# RAG-SR: Retrieval-Augmented Generation for Neural Symbolic Regression

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## Outline

# Introduction

## Symbolic Regression

- **Symbolic Regression (SR)** discovers mathematical expressions that best describe a dataset
- Automatically determines both the **structure** $f$ and **parameters** $\theta$ of the model
- Offers both **high accuracy** and **interpretability**
- Applications: physics, biology, finance, scientific discovery

**Mathematical Definition:**

$$(f^*, \theta^*) = \underset{f \in F, \theta}{\operatorname{argmin}} \sum_{i=1}^{n} L(f(x_i, \theta), y_i) \tag{1}$$

## Problem Formulation: Feature Construction Approach

- Generate a set of symbolic trees/features $\Phi = \{\phi_1, \ldots, \phi_m\}$ from dataset $(X, Y)$
- Enhance interpretable model $M$ (e.g., linear regression)
- Objective: Minimize loss function

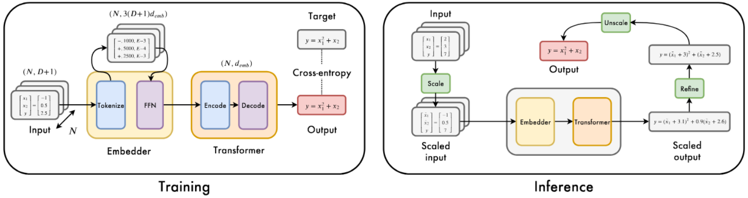
$$L(\Phi; X, Y) = \frac{1}{N} \sum_{i=1}^{N} \ell\left(M\left(\phi_1(X_i), \ldots, \phi_m(X_i)\right), Y_i\right) \tag{2}$$

**Advantages:**

- Effective for complex real-world problems
- Multiple weak features can collectively work well

## Pre-trained Models

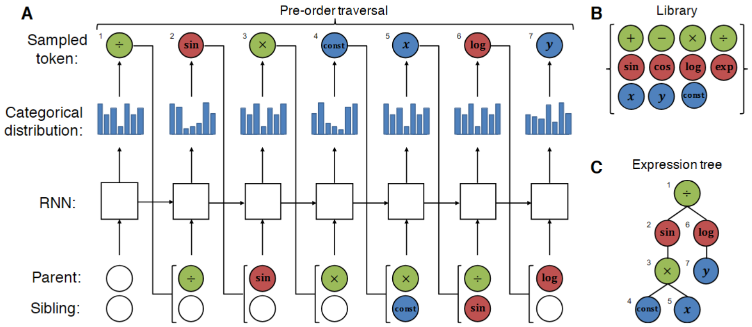
- Limited to seen functions
- Struggles with new variables
- Requires large pre-training



# Limitations of Current Approaches: Reinforcement Learning

## Reinforcement Learning

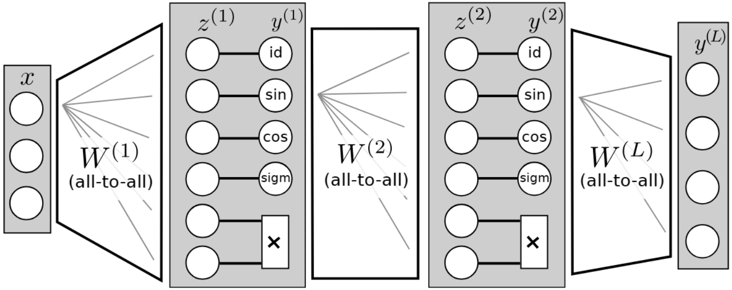
- Low sample efficiency
- Limited feedback
- Slow convergence



## Limitations of Current Approaches: Sparse Supervised Learning

**Sparse Supervised Learning**

- Relies on heuristic pruning
- Produces potentially large solutions
- Requires differentiable activation functions



## Related Work

**Neural Symbolic Regression**

- Pre-trained models (DSR, E2E) struggle with unseen functions/variables
- RL approaches have low sample efficiency
- Sparse supervised learning requires differentiable activation functions

**Evolutionary Symbolic Regression**

- Traditional GP lacks search effectiveness
- Semantic GP is effective but relies solely on existing building blocks
- Limited knowledge retention during evolution

## Key Insight: Guiding Neural Generation with Good Solutions

### Key Insight

**From LM perspective:**

- Using neural networks to directly improve solutions leads to hallucination
- Better approach: Show the model potentially good improvements and ask it to generate better ones

**From EA perspective:**

- Instead of asking ”give me a good mutation,” we show examples of good mutations and say ”a good mutation is like this, give me a better one”

**When using LLMs like ChatGPT:**

- Don’t ask: ”The current program only does B, but I want it to do A”
- Instead ask: ”The current program only does B, I want it to do A, and I think a potential direction is...”

## RAG-SR: A Novel Semantic-to-Symbolic Learning Framework

**Our Approach:** Integrating evolutionary feature construction with neural networks through online learning

- **Semantic Descent:** Adaptively generates symbolic trees aligned with desired semantics in real-time through online supervised learning
- **Retrieval-Augmented Generation:** Mitigates hallucinations by leveraging symbolic expressions in a library
- **Masked Contrastive Learning:** Captures semantically equivalent but syntactically different symbolic expressions
- **Scale-invariant Data Augmentation and Double Query Strategy:** Improves robustness to linear regression

# Methodology

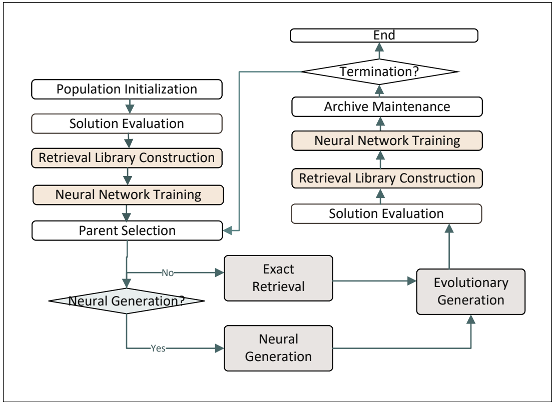
## RAG-SR: Solution Initialization & Evaluation

**Step 1: Solution Initialization**

- Random symbolic trees using ramped half-and-half

**Step 2: Solution Evaluation**

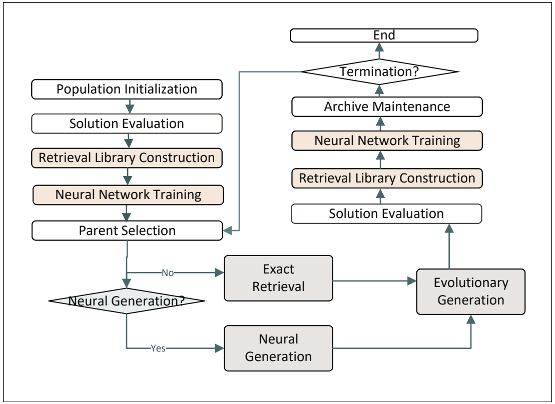
- Features evaluated via ridge regression with LOOCV



## RAG-SR: Semantic Library Construction

**Step 3: Semantic Library Construction**

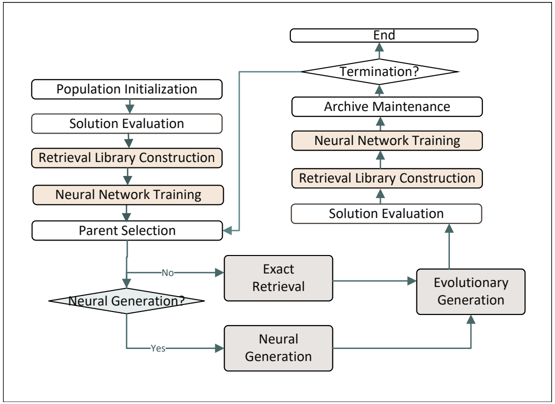
- **Retrieval Library:** FIFO queue with KD-Tree for efficient retrieval
  - Semantics are normalized before storing because feature construction is insensitive to scale
- **Neural Semantic Library:** Trained using pairs from retrieval library



## RAG-SR: Solution Selection Process

**Step 4: Solution Selection**

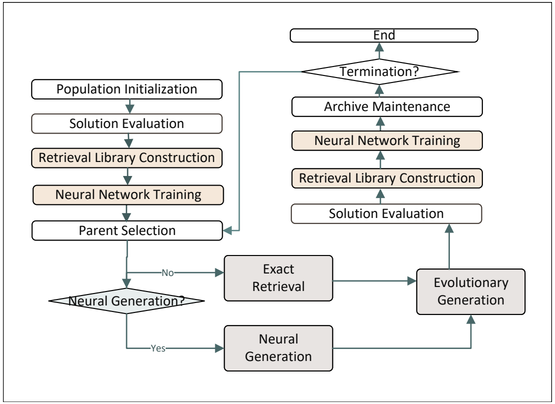
- Lexicase selection to select promising parents



## RAG-SR: Solution Generation

**Step 5: Solution Generation**

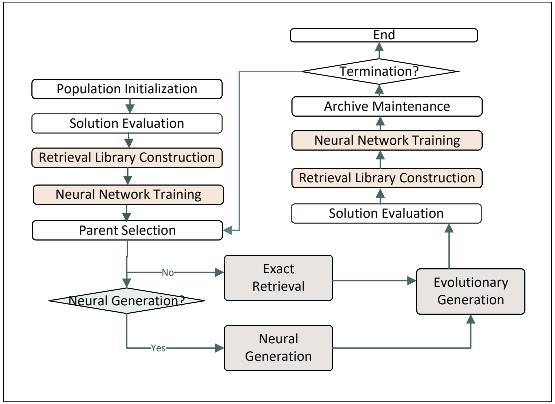
- **Semantic Descent:** Local search to improve solutions
- **Evolutionary Search:** Global exploration with GP operators



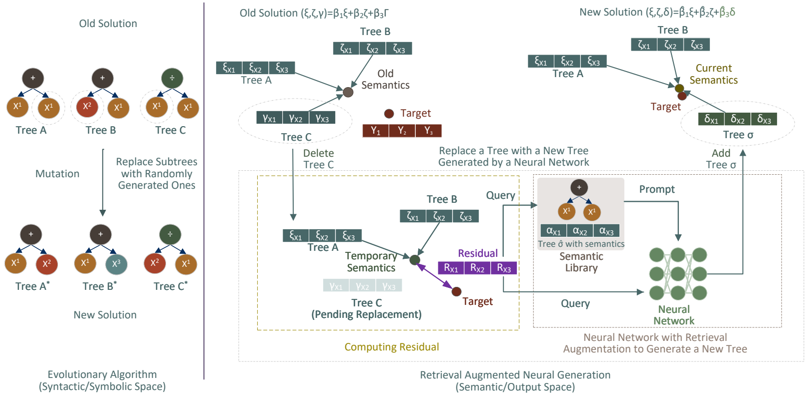
## RAG-SR: Archive Maintenance

### Step 6: Archive Maintenance

- Store best-performing solution



## Semantic Descent: Overview


Old Solution
Tree A
Tree B
Tree C
Mutation
Replace Subtrees with Randomly Generated Ones
Tree A*
Tree B*
Tree C*
New Solution
Evolutionary Algorithm (Syntactic/Symbolic Space)
Old Solution (ξ,ζ,γ)=β₁ξ+β₂ζ+β₃Γ
Old Semantics
Target
Delete Tree C
Replace a Tree with a New Tree Generated by a Neural Network
New Solution (ξ,ζ,δ)=β̂₁ξ+β̂₂ζ+β̂₃δ
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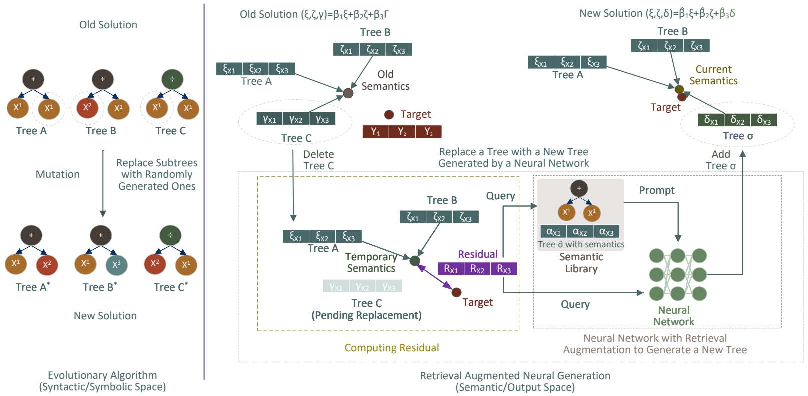
Add Tree σ
Temporary Semantics
Tree C (Pending Replacement)
Residual
Query
Prompt
Tree ô with semantics
Semantic Library
Neural Network
Computing Residual
Neural Network with Retrieval Augmentation to Generate a New Tree
Retrieval Augmented Neural Generation (Semantic/Output Space)

**Key Principle:**

- Iterative optimization replacing suboptimal features while maintaining a constant feature count

## Semantic Descent: Step 1-2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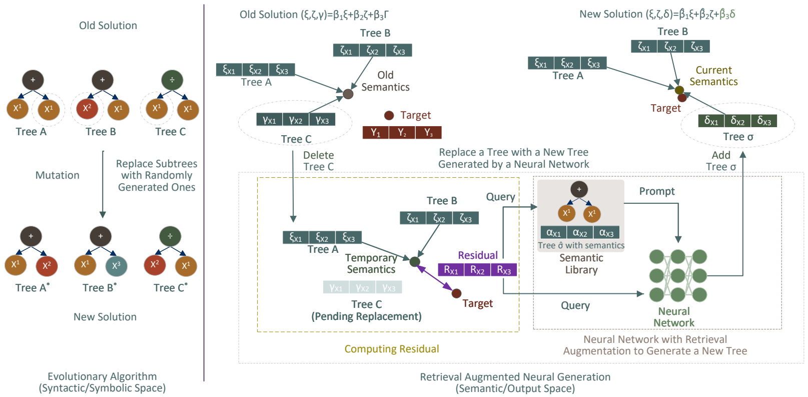
**For each tree $\phi_i$ in solution $\{\phi_1, \dots, \phi_m\}$:**

1. Temporarily remove contribution of $\phi_i$: $\Phi^{temp}(X) = \Phi(X) - \beta_i \phi_i(X)$
2. Compute residual $R = Y - \Phi^{temp}(X)$

## Semantic Descent: Step 3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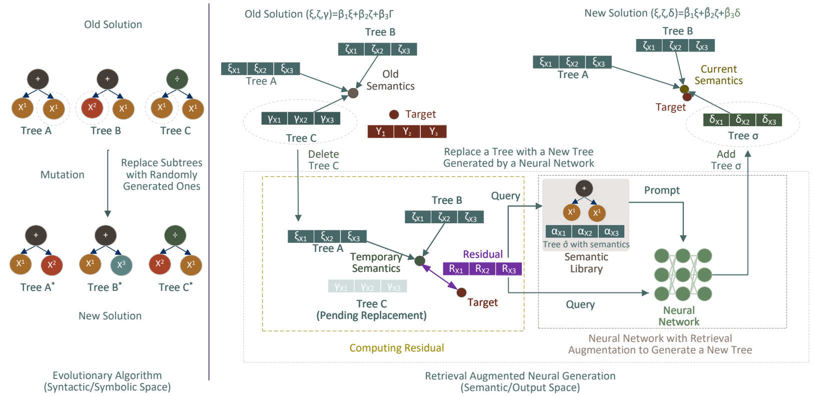
**Generate a new tree to fill this gap using:**

- Neural generation with probability $P_{neural}$: "Here's a pattern that worked before, generate something better"
- Retrieval from semantic library with probability $1 - P_{neural}$: "Find the best matching pattern we've seen before"

## Semantic Descent: Step 4



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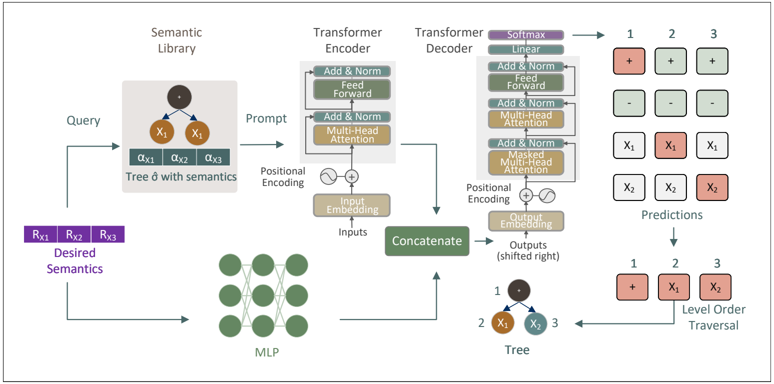
**Final Step:**

- Accept new tree if it reduces error for Retrieval, directly accept if Neural generation
- Continue process iteratively for all trees in the solution

# Retrieval-Augmented Generation

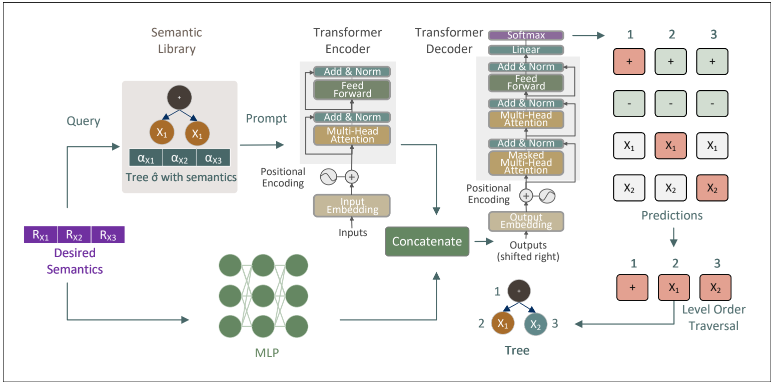


**Challenge:** Language model can always generate something, but may be irrelevant to the given task

**Key Idea:** Retrieval-augmented generation to reduce hallucination

- **Data Collection:** Store evaluated subtrees and semantics in a library
- **Network Training:** Map semantics to symbolic expressions
- **Retrieval:** Provide context from promising expressions

## NEURAL NETWORK ARCHITECTURE



- **MLP with Residual Connections:** Processes desired semantics $R$
- **Transformer Encoder:** Processes nearest symbolic tree $\hat{\phi}$
- **Transformer Decoder:** Generates sequence of tokens for new tree
- **Output:** Valid symbolic tree $\phi$ with semantics aligned to $R$

## Loss Function

**Dual-objective loss function:**

$$L = L_{\text{cross-entropy}} + \lambda \cdot L_{\text{InfoNCE}} \tag{3}$$

**Cross-Entropy Loss:** Traditional objective for sequence generation
**InfoNCE Loss:** Contrastive learning to capture semantic equivalence

## Masked Contrastive Loss

**Objective:** Align embeddings from intention encoding and retrieval-augmented encoding

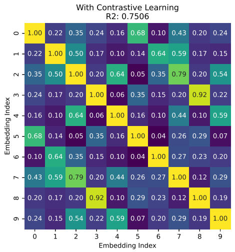
**Process:**

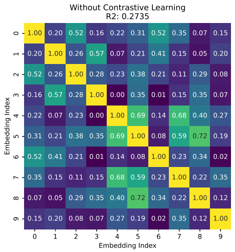
- Nearest semantics $\hat{\phi}(X) \in \mathbb{R}^{B \times N} \rightarrow \text{MLP} \rightarrow \mathbf{F}_{\text{nearest}} \in \mathbb{R}^{B \times K}$
- Symbolic embedding $\mathbf{H}_{\text{Transformer}} \in \mathbb{R}^{B \times L \times D} \rightarrow \text{Average} \rightarrow \mathbf{H}_{\text{avg}} \in \mathbb{R}^{B \times D}$

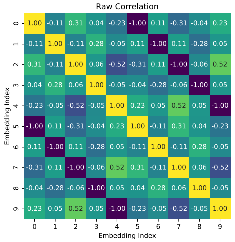
**InfoNCE Loss with Masking:**

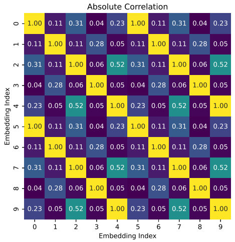
$$L_{\text{InfoNCE}} = -\frac{1}{B} \sum_{i=1}^{B} \log \frac{\exp\left(\text{sim}(\mathbf{F}_{\text{nearest}}[i], \mathbf{H}_{\text{avg}}[i])/\tau\right)}{\sum_{j=1}^{B} \exp\left(\text{sim}(\mathbf{F}_{\text{nearest}}[i], \mathbf{H}_{\text{avg}}[j]) \cdot \text{mask}/\tau\right)} \tag{4}$$

# Effect of Contrastive Learning









**Mask Strategy:**

- Mask matrix eliminates false negatives (cosine similarity > 0.99)
- Prevents penalizing semantically similar expressions
- Improves discrimination between truly different expressions

**Key Findings:**

- Captures different expressions with the same semantics as equivalent
- Without it: different embeddings for equivalent semantics

## Data Augmentation & Double Query

**Sign-invariant Property:** In linear regression, sign of coefficients is automatically adjusted
**Data Augmentation:** Include both the original feature pairs $(\psi, \psi(X))$ and their negations $(\psi, -\psi(X))$

$$T \leftarrow T \cup \{(\psi, -\psi(X)) \mid (\psi, \psi(X)) \in T\} \tag{5}$$

**Double Query:**

- Query the neural network with both the desired semantics $R$ and its negation $-R$
- Generate candidate trees $\phi$ and $\phi'$
- Select tree with highest probability

## Experiments

## Experimental Setup

**Datasets:**

- 120 black-box datasets from PMLB benchmark
- 119 Feynman equations and 14 Strogatz datasets

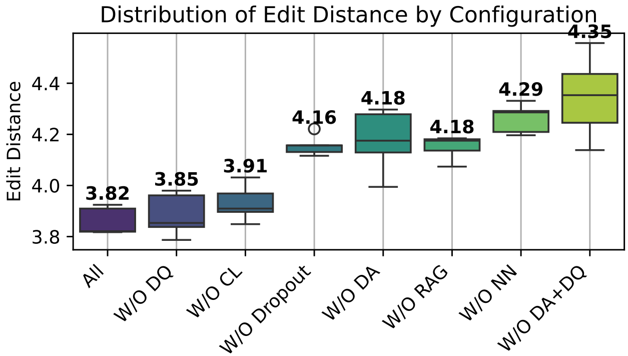
**Evaluation Protocol:**

- 75:25 train-test split
- 10 repetitions for robustness
- $R^2$ score on test set as metric
- Min-max scaling of input features

**Configuration:**

- Population size: 200
- Generations: 100
- Solutions of 10 trees each
- $P_{neural} = 0.1$

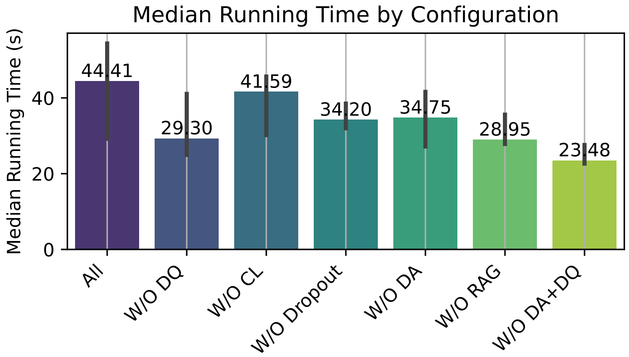
## Component Evaluation: Edit Distance



**Observations:**

- Neural generation outperforms simple retrieval (W/O NN)
- All components together achieve lowest edit distance
- RAG has most significant impact, followed by data augmentation
- Dropout, contrastive learning, and double query show moderate benefits

## Component Evaluation: Running Time



**Observations:**

- RAG moderately increases running time
- Removing DA and DQ reduces time but sacrifices accuracy
- Trade-off between computational cost and performance
- Acceptable overhead given accuracy improvements

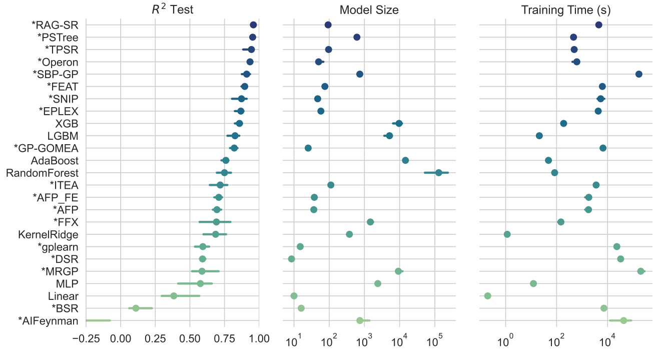
## Generated Trees Examples

| RAG-NN Generated Tree (Distance) | Simple NN Generated Tree (Distance) |
|---|---|
| Sin(Sin(ARG3)) (0) | Cos(Cos(Cos(ARG9))) (4) |
| AQ(ARG7, ARG8) (0) | Log(Max(ARG7, ARG7)) (3) |
| Max(ARG1, ARG8) (0) | Subtract(ARG1, ARG1) (2) |
| Sqrt(Sqrt(ARG2)) (0) | Log(Log(ARG2)) (2) |
| Subtract(ARG6, ARG7) (0) | Max(ARG7, ARG7) (2) |

| Retrieval Tree (Distance) | Ground Truth Tree |
|---|---|
| Sin(ARG3) (1) | Sin(Sin(ARG3)) |
| Log(Neg(Max(AQ(ARG8, ARG0), AQ(ARG7, ARG8)))) (6) | AQ(ARG7, ARG8) |
| Max(add(Abs(Sin(Cos(ARG6))), ARG8), ARG1) (6) | Max(ARG1, ARG8) |
| Square(Log(ARG2)) (2) | Sqrt(Sqrt(ARG2)) |
| Subtract(ARG7, ARG6) (2) | Subtract(ARG6, ARG7) |

**Observations:** RAG significantly improves the neural network’s ability to generate correct expressions

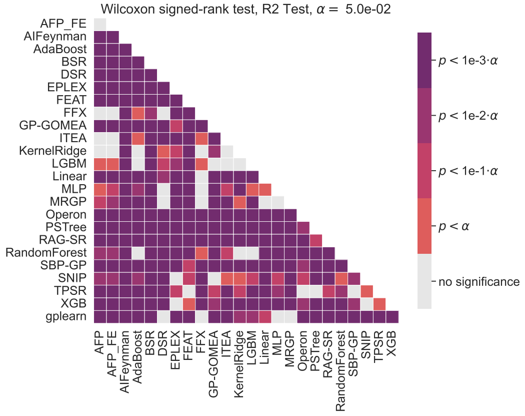
## Performance on SR Benchmark



**Observations:**

- RAG-SR outperforms all 25 algorithms in $R^2$ scores
- Produces models an order of magnitude smaller than SBP-GP
- Training time comparable to FEAT
- Best balance between accuracy, complexity, and efficiency

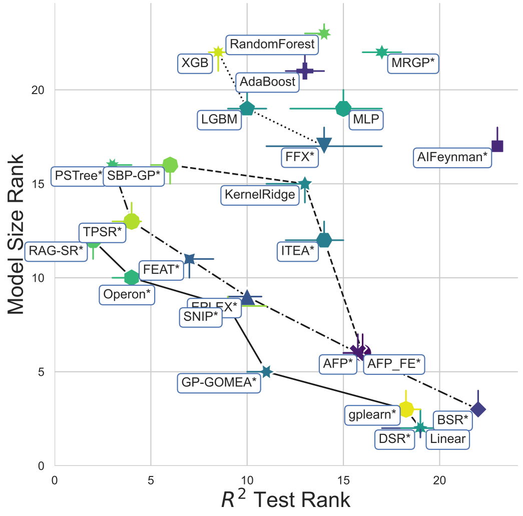
## Statistical Significance



**Observations:**

- RAG-SR significantly outperforms all other methods
- Improvement over TPSR confirms effectiveness of online learning vs. pre-training
- Advantage over SBP-GP shows value of integrating a neural network component

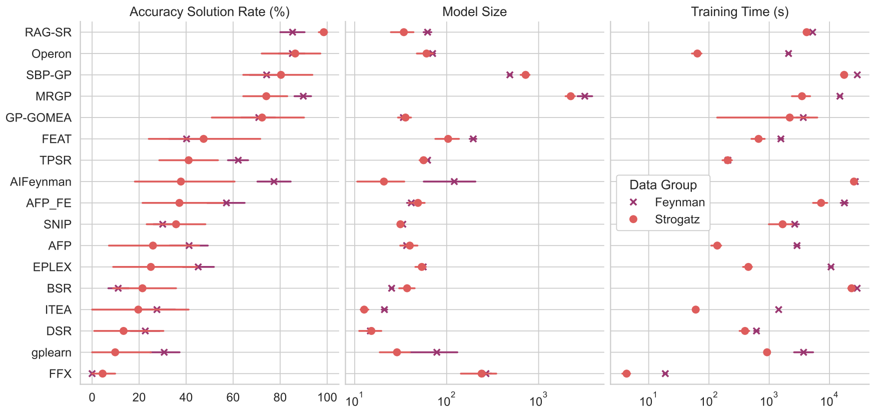
## Pareto Front Analysis



**Observations:**

- RAG-SR appears on the first Pareto front
- Excellent balance between accuracy and model complexity

## Feynman and Strogatz Results



**Observations:**

- Highest test $R^2$ scores on Strogatz datasets
- Second-best on Feynman datasets (after MRGP)
- MRGP models are an order of magnitude larger
- Significantly outperforms deep learning-based SR methods

## Conclusion

## Conclusion

**Contributions:**

- Novel symbolic regression with retrieval-augmented neural semantic library
- Effective online learning approach without pre-training
- Retrieval augmentation that effectively mitigates hallucination
- Contrastive learning that considers semantic equivalence, improving effectiveness
- Data augmentation and double query that leverage sign-invariance, enhancing performance

**Future Directions:**

- Extending to noisy datasets with limited samples
- GPU acceleration for combining pre-training and online learning

## Key Takeaway

Key Innovation of RAG-SR:

Don’t ask the NN to generate good improvements.

Instead, show examples of good improvements and say: ’A good improvement is like this, now give a better one.’

## Thank You!

**Questions?**

Source Code: `https://github.com/hengzhe-zhang/RAG-SR`