK^T}{\sqrt{d_k}} \right) V$$  \hspace{1cm} (2)

The symbols $Q$, $K$, and $V$ represent the matrix of the query vector of each token or subtree of the input functions, the matrix of the key vector, and the matrix of the value vector, respectively. If $Q$, $K$, and $V$ are the first stage of the encoder, the first stage represents the matrix $X$ of distributed representations of the input tokens or subtrees multiplied by the weights $W^Q$, $W^K$, and $W^V$, respectively (i.e., $XW^Q$, $XW^K$, and $XW^V$). $K^T$ means the transpose of matrix $K$, and $d_k$ is the dimensionality of the key vector. The second and subsequent layers of the encoder were obtained by multiplying the output of the previous layer by another weight, $W^Q$, $W^K$, or $W^V$, specific to that layer. The dimensions of $Q$ and $K$ are the numbers of series tokens or subtrees multiplied by $d_k$. The dimension of $V$ is the number of series tokens or subtrees multiplied by $d_v$. The number of dimensions of the value vector. By making a heat map of the weight values, which were the output of the softmax function expressed by (2) in self-attention, we could verify for a given head which token or subtree of the given integrand in self-attention was targeted and how the targets were sequentially updated. In this study as well as in previous studies, we used Multi-head attention [22], a method that computes the value from (2) in multiple parallels to learn more diverse expressions, as follows:

$$\text{MultiHead}(Q, K, V) = \text{concat}(\text{head}_1, \cdots, \text{head}_h)W^O$$  \hspace{1cm} (3)

where $\text{head}_i = \text{Attention}(QW^Q_i, KW^K_i, VW^V_i)$

In (3), the dimensionalities of the weights are $W^Q \in \mathbb{R}^{d_{model} \times d_k}$, $W^K \in \mathbb{R}^{d_{model} \times d_k}$, $W^V \in \mathbb{R}^{d_{model} \times d_v}$, and $W^O \in \mathbb{R}^{d_v \times d_{model}}$, where $h$ is the number of attention heads, and $d_{model}$ is the maximum series length that the model could receive. In this way, we tested whether the coordinates on the two-dimensional space of each attention-head in the self-attention layer were close together (i.e., similar in their role assignment) or far apart (i.e., different in their role assignment).

We then calculated the average entropy of the attention map of the self-attention layer proposed previously to test whether the attention map of the head was homogeneous across layers [23]. In this study, we calculated the entropy of the attention map for each token or subtree in the attention head, and the average entropy of the attention map of the head in the same layer was calculated as the mean entropy. The increase in the average entropy through the layers was used to determine whether the attention map was homogenous through the layers.

F. MEASUREMENT OF THE RUNTIME OF EACH LEARNING MODEL AND EXISTING NON-LEARNING BASED SYMBOLIC INTEGRATION TOOLS

To verify that the symbolic integration based on the learning models developed in this study did not result in unrealistic execution times, we checked the average execution time for a single symbolic integration of the test data using the eight learning models and existing symbolic integration tools. Symbolic integration in the learning model was performed on an NVIDIA Tesla V100. Symbolic integration in existing non-learning-based tools was performed on a macOS High Sierra 2.2 GHz Intel Core i7.

G. DATA AVAILABILITY

All of the pairing functions of integrands and primitive functions (i.e., 2,425 couples of functions) of the test dataset and details of that dataset can be accessed at https://github.com/funalab/SymbolicIntegrator. In addition, 20 pairing functions for the training and validation dataset are available from the above URL. The remaining training dataset (i.e., 9,677 couples of functions) is available upon request.

H. CODE AVAILABILITY

The code created and used in this research is available at https://github.com/funalab/SymbolicIntegrator and the learned models based on LSTM and Transformer can be accessed via the above URL.

III. RESULTS

A. EVALUATION OF SYMBOLIC INTEGRATION METHODS

First, we constructed eight learning models with the integrand as input and the primitive function as output (see II-B). Each model was then trained using 10-fold cross-validation on the created training data (Supplementary Table 3). For these trained models, we used the integrands of the test data as input and evaluated the rate of correct answers, i.e., the percentage of matches between the derivative of the output primitive function and the integrand (Table 1). The LSTM model with string and polish showed the highest correct answer rate as a stand-alone learning model (98.80%).

To assess the superiority of this learning model for symbolic integration, we calculated the correct answer rate for 2,425 test functions in mathematical integration tools such as Mathematica, Maxima, Rubi, and Matlab (Table 1). We found that LSTM with string and polish outperformed Mathematica (98.30%), which achieved the highest correct answer rate of any previous symbolic integration tool.
B. IMPROVEMENT BASED ON INTEGRATION OF THE LEARNING MODELS’ OUTPUTS

The correctness of the algorithm for symbolic integration can be verified by comparing the derivative of the output primitive function with the integrand. We constructed a model that generated a primitive function, the derivative of which consistently equaled the integrand for the eight learning models constructed in this study (Fig. 1, Integrated All models). The correct answer rate of the Integrated All models on the test data was 99.79%, an improvement of 0.99% (24 functions) over the highest accuracy of the stand-alone models. The improvement of the best stand-alone learning model (LSTM string polish model) over Mathematica was 0.5%. In addition, we verified whether there were any functions that could be correctly integrated only by the Integrated All model. We discovered that there were 41 functions that were incorrectly integrated by all of the mathematical integration tools (Mathematica, Maxima, Rubi, and Matlab) but correctly integrated by the Integrated All model (Supplementary Table 4). Therefore, the result with the Integrated All models was an even more remarkable improvement.

C. REASON FOR INTEGRATING LEARNING MODELS TO IMPROVE ACCURACY

Integrating the output of the learning models that answered correctly produced a significant improvement in the accuracy of the Integrated All models for the test data. The main reason for this improvement was the significant differences in the correctness of the answers between learning models. We determined the number of integrands that were calculated incorrectly among the symbolic integration results with test data (Fig. 3). We confirmed that the integrands that were incorrectly calculated depended very much on the learning model (LSTM/Transformer) and input-output schemes of the datasets (string/subtree and polish/IRPP) (Fig. 3a, b). Because the number of incorrectly calculated integrands for any input-output scheme or learning model was no greater than five (Fig. 3c), the Integrated All models allowed the adoption of correctly answered questions and avoided incor-

right answers.

D. CHARACTERIZATION OF THE SYMBOLIC INTEGRATION MECHANISM

The reason that the integration of the output results by the learning models improved the accuracy was that each learning model could answer different integrands correctly; each learning model performed the symbolic integrations based on different symbolic integration methods. To elucidate these differences, we analyzed the attention layer of each learning model, which represents the part of the integrand and the primitive function on which each learning model focuses.

For the LSTM-based learning model, we focused on the attention map when the primitive functions were \( \frac{\cos^3 x}{x} \) and \( \frac{\cos^4 x}{x} \) in the learning model with string and polish, and in the learning model with subtree and polish. The functions where the primitive functions were \( \frac{\cos^3 x}{x} \) and \( \frac{\cos^4 x}{x} \) were generalized to the problem of turning the integrand \( -\frac{\cos^{1+n}(x)(\cos(x)+nx\sin(x))}{x^2} \) into the primitive function \( \frac{\cos^n x}{x} \). In other words, the symbolic integration of this integrand is a problem that can be solved based on the formula with attention to the constant \( n \). By measuring the similarity of the attention maps generated from the input of these two functions, we could verify whether LSTM was able to evaluate the integrals in accordance with the integration formula. Visualization of the attention maps made it clear that the attention maps were similar to each other in both learning models with string and polish as well as with subtree and polish (Fig. 4a, b, d, e). However, a comparison of the LSTM’s attention map with string and polish based on the JS divergence [24] revealed that the JS divergence of the attention map for the constant 3, 4 was much larger than the JS divergence for the other expressions (Fig. 4c). The implication was that the learning model could perform the symbolic integration based on the integration formula while
giving appropriate attention to the constant \( n \). A comparison of the LSTM’s attention maps with subtree and polish using JS divergence showed that in addition to the JS divergence of the attention map of the different subtrees in the primitive function (between “\( \cos x \)" and “\( \cos 3 x \)" subtrees, and “4 EOS [End of Sentence] EOS” and “3 EOS EOS” subtrees), the JS divergence of the attention map of the common subtrees (between the “divide \( x \)” subtree for these two integrands and the “\( \cos x \) EOS” subtree for these two integrands) was much larger than that of other subtrees (Fig. 4f). The implication was that in addition to gazing at the constant \( n \) based on the integration formula, the learning model was able to perform the mathematical integrals of gazing that went beyond the integration formulas. These results revealed that the learning models based on LSTM learned different methods of symbolic integration from each other because of the differences in input-output schemes and that each model produced different results in terms of the correctness or incorrectness of the primitive function.

Next, for the Transformer-based learning model, we focused on the self-attention layer of the encoder when the integrand was \( e^x \times n \times \cos^3 x (\cos x - 4 \sin x) \) in the learning model with string and polish as well as subtree and polish. The Transformer model consisted of six self-attention layers for each of the encoder and decoder parts, and there were eight multi-heads in each layer. We attempted to clarify the symbolic integration mechanism of the Transformer model by uncovering the part of the integrand on which the model focused for each head in this self-attention layer and for each layer. To clarify the relationship between the gazed part of the integrand in each head, we mapped the attention maps of the heads to the two-dimensional space using the multidimensional scaling method based on the JS divergence between the attention maps of the 48 heads (Fig. 5). The results showed that the attention maps of the heads in the same layer tended to become similar in deeper layers, regardless of whether the string and polish or the subtree and polish were used (Fig. 5a, c). Regardless of the input-output schemes, the Transformer model paid attention only to the part of the function to which it decided to pay attention in each deep layer of the self-attention layer. In the shallow layers, however, each head apparently had a very different attention map for both input-output schemes. The implication is that, depending on the input-output schemes, the Transformer model focused on each unique part of the integrand on a shallow layer, i.e., various parts of the integrand for each head in the initial processing stage of the symbolic integration. To further assess the similarity of the attention maps between the heads in each of these layers, we calculated the average entropy of the attention maps of the eight heads in each layer (Fig. 6). The result showed that the average entropy, which is the homogeneity between attention maps, was low in the shallow layers, but an increase of the average entropy in the deeper layers indicated that the difference in the attention maps between the heads had disappeared. The more pronounced increase of average entropy with each layer for the subtree and polish input-output schemes (Fig. 6a) than for the string and polish input-output schemes (Fig. 6b) indicated that the model with string and polish specified the parts of the integrand on which to concentrate from the beginning of the input of the integrand throughout the head. In contrast, the model with subtree and polish concentrated on a part of the integrand specific to each head and performed symbolic integration based on a wide range of information. In the case of the string and polish input-output schemes, the attention maps of each head were similar to each other (Fig. 5c), but in the case of the subtree and polish input-output schemes, the attention maps of each head differed (Fig. 5d). In other words, in the case of the string and polish, the role of each head was firmly fixed to the part of the integrand that was the focus of attention across the layers in the self-attention layer, but in the case of the subtree and polish, the part of the integrand on which attention was focused was more flexible and was determined for each head without being bound by the relationship between the heads of the layers.

There were thus differences in the (i) relationships between the paired mathematical expressions that depended on the input-output schemes and the learning models, (ii) mathematical expressions of the integrand, and (iii) processing methods in the model. Attention should be paid to these differences in the conversion from the integrand to the primitive function because the differences they created caused the functions to be integrated to be correct or incorrect. The integration of the output results of the learning models consequently improved the rate of correct answers.

**E. EVALUATION OF THE EXECUTION TIME FOR SYMBOLIC INTEGRATION**

To determine whether the execution times of symbolic integration for the eight learning models were realistic, we measured the average runtime for a single integration of
A. OPTIMAL INPUT-OUTPUT SCHEMES AND LEARNING MODEL

In this study, we pointed out various problems in the learning model for symbolic integration developed by Lample et al. [11] We developed eight learning models based on combinations of each input-output scheme or learning model, and we showed that the learning model with string and polish and LSTM achieved the highest complete correct answer rate of all learning models and existing symbolic integration tools (Table 1, 98.80%, LSTM string polish).

The main difference between this model and that of Lample et al. [11] was the use of LSTM instead of Transformer as the learning model. The superior performance of LSTM reflected the difference in the way LSTM and Transformer learn the location of the tokens in the input integrands. The LSTM model learns the relative positions of the tokens in the input integrands as it sequentially updates the memory cells inside LSTM by sequentially feeding the input tokens as time-series data into the model. In contrast, the Transformer adds positional information about the order of the tokens of the integrands before they are input to the model. In addition, the biased length of one of the functions in the dataset used in this study (Supplementary Fig. 4) caused the learning model to take a variety of long and short functions as input and processed them appropriately to convert them into primitive functions. When the input consists of such a variety of long and short functions, the use of absolute positioning of mathematical symbols is detrimental. For example, if the learning model is good at integrating over short functions, it will have to integrate over long functions by anticipating unpredictable information about the positions of function symbols. If it is good at integrating over long functions, it will fail to integrate over short functions because it will not be able to use enough information about the positions of function symbols. However, if a learning model is based on the relative positions of mathematical symbols, these adverse effects apparently do not exist, and for this reason LSTM outperforms Transformer. It was thus useful to adopt a learning model that could learn the order of the tokens in the input functions as relative positions in the symbolic integration. This utility was confirmed by the fact that the proposed subtree input-output schemes improved the accuracy of the Transformer model compared to the string input-output scheme by considering the relative input order (Table 1, 97.48%, Transformer string polish, 97.73%, Transformer subtree polish).

It is interesting to note, however, that the accuracy was lower when the subtree input-output scheme was used with LSTM than when the string scheme was used (Table 1, 98.14%, LSTM subtree polish), probably because the attention from the decoder part to the output of the encoder part of the model in LSTM is performed only once for each token in the input function and only for one context. In addition, the IRPP input-output scheme, which tries to make the output of the symbolic integration consider the rules of operation, did not improve the accuracy of the LSTM symbolic integration with string input (Table 1, 97.98%, LSTM string IRPP). We

IV. DISCUSSION

the test data using these models and existing integration tools (Supplementary Fig. 3). The average execution time for integration varied from 0.062 seconds (LSTM with string and polish) to 1.059 seconds (Transformer with subtree and polish) and was shorter than the time required for the existing symbolic integration tools, except for Matlab. To evaluate the complexity of the models, we counted the number of parameters in each of the eight learning models (Supplementary Table 5). The discovery that the number of parameters in the models was on the order of about 40 to 800 million was consistent with a comparison of the results to the execution times.
considered that this failure was due mainly to the use of different ways to describe the inputs and outputs, which are both homogeneous in terms of functions. The effort required to learn the different rules of arithmetic consequently increases, and this increased effort leads to more errors in symbolic integration. If the implications of the input and output are essentially homogeneous, as in symbolic integration, then the improved accuracy could probably be attributed to the unification of notation.

B. AFFINITY OF INPUT-OUTPUT SCHEMES AND LEARNING MODELS

In this study, we achieved a 99.79% correct answer rate with an integrated model that chose the output of the model that answered correctly. This improvement was achieved because there was a difference in the integrands that each learning model could correctly integrate (Fig. 3). To explore this issue in more depth, we tried to elucidate the symbolic integration of the integrands that each learning model incorrectly integrated by focusing on the integrands that were integrated incorrectly by each learning model.

We aimed to elucidate the characteristics of integrands that were incorrectly integrated by focusing on the wrong answers caused by the difference between string and subtree input-output schemes. We investigated the functions that were incorrectly answered by the four learning models with string and the four learning models with subtree (Supplementary Table 6). The results confirmed that the learning model with string tended to produce results contrary to the rules of mathematical operation grammar. In those results, extra mathematical symbols were present or some mathematical symbols were missing when the input was an integrand composed of long mathematical expressions (Supplementary Table 7). The missing symbols were probably due to the fact that the operators and operands of the arithmetic relationships were located far from each other, and it was consequently impossible to fully grasp the arithmetic rules. We confirmed that in the learning model with subtree, only the symbol of one node in the subtree was wrong in the output primitive function when the input was an integrand composed of short mathematical expressions (Supplementary Table 8). For example, when integrating the function \(-\csc^2 x\), the primitive function is \(\cot x\). However, in the output of the learning model, it was seen that cot in this primitive function was mistaken as a different operator such as \(\csc\) or \(\ln\). This result likely reflected the requirement of the learning model with subtree for the output of a large amount of information from a small amount of information when integrating the functions, because its output was the mathematical symbols of the three nodes of the subtree from one hidden vector propagated from the input. This lack of information may have led to errors in the mathematical symbols of only one node of the subtree.

By focusing on the difference between LSTM and Transformer in terms of wrong answers, we hoped to identify the characteristics of the integrands that were incorrectly integrated. We investigated the functions that were incorrectly integrated by the four models that adopted LSTM and by the four models that adopted Transformer (Supplementary Table 9). We confirmed in the case of the LSTM-based learning model that the model evaluated the integral incorrectly when the lengths of the integrand and the primitive function were similar (Supplementary Table 10). For example, it was confirmed that the learning model answered incorrectly in problems where the integral of the function \(-\frac{\cot x \csc^2 x}{n}\) became \(\frac{\cot x \csc^2 x}{n}\). This pattern resulted from the fact that the propagation of information inherited from the encoder was insufficient for the output of a primitive function of similar length, and consequently the information added by the attention layer could not be used effectively. In the case of the Transformer-based learning model, the answers tended to be wrong when the length of the integrand and the primitive function were significantly different (Supplementary Table 11). For example, it was confirmed that the learning model answered incorrectly in problems where the integral of the function \(-\frac{\cot x \csc x \log x (\cos (2x) + \log x + 2x \csc x \log x)}{x^2}\) became \(\frac{\cot x \csc x \log^2 x}{x}\). In the Transformer model, the same number of self-attentions were set in the encoder and decoder part, and when the information contents of the input and output functions were similar, the encoding and decoding worked effectively. However, when the information content differed significantly, wrong answers were produced because of the imbalance in the accuracy of the encoding and decoding.

We aimed to clarify the characteristics of integrands that were incorrectly integrated by focusing on the problem of wrong answers due to the difference between the polish and IRPP input-output schemes. We investigated the number of wrong answers in four learning models with polish and four learning models with IRPP (Supplementary Table 12). The learning models with polish tended to produce incorrect answers for functions with few operators (Supplementary Table 13). For example, it was confirmed that the learning model answered incorrectly in problems where the integral of the function \(-\frac{3}{2x^2}\) became \(x^{-2}\). The use of Polish notation for both the input and output functions meant that the operators in the input integrands and in the relevant output primitive function were situated distally. The high probability that the few operators in the integrand and primitive function were strongly related to each other suggested that use of the polish input-output scheme to configure these operators distally was detrimental and led to incorrect integrands. We confirmed, however, that the large number of operators in the learning model with IRPP caused erroneous answers, especially in functions containing a large number of constants (Supplementary Table 14). For example, it was confirmed that the learning model answered incorrectly in problems where the integral of the function \(\frac{n^2 \sec x (3x + x \cos (2x) - \sin (2x)) \tan x}{2x^2}\) became \(\frac{n^2 \sin x \tan x}{x}\), i.e., there were too many constants such as 2 or 3. In the IRPP input-output scheme, the integrand and primitive function were written in reverse Polish notation and Polish notation. The initial parts of both functions were thus proximal to each other. However, if the function was
a relatively long mathematical expression with many operators, there would be many constants, and the input-output relationship of these operators would be distal. This condition may have been detrimental and have led to erroneous answers when the learning model processed functions composed of numerous operators and constants.

In summary, it was clear that the symbolic integrations that were problematic differed among the different input-output schemes and learning models. The integrated model took these considerations into account and selected results in a cross-subsidized manner that led to dramatically improved accuracy. In this study, LSTM and Transformer were used as the learning machines to perform symbolic integration. Recently, it has been widely reported that adaptive machine translation and learning machines that use adversarial learning methods show high accuracy in the fields of machine translation and image analysis [25]–[27]. It is hoped that by learning symbolic integration based on these learning machines and adding them to our integrated learning model, we can achieve even higher accuracy in symbolic integration.

C. USEFULNESS OF ELUCIDATING SYMBOLIC INTEGRATION MECHANISMS

In addition to these analyses of wrong answers, we also conducted analyses focused on the attention layer of each learning model to elucidate the mechanism of symbolic integration specific to each model and to clarify differences between them. We found that LSTM with string and polish was good at performing formula-compliant integrals, and the Transformer with string and polish could precisely determine the roles played by functions of interest for each head. These findings could not only contribute to the discovery of new symbolic integration theorems but also facilitate the construction of more accurate symbolic integration learning models. For example, the performance of formula-compliant symbolic integration by LSTM with string and polish made it possible to input an unsolved integrand and analyze the attention layer to clarify the variables and mathematical symbols of interest. The knowledge forthcoming from this discovery should greatly facilitate the application of symbolic integration theory. The discovery that the role of each head in the Transformer with string and polish facilitated integration of mathematical expressions could enable improvement of the learning model via adoption of information about the substructure of the essential mathematical expression in a way that promotes this mechanism. We were thus convinced that characterization of learning models provides the seeds for new mathematical knowledge and very useful insights into how to devise better learning models.

D. IMPROVEMENT BASED ON INTEGRATION OF THE OUTPUTS OF THE LEARNING MODELS

In this study, we developed a learning machine to perform integration and showed that it could perform integration with greater accuracy than any other integration method proposed so far. We considered the performance of the model for primitive functions corresponding to integrands containing up to five elementary functions and operators. However, in this research, we have only verified whether the integration of functions generated by the aforementioned rules was possible or not, and we have not yet verified whether the integration itself, which is used in various engineering fields, is possible or not. In other words, to apply the learning machine to simulations that are widely used in engineering fields, it will be necessary to verify the integrability of functions used in each field.

In addition, other than examining the possibility of integration in these individual fields, we should ask whether it is possible to make integration of all general integrands possible through machine learning. In machine learning, accurate problem processing can be achieved by preparing training data that sufficiently cover the input space of the target problem, but the number of integrands targeted by integration in general mathematics is infinite, and it is impossible to prepare sufficient training data in an infinitely large space. However, if we limit this problem to integrals in the field of engineering, the space is presumably finite. This can be easily imagined from the perspective of the length of the functions, as we have done in our verification. In other words, in the future, based on the rules for constructing integrands in engineering, we can derive an upper limit for the input space and consider a method to enable symbolic integration in an arbitrary field like engineering by specifying a sufficient amount of training data.

V. CONCLUSION

Integration is a mathematical problem that is essential in a wide range of engineering fields, and the development of a method for symbolic integration has been desirable, especially because it derives exact solutions without errors. Here, we developed eight learning models for symbolic integration that were combinations of input-output schemes (string/subtree, polish/IRPP) and learning models (LSTM/Transformer). Among these models, the learning model that adopted string and polish as input-output schemes and LSTM as its learning model achieved the highest correct answer rate (98.80%) based on the agreement between the derivative of the output primitive function and the integrands that were not involved in the learning process. This learning model surpassed all existing symbolic integration methods. If the metric of the accuracy of symbolic integration is the agreement between the derivative of the output primitive function and the input integrand, we succeeded in constructing a symbolic integration algorithm that raised the correct answer rate of the stand-alone learning model by ~1.0% to 99.79%. In summary, we have developed a more accurate method of selecting the correct model than the existing method by requiring that the result of symbolic integration be assessed based on whether the output of the model is consistent with the input formula when the output is differentiated. The symbolic integration method we have developed not only enables rigorous simulations for error-free integration in the
engineering field, but it is also expected to contribute to the discovery of new theorems in integration by using feature analysis for the learning machine.

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