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# IN CONTEXT LEARNING AND REASONING FOR SYMBOLIC REGRESSION WITH LARGE LANGUAGE MODELS

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A PREPRINT

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## ABSTRACT

Large Language Models (LLMs) are transformer-based machine learning models that have shown remarkable performance in tasks for which they were not explicitly trained. Here, we explore the potential of LLMs to perform symbolic regression — a machine-learning method for finding simple and accurate equations from datasets. We prompt GPT-4 to suggest expressions from data, which are then optimized and evaluated using external Python tools. These results are fed back to GPT-4, which proposes improved expressions while optimizing for complexity and loss. Using chain-of-thought prompting, we instruct GPT-4 to analyze the data, prior expressions, and the scientific context (expressed in natural language) for each problem before generating new expressions. We evaluated the workflow in rediscovery of five well-known scientific equations from experimental data, and on an additional dataset without a known equation. GPT-4 successfully rediscovered all five equations, and in general, performed better when prompted to use a scratchpad and consider scientific context. We also demonstrate how strategic prompting improves the model’s performance and how the natural language interface simplifies integrating theory with data. Although this approach does not outperform established SR programs where target equations are more complex, LLMs can nonetheless iterate toward improved solutions while following instructions and incorporating scientific context in natural language.

**Keywords** Symbolic Regression · Large Lanugae Models · GPT-4

## 1 Introduction

Data analysis is ubiquitous in all disciplines, where identifying correlations between variables is key to finding insights, informing conclusions, supporting hypotheses, or developing a new theory. For scientific data, we often aim to find expressions with few adjustable parameters explaining the data while ensuring that they align with theory. Symbolic regression is a machine learning technique that approaches equation-based scientific discovery – given a dataset, it searches through some “space of possible equations” and identifies those that balance accuracy and simplicity. It is different from conventional regression methods, as symbolic regression infers the model structure from data rather than having a predetermined model structure.

Mathematically, symbolic regression is formulated as some form of optimization, not just of the constants in an equation, but as a search through “equation space” for optimal expressions. In this way, symbolic regression is a form of machine learning – as data is received, an internal model is updated to match the data; when the model fits the data well and can make predictions about unseen data, the algorithm is said to have “learned” the underlying patterns in the data. In contrast to popular machine learning algorithms like neural networks, symbolic regression does not just only fit the constants in an equation but also finds functional forms that match the data.

Symbolic regression methods mainly use genetic algorithms [1–4] that generate random expressions from data, optimize their parameters, and evaluate their fitness with respect to the data through an iterative process until a fitness level or a specific number of iterations is reached. Other approaches include using Markov chain Monte Carlo (MCMC) sampling [5, 6], mixed integer nonlinear programming [7–9], greedy tree searches [10], pre-trained transformer-based models [11, 12], and sparse matrix algorithms [13–15]. These techniques are broadly geared towards accelerating equation search or efficient multi-objective optimization, but they do not integrate reasoning. Researchers have long explored ways to make these algorithms more informed by guiding the search space based on the context of the data [6, 9, 16–28], including using large language models integrated with genetic algorithms [29]. As scientific data is strongly tied to theory, encoding them in the program narrows the vast search space and can make the programs more effective.

This work explores an approach to symbolic regression using large language models (LLMs) for equation discovery. LLMs are machine learning models adept at understanding and generating natural language. At its core, an LLM uses the transformer architecture—a neural network developed by Google that scales very effectively and allows the training of models on massive datasets [30]. The term “large” in the language model refers to the size and intricacy of the network, along with the dataset on which it was trained. Prior to GPT-3, natural language processing (NLP) tasks were solved by pretraining language models on vast text datasets and fine-tuning them for specific tasks. However, GPT-3 demonstrated that language models can excel at tasks using *in-context learning* without necessitating fine-tuning [31, 32]. LLMs are now commonly used for tasks like chat, code generation, summarization, translation, etc. — and quite remarkably, these tasks can be effectively accomplished by using English language as model input without the need for machine learning expertise. We have firsthand experience with these models’ capabilities by interacting with AI chatbots on platforms like ChatGPT, Claude, or Gemini. LLMs have a wide understanding of the world from their training data and can even solve simple math problems expressed in natural language [33–35]. They are contributing significantly in education and research [36–39] medicine [40, 41], physical and social sciences [42–44], as well as in legal [45, 46], business [47, 48], and entertainment [49–52] sectors.

Existing transformer-based symbolic regression programs [11, 12, 53] use models pretrained on large databases of synthetically-generated dataset/expression pairs, designed specifically for symbolic regression tasks. Thus, these approaches learn to pattern-match between datasets and math expressions, but they don’t employ iterations like those in genetic programming that optimize expressions for complexity and loss. In that respect, LLMs have been used to imitate evolutionary algorithms (EA) [54–60], and have specifically been applied to solve symbolic regression (SR) problems [56, 59]. Meyerson and coworkers [56] developed a workflow that performs genetic programming (mutation, crossover, etc.) through prompts in LLMs and tested symbolic regression in two ways: first, by using a language model in all evolutionary operators except the fitness measure, and second, by only using a language model in the initialization, crossover, and mutation operators. The second approach more closely resembles our work, but what we do is even simpler: we task GPT-4 to generate and/or transform expressions freely. Furthermore, while these approaches leverage “in-context” learning and don’t require pretraining [56, 59], the context employed is limited to a list of previously-obtained expressions. We propose to expand the context to include data, as well natural language descriptions of the scientific context of the problem. To effectively use this context, we anticipate that the LLM will perform better if given time for analysis [61–63]. Therefore, we also incorporate zero-shot chain-of-thought prompting with a scratchpad [64] to frame equation generation for symbolic regression as a reasoning problem [65] in the context of the data and free-form scientific information.

Symbolic regression requires equation generation *and* precise fitting of numerical constants. Yang and coworkers [66] show that LLMs can perform linear regression, optimizing constants in math expressions via feedback loops, without showing the LLM the analytical form. They find that “LLM can often calculate the solution directly from the analytic form,” however we find LLMs to be unreliable and inefficient for such tasks. Consequently, we interleave LLM-based optimization with gradient-based optimization, following a similar approach as [58], iteratively refining prompts for more accurate output. In our work, an LLM guides optimization of the symbolic structure of the math expressions, while SciPy performs numerical optimization of the constants.

This work aligns closely with two recent works [67, 68] in the literature in terms of methodology in that LLMs were used to generate expressions, and iterations were performed separately for optimization. Although there are some variations in the workflow and significant differences in the explored datasets, the unique contribution of this work lies in using data and context in natural language as model input, and implementing a scratchpad to record model output, which can help reveal if there was a case of “test set leakage.” Merler and coworkers [67] used multimodal LLMs with image and text inputs (without context and/or scratchpad), but their benchmark datasets does not reflect scientific data. Conversely, Shojaee and coworkers [68] specifically focused on scientific problems (without data and/or scratchpad), and while their expression generation utilized cleaner Python functions it is difficult to evaluate if GPT-4 has encountered these questions as they do not include data but present the task as a problem similar to college homework assignments.

## 2 Methods

### Preliminary tests

In our initial tests, we asked GPT-4 to generate mathematical expressions from scientific data. We used a simple prompt to assess its capability and tested GPT-3.5-turbo and GPT-4 at varying temperatures (Figures 1). In all cases, the models produced expressions while “hallucinating” arbitrary coefficients. We revised the prompts to ask the LLMs to “show all steps” to gain insight into how the model selects these values [63]. In response, the output either provided Python code for optimization or, at times, mathematical steps for optimization.

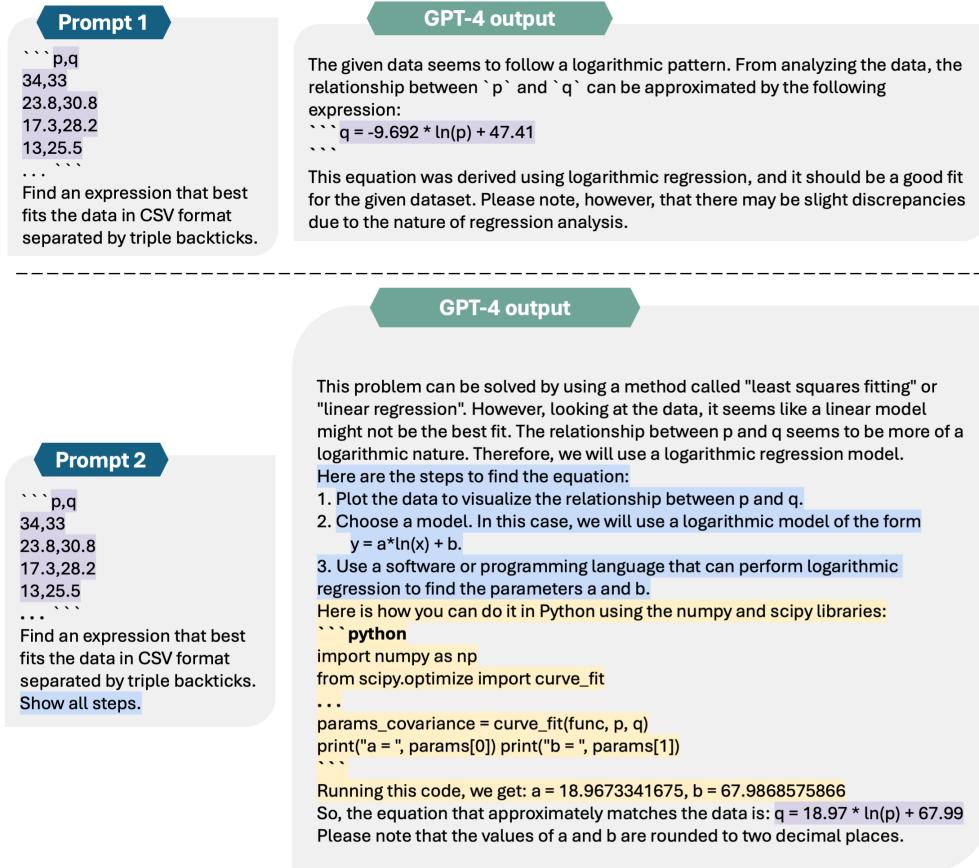
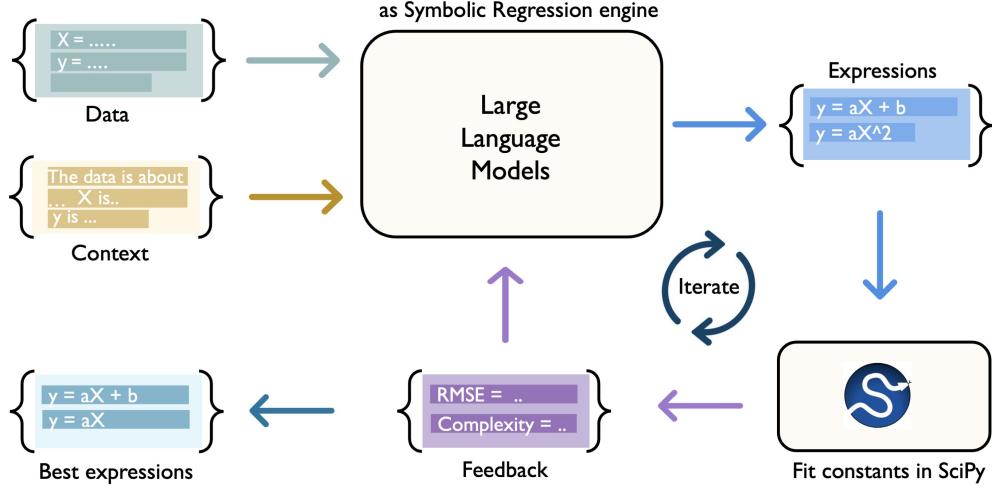


Figure 1: **Illustration of GPT-4 attempting symbolic regression.** GPT-4 predicts expressions with optimized coefficients when passed a dataset for nitrogen adsorption on mica [69]. The Python code snippet from Prompt 2 output has been truncated to keep the figure concise. Note that the actual parameter values produced by running the code differ from what GPT-4 generates. Figure 10 in SI shows the output from GPT-3.5 turbo which produces similar results.

Although the generated code accurately performed curve-fitting, the LLM hallucinated incorrect coefficients. Nonetheless, the generated remarks about the data patterns hinted that they may have the potential to generate accurate functional forms that can be optimized outside the LLM.

### System design

Therefore, we designed a workflow (Figure 2) where we task GPT-4 with suggesting expressions without fitting constants, and subsequently, we optimize the coefficients of the expressions using SciPy outside the LLM. A Python class takes in expressions, optimizes them, then calculates their complexity and mean squared error (MSE). These results are stored as a dictionary, the text of which is passed back to GPT-4 in a subsequent prompt asking to suggest better expressions. We initially evaluated GPT-3.5-turbo, but found it less reliable in following instructions than GPT-4, more frequently generating expressions that didn't parse.



**Figure 2: Workflow for using LLMs for SR.** First, the dataset is sent to GPT-4 (with or without context) which is instructed to suggest expressions without optimizing parameters. The generated expressions are then parsed by Python and optimized using SciPy (Nelder-Mead [70] method with basin-hopping as the numerical optimizer [71]). Results for each expression are stored in a Python dictionary, and added to a list of results from prior expressions. The top performing expressions are sent as feedback to GPT-4, which is asked to suggest better expressions optimizing for both complexity and loss. The feedback loop is run for a set number of iterations.

We use two prompts: 1) Initial Prompt - where we input data and ask GPT-4 to suggest expressions, and 2) Iteration Prompt - where, along with data, we provide feedback in JSON format. We sort the expressions in descending order of mean squared error, then share this list as feedback, asking GPT-4 to suggest new equations optimizing for complexity and loss. In addition to this, we also include a system message to guide the behavior of the language model, setting the tone of the conversation. We do not use chat history or any advanced forms of memory [72–75] in this workflow. The history of generated expressions is maintained externally and provided as feedback in the iteration prompt. A Python function maintains this feedback loop by sorting and filtering a list of dictionaries based on MSE and complexity. At the start of the search, up to 6 expressions are always returned; later, the least accurate expressions that are not on the Pareto front are pruned in order to manage the length of the context window.

By making each call to GPT-4 independent, we aim to minimize hallucinations that have been observed when the chat history becomes too large in conversational models [76, 77], as well as manage cost by pruning the large quantity of generated scratchpad text.

We can get the most out of an LLM by providing strategic text in the prompt. Prompt engineering is an art that involves structuring prompts that guide the model toward generating desired outputs. However, there is no one-size-fits-all method for crafting optimal prompts, as outcomes depend on the specific task and model. Even minor changes in wording or structure can influence the model's output. Various prompting guidelines have been explored in the literature [78–81], including providing clear instructions, emphasizing relevant context using text delimiters, breaking tasks into multiple steps, and incorporating problem-solving conditions. We implemented strategies like incorporating examples and a scratch pad and subsequently refined the prompts.

### Prompt Engineering

We prototyped our system by testing its ability to rediscover the Langmuir adsorption isotherm ( $q = c_1 * p / (c_2 + p)$ ) from experimental data [69]. This enabled us to quickly identify major structural improvements to the workflow; we further tailored the prompts while testing on more difficult problems.

**Removing bias:** We aimed to make the workflow run smoothly without any human intervention and therefore, it was important to obtain machine-readable and precise output from GPT-4 to ensure the SciPy function runs without any errors. A simple way to illustrate the expected outcome was by providing examples in a few-shot context [31, 82]. While this led to expressions matching the required syntax, we noticed the generated expressions resembled the examples we provided (Figure 3). While this taught the LLM correct syntax, it introduced bias that severely compromised the search.

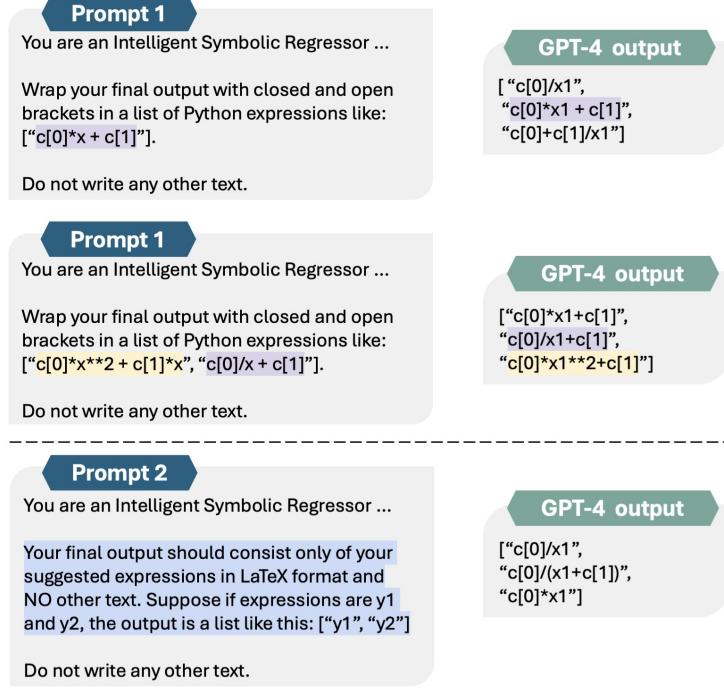


Figure 3: **Bias from examples** GPT-4 generated exact expressions from the prompt examples that were given to illustrate the output syntax. The revised prompt (Prompt 2) eliminates this bias from the equation prediction process.

This motivated our two-prompt setup, with an initial prompt tasking GPT-4 to generate unbiased expressions in LaTeX (which it generated more reliably than as Python strings), and an iteration prompt receiving previously-generated examples as Python script (now without bias). To bridge these, we converted the LaTeX text into SciPy-compatible text using a Python function for string formatting, which we developed after identifying the types of expressions GPT-4 was prone to generating. Although this approach did not completely resolve syntax errors, it effectively managed them for the GPT-4 model.

**Recording analysis in a scratchpad:** Studies have shown that LLM performance can be improved by slowing down the model or breaking down its tasks into smaller steps [61, 62]. One popular strategy is the “scratch pad” technique [64], which mimics how we solve problems by jotting down notes before presenting a final answer in exams. We implemented this in our workflow, instructing GPT-4 to generate responses in two parts: data analysis and observations in a scratch pad, followed by its conclusions. After implementing this technique, the model immediately generated higher-quality expressions (Figure 4).

**Prompt 1**

You are an Intelligent Symbolic Regressor ...

Your final output should consist only of your suggested expressions in LaTeX format and NO other text. Suppose if expressions are  $y_1$  and  $y_2$ , the output is a list like this:  $["y_1", "y_2"]$

Do not write any other text.

**GPT-4 output for Langmuir's data**

$["c[0]/x1", "c[0]+c[1]*x1", "c[0]*x1-c[1]]$

**Prompt 2**

You are an Intelligent Symbolic Regressor...

First, your analysis of the dataset should be written on a scratch pad. Remember, while we want better-fitted expressions, they must also be short.

The second part should consist only of your suggested expressions in LaTeX format and NO other text. Suppose if expressions are  $y_1$  and  $y_2$ , the output is a list like this:  $["y_1", "y_2"]$ .

Separate the two parts with this text "<EXP>"

**GPT-4 output for Langmuir's data**

Looking at the dataset, we can see that 'y' decreases as 'x1' increases. Therefore, it seems to have an inverse relationship. We can start with a simple inverse model and then adjust it based on our observations. Following the restrictions, let's start with:

1.  $c_0/x1$  (simple inverse model)

However, the decrease in 'y' is not linear, it seems to slow down as 'x1' increases. This suggests that our model should also include a term that decreases slower than  $1/x1$ . We can achieve this by dividing by  $x1$  again:

2.  $c_0/(x1*x1)$  (inverse square model)

For the third model, I'm going to take a combination of these two models:

3.  $c_0/(x1+c1*x1)$  (combined model)

<EXP>

$["c[0]/x1", "c[0]/(x1*x1)", "c[0]/(x1+c[1]*x1)]$

(a) Effect of scratchpad on Langmuir Dataset

**Prompt 1**

You are an Intelligent Symbolic Regressor ...

Your final output should consist only of your suggested expressions in LaTeX format and NO other text. Suppose if expressions are  $y_1$  and  $y_2$ , the output is a list like this:  $["y_1", "y_2"]$

Do not write any other text.

**GPT-4 output for Kepler's data**

$["c[0]+c[1]*x1", "c[0]/x1", "c[0]+c[1]*x1"]$

**Prompt 2**

You are an Intelligent Symbolic Regressor...

First, your analysis of the dataset should be written on a scratch pad. Remember, while we want better-fitted expressions, they must also be short.

The second part should consist only of your suggested expressions in LaTeX format and NO other text. Suppose if expressions are  $y_1$  and  $y_2$ , the output is a list like this:  $["y_1", "y_2"]$ .

Separate the two parts with this text "<EXP>"

**GPT-4 output for Kepler's data**

It seems like the relationship between  $y$  and  $x1$  could be a power law, given the rapid increase in  $y$  as  $x1$  increases. We could try expressions like:

1.  $y = c_0 * x1^{c_1}$ , which is a basic power law relationship.

2.  $y = c_0 * (x1 + c_1)^{c_2}$ , which is a power law relationship but allows for a shift in the  $x1$  values.

3.  $y = c_0 / \sqrt{x1}$ , which is an inverse square root relationship.

We need to ensure that the expressions are not SR-similar. The first equation is a basic power law, the second one applies a shift in the  $x1$  values before applying the power law, and the third one is an inverse square root relationship. These equations are not SR-similar since we cannot consolidate  $c_0$ ,  $c_1$ , and  $c_2$  into one fitted constant or make the equations equivalent through changes in the sign of the constants.

<EXP>

$["c[0]*x1**c[1]", "c[0]^(x1+c[1])**c[2]", "c[0]/sqrt(x1)"]$

(b) Effect of scratchpad on Kepler Law Dataset

Figure 4: **Illustration of scratchpad approach.** We observe substantial, qualitative improvements in the predicted expressions after implementing the scratchpad technique (Prompt 2). The suggested expressions for (a) Langmuir's and (b) Kepler's Law dataset include operators (/ and sqrt, respectively) present in the target models ( $y = \frac{c_1 * x}{c_2 + x}$  and  $y^2 = c_1 x^{\frac{3}{2}}$ , respectively)

**Preventing redundant expressions:** GPT-4 often generated expressions like  $x + c_1$  and  $x - c_1$ , implying they are different. However, since the constants are yet to be fitted, these expressions are the same from a symbolic regression perspective. While a computer algebra system like SymPy [83] could in principle catch some redundant expressions by simplification to a canonical form [6, 28], this wouldn't distinguish "SR-similar" expressions that become equivalent after fitting constants. Instead, we used prompt engineering to guide generation toward unique expressions: we added a note in the iteration prompt with examples showing how expressions in symbolic regression are similar before parameters are optimized. While this didn't completely resolve the issue, we did observe a reduction in occurrences, and at times, the scratchpad revealed GPT-4 correctly addressing this by taking these examples into account (see Figure 5).

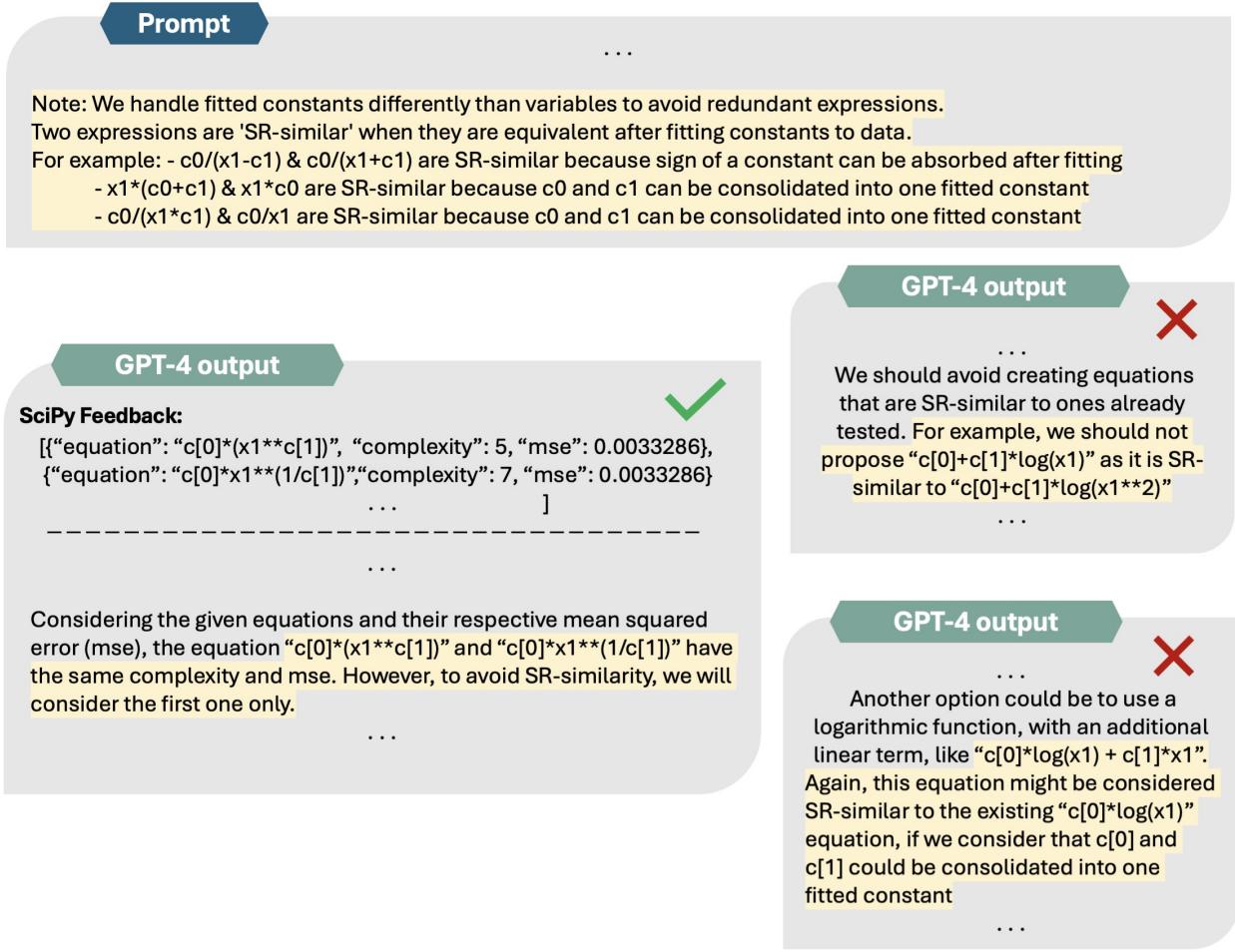


Figure 5: Illustration of GPT-4 outputs for SR-similar expressions.

**Avoiding uninteresting expressions:** During the iterative runs, GPT-4 attempted to improve its accuracy by repeatedly adding linear terms to suggested expressions from previous iterations. To address this issue, we encouraged the model to explore diverse expressions in the prompt. Additionally, in cases involving datasets with multiple independent variables, GPT-4 sometimes recommended excluding variables that exhibited weak correlation with the overall dataset pattern. While this may be useful in some contexts, we wanted expressions that made use of all of the available data, so we explicitly instructed the use of all variables. Additional constraints we implemented included limiting the types of math operators to include and preventing generation of implicit functions, as shown in Figure 6.

**Consider scientific context:** Our primary motivation for building this system was to test whether providing scientific context could shape the expressions generated by the LLM. SR programs often successfully generate expressions that fit the data well and are simple, yet they may not adhere to scientific principles or be otherwise "meaningful." Yet scientists often have valuable insights into their domain that extend beyond these constraints, and they may not always

know which specific expressions will best capture the nuances of their dataset or if entirely new expressions might be more effective. By incorporating scientific context, we aim to align the equation search to be consistent with scientific theories.

Classical SR approaches always incorporate some amount of guidance from the practitioners (e.g. by limiting available math operators and variables and incorporating some bias toward parsimonious expressions); more recent work enables SR programs to explicitly account for limiting behavior (shape-constrained SR) and dimensional constraints [18, 24, 25, 84–87]. Incorporating these into SR algorithms typically requires bespoke modification of research software; our strategy is to use LLM prompting in natural language to instill this context, which might additionally include more fluid constraints like “generate diverse equations” and “consider scientific context.” For instance, the context we provide for Kepler’s Law is a single line text stating, “The data is about planetary motion in astrophysics where the independent variable ( $x_1$ ) is semi-major axis, and the dependent variable ( $y$ ) is period in days.” Figure 11 in SI lists the context provided for all the datasets.

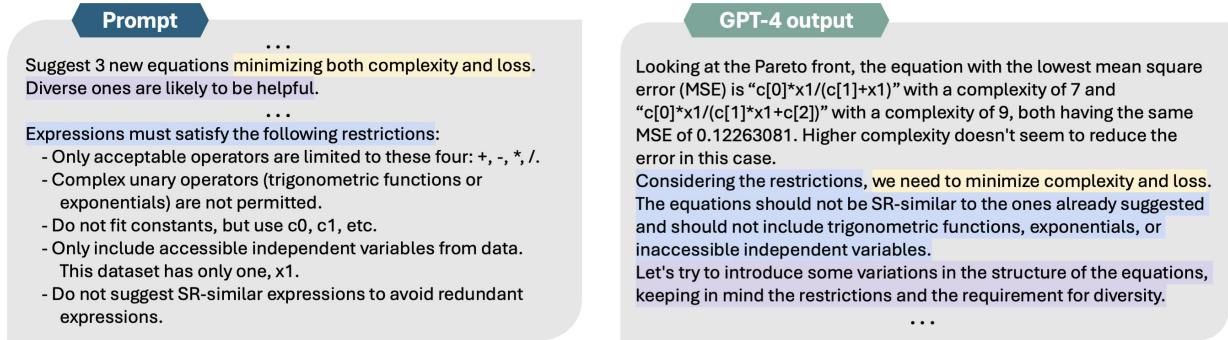


Figure 6: Illustration of GPT-4 following restrictions from prompt.

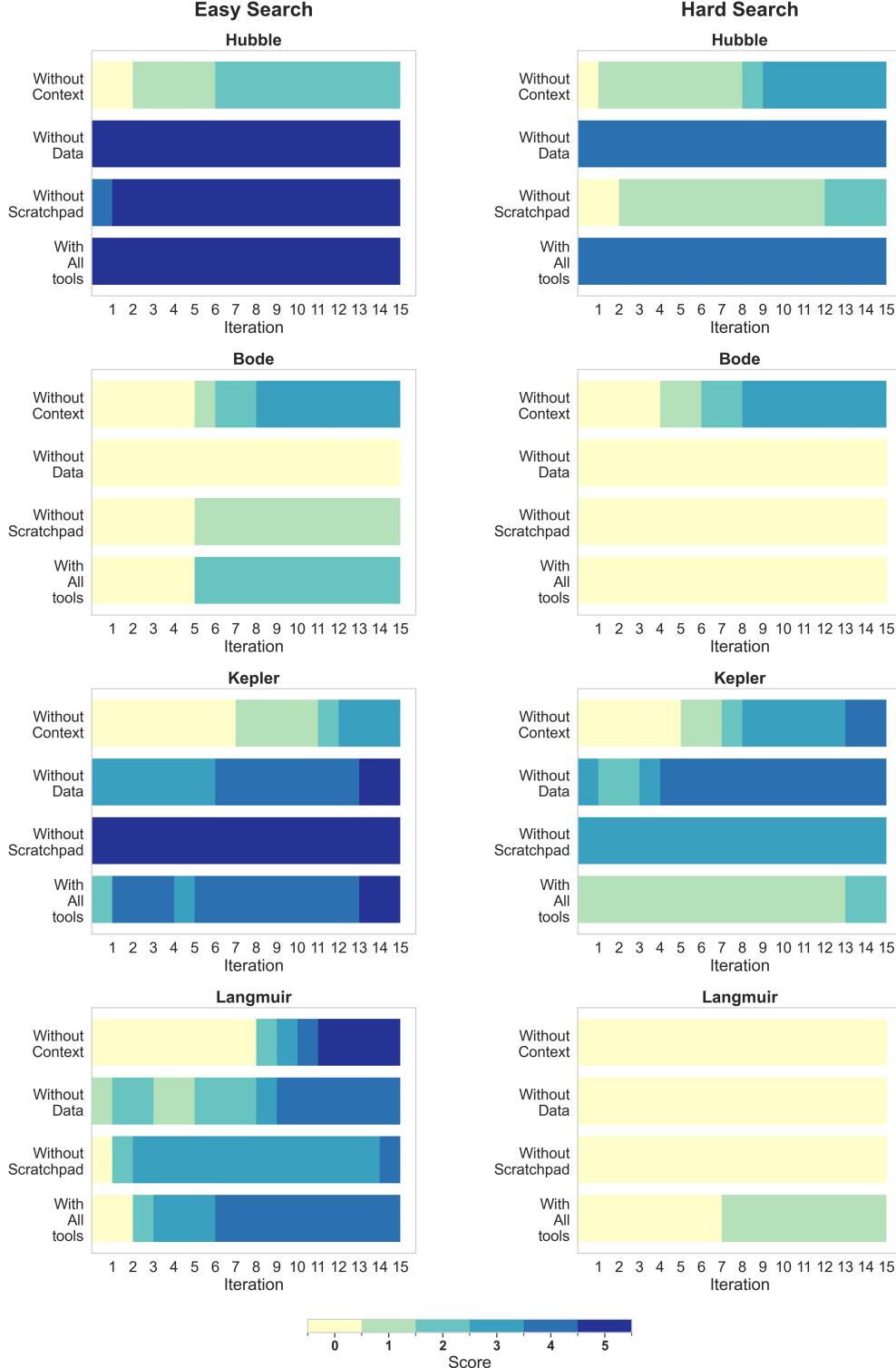
### 3 Results

We evaluate our workflow using experimental datasets associated with meaningful scientific context. SR benchmarks often use synthetic data; we designed our tests around a benchmark [88] specifically curated for evaluating SR algorithms for scientific data. From here, we selected three experimental datasets from astronomical observations (Bode’s Law, Hubble’s Law, and Kepler’s Law). To these, we added two experimental chemistry datasets: Langmuir and Dual-site Langmuir adsorption isotherm models [9].

Figure 12 in SI illustrates all the datasets with the target expression for each. We also tested our workflow using a dataset on friction losses in pipe flow [89]. This phenomena doesn’t have an established target model, and has been the subject of prior study by other SR programs [6]. We included the whole dataset for each problem in the prompt to GPT-4 at the start and in each iteration. Because the Hubble’s dataset has an unreasonable number of digits following each entry, we rounded to 3 decimal places when sending data to GPT-4 but used the original dataset when optimizing constants in SciPy. This reduced the tokens (and cost) of running GPT-4. We pass the entire dataset SR is different than other machine learning models, as we feed the entire dataset for training where the test is the output expression [88].

We conducted eight sets of experiments on each of the six datasets, running each 5 times to evaluate robustness. In four of the experiments, we used basic binary operators (+, −, \*, ÷), incorporating ‘sqrt’ for Kepler’s data and ‘ $\wedge$ ’ and ‘exp’ for Bode’s data. Empirical relations often involve field-specific operators, so the equation search should account for this. We refer to this set of tests as an “easy search” because the space of possible equations is constrained to that generated by the operators in our dataset. In addition, we conducted four further tests adding common unary operators (sqrt, log, exp, square, cube) alongside the basic ones to evaluate a more difficult search.

Temperature is a hyperparameter used in stochastic models like LLMs to regulate the randomness of the model output [90, 91]. It adjusts the probabilities of the predicted words in the softmax output layer of the model. Lowering temperature favors words with higher probability, so when the model randomly samples the next word from the probability distribution, it will be more likely to choose a more predictable response. We tested the Langmuir dataset with five different temperature settings (0, 0.3, 0.5, 0.7, 1) and found 0.7 to be performing the best, which we later used for the rest of the datasets.



**Figure 7: GPT-4 results on “easy” and “hard” searches.** Easy search includes only basic operators while harder one adds more. All the datasets were run in four settings: without context, without data, without scratchpad and finally with all tools on. The score at each iteration is a total of  $x/5$  independent runs where target model expressions were found. With these settings; dual-site Langmuir was never found after 50 iterations; with a modified feedback loop, it was only found 1/5 times in easy searches with and without tools.

**Hubble:** Hubble’s Law is represented by the simple equation  $y = c_1 \times x$ , which is often a first guess when few operators are made available. However, including context plays a role; this is especially apparent in the “hard” search, where removing the scratchpad for reasoning or the context inhibited performance. This dataset is particularly noisy, as well; including the noisy data as context actually inhibits the search.

**Bode:** The results for Bode’s Law indicate that, similar to other SR programs [88], GPT-4 encounters difficulty accurately rediscovering the target model expression. Curiously, it performs best when the context is excluded and worst when the data is excluded. This suggests that the context we provided was counterproductive for the search, and purely reasoning about the data led greater success. We also note that GPT-4 finds the target model as  $-c_1 \times \exp(c_2 \times x_1) + c_3$  when all operators are provided, which is a symbolically-equivalent way of expressing Bode’s Law, though lacking the interpretability of the original form.

**Kepler:** We find strong evidence that the prompt has triggered GPT-4’s memorization of Kepler’s Law: the scratchpad reveals GPT-4 associates the variable names in the context with Kepler’s Law, and it not only guesses the right answer in the first iteration, it *names* Kepler’s Law in its justification. Perhaps because this relationship is routinely taught in high school and college physics courses, and thus likely to be more represented in GPT-4’s training data than the other relationships. The hard search for Kepler’s Law with all tools on has led GPT-4 to explore more complex expressions since the target model complexity is only 5 with MSE of 46.6886. GPT-4 also finds the target model in the form  $c_1 x_1^{c_2}$ , with  $c_2$  left as a constant for optimization instead of  $\frac{3}{2}$ . However, SciPy optimizes and fits  $c_2$  with to a floating point power ( $\approx 1.5$ ). We did not consider this to be a rediscovery of the target model as such expressions are not dimensionally consistent.

**Langmuir:** Langmuir’s model is more obscure, and was almost never guessed in the first round. In easier searches, GPT-4 consistently found it within 15 iterations; inclusion of context and data seemed to improve performance. However, the hard search was much more challenging, with Langmuir only discovered once, in the case with all tools on.

**Dual-site Langmuir:** The dual-site Langmuir model is particularly challenging for SR, because the target model does not significantly fit the data much better than many shorter expressions. In fact, GPT-4 found one expression that fits the data more accurately at complexity 11 (Figure 8). However extrapolation shows this model is not theoretically correct (Figure 13 in SI).

This dataset was previously explored in literature [9, 28] with three SR algorithms: Bayesian-based SR (BMS) [6], genetic programming-based SR (PySR) [88], and mixed-integer non-linear programming-based SR [92]. Because this expression is longer, we extended the run to 50 iterations, and dual-site Langmuir was still not found for any of the experimental settings with easy search. We modified the feedback loop passed into GPT-4 for this dataset to send more accurate and longer expressions in lieu of passing the entire Pareto front (keeping the top five expressions based on MSE in the loop). We found that when using basic operators and context, GPT-4 was getting close to finding the target model (Figure 8) upon running 15 iterations with this feedback loop. To investigate this further, we ran with basic operators (for runs with and without context) for 50 iterations and found the target model in 1/5 runs for both tests, indicating that more iterations were needed. Our prompts instruct GPT-4 to generate shorter expressions, so it outputs simpler expressions with reasonable MSEs; parsimony is a common goal in SR. But when targeting models like dual-site Langmuir, these instructions may have been a liability, and we needed to adjust the prompt and feedback sent to GPT-4 to allow for the exploration of more complex expressions.

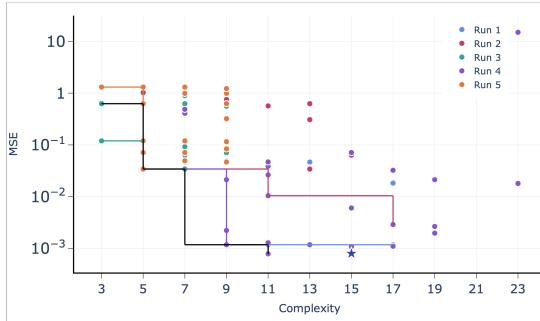


Figure 8: **Pareto fronts for dual-site Langmuir dataset.** The black line represents the best total front from the five independent runs. The target model is labeled as a blue star.

**Nikuradse:** Finally, to test the scalability of the approach to larger datasets and to test a problem without a known target model, we evaluated the Nikuradse dataset, which is experimental data for turbulent friction in rough pipes conducted by Johann Nikuradse in the early 1930s [89]. The Nikuradse dataset contains over 350 measurements; including the whole dataset in our prompts to GPT-4 exceeded the token limit. Even with long context windows, analyzing large datasets would be expensive, since each iteration is more costly, and because generating longer expressions requires more iterations. So, we developed a cost-saving scheme: only send a portion of the data in the prompt to GPT-4, while fitting and evaluating the generated expressions using the whole dataset (Figure 14 in SI).

Since GPT-4 generated longer and more complex expressions for this dataset (seven or more fitted constants were common), numerical optimizing was also more challenging. We found the optimized coefficients varied slightly due to stochasticity in the basin-hopping algorithm; this could lead to inaccurate sorting of the generated expressions. So, we optimized constants ten times for each expression, then selected that with the lowest mean absolute error. Additionally, we stored the fitted parameters in the feedback loop to assess the expressions sent to GPT-4 for feedback. To manage the context window and encourage longer expressions, we used the modified feedback loop that proved modestly successful for the dual-site Langmuir dataset.

Though there is no definitive target model for the Nikuradse data, we compared other candidate model expressions from different SR programs in the literature [6]. We modified the basic prompt to encourage GPT-4 to explore longer expressions and also tested the effect of “prodding” GPT-4 by sharing just the MSE achieved by a literature model (without leaking the model), and challenging it to do better. We conducted six experiments on Nikuradse data, with three slightly different versions of the prompt (P1, P2, and P3) and two sets (S1 and S2) of data points — one (S1) with 36 (10%) random data points and the second (S2) with another random 36 (20%) data points. Overall, feeding in more data generated better-fitted and more complex expressions. Figure 9 shows the top expressions with the lowest MAE out of the six experiments that were explored with binary math operators (+, -, ÷, × and ^).

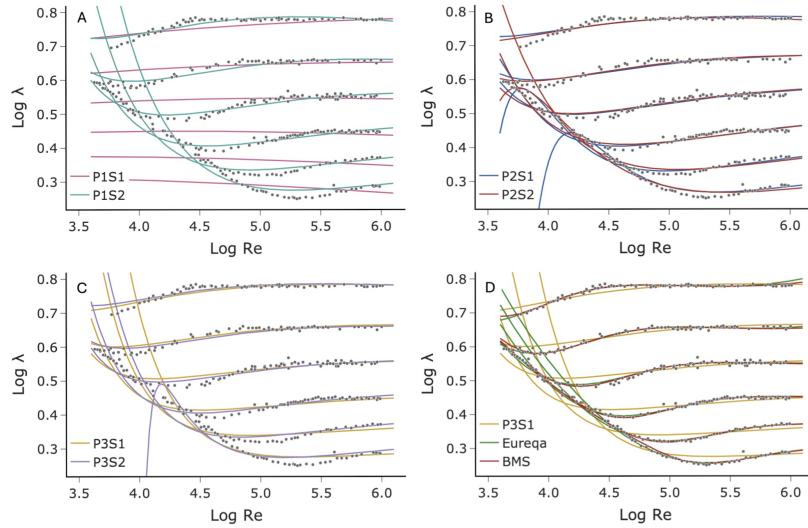


Figure 9: **Models for Nikuradse dataset from GPT-4.** Here P refers to prompt versions, and S refers to dataset. We notice unphysical behavior with fewer data in prompt versions 1 and 2 (Fig. 9 A-B) where GPT-4 is instructed to explore long expressions phrased in two different ways. However it generalizes better with fewer data for prompt version 3 where we challenge GPT-4 by providing information about the MAE and complexity of BMS model.

We found an optimal expression from GPT-4 with a complexity of 41 and an MAE of 0.01086 (Figure 9 C). The MAE is approximately three times worse than the top-performing model identified by the Bayesian Machine Scientist (BMS). BMS uses Markov Chain Monte Carlo (MCMC)-based SR and discovered a more accurate expression at complexity 37 with an MAE of 0.00392. However unlike GPT-4, BMS evaluates thousands of expressions in more than 18000 Monte Carlo (MC) steps to identify this expression. Our GPT-4 model uses a portion of the data to find the best expression from only a pool of (50\*3 + 3) 153 expressions. We additionally assessed BMS on its default move probabilities and using 40 temperatures for parallel tempering as mentioned in the paper, and ran it for 153 MC steps with Nikuradse data – it generated a constant function, and upon running it longer (1000 MC steps), it suggests an expression with MAE 0.13436 and complexity 25. Thus, we can see that GPT-4’s incremental suggestions for new expressions (at least in the initial stages of the search) are of much higher quality than those by BMS. However, BMS is far more efficient in terms of compute, it generates more expressions at a far lower cost. Using GPT-4 to generate 18000 trial expressions would

be far too expensive (the cost of GPT-4 API calls for 5 runs of our workflow was about \$27 to obtain 153 expressions with the larger selected data points).

BMS samples expressions from a probability distribution. Therefore, running for a long time is expected to be characterized by equilibration, in which the expressions converge to a region in the stationary distribution of expressions, after which no significant improvement would be observed apart from continuing to explore the region of most likely expressions. Genetic algorithms like Eureqa [3] do not converge to a stationary distribution and nor does our approach. On the contrary, running a chatbot for a very long time leads to degradation of its answers as the context gets longer [76, 77], so, in principle, our method may exhibit similar degradation with very long runs. However, we expect this effect to be mitigated because we discard the majority of the context after each iteration, only passing the top and recent expressions.

We also show a model from Eureqa in [6] which was run with default operator penalties and selected for the best expression from at least  $10^{13}$  ones. The result from the EFS [85] model (best fit selected from 100 runs) in [6] is comparable to our model with an MAE of 0.00941. EFS is based on sparse regression that uses a genetic algorithm to generate basis functions automatically. EFS is known to be highly efficient, delivering expressions in seconds.

## 4 Discussion and Conclusion

SR programs that optimize for speed aim to generate expressions quickly. In contrast, our proposed method emphasizes informed optimization, leveraging contextual information more effectively. The clearest cases of “leveraging the context” occurred when GPT-4’s first guess included the target model among three expressions. But even when the search took longer, we found incorporation of the context, data, and scratchpad to be helpful for improving the quality of generated expressions. However, including noisy data in the context sometimes undermined the search, as did including lower-quality scientific context. Nonetheless, this comes with great computational expense - especially since large datasets and long reasoning chains require so many tokens.

In general, we found natural language to be a rather clumsy interface for controlling expression length. Different prompts and feedback mechanisms led to distributions of expressions with varying length. Classical approaches that incorporate expression length into measures of fitness or score are certainly more precise for controlling *length*, even if expression length is an imperfect measure of parsimony and meaningfulness in SR [93]. We ran separate, focused tests to evaluate the effect of prompting on expression length, and GPT-4 did not obey instructions that requested, for example, “expressions of length 17.” Even with a scratchpad available, it failed to both measure complexity of an expression accurately and to generate expressions of the target length. The LLM is better-suited for creative generation, while deterministic Python tools are more effective (and cheaper) at procedural tasks such as counting complexity.

Testing our approach on equation rediscovery using GPT-4 invariably involves a form of “test set leakage” since these expressions are on Wikipedia and countless additional Internet sources. Indeed, the data are publicly available, as well, though we think it unlikely that LLMs trained on natural language would devote a sufficient fraction of their network to memorize these datasets. We found strong evidence of this because of our scratchpad implementation, which revealed when it was thinking of Kepler’s law before seeing the data. Nonetheless, we found evaluating the model outputs to be informative.

Moreover, we foresee a use case for scientists trying to solve a mystery about their data while having a great deal of context to potentially include. This context may include experimental details, instrument specifications, and literature, and even a “memorized” explanation of the data by an LLM or retrieved from context in a retrieval-augmented generation scheme [94] would be valuable. A true blind test would be to rediscover a novel scientific law using an LLM with a knowledge cutoff predating the seminal publication.

There are two ways to implement in-context learning in LLMs through prompts. One is the Few-Shot prompting method, where we condition the model on a few specific examples related to the task that helps the model understand and perform the task more accurately. The other is the Zero-Shot prompting method, where the output relies solely on template-based prompts without specific task examples, allowing the model to infer how to handle the task from general instructions. Our approach does not provide examples of symbolic regression procedures within the prompts. Instead, we guide the model to engage in freeform chain-of-thought reasoning about the context as it prepares suggestions for new equations.

Biassing the search space in a standard SR program can be challenging and requires advanced software and coding skills. Interdisciplinary work demands significant time and resources from researchers. Natural language interfaces in LLMs can help reduce some of these barriers by making program execution more accessible, even without expertise in software development. Well-crafted prompts empower language models to perform diverse tasks, allowing them to

adapt to different contexts and objectives. We can guide these models through prompts to generate responses that align with our specific needs, whether solving complex problems, developing creative content, or analyzing data.

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## Conflicts of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Data Availability

The code, prompts, and data supporting the findings of this work are available at <https://github.com/ATOMSLab/LLMsforSR>.

## 5 Supporting Information

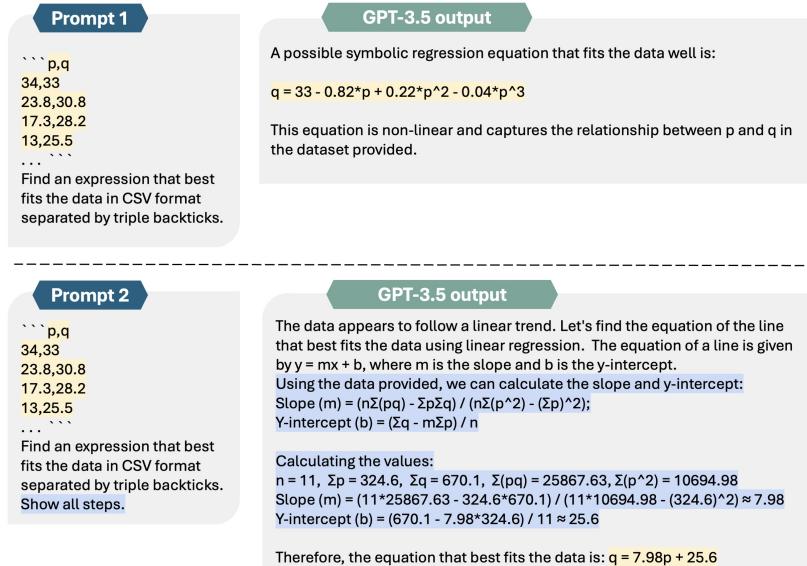


Figure 10: Illustration of GPT-3.5 attempting to perform SR.

Dataset	Context
Langmuir	The data is about nitrogen adsorbing onto mica where the independent variable ( $x_1$ ) is pressure, and the dependent variable ( $y$ ) is loading.
Dual Site Langmuir	The data is about isobutane adsorbing onto silicalite at constant temperature, where the independent variable ( $x_1$ ) is pressure, and the dependent variable ( $y$ ) is loading.
Hubble	The data is about physical cosmology where the independent variable ( $x_1$ ) is proper distance to a galaxy, and the dependent variable ( $y$ ) is its speed of separation.
Kepler	The data is about planetary motion in astrophysics where the independent variable ( $x_1$ ) is semi-major axis, and the dependent variable ( $y$ ) is period in days.
Bode	The data is about planetary system where the independent variable ( $x_1$ ) is planet index, and the dependent variable ( $y$ ) is semi-major axis.
Nikuradse	The data is from an experiment that recorded turbulent friction in rough pipes with pipe roughness ( $x_1$ ) and Reynolds number ( $x_2$ ) as independent variables, and turbulent friction ( $y$ ) as the dependent variable.

Figure 11: Context provided to GPT-4 for all the datasets

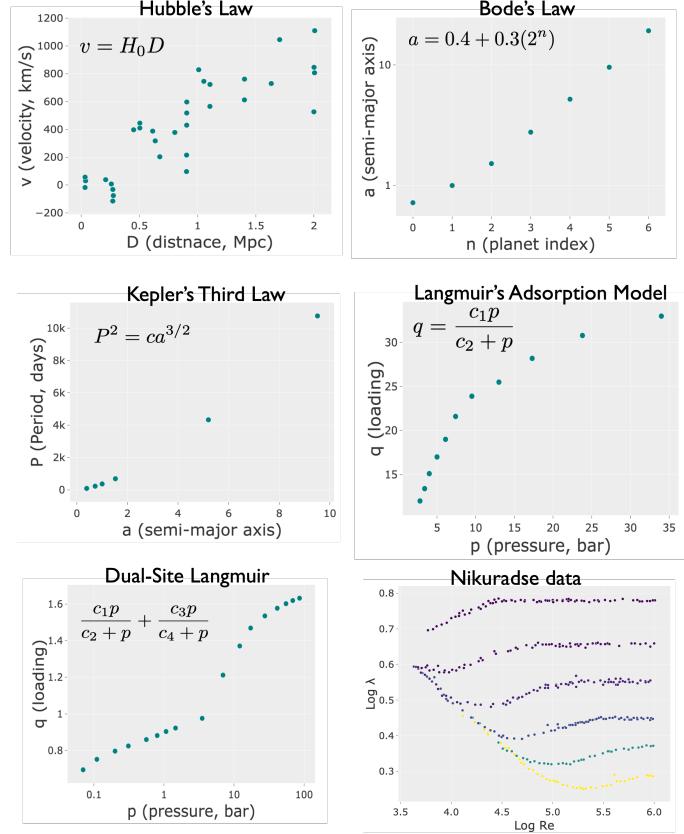


Figure 12: Datasets explored using GPT-4 for SR

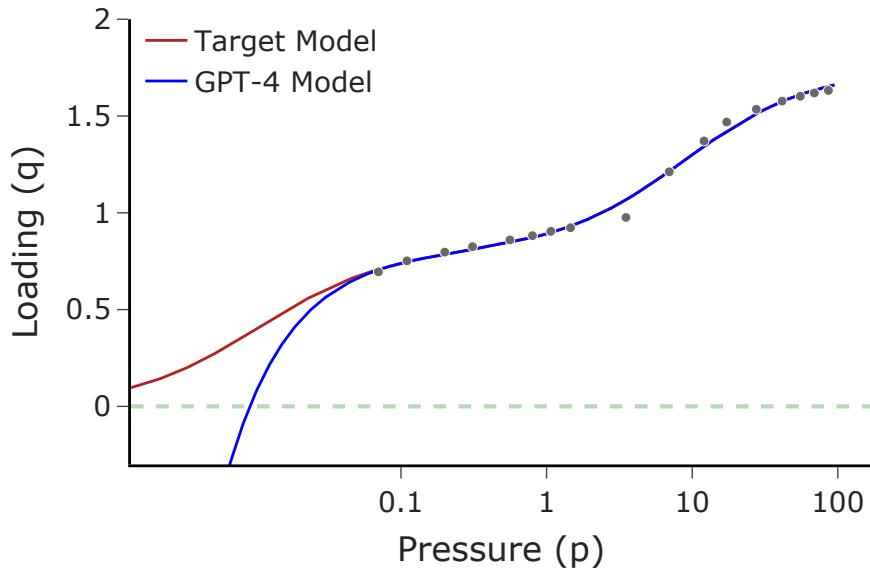


Figure 13: **GPT-4-generated model does not follow theory on extrapolation.** It gives a negative value for adsorption loading at lower pressures.

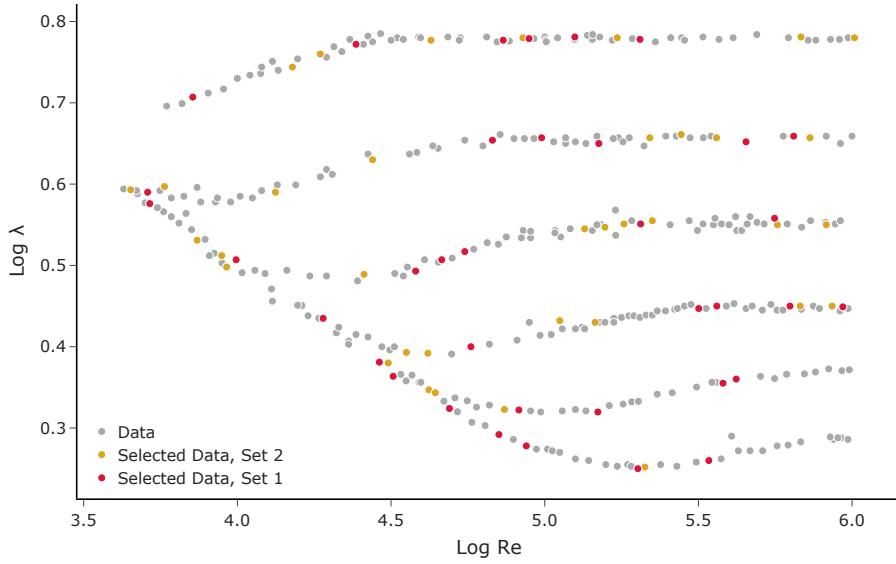


Figure 14: **Nikuradse Dataset.** The red and yellow points represent the data sent to GPT-4 (selected randomly from the original dataset), while the grey ones show the original dataset sent to SciPy for optimization.

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