
A Transformer Model for Symbolic Regression towards Scientific Discovery

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Abstract

Symbolic Regression (SR) searches for mathematical expressions which best describe numerical datasets. This allows to circumvent interpretation issues inherent to artificial neural networks, but SR algorithms are often computationally expensive. This work proposes a new Transformer model aiming at Symbolic Regression particularly focused on its application for Scientific Discovery. We propose three encoder architectures with increasing flexibility but at the cost of column-permutation equivariance violation. Training results indicate that the most flexible architecture is required to prevent from overfitting. Once trained, we apply our best model to the SRSD datasets (Symbolic Regression for Scientific Discovery datasets) which yields state-of-the-art results using the normalized tree-based edit distance, at no extra computational cost.

1 Introduction

Machine Learning methods allow to infer relationships in datasets and replicate them, but they are often criticized for being black-box models, preventing from understanding the assumptions and discoveries of the model. Symbolic Regression (SR) aims at addressing this problem by searching the space of mathematical expressions and find an interpretable analytical model to explain a given dataset. SR originated in the field of Genetic Programming [1], and most state-of-the-art methods still use this approach. However, Genetic Programming algorithms tend to be computationally expensive, and deep learning methods have recently attracted attention from the SR community due of their almost instantaneous inference [2–10]. Notably, the “End-to-End Symbolic Regression with Transformer” model of Kamienny et al. [8] provides close to state-of-the-art performances (when using the R^2 accuracy metric) at virtually no extra computational time.

Because of its interpretability, SR has been extensively applied in various scientific domains. A pioneer study by Schmidt and Lipson [11] proposed to automatically rediscover physical laws by

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only providing experimental data on the position and velocity of objects. Since then, the sub-field of Symbolic Regression for Scientific Discovery (SRSD) tries to draw the line between SR seen as an exercise for Machine Learning research on one side, and its potential for automated or assisted scientific discovery on the other.

As the SR community was growing, La Cava et al. [12] proposed SRBench, a modern, living, and unified framework to benchmark SR methods. However, although they used physically-motivated equations, Matsubara et al. [13] point out that existing SR datasets have several important shortcomings: unrealistic sampling process, inappropriate handling of physical constants (e.g. the speed of light is sampled in the range $[1, 5]$), lack of diversity in orders of magnitude, the systematic treatment of integer variables as continuous variables, or the fact only relevant variables are provided in the input dataset. Another problem of SR tasks lies in the lack of meaningful evaluation metrics specifically for SRSD. To tackle these issues, Matsubara et al. [13] propose SRSD datasets based on the 120 equations from the Feynman SR datasets [14], meticulously reviewing and highlighting properties for each dataset, and split into three categories: 30 easy, 40 medium, and 50 hard datasets. They also propose the use of the normalized tree-based edit distance to better assess how structurally close from the ground-truth the predicted equations are.

This work introduces a new Transformer model tailored for SR in the context of scientific discovery. We propose three encoder architectures and train our model using generated datasets. We then evaluate our best model on the SRSD datasets using the normalized tree edit distance. We show that our best model achieves state-of-the-art results on the SRSD datasets at almost immediate inference time. We also publish our code repository for future studies¹.

2 Methodology – Symbolic Regression with Transformers

This section introduces the architecture for our Transformer model, the methodology used to generate the training dataset, and the adopted training strategy.

2.1 Architecture of our Transformer model

Our model is a Transformer model [15] adapted to the problem of SR (see Figure 1). It comprises an encoder, which receives a numerical tabular dataset as input, and a decoder, whose task is to predict a sequence of tokens corresponding to the ground-truth equation. The role of the encoder is to convert the tabular dataset of numerical values into meaningful features. We propose and analyze the performances of three architectures for the encoder.

We keep in mind that the features of the numerical tabular datasets (i.e. the output of the encoder) are expected to be permutation invariant with respect to the rows (the observations), and permutation equivariant with respect to the columns (the variables). On one hand, row-permutation invariance requires that the features do not change when the rows of the tabular dataset are shuffled. On the other hand, column-permutation equivariance calls for similar changes between the input and the output. For example, if the ground-truth equation is $\log(x_1 - x_2)$ and the variables x_1 and x_2 are switched in the original tabular dataset, we expect the features to change accordingly such that our model should predict $\log(x_2 - x_1)$.

The encoder of our Transformer model starts with a Cell MLP, followed by a stack of N_{enc} identical layers, where we propose three architectures for the encoder layers (see items below, and architecture details in Appendix A). A final MLP layer followed by MaxPooling allows to build features that are permutation invariant with respect to the rows.

- **MLP encoder layer** is made of a MLP, a row-wise Max-Pooling, another MLP, and a column-wise Max-Pooling. This architecture preserves both row-permutation invariance and the column-permutation equivariance.
- **Att encoder layer** uses a multi-head self-attention mechanism layer between variable features. Like the MLP architecture, this encoder layer type preserves both the row-wise permutation invariance and the column-wise permutation equivariance properties.
- **Mix encoder layer** starts by blending the column features using a standard MLP layer. This layer is inspired by PointNets [16], an artificial neural network architecture satisfying

¹<https://github.com/omron-sinicx/transformer4sr>

row-permutation invariance and taking point clouds as input. The output of this first layer is then passed to a multi-head self-attention mechanism layer to look at other observations (rows) in the numerical dataset. While the row-permutation invariance is preserved, the MLP operation breaks the column-permutation equivariance property.

The decoder of our model first combines (learnable) token embeddings and (fixed) token positional encodings. The main part of the decoder is composed of N_{dec} stacked identical layers. Following the typical architecture for the decoder of the Transformer model, each layer has: (i) a masked multi-head self-attention layer, (ii) another multi-head attention layer where the queries and the keys come from the output of the encoder and the values come from the previous layer, and (iii) a final standard MLP layer. An additional MLP layer outputs a matrix of dimension $(M \times v)$, where M is the maximum number of tokens allowed and v is the vocabulary size. As a Transformer model, the decoder of our model is auto-regressive, i.e. the first n outputs of the decoder are fed back into the decoder itself to produce output $n + 1$ during inference.

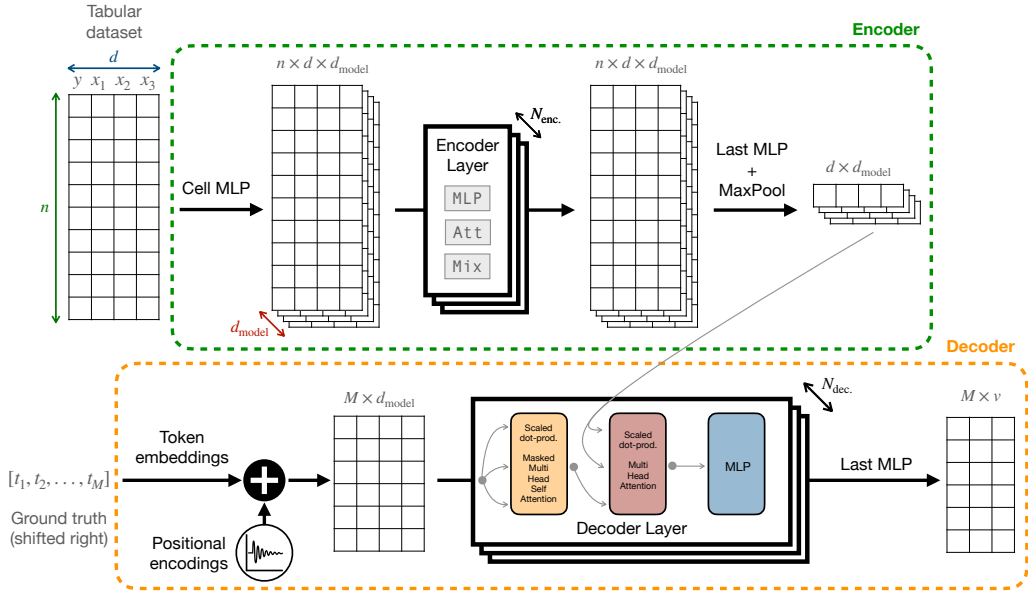


Figure 1: **Architecture of our Transformer model for Symbolic Regression.** We propose three encoder architectures: MLP, At t, or Mix. The decoder is a standard Transformer decoder and is the same in all cases. During training, the encoder receives the tabular dataset and the decoder receives the ground-truth sequence of tokens, used with teacher-forcing method. During inference, the decoder is on its own and predicts tokens in an auto-regressive manner.

We introduce d_{model} , the innermost dimension of our model, which corresponds to the dimension of the feature space used for internal representations. After few trials and errors, and given our computational limitations, we fix $d_{\text{model}} = 256$ as well as $N_{\text{enc}} = 4$, $N_{\text{dec}} = 8$, and the number of independent heads for the multi-head attention layers is $h = 4$. Given these hyperparameters, the MLP, At t, and Mix models respectively have 6, 863, 892, 7, 523, 348, and 9, 622, 548 trainable parameters (more on that in Appendix A).

2.2 Generating synthetic training datasets

The model is trained using synthetic tabular datasets, aimed at representing the diversity of real world data typically collected during scientific experiments. We first generate a large variety of skeleton equations using SymPy [17] which we then sample from.

We begin by generating ground-truth equations, by sampling tokens from a fixed predefined vocabulary composed of the following tokens: [add, mul, sin, cos, log, exp, neg, inv, sq, cb, sqrt, C, x1, x2, x3, x4, x5, x6]. Tokens sq and cb respectively denote squared and cubed values. Token C denotes a constant whose value will be later sampled. Expressions can include

up to six variables, denoted from x_1 to x_6 . Each token is given a sampling weight (see the code) to account for typical frequencies of operators, e.g. `mul` is more common than `cos`. Note that we do not include the binary operations corresponding to division and subtraction, but instead use `inv` and `neg` to represent the unary operation of inverse and negative.

Equations are represented as trees in SymPy. The two tokens `add` and `mul` represent binary operators and correspond to binary nodes requiring two children. Tokens `sin`, `cos`, `log`, `exp`, `neg`, `inv`, `sq`, `cb`, and `sqrt` are unary operators, represented as nodes needing one child. The remaining tokens `C`, `x1`, `x2`, `x3`, `x4`, `x5`, and `x6` represent constant or variables, and correspond to the tree leaves. We start by sampling a token from the vocabulary, and continue the sampling process until the tree is completed, i.e. when all nodes have all their children.

We generate $N_{\text{sample}} = 1,000,000$ random equations. These equations are simplified in a consistent way using SymPy. Besides, we discard equations made of a single leaf, equations that do not make use of the constant C in their skeleton, and equations that do not have a single variable. We also discard expressions that have more than 30 tokens. We are left with 112,944 valid expressions, from which we finally discard duplicates and end up with 17,438 unique valid expressions. For each remaining equation, the ground-truth is stored as a sequence of tokens from the equation tree, using the pre-order traversal algorithm allowing to maintain a one-to-one correspondence between equation tree and sequence of tokens. For example, the skeleton of the equation $y = 10x_1 + x_2 \log(x_1)$ will be stored as the sequence `[add, mul, C, x1, mul, x2, log, x1]`.

For each unique valid expression, we uniformly sample a value for the constant C in the range $[-100; +100]$, and we log-uniformly sample 50 times the values for the variables x_1, \dots, x_K (where $K \leq 6$) in the range $[10^{-1}; 10^1]$. The log-uniform range for the variables is chosen to represent the natural variability of physical phenomena. This sampling process generates a tabular dataset of size $(50, 7)$, where 50 is the number of observations and 7 corresponds to the response variable followed by the maximum number of variables allowed $(y, x_1, x_2, x_3, x_4, x_5, x_6)$, possibly padded with zeros.

The whole sampling process is repeated 100 times, such that there exist several tabular datasets corresponding to the same ground-truth, but with different values for the constants and the variables. Lastly, we discard datasets from which sampling was impossible (e.g. $\log(-x_1x_2)$, because $x_i \geq 0$) or datasets where $|y| > 10^9$. We are left with 1,494,588 tabular datasets for training.

2.3 Model training

Our model is fed numerical tabular datasets and is tasked to output tokens. In the beginning, we initiate the decoder with the start of sequence `<SOS>` token. Besides, the ground-truth sequences are padded with the `<PAD>` token, so that all ground-truths have size $M = 31$ (including the `<SOS>` token). Our vocabulary of tokens is the same as the one used for equation generation (see previous subsection) with the addition of the `<SOS>` and `<PAD>` tokens. The vocabulary size is $v = 20$.

We use the categorical cross-entropy loss function with the Teacher Forcing method during training. We also test with and without label-smoothing for the loss function (label-smoothing of $\epsilon = 0.1$) when training, and compare results in the next section.

Following the default parameters of Vaswani et al. [15], the parameters of our Transformer model are updated with the Adam optimizer [18], with an initial learning rate $\gamma = 1$, decay factors of $\beta_1 = 0.9$ and $\beta_2 = 0.98$ and small scalar $\epsilon = 10^{-9}$. Besides, we use the same learning rate scheduler as [15] with 4,000 warm-up steps followed by an inverse square-root decay. During training, we monitor the loss function as well as the token-wise accuracy (seen as a v -class classification problem). Finally, we use dropout regularization with $p_{\text{drop}} = 0.25$.

The entire training dataset is split into train, validation, and test subsets with proportions 80%, 10% and 10% respectively. We provide batches of size 1,024, which corresponds to 1,168 training iterations to complete an epoch. We train for 100 epochs using 4 NVIDIA Tesla V100 GPUs with 16GB memory. One epoch takes about 8 min to be completed, such that the whole training process was completed in approximately 13 hours.

3 Results

This section first introduces the results regarding training our Transformer model with respect to the proposed encoder architectures and training loss functions, and then presents the performances of our best model on the SRSD datasets [13].

3.1 Training results with respect to encoder architectures

We present the training results obtained for different training scenarios. Figures 2 and 3 show the evolution of the loss function and the token-wise accuracy (v -class classification) with respect to training epochs for all three proposed architectures. Figure 2 corresponds to the case without label-smoothing and Figure 3 to the case with label-smoothing $\epsilon = 0.1$.

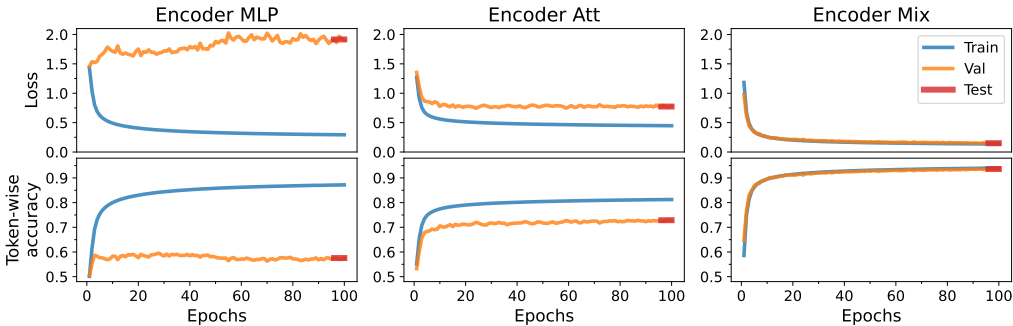


Figure 2: **Loss function and token-wise accuracy during training without label-smoothing.** The MLP encoder architecture strongly overfits the training set and cannot generalize to the validation/test sets. The Att encoder architecture can somehow generalize to the validation/test sets but still shows some overfitting. The Mix architecture shows no overfit sign at all.

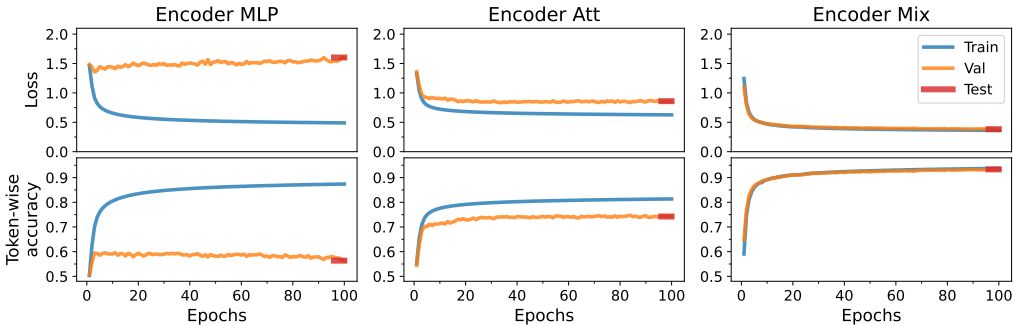


Figure 3: **Loss function and token-wise accuracy during training with $\epsilon = 0.1$ label-smoothing.** The same statement as Figure 2 applies. Label-smoothing does not resolve the overfitting problem.

As can be seen on Figure 2, the MLP and Att encoder architectures overfit the training set and do not generalize their learning to the validation and test sets. The overfit is much stronger for the MLP architecture. In contrast, the Mix encoder architecture do not show any sign of overfitting, and both the loss function and the token-wise accuracy computed on the validation or test sets match with the train set. The validation and the test sets are statistically equivalent, and therefore exhibit similar performances at epoch 100 because we do not use early-stopping with the validation set.

An intuitive justification for this state of affairs is that the Mix architecture allows for arbitrary interactions between the variables x_1, \dots, x_6 and y , by blending them together. The subsequent self-attention layer of the Mix encoder allows to look for relations between observation-wise features and therefore build an internal representation of the whole tabular dataset. On the other hand, the MLP and Att architectures dedicate most of their parameters to computing variable-only features.

Their encoder crosses the information between variables only through few MaxPooling operations (for the MLP architecture) or self-attention layers (for the Att architecture). In other words, trying to preserve the permutation equivariance property with respect to variables is too restrictive and hinders the flexibility of the encoder, while violating this property with the Mix architecture instead allows for building more meaningful features.

Introducing label-smoothing does not change the relative behaviour of the three proposed architectures. However, we can see on Figure 3 that the loss function plateaus at higher values (which makes sense because of label-smoothing), while the token-wise accuracy appears to be unaffected.

3.2 Performances on SRSD datasets

Now, we move to the evaluation of our best Transformer model using the SRSD datasets proposed to evaluate SR methods tailored for scientific purposes. The set of the 120 SRSD problems is available online² and is split into three subsets: 30 easy, 40 medium, and 50 hard equations [13].

Each equation in the SRSD dataset is comprised of 10,000 observations, divided into 8,000 training, 1,000 validation, and 1,000 test observations. As our model is already pre-trained using the generated training dataset presented in Section 2.2, we only use the 1,000 observations from the test set for each equation in the SRSD dataset.

There exist several heterogeneous metrics to assess the performances of SR algorithms. Notably, La Cava et al. [12] propose to use three metrics in their open-source benchmark, called SRBench. These are (i) the R^2 test for the accuracy, (ii) the formula complexity for the interpretability, and (iii) the inference time for the rapidity. However, these metrics do not assess how structurally close to the ground-truth equation the model prediction is, and are mostly useful when the ground-truth equations are unknown.

For this reason, and because the ground-truth equations are available, we decide to focus on the estimation of the correct skeleton equation, considered to be the hardest problem. We use the normalized tree-based edit distance proposed by Matsubara et al. [13] defined as:

$$\tilde{d}(f_{\text{pred}}; f_{\text{true}}) = \min \left(1; \frac{d(f_{\text{pred}}; f_{\text{true}})}{|f_{\text{true}}|} \right)$$

where $d(f_{\text{pred}}; f_{\text{true}})$ is the tree edit distance computed with the Zhang and Shasha algorithm [19] between the predicted f_{pred} and the ground-truth f_{true} equations represented as trees, and $|f_{\text{true}}|$ is the number of tokens (or tree nodes) for the ground-truth equation. It has been shown that this metric is more aligned with human judgment than the R^2 scores in cases where the ground-truth is known [13].

During evaluation, we start with formatting the SRSD datasets such that the variables x_1 to x_6 lie in the range $[10^{-1}; 10^1]$ to match the range of the generated datasets used during training. We also log-normalize the response variable y and compensate it by adding an extra token C in the ground-truth to take the scaling factor into account. Because there exist several ways of expressing the same mathematical expression, we standardize the ground-truth equations using the `simplify` and `factor` SymPy functions, which are the same conventions used during training (see Section 4 for details). Finally, recall that our model takes as input tabular numerical datasets of size (50, 7). Therefore, we randomly sample $N = 50$ valid observations from the 1,000 available observations in the test sets, and we repeat this sampling process 30 times for each SRSD dataset.

Table 1 presents the mean of the normalized tree-edit distance for each SRSD dataset category and each of our six trained models. These results indicate that the Mix encoder architecture provides best solutions when applied to the SRSD datasets. The use of label-smoothing in the loss function does not seem to significantly affect the performances of our model, except maybe on the easy SRSD datasets. Therefore, we select the Mix Transformer model trained with label-smoothing as our best model.

3.3 Comparison with state-of-the-art Symbolic Regression methods

We compare these results with the performances of six baseline SR algorithms used in [13], where five of the baselines are state-of-the-art SR methods, according to the SRBench study [12].

²huggingface.co/datasets/yoshitomo-matsubara/srsd-feynman_{easy;medium;hard}

	No label smoothing			With label smoothing		
	MLP	Att	Mix	MLP	Att	Mix
easy	0.975	0.821	0.740	0.896	0.896	0.686
medium	0.938	0.795	0.678	0.885	0.799	0.697
hard	0.857	0.778	0.732	0.840	0.800	0.747

Table 1: **Normalized tree edit distance for the proposed Transformer models.** The Mix encoder architecture provides best results on the SRSD datasets, regardless of the use of label-smoothing in the loss function.

- gplearn, a Genetic Programming Python library built with Scikit-Learn [20].
- Age-Fitness Pareto (AFP), a Genetic Programming method using Pareto optimization which takes into account the model’s age (epoch) when training [21].
- AFP-FE, which corresponds to AFP using Eureqa for fitness estimation [11]. As a commercial platform, Eureqa cannot be easily integrated in the benchmark.
- AI-Feynman (AIF), a physics-driven SR algorithm using successive divide and conquer fixed rules. They also introduce the Feynman datasets [14].
- Deep Symbolic Regression (DSR), using recurrent neural networks [3].
- End-to-End Symbolic Regression with Transformer (E2E), another Transformer-based model considered state-of-the-art for SR [8]. They use the scientific notation for tokens even within the encoder, unlike our model which uses the raw numerical values.

Table 2 presents the results of our best model (Best m.) against other traditional baselines for SR tasks, where the scores have been taken from [13]. We can see that our best Transformer model provides the lowest normalized tree-edit distance results among all methods when evaluated on the SRSD medium and hard datasets. For the easy SRSD datasets, DSR and AI-Feynman achieve the best solutions.

	gplearn	AFP	AFP-FE	AIF	DSR	E2E	Best m.
easy	0.876	0.703	0.712	0.646	0.551	1.000	0.686
medium	0.939	0.873	0.897	0.936	0.789	1.000	0.697
hard	0.978	0.960	0.956	0.930	0.833	0.981	0.747

Table 2: **Aggregated performances on the SRSD datasets.** Our best Transformer model (Mix encoder with label-smoothing) outperforms other traditional SR methods on the medium and hard SRSD datasets, and provides competitive performances on the easy SRSD datasets.

It is worth mentioning that our Transformer model being already trained, the inference is almost instantaneous at test time, unlike the first five SR algorithms. Therefore, it benefits from the same advantage as the End-to-End Transformer for (E2E) SR proposed by Kamienny et al. [8] while providing better results on unseen datasets coming from various scientific fields.

4 Discussion

Because of the token-wise accuracy close to 93% during training (see Figures 2 and 3), we might expect even lower normalized tree-edit distance results. However, the normalized edit distance results during evaluation with the SRSD datasets are worse than what they would be if computed over the generated tabular numerical datasets used for training. This is because of at least two reasons. The first one is that the Transformer model is now on its own in an auto-regressive manner during inference, as the Teacher Forcing method cannot be used during test on the SRSD datasets. This means that early errors get propagated and amplified during decoding. The second one is that as we increase the ground-truth equation complexity (typically its number of tokens) there is exponentially more and more possible equations. As a result, the medium and hard SRSD equations most likely do not appear in the generated datasets used during training. And while some equations of the easy

SRSD datasets might be in the training set, typical equations with small length (less than 10 tokens) are underrepresented in the training set, which leads our model to often output more than necessary tokens.

This observation leads to the discussion of an important problem when training Transformer models tailored for SR: the difference between in-domain performance versus out-of-domain generalization. While one can easily overfit the training set with enough parameters and computing time, this does not guarantee that the Transformer model can extrapolate its learning to out-of-domain datasets. When they introduced their “End-to-End Symbolic Regression with Transformers” (E2E), Kamienny et al. [8] explained that memorization of the training set does not occur based on a statistical reasoning (see Appendix C of [8]). We would instead argue that memorization does occur, and there is no point trying to prevent this from happening. Memorization at least guarantees that the tabular datasets presented to the Transformer during training will be correctly identified during inference at test time. The actual hurdles instead include: building diverse and representative tabular datasets, handling constants and variables frequency, choosing appropriate sampling ranges, or finding ways to represent ground-truth equations coherently – e.g. which of $y = (x_1 - x_2)^2$, $y = x_1^2 + x_2^2 - 2x_1x_2$, or $y = x_2^2 - 2x_1x_2 + x_1^2$ should the Transformer model predict, although all correct?

As most traditional SR algorithms can be computationally expensive, Transformer models take advantage of prior GPU training to allow for almost instantaneous inference results later on. However, further improvements and new research should still be done as to what architectures and training strategies are optimal. In particular, we showed here that trying to preserve the permutation invariance and equivariance properties might be unreasonably restrictive constraints, potentially hindering the flexibility of the artificial neural network models. We also note that depending on the chosen metric(s), ranking of methods can greatly vary. While SRBench [12] discuss the performance of SR methods focused on the R^2 , the model complexity, and the inference time, we decide to use the normalized edit distance as suggested by Matsubara et al. [13] as this metric allows to quantify how structurally close to the ground-truth the estimation is. It should be an important metric to discuss the potential of symbolic regression for scientific discovery as the metric considers both the interpretability and structural similarity between the true and predicted equations.

5 Conclusion

Because of the vast searching space, Symbolic Regression (SR) is a very complicated problem, and its real-world application towards scientific discovery is even more complex. Now, a major strength of Transformer models for SR is that their inference is almost instantaneous, because they have already been trained for long hours beforehand. In this work, we proposed several Transformer model architectures tailored for SR and aiming to solve automatic scientific discovery tasks. Our best model demonstrates strong performances on the SRSD datasets, a large dataset for SR in the context of scientific discovery. It already improves over the results of E2E, another Transformer model for SR, and there is still much room for improvement. In particular, generating more diverse training datasets, allowing for more flexibility with the constants, having a more flexible vocabulary of allowed tokens, or bigger/more refined Transformer architectures could improve our proposed Transformer model. Our code is open-sourced and can be accessed at the following repository¹.

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References

- [1] John R. Koza. *Genetic Programming*. The MIT Press, 1992.

- [2] Allan Costa, Rumen Dangovski, Owen Dugan, Samuel Kim, Pawan Goyal, Marin Soljačić, and Joseph Jacobson. Fast Neural Models for Symbolic Regression at Scale. *arXiv e-prints*, art. arXiv:2007.10784, July 2020. doi: 10.48550/arXiv.2007.10784.
- [3] Brenden K Petersen, Mikel Landajuela Larma, Terrell N. Mundhenk, Claudio Prata Santiago, Soo Kyung Kim, and Joanne Taery Kim. Deep symbolic regression: Recovering mathematical expressions from data via risk-seeking policy gradients. In *International Conference on Learning Representations*, 2021. URL <https://openreview.net/forum?id=m5Qsh0kBQG>.
- [4] Samuel Kim, Peter Y. Lu, Srijon Mukherjee, Michael Gilbert, Li Jing, Vladimir Čeperić, and Marin Soljačić. Integration of neural network-based symbolic regression in deep learning for scientific discovery. *IEEE Transactions on Neural Networks and Learning Systems*, 32(9): 4166–4177, 2021. doi: 10.1109/TNNLS.2020.3017010.
- [5] Mikel Landajuela, Brenden K Petersen, Sookyung Kim, Claudio P Santiago, Ruben Glatt, Nathan Mundhenk, Jacob F Pettit, and Daniel Faissol. Discovering symbolic policies with deep reinforcement learning. In Marina Meila and Tong Zhang, editors, *Proceedings of the 38th International Conference on Machine Learning*, volume 139 of *Proceedings of Machine Learning Research*, pages 5979–5989. PMLR, 18–24 Jul 2021. URL <https://proceedings.mlr.press/v139/landajuela21a.html>.
- [6] Luca Biggio, Tommaso Bendinelli, Alexander Neitz, Aurelien Lucchi, and Giambattista Parascandolo. Neural symbolic regression that scales. In Marina Meila and Tong Zhang, editors, *Proceedings of the 38th International Conference on Machine Learning*, volume 139 of *Proceedings of Machine Learning Research*, pages 936–945. PMLR, 18–24 Jul 2021. URL <https://proceedings.mlr.press/v139/biggio21a.html>.
- [7] Mojtaba Valipour, Maysum Panju, Bowen You, and Ali Ghodsi. Symbolicgpt: A generative transformer model for symbolic regression. In *Preprint Arxiv*, 2021. URL <https://arxiv.org/abs/2106.14131>. Under Review.
- [8] Pierre-Alexandre Kamienny, Stéphane d’Ascoli, Guillaume Lample, and Francois Charton. End-to-end symbolic regression with transformers. In Alice H. Oh, Alekh Agarwal, Danielle Belgrave, and Kyunghyun Cho, editors, *Advances in Neural Information Processing Systems*, 2022. URL https://openreview.net/forum?id=Go0uIrDHG_Y.
- [9] Julia Balla, Sihao Huang, Owen Dugan, Rumen Dangovski, and Marin Soljagic. AI-Assisted Discovery of Quantitative and Formal Models in Social Science. *arXiv e-prints*, art. arXiv:2210.00563, October 2022. doi: 10.48550/arXiv.2210.00563.
- [10] Luca Biggio, Bendinelli Tommaso, and Pierre-Alexandre Kamienny. Privileged deep symbolic regression. In *NeurIPS 2022 AI for Science: Progress and Promises*, 2022. URL <https://openreview.net/forum?id=Dzt-AGgpF0>.
- [11] Michael Schmidt and Hod Lipson. Distilling free-form natural laws from experimental data. *Science*, 324, 2009. ISSN 00368075. doi: 10.1126/science.1165893.
- [12] William La Cava, Patryk Orzechowski, Bogdan Burlacu, Fabricio Olivetti de Franca, Marco Virgolin, Ying Jin, Michael Kommenda, and Jason H. Moore. Contemporary symbolic regression methods and their relative performance. In *Thirty-fifth Conference on Neural Information Processing Systems Datasets and Benchmarks Track (Round 1)*, 2021. URL <https://openreview.net/forum?id=xVQMrDLyGst>.
- [13] Yoshitomo Matsubara, Naoya Chiba, Ryo Igarashi, and Yoshitaka Ushiku. Rethinking symbolic regression datasets and benchmarks for scientific discovery. *arXiv preprint arXiv:2206.10540*, 2022.
- [14] Silviu Marian Udrescu and Max Tegmark. Ai feynman: A physics-inspired method for symbolic regression. *Science Advances*, 6, 2020. ISSN 23752548. doi: 10.1126/sciadv.aay2631.
- [15] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Ł ukasz Kaiser, and Illia Polosukhin. Attention is all you need. In I. Guyon,

- U. Von Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 30. Curran Associates, Inc., 2017. URL https://proceedings.neurips.cc/paper_files/paper/2017/file/3f5ee243547dee91fbd053c1c4a845aa-Paper.pdf.
- [16] Charles R. Qi, Hao Su, Kaichun Mo, and Leonidas J. Guibas. Pointnet: Deep learning on point sets for 3d classification and segmentation. In *Proceedings - 30th IEEE Conference on Computer Vision and Pattern Recognition, CVPR 2017*, volume 2017-January, 2017. doi: 10.1109/CVPR.2017.16.
- [17] Aaron Meurer, Christopher P. Smith, Mateusz Paprocki, Ondřej Čertík, Sergey B. Kirpichev, Matthew Rocklin, AMiT Kumar, Sergiu Ivanov, Jason K. Moore, Sartaj Singh, Thilina Rathnayake, Sean Vig, Brian E. Granger, Richard P. Muller, Francesco Bonazzi, Harsh Gupta, Shivam Vats, Fredrik Johansson, Fabian Pedregosa, Matthew J. Curry, Andy R. Terrel, Štěpán Roučka, Ashutosh Saboo, Isuru Fernando, Sumith Kulal, Robert Cimrman, and Anthony Scopatz. Sympy: symbolic computing in python. *PeerJ Computer Science*, 3:e103, January 2017. ISSN 2376-5992. doi: 10.7717/peerj-cs.103. URL <https://doi.org/10.7717/peerj-cs.103>.
- [18] Diederik P. Kingma and Jimmy Lei Ba. Adam: A method for stochastic optimization. *3rd International Conference on Learning Representations, ICLR 2015 - Conference Track Proceedings*, pages 1–15, 2015.
- [19] Kaizhong Zhang and Dennis Shasha. Simple fast algorithms for the editing distance between trees and related problems. *SIAM Journal on Computing*, 18, 1989. ISSN 00975397. doi: 10.1137/0218082.
- [20] GPLEarn. Gplearn, genetic programming in python. <https://gplearn.readthedocs.io/en/stable>, 2023. Accessed: 2023-09-01.
- [21] Michael D. Schmidt and Hod Lipson. Age-fitness pareto optimization. In *Genetic Programming Theory and Practice VIII*, 2010. doi: 10.1145/1830483.1830584.

A Proposed encoder architectures

This appendix provides additional information regarding the proposed three encoder architectures and their properties. Figures 4, 5, and 6 respectively represent the MLP, the Att, and the Mix encoder architectures.

The MLP encoder architecture is the first we propose, and is shown on Figure 4. This encoder architecture has desirable properties regarding numerical tabular datasets. The ‘‘Cell MLP’’ allows to preserve the row permutation invariance and column permutation equivariance. Dataset-wise features are constructed using the ‘‘Row MaxPool’’ and the ‘‘Column MaxPool’’ operations. Note that the innermost dimension (the dimension of the Cell MLP) has been divided by two in order to conserve the same dimension after concatenations with the MaxPooling outputs. While this architecture preserves interesting properties, it shows the worst results during training and evaluation on the SRSD datasets. This is because most of the MLP encoder parameters are dedicated to construct cell representations, but only few of them allow for interactions between variables (the columns of the dataset).

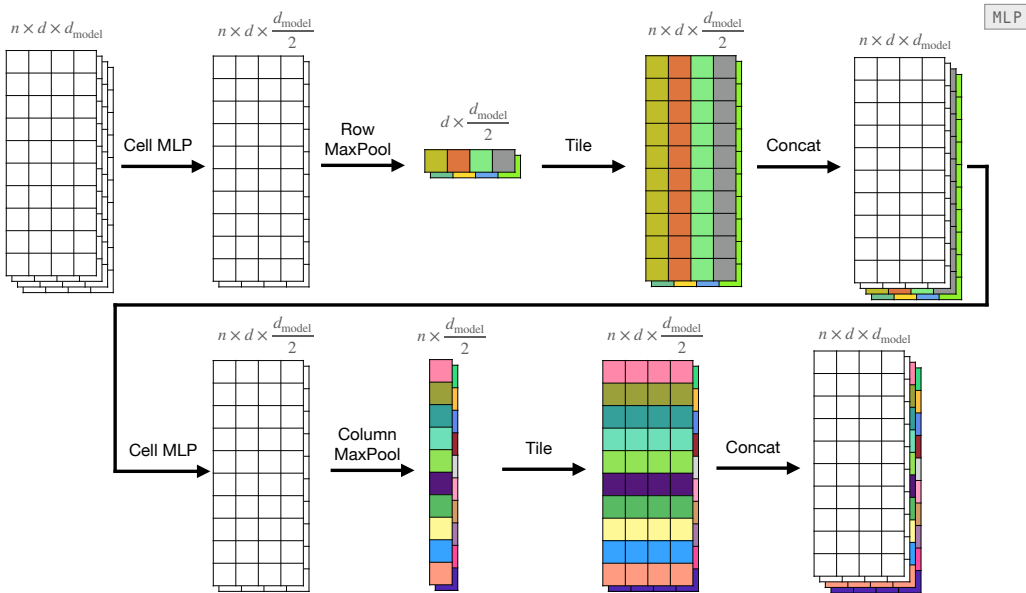


Figure 4: **Encoder architecture – MLP version.** This encoder architecture preserves row permutation invariance and column permutation equivariance. After MaxPooling, the features are tiled and concatenated to the original tensor. This architecture does not allow for much flexibility in feature design between variables.

In light of the shortcomings of the MLP encoder architecture, we then propose the Att encoder architecture (c.f. Figure 5) which utilizes multi-head self-attention mechanisms to build more flexible features from the input tabular dataset. The Att encoder architecture conserves the same properties as the previous encoder architecture, because self-attention layers do not break the row permutation invariance or the column permutation equivariance when applied on the innermost dimension (the feature dimension, see Figure 5). This means that the self-attention mechanism is applied on a cell basis and across variables, i.e. seeking relevant information in other columns (other variables) but not across different samples. As could be seen in Section 3, this architecture also allows for better generalization: the validation and test loss/accuracy are closer to the train loss/accuracy with the Att encoder than with the MLP encoder. However, we can still observe some overfitting and the small gap between train and validation or test metrics indicate that there is additional room for improvement.

Finally, the Mix encoder architecture offers the most flexible design at the expense of violating the column permutation equivariance properties. This architecture has been inspired by PointNets, an artificial neural network architecture to work with point clouds classification and segmentation tasks [16]. As can be seen on Figure 6, the Mix encoder architecture starts by flattening the columns features altogether, such that original 3D feature tensors become 2D feature tensors. The following

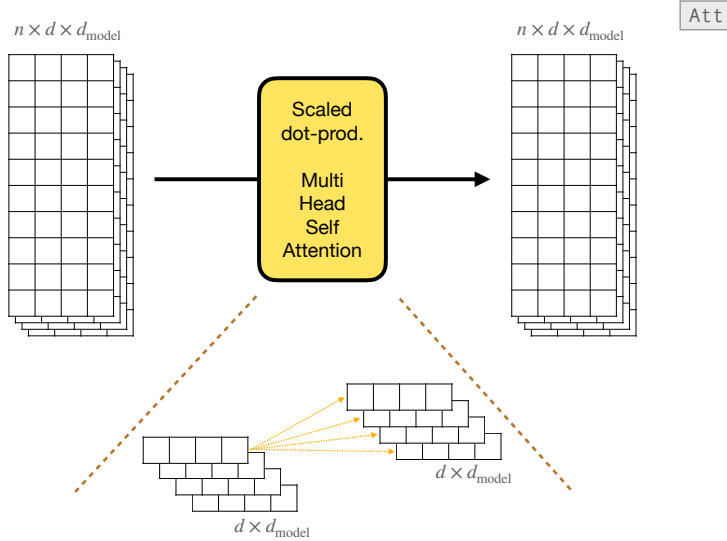


Figure 5: **Encoder architecture – Att version.** The self-attention mechanism preserves row permutation invariance and column permutation equivariance, and is more flexible in feature design.

MLP is not a “Cell MLP” anymore, but instead blends information from all columns: this allows for arbitrary relations between the input variables x_k and the response variable y . Next, a multi-head self-attention mechanism layer is applied onto the $(n \times d_{\text{model}})$ tensor, which allows to compare and match sample features across the whole dataset. This step preserves the row permutation invariance and allows for greater flexibility in feature design. Finally, we add and normalize (residual connection) the original dataset with its new features (after being broadcasted), which restores the original shape.

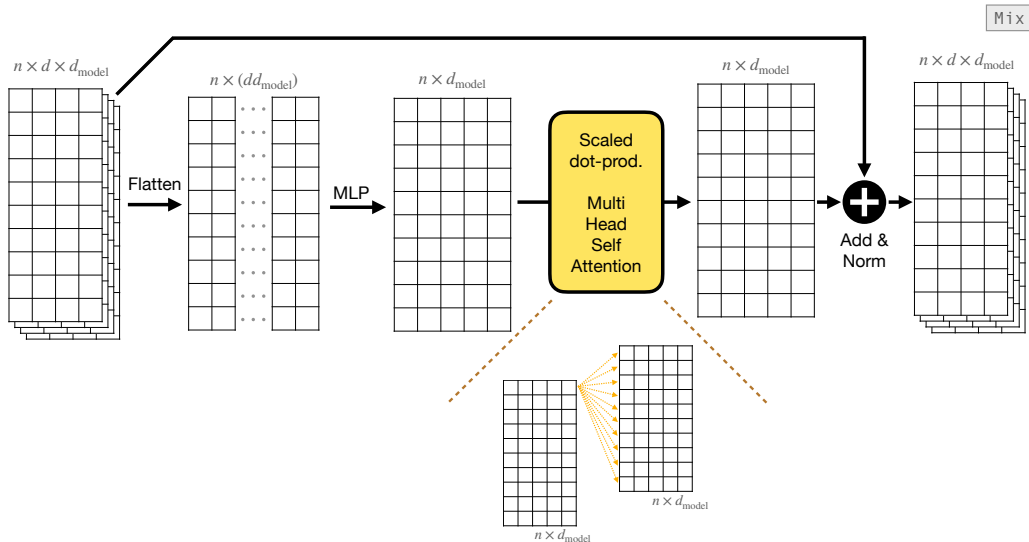


Figure 6: **Encoder architecture – Mix version.** This architecture violates column permutation equivariance, but allows for the computation of arbitrary relationships between variables.

During the review process of this manuscript, it has been brought to our attention that column-permutation equivariance could still be enforced during training by using data-augmentation strategies. Indeed, for each equation in our synthetic training dataset, we could draw random column permutations and change the ground truth accordingly. For example, suppose the ground-truth equation is given by $y = \log(x_1) + x_1x_2$, we could then swap ground-truth to $\log(x_2) + x_2x_1$ accordingly in the tabular dataset and convert the ground-truth to $\log(x_2) + x_2x_1$ accordingly.

For the three proposed architectures, the number of trainable parameters varies depending on the chosen hyper-parameters. Table 3 presents the number of parameters for each building block.

		Number of parameters	
Encoder	First Cell MLP		$d_{\text{model}}^2 + 3d_{\text{model}}$
	One Encoder Layer	MLP	$\frac{3}{2}d_{\text{model}}^2 + 2d_{\text{model}}$
		Att	$4d_{\text{model}}^2 + 6d_{\text{model}}$
		Mix	$(5 + d)d_{\text{model}}^2 + 8d_{\text{model}}$
	Last MLP		$d_{\text{model}}^2 + d_{\text{model}}$
Decoder	Token Embeddings		vd_{model}
	One Decoder Layer		$12d_{\text{model}}^2 + 17d_{\text{model}}$
	Last MLP		$vd_{\text{model}} + v$

Table 3: **Number of trainable parameters per building block.** The overall number of trainable parameters scales quadratically with d_{model} , the innermost dimension of our Transformer model. For the **Mix** encoder architecture, the number of trainable parameters also scales linearly with the number of columns d in the tabular datasets. Finally for the decoder, the number of trainable parameters depends on the vocabulary size v .

Note that for the encoder and decoder parts, the number of trainable parameters is given for a single layer. They should be multiplied by the number of encoder layers N_{enc} and decoder layers N_{dec} before being added to obtain the total number of trainable parameters $N_{\theta, \text{xxx}}$ for each architecture.

$$N_{\theta, \text{MLP}} = (1.5N_{\text{enc}} + 12N_{\text{dec}} + 2)d_{\text{model}}^2 + (2N_{\text{enc}} + 17N_{\text{dec}} + 2v + 4)d_{\text{model}} + v$$

$$N_{\theta, \text{Att}} = (4N_{\text{enc}} + 12N_{\text{dec}} + 2)d_{\text{model}}^2 + (6N_{\text{enc}} + 17N_{\text{dec}} + 2v + 4)d_{\text{model}} + v$$

$$N_{\theta, \text{Mix}} = ((5 + d)N_{\text{enc}} + 12N_{\text{dec}} + 2)d_{\text{model}}^2 + (8N_{\text{enc}} + 17N_{\text{dec}} + 2v + 4)d_{\text{model}} + v$$

As a sanity check, we can plug the values used in this work, i.e. $N_{\text{enc}} = 4$, $N_{\text{dec}} = 8$, $d = 7$, $v = 20$, and $d_{\text{model}} = 256$. We can verify that $N_{\theta, \text{MLP}} = 6,863,892$, $N_{\theta, \text{Att}} = 7,523,348$, and $N_{\theta, \text{Mix}} = 9,622,548$, as introduced at the end of Section 2.1 in the main text.