

GEOBENCH: A NEW BENCHMARK ON SYMBOLIC REGRESSION WITH GEOMETRIC EXPRESSIONS

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ABSTRACT

Symbolic regression (SR) is a highly effective approach for discovering mathematical expressions directly from data. With the proliferation of various SR methods, SRBench (La Cava et al., 2021) has made an important contribution by offering a standardized evaluation framework that includes 130 SR datasets and assesses 14 SR methods. Nevertheless, the methods incorporated in SRBench are somewhat outdated, and the benchmark dataset does not encompass results from more recent approaches, such as SNIP (Meidani et al., 2024). Furthermore, the evaluation metrics employed in SRBench fail to fully capture the breadth of symbolic regression capabilities, and the benchmark data itself exhibits scientific inconsistencies. Although Matsubara et al. (2022) address some of these issues, their approach remains incomplete. In response, we propose a novel benchmark consisting of 71 expressions derived from geometric contexts, which are categorized into three difficulty levels: easy, medium, and hard. We conduct an evaluation of 20 SR methods on these expressions, focusing exclusively on the symbolic regression capabilities of each model. These capabilities are measured in terms of recovery rates across the different difficulty levels and in aggregate. Our study provides a comprehensive methodology for reproducing the experiments and includes results for newly developed SR methods using this updated benchmark. The findings reveal significant variability in the symbolic regression performance across the evaluated models.

1 INSTRUCTION

In many aspects of life, various phenomena can be described by mathematical equations, such as Newton’s Second Law and the law of gravity. Symbolic regression (SR) is a powerful tool for uncovering these underlying relationships. Specifically, SR seeks to discover a mathematical expression that links input and output data. Unlike traditional machine learning techniques, such as neural networks, SR offers greater interpretability and superior generalization, avoiding the complexity often associated with opaque models. Due to these advantages, symbolic regression has been applied across diverse fields, including physics (Sun et al., 2021; Udrescu & Tegmark, 2020; Schmidt & Lipson, 2009), network control (Sharan et al., 2022), finance (La Malfa et al., 2021), and material science (Wang et al., 2019).

However, symbolic regression (SR) poses significant challenges due to its expansive search space. The inclusion of constants further complicates the task, as they increase the complexity of potential solutions. In fact, SR has been formally proven to be an NP-complete problem (Virgolin & Pissis, 2022; Song et al., 2024).

Historically, SR originated with polynomial fitting, where early approaches focused on extracting equations through linear regression. To improve accuracy, researchers incorporated more complex input features, such as Fourier bases. However, this method compromised the interpretability of the results and increased the risk of overfitting.

Subsequently, expression trees became a popular approach for tackling SR tasks. An expression tree consists of *internal nodes* representing mathematical operators (e.g., $+$, $-$, \times , \div , \log , \exp , \sin , \cos) and *leaf nodes* that represent constants (e.g., 1, 2) or variables (e.g., x). By recursively evaluating sub-trees, the expression tree generates a corresponding mathematical expression. The construction of an expression tree typically follows a recursive method, where operators are added in pre-order

054 traversal until no further additions are possible. This transforms SR into a sequence generation
055 problem, akin to tasks in natural language processing (NLP).
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057 Symbolic regression involving constants presents a particularly challenging task. Traditional meth-
058 ods often treat constants within equations as parameters in a linear regression framework, allowing
059 them to be estimated by solving the associated function. In subsequent stages, models typically sam-
060 ple random values to substitute for constants in the generated expressions. If an expression yields
061 a high loss value, the corresponding random constant is discarded, while constants producing lower
062 losses are retained. In more recent approaches, constants are preserved by introducing a constant
063 token. This allows the model to solve for the constant value during the error calculation phase. At
064 this stage, the constants are treated as input variables, and the error is treated as the target value.
065 Optimization algorithms, such as BFGS (Roger Fletcher & Sons, 2013), are commonly employed to
066 fine-tune the constants and minimize error.

067 With the development of SR methods came the emergence of benchmarks. Nyugen (Uy et al.,
068 2011) introduced one of the early symbolic regression benchmarks, comprising 12 short expressions
069 designed to evaluate SR techniques across a range of simple to moderately complex equations.
070 Similarly, Jin (Jin et al., 2019), Neat, and Keijzer (Keijzer, 2003) created their own datasets to
071 test the symbolic regression abilities of their models. However, the data in these benchmarks have
072 limitations, as they often involve non-prime functions, such as the expression $\sum_{i=1}^{x_1} \frac{1}{i}$, rather than
073 more fundamental mathematical expressions. Consequently, these datasets are sometimes more
074 suited to assessing curve-fitting abilities rather than the capacity to discover underlying symbolic
075 functions.

076 As well, some benchmarks have been developed to assess specific aspects of symbolic regres-
077 sion capabilities. For example, Nyugen^c primarily evaluates SR models’ ability to handle con-
078 stants, as all its equations include constant parameters. The R rationals and R* benchmarks
079 (McDermott et al., 2012) are designed to test models’ abilities to solve complex fractional equa-
080 tions, while the Livermore benchmark (Mundhenk et al., 2021b) focuses on equations containing
081 cos, sin, log, exp, and power functions. However, these benchmarks often lack real-world applica-
082 bility, as expressions like $\log(x_1 + 1) + \log(x_1^2 + x_1) + \log(x_1)$ are primarily suited for testing,
083 not use in real world. As well, these benchmarks has no uniform metric since some models tests for
084 R^2 and the other uses it for symbolic recovery rate.

085 The introduction of the AIFeynman dataset (Udrescu & Tegmark, 2020) marked a significant step
086 forward in SR benchmarking. This dataset comprises 120 equations derived from the Feynman
087 Lectures on Physics (Feynman et al., 2015) and serves as a robust benchmark for SR tasks. Re-
088 cently, the SRBench team (La Cava et al., 2021) has combined 118 equations from this dataset with
089 the Strogatz dataset (Strogatz, 2018), which includes 14 equations modeling nonlinear and chaotic
090 dynamical processes, providing a more comprehensive evaluation of SR methods. Additionally, SR-
091 Bench includes different noise levels ranging from 0.0, 0.1, 0.01, 0.001, to assess the models’ ability
092 to handle noisy data. This benchmark evaluates 14 SR methods as baselines, resolving issues seen
093 in earlier datasets, such as a focus on equations primarily suited for testing and not for real-world
094 scientific experiments. It also provides a framework to reproduce results and test new models. How-
095 ever, SRBench has some limitations, as more than half of the evaluated methods are based on genetic
096 programming (GP) approaches, and many are from before 2022. Furthermore, the benchmark in-
097 cludes some scientifically unrealistic assumptions, such as treating the gravitational constant as a
098 variable, and has been criticized for its oversimplified sampling process and inappropriate formulas
099 (Matsubara et al., 2022).

100 Subsequently, Matsubara et al. (2022) attempted to address some of the existing issues; however,
101 their evaluation was restricted to only six methods. This limited selection of baselines may result in
102 an insufficient comparison, particularly when assessing the performance of new models introduced
103 into the field.

104 To address these issues, we propose our geometric dataset. It consists of 2D and 3D geometric
105 problems, such as calculating the area of a triangle given the lengths of its three sides. These
106 problems are meaningful in real-world applications and complement existing physical symbolic
107 regression datasets. We categorize these datasets into three difficulty levels: easy, medium, and
hard. We evaluate our 71 datasets using 20 SR baselines from 8 different approaches. The metrics of
our benchmark are twofold: (1) the symbolic recovery rate across each difficulty level and overall,

108 and (2) the number of expressions that can be discovered when models are allowed to run for an
109 extended period.
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111 2 DIFFERENT APPROACH OF SYMBOLIC REGRESSION 112

113 **Linear Methods:** The SINDy method (Kaiser et al., 2018) applies the L1 Loss to reduce the number
114 of active basis functions in a linear regression framework, thereby distilling a simple equation as a
115 linear combination of candidate terms from a predefined library. Although SINDy is known for
116 its interpretability and speed, its performance heavily depends on the selection of the predefined
117 library. If the true solution is not a combination of terms in the library, SINDy is unable to identify
118 it. Recently, the KAN model (Liu et al., 2024) has emerged using spline methods as an alternative
119 to improve upon these limitations.
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121 **Genetic Programming:** The genetic programming method (Schmidt & Lipson, 2009; Augusto &
122 Barbosa, 2000; Gustafson et al., 2005) represents expressions as trees, which serve as the populations
123 in the algorithm. Mutation and crossover operations modify the trees by changing sub-trees or
124 exchanging parts of the tree. The advantage of genetic algorithms in symbolic learning is their
125 ability to iteratively modify the expression tree via genetic recombination, enabling the model to
126 explore a wide range of expressions. However, a significant disadvantage is the tendency of genetic
127 algorithms to overfit; once the algorithm veers toward an incorrect solution, it is often difficult
128 to recover a correct path to the truth.
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130 **Deep Learning Methods:** There are two main approaches to using deep learning in symbolic re-
131 gression. One approach leverages neural networks to identify relationships between variables and
132 merge them to reduce the search space (Udrescu & Tegmark, 2020; Udrescu et al., 2020). While
133 this method simplifies the search, it requires large amounts of data and does not always succeed
134 in fitting the correct equations. The other approach replaces traditional network components (e.g.,
135 linear layers or activation functions) with symbolic functions and applies L1 loss to reduce active
136 modules, thus simplifying the output (Martius & Lampert, 2016; Sahoo et al., 2018). This approach
137 achieves lower MSE, but optimizing the sparse network to precisely recover the correct equation is
138 extremely challenging.

139 **Deep Reinforcement Learning Methods:** The deep reinforcement learning approach (Petersen
140 et al., 2019) frames symbolic regression as a sequential decision-making problem, where models
141 take actions at each step (e.g., adding or modifying terms) based on the current state, which is
142 evaluated using a recurrent neural network (or LSTM). After each generation, the models learn from
143 the best-generated expressions, guided by a reward function. This method effectively narrows the
144 search space but can suffer from overfitting and lack of exploration.

145 **Traditional Machine Learning Methods:** This approach (Sun et al., 2022; Xu et al., 2024) is
146 similar to deep reinforcement learning but uses Monte Carlo Tree Search (MCTS) instead of neural
147 networks to guide the search process. By avoiding the need for neural network training, this method
148 is faster for smaller problems but struggles with more complex equations.

149 **Transformer-Based Pretrain Methods:** Inspired by the GPT models (Radford et al., 2018),
150 transformer-based symbolic regression models (Kamienny et al., 2022) pretrain on large sets of
151 artificial expressions and use this pretraining to generate expressions from input data. Subsequently,
152 genetic programming or reinforcement learning (Holt et al., 2022; Landajuela et al., 2022) is em-
153 ployed to refine the output of the transformer models. While transformers provide excellent initial
154 solutions, they may struggle with out-of-distribution data, leading to overfitting or poor performance
155 on unseen tasks.

156 **Bayesian Methods:** Bayesian symbolic regression (Jin et al., 2019; Guimerà et al., 2020) leverages
157 prior knowledge (e.g., preferences for basis functions, operators, or original features) and produces
158 symbolic expressions as a linear combination of concise terms, controlled by a prior distribution.
159 The symbolic regression problem is solved by sampling expression trees from the posterior distri-
160 bution using a Markov Chain Monte Carlo (MCMC) algorithm. Although this method conserves
161 memory, it can be computationally expensive and may struggle to produce accurate results due to
the limitations of MCMC sampling.

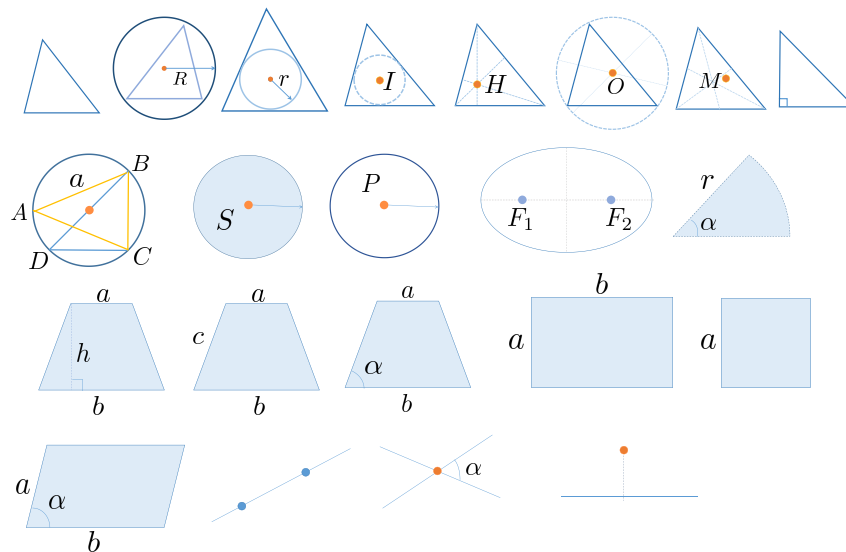


Figure 1: the 2D geometric objects in our dataset including triangles, circles, trapezoids, elliptic, squares, rectangles, lines and point.

Brute-Force Search Methods: Given that symbolic regression seeks simple expressions to describe phenomena, the true expression trees often have limited depth (e.g., maximum 6 layers). This observation motivates brute-force methods, which enumerate possible expressions layer by layer (Ruan et al., 2024), as the $n + 1$ -th layer can be constructed by combining elements from the n -th layer. GPU-based implementations can accelerate this search process, making brute-force methods effective for finding simple expressions with few variables, although they struggle with larger and more complex problems because of GPU’s memory.

3 GEOMETRIC DATASET

3.1 DATASETS

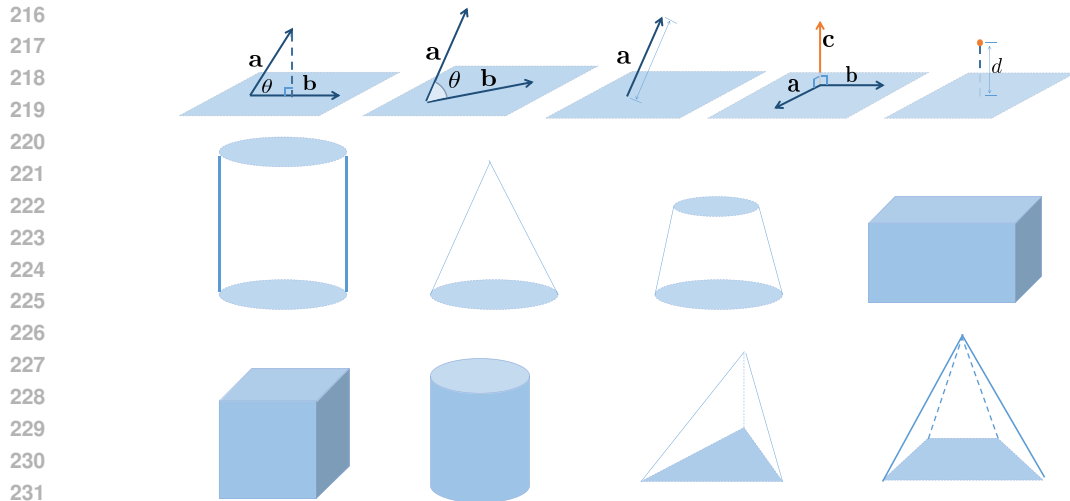
Diving into the details of our geometry dataset, it’s divided into two main sections: 2-D and 3-D geometry. The first section is a thorough compilation of 2-D geometrical shapes such as triangles, rectangles, squares, and circles, complete with their corresponding equations. In the second section, the dataset expands into the realm of 3-D geometry, presenting a wide array of shapes including vectors, spheres, various solids, and pyramids, each paired with their relevant equations.

2-D part: The dataset begins with various types of triangles. We assess the ability to determine the perimeter and area of triangles given different sets of known values: three sides (SSS), two sides with the included angle (SAS), and two angles with the included side (AAS) or the opposite sides (ASA). These four methods constitute the foundational techniques for establishing triangle congruence and equality.

For right-angled triangles, the dataset facilitates the calculation of the perimeter and area using the lengths of the right sides and the hypotenuse, or by employing the length of one right side and the angle opposite to it.

Incorporated into this dataset are three pivotal laws of trigonometry: the Cosine Theorem (Law of Cosines), the Pythagorean Theorem, and the Sine Theorem (Law of Sines). Utilization of these theorems allows for the resolution of the perimeter and area for a variety of straightforward geometrical constructs.

Moreover, the dataset tackles more challenging computations such as determining the circumcircle and incircle radius of a triangle based solely on its three side lengths.



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Figure 2: the 3D geometric objects in our dataset including three-dimensional vectors, cylinder, cones, frustums, sphere, cuboids, cubes, pyramids and tetrahedrons.

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Expanding beyond simple measurements, we also delve into coordinate geometry. The dataset includes the calculation of the horizontal coordinates for four significant points within a triangle: the centroid (center of mass), the incenter (intersection of angle bisectors), the circumcenter (intersection of perpendicular bisectors), and the orthocenter (intersection of altitudes). These calculations are vital for a deeper understanding of a triangle’s geometric properties and their applications.

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Venturing beyond triangular shapes, our collection encompasses trapezoids, specifically focusing on isosceles trapezoids. By utilizing the dimensions of the upper and lower bases, height, sides, or the angles adjacent to the base, one can deduce both the perimeter and area of these quadrilaterals.

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The dataset also embraces the circular and elliptical geometries. It allows for the calculation of a circle’s perimeter (or circumference) using its radius, as well as the perimeter and area of a sector by its central angle and radius. For ellipses, the major and minor axes serve as the basis for determining the area and locating the focal points.

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Additionally, the dataset includes rectangles and squares. Given the lengths of their edges, we can easily determine their perimeter and area.

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Lastly, the dataset serves as a resource for analytical geometry concerning lines and points. It enables the determination of the horizontal and vertical coordinates where two lines intersect, based on their slopes and intercepts. It further aids in calculating the slope and intercept of a line passing through two points, given their horizontal and vertical coordinates. Additionally, it provides the tools to find the directed distance from a point to a line, integrating the line’s slope and intercept with the point’s coordinates.

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3-D part: For three-dimensional vectors, the dataset includes methods for calculating their magnitude, the cosine of the angle between two vectors, their dot product, and the horizontal coordinate of their cross product. In conjunction with point coordinates, it facilitates the calculation of the directed distance from a point to a plane, essential for spatial analysis.

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In terms of solids, the dataset aids in finding the surface area and volume of cylinders using their base radius and height. The same parameters are used for cones, with additional calculations for their surface area and volume. For frustums, the dataset provides a method to determine the surface area and volume from the radii of the upper and lower bases and the height.

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Spherical geometry is also covered, with the dataset enabling the calculation of a sphere’s surface area from its radius. In the study of cuboids, the dataset allows for the determination of the sum of edge lengths, surface area, and volume from the lengths of the three edges. Similarly, for cubes, the side length can be used to find the sum of edge lengths, surface area, and volume.

The dataset also includes calculations for pyramids, using the base area and height to find the volume. For regular tetrahedrons, the base edge and height, or the base edge and side, provide the necessary measurements to calculate surface area and volume. In addition, the hardest ones show that the volume of an arbitrary tetrahedron can be calculated using two equations.

The complete set of symbolic equations can be found in Table 2, Appendix Section A.

To delve deeper into this dataset, we observe that many equations are derived using Helen’s law or other complex expressions. However, a significant portion can be simplified to the determinant of a square matrix, exemplified by the equation for the horizontal coordinate of the circumcenter below. This simplification is noteworthy as determinants are not commonly employed in symbolic regression methods.

$$x_c = \frac{\begin{vmatrix} x_1^2 + y_1^2 & y_1 & 1 \\ x_2^2 + y_2^2 & y_2 & 1 \\ x_3^2 + y_3^2 & y_3 & 1 \end{vmatrix}}{2 \begin{vmatrix} x_1 & y_1 & 1 \\ x_2 & y_2 & 1 \\ x_3 & y_3 & 1 \end{vmatrix}}$$

Furthermore, the result from the determinant calculation may lead to misconceptions regarding the polynomial order within the models. A third-order determinant consists of three positive and three negative polynomials. The interplay between these positive and negative elements often misleads the model’s search direction. Therefore, searching ability against bad equations are useful in this benchmark.

We categorized all datasets into three difficulty levels:

- **Easy:** This category contains the simplest equations, such as the perimeter of a triangle given the lengths of its three edges ($P = a + b + c$) and the volume of a pyramid given the base area and height ($V = \frac{1}{3}Sh$). In summary, this level comprises combinations of basic polynomial equations, making them relatively easy to solve. Each equation in this category can typically be solved within one hour.
- **Medium:** This category includes equations involving non-linear terms. Examples include the Pythagorean theorem ($c = \sqrt{a^2 + b^2}$) and finding the vertical coordinate of the intersection of two lines given their slopes and intercepts ($y = \frac{k_2b_1 - k_1b_2}{k_2 - k_1}$). While these equations introduce non-linear components, they remain closely related to basic polynomial structures. Solving each equation in this category typically requires approximately five hours.
- **Hard:** This category features the most complex equations, such as the volume of an arbitrary tetrahedron and Heron’s formula for the area of a triangle based on the lengths of its three sides ($S = \sqrt{\frac{(a+b+c)(a+b-c)(a+c-b)(b+c-a)}{16}} = \sqrt{2a^2b^2 + 2a^2c^2 + 2b^2c^2 - a^4 - b^4 - c^4}/4$). These equations are characterized by longer and deeper mathematical structures, making them significantly more challenging to solve. Each equation in this category typically requires up to one day to solve. And, there are hard equations in our dataset is the cosine value of angle between two vectors $\cos \theta = \frac{x_1x_2 + y_1y_2 + z_1z_2}{\sqrt{(x_1^2 + y_1^2 + z_1^2) \times (x_2^2 + y_2^2 + z_2^2)}}$, which is composed by 6 variables.

And our dataset contains two different sizes: 500 for normal model and 100000 for machine learning models that need to fit the curve.

3.2 METRICS

We use the symbolic recovery rate as the primary metric for evaluating performance, calculated as follows:

$$\text{recovery rate} = \frac{\text{count of successful discoveries}}{\text{count of total roll-outs}} \quad (1)$$

Algorithm 1 Algorithm for Discriminating the Correct Expression**Input:** dataset $\mathcal{S}_{data} = (X, y)$, ground truth expression \mathcal{F} , input expression \mathcal{F}_i , simplify function.**Output:** Boolean value representing whether the input expression is correct.

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327  $\mathcal{F}_i(X) \rightarrow \hat{y}$  ▷ Evaluate the input expression  $\mathcal{F}_i$  on  $X$  to obtain  $\hat{y}$ 
328  $\|y - \hat{y}\| \rightarrow err$  ▷ Compute error between predicted and actual values
329 if  $err \geq 10^{-5}$  then
330     return false ▷ Return false if error exceeds threshold
331 end if
332  $simplify(\mathcal{F}_i) \rightarrow \mathcal{F}_i$  ▷ Simplify the input expression
333  $\mathcal{F}_i - \mathcal{F} \rightarrow \mathcal{G}$  ▷ Compute the difference functions between input and ground truth expressions
334  $simplify(\mathcal{G}) \rightarrow \mathcal{G}$  ▷ remove redundant sub-expressions
335 replace constants below  $10^{-5}$  in  $\mathcal{G}$  with 0
336 if  $\mathcal{G}$  is empty then
337     return true ▷ Return true if the expressions are equivalent
338 end if
339  $\mathcal{G}(X) \rightarrow \hat{z}$  ▷ Evaluate  $\mathcal{G}$  on  $X$  to obtain  $\hat{z}$ 
340  $\|\hat{z}\| \rightarrow err$  ▷ Compute error for the difference expression
341 if  $err \geq 10^{-20}$  then
342     return human_justify( $\mathcal{G}$ ) ▷ If error is still significant, defer to human justification
343 end if
344 return true ▷ Return true if the difference is negligible

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The method for distinguishing a successful discovery is outlined in Algorithm 1. We choose sympy (Meurer et al., 2017) to simplify the expression and human justify. We conduct 100 independent runs with different random seeds, and the time limits for the easy, medium, and hard problems are set to 1 hour, 5 hours, and 24 hours, respectively. Additionally, the hardware constraints include 10 CPU cores and one A100 GPU.

The metrics used for evaluating our benchmark are as follows:

- **Overall Recovery Rate:** The average recovery rate across all 71 datasets. This metric is designed to test the symbolic regression ability among all models.
- **Categorized Recovery Rate:** This metric allows for performance evaluation within specific difficulty levels (easy, medium, hard). By focusing on one category at a time, models can demonstrate their stability on easy problems and their capacity for exploration on hard problems.
- **Result-Oriented Recovery Rate:** Additional sub-categories can be created based on different dimensions, such as 2D versus 3D problems, the type of object studied (e.g., triangle, circle, sphere), and the type of result (e.g., perimeter, area, volume). This allows models to be compared within specific domains and contexts to highlight their performance in particular scenarios.
- **Number of Discovered Equations:** Since multiple runs can be performed for each algorithm, we also calculate the number of distinct expressions successfully discovered, where the recovery rate is greater than 0%. A higher number of discovered expressions reflects the model’s ability to search effectively across different problem spaces.

3.3 SYMBOLIC REGRESSION METHODS

We use 20 different symbolic method based on 8 different approach. The correspondence is shown in the table below Table 1 and all parameter setting is at Table 5 in Appendix Section B:

- **Bayesian Machine Scientist** (Guimerà et al., 2020): This model determines the posterior probability of each expression from a corpus of mathematical expressions compiled from Wikipedia. The MCMC algorithm is then used to sample from the posterior distribution of expressions, generating new expressions based on these probabilities.
- **PSRN** (Ruan et al., 2024): A symbolic regression model that utilizes parallelized tree search (PTS) to discover mathematical expressions from data. PSRN employs GPU-

Table 1: Correspondence between symbolic regression methods and approaches. BF stands for Brute Force Searching, DL denotes Deep Learning methods, DRL stands for Deep Reinforcement Learning methods, GP refers to Genetic Programming, Pretrain refers to methods using transformer modules for pretraining, Dimension refers to special methods targeting dimensional constraints and MCTS refers to machine learning models using the Monte Carlo Tree Search algorithm.

Symbolic Regression Method	Category
Bayesian Machine Scientist	Bayesian
PSRN	BF
EQL	DL
AI Feynman	DL
NGGP	DRL, GP
uDSR	DRL, GP, Pretrain
PhySO	DRL, GP, Dimension
gplearn	GP
DEAP	GP
pysr	GP, Dimension
Sindy	Linear
SymINDy	Linear, GP
KAN	Linear
SPL	MCTS
RSRM	MCTS, GP
NeSymReS	Pretrain
E2E	Pretrain
DGSR	Pretrain, GP
TPSR	Pretrain, MCTS
SNIP	Pretrain

accelerated parallel evaluation of symbolic expressions and implements efficient subtree reuse and caching. The model features a unique approach of selecting expressions based on minimum loss, followed by recursive symbolic backward derivation. Its core parallel symbolic regression module can integrate with various token generation methods.

- **EQL** (Coulom, 2006; Kim et al., 2020): This model uses multiplication units and nonlinear activation functions (e.g., sine and cosine) in its neural network. Each layer contains linear mappings and nonlinear transformations, and the network is trained using a Lasso-like objective function, combining L2 loss and L1 regularization.
- **AI Feynman** (Udrescu & Tegmark, 2020; Udrescu et al., 2020): This model employs a neural network to fit the data, then uses the network to identify relationships between variables, such as symmetry. After this, AiFeynman runs a brute-force search based on the extracted knowledge.
- **NGGP** (Mundhenk et al., 2021a): An upgraded version of DSR (Petersen et al., 2019), NGGP uses an RNN-based model through deep reinforcement learning to learn the distribution of expressions. It then fine-tunes these expressions using GP methods, focusing only on those that have been improved through fine-tuning.
- **uDSR** (Landajuela et al., 2022): An upgraded version of NGGP (Mundhenk et al., 2021a), this model incorporates the AiFeynman module to reduce the number of variables. It also introduces a linear token for generating polynomials and utilizes large-scale pretraining.
- **PhySO** (Tenachi et al., 2023): This model applies dimensional constraints to the NGGP (Mundhenk et al., 2021a) module. If a generated token violates dimensional constraints (e.g., summing variables with different dimensions), the generation probability is set to zero.
- **pysr** (Cranmer, 2023): Considered one of the best GP models, pysr optimizes hyperparameters algorithmically and supports dimensional constraints. When an expression violates dimensional constraints, its fitness is significantly penalized.
- **gplearn** (Stephens, 2016): This model retains the familiar scikit-learn fit/predict API, allowing it to work seamlessly with existing scikit-learn pipelines and grid search modules.

- 432 • **DEAP** (d’Ascoli et al., 2022): A novel evolutionary computation framework designed for
433 rapid prototyping and testing of ideas. It seeks to make algorithms explicit and data struc-
434 tures transparent. Many models using GP (Mundhenk et al., 2021a; Holt et al., 2022; Xu
435 et al., 2024) rely on DEAP as their foundation.
- 436 • **Sindy** (Kaheman et al., 2020): The original SINDy model uses sparse regression tech-
437 niques, such as LASSO, to obtain expressions from linear combinations of functions in a
438 predefined library of candidate functions.
- 439 • **SymINDy** (Kitaitsev & Manzi, 2022): This model uses GP to generate libraries of candi-
440 date functions and integrates them with the SINDy method. The fitness value is positively
441 correlated with the error produced by SINDy.
- 442 • **KAN** (Liu et al., 2024): In KAN, traditional weight parameters at the network’s edges
443 are replaced by univariate function parameters. Each node aggregates the outputs of these
444 functions without any nonlinear transformations, relying on spline methods to replace tra-
445 ditional weight parameters.
- 446 • **SPL** (Sun et al., 2022): This model contains many predefined simple expressions as mod-
447 ules and uses the MCTS method to combine these modules into full expressions. After
448 each roll-out, the best result is used as one of the modules for future iterations.
- 449 • **RSRM** (Xu et al., 2024): This model combines MCTS and GP to generate functions. It
450 employs double Q-learning to initialize probabilities in the MCTS module, enabling the
451 model to learn from previous roll-outs. The model also uses spline fitting to determine
452 whether functions are odd or even and includes an MSDB block to extract useful modules
453 from the best expressions for use in subsequent roll-outs.
- 454 • **NeSymReS** (Biggio et al., 2021): This model uses a pre-trained Transformer during the
455 pre-training phase, trained on hundreds of millions of equations specifically generated for
456 each batch. In the test step, an encoder encodes input expressions into latent vectors, from
457 which the decoder iteratively samples candidate skeletons for the symbolic equation. For
458 each candidate, numerical constants are fitted by treating them as independent parameters.
- 459 • **E2E** (Kamienny et al., 2022): This model trains a Transformer on a synthetic dataset
460 to perform end-to-end (E2E) symbolic regression, directly predicting solutions without
461 relying on skeletons. The predicted constants are refined using the BFGS algorithm
462 (Roger Fletcher & Sons, 2013) as an informed starting point. Additionally, generative
463 and inference techniques are introduced to allow the model to scale to larger problems.
- 464 • **DGSR** (Holt et al., 2022): This model trains a Transformer on a synthetic dataset, out-
465 putting expressions end-to-end, which are then refined using a GP module. The framework
466 can perform symbolic regression on a large number of input variables while reducing com-
467 putational cost during inference, as it encodes the data itself rather than the entire symbolic
468 expression tree. This is achieved by learning representations of equations that capture in-
469 variant structures across different equations.
- 470 • **TPSR** (Shojaee et al., 2023): TPSR utilizes a forward planning algorithm that incorpo-
471 rates Monte Carlo Tree Search (MCTS) as a decoding strategy on top of a pre-trained
472 Transformer-based SR model. This guides the generation of equation sequences. TPSR re-
473 duces overall inference time by incorporating feedback during the generation process and
474 using an efficient caching mechanism.
- 475 • **SNIP** (Meidani et al., 2024): SNIP (Symbolic-Numeric Integrated Pre-training) bridges
476 symbolic mathematical expressions and their corresponding numeric representations. The
477 model employs dual Transformer encoders: one dedicated to learning symbolic represen-
478 tations and the other for numeric representations. Task-independent comparison targets
479 enhance the similarity between the two representations. The multimodal pretraining of
480 SNIP enables cross-modal understanding and generation of content.

482 4 RESULTS

483 We present two primary results derived from the measured datasets in Figure 3. Further details and
484 additional results can be found in Appendix Section C Figure 4.

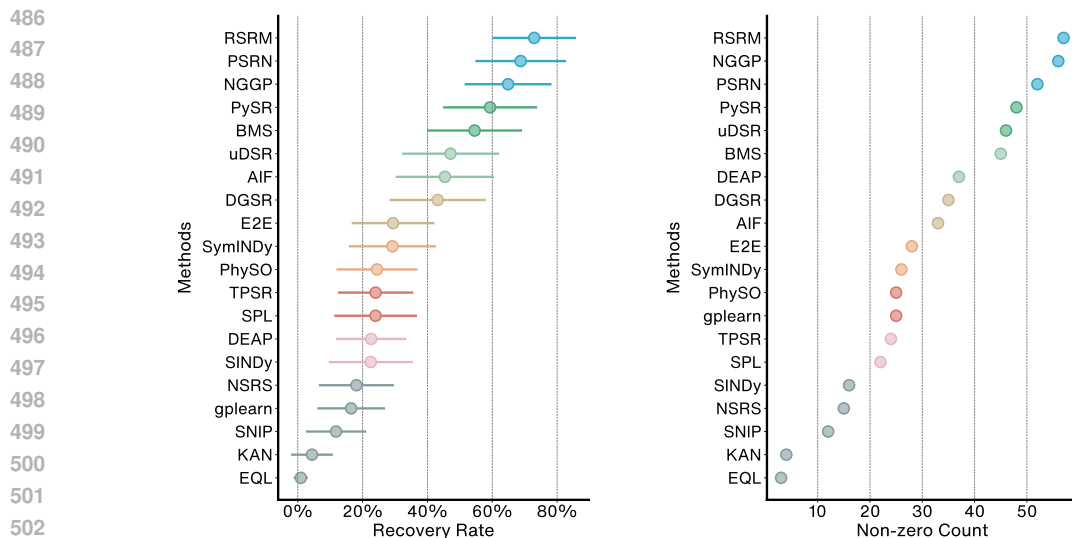


Figure 3: Results on the geometric dataset: the left panel illustrates the average recovery rate across all 71 equations, while the right panel displays the number of equations successfully discovered by the models. BMS, AIF and NGNS refer to the Bayesian Machine Scientist, AIFeynman and NeSymReS, respectively.

In the left panel, it is observed that the top five models in terms of recovery rate are RSRM (Xu et al., 2024), PSRN (Ruan et al., 2024), NGGP (Mundhenk et al., 2021a), PySR (Cranmer, 2023), and Bayesian Machine Scientist (Guimerà et al., 2020). Notably, methods based on deep learning and transformer-based pretraining tend to perform below these models.

A comparison within the same methodological class reveals consistent improvements in performance over time. However, in the case of transformer-based pretraining methods, newer models such as SNIP (Meidani et al., 2024) demonstrate weaker performance compared to earlier models like End2End Transformers (Kamienny et al., 2022). This discrepancy could be attributed to a focus on optimizing the R^2 score, potentially at the expense of true symbolic regression capabilities.

In the genetic programming domain, PySR (Cranmer, 2023) significantly outperforms other models such as DEAP (Fortin et al., 2012) and gplearn (Stephens, 2016). While hyperparameter tuning may contribute to this performance difference, dimensional analysis also plays a crucial role. Specifically, PySR applies penalties to expressions that violate dimensional consistency, which improves the model’s robustness. In contrast, PhySO (Tenachi et al., 2023) performs less effectively, ranking lower than both NGGP (Mundhenk et al., 2021a) and uDSR (Landajuela et al., 2022). PhySO’s strict adherence to dimensional consistency dramatically reduces its search space, potentially leading to overfitting early in the training process.

The right panel of Figure 3 mirrors the trends observed in the left panel. While some models exhibit low recovery rates, they still manage to discover a significant number of equations, as exemplified by gplearn (Stephens, 2016).

5 CONCLUSION

In conclusion, we introduce a novel symbolic regression dataset, comprising a refined version of the SRBench dataset. We evaluate the performance of 20 different models across 8 methodological categories. Our analysis indicates that Monte Carlo Tree Search (MCTS) methods are particularly well-suited to this task, due to their broad search capabilities. Parallel search algorithms and deep reinforcement learning methods also demonstrate strong performance.

Furthermore, we highlight that an exclusive focus on optimizing the R^2 score can result in diminished symbolic recovery rates. As future work, we aim to identify additional symbolic equations for benchmarking and investigate optimal approaches for selecting equations under noisy conditions.

540 ETHICS STATEMENT

541

542 Our studies does not involve human subjects, practices to data set releases, potentially harmful
 543 insights, methodologies and applications, pontential conflicts of interest and sponsorship, discrim-
 544 ination/bias/fairness concerns, privacy and security issues, legal compliance, and research integrity
 545 issues.

546

547 REPRODUCIBILITY STATEMENT

548

549 Codes and models of Geometric Benchmark will be available at github upon the paper’s publication.
 550 Details about experiments mentioned is at appendix section A, B.

551

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A DATASET DETAILS

This section provides a detailed description of the geometric dataset. The complete dataset is presented in Tables 2, 3, and 4. The dataset comprises 8 parts: Dataset name, Equation, Category, Input data label, Input dimension, Output data label, Output dimension and Limitations. And our dataset contains two different sizes: 500 for normal model and 100000 for machine learning models that need to fit the curve.

- **Dataset Name:** This part specifies the name or identifier of the dataset, providing a clear reference for the specific set of geometric data being described according to the type of geometric shapes or phenomena it covers.
- **Category:** This section categorizes the dataset’s difficulties. Easy polynomial expressions are classified to easy and complex polynomial with few non-linear tokens are classified to medium and other hard equations are classified to hard.
- **Equation:** This section lists the mathematical equations associated with the geometric shapes or phenomena covered in the dataset. These equations are used to compute various properties, such as volume, area, or perimeter, based on the input data.
- **Input Data Label:** This part describes the labels or names of the input variables. These labels indicate what each input represents, such as the length of an edge, the height, or the angles between edges in geometric shapes.
- **Input Dimension:** This section provides the dimensionality of the input data. It specifies the number of input variables or parameters required for the equations. For instance, a triangle might require two side lengths with m dim and an angle between them with rad dim.
- **Output Data Label:** This part describes the labels or names of the output variables. These labels indicate the properties being calculated, such as area, volume, or perimeter.
- **Output Dimension:** This section provides the dimensionality of the output data. It specifies the results generated by the equations. For instance, calculating the area of a rectangle results in output dimensions of m^2 .
- **Limitations:** This part outlines any constraints or limitations associated with the dataset or the equations. These might include restrictions on the values of input parameters or specific conditions under which the equations are valid like the sum of two edges can not be larger than the other one in triangles.

The generation process follows this logic: values are randomly generated, with angles sampled uniformly from the interval $[0, \pi]$, and other values sampled uniformly from the range $[1, 5]$. The generated values are then evaluated against predefined constraints (Limitation from dataset). If any of these constraints are violated, new values are generated, and this process continues until the dataset size reaches either 500 or 100,000, depending on the specified target.

Table 2: 1 part/3 part of geometric dataset.

Dataset name	category	Equation
756 triangle-1	easy	$x_1 + x_2 + x_3$
757 triangle-2	hard	$\sqrt{-x_1^4 + 2x_1^2x_2^2 + 2x_1^2x_3^2 - x_2^4 + 2x_2^2x_3^2 - x_3^4}/4$
758 triangle-3	hard	$x_1 + x_2 + \sqrt{x_1^2 - 2x_1x_2 \cos(x_3) + x_2^2}$
759 triangle-4	medium	$(x_1x_2 \sin(x_3))/2$
760 triangle-5	hard	$x_1 \sin(x_2)/\sin(x_2 + x_3) + x_1 \sin(x_3)/\sin(x_2 + x_3) + x_1$
761 triangle-6	hard	$x_1^2 \sin(x_2) \sin(x_3)/(2 \sin(x_2 + x_3))$
762 triangle-7	medium	$x_1 + x_1 \sin(x_3)/\sin(x_2) + x_1 \sin(x_2 + x_3)/\sin(x_2)$
763 triangle-8	medium	$x_1^2 \sin(x_3) \sin(x_2 + x_3)/(2 \sin(x_2))$
764 triangle-9	medium	$x_1 + x_2 + \sqrt{(-x_1^2 + x_2^2)}$
765 triangle-10	medium	$\sqrt{-x_1^4 + x_1^2x_2^2}/2$
766 triangle-11	medium	$x_1 + x_1 \tan(x_2) + x_1/\cos(x_2)$
767 triangle-12	medium	$x_1^2 \tan(x_2)/2$
768 triangle-13	medium	$x_1 \sin(x_3)/\sin(x_2)$
769 triangle-14	hard	$\sqrt{x_1^2 - 2x_1x_2 \cos(x_3) + x_2^2}$
770 triangle-15	medium	$\sqrt{x_1^2 + x_2^2}$
771 triangle-16	hard	$(x_1x_2x_3)/\sqrt{-x_1^4 + 2x_1^2x_2^2 + 2x_1^2x_3^2 - x_2^4 + 2x_2^2x_3^2 - x_3^4}$
772 triangle-17	hard	$\sqrt{-x_1^4 + 2x_1^2x_2^2 + 2x_1^2x_3^2 - x_2^4 + 2x_2^2x_3^2 - x_3^4}/(2x_1 + 2x_2 + 2x_3)$
773 triangle-18	easy	$(x_1 + x_3 + x_5)/2$
774 triangle-19	hard	$(x_1 \sqrt{x_3^2 + x_4^2} + x_3 \sqrt{(x_1 - x_3)^2 + (x_2 - x_4)^2})/(\sqrt{x_1^2 + x_2^2} + \sqrt{x_3^2 + x_4^2} + \sqrt{(x_1 - x_3)^2 + (x_2 - x_4)^2})$
775 triangle-20	hard	$(x_1^2x_4 + x_2^2x_4 - x_2x_3^2 - x_2x_4^2)/(2(x_1x_4 - x_2x_3))$
776 triangle-21	hard	$(-x_1x_2x_3 + x_1x_3x_4 - x_2^2x_4 + x_2x_4^2)/(x_1x_4 - x_2x_3)$
777 circle-1	easy	$2\pi x_1$
778 circle-2	easy	πx_1^2
779 circle-3	easy	πx_1x_2
780 circle-4	medium	$\sqrt{x_1^2 - x_2^2}$
781 circle-5	easy	$(x_2 + 2)x_1$
782 circle-6	easy	$x_2x_1^2/2$
783 trapezoid-1	hard	$x_1 + x_2 + \sqrt{x_1^2 - 2x_1x_2 + x_2^2 + 4x_3^2}$
784 trapezoid-2	easy	$x_1x_3/2 + x_2x_3/2$
785 trapezoid-3	easy	$x_1 + x_2 + 2x_3$
786 trapezoid-4	hard	$(x_1 + x_2)\sqrt{-x_1^2 + 2x_1x_2 - x_2^2 + 4x_3^2}/4$
787 trapezoid-5	medium	$x_1 - 2x_1/\cos(x_3) + x_2 + 2x_2/\cos(x_3)$
788 trapezoid-6	medium	$-x_1^2 \tan(x_3)/4 + x_2^2 \tan(x_3)/4$
789 rectangle-1	easy	$2x_1 + 2x_2$
790 rectangle-2	easy	x_1x_2
791 rectangle-3	easy	$4x_1$
792 rectangle-4	easy	x_1^2
793 rectangle-5	easy	$2x_1 + 2x_2$
794 rectangle-6	medium	$x_1x_2 \sin(x_3)$
795 line-1	medium	$(x_2 - x_4)/(x_3 - x_1)$
796 line-2	medium	$(x_3x_2 - x_1x_4)/(x_3 - x_1)$
797 line-3	medium	$(x_1 - x_3)/(1 - x_1x_3)$
798 line-4	medium	$(x_3 - x_1)/(x_4 - x_2)$
799 line-5	medium	$(x_4x_1 - x_2x_3)/(x_1 - x_3)$
800 line-6	hard	$(x_2 - x_3x_1 - x_4)/\sqrt{x_3^2 + 1}$
801 vector3d-1	medium	$\sqrt{x_1^2 + x_2^2 + x_3^2}$
802 vector3d-2	hard	$(x_1x_2 + x_3x_4 + x_5x_6)/\sqrt{(x_1^2 + x_2^2 + x_3^2)(x_2^2 + x_4^2 + x_6^2)}$
803 vector3d-3	medium	$x_1x_2 + x_3x_4 + x_5x_6$
804 vector3d-4	easy	$x_3x_6 - x_4x_5$
805 vector3d-5	hard	$(x_1x_4 + x_2x_5 + x_3x_6)/\sqrt{x_4^2 + x_5^2 + x_6^2}$
806 sphere-1	easy	$\pi x_1^2 + 2\pi x_1x_2$
807 sphere-2	easy	$\pi x_1^2x_2$
808 sphere-3	hard	$\pi x_1^2 + 2\pi x_1\sqrt{x_1^2 + x_2^2}$
809 sphere-4	easy	$\pi/3x_1^2x_2$
810 sphere-5	hard	$\pi(x_1^2 + x_2^2 + \sqrt{x_3^2 + (x_2 - x_1)^2})(x_1 + x_2)$
811 sphere-6	medium	$\pi(x_1^2 + x_1x_2 + x_1^2)x_3$
812 sphere-7	easy	$4\pi/3x_1^3$
813 sphere-8	easy	$4\pi x_1^2$
814 cuboid-1	easy	$4x_1 + 4x_2 + 4x_3$
815 cuboid-2	easy	$2x_1x_2 + 2x_1x_3 + 2x_2x_3$
816 cuboid-3	easy	$x_1x_2x_3$
817 cuboid-4	easy	$12x_1$
818 cuboid-5	easy	$6x_1^2$
819 cuboid-6	easy	x_1^3
820 regular-tetrahedron-1	medium	$x_1\sqrt{4x_2^2 + x_1^2 + x_1^2}$
821 regular-tetrahedron-2	medium	$1/3x_1^2\sqrt{x_2^2 - \frac{1}{2}x_1^2}$
822 regular-tetrahedron-3	easy	$1/3x_1^2x_2$
823 tetrahedron-1	hard	$1/12x_4\sqrt{-x_1^4 + 2x_1^2x_2^2 + 2x_1^2x_3^2 - x_2^4 + 2x_2^2x_3^2 - x_3^4}$
824 tetrahedron-2	easy	$x_1x_2/3$
825 tetrahedron-3	hard	$1/6x_1x_2x_3\sqrt{\sin(x_4)^2 + \sin(x_5)^2 + \sin(x_6)^2 + 2\cos(x_4)\cos(x_5)\cos(x_6)} - 2$
826 tetrahedron-4	hard	$1/3\sqrt{(-x_1^2/2 + x_2^2/2 + x_3^2/2)(x_1^2/2 - x_2^2/2 + x_3^2/2)(x_1^2/2 + x_2^2/2 - x_3^2/2)}$

Table 3: 2 part/3 part of geometric dataset.

Dataset name	Input data label	Input dimensions
triangle-1	Triangle three sides	m m m
triangle-2	Triangle three sides	m m m
triangle-3	Triangle two sides and the included angle	m m r
triangle-4	Triangle two sides and the included angle	m m r
triangle-5	Triangle two angles and the included side	m r r
triangle-6	Triangle two angles and the included side	m r r
triangle-7	Triangle two angles and the opposite sides	m r r
triangle-8	Triangle two angles and the opposite sides	m r r
triangle-9	Right-angled triangle right sides and hypotenuse	m m
triangle-10	Right-angled triangle right sides and hypotenuse	m m
triangle-11	Right-angled triangle right side and opposite angle	m r
triangle-12	Right-angled triangle right side and opposite angle	m r
triangle-13	Triangle two angles and the opposite sides	m r r
triangle-14	Triangle two sides and the included angle	m m r
triangle-15	Right-angled triangle two right sides	m m
triangle-16	Triangle three sides	m m m
triangle-17	Triangle three sides	m m m
triangle-18	Triangle three points' coordinates	m m m m m m
triangle-19	Triangle two points' coordinates	m m m m
triangle-20	Triangle two points' coordinates	m m m m
triangle-21	Triangle two points' coordinates	m m m m
circle-1	Circle radius	m
circle-2	Circle radius	m
circle-3	Ellipse major and minor axis	m m
circle-4	Ellipse major and minor axis	m m
circle-5	Sector radius and angle	m r
circle-6	Sector radius and angle	m r
trapezoid-1	Isosceles trapezoid upper base lower base and height	m m m
trapezoid-2	Isosceles trapezoid upper base lower base and height	m m m
trapezoid-3	Isosceles trapezoid upper base lower base and side	m m m
trapezoid-4	Isosceles trapezoid upper base lower base and side	m m m
trapezoid-5	Isosceles trapezoid upper base lower base and side angle	m m r
trapezoid-6	Isosceles trapezoid upper base lower base and side angle	m m r
rectangle-1	Rectangle two sides	m m
rectangle-2	Rectangle two sides	m m
rectangle-3	Square side length	m
rectangle-4	Square side length	m
rectangle-5	Parallelogram two sides and included angle	m m r
rectangle-6	Parallelogram two sides and included angle	m m r
line-1	Two lines slope and intercept	l m l m
line-2	Two lines slope and intercept	l m l m
line-3	Two lines slope and intercept	l m l m
line-4	Two points horizontal and vertical coordinates	m m m m
line-5	Two points horizontal and vertical coordinates	m m m m
line-6	Point horizontal and vertical coordinate and Line slope and intercept	m m l m
vector3d-1	Three-dimensional vector	m m m
vector3d-2	Two three-dimensional vectors	m m m m m m
vector3d-3	Two three-dimensional vectors	m m m m m m
vector3d-4	Two three-dimensional vectors	m m m m m m
vector3d-5	Three-dimensional vector and point coordinates	m m m l l l
sphere-1	Cylinder base radius and height	m m
sphere-2	Cylinder base radius and height	m m
sphere-3	Cone base radius and height	m m
sphere-4	Cone base radius and height	m m
sphere-5	Frustum upper and lower base radius and height	m m m
sphere-6	Frustum upper and lower base radius and height	m m m
sphere-7	Sphere radius	m
sphere-8	Sphere radius	m
cuboid-1	Cuboid three edge lengths	m m m
cuboid-2	Cuboid three edge lengths	m m m
cuboid-3	Cuboid three edge lengths	m m m
cuboid-4	Cube side length	m
cuboid-5	Cube side length	m
cuboid-6	Cube side length	m
regular tetrahedron-1	Regular tetrahedron base edge and height	m m
regular tetrahedron-2	Regular tetrahedron base edge and side	m m
regular tetrahedron-3	Regular tetrahedron base edge and height	m m
tetrahedron-1	tetrahedron three edges and height	m m m m
tetrahedron-2	tetrahedron base area and height	m ² m
tetrahedron-3	tetrahedron three edges and three angles from one point	m m m r r r
tetrahedron-4	isohedral tetrahedron 3 edges	m m m

Table 4: 3 part/3 part of geometric dataset.

Dataset name	Output data label	Output dimension	Limitations	
triangle-1	Perimeter	m	$x_1 + x_2 > x_3, x_1 + x_3 > x_2, x_2 + x_3 > x_1$	
triangle-2	Area	m^2		
triangle-3	Perimeter	m		
triangle-4	Area	m^2		
triangle-5	Perimeter	m		$x_2 + x_3 < \pi$
triangle-6	Area	m^2		$x_2 + x_3 < \pi$
triangle-7	Perimeter	m		$x_2 + x_3 < \pi$
triangle-8	Area	m^2		$x_2 + x_3 < \pi$
triangle-9	Perimeter	m	$x_1 < x_2$	
triangle-10	Area	m^2	$x_1 < x_2$	
triangle-11	Perimeter	m	$x_2 < \pi/2$	
triangle-12	Area	m^2	$x_2 < \pi/2$	
triangle-13	Another side	m	$x_2 + x_3 < \pi$	
triangle-14	Another side	m		
triangle-15	Hypotenuse	m	$x_1 + x_2 > x_3, x_1 + x_3 > x_2, x_2 + x_3 > x_1$	
triangle-16	Circumcircle radius	m		
triangle-17	Incircle radius	m		
triangle-18	Centroid horizontal coordinate	m	$x_1 + x_2 > x_3, x_1 + x_3 > x_2, x_2 + x_3 > x_1$	
triangle-19	incenter horizontal coordinate	m		
triangle-20	circumcenter horizontal coordinate	m		
triangle-21	orthocenter horizontal coordinate	m		
circle-1	Perimeter	m		
circle-2	Area	m^2		
circle-3	Area	m^2	$x_1 > x_2$	
circle-4	Focal point	m	$x_1 > x_2$	
circle-5	Perimeter	m		
circle-6	Area	m		
trapezoid-1	Perimeter	m	$x_3 > (x_1 - x_2)/2, x_3 > (x_2 - x_1)/2$	
trapezoid-2	Area	m^2		
trapezoid-3	Perimeter	m		
trapezoid-4	Area	m^2		
trapezoid-5	Perimeter	m		$x_1 < x_2, x_3 < \pi/2$
trapezoid-6	Area	m^2		$x_1 < x_2, x_3 < \pi/2$
rectangle-1	Perimeter	m		
rectangle-2	Area	m^2		
rectangle-3	Perimeter	m		
rectangle-4	Area	m^2		
rectangle-5	Perimeter	m		
rectangle-6	Area	m^2		
line-1	Intersection horizontal coordinate	m		
line-2	Intersection vertical coordinate	m		
line-3	Angle tangent value	l		
line-4	Slope of the line through two points	l		
line-5	Intercept of the line through two points	m		
line-6	Point to line distance (directed)	m		
vector3d-1	Magnitude	m		
vector3d-2	Cosine value of the angle	m		
vector3d-3	Dot product	m		
vector3d-4	Cross product horizontal coordinate	m		
vector3d-5	Point to plane distance (directed)	m		
sphere-1	Surface Area	m^2		
sphere-2	Volume	m^3		
sphere-3	Surface Area	m^2		
sphere-4	Volume	m^3		
sphere-5	Surface Area	m^2		
sphere-6	Volume	m^3		
sphere-7	Surface Area	m^2		
sphere-8	Surface Area	m^2		
cuboid-1	Sum of edge lengths	m		
cuboid-2	Surface Area	m^2		
cuboid-3	Volume	m^3		
cuboid-4	Sum of edge lengths	m		
cuboid-5	Surface Area	m^2		
cuboid-6	Volume	m^3		
regular tetrahedron-1	Surface Area	m^2	$x_2 > \frac{1}{2}x_1^2$	
regular tetrahedron-2	Volume	m^3		
regular tetrahedron-3	Volume	m^3		
tetrahedron-1	Volume	m^3	$x_1 + x_2 > x_3, x_1 + x_3 > x_2, x_2 + x_3 > x_1$	
tetrahedron-2	Volume	m^3		
tetrahedron-3	Volume	m^3		$x_4 + x_5 + x_6 < \pi$
tetrahedron-4	Volume	m^3		$x_1 + x_2 > x_3, x_1 + x_3 > x_2, x_2 + x_3 > x_1$

B MODEL DETAILS

In this section, we give hyper-parameters of all 20 models at Table 5. The other parameters not mentioned in table is set as default value. In most models, the token set is $+$, $-$, \times , \div and \cos , \sin , $\sqrt{\cdot}$ and X , $const$.

Table 5: Hyper-parameter setting of all 20 models.

Model	Hyper-parameters
Bayesian Machine Scientist	{ Drtarget: 60, nsample: 1000, anneal: 20, burnin: 5000, annealf: 6 }
PSRN	{ trying_const_num: 2, trying_const_range: [0,4], trying_const_n_try: 3 }
EQL	{ l ₀ _reg: 0.0001, iterations: 10 }
AlFeynman	{ BF_try_time: 60, BF_ops_file_type: "14ops", polyfit_deg: 3, NN_epochs: 1000 }
NGGP	{ gp_population_size: 500, generations: 20, p_crossover: 0.5, p_mutate: 0.5, tournament_size: 5, train_n: 50, mutate_tree_max: 3, n_samples: 200000, batch_size: 500 }
uDSR	{ function_set: [add, sub, mul, div, sin, cos, sqrt, const, poly], poly_degree: 3, gp_population_size: 500, generations: 20, p_crossover: 0.5, p_mutate: 0.5, tournament_size: 5, train_n: 50, mutate_tree_max: 3, n_samples: 200000, batch_size: 500 }
PhySO	{ fixed_consts: [1, pi], fixed_consts_units: [[0], [0]], free_consts_names: [], free_consts_units: [], op_names: [mul, add, sub, div, inv, n2, sqrt, neg, sin, cos], run_config: config2.config2 }
gplearn	{ population_size: 1000, generations: 20, p_crossover: 0.7, max_samples: 0.9, parsimony_coefficient: 0.01 }
DEAP	{ const_range: (0,4), generations: 400, p_crossover: 0.3, p_mutate: 300 }
pysr	{ iterations: 200, weight_optimize: 0.001, adaptive_parsimony_scaling: 1000, parsimony: 0.0 }
Sindy	{ library: GeneralizedLibrary([PolynomialLibrary, FourierLibrary]) degree: [2,3,4,5] }
SymINDy	{ sparsity_coef: 0.01, library_name: "generalized", ngen: 20 }
KAN	{ width: [num_of_inputs, 2, 1], grid: 3, k: 3 }
SPL	{ transplant_step: 10000 }
RSRM	{ tournsize: 10, max_height: 10, max_const: 6, cspb: 0.1, mutpb: 0.5, pops: 500, times: 30, hof_size: 20, token_discount: 0.99, max_expr_num: 20, expr_ratio: 0.1, token_ratio: 0.5, form_type: [Add] }
NeSymReS	{ config_file: "100M/eq_setting.json" }
E2E	{ beam_size: 10, n_trees_to_refine: 10 max_input_points: 200, eval_input_length_modulo 50, prediction_sigmas: 1, 2, 4, 8, 16 }
DGSR	{ training_equations: 200000, training_epochs: 20, batch_outer_datasets: 24, batch_inner_equations: 100, other_setting_file: "config.yaml" }
TPSR	{ lam: 0.1, horizon: 200 width: 5 num_beams: 2, rollout: 5 max_input_points :200, max_number_bags :10 }
SNIP	{ max_input_points: 200, lso_optimizer: gwo, lso_pop_size: 50, lso_max_iteration: 10, lso_stop_r2: 0.999, beam_size: 2 }

C EXTRA RESULT

In this section, we present additional results from the geometric dataset. As shown in Figure 4, the performance of many models across the three difficulty levels—easy, medium, and hard—appears consistent. The strong symbolic regression capabilities demonstrated by models such as RSRM and PSRN can be attributed to their proficiency in handling medium and hard-level expressions. RSRM utilizes MSDB, a mechanism for storing previously encountered failure cases, while PSRN systematically explores a vast array of potential equations. This figure illustrates that both strategies are effective in improving symbolic regression performance.

Additionally, Bayesian models, such as the Bayesian Machine Scientist, achieve a 100% success rate in the easy category, highlighting their stability and reliability in simpler tasks.

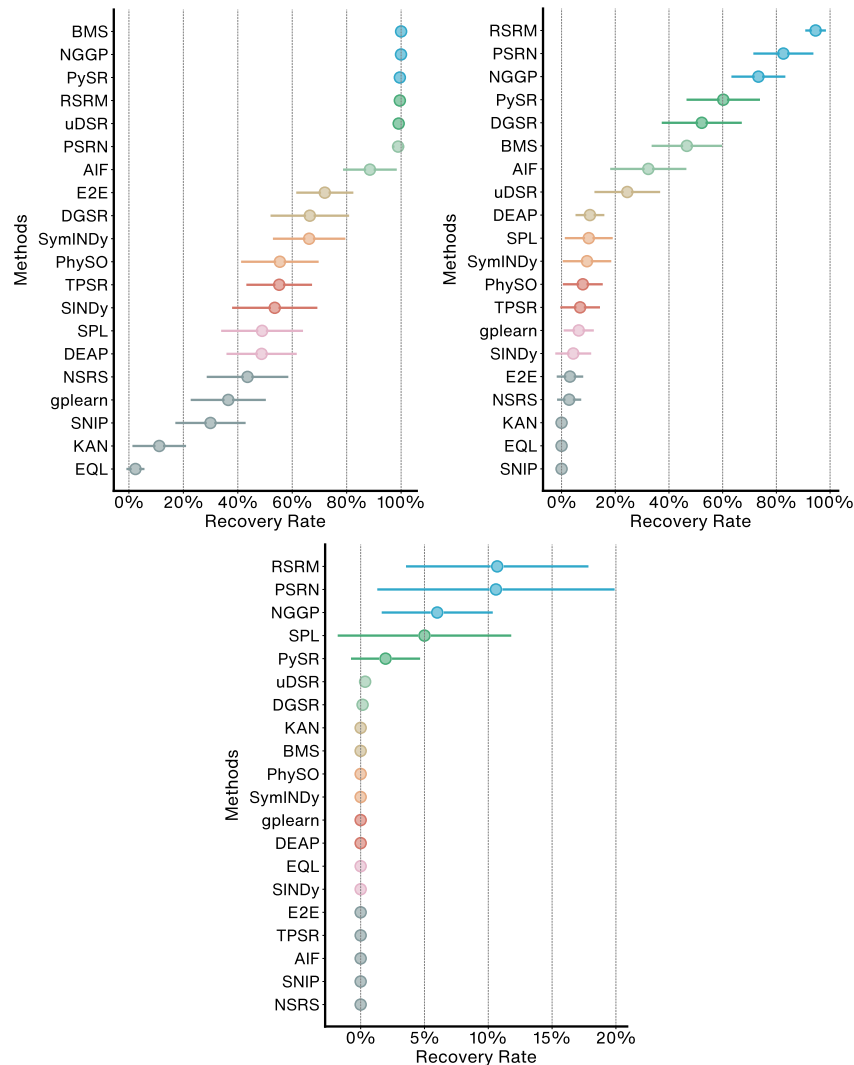


Figure 4: extra result within three different category.

D FULL RECOVERY SCORE OF EACH MODEL

In this section, we provide the recovery rate within each method and each model in Table 6.

Table 6: The recovery rate within each method and each model. BMS, AIF and NGNS refer to the Bayesian Machine Scientist, AIFeynman and NeSymReS, respectively.

Dataset name	PSRN	psyr	NGGP	uDSR	RSRM	KAN	BMS	phySO	SymINDy	gplearn	DEAP	EQL	Sindy	SPL	E2E	TPSR	AIF	SNIP	DGSR	NSRS
triangle-1	1	1	1	1	1	1	1	1	1	1	0.95	0.5	1	1	1	1	1	1	1	1
triangle-2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
triangle-3	0	0	0	0	0.12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
triangle-4	1	1	1	0.2	1	0	0.95	0	1	0.1	0.21	0	0	0.43	0	0	1	0	0.93	0
triangle-5	0.12	0	0	0	0.19	0	0	0	0	0	0	0	0	0	0	0	0	0	0.03	0
triangle-6	1	0	0.07	0	0.17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
triangle-7	0.07	0.78	0.21	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0.65	0
triangle-8	1	0.12	0.18	0	1	0	0	0	0	0	0.02	0	0	0	0	0	0	0	0.03	0
triangle-9	0.67	0.27	1	0.04	0.71	0	0.05	0	0	0	0	0	0	0	0	0	0	0	0	0
triangle-10	1	1	1	0.22	1	0	0.56	0	0	0	0	0	0	0	0	0	0.73	0	0	0
triangle-11	1	0.93	0.99	0.01	0.66	0	0.71	0	0	0.01	0	0	0	0	0	0	0	0	1	0
triangle-12	1	0.12	0.95	0	1	0	1	0	0	0.01	0.02	0	0	0	0	0	0	0	1	0
triangle-13	1	0.78	0.97	0.02	1	0	0.75	0.06	0.1	0.2	0.29	0	0	0	0	0	0	0	1	0
triangle-14	0	0	0.01	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
triangle-15	1	0.83	1	1	1	0	0.95	0.71	0	0.07	0	0	0	1	0	0	1	0	0	0
triangle-16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
triangle-17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
triangle-18	0.69	0.98	1	1	1	1	1	0	0.45	0	0	0.05	1	0	0.21	0	0	0	0.03	0
triangle-19	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
triangle-20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
triangle-21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
circle-1	1	1	1	1	1	0	1	0.93	0	0	0.15	0	0	1	0.77	1	1	1	0	1
circle-2	1	1	1	1	1	0	1	1	0	0	0.06	0	0	1	0.95	0.73	1	1	0	0.34
circle-3	1	1	1	1	1	0	1	1	0	0	0.02	0	0	1	1	0.87	1	0	0	0.12
circle-4	1	1	1	1	0.76	0	0.71	0.15	0	0.13	0.07	0	0	0.9	0	0	1	0	0	0
circle-5	1	1	1	1	1	0	1	0.92	1	0.89	0.85	0	1	0.1	0.99	0.53	1	0	1	0
circle-6	1	1	1	0.94	1	0	1	0.17	1	0.02	0.57	0	0	0	0.17	0.53	1	0	1	0
trapezoid-1	0	0	0.26	0.03	0.79	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
trapezoid-2	1	1	1	1	1	0	1	0	1	0	0.13	0	1	0	1	0.27	1	0	0.73	0
trapezoid-3	1	1	1	1	1	0	1	1	1	0.96	0.87	0	1	1	0.82	0.67	1	0.17	1	0
trapezoid-4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
trapezoid-5	1	0	0.31	0	1	0	0	0	0	0	0.09	0	0	0	0	0	0	0	0.45	0
trapezoid-6	1	0	0.24	0	1	0	0.22	0	0	0	0	0	0	0	0	0	0	0	0	0
rectangle-1	1	1	1	1	1	1	1	0.9	1	0.95	0.94	0.12	1	1	0.61	0.4	1	0.17	1	1
rectangle-2	1	1	1	1	1	0	1	1	1	0.98	0.96	0	1	1	0.99	0.87	1	0	1	1
rectangle-3	1	1	1	1	1	0	1	0.8	1	0.76	0.98	0	1	1	0.86	0.8	1	0.75	1	1
rectangle-4	1	1	1	1	1	0	1	1	1	0.98	1	0	1	1	0.71	1	1	0.4	1	1
rectangle-5	1	1	1	1	1	0	1	1	1	0.93	0.96	0	1	1	0.12	0	1	0.5	1	0.74
rectangle-6	1	1	1	0.26	1	0	1	0.9	1	0.82	0.72	0	0	0	0	0	1	0	1	0.65
line-1	0.98	0.76	0	1	0	0	0.15	0	0	0.02	0.09	0	0	0	0	0	0	0	1	0
line-2	1	1	0.56	0	1	0	0.15	0	0	0	0.24	0	0	0	0	0	0	0	1	0
line-3	1	0.95	1	0.01	1	0	0.33	0	0	0	0.2	0	0	0	0	0	0	0	0.95	0
line-4	1	1	0.93	0.01	1	0	0	0	0	0.03	0.19	0	0	0	0	0	0	0	1	0
line-5	1	0.97	0.44	0.02	1	0	0	0	0	0	0.08	0	0	0	0	0	0	0	1	0
line-6	1	0.39	0.51	0.04	0.12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
vector3d-1	0.26	0.03	0.32	1	0.93	0	0.2	0	0	0	0	0	0	0	0	0	1	0	0	0
vector3d-2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
vector3d-3	1	0.12	0.42	1	1	0	1	0	0.08	0.08	0.21	0	1	0	0.72	0.92	1	0	1	0
vector3d-4	1	0.98	1	1	1	0	1	0	0.23	0.15	0.36	0	1	0	0.01	0	0	0	1	0
vector3d-5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
sphere-1	1	1	1	1	1	0	1	0.29	0.75	0	0	0	0	0	0.9	0.6	1	0	0	0
sphere-2	1	1	1	0.95	1	0	1	1	0.43	0	0.04	0	0	0.2	0.68	1	1	0	0	0
sphere-3	0	0	0.35	0	0.75	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
sphere-4	1	1	1	0.99	1	0	1	0	0	0	0	0	0	0	0.59	0.6	1	0	0	0
sphere-5	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
sphere-6	1	0.97	1	0.79	1	0	1	0	0	0	0	0	0	0	0	0.67	0.7	0	0	0
sphere-7	1	1	1	1	1	0	1	0	0.45	0	0	0	0	0	0.96	0.07	1	0	0	1
sphere-8	1	1	1	0.99	1	0	1	1	0.23	0	0.02	0	0	1	0.98	0	1	1	0	0
cuboid-1	1	1	1	1	1	0	1	0.13	1	0	0.38	0	1	0	0.72	0.13	1	0.4	1	0
cuboid-2	1	0.91	0.99	1	1	0	1	0	1	0.06	0.13	0	1	0.1	0	0	0.79	0	1	0
cuboid-3	1	1	1	0.92	1	0	1	1	1	0.98	1	0	0	0	1	1	1	0	1	1
cuboid-4	1	1	1	1	1	0.12	1	0.13	1	0	0.87	0	1	0.1	0.88	0.93	1	1	1	1
cuboid-5	1	1	1	1	1	0	1	0.13	1	0.13	0.96	0	1	0.2	0.99	0.73	1	1	1	0
cuboid-6	1	1	1	1	1	0	1	1	1	0.93	0.83	0	0	1	0.93	0	1	0	1	1
regular-1	0	0	0	0.04	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
regular-2	0	0	0.58	0.01	0.7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
regular-3	1	1	1	0.96	0.87	0	1	0	0	0	0	0.17	0	0	1	0.33	0.73	1	0	0.85
tetrahedron-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
tetrahedron-2	1	1	1	1	1	0	1	0.13	0	0.5	0.45	0	0	0	0.98	1	0	0	1	1
tetrahedron-3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
tetrahedron-4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
zero count	19	23	15	25	14	67	26	46	45	46	34	68	55	49	43	47	48	59	36	56
average	68.75%	59.31%	64.86%	47.11%	72.92%	4.39%	54.55%	24.44%	29.18%	16.46%	22.65%	0.94%	22.54%	23.99%	29.39%	24.01%	25.13%	11.82%	43.17%	18.10%
average-easy	98.89%	99.54%	99.96%	99.11%	99.54%	11.14%	100.00%	55.46%	66.21%	36.50%	48.75%	2.39%	53.57%	48.93%	71.96%	55.21%	44.07%	29.96%	66.46%	43.57%
average-medium	82.61%	60.22%	73.30%	24.48%	94.61%	0.00%	46.65%	7.91%	9.48%	6.39%	10.57%	0.00%	4.35%	10.13%	3.13%	6.91%	23.91%	0.00%	52.22%	2.83%
average-hard	10.60%	1.95%	6.00%	0.35%	10.70%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	5.00%	0.00%	0.00%	0.00%	0.00%	0.15%	0.00%