Neural-Guided Symbolic Regression with Semantic Prior

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Abstract
Symbolic regression has been shown to be quite useful in many domains from discovering scientific laws to industrial empirical modeling. Existing methods focus on numerically fitting the given data. However, in many domains, symbolically derivable properties of the desired expressions are known. We illustrate these “semantic priors” with leading powers (the polynomial behavior as the input approaches 0 and ∞). We introduce an expression generating neural network that significantly favors the generation of expressions with desired leading powers, even generalizing to powers not in the training set. We then describe our Neural-Guided Monte Carlo Tree Search (NG-MCTS) algorithm for symbolic regression. We extensively evaluate our method on thousands of symbolic regression tasks and desired expressions to show that it significantly outperforms baseline algorithms and exhibits discovery of novel expressions outside of the training set.

1. Introduction
Symbolic regression is the problem of finding a mathematical expression from a discrete space of expressions that conforms to a set of data points. Some of the most common methods for symbolic regression are based on evolutionary algorithms (EA) (Forrest, 1993), which have been used to find natural laws in some prototype physical systems from experimental data (Schmidt & Lipson, 2009). Recently, several new learning algorithms have been proposed for symbolic regression based on grammar variational autoencoder (Kusner et al., 2017), compressed-sensing (Ouyang et al., 2018), and proximal policy optimization (Ramachandran et al., 2017).

However, all these methods fail to take advantage of a key value provided by symbolic expressions. We can extract mathematical facts from the symbolic expression that have real meaning in many domains. In this paper, we consider the asymptotic behaviors of leading powers. For example, most materials have a heat capacity proportional to $T^3$ at low temperatures $T$, and the gravitational field of planets (at distance $r$) should behave as $1/r$ as $r \to \infty$. These leading powers can be derived from the expressions automatically without numeric evaluation on specific data points. These “semantic priors” provide a very different constraint on the desired output expressions and can provide significant utility for symbolic regression, especially for extrapolation far from the training data and for efficient learning from a small number of data points.

We first develop an expression generating neural network (NN) to produce expressions that match given leading powers. We then introduce Neural-Guided Monte Carlo Tree Search (NG-MCTS) which uses this expression generating NN with Monte Carlo Tree Search (MCTS) for effective symbolic regression on a variety of tasks.

The expression generating NN learns a distribution over a family of mathematical expressions (belonging to a grammar of expressions) conditioned on the leading power specifications. The model generates an expression as a sequence of grammar production rules by incrementally expanding partial grammar derivations. The model encodes the leading power specification together with a partial parse tree, and induces a distribution over the next grammar production rule. We then develop the NG-MCTS algorithm to efficiently search the space of expressions given a set of data points and the desired leading powers. The algorithm uses the learned model to predict the grammar production probabilities from the leading powers to guide the exploration.

We evaluate our approach in two parts. We first demonstrate that our expression generating NN can significantly favor generation of expressions matching the given leading powers, and generate syntactically and semantically novel expressions. Further, we show it can generalize to leading powers not present in the training data. We then demonstrate, on a large set of thousands of desired expressions, that NG-MCTS can successfully solve significantly more symbolic regression tasks (71.22%) compared to baseline approaches such as MCTS (0.54%) and EA (23.37%). This extensive evaluation is important to judge the robustness of techniques, which is difficult to judge with only the handful of desired expressions typically examined.
In summary, this paper makes the following key contributions:

- We propose a new strategy to incorporate semantic prior knowledge such as leading powers to specify symbolic regression tasks.
- We develop an expression generating NN to learn a distribution over (syntactically-valid) mathematical expressions conditioned on the leading powers.
- We develop the NG-MCTS algorithm that uses the expression generating NN to guide the MCTS to efficiently identify the desired symbolic expression.
- We extensively evaluate our expression generating NN to demonstrate generalization for leading powers, and the NG-MCTS algorithm to show that our approach significantly outperforms many baseline techniques on thousands of tasks.

2. Related Work

We briefly discuss the related works in the areas of symbolic regression and neural program synthesis. One key difference between these works and ours is that instead of only embedding numerical data points (or input-output examples), we introduce semantic properties of symbolic expressions (such as leading powers) as an additional specification mechanism, and develop algorithms to use such specifications to efficiently guide the search of desired expressions.

2.1. Symbolic Regression

A symbolic regression method can be characterized using three key aspects: the symbolic space of expressions, a scoring function, and the search algorithm. The symbolic space is defined using a set of discrete symbols including the algebraic operators, functions, coefficients, and variables. The scoring function is used to evaluate expressions in the symbolic space and the search algorithm decides the exploration of expressions in the space. Symbolic regression is a large area and we highlight only a few past papers here.

Schmidt & Lipson (2009) present a symbolic regression technique to learn natural laws from experimental data. The symbolic space is defined using operators $+,-,\times,/,$ sin, cos, constants, and variables. An expression is represented as a graph, where intermediate nodes represent operators and leaves represent coefficients and variables. The EA varies the structures to search new expressions using a score that accounts for both accuracy and the complexity of the expression. This approach has been further used to get empirical expressions in electronic engineering (Ceperic et al., 2014), water resources (Klotz et al., 2017), and social science (Truscott & Korns, 2014).

Another approach based on grammar variational autoencoder (Kusner et al., 2017) was recently proposed to learn a generative model of structured arithmetic expressions and molecules, where the latent representation captures the underlying grammatical structure. This ensures that only syntactically valid expressions are generated by the decoder. This approach was further shown to improve a Bayesian optimization based method for symbolic regression.

Similar to these approaches, most other approaches search for expressions from scratch using only data points (Schmidt & Lipson, 2009; Ramachandran et al., 2017; Ouyang et al., 2018) without prior knowledge. Abu-Mostafa (1994) suggests incorporating prior knowledge of a similar form to our semantic priors, but actually implements those priors by adding additional data points and terms in the loss function.

2.2. Neural Program Synthesis

Program synthesis is the task of learning programs in a domain-specific language (DSL) that satisfy a given specification (Gulwani et al., 2017). It is closely related to symbolic regression, where the DSL can be considered as a grammar defining the space of valid expressions. There have been some recent works that use neural networks for learning programs (Devlin et al., 2017; Balog et al., 2016; Parisotto et al., 2017; Vijayakumar et al., 2018). Robust-Fill (Devlin et al., 2017) trains an encoder-decoder model that learns to decode programs as a sequence of tokens given a set of input-output examples. Since it decodes program tokens directly, there is no guarantee that the output programs are going to be grammatically valid. For more complex DSL grammars such as Karel that consists of nested control-flow, an additional grammar mask is used to ensure syntactic validity of the decoded programs (Bunel et al., 2018). However, these approaches only use examples as specification.

3. Problem Definition

In order to demonstrate how prior knowledge can be incorporated into symbolic regression, we construct a symbolic space using a context-free grammar $G$:

$$
O \rightarrow S \\
S \rightarrow S + T | S - T | S^* T | S^/ T | T \\
T \rightarrow \left(\langle S \rangle \right) | \langle x \rangle | \langle 1 \rangle
$$

This expression space covers a rich family of rational expressions, and the size of the space can be further parameterized by a bound on the maximum expression length. Many symbolic and numerical properties can be considered as prior knowledge. For example, monotonicity or convexity for the whole function or in certain intervals; constraints of differentials and integrations; asymptotic behavior at infinity or fixed points, etc. Asymptotic behaviors such as leading powers are important properties for physicists and mathematicians constructing expressions for their problems. For
an expression $f(x)$, the leading power at $x_0$ is defined as
\[
P_{x \to x_0}[f] = p \quad \text{s.t.} \quad \lim_{x \to x_0} \frac{f(x)}{x^p} \text{ non-zero constant.}
\] (2)

In this paper, the leading powers at $x_0 \in \{0, \infty\}$ are taken as an example of prior knowledge for an expression.

Let $S(G, k)$ denote the space of all expressions in the Grammar $G$ with a maximum expression length of $k$. Conventional symbolic regression searches for a desired expression $f(x)$ in the space of expressions $S(G, k)$ that conforms to a set of data points $\{(x, f(x)) \mid x \in D_{\text{train}}\}$, i.e. find a $g(x) \in S(G, k) : \phi(g(x), D_{\text{train}})$, where $\phi$ denotes the acceptance criterion, usually root mean square error (RMSE). With the additional semantic prior specification of leading powers $c^{(0)}$ and $c^{(\infty)}$ at 0 and $\infty$, the symbolic regression problem becomes: find a $g(x) \in S(G, k) : \phi(g(x), D_{\text{train}}) \land (P_{x \to 0}[g] = c^{(0)}) \land (P_{x \to \infty}[g] = c^{(\infty)})$.

4. Expression Generating Neural Network

![Figure 1](image.png)

**Figure 1. Model architecture.** (a) Exemplary expression. (b) Leading powers of $1/(x + 1)$ at 0 and $\infty$. (c) Parse tree of $1/(x + 1)$. (d) Production rule sequence, the preorder traversal of production rules in the parse tree. (e) Architecture of the model to predict the next production rule from the partial sequence.

Figure 1(a) and (c) show an example of how an expression is parsed as a parse tree by the grammar defined in Eq. (1). The parse tree in Figure 1(c) can be serialized into a production rule sequence $r_1, \ldots, r_L$ by preorder traversal, as shown in Figure 1(d). Let $L$ denote the length of the production rule sequence, which varies for different expressions. Figure 1(b) shows the leading powers of the exemplary expression in Figure 1(a). The conditional distribution of an expression is parameterized as a sequential model
\[
p_\theta(f[c^{(0)}, c^{(\infty)}]) = \prod_{t=1}^{L-1} p_\theta(r_{t+1} | r_1, \ldots, r_t, c^{(0)}, c^{(\infty)}).
\] (3)

We build a NN (as shown in Figure 1(e)) to predict the next production rule $r_{t+1}$ from a partial sequence $r_1, \ldots, r_t$ and conditions $c^{(0)}, c^{(\infty)}$.

In training, each expression in the training set is first parsed as a production rule sequence. Then a partial sequence of length $t \in \{1, \ldots, L - 1\}$ is sampled randomly as the input and the $(t + 1)$-th production rule is selected as the output (see blue and orange text in Figure 1(d)). Each production rule of the partial sequence is represented as an embedding vector of size 10. The conditions are concatenated with each embedding vector. This sequence of embedding vectors are fed into a bidirectional Gated Recurrent Units (GRU) (Cho et al., 2014) with 1000 units. A softmax layer is applied to the final output of GRU to obtain the raw probability distribution over the next production rules in Eq. (1).

Note that not all the production rules are grammatically valid as the next production rule for a given partial sequence. The partial sequence is equivalent to a partial parse tree. The next production rule expands the leftmost non-terminal symbol in the partial parse tree. For the partial sequence in Figure 1, the next production rule expands non-terminal symbol $T$, which constrains the next production rule to only those with left-hand-side symbol $T$.

We use a stack to keep track of non-terminal symbols in a partial sequence as described in grammar variational autoencoder (Kusner et al., 2017). A mask of valid production rules is computed from the input partial sequence. This mask is applied to the raw probability distribution and the result is normalized to 1 as the output probability distribution. The loss is the cross entropy between the output probability distribution and the next production rule.

5. Neural-Guided Monte Carlo Tree Search

We now briefly describe the NG-MCTS algorithm that uses the expression generating NN to guide the symbolic regression search. The discrepancy between the best found expression $g(x)$ and the desired $f(x)$ is evaluated on data points and leading powers. The error on data points is measured by RMSE $\Delta g(x) = \sqrt{\frac{1}{|D_{\text{eval}}|} \sum_{x \in D_{\text{eval}}} (f(x) - g(x))^2}$ on training points $D_{\text{train}} : \{1, 2, 1.6, 2.0, 2.4, 2.8\}$, points in interpolation region $D_{\text{interpolation}} : \{1.4, 1.8, 2.2, 2.6\}$ and points in extrapolation region $D_{\text{extrapolation}} : \{5, 6, 7, 8, 9\}$. The error on leading powers is measured by sum of abso-
lute errors at 0 and \( \infty \), \( \Delta P[g] = |P_{x\rightarrow0}[f] - P_{x\rightarrow0}[g]| + |P_{x\rightarrow\infty}[f] - P_{x\rightarrow\infty}[g]| \). The default choice of objective function for symbolic regression algorithms is \( \Delta g_{\text{train}} \) alone. When additional conditions such as leading powers need to be taken into consideration, the objective function can be defined as \( \Delta g_{\text{train}} + \Delta P[g] \), which minimizes both the RMSE on the training points and the absolute difference of the leading powers.

Most symbolic regression algorithms are based on EA, e.g. Schmidt & Lipson (2009), where it is nontrivial to incorporate our expression generating NN to guide the generation strategy in a step-by-step manner, as the mutation and cross-over operators perform transformations on fully completed expressions. However, it is possible to incorporate a probability distribution over expressions for many heuristic search algorithms such as Monte Carlo Tree Search (MCTS). MCTS is a heuristic search algorithm that has been shown to perform exceedingly well in problems with large combinatorial space, such as mastering the game of Go (Silver et al., 2016) and planning chemical syntheses (Segler et al., 2018). In MCTS for symbolic regression, a partial parse tree sequence \( r_1, \ldots, r_t \) can be defined as a state \( s_t \) and the next production rule is a set of actions \( \{a\} \). In the selection step, we use a variant of the PUCT algorithm (Silver et al., 2016; Rosin, 2011) for exploration. For MCTS, the prior probability distribution \( p(a_i | s_t) \) is uniform among all valid actions.

We develop NG-MCTS by incorporating the expression generating NN into the MCTS for symbolic regression. In particular, the prior probability distribution \( p(a_i | s_t) \) is computed by our expression generating NN conditioned on the partial sequence and the desired condition. We run MCTS for 500 simulations for each desired expression \( f(x) \). The exploration strength is set to 50 and the length limit of the production rule sequence is set to 100.

For comparison, we also search expressions using the conventional symbolic regression approach with EA. We use implementation from DEAP (Fortin et al., 2012), a popular package for symbolic regression research (Quade et al., 2016; Claveria et al., 2016). We define a set of required primitives: +, −, *, /, x and 1. The expression is represented as a tree where all the primitives are nodes. We start with a population of 10 individual trees. The maximum height of a tree is set to 50. The probability of mating two individuals is 0.1, and the probability of mutating an individual is 0.5 (chosen based on a hyperparameter search, see Appendix G). The limit of number of evaluations for a new offspring is set to 500 so that it is comparable to the number of simulations in MCTS.

6. Evaluation

We now present the evaluation of our technique on thousands of symbolic regression tasks. We first evaluate our expression generating NN model on a set of expression generation tasks conditioned on leading powers. We show that the NN model not only learns to generate expressions for conditions in the training set, but also generalizes to some new conditions. We also present a qualitative evaluation of the NN model to better comprehend its learned behavior. Finally, we evaluate the NG-MCTS algorithm that uses the expression generating NN to guide the exploration in a step-by-step manner, and show that it significantly outperforms baseline MCTS and EA algorithms even with the leading power conditions added to their objective functions.

6.1. Dataset

We denote the condition of an expression as a pair of integer leading powers \( (P_{x\rightarrow0}[f], P_{x\rightarrow\infty}[f]) \) and define the complexity of a condition by \( M[f] = |P_{x\rightarrow0}[f]| + |P_{x\rightarrow\infty}[f]| \). Obviously, expressions with \( M[f] = 4 \) are more complicated to construct than those with \( M[f] = 0 \). We create a dataset balanced on each condition (submitted as supplementary materials), as described in Appendix A. For each pair of integer leading powers satisfying \( M[f] \leq 4 \), 1000 shortest expressions are selected so that there are 41000 expressions in total. They are randomly split into three sets. The first two are training (28837) and validation (4095) sets. For the remaining expressions, 50 expressions with unique simplification expressions are sampled from each condition for \( M[f] \leq 4 \), to form a holdout set with 2050 expressions. In the same way, we also create a holdout set of 1000 expressions for \( M[f] = 5 \) and 1200 expressions for \( M[f] = 6 \). These conditions do not exist in training and validation sets.

6.2. Evaluation of Expression Generating NN

The NN model described in Section 4 is implemented in TensorFlow (Abadi et al., 2016) (code submitted as supplementary materials). It is trained from partial sequences sampled from expressions in the training set. The loss on validation set is computed to avoid model overfitting. In the generation stage, the model predicts the probability distribution over the next production rules from the starting rule \( r_1 : O \rightarrow S \) and desired condition \( c^{(0)}, c^{(\infty)} \). The next production rule is sampled from distribution \( p_0(r_2 | r_1, c^{(0)}), c^{(\infty)} \) and then appended to \( r_1 \). Then \( r_3 \) is sampled from \( p_0(r_3 | r_1, r_2, c^{(0)}, c^{(\infty)}) \) and appended to \( [r_1, r_2] \). This procedure is repeated until \( [r_1, \ldots, r_L] \) form a parse tree where all the leaf nodes are terminal, or the length of generated sequence reaches the prespecified limit, which is set to 100 for our experiments.

Baseline Models  We compare NN with a number of base-
line models that provide a probability distribution over the next production rules. All these distributions are masked by the valid production rules computed from the partial sequence before sampling. For each desired condition within $|P_{x \to 0}^0(f)| \leq 9$ and $|P_{x \to \infty}^\infty(f)| \leq 9$, $k = 100$ expressions are generated.

Neural Network No Condition (NNNC) A model with the same setup as NN except not conditioning on $c(0)$, $c(\infty)$.

Random The next production rule $r_{t+1}$ is sampled uniformly from all the valid production rules given a partial sequence $r_1, \ldots, r_t$.

Full History (FH) The next production rule $r_{t+1}$ is sampled from its empirical distribution given the full partial sequence and the desired condition.

Full History No Condition (FHNC) The next production rule $r_{t+1}$ is sampled from its empirical distribution given the full partial sequence only.

Limited History (LH) $l$ The next production rule $r_{t+1}$ is sampled from its empirical distribution given the last $l$ production rules of the partial sequence and desired condition.

Limited History No Condition (LHNC) $l$ The next production rule $r_{t+1}$ is sampled from its empirical distribution given the last $l$ production rules of the partial sequence.

Note that all the aforementioned empirical distributions are derived from the training set $\{f\}$. For limited history models, if $l$ exceeds the length of the partial sequence, we instead take the full partial sequence. Intuitively, a model that does not depend on condition and uses little amount of history would be close to the Random model, while a model that depends on condition and uses the full history would be equivalent to sampling from the training set.

Metrics We propose four metrics to evaluate the performance. For each condition $(c(0), c(\infty))$, $k$ expressions $\{g_i\}$ are generated from model $p_{\theta}(f|c(0), c(\infty))$.

Success Rate We compute the leading powers $(P_{x \to 0}^0[g_i], P_{x \to \infty}^\infty[g_i])$ of the generated expression and check whether they match the desired condition. Success rate is defined as the proportion of the generated expressions satisfying the condition.

Mean L1-distance Success rate measures how many generated expressions match the condition exactly. We also measure how close $(P_{x \to 0}^0[g_i], P_{x \to \infty}^\infty[g_i])$ are to $(c(0), c(\infty))$ by the mean L1-distance.

Syntactic Novelty Rate Generalization can be measured by how many generated expressions do not appear in the training set $\{f\}$. A direct criterion is whether one expression has syntactic duplicates in the training set. For example, if $x + 1$ is in the training set and $(1) + x$ is not, then $(1) + x$ is a syntactically novel expression generated by the model. The rate of syntactic novelty is defined as the proportion of the generated expressions that satisfy the condition and are syntactically novel.

Semantic Novelty Rate Another perspective of generalization beyond syntactic novelty is semantic novelty. We use simplify function in SymPy (Meurer et al., 2017) to normalize expressions. Two expressions are semantically identical if they can be simplified to the same expression. The rate of semantic novelty is defined as the proportion of the generated expressions that satisfy the condition and are semantically novel.

To avoid inflating the rates of syntactic and semantic novelty, we only count the number of unique syntactic and semantic novelties in terms of their expressions and simplified expressions, respectively.

Quantitative Evaluation We first demonstrate that our expression generating NN can learn to generalize to new expressions with syntactic and semantic novelties, as well as new conditions not seen in the training set. Table 1 shows a comparison of the model performance between baseline and NN models measured by the metrics. We define $M[f] \leq 4$ as in-sample condition region and $M[f] > 4$ as out-of-sample condition region. In both regions, the generalization ability of the model is reflected by the number of syntactic and semantic novelties it generates, not just the number of successes. For example, NN prefers expressions with leading powers closer to the desired condition. This suggests that for the unmatched expressions, NN performs better for individual conditions. Figure 2 shows the metrics for NN and LHNC (8) on each condition. NN performs better in the in-sample condition region (inside the red boundary) and also generalizes to more conditions in the out-of-sample condition region (outside the red boundary).
Table 1. Metrics for expression generating NN and baseline models. We compute the average of syntactic novelty rates and semantic novelty rates over all the conditions in $M[f] \leq 4$ (in-sample). We compute the total number of success, syntactic novelty and semantic novelty expressions over all the conditions in $M[f] > 4$ (out-of-sample). Details of why the metrics are aggregated on different levels in the two regions are explained in Appendix C. We also count the number of conditions with non-zero success rates in the out-of-sample condition region. The mean L1-distances are averaged over all the conditions in $M[f] \leq 4$, and conditions in $M[f] = 5, 6, 7$, respectively.

| MODEL | $M[f] \leq 4$ | $M[f] > 4$ | $M[f] = 5$ | $M[f] = 6$ | $M[f] = 7$ |
|-------|---------------|-------------|-------------|-------------|-------------|
|       | SYN (%) | SEM (%) | TOTAL | NUM EXPRESSIONS | NUM CONDITIONS | L1-DIST |
| NN    | 35.0  | 2.7   | 1465  | 1416  | 1084  | 115  | 0.8  | 1.4  | 2.5  | 4.3  |
| NNNC  | 1.8   | 0.2   | 0.7   | 0     | 0     | 0    | 0.0  | 18.0 | 18.0 | 18.0 |
| RANDOM| 0.0   | 0.0   | 0     | 0     | 0     | 0    | 0.0  | 18.0 | 18.0 | 18.0 |
| FH    | 0.0   | 0.0   | 0     | 0     | 0     | 0    | 0.0  | 18.0 | 18.0 | 18.0 |
| FHNC  | 5.0   | 1.1   | 0     | 0     | 0     | 0    | 0.0  | 18.0 | 18.0 | 18.0 |
| LH (2)| 10.3  | 3.1   | 0     | 0     | 0     | 0    | 0.0  | 18.0 | 18.0 | 18.0 |
| LH (4)| 14.6  | 2.4   | 0     | 0     | 0     | 0    | 0.0  | 18.0 | 18.0 | 18.0 |
| LH (8)| 1.2   | 0.1   | 0     | 0     | 0     | 0    | 0.0  | 18.0 | 18.0 | 18.0 |
| LH (16)|1.5  | 0.3   | 3     | 3     | 3     | 3    | 0.0  | 18.0 | 18.0 | 18.0 |

Figure 2. Metrics for expression generating NN and LHNC (8) on each condition within $|P_{x \rightarrow 0}[f]| \leq 9$ and $|P_{x \rightarrow \infty}[f]| \leq 9$. Similar plots for other baselines are shown in Appendix E. Each column corresponds to one of the metrics. Conditions with $M[f] \leq 4$ are inside the red boundary. Conditions with zero success rate, syntactic novelty rate or semantic novelty rate are left blank.

Qualitative Evaluation  Besides quantitative evaluation, we also perform a qualitative evaluation to better comprehend the learned NN model and its generative behavior.

Syntactic Novelty Examples  For ease of presentation, we show syntactic novelties generated by NN that only have one semantically identical expression (i.e., the expression that shares the same simplified expression) in the training set. By comparing each syntactic novelty and its semantically identical expression in the training set (shown in Table 2), we can observe that the model generates some nontrivial syntactic novelties. For humans to propose such syntactic novelties, they would need to know and apply the corresponding nontrivial mathematical rules (shown in the first column of Table 2) to derive the expressions from those already known in the training set. On the contrary, NN generates the syntactic novelties without being explicitly taught these mathematical rules.

Expression Completion  We also perform a task of expres-
and a variety of desired conditions in Ta-

We now present the evaluation of our NG-MCTS method, where each step in the search is guided by our expression as the corresponding syntactic novelty. The first column shows the mathematical rules a human needs to know and apply to derive each syntactic novelty from its semantically identical expression in the training set.

A mathematical rule
| SYNTACTIC NOVELTY | SEM-IDENTICAL EXPRESSION |
|-------------------|--------------------------|
| $1/(A/B) = B/A$   | $1+1/(1+(x/(1+x)))/1+(1+x)/(1+(1+x))$ |
| $A/(B+B) = A/B+1/2$ | $1 - x/(1+(x/1+x))$ |
| $A + B = B + A$   | $x/(1+(x/1+x))$ |
| $A/(B + C) = A/B/C$ | $(1 - (x/1+x))/((x+x+x) - (1 - (x/1+x)))$ |
| $A/C + B/C = (A + B)/C$ | $(1 + (1/(1+x)))/((x + x - x) - 1) - (1 + x)/((x - 1) - (x + x))$ |

Top three probable expressions are presented for each exemplary condition. Column Match indicates whether the generated expression matches the desired condition.

Top three probable expressions are presented for each exemplary condition. Column Match indicates whether the generated expression matches the desired condition.

### Table 3. Examples of expression completion of $1/\boxed{\square} - \boxed{\square}$

| $M[f]$ | $c^{(0)}$ | Expression | Probability | Match |
|--------|-----------|------------|-------------|-------|
| 1      | 0         | $1/(1+x)$  | $7.8%$      | ✓     |
| 1      | 0         | $1/(1+x)$  | $7.7%$      | ✓     |
| 1      | 0         | $1/(1+x)$  | $7.0%$      | ×     |
| 2      | -1        | $x/(x+x)$  | $17.3%$     | ✓     |
| 1      | 0         | $x/(x+x)$  | $12.0%$     | ✓     |
| 1      | -1        | $x/(x+x)$  | $6.8%$      | ×     |
| 4      | -2        | $x/(x+x)$  | $48.5%$     | ✓     |
| 1      | 0         | $x/(x+x)$  | $12.5%$     | ×     |
| 1      | 0         | $x/(x+x)$  | $7.6%$      | ×     |
| 5      | -3        | $x/(x+x)$  | $29.5%$     | ×     |
| 1      | 0         | $x/(x+x)$  | $19.3%$     | ×     |
| 1      | 0         | $x/(x+x)$  | $12.9%$     | ✓     |

$D_{\text{train}}$. EA solves 12.83% expressions, while MCTS only solves 0.54% expressions. This suggests that compared to EA, MCTS is not efficient in searching a large space with limited number of simulations. We also examine the errors on hard expressions, the intersection of unsolved expressions of all methods. The medians of $\Delta P[g]$ are both 3, which are large as the maximum $M[f]$ in this set is 4.

In order to examine the effect of leading powers, we use leading powers alone in MCTS (PW-ONLY). The median of $\Delta P[g]$ for hard expressions is reduced to 1 but the medians of $\Delta g_{\text{int}}$ and $\Delta g_{\text{ext}}$ are significantly higher. We then add leading powers to the objective function together with data points. MCTS + PW does not have a notable difference to MCTS. However, EA + PW improves solved expressions to 23.37% and $\Delta P[g]$ of hard expressions are zero. This indicates adding semantic prior knowledge in the objective function is helpful for symbolic regression. More importantly, we demonstrate step-wise guidance of semantic prior from NN can lead to even more significant improvements. NG-MCTS solves 71.22% expressions in the holdout set, three times over the best EA + PW. ALthough EA has the lowest medians of $\Delta g_{\text{train}}$ and $\Delta g_{\text{ext}}$, NG-MCTS is only slightly worse. On the other hand, NG-MCTS outperforms on $\Delta g_{\text{ext}}$ and $\Delta P[g]$, which indicates that step-wise guidance of semantic prior helps to generalize better in extrapolation than all the other methods.

We also apply the aforementioned methods to search expressions in holdout sets $M[f] = 5$ and $M[f] = 6$. The percentage of solved expressions decreases as $M[f]$ increases. This is reasonable because larger $M[f]$ requires more complicated syntactic structure, which makes the search more difficult. The median of $\Delta P[g]$ also increases with larger $M[f]$ for the other methods, but the value for NG-MCTS is
Table 4. Results of symbolic regression methods. Search expressions in holdout sets $M[f] \leq 4$, $M[f] = 5$ and $M[f] = 6$ with data points on $D_{train}$ and/or leading powers $P_{x \rightarrow 0}[f]$ and $P_{x \rightarrow \infty}[f]$. The options are marked by on ($\sqrt{ }$), off ($\times$) and not available ($–$). If the RMSEs of the best found expression $g(x)$ in interpolation and extrapolation are both smaller than $10^{-6}$ and $\Delta P[g] = 0$, it is solved. If $g(x)$ is non-terminal or $\infty$, it is invalid. Hard includes expressions in the holdout set which are not solved by any of the six methods. The medians of $\Delta g_{train}$, $\Delta g_{int}$, $\Delta g_{ext}$, and the median absolute errors of leading powers $\Delta P[g]$ for hard expressions are reported.

| $M[f]$ | METHOD | NEURAL OBJECTIVE FUNCTION | SOLVED | INVALID | PERCENT | HARD |
|--------|--------|---------------------------|--------|---------|---------|------|
|        |        | $D_{train}$ $P_{x \rightarrow 0}[f]$ |        |         |         |      |
| $\leq 4$ | MCTS | $\times$ $\sqrt{ }$ $\times$ | 0.54% | 2.93% | 0.728 | 0.598 | 0.723 | 3 |
| | MCTS (PW-ONLY) | $\times$ $\times$ $\times$ | 0.24% | 0.00% | 2.069 | 2.823 | 1 |
| | NG-MCTS | $\sqrt{ }$ $\sqrt{ }$ $\times$ | 0.20% | 0.39% | 0.967 | 0.836 | 0.541 | 2 |
| | EA | $\sqrt{ }$ $\sqrt{ }$ $\times$ | 71.22% | 0.00% | 0.225 | 0.194 | 0.084 | 0 |
| | EA + PW | $\sqrt{ }$ $\times$ $\times$ | 12.83% | 3.32% | 0.186 | 0.162 | 0.358 | 3 |
| $= 5$ | MCTS | $\times$ $\sqrt{ }$ $\times$ | 0.00% | 3.90% | 0.857 | 0.738 | 0.950 | 5 |
| | MCTS (PW-ONLY) | $\times$ $\times$ $\times$ | 0.00% | 0.00% | 1.890 | 1.027 | 1 |
| | NG-MCTS | $\sqrt{ }$ $\sqrt{ }$ $\times$ | 0.10% | 3.50% | 1.105 | 0.914 | 0.500 | 4 |
| | EA | $\sqrt{ }$ $\sqrt{ }$ $\times$ | 32.10% | 0.00% | 0.247 | 0.229 | 0.020 | 0 |
| | EA + PW | $\sqrt{ }$ $\times$ $\times$ | 2.90% | 4.20% | 0.227 | 0.204 | 0.155 | 4 |
| $= 6$ | MCTS | $\times$ $\sqrt{ }$ $\times$ | 0.00% | 6.33% | 0.366 | 0.365 | 0.109 | 0 |
| | MCTS (PW-ONLY) | $\times$ $\times$ $\times$ | 0.00% | 0.00% | 1.027 | 0.819 | 0.852 | 6 |
| | NG-MCTS | $\sqrt{ }$ $\sqrt{ }$ $\times$ | 0.08% | 7.33% | 1.228 | 1.051 | 0.391 | 4 |
| | EA | $\sqrt{ }$ $\sqrt{ }$ $\times$ | 17.33% | 0.17% | 0.236 | 0.209 | 0.008 | 0 |
| | EA + PW | $\sqrt{ }$ $\times$ $\times$ | 1.25% | 5.08% | 0.219 | 0.191 | 0.084 | 5 |

always zero. This demonstrates that our NN model is able to successfully guide the NG-MCTS even for leading powers not appearing in the training set. Overall, NG-MCTS still significantly outperforms other methods in solved percentage and extrapolation. Figure 3 compares $\Delta g_{ext}$ for each expression among different methods in holdout set $M[f] = 5$. The upper right cluster in each plot represents expressions unsolved by both methods. Most of the plotted points are above the 1:1 line (dashed), which shows that NG-MCTS outperforms the others for most unsolved expressions in extrapolation. Examples of expressions solved by NG-MCTS but unsolved by EA + PW and vice versa are presented in Appendix H.

Since noise may exist in realistic applications of symbolic regression, we repeat the same experiment with Gaussian noise on $D_{train}$ in Appendix I. The percentage of solved expressions decreases for all methods but NG-MCTS still solves significantly more tasks.

7. Conclusion

In this work, we introduce the idea of semantic priors as represented by leading powers as a powerful concept for symbolic regression. Our expression generating NN successfully favors generating expressions with the desired leading powers, generalizing syntactically and semantically, and to more complex leading powers. This model is used in Neural Guided Monte Carlo Tree Search (NG-MCTS) to effectively perform symbolic regression. Our experiments demonstrate the robustness and superiority of our technique on thousands of desired expressions, which are a much larger evaluation set than the benchmarks considered in earlier symbolic regression approaches.

One of the surprising aspects of this work is the generalization of our expression generating NN to more complex leading powers. We hope to further extend the applicability of this model to more robustly cover the leading powers relevant for realistic modeling problems. Further, our work highlights the importance of guiding the search in symbolic regression using a neural network with semantic prior knowledge. Producing new models for generation that take other forms of semantic priors besides leading powers is an important area of further research.
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A. Dataset

In order to create a dataset balanced on each condition, we first enumerate all possible parse trees from

\[ O \rightarrow S \]
\[ S \rightarrow S^* + T | S^* - T | S^* T | S^* / T | T \]
\[ T \rightarrow ('S') | 'x' | '1' \]

within ten production rules. Then we repeat downsampling and augmentation operations for four times.

**Downsampling** Expressions are grouped by their simplified expressions computed by SymPy (Meurer et al., 2017). For each group, we select 20 shortest expressions in terms of string length.

**Augmentation** For each expression, five new expressions are created by randomly replacing one of the 1 or x symbols by \((1/x), (x/(1+x)), (x/(1-x)), (1/(1+x)), (1/(1-x)), (1-x), (1+x), (x * x), (x * (1+x)), (x * (1-x))\).

B. Details of the Baseline Models

We provide more details of the baseline models we proposed to be compared with our NN model. Using the same notation as in Eq. (3), the conditional distribution of the next production rule given the partial sequence and the desired condition is denoted by

\[ p(r_{t+1}|r_1, \ldots, r_t, c^{(0)}, c^{(\infty)}) \]

The baseline models are essentially different ways to approximate the conditional distribution using empirical distributions.

**Limited History (LH) (l)\)** The conditional distribution is approximated by the empirical conditional distribution given at most the last \(l\) production rules of the partial sequence and the desired condition. We derive the empirical conditional distribution from the training set by first finding all the partial sequences therein that match the given partial sequence and desired condition. Then we compute the proportion of each production rule that appears as the next production rule of the found partial sequences. The proportion is therefore the empirical conditional distribution. To avoid introducing an invalid next production rule, the empirical conditional distribution is multiplied by the production rule mask of valid next production rules, and renormalized.

\[ p_{\text{LH}}^{(l)} = \hat{p}(r_{t+1}|r_{t-l+1}, \ldots, r_t, c^{(0)}, c^{(\infty)}) \]

**Full History (FH)** The conditional distribution is approximated by the empirical conditional distribution given the full partial sequence and the desired condition. The empirical conditional distribution is derived from the training set similarly as the LH model.

\[ p_{\text{FH}} = \hat{p}(r_{t+1}|r_1, \ldots, r_t, c^{(0)}, c^{(\infty)}) \]

**Limited History No Condition (LHNC) (l)** The conditional distribution is approximated by the empirical conditional distribution given at most the last \(l\) production rules of the partial sequence only, where the desired condition is ignored. The empirical conditional distribution is derived from the training set similarly as the LH model.

\[ p_{\text{LHNC}}^{(l)} = \hat{p}(r_{t+1}|r_{t-l+1}, \ldots, r_t) \]

**Full History No Condition (FHNC)** The conditional distribution is approximated by the empirical conditional distribution given the full partial sequence only, where the desired condition is ignored. The empirical conditional distribution is derived from the training set similarly as the LH model.

\[ p_{\text{FHNC}} = \hat{p}(r_{t+1}|r_1, \ldots, r_t) \]

C. Details of Aggregating Metrics on Different Levels

The metrics are aggregated on different levels. We compute the average of success rates, syntactic novelty rates and semantic novelty rates over all the conditions in the in-sample condition region. The out-of-sample condition region is not bounded, and hence we consider the region within \([P_{x \rightarrow 0}[f]] \leq 9\) and \([P_{x \rightarrow \infty}[f]] \leq 9\). Since the average can be arbitrarily small if the boundary is arbitrarily large, instead we compute the total number of success, syntactic novelty and semantic novelty expressions over all the conditions in the out-of-sample region.

The L1-distance is not well defined for an expression which is non-terminal or \(\infty\). For both cases, we specify the L1-distance as 18, which is the L1-distance between conditions \((0, 0)\) and \((9, 9)\).

D. Diversity of Generated Expressions

A model that generates expressions with a high success rate (i.e., satisfying the desired condition most of the times) but lacking of diversity is problematic. To demonstrate the diversity of expressions generated by our NN model, we generate 1000 expressions on each desired condition, and compute the cumulative counts of unique expressions and unique simplified expressions that satisfy the desired condition among the first number of expressions of the 1000 generated expressions, respectively. Figure D.1 shows the cumulative counts on three typical desired conditions \((c^{(0)}, c^{(\infty)}) = (0, 0), (5, 5), (-2, -3)\). We can observe that the counts steadily increase as the number of generated expressions under consideration increases. Even with 1000 expressions, the counts have not been saturated.
E. Additional Plots of Metrics for Expression Generating NN and Baseline Models

Due to the space limit of the paper, Figure 2 in the main text only contains the plots of metrics on each condition for LHNC (8) and NN. Additional plots of all the baseline models in Table 1 are presented in this section. Figure E.1 contains NN, NNNC and Random. Figure E.2 contains FH and FHNC. Figure E.3 contains LH (2), LH (4), LH (8) and LH (16). Figure E.4 contains LHNC (2), LHNC (4), LHNC (8) and LHNC (16).

F. Selection Step in Monte Carlo Tree Search

In the selection step, we use a variant of the PUCT algorithm (Silver et al., 2016; Rosin, 2011) for exploration,

$$U(s_t, a) = c_{puct} P(s_t, a) \sqrt{\frac{\sum_b N(s_t, b)}{1 + N(s_t, a)}},$$  \hspace{0.5cm} (4)

where $N(s_t, a)$ is the number of visits to the current node, $\sum_b N(s_t, b)$ is the number of visits to the parent of the current node, $c_{puct}$ controls the strength of exploration and $P(s_t, a)$ is the prior probability of action $a$. This strategy initially prefers an action with high prior probability and low visits for similar tree node quality $Q(s_t, a)$.

G. Choice of Hyperparameters

NN is trained with batch size 256 for $10^7$ steps. The initial learning rate is 0.001. It decays exponentially every $10^5$ steps with a base of 0.99.

The hyperparameters of MCTS (exploration strength = 50) and EA (the probability of mating two individuals = 0.1, the probability of mutating an individual = 0.5) are selected by hyperparameter searching to maximize the solved percentage in holdout set $M[f] \leq 4$ with both $D_{train}$ and $P_{x \rightarrow 0}[f]$, $P_{x \rightarrow 0}[f]$ provided.

H. Examples of Symbolic Regression Results

In this section, we select expressions solved by NG-MCTS but unsolved by EA + PW in Table 4 as examples of symbolic regression results. Figure H.1, Figure H.2 and Figure H.3 show eight expressions with $M[f] \leq 4$, $M[f] = 5$ and $M[f] = 6$, respectively. The symbolic expressions, leading powers, interpolation errors and extrapolation errors of these 24 desired expressions $f(x)$, as well as their corresponding best expressions found by NG-MCTS, denoted by $g^{NG-MCTS}(x)$, and by EA + PW, denoted by $g^{EA+PW}(x)$, are listed in Table H.1.

We also select expressions solved by EA + PW but unsolved by NG-MCTS in Table 4 as examples of symbolic regression results. Figure H.4, Figure H.5 and Figure H.6 show eight expressions with $M[f] \leq 4$, $M[f] = 5$ and $M[f] = 6$, respectively. The symbolic expressions, leading powers, interpolation errors and extrapolation errors of these 24 desired expressions $f(x)$, as well as their corresponding best expressions found by NG-MCTS and EA + PW are listed in Table H.2.

I. Symbolic Regression with Noise

In the main text, the training points $D_{train}$ from the desired expression is noise-free. However, in realistic applications of symbolic regression, measurement noise usually exists. We add a random Gaussian noise with standard deviation 0.5 to expression evaluations on $D_{train}$ and compute $\Delta g_{int.}$ and $\Delta g_{text}$ using evaluations without noise. The results are summarized in Table I.1. The performance of all the methods is worse than that in the noise-free experiments,
but the relative relationship still remains. NG-MCTS solves the most expressions than all the other methods. It has the lowest medians of $\Delta g_{\text{ext}}$ and $\Delta P[g]$, suggesting good generalization in extrapolation even with noise on training points.
Figure E.1. Metrics for NN, NNNC and Random models on each condition within \(|P_{x \to 0}[f]| \leq 9\) and \(|P_{x \to \inf}[f]| \leq 9\). Each column corresponds to a metric: success rate, mean L1-distance, syntactic novelty rate and semantic novelty rate, respectively. Conditions with \(M[f] \leq 4\) are inside the red boundary. Conditions with zero success rate, syntactic novelty rate or semantic novelty rate are left blank in the corresponding plots.
Figure E.2. Metrics for FH and FHNC models on each condition within $|P_{x\rightarrow 0}[f]| \leq 9$ and $|P_{x\rightarrow \infty}[f]| \leq 9$. Each column corresponds to a metric: success rate, mean L1-distance, syntactic novelty rate and semantic novelty rate, respectively. Conditions with $M[f] \leq 4$ are inside the red boundary. Conditions with zero success rate, syntactic novelty rate or semantic novelty rate are left blank in the corresponding plots.
Figure E.3. Metrics for LH models with different history length on each condition within $|P_{x \to 0}[f]| \leq 9$ and $|P_{x \to \infty}[f]| \leq 9$. Each column corresponds to a metric: success rate, mean L1-distance, syntactic novelty rate and semantic novelty rate, respectively. Conditions with $M[f] \leq 4$ are inside the red boundary. Conditions with zero success rate, syntactic novelty rate or semantic novelty rate are left blank in the corresponding plots.
Figure E.4. Metrics for LHNC models with different history length on each condition within $|P_{x \rightarrow 0}f| \leq 9$ and $|P_{x \rightarrow \infty}f| \leq 9$. Each column corresponds to a metric: success rate, mean L1-distance, syntactic novelty rate and semantic novelty rate, respectively. Conditions with $M[f] \leq 4$ are inside the red boundary. Conditions with zero success rate, syntactic novelty rate or semantic novelty rate are left blank in the corresponding plots.
Figure H.1. Examples of expressions solved by NG-MCTS but unsolved by EA + PW with $M[f] \leq 4$. Each subplot of (a)-(h) demonstrates an expression solved by NG-MCTS but unsolved by EA + PW. Grey area is the region to compute interpolation error $\Delta g_{\text{int}}$, and light blue area is the region to compute extrapolation error $\Delta g_{\text{ext}}$. The display range of y-axis is $[-5, 5]$ for the four subplots in the first row and $[-200, 200]$ for the four subplots in the second row to show the discrepancy of expressions on two different scales.

Figure H.2. Examples of expressions solved by NG-MCTS but unsolved by EA + PW with $M[f] = 5$. Each subplot of (a)-(h) demonstrates an expression solved by NG-MCTS but unsolved by EA + PW. Grey area is the region to compute interpolation error $\Delta g_{\text{int}}$, and light blue area is the region to compute extrapolation error $\Delta g_{\text{ext}}$. The display range of y-axis is $[-5, 5]$ for the four subplots in the first row and $[-200, 200]$ for the four subplots in the second row to show the discrepancy of expressions on two different scales.
Figure H.3. Examples of expressions solved by NG-MCTS but unsolved by EA + PW with $M[f] = 6$. Each subplot of (a)-(h) demonstrates an expression solved by NG-MCTS but unsolved by EA + PW. Grey area is the region to compute interpolation error $\Delta g_{int}$, and light blue area is the region to compute extrapolation error $\Delta g_{ext}$. The display range of y-axis is $[-5, 5]$ for the four subplots in the first row and $[-200, 200]$ for the four subplots in the second row to show the discrepancy of expressions on two different scales.

Figure H.4. Examples of expressions solved by EA + PW but unsolved by NG-MCTS with $M[f] \leq 4$. Each subplot of (a)-(h) demonstrates an expression solved by EA + PW but unsolved by NG-MCTS. Grey area is the region to compute interpolation error $\Delta g_{int}$, and light blue area is the region to compute extrapolation error $\Delta g_{ext}$. The display range of y-axis is $[-5, 5]$ for the four subplots in the first row and $[-200, 200]$ for the four subplots in the second row to show the discrepancy of expressions on two different scales.
| θ | P_{\text{true}} | P_{\text{est}} | Δ | Δ_{\text{true}} |
|---|---|---|---|---|
| θ_1 | -2 | -2 | 0.000 | 0.000 |
| θ_2 | -2 | -2 | 0.324 | 0.025 |
| θ_3 | -4 | 0 | 0.000 | 0.000 |
| θ_4 | -4 | 0 | 0.493 | 0.155 |
| θ_5 | -1 | -2 | 0.000 | 0.000 |
| θ_6 | -1 | -1 | 0.153 | 0.000 |
| θ_7 | -2 | -2 | 0.000 | 0.000 |
| θ_8 | -2 | -2 | 2.076 | 0.000 |
| θ_9 | 1 | 0 | 0.000 | 0.000 |
| θ_10 | 3 | 1 | 0.382 | 0.000 |
| θ_11 | 3 | 0 | 0.746 | 0.000 |
| θ_12 | -3 | -2 | 0.000 | 0.000 |
| θ_13 | -3 | -2 | 0.211 | 0.008 |
| θ_14 | 4 | 1 | 0.000 | 0.000 |
| θ_15 | 4 | 1 | 0.053 | 0.309 |
| θ_16 | 0 | -5 | 0.000 | 0.000 |
| θ_17 | 0 | -2 | 0.000 | 0.000 |
| θ_18 | -3 | 2 | 0.000 | 0.000 |
| θ_19 | 2 | 2 | 2.289 | 22.530 |
| θ_20 | -1 | -2 | 0.000 | 0.000 |
| θ_21 | -2 | -2 | 0.753 | 247.637 |
| θ_22 | -2 | -3 | 0.000 | 0.000 |
| θ_23 | -2 | -2 | 0.000 | 0.000 |
| θ_24 | -2 | -2 | 2.203 | 343.242 |
| θ_25 | -3 | -3 | 0.000 | 0.000 |
| θ_26 | -3 | -3 | 0.000 | 0.000 |
| θ_27 | -3 | -1 | 2.086 | 0.303 |
| θ_28 | -3 | -3 | 0.000 | 0.000 |
| θ_29 | -3 | -2 | 0.000 | 0.000 |
| θ_30 | -3 | -2 | 0.000 | 0.000 |

Table H.1: Examples of expressions solved by NG-MCTS out unovel by EA + PW. This table shows the desired expressions found by NG-MCTS, θ_{\text{true}} (‘θ’), and by EA + PW, θ_{\text{est}} (‘θ’), and their corresponding best expressions found by NG-MCTS, θ_{\text{true}} (‘θ’), and by EA + PW, θ_{\text{est}} (‘θ’). The leading powers θ_{\text{true}} (‘θ’) and θ_{\text{est}} (‘θ’) are marked for each expression.
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Figure H.5. **Examples of expressions solved by EA + PW but unsolved by NG-MCTS with** $M[f] = 5$. Each subplot of (a)-(h) demonstrates an expression solved by EA + PW but unsolved by NG-MCTS. Grey area is the region to compute interpolation error $\Delta g_{\text{int}}$, and light blue area is the region to compute extrapolation error $\Delta g_{\text{ext}}$. The display range of y-axis is $[-5, 5]$ for the four subplots in the first row and $[-200, 200]$ for the four subplots in the second row to show the discrepancy of expressions on two different scales.

Figure H.6. **Examples of expressions solved by EA + PW but unsolved by NG-MCTS with** $M[f] = 6$. Each subplot of (a)-(h) demonstrates an expression solved by EA + PW but unsolved by NG-MCTS. Grey area is the region to compute interpolation error $\Delta g_{\text{int}}$, and light blue area is the region to compute extrapolation error $\Delta g_{\text{ext}}$. The display range of y-axis is $[-5, 5]$ for the four subplots in the first row and $[-200, 200]$ for the four subplots in the second row to show the discrepancy of expressions on two different scales.
### Table H.2: Examples of expressions solved by EA + PW but unsolved by NG-MCTS (\(g\)) and by EA + PW \& MCTS (\(f\)). The leading powers \(P_{\nu=1}\) and \(P_{\nu=0}\), interpolation error \(\Delta x\nu\), and extrapolation error \(\Delta x\nu\).

| EXPRESSION | \(P_{\nu=1}\) | \(P_{\nu=0}\) | \(\Delta x\nu\) | \(\Delta x\nu\) |
|------------|----------------|----------------|----------------|----------------|
| \(g_0\)   | -3             | -3             | 0.026          | 0.053          |
| \(g_0\)   | 3              | 3              | 0.000          | 0.000          |
| \(g_0\)   | 3              | 3              | 0.000          | 0.000          |
| \(g_0\)   | 3              | 3              | 0.000          | 0.000          |
| \(g_0\)   | 3              | 3              | 0.000          | 0.000          |
| \(g_0\)   | 3              | 3              | 0.000          | 0.000          |
| \(g_0\)   | 3              | 3              | 0.000          | 0.000          |
| \(g_0\)   | 3              | 3              | 0.000          | 0.000          |
| \(g_0\)   | 3              | 3              | 0.000          | 0.000          |
| \(g_0\)   | 3              | 3              | 0.000          | 0.000          |

Note: The table shows the leading expressions found by NG-MCTS (\(g\)) and by EA + PW \& MCTS (\(f\)). The leading powers \(P_{\nu=1}\) and \(P_{\nu=0}\) are given, along with interpolation and extrapolation errors.
Table I.1. Results of symbolic regression methods with noise. Search expressions in holdout sets $M[f] \leq 4$, $M[f] = 5$ and $M[f] = 6$ with data points on $D_{\text{train}}$ and / or leading powers $P_{x \rightarrow 0}[f]$ and $P_{x \rightarrow \infty}[f]$. The options are marked by on (✓), off (×) and not available (–). If the RMSEs of the best found expression $g(x)$ in interpolation and extrapolation are both smaller than $10^{-9}$ and $\Delta P[g] = 0$, it is solved. If $g(x)$ is non-terminal or $\infty$, it is invalid. Hard includes expressions in the holdout set which are not solved by any of the six methods. The medians of $\Delta g_{\text{train}}$, $\Delta g_{\text{int}}$, $\Delta g_{\text{ext}}$ and the median absolute errors of leading powers $\Delta P[g]$ for hard expressions are reported.

| $M[f]$ | METHOD | NEURAL OBJECTIVE FUNCTION | SOLVED | INVALID | PERCENT | $\Delta g_{\text{train}}$ | $\Delta g_{\text{int}}$ | $\Delta g_{\text{ext}}$ | $\Delta P[g]$ |
|--------|--------|---------------------------|--------|---------|---------|-----------------|-----------------|-----------------|---------|
| ≤ 4    | MCTS   | × ✓ ×                     | 0.39%  | 0.54%   | 0.689  | 0.351 | 0.371 | 3 |
|        | MCTS (PW-ONLY) | × × ✓ | 0.34% | 0.00% | 1.003 | 0.865 | 1 |
|        | MCTS + PW | ✓ ✓ ✓ | 0.34% | 0.49% | 0.887 | 0.643 | 0.825 | 2 |
|        | NG-MCTS | ✓ ✓ ✓ | 24.29% | 0.05% | 0.452 | 0.449 | 0.256 | 0 |
|        | EA     | ✓ ✓ ×                     | 4.44%  | 3.95%   | 0.399  | 0.223 | 0.591 | 3 |
|        | EA + PW | ✓ ✓ ✓ | 4.34%  | 0.39%   | 0.385  | 0.489 | 0.260 | 0 |
| = 5    | MCTS   | × ✓ ×                     | 0.00%  | 4.00%   | 0.931  | 0.599 | 0.972 | 5 |
|        | MCTS (PW-ONLY) | × × ✓ | 0.00% | 0.00% | 1.394 | 1.000 | 3 |
|        | MCTS + PW | ✓ ✓ ✓ | 0.00% | 3.00% | 0.944 | 0.817 | 0.727 | 5 |
|        | NG-MCTS | ✓ ✓ ✓ | 10.80% | 0.10% | 0.558 | 0.430 | 0.103 | 0 |
|        | EA     | ✓ ✓ ×                     | 1.00%  | 3.10%   | 0.480  | 0.256 | 0.266 | 4 |
|        | EA + PW | ✓ ✓ ✓ | 1.80%  | 1.80%   | 0.448  | 0.382 | 0.122 | 0 |
| = 6    | MCTS   | × ✓ ×                     | 0.00%  | 9.75%   | 0.960  | 0.762 | 0.888 | 6 |
|        | MCTS (PW-ONLY) | × × ✓ | 0.00% | 0.00% | 1.024 | 0.861 | 4 |
|        | MCTS + PW | ✓ ✓ ✓ | 0.00% | 8.83% | 1.122 | 0.807 | 0.163 | 4 |
|        | NG-MCTS | ✓ ✓ ✓ | 10.33% | 0.08% | 0.426 | 0.205 | 0.009 | 0 |
|        | EA     | ✓ ✓ ×                     | 0.67%  | 4.58%   | 0.463  | 0.427 | 0.852 | 5 |
|        | EA + PW | ✓ ✓ ✓ | 1.42%  | 6.50%   | 0.388  | 0.369 | 0.065 | 0 |