
HARDMATH: A Benchmark Dataset for Challenging Problems in Applied Mathematics

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Abstract

Advanced applied mathematics problems are not well-represented in existing benchmark datasets used to evaluate Large Language Models (LLMs). To address this, we introduce **HARDMATH**, a dataset of difficult problems inspired by Harvard University’s graduate course on asymptotic methods. The dataset contains a diverse set of challenging applied mathematics problems with worked solutions that use various analytical approximation methods. Developing such solutions typically requires multiple modes of analysis—including mathematical reasoning, the use of computational tools, and subjective judgment—making this a challenging problem for LLMs. We establish a framework that auto-generates an arbitrarily large number of ‘hard’ applied mathematics problems with solutions and includes validity checks against numerical ground-truth calculations. Additionally, we report quantitative and qualitative evaluation results on frontier open- and closed-source models using a test set of 366 sampled from the main dataset, as well as a “Word problems in context” test set of 40 problems. Leading closed-source models, such as GPT-4, achieve only around 50% accuracy even with few-shot Chain-of-Thought prompting, which is considerably lower than performance on existing mathematics benchmark datasets. Open-source models demonstrate an even larger performance gap, suggesting room for model fine-tuning. Our findings demonstrate the limitations of current LLMs in solving advanced graduate-level applied mathematics problems and highlight the need for datasets like **HARDMATH** to further improve LLM mathematical capabilities.

1 Introduction

The mathematical equations that arise in practical, scientific, and engineering problems can rarely be solved analytically. Traditional mathematics courses typically focus on equations that have exact, analytical solutions and only teach a limited set of techniques for solving them. The mathematical reasoning datasets used to benchmark large language models (LLMs) are predominantly restricted to these types of problems and techniques. However, many practical mathematics problems involve integrals, ordinary differential equations (ODEs), and partial differential equations (PDEs) that do not admit closed-form solutions and must be approached with a different set of techniques. Numerical solutions reveal insights, but do not provide intuition as to *why* solutions behave as they do. A paradigmatic approach seeks *approximate* analytical solutions to complex mathematics problems using tools from applied mathematics, such as asymptotic and applied analysis, which are currently

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not well-represented in existing mathematics benchmark datasets for LLMs. To address this gap, we present **HARDMATH**, the Harvard Asymptotic Reasoning Dataset for Mathematics². This dataset captures a fundamentally different type of mathematical reasoning than other benchmarks, and it can be useful for evaluating LLMs’ proficiency in making research-relevant approximations.

HARDMATH contains 1,466 problems modeled after those from Harvard University’s graduate course on asymptotic methods, which covers algebraic equations, ODEs, and integrals that often arise in real scientific and engineering contexts but that cannot be solved exactly. To find approximate but accurate solutions to these ‘messy’ mathematical problems, we leverage various asymptotic reasoning techniques to create this dataset.

A primary motivation for developing **HARDMATH** is the lack of benchmark datasets targeting the mathematical approximation methods required in many applications. While some recent works have begun to include university-level problems [11], most datasets focus on grade school- to high school-level mathematics problems [3, 10, 6] whose solution methods only involve direct, ‘clean’ calculations. In contrast, **HARDMATH** targets applied mathematics problems that require approximate solutions, which is an equally important area of mathematical reasoning. Finding approximate analytical solutions can be challenging even for those with high levels of mathematical proficiency, as it requires advanced techniques from calculus, differential equations, and complex analysis. Computational tools are also needed to explore the behavior of different terms in each equation and to find numerical solutions that can be compared with approximate solutions. Given the difficulty of these problems and their prevalence across science and engineering—often confronting researchers without a strong background in advanced mathematics—we contend that this level of difficulty and style of mathematics *must not be excluded* from LLM evaluations.

Rather than the typical procedure of collecting problems from textbooks, standardized tests, or competitions like most existing datasets, we develop algorithms to automatically generate problems and step-by-step solutions. We design a comprehensive testing methodology to assess leading LLMs’ mathematical reasoning abilities in this approximation methods domain. Our dataset consists of a larger set that can be used for fine-tuning, and two test sets that we use to evaluate leading LLMs. We present evaluation accuracy and error modes analysis for these test sets. Specifically, we show that the *current* performance of existing LLMs on these problems is poor, leaving much room for future improvement.

2 Related work

LLMs have shown promising capabilities in mathematics. However, evaluating and expanding the full extent of these abilities requires diverse datasets with problems that go beyond basic arithmetic or elementary word problems. Existing benchmarks often focus on these simpler domains, with a gap in addressing graduate-level applied mathematics problems that demand a deeper understanding and diverse, multi-modal analytical skills. Most mathematics datasets for evaluating or training LLMs contain samples that either present the problem directly or within a constructed narrative context. Notable examples of these datasets include **MATH** (12,500 high school competition-style problems) [10], **GSM8K** (8,500 multistep grade-school problems) [6], **MATHQA** (37,000 GRE/GMAT-level multiple-choice problems) [3], **ODYSSEY-MATH** (387 hand-curated problems across various difficulty levels) [14], and [23] (a bilingual concept-wise mathematical dataset). While these existing datasets are valuable for assessing LLM math performance in certain areas, most are limited in scope and complexity.

Recent efforts target more advanced problems that are most often manually-sourced. Relevant works include **JEEBENCH** [4] and a subset of the **MATHBENCH** dataset [11], both of which cover some college-level topics including simple ordinary differential equations and multivariable calculus. More advanced-level problems are presented in **GHOSTS**, which includes more advanced-level problems in its **GRAD-TEXT** subset—a collection of 130 exercises from graduate-level mathematics

²The dataset and code used to generate it are available at <https://github.com/sarahmart/HARDMath>.

Table 1: Comparison of **HARDMATH** with related datasets. Note that for all the datasets excluding **MATH** and **GSM8K**, we report the number of relevant problems at a comparable difficulty to our dataset (e.g., **THEORY-KNOWLEDGE-COLLEGE** in **MATHBENCH**, and **GRAD-TEXT** and **HOLES-IN-PROOFS** from **GHOSTS**.) **HARDMATH** is the largest graduate-level dataset.

Dataset	Size	Data Generation	Difficulty
MATH (Hendrycks et al., 2021)	12.5K	Manual	High School
GSM8K (Cobbe et al., 2021)	8.5K	Manual	Grade School
MATHBENCH-T (Liu et al., 2024)	632	Manual, Algorithmic	Undergraduate
JEEBENCH (Arora et al., 2023)	236	Manual	High School
GHOSTS (Frieder et al., 2023)	190	Manual	Graduate
ARB (Sawada et al., 2023)	34	Manual	Graduate
HARDMATH (Ours)	1.4K	Algorithmic	Graduate

81 textbooks in functional analysis, topology, and probability theory [8]—and in **ARB**, which features
82 a small set of university-level formal mathematics problems from prior qualifying examinations in
83 the mathematics departments at Harvard University and the University of California, Berkeley [19].
84 However, these datasets have several limitations, such as their size and scalability; datasets created
85 by scraping textbooks or similar resources are generally quite small and difficult to expand easily.
86 Most of these challenging datasets also only focus on abstract, formal mathematics and exclude other
87 forms of mathematical reasoning. Finally, textbook problems are often protected by copyright, which
88 can complicate their public use.

89 Existing datasets (summarized in Table 1) thus lack the scale and specific focus needed to evalu-
90 ate LLMs on advanced mathematical problems that may be highly useful for scientific research.
91 **HARDMATH** aims to address these limitations by offering a large collection of challenging applied
92 mathematics problems inspired by a graduate-level course on asymptotic methods. It emphasizes
93 problems that require diverse mathematical approaches, numerical calculations, and subjective judg-
94 ment, mirroring the complexity of problems faced by researchers in a variety of domains. Code for
95 auto-generating the problems in **HARDMATH** can be used to generate any number of additional
96 problems, which is a unique and powerful feature for scaling LLM benchmarking and model develop-
97 ments like novel prompting techniques or fine-tuning. A key area of interest in current LLM research
98 is developing models that can effectively use external tools. The problems in our dataset are unique
99 because they involve approximate solutions that cannot be formalized using tools like Lean or similar
100 software. To excel in this benchmark, LLMs must integrate tool use with sophisticated reasoning.
101 This makes **HARDMATH** particularly valuable for benchmarking and advancing LLMs capable of
102 effective tool use, setting it apart from other mathematical datasets.

103 3 Datasets

104 3.1 **HARDMATH** design choices

105 Here, we detail the **HARDMATH** dataset, which contains problems on polynomial nondimension-
106 alization, polynomial root-finding, ODEs, integrals, and word problems that contextualize each of
107 these. **HARDMATH** contains four problem classes with seven distinct problem types, as well as
108 40 handwritten word problems contextualizing the problem types. The main **HARDMATH** dataset,
109 which can be used for fine-tuning, contains 1,060 problems, and the evaluation dataset **HARDMATH-**
110 **mini**, which we use in this paper to benchmark LLM performance, contains 366 problems. Figure 1
111 provides a detailed breakdown of these datasets.

112 One key commonality between all **HARDMATH** problems is the use of the *Method of Dominant*
113 *Balance* in calculating solutions. This reduces an equation to only the terms that ‘dominate’ the
114 behavior of the solution and can significantly simplify the equation [5]. In addition to the Method
115 of Dominant Balance, our problems also involve other sophisticated mathematical techniques, such

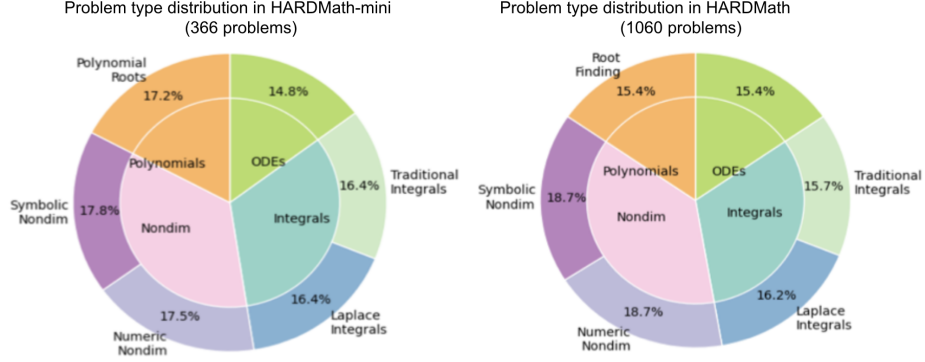


Figure 1: Breakdowns of the **HARDMath-mini** (left) and the **HARDMATH** (right) datasets.

as checks for self-consistency and the use of numerical methods. The combination of these tools captures several key aspects of mathematical modeling, including the combined use of computational and analytical techniques. Additionally, subjective choices about the regimes of solution space to consider, the number of terms to include in approximate expressions, and the approximation methods themselves must be made on a case-by-case basis with rigorous mathematical justification. Both of these aspects are potentially difficult tasks for existing LLMs.

3.2 Dataset generation and verification

The data generation code uses SymPy [13], a library for symbolic mathematics, and SciPy, a library for scientific computing [21], to implement the mathematical procedures required for obtaining approximate, analytical solutions. Problems are generated by combining randomly selected coefficients, functional forms, and initial conditions uniquely defined for each problem (described in Appendix A)—no duplicate problems are included. Solutions are generated by navigating through a set of possible cases during the algorithmic problem-solving strategy. Each mathematical step is embedded in explanatory text so **HARDMATH** solutions match the style and rigor of traditional problem set solutions. The main results for all problems are included in boxed environments in the solution explanations to distinguish them from the rest of the text. This follows the formatting convention used in other mathematics datasets designed for LLM benchmarking, such as the **MATH** dataset [10].

For each problem type, the dataset includes: 1) \LaTeX -formatted problem statements with prompts, 2) \LaTeX -formatted solution steps and final analytical answer(s), 3) Demonstration of the accuracy of the analytical results by comparing with numerical solutions, and 4) Metadata descriptors of the problem and solution types.

For every problem type, we select evaluation points in each solution regime and calculate the relative error between the analytical solution and the numerical solution at these points. Problems were included in **HARDMATH** only if their approximate solutions had less than 10% error from the numerically calculated ground-truths. For the polynomial root correction problems, we also confirm that the corrections improve the original approximation. Manually verifying solutions step-by-step is not feasible for a dataset of this size, but this verification procedure provides a high degree of confidence in the accuracy of the solutions in the dataset.

3.3 Problem types

3.3.1 Nondimensionalization of polynomials

Nondimensionalization is a technique to simplify equations by reducing the number of parameters [7]. In **HARDMATH**, the first type of polynomial used for nondimensionalization demonstration

149 contains symbolic coefficients and is of the form

$$a_1x^{n_1} + a_2x^{n_2} + a_3, \quad n_1 > n_2 > 0. \quad (1)$$

Nondimensionalization converts this to the form $\epsilon y^{n_1} + y^{n_2} + 1$. The second type contains numerical coefficients and are of the form

$$\pm a_1x^{n_1} \pm a_2x^{n_2} \pm a_3, \quad n_1 > n_2$$

150 which can be simplified to $\epsilon y^{n_1} \pm y^{n_2} \pm 1$ given a specific *numerical* value of ϵ .

151 For all problem types described in this section, we provide details about the parameters used to
152 generate problems and the mathematical techniques used to solve them in Appendix A.

153 3.3.2 Polynomial root-finding

154 Exact formulas exist for quadratic, cubic, and quartic equations, but deriving them for quintic or
155 higher-order polynomials is not possible [20]. **HARDMATH** includes approximate root-finding
156 examples for higher order polynomials of the form $\epsilon x^{n_1} \pm x^{n_2} \pm 1$ (example in Appendix A.1.2).
157 The goal is to solve for roots in terms of ϵ using the method of dominant balance for small and large
158 positive ϵ regimes.

159 3.3.3 Polynomial root correction terms

160 The use of two-term dominant balances—such as in the previous problem type—neglects terms
161 and introduces an error. We can calculate a correction term δ to reduce this error via the following:
162 suppose the true roots x^* of a polynomial are given by $x^*(\epsilon) = \bar{x}(\epsilon) + \delta$, where \bar{x} is our approximation
163 to the root and δ is the error term. Plugging the roots $x^*(\epsilon) = \bar{x}(\epsilon) + \delta$ into the polynomial allows
164 one to use a Taylor expansion of δ around \bar{x} and solve for the correction δ .

165 3.3.4 Nonlinear ordinary differential equations

166 We generate nonlinear third-order ODEs for which there do not exist exact analytical solutions and
167 provide approximate formulae for small and large x regimes, where the small x regime is near $x = 0$
168 and the large x regime typically involves the solution diverging (example in Appendix A.1.4). The
169 method is robust for higher-order problems, but for simplicity we include only third-order ODEs.

170 3.3.5 Traditional integrals

171 We consider integrals of the form $I(\epsilon) = \int_0^a \frac{1}{\epsilon + P(x)} dx$, where $P(x)$ is an arbitrary polynomial. The
172 dataset provides approximations of each integral in three regimes (small, intermediate, and large ϵ).

173 3.3.6 Laplace integrals

We consider integrals of the form $I(x) = \int_a^b g(t)e^{\pm x f(t)} dt$, which can be approximated using Laplace's Method when x is very large because the integral's value is dominated by the region around t_0 [5]. Depending on where the minimum is, the approximation is either

$$I(x) \approx g(t_0)e^{\pm x f(t_0)} \sqrt{\frac{2\pi}{x|f''(t_0)|}} \quad \text{or} \quad I(x) \approx \frac{g(t_0)e^{\pm x f(t_0)}}{x|f''(t_0)|}.$$

1. Sample Laplace Integral Problem and Final Analytical Solution

Problem: Consider the integral

$$I(x) = \int_{0.4}^{0.8} (-2.4t^2 - 2.8 \tan^{-1}(t)) e^{-x(1.4t^3 - 2.6 \cos(t) + 1.3 \tan^{-1}(t) + 0.4)} dt.$$

Develop an analytical formula for $I(x)$ that is accurate as x becomes large.

174

Final Analytical Solution:

$$I(x) \approx -\frac{0.517e^{1.411x}}{x}$$

3.4 Word problems in context

One motivation for creating **HARDMATH** is to help LLMs recognize and solve problems where approximation techniques are needed. To evaluate how LLMs perform on such problems in realistic scenarios, we develop a smaller dataset of 40 word problems, written manually (see example in Box 2). Although this dataset is smaller than our hand-verified evaluation set, it is large enough to evaluate the effect of additional context in the problem statement on LLM accuracy.

2. Sample Word Problem with Context

The density of fish at different points along a certain path in a lake can be modeled as $(\epsilon + x^2 + x^5)^{-1}$, where x represents the distance from the shore in kilometers (ranging from 0 to 100 km), and ϵ represents environmental factors that affect the fish density. To study the total presence of fish along the path, develop an approximate analytical formula for $I(\epsilon)$ given below:

$$I(\epsilon) = \int_0^{100} \frac{1}{\epsilon + x^2 + x^5} dx.$$

4 Evaluation

4.1 Evaluation protocols

We carry out LLMs evaluations on **HARDMath-mini**, a carefully selected test set of 366 problems that matches the composition statistics of **HARDMATH** (Fig. 1) to optimize computational resources. Despite its reduced size, this subset includes a sufficient number of questions to ensure consistent and reliable testing results, maintaining the integrity of our evaluation. We separately evaluate four problem types: 1) *Nondim* includes nondimensionalization in symbolic and numerical form; 2) *Roots* includes polynomial root-finding; 3) *ODEs* includes nonlinear ODEs; and 4) *Integrals* includes traditional and Laplace integrals. The input prompt contains the essential problem setup and a description of the question, supplemented with problem type-specific hints for answer formatting. Few-shot prompting adds a fixed set of paired problem-solution examples from the corresponding problem types. Example prompts can be found in Appendix A.2.1, Table 6.

Model-generated responses are evaluated and scored for accuracy using a protocol combining automatic assessment of final answers and procedural LLM-based grading. Automatic assessment follows Hendrycks et al. [10], prompting models to wrap the final answer with the LaTeX `\boxed{}` command (Table 6). Evaluation then compares the model’s output within `\boxed{}` command to **HARDMATH** solution. To handle different mathematical expression formats, we implement both SymPy-based [13] equivalence checks, as well as numerical evaluations.

In addition to the standard automatic assessment of final answers, we developed a novel procedural grading approach leveraging LLMs, tailored to the unique nature of our dataset. Our dataset presents two unique challenges compared to existing mathematics datasets: 1) Some problem types require complex, multi-step solution procedures where a single cut-off criterion at the final answer cannot capture the full spectrum of model performance. Thus, grading intermediate steps in the solving procedure are necessary for comprehensive assessment. 2) **HARDMATH** targets the model’s ability to make human-like abstraction and approximation judgments. Some problem types allow a narrow range of solutions rather than a single exact one, as long as the reasoning is self-consistent and the final result agrees with the numerical ground truth.

Inspired by LLMs’ ability to generate consistent ratings for response content and style [9], we use GPT-4o as a procedural grader, prompted with the ground truth answer key and clear grading rubrics adapted from the course’s grading guidelines for each problem type (example grading prompts in Appendix A.2.2 Table 4). We hand-verified a subset of grading responses and found that LLM-based grading is closely aligned with human grading used in the graduate course. Average score adjustment for each model and problem type is summarized in Appendix A.2.3 Table 5. We implemented this procedural grading alongside automatic final answer assessment for the problem types *Roots*, *ODEs*, and *Integrals*.

4.2 Model choice

We compare the performance of several closed- and open-source models with different prompting methods on **HARDMATH**: 1) Closed-source LLMs include GPT-3.5 [17, 18, 16] and GPT-4 [1] in zero- and few-shot settings with the Chain-of-Thought (CoT) [22] prompting, and 2) Open-source LLMs include Llama 3 [2] and CodeLlama [12] in zero- and few-shot settings with CoT prompting. We provide the prompts and hyper-parameters for LLMs evaluations in Appendix A.2.4 Table 6.

4.3 Quantitative results

We present the accuracy of the models and prompting settings for each problem type and the combined test set (Table 2, Figure 4). Few-shot CoT prompting significantly boosts performance for all models, with GPT-4 showing the greatest improvement, consistent with [22] (Figure 4a). We do observe that such performance increase upon prompting behavior shows problem type specific patterns: Figure 5 demonstrates that it saturates quickly for harder problem types like *ODEs*. The varying performance increases among different problem types may be due to different error modes in model answers, which we discuss in the following section. Among closed-source models, GPT-4 with 5-shot CoT prompting achieves the highest overall accuracy of 44.6%. Among open-source models, Llama3-8b with 5-shot CoT prompting achieves the highest overall accuracy of 19.9%. We discuss the performance of these representative models—GPT-4 and Llama3—on **HARDMath-mini** in comparison with established datasets, including **GSM-8K** [6], **MATH** [10], and more advanced mathematics datasets like **GHOSTS** [8].

Llama3-8b achieves a test accuracy of 30.0% on the **MATH** dataset with 4-shot CoT and 79.6% on the **GSM-8K** dataset with 8-shot CoT prompting [2]. Testing Llama3-8b on **HARDMath-mini** resulted in an overall accuracy of 19.9% with 5-shot CoT prompting. GPT-4 (gpt-4-turbo-2024-04-09) is reported to achieve 72.2% accuracy on the **MATH** dataset with 0-shot CoT prompting [15] and 92.0% on the **GSM-8K** dataset with 5-shot CoT prompting [1]. On a recently released dataset **MINIGHOSTS**, which measures the advanced mathematical abilities of LLMs, GPT-4 reaches an average score of 4.15 out of 5. We tested GPT-4 on our **HARDMath-mini** dataset and obtained an overall accuracy of 44.6% with 5-shot CoT prompting. Even with few-shot CoT prompting, the test accuracy of both models on all **HARDMATH** problem types is considerably lower than on existing benchmark mathematics datasets. This suggests that our problems are more challenging particularly in the domains of mathematical reasoning required by our dataset. Notably, GPT-4 also performs poorly on a subset of **MINIGHOSTS** taken from graduate mathematics textbooks, scoring only 3.5 out of 5. These results highlight the value of **HARDMATH** as a challenging benchmark for evaluating the mathematical capabilities of LLMs.

4.3.1 Extensions to word problems

We test the best-performing model, GPT-4, on a set of word problems that included a mixture of *Nondim*, *Roots*, *ODEs*, and *Integrals*. To assess the model’s ability to solve problems in relevant research contexts, we avoided additional prompt engineering and used only the questions as prompts, omitting the problem-specific hints listed in Table 3. This evaluation resulted in an overall accuracy of 28.1%.

Table 2: Evaluation Accuracy (percentage) on the **HARDMATH** evaluation set.

Model	ALL	Nondim	Roots	ODEs	Integrals
Closed-source models					
GPT-3.5 (0 shot)	7.30	5.05	17.2	12.9	3.33
GPT-3.5 (1 shot CoT)	13.8	6.11	29.3	14.8	18.2
GPT-3.5 (5 shot CoT)	25.0	24.3	35.0	20.4	23.1
GPT-4 (0 shot)	13.6	6.04	33.7	15.7	14.9
GPT-4 (1 shot CoT)	37.9	36.5	52.8	20.3	40.5
GPT-4 (5 shot CoT)	44.6	48.6	57.3	21.7	41.4
Open-source models					
Llama3-8b (0 shot)	3.90	0.50	11.5	10.7	2.52
Llama3-8b (5 shot CoT)	19.9	17.9	17.1	12.04	28.1
CodeLlama-13b (0 shot)	1.62	0.00	8.73	1.85	0.50
CodeLlama-13b (5 shot CoT)	9.56	8.41	13.1	9.7	9.57

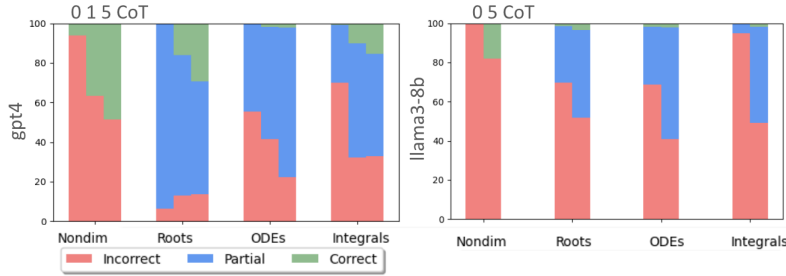


Figure 2: Percentage of correct, partial, and incorrect responses for GPT-4 and Llama3, prompting conditions, and problem types.

4.4 Fine-grained results

In addition to reporting the summarized test accuracy, we study the detailed breakdown of model responses at different correctness level and summarize specific error modes of LLMs solving these challenging applied mathematics questions. This analysis helps us compare the performance nuances and understands reasoning paths from axes of model, prompting technique and question type.

We first break down model performance by percentage of correct, partial and incorrect responses (Figure 2). This analysis reveals how few-shot prompting enhances model performance across varying problem types but through different strategy. Overall quantitative results already shows that *ODEs* and *Integrals* are comparatively harder for all models (Figure 4b). For these complex problems, full correctness is rare. Correctness level analysis shows that models tend to increase partial credit responses with CoT prompting, as they struggle to solve the problems entirely but manage to partially address them. In contrast, for simpler problems like *Roots*, advanced models like GPT-3.5 and GPT-4 get more fully correct responses with increasing CoT shot number (Fig. 6).

We second summarize the error modes of partial and incorrect responses to better understanding the model’s reasoning pitfalls. Particularly, we want to dissect how CoT changes model performance on the level of detailed errors. Figure 3 uses GPT-4’s responses at 0 vs. 5 shots on problem type *Roots* as an analysis example. It illustrates how 5-shot CoT prompting significantly alters the error structure compared to 0-shot. The most common error mode—incorrectly setting up dominant balance by considering only the leading term—diminishes substantially. Instead, errors shift to more nuanced issues: 1) setting up correct dominant balances but missing certain cases, or 2) failing to calculate complex roots (examples of those error modes included in Appendix A.3.2). This shift indicates that CoT prompting improves the model’s understanding and application of dominant balance techniques, enabling it to move beyond intuitive yet incorrect simplifications.

Above analysis demonstrates that our unique dataset provides rich insights into the strengths and weaknesses of LLM reasoning in mathematical contexts that demand approximation skills.

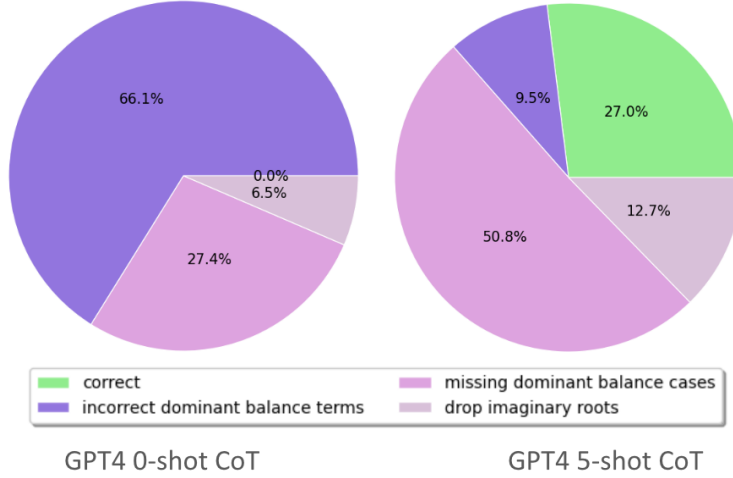


Figure 3: GPT-4 error modes for problem type *Roots* at 0 vs. 5 shot CoT prompting

3. Grading Response: *Roots*

Question: Consider the polynomial $P(x) = \epsilon x^8 + x^4 - 1$. Find approximate expressions for all roots of the polynomials in the limit of small positive ϵ and large positive ϵ . Only a single term approximation to the root is required.

Grading for Small Positive ϵ :

Model Response: For small $\epsilon : [1, -1, i, -i]$

Ground Truth:

$$\text{For small positive } \epsilon : \left[-\sqrt[4]{-\frac{1}{\epsilon}}, \sqrt[4]{-\frac{1}{\epsilon}}, -i\sqrt[4]{-\frac{1}{\epsilon}}, i\sqrt[4]{-\frac{1}{\epsilon}}, -1, 1, -i, i \right]$$

The response only includes the roots from the balance $B + C = 0$ and completely misses the roots from the balance $A + B = 0$. Therefore, score for small positive ϵ is 0.5

5 Conclusion

We introduce **HARDMATH**, a new dataset that covers several problem types from an advanced applied mathematics course that can be used to benchmark LLMs mathematical capabilities and perform model developments including fine-tuning. This dataset consists of 1060 examples and we include additionally 366 verified examples in **HARDMath-mini** and 40 verified ‘problems in context’ that we evaluate various leading LLMs on. **HARDMATH** is unique in several ways. First, there do not exist large-scale mathematical datasets covering problems of similar difficulty from applied mathematics. Second, the dataset’s problems and solutions are algorithmically generated, meaning that one could produce datasets of arbitrary size using our framework. This feature of **HARDMATH** is especially unique, since most existing mathematical datasets require manual problem-setting or curation from other sources (many of which are not publicly accessible).

Our evaluation results use **HARDMATH-MINI** as a comprehensive test set, but future work will fine-tune LLMs on our train set. If a fine-tuned LLM could achieve mastery on **HARDMATH**, it could replace or aid human teaching assistants. This type of “LLM-assistant” could help students determine which approximation methods to use, how to apply them, and even grade homework using our procedural evaluation framework. The course also covered several other topics that are not included in this initial dataset, such as boundary value problems and PDEs, which can also be algorithmically generated following our framework.

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Checklist

1. For all authors...
 - (a) Do the main claims made in the abstract and introduction accurately reflect the paper’s contributions and scope? [Yes] See Section 1.
 - (b) Did you describe the limitations of your work? [Yes] See Section 3 and Section 5
 - (c) Did you discuss any potential negative societal impacts of your work? [N/A] We discuss potential societal impacts but do not consider them to be negative.
 - (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
 - (a) Did you state the full set of assumptions of all theoretical results? [N/A]
 - (b) Did you include complete proofs of all theoretical results? [N/A]
3. If you ran experiments (e.g. for benchmarks)...

- 393 (a) Did you include the code, data, and instructions needed to reproduce the main experi-
 394 mental results (either in the supplemental material or as a URL)? [Yes] The data, code
 395 used for data generation, evaluation, and corresponding documentation are available at
 396 at this GitHub repository, which is also linked in the paper text.
- 397 (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they
 398 were chosen)? [Yes] See Appendix and GitHub repository for all code generation
 399 details.
- 400 (c) Did you report error bars (e.g., with respect to the random seed after running experi-
 401 ments multiple times)? [N/A]
- 402 (d) Did you include the total amount of compute and the type of resources used (e.g., type
 403 of GPUs, internal cluster, or cloud provider)? [Yes] See Section A.2.5
- 404 4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
- 405 (a) If your work uses existing assets, did you cite the creators? [Yes] Section 3 cites
 406 relevant code assets and Section 4.2 cites LLMs used.
- 407 (b) Did you mention the license of the assets? [Yes] Llama3 and CodeLlama models
 408 and weights are released under the Meta AI license and used for both researchers and
 409 commercial entities. For detailed licensing information, refer to <https://github.com/meta-llama>.
- 410 (c) Did you include any new assets either in the supplemental material or as a URL? [Yes]
 411 The dataset and codebase are available on GitHub. They are also described in the
 412 Supplementary Material.
- 413 (d) Did you discuss whether and how consent was obtained from people whose data you're
 414 using/curating? [N/A]
- 415 (e) Did you discuss whether the data you are using/curating contains personally identifiable
 416 information or offensive content? [N/A]
- 417 5. If you used crowdsourcing or conducted research with human subjects...
- 418 (a) Did you include the full text of instructions given to participants and screenshots, if
 419 applicable? [N/A]
- 420 (b) Did you describe any potential participant risks, with links to Institutional Review
 421 Board (IRB) approvals, if applicable? [N/A]
- 422 (c) Did you include the estimated hourly wage paid to participants and the total amount
 423 spent on participant compensation? [N/A]
- 424

425 A Appendix

426 A.1 Implementation and method details for data generation

427 The following subsections detail the process used to generate the problems and solutions for each
 428 problem type.

429 A.1.1 Nondimensionalization of polynomials

430 The first nondimensionalization sub-type is generalized by varying the integer values for the degrees
 431 n_1 and n_2 within the range $0 < n_2 < n_1 < 10$, while keeping $a_1, a_2, a_3 > 0$ symbolic. Solutions to
 432 these problems express the dimensionless parameter ϵ in terms of these three coefficients.

Sample Symbolic Nondimensionalization Problem and Full Solution

Problem: Nondimensionalize the polynomial

$$a_1 x^{10} + a_2 x^9 + a_3$$

into one of the form $\epsilon y^{10} + y^9 + 1$. Express ϵ as a function of a_1, a_2 , and a_3 .

433

Solution: We begin with the substitution

$$x = y \sqrt[9]{\frac{a_3}{a_2}}$$

This gives the expression

$$a_1 y^{10} \left(\frac{a_3}{a_2} \right)^{\frac{10}{9}} + a_3 y^9 + a_3$$

Divide by the coefficient remaining in front of the constant, leaving us with the nondimensionalized polynomial with coefficients in terms of a_1 , a_2 , and a_3 :

$$\frac{a_1 y^{10} \left(\frac{a_3}{a_2} \right)^{\frac{10}{9}}}{a_3} + y^9 + 1.$$

By inspection, we can see that

$$\epsilon = \frac{a_1 \left(\frac{a_3}{a_2} \right)^{\frac{10}{9}}}{a_3}.$$

434

435 The second subtype implements integer numerical values for the coefficients a_1 , a_2 , a_3 that are are
436 randomly chosen from $[-10, 10]$.

Sample Numeric Nondimensionalization Problem and Full Solution

Problem: Nondimensionalize the polynomial

$$P(x) = 2x^7 + 8x^2 + 5$$

into a polynomial of the form $\epsilon y^7 \pm y^2 \pm 1$. Solve for ϵ .

Solution: For now, we ignore the numeric values of the coefficients and instead call them a_1 , a_2 , a_3 . Our polynomial is then:

$$a_1 x^7 + a_2 x^2 + a_3.$$

Use the substitution

$$x = y \sqrt[7]{\frac{a_3}{a_2}},$$

which gives the expression

$$a_1 y^7 \left(\frac{a_3}{a_2} \right)^{\frac{7}{7}} + a_3 y^2 + a_3.$$

Divide all terms by the coefficient remaining in front of the constant term, giving us the nondimensionalized polynomial with coefficients in terms of a_1 , a_2 , a_3 :

$$\frac{a_1 y^7 \left(\frac{a_3}{a_2} \right)^{\frac{7}{7}}}{a_3} + y^2 + 1$$

Substituting in the known numeric values for a_1 , a_2 , a_3 (using their absolute values as we have already accounted for sign), we get:

$$\frac{25\sqrt{10}y^7}{1024} + y^2 + 1$$

From inspection of this nondimensionalized equation, we can now identify ϵ :

$$\epsilon = \frac{25\sqrt{10}}{1024} \Rightarrow \boxed{\epsilon \approx 0.08.}$$

437

438 **A.1.2 Polynomial root-finding**

439 As with the nondimensionalization problems, degrees in the polynomial are randomly generated with
 440 maximum order ten and $0 < n_2 < n_1$. See a full problem and solution below.

Sample Polynomial Root-finding Problem and Full Solution

Problem: Consider the polynomial

$$P(x) = \epsilon x^6 - x^5 + 1.$$

Find first order approximations for all roots of the polynomials in the limit of small positive ϵ and large positive ϵ .

Solution: We begin by equating the polynomial to zero to solve for the roots: $P(x) = 0$. This problem can be rewritten in the form $A + B + C = 0$, where: $A = \epsilon x^6$; $B = -x^5$; $C = 1$.

This problem has no analytical solutions, so we find approximate solutions to the roots by considering the three possible dominant balances. For each dominant balance, we find the roots of the resulting equation and evaluate whether each balance is self-consistent for small or large positive ϵ .

We start with the balance $A + B = 0$, assuming that $|C|$ is negligible when compared to $|A|$ and $|B|$. Solving this for x in terms of ϵ then gives us 1 non-zero root:

$$\begin{aligned} \epsilon x^6 - x^5 &= 0 \\ \Rightarrow x &= \left[\frac{1}{\epsilon} \right]. \end{aligned}$$

To verify that these roots are consistent with the assumption that $|A|, |B| \gg |C|$, we substitute these found roots back into the terms A , B , and C and compare their magnitudes. Using this method, we find that it is true that these roots are valid for small ϵ , while validity for large ϵ is false.

Therefore, these roots are valid in the limit of small positive ϵ only.

Next we examine the balance $B + C = 0$, assuming that $|A|$ is negligible when compared to $|B|$ and $|C|$. Solving this for x in terms of ϵ gives us 5 non-zero roots:

$$\begin{aligned} 1 - x^5 &= 0 \\ \Rightarrow x &= 1, -\frac{1}{4} + \frac{\sqrt{5}}{4} - \frac{i\sqrt{2\sqrt{5}+10}}{4}, -\frac{1}{4} + \frac{\sqrt{5}}{4} + \frac{\sqrt{-10-2\sqrt{5}}}{4}, \\ &\quad -\frac{\sqrt{5}}{4} - \frac{1}{4} - \frac{i\sqrt{10-2\sqrt{5}}}{4}, -\frac{\sqrt{5}}{4} - \frac{1}{4} + \frac{i\sqrt{10-2\sqrt{5}}}{4}. \end{aligned}$$

To verify that these roots are consistent with the assumption that $|B|, |C| \gg |A|$, we substitute these found roots back into A , B , and C and compare their magnitudes. Using this method, we find that it is true that these roots are valid for small ϵ , while validity for large ϵ is false.

Therefore, these roots are valid in the limit of small positive ϵ only.

Finally, we examine the balance $A + C = 0$, assuming that $|B|$ is negligible when compared to $|A|$ and $|C|$. Solving this for x in terms of ϵ gives us 6 non-zero roots:

$$\begin{aligned} \epsilon x^6 + 1 &= 0 \\ \Rightarrow x &= \left[-\sqrt[6]{-\frac{1}{\epsilon}}, \sqrt[6]{-\frac{1}{\epsilon}}, \frac{\sqrt[6]{-\frac{1}{\epsilon}}(-1-\sqrt{3}i)}{2}, \right. \\ &\quad \left. \frac{\sqrt[6]{-\frac{1}{\epsilon}}(-1+\sqrt{3}i)}{2}, \frac{\sqrt[6]{-\frac{1}{\epsilon}}(1-\sqrt{3}i)}{2}, \frac{\sqrt[6]{-\frac{1}{\epsilon}}(1+\sqrt{3}i)}{2} \right]. \end{aligned}$$

To verify that these roots are consistent with the assumption that $|A|, |C| \gg |B|$, we substitute these found roots back into A , B , and C and compare their magnitudes. Using this method, we find that it is false that these roots are valid for small ϵ , while validity for large ϵ is true. Therefore, these roots are valid in the limit of large positive ϵ only.

By the Fundamental Theorem of Algebra, a polynomial of degree 6.0 has exactly 6.0 roots. We have found 6.0 roots that are valid in the limit of small positive ϵ and 6.0 roots valid in the limit of large positive ϵ . Our method therefore provides a complete solution to the problem, finding the correct number of roots in each ϵ regime.

The roots of $P(x)$ for large positive ϵ are

$$\begin{aligned} & -\sqrt[6]{-\frac{1}{\epsilon}}, \sqrt[6]{-\frac{1}{\epsilon}}, \frac{\sqrt[6]{-\frac{1}{\epsilon}}(-1 - \sqrt{3}i)}{2}, \\ & \frac{\sqrt[6]{-\frac{1}{\epsilon}}(-1 + \sqrt{3}i)}{2}, \frac{\sqrt[6]{-\frac{1}{\epsilon}}(1 - \sqrt{3}i)}{2}, \frac{\sqrt[6]{-\frac{1}{\epsilon}}(1 + \sqrt{3}i)}{2} \end{aligned}$$

and the roots of $P(x)$ for small positive ϵ are

$$\begin{aligned} & \frac{1}{\epsilon}, 1, -\frac{1}{4} + \frac{\sqrt{5}}{4} - \frac{i\sqrt{2\sqrt{5}+10}}{4}, -\frac{1}{4} + \frac{\sqrt{5}}{4} + \frac{\sqrt{-10-2\sqrt{5}}}{4}, \\ & -\frac{\sqrt{5}}{4} - \frac{1}{4} - \frac{i\sqrt{10-2\sqrt{5}}}{4}, -\frac{\sqrt{5}}{4} - \frac{1}{4} + \frac{i\sqrt{10-2\sqrt{5}}}{4} \end{aligned}$$

442

443 A.1.3 Polynomial root correction terms

444 The true roots x^* of a polynomial are given by $x^*(\epsilon) = \bar{x}(\epsilon) + \delta$, where \bar{x} is our existing approximation
445 to the root as found in Appendix A.3 and δ is the error term. This requires us to solve

$$\epsilon(\bar{x} + \delta)^{n_1} \pm (\bar{x} + \delta)^{n_2} \pm 1 = 0$$

446 for δ by equating coefficients of ϵ terms of the same order, as detailed in the worked solution below.

Sample Numeric Nondimensionalization Problem and Full Solution

Problem: Consider the polynomial

$$P(x) = \epsilon x^3 - x + 1.$$

Find approximate expressions for all roots of the polynomial in the limit of small positive ϵ and large positive ϵ . Use a series expansion to calculate improved formulae for these roots to order 1 i.e. calculate $\mathcal{O}(1)$ corrections for each root.

Solution: Note: The root calculation in this problem follow the same method as those demonstrated in the A.3, so they has been omitted here. We include only correction term calculations for the sake of brevity.

We now need to calculate correction terms for these roots to give us better approximations. We consider the ansatz that the root is given by $\bar{x} + \delta$, where the correction term δ is the sum of higher order terms of ϵ that we initially neglected in our approximation \bar{x} . By definition, $\delta < \bar{x}$. We plug this ansatz into the polynomial and perform a series expansion in δ . We keep terms only up to $\mathcal{O}(1)$ in δ . Then, we set the expression equal to 0 and solve for δ .

Regime 1: valid for small ϵ

447

Root 1: $-\sqrt{\frac{1}{\epsilon}}$

$$\bar{x} + \delta = -\sqrt{\frac{1}{\epsilon}} + \delta$$

Substitute this into $P(x)$ for x and equate to 0:

$$-\delta + \epsilon \left(\delta - \sqrt{\frac{1}{\epsilon}} \right)^3 + \sqrt{\frac{1}{\epsilon}} + 1 = 0.$$

We then expand this expression to get

$$\delta^3 \epsilon - 3\delta^2 \epsilon \sqrt{\frac{1}{\epsilon}} + 2\delta - \epsilon \left(\frac{1}{\epsilon} \right)^{\frac{3}{2}} + \sqrt{\frac{1}{\epsilon}} + 1 = 0$$

and represent it as a series of $\mathcal{O}(1)$ in δ , discarding higher order δ terms

$$2\delta - \epsilon \left(\frac{1}{\epsilon} \right)^{\frac{3}{2}} + \sqrt{\frac{1}{\epsilon}} + 1 \approx 0.$$

We can then solve the expression for the correction δ to $\mathcal{O}(1)$, and get

$$\delta \approx \frac{\epsilon \left(\frac{1}{\epsilon} \right)^{\frac{3}{2}}}{2} - \frac{\sqrt{\frac{1}{\epsilon}}}{2} - \frac{1}{2}.$$

Root 2: $\sqrt{\frac{1}{\epsilon}}$

$$\bar{x} + \delta = \sqrt{\frac{1}{\epsilon}} + \delta$$

Substitute this into $P(x)$ for x and equate to 0:

$$-\delta + \epsilon \left(\delta + \sqrt{\frac{1}{\epsilon}} \right)^3 - \sqrt{\frac{1}{\epsilon}} + 1 = 0.$$

We then expand this expression to get

$$\delta^3 \epsilon + 3\delta^2 \epsilon \sqrt{\frac{1}{\epsilon}} + 2\delta + \epsilon \left(\frac{1}{\epsilon} \right)^{\frac{3}{2}} - \sqrt{\frac{1}{\epsilon}} + 1 = 0$$

and represent it as a series of $\mathcal{O}(1)$ in δ , discarding higher order δ terms

$$2\delta + \epsilon \left(\frac{1}{\epsilon} \right)^{\frac{3}{2}} - \sqrt{\frac{1}{\epsilon}} + 1 \approx 0.$$

We can then solve the expression for the correction δ to $\mathcal{O}(1)$, and get

$$\delta \approx -\frac{\epsilon \left(\frac{1}{\epsilon} \right)^{\frac{3}{2}}}{2} + \frac{\sqrt{\frac{1}{\epsilon}}}{2} - \frac{1}{2}.$$

Regime 2: valid for small ϵ

Root 1: 1

$$\bar{x} + \delta = 1 + \delta$$

Substitute this into $P(x)$ for x and equate to 0:

$$-\delta + \epsilon (\delta + 1)^3 = 0.$$

We then expand this expression to get

$$\delta^3 \epsilon + 3\delta^2 \epsilon + 3\delta \epsilon - \delta + \epsilon = 0$$

and represent it as a series of $\mathcal{O}(1)$ in δ , discarding higher order δ terms

$$\delta(3\epsilon - 1) + \epsilon \approx 0.$$

We can then solve the expression for the correction δ to $\mathcal{O}(1)$, and get

$$\delta \approx -\frac{\epsilon}{3\epsilon - 1}.$$

Regime 3: valid for large ϵ

Root 1: $\sqrt[3]{-\frac{1}{\epsilon}}$

$$\bar{x} + \delta = \sqrt[3]{-\frac{1}{\epsilon}} + \delta$$

Substitute this into $P(x)$ for x and equate to 0:

$$-\delta + \epsilon \left(\delta + \sqrt[3]{-\frac{1}{\epsilon}} \right)^3 - \sqrt[3]{-\frac{1}{\epsilon}} + 1 = 0.$$

We then expand this expression to get

$$\delta^3\epsilon + 3\delta^2\epsilon\sqrt[3]{-\frac{1}{\epsilon}} + 3\delta\epsilon\left(-\frac{1}{\epsilon}\right)^{\frac{2}{3}} - \delta - \sqrt[3]{-\frac{1}{\epsilon}} = 0$$

and represent it as a series of $\mathcal{O}(1)$ in δ , discarding higher order δ terms

$$\delta \left(3\epsilon \left(-\frac{1}{\epsilon} \right)^{\frac{2}{3}} - 1 \right) - \sqrt[3]{-\frac{1}{\epsilon}} \approx 0.$$

We can then solve the expression for the correction δ to $\mathcal{O}(1)$, and get

$$\delta \approx \frac{\sqrt[3]{-\frac{1}{\epsilon}}}{3\epsilon \left(-\frac{1}{\epsilon} \right)^{\frac{2}{3}} - 1}.$$

Root 2: $\frac{\sqrt[3]{-\frac{1}{\epsilon}}(-1-\sqrt{3}i)}{2}$

$$\bar{x} + \delta = \frac{\sqrt[3]{-\frac{1}{\epsilon}}(-1-\sqrt{3}i)}{2} + \delta$$

Substitute this into $P(x)$ for x and equate to 0:

$$-\delta + \epsilon \left(\delta + \frac{\sqrt[3]{-\frac{1}{\epsilon}}(-1-\sqrt{3}i)}{2} \right)^3 - \frac{\sqrt[3]{-\frac{1}{\epsilon}}(-1-\sqrt{3}i)}{2} + 1 = 0.$$

We then expand this expression to get

$$\begin{aligned} \delta^3\epsilon - \frac{3\delta^2\epsilon\sqrt[3]{-\frac{1}{\epsilon}}}{2} - \frac{3\sqrt{3}i\delta^2\epsilon\sqrt[3]{-\frac{1}{\epsilon}}}{2} - \frac{3\delta\epsilon\left(-\frac{1}{\epsilon}\right)^{\frac{2}{3}}}{2} \\ + \frac{3\sqrt{3}i\delta\epsilon\left(-\frac{1}{\epsilon}\right)^{\frac{2}{3}}}{2} - \delta + \frac{\sqrt[3]{-\frac{1}{\epsilon}}}{2} + \frac{\sqrt{3}i\sqrt[3]{-\frac{1}{\epsilon}}}{2} = 0 \end{aligned}$$

and represent it as a series of $\mathcal{O}(1)$ in δ , discarding higher order δ terms

$$\delta \left(-\frac{3\epsilon\left(-\frac{1}{\epsilon}\right)^{\frac{2}{3}}}{2} + \frac{3\sqrt{3}i\epsilon\left(-\frac{1}{\epsilon}\right)^{\frac{2}{3}}}{2} - 1 \right) + \frac{\sqrt[3]{-\frac{1}{\epsilon}}}{2} + \frac{\sqrt{3}i\sqrt[3]{-\frac{1}{\epsilon}}}{2} \approx 0.$$

We can then solve the expression for the correction δ to $\mathcal{O}(1)$, and get

$$\delta \approx \frac{\sqrt[3]{-\frac{1}{\epsilon}}(1 + \sqrt{3}i)}{3\epsilon\left(-\frac{1}{\epsilon}\right)^{\frac{2}{3}} - 3\sqrt{3}i\epsilon\left(-\frac{1}{\epsilon}\right)^{\frac{2}{3}} + 2}.$$

Root 3: $\frac{\sqrt[3]{-\frac{1}{\epsilon}}(-1 + \sqrt{3}i)}{2}$

$$\bar{x} + \delta = \frac{\sqrt[3]{-\frac{1}{\epsilon}}(-1 + \sqrt{3}i)}{2} + \delta$$

Substitute this into $P(x)$ for x and equate to 0:

$$-\delta + \epsilon \left(\delta + \frac{\sqrt[3]{-\frac{1}{\epsilon}}(-1 + \sqrt{3}i)}{2} \right)^3 - \frac{\sqrt[3]{-\frac{1}{\epsilon}}(-1 + \sqrt{3}i)}{2} + 1 = 0.$$

We then expand this expression to get

$$\begin{aligned} \delta^3 \epsilon - \frac{3\delta^2 \epsilon \sqrt[3]{-\frac{1}{\epsilon}}}{2} + \frac{3\sqrt{3}i\delta^2 \epsilon \sqrt[3]{-\frac{1}{\epsilon}}}{2} - \frac{3\delta \epsilon \left(-\frac{1}{\epsilon}\right)^{\frac{2}{3}}}{2} \\ - \frac{3\sqrt{3}i\delta \epsilon \left(-\frac{1}{\epsilon}\right)^{\frac{2}{3}}}{2} - \delta + \frac{\sqrt[3]{-\frac{1}{\epsilon}}}{2} - \frac{\sqrt{3}i \sqrt[3]{-\frac{1}{\epsilon}}}{2} = 0 \end{aligned}$$

and represent it as a series of $\mathcal{O}(1)$ in δ , discarding higher order δ terms

$$\delta \left(-\frac{3\epsilon \left(-\frac{1}{\epsilon}\right)^{\frac{2}{3}}}{2} - \frac{3\sqrt{3}i\epsilon \left(-\frac{1}{\epsilon}\right)^{\frac{2}{3}}}{2} - 1 \right) + \frac{\sqrt[3]{-\frac{1}{\epsilon}}}{2} - \frac{\sqrt{3}i \sqrt[3]{-\frac{1}{\epsilon}}}{2} \approx 0.$$

We can then solve the expression for the correction δ to $\mathcal{O}(1)$, and get

$$\delta \approx \frac{\sqrt[3]{-\frac{1}{\epsilon}}(1 - \sqrt{3}i)}{3\epsilon\left(-\frac{1}{\epsilon}\right)^{\frac{2}{3}} + 3\sqrt{3}i\epsilon\left(-\frac{1}{\epsilon}\right)^{\frac{2}{3}} + 2}.$$

450

451 A.1.4 ODEs

We generate third-order ordinary differential equations of the form

$$y''' = f_1(x)(y'')^a + f_2(x)(y')^b + f_3(x)y^c + f_4(x),$$

452 where $f_1(x), f_2(x), f_3(x), f_4(x)$ are rational functions with integer coefficients. The initial condi-
453 tions are randomly selected integers from $[0, 3]$. The dataset excludes problems with a function of x
454 as a dominant term because of the difficulty of deriving power law expressions in these cases.

Approximate solutions at small x can be derived using a Taylor series expansion (up to the third order) around $x = 0$. Solving ODEs in the large x regime involves determining the two largest terms, assuming a divergence at some large x^* , and solving the dominant balance between these terms to create a power law approximation of the form

$$y(x) = A(x^* - x)^P.$$

ODE Problem and Solution

Problem: Consider the following third-order ordinary differential equation:

$$y''' = -\frac{y}{24x^4 + 6x^2 + 3} + y'^2 - \frac{y''}{5x^3 - 2x^2 - x + 2} - \frac{1}{12x^2 - \cos(x) + 11}$$

with initial conditions at $x = 0$:

$$y(0) = 1.00$$

$$y'(0) = 0.00$$

$$y''(0) = 0.00$$

Find analytical expressions that approximate the solution of $y(x)$ at small and large x .

Solution:

The dominant balance in the large x regime is given by

$$\frac{d^3}{dx^3}y = \left(\frac{d}{dx}y\right)^2.$$

We recognize that the solution of this ODE will diverge at finite x and that divergences typically follow a power law of the form

$$y = \alpha(x - x^*)^p,$$

where x^* is the divergence point. The divergence point can be determined by estimated by examining the numerical solution generated by code.

Plugging in the dominant terms we found previously yields the following equation:

$$\alpha p(p-2)(p-1)(x-11.45)^{p-3} = \alpha^2 p^2 (x-11.45)^{2p-2}.$$

After substituting the derivatives, the equation is reorganized to collect terms with respect to $(x - x^*)$. This leads to an equation where the coefficients and powers of $(x - x^*)$ are equated on both sides. Simplifying the equation gives us two separate equations, one for the coefficients and another for the powers of $(x - x^*)$. There is now a system of equations, where the coefficients' equation is

$$\alpha p(p-2)(p-1) = \alpha^2 p^2$$

and the powers' equation is:

$$p-3 = 2p-2.$$

Solving this system of equations provides the values of α and p . A valid solution is identified if α and p are both nonzero. Here, the solution for α and p is found to be:

$$\alpha = -6, \quad p = -1$$

With these values, the analytical approximation for the solution at large x (near the divergence point) is given by

$$y = -6(x - 11.45)^{-1}.$$

The approximate solution at small x can also be solved used dominant balance, but one can take advantage of the initial conditions and form a Taylor series instead around $x = 0$, which is given by

$$y(x) \approx y(0) + y'(0)x + \frac{y''(0)}{2!}x^2 + \frac{y'''(0)}{3!}x^3.$$

Plugging in the initial conditions, we get the following expression at small x :

$$y(x) = 1 - \frac{13}{180}x^3$$

Thus, with rounding for clarity, the solution is given by

$$y(x) = 1 - \frac{13}{180}x^3, \quad y = -6(x - 11.45)^{-1}.$$

456 A.1.5 Integrals

457 The polynomial $P(x)$ is randomly generated to consist of up to ten terms, where each term is a power
 458 function of x with an integer power randomly sampled from 1 and 20 and an integer coefficient
 459 sampled from 1 to 10. The integration bound $a \in [0, 100]$ is also randomly selected. This form
 460 ensures that the integral does not oscillate.

The height is approximated as the maximum value of the integrand, which is $\frac{1}{\epsilon}$, and the width can be estimated as the distance over which the integrand decreases from its maximum value by a factor of 2, which implies that the width x obeys the equation

$$\frac{1}{\epsilon + P(x)} = \frac{1}{2\epsilon} \Rightarrow P(x) = \epsilon.$$

461 In the regime of small ϵ , the term with the smallest degree and ϵ are the dominant terms, and in the
 462 regime of intermediate ϵ , the term with the largest degree and ϵ are dominant. There exists one more
 463 solution regime when the width of the integral exceeds the limits of integration, or when ϵ is "very
 464 large." In this case, the integral is approximated by L/ϵ , where L is the integration range.

Sample Integral Problem and Full Solution

Problem:

Consider the integral $I(\epsilon) = \int_0^{56.00} \frac{1}{\epsilon + 2.0x^{6.0} + 2.0x^{9.0} + 5.0x^{11.0} + 5.0x^{13.0}} dx$. Develop analytical formulas that approximate $I(\epsilon)$ for different regimes of ϵ .

Solution: The integral is of the form $I(\epsilon) = \int_0^{56} \frac{1}{\epsilon + P(x)} dx$ where $P(x)$ is a polynomial. Thus, its value can be estimated as the product between a height and a width.

Since the integrand is maximized at $x = 0$, the height can be set to $\frac{1}{\epsilon}$.

For small ϵ , we define the width as the point where the integrand becomes half of its maximum height. This corresponds to solving for x given $P(x) = \epsilon$. Applying dominant balance, considering the term in $P(x)$ with the smallest degree, the width is approximated as $\left(\frac{1}{2.0*\epsilon}\right)^{1/6.0}$. Therefore, the analytical approximation of the integral for small ϵ is $I(\epsilon) = \frac{0.8909}{\epsilon^{0.8333}}$.

For an intermediate regime where ϵ is large, we also define the width based on the term with the largest degree. The width is approximated as $\left(\frac{1}{5.0*\epsilon}\right)^{1/13.0}$. Therefore, the analytical approximation of the integral for large ϵ is $I(\epsilon) = \frac{0.7647}{\epsilon^{0.8333}}$.

If the width of the integral exceeds the range of integration, we consider one more regime for very large ϵ . The width is then just the range of integration, so in this regime, the integral can be approximated as $\frac{L}{\epsilon}$. Therefore, the analytical approximation of the integral for very large ϵ is $I(\epsilon) = \frac{56}{\epsilon}$.

Altogether, the solutions at small, large, and very large ϵ are $\frac{0.89}{\epsilon^{0.83}}, \frac{0.76}{\epsilon^{0.83}}, \frac{56}{\epsilon}$.

465

466 A.1.6 Laplace integrals

467 Laplace integrals of the form $I(x) = \int_a^b g(t)e^{\pm x f(t)} dt$ assume that $f(t) > 0$, is never a constant, and
 468 has an absolute minimum at a point t_0 either in the interior of or on the bounds of the interval $[a, b]$.

469 The set of possible Laplace integrals $I(x)$ in our dataset are parameterized by four parameters:
 470 the bounds $[a, b]$, $g(t)$, $f(t)$, and the sign in front of x . To generate the dataset, the bounds for
 471 each problem were randomly sampled from the $[-1, -0.9, \dots, 0.9, 1]$, and the sign was uniformly
 472 sampled from $\{-1, 1\}$. The functions $f(t)$ and $g(t)$ were generated by randomly selecting a linear
 473 combination of polynomials up to fifth order and basic trigonometric functions.

474 Our solution uses SymPy under the hood to find the minima of $f(t)$ (or the dual annealing algorithm
 475 if SymPy fails to return the minima).

Problem: Consider the integral

$$I(x) = \int_{-0.9}^{0.3} (-1.6t^2 - 0.5 \sin(t) - 1.9)e^{+x(-2.5t^4 - 0.8t^3 + 1.4t^2)} dt \quad (2)$$

Develop an analytical formula for $I(x)$ that is accurate as $x \rightarrow \infty$.

Solution:

The integral is of the form

$$I(x) = \int_a^b g(t)e^{+xf(t)} dt \quad (3)$$

where $a = -0.9$, $b = 0.3$, $g(t) = -1.6t^2 - 0.5 \sin(t) - 1.9$, and $f(t) = -2.5t^4 - 0.8t^3 + 1.4t^2$. This means we can use Laplace's method to develop an analytical approximation in the limit that $x \rightarrow \infty$. In this limit, the integral will be dominated by the integrand near the maximum of $f(t)$ within the bounds $[-0.9, 0.3]$. So, to simplify the integral, we will expand the integrand around this maximum. In this case, we can find the maximum of $f(t) = -2.5t^4 - 0.8t^3 + 1.4t^2$ on the interval analytically. We begin by looking for critical point(s) t_{crit} of $f(t)$ by solving $f'(t) = -10.0t^3 - 2.4t^2 + 2.8t = 0$ for t . This gives us that $t_{crit} = [-0.66, 0]$. To find the maximum on this interval, we evaluate $f(t)$ at the critical point(s) t_{crit} and the bounds -0.9 and 0.3 . We take the t that gives the largest value. Here, this maximum $t_0 = [-0.66]$. Since the integral is dominated by the value of the integrand near -0.66 , we Taylor expand the integrand around this point.

$$I(x) = \int_a^b (g(-0.66) + (t + 0.66)g'(-0.66) + \dots) \\ * e^{+x(f(-0.66) + (t+0.66)f'(-0.66) + \frac{(t+0.66)^2}{2}f''(-0.66) + \dots)} dt \quad (4)$$

But $f'(-0.66) = 0$ by definition, so we can remove this term from the exponent. We can then approximate

$$I(x) \approx \int_a^b g(-0.66)e^{+x(f(-0.66) + \frac{(t+0.66)^2}{2}f''(-0.66))} dt, \quad (5)$$

which equals

$$g(-0.66)e^{+xf(-0.66)} \int_a^b e^{+x(\frac{(t+0.66)^2}{2}f''(-0.66))} dt \quad (6)$$

We perform the change of variables $u = \sqrt{x \frac{|f''(-0.66)|}{2}}(t + 0.66)$, rewriting the integral as

$$g(-0.66)e^{+xf(-0.66)} \int_{\sqrt{x \frac{|f''(-0.66)|}{2}}(a+0.66)}^{\sqrt{x \frac{|f''(-0.66)|}{2}}(b+0.66)} \sqrt{\frac{2}{x|f''(-0.66)|}} e^{-u^2} du \quad (7)$$

Since $x \rightarrow \infty$, we approximate this as

$$g(-0.66)e^{+xf(-0.66)} \sqrt{\frac{2}{x|f''(-0.66)|}} \int_{-\infty}^{\infty} e^{-u^2} du \quad (8)$$

Solving the integral and evaluating, we find that

$$I(x) \approx -1.21 \sqrt{\frac{\pi}{x}} e^{0.37x} \quad (9)$$

477 A.2 Evaluation setup

478 A.2.1 Prompts for response generation

Table 3: Problem type specific hints by Question and Answer Type

Question Type	Answer Type	Task instruction
Nondim-symbolic	SymPy	Please answer the question requiring an answer in a SymPy convertible formula containing variables and math operation expressions and provide the final answer, e.g., x^3 , $\frac{x}{y}$ inside a Latex boxed format <code>\boxed{}</code> .
Nondim-numerical	Float (2)	Please answer the question requiring a floating-point number with two decimal places and provide the final value, e.g., 0.80, 3.12, inside a Latex box <code>\boxed{}</code> .
Polynomial Roots	SymPy List	Please answer the question requiring a Python list containing SymPy convertible formulas of variable ϵ and math operation expressions and provide the final list, e.g., $[\epsilon^3, \frac{1}{\epsilon}]$ inside a Latex boxed format <code>\boxed{}</code> .
ODEs	SymPy List	Please answer the question requiring a Python list containing SymPy convertible formula of $y = f(x)$ and provide the final list, e.g., $[y = 1 - x^3, y = -6/(x - 5)]$, inside a Latex boxed format <code>\boxed{}</code> .
Integrals	SymPy	Please answer the question requiring an answer in a SymPy convertible formula containing formulas of variable x and math operation expressions and provide the final answer, e.g., x^3 inside a Latex boxed format <code>\boxed{}</code> .

Table 4: LLM-based grading prompts by Question and Answer Type

Question type	Answer type	Task instruction
Polynomial Roots	SymPy List	Please take this response {response} and this answer key {answer key} and grade the response based on the following criteria: 1) Check both the small and large ϵ solutions. 2) For each solution, give full credit if it completely matches the elements in the answer key; give partial credit proportional to the number of matching roots between the response and the answer key; give no credit if it is completely wrong. 3) For both partial and no credit briefly state the error reason. 4) Average the scores for the small and large epsilon solutions to obtain a final score between 0 and 1. 5) Give the final grading as a float in Latex boxed format \boxed{ }.
ODEs	SymPy List	Please take this response {response} and this solution {answer key} and grade the response based on the following criteria: 1) Check both the small and large ϵ solutions. 2) For each solution, give full credit if it matches the formula in the answer key; give no credit if it is completely wrong and briefly state the reason for the error. 3) Average the scores for the small and large epsilon solutions to obtain a final score between 0 and 1. 4) Give the final grading as a float in Latex boxed format \boxed{ }.
Integrals (tradi- tional)	SymPy List	Please take this response {response} and this solution {answer key} and grade the response based on the following criteria: 1) Check both the small and large ϵ solutions. 2) For each solution, give full credit if it matches the formula in the answer key; give no credit if it is completely wrong and briefly state the reason for the error. 3) Average the scores for the small and large epsilon solutions to obtain a final score between 0 and 1. 4) Give the final grading as a float in Latex boxed format \boxed{ }.
Integrals (Laplace)	SymPy	Please take this response {response} and this solution {answer key} and grade the response based on the following criteria: 1) Check the large x final solution. 2) Give full credit if it matches the formula in the answer key; give half credit if the {response} get to the checkpoint where it correctly identifies t_0 where f attains its maximum and attempt performing Taylor's expansion around it but the final answer is wrong; give no credit if it is completely wrong. 3) For both partial and no credit briefly state the error reason. 4) Give the final grading as a float in Latex boxed format \boxed{ }.

480 A.2.3 GPT grading human verification

Model	Roots	ODEs	Integrals
GPT3.5 (0)	0	0	0
GPT3.5 (1)	0	-0.09	-0.02
GPT3.5 (5)	+0.02	+0.07	+0.02
GPT4 (0)	0	-0.02	0
GPT4 (1)	0	-0.04	-0.02
GPT4 (5)	+0.07	-0.07	-0.15
Llama3-8b (0)	0	0	-0.02
Llama3-8b (5)	-0.07	-0.02	-0.02
Codellama3-14b (0)	0	-0.02	0
Codellama3-14b (5)	0	-0.02	0

Table 5: Average adjusted points using human judgment from GPT-based grading. Rows with score adjustments of 0.1 or more are highlighted in pink.

481 A.2.4 Model hyper-parameters

Table 6: Generating parameters for various LLMs.

Model	Generation Setup
GPT-3.5	model = gpt-3.5-turbo, temperature = 0, max_tokens = 4000
GPT-4	model = gpt-4-turbo, temperature = 0, max_tokens = 4000
Llama3	model = llama3:8b, temperature = 0
CodeLlama	model = codellama:13b, temperature = 0

482 A.2.5 Computing resource

483 Evaluations of open-source models on **HARDMATH** are conducted on the O2 High Performance
484 Compute Cluster, supported by the Research Computing Group, at Harvard Medical School. See
485 <https://it.hms.harvard.edu/our-services/research-computing> for more information.
486 We would like to thank the HMS Research Computing Consultant Group for their consulting services,
487 which facilitated the computational analyses detailed in this paper.

488 A.3 Extended experimental results

489 A.3.1 Extended evaluation results

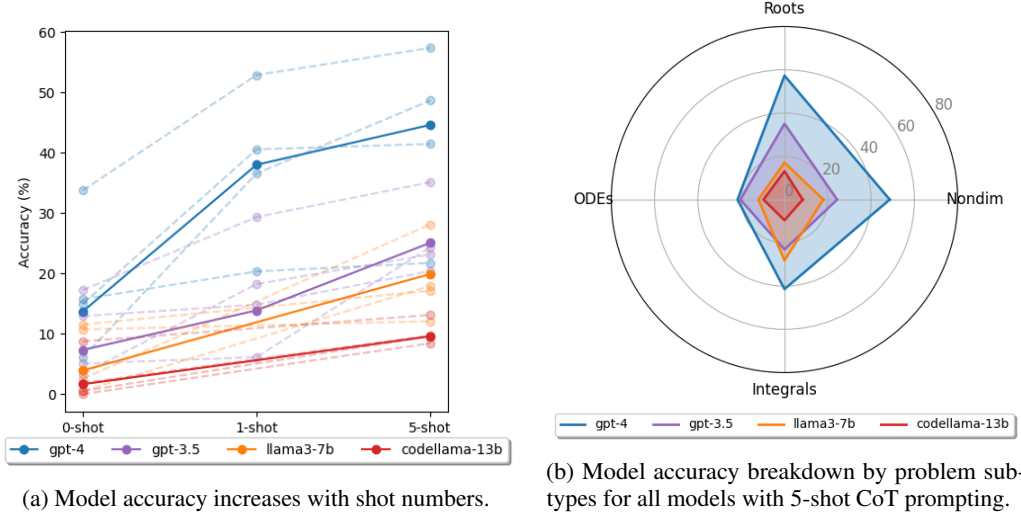


Figure 4: Model evaluation accuracy breakdown by shot number and problem sub-types. (a) evaluation accuracy for all models increases with shot numbers for CoT prompting with GPT-4 having the largest improvement; (b) evaluation accuracy breakdown for all models on all problem sub-types under the 5-shot CoT condition.

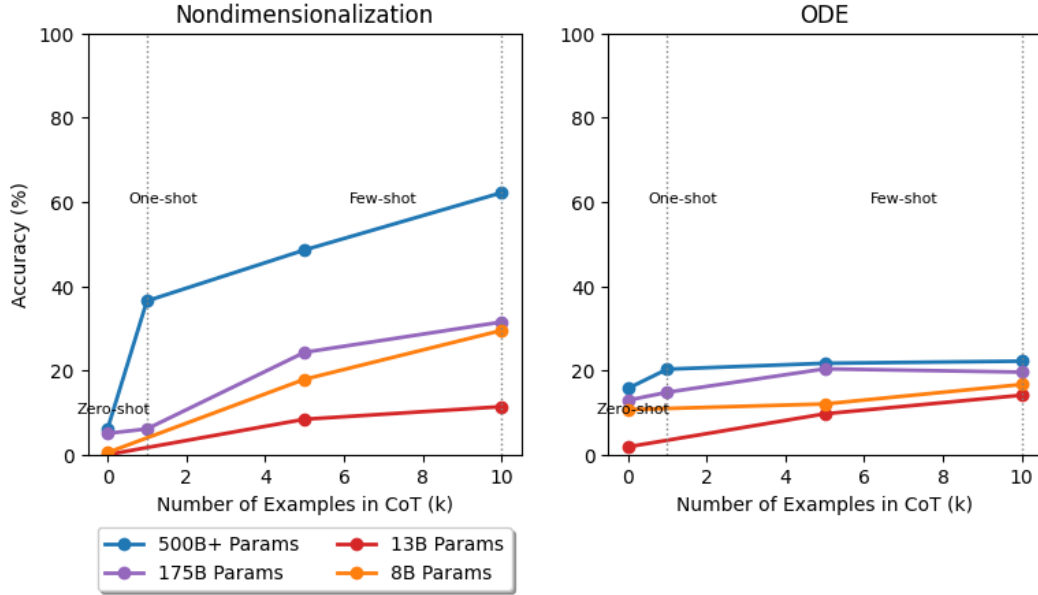


Figure 5: Model performance scaling upon few-shot prompting (0, 1, 5, 10) for problem type *Nondim* and *ODEs*

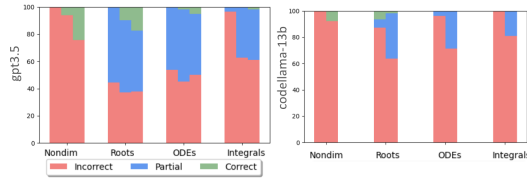


Figure 6: Percentage of correct, partial, and incorrect responses for GPT-3.5 and CodeLlama using CoT.

A.3.2 Extended error mode analysis

Problem 206 Grading Response: *Roots* (error mode: incorrect dominant balance setup)

Question: Consider the polynomial $P(x) = \epsilon x^6 + x^4 - 1$. Find approximate expressions for all roots of the polynomials in the limit of small positive ϵ and large positive ϵ . Only a single term approximation to the root is required.

Grading for Large Positive ϵ :

Model Response: For large ϵ When ϵ is large, the term ϵx^6 dominates the polynomial for most x , except for potentially small x where x^4 might still be relevant. However, focusing on the dominant term gives: $P(x) \approx \epsilon x^6$. Setting this equal to zero for an approximation (acknowledging that we're looking for non-trivial roots of the overall polynomial, but focusing on dominance to guide our approximation), suggests that we don't get meaningful roots from this term alone since $x^6 = 0$ doesn't provide roots that satisfy the original polynomial's requirement for non-zero roots.

Reference Solution: Finally, we examine the balance $A + C = 0$, assuming that $|B|$ is negligible when compared to $|A|$ and $|C|$. Solving this for x in terms of ϵ gives us 6 non-zero

roots: $\epsilon x^6 - 1 = 0$ implies $x = \left[\frac{(-1 \pm \sqrt{3}i) \sqrt[6]{\frac{1}{\epsilon}}}{2}, \frac{(1 \pm \sqrt{3}i) \sqrt[6]{\frac{1}{\epsilon}}}{2}, -\sqrt[6]{\frac{1}{\epsilon}}, \sqrt[6]{\frac{1}{\epsilon}} \right]$. To

verify the roots found for consistency with our initial assumption, we check that $|A|, |C| \gg |B|$ holds for this root by substituting our found root expression for x back into A, B , and C and comparing their magnitudes. Using this method, we find that validity for small ϵ is False and validity for large ϵ is True.

Grading: The response wrongly sets up the dominant balance as $A = 0$ and does not provide a concrete list of roots for large ϵ . Therefore, score for large positive ϵ is 0.0

Problem 203 Grading Response: *Roots* (error mode: drop imaginary roots)

Question: Consider the polynomial $P(x) = \epsilon x^3 + x^2 - 1$. Find approximate expressions for all roots of the polynomials in the limit of small positive ϵ and large positive ϵ . Only a single term approximation to the root is required.

Grading for Large Positive ϵ :

Model Response: To find the approximate expressions for all roots of the polynomial $P(x) = \epsilon x^3 + x^2 - 1$ in the limits of small and large ϵ , we will consider the two cases separately. For Large ϵ When ϵ is large, the term ϵx^3 dominates the polynomial. Thus, the polynomial can be approximated by ignoring the x^2 term, leading to $\epsilon x^3 - 1 \approx 0$. Solving for x gives us an approximation for the root: $x \approx \left(\frac{1}{\epsilon}\right)^{\frac{1}{3}}$. The other roots in this limit are complex and given the scope, we'll focus on this real root approximation.

Reference Solution: Finally, we examine the balance $A + C = 0$, assuming that $|B|$ is negligible when compared to $|A|$ and $|C|$. Solving this for x in terms of ϵ gives us 3 non-zero roots:

$$\epsilon x^3 - 1 = 0 \text{ implies } x = \left[\frac{(-1 - \sqrt{3}i) \sqrt[3]{\frac{1}{\epsilon}}}{2}, \frac{(-1 + \sqrt{3}i) \sqrt[3]{\frac{1}{\epsilon}}}{2}, \sqrt[3]{\frac{1}{\epsilon}} \right]. \text{ To verify the}$$

roots found for consistency with our initial assumption, we check that $|A|, |C| \gg |B|$ holds for this root by substituting our found root expression for x back into A , B , and C and comparing their magnitudes. Using this method, we find that validity for small ϵ is False and validity for large ϵ is True. Therefore, these roots are valid in the limit of large positive ϵ only.

Grading: The response makes additional assumptions to drop the two other complex roots for large ϵ regime without the question asking it to do so. Therefore, score for large positive ϵ is 0.5

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495 A.3.3 Extended example GPT-4o grading responses

Grading Response: ODEs (incorrect)

To grade the response, we will compare the provided solutions in the response with the ground truth solutions in both the small x and large x regimes.

Small x Regime

Response: $y(x) = 1 - 5e^{-x}$

Ground Truth: $y(x) = 1 - \frac{5x^3}{6}$

The response and the ground truth solution for small x are significantly different. The ground truth solution is a polynomial in x , while the response includes an exponential term. They do not match at all, so the solution for the small x regime is completely wrong.

Large x Regime

Response: $y(x) = \text{"Assumed rapid growth form due to } y'^4 \text{ term."}$

Ground Truth: $y = \sqrt[3]{30}(x - 2.68)^{\frac{1}{3}} + (1.84)$

The response does not provide a specific analytical expression for the large x regime, while the ground truth does provide a specific form. The response mentions rapid growth due to y'^4 , but without a clear analytical form, this response doesn't match the ground truth solution. This indicates that the solution for the large x regime is also completely wrong.

Given the evaluation criteria, both solutions do not match or are incomplete compared to the ground truth. Therefore, each solution gets no credit.

The final grading is 0.0.

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Box 3: Example grading response for a ODEs problem that gets zero point.

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Grading Response: *Integrals* (correct)

The model response approximates the integral for small ϵ as $\frac{1}{6^{1/4}}\epsilon^{-3/4}$ and for large ϵ as

$$\frac{1}{8^{1/18}}\epsilon^{-17/18}.$$

Now, let's compare these results with the ground truth solutions:

For small ϵ : - The ground truth solution is $I(\epsilon) = \frac{0.64}{\epsilon^{0.75}}$. - The model's result is

$$\frac{1}{6^{1/4}}\epsilon^{-3/4}.$$

Both results for small ϵ are essentially the same, with:

$$\frac{1}{6^{1/4}} \approx 0.64$$

For large ϵ : - The ground truth solution is $I(\epsilon) = \frac{0.89}{\epsilon^{0.94}}$. - The model's result is

$$\frac{1}{8^{1/18}}\epsilon^{-17/18}.$$

Both results for large ϵ are essentially the same, with:

$$\frac{1}{8^{1/18}} \approx 0.89$$

Since the model's response closely matches the ground truth solutions in both regimes (small and large ϵ) and provides essentially the same approximations, I would give full credit $\boxed{1.0}$

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Box 4: Example grading response for a *Integrals* sub-type simple integral problem that gets full points.

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Grading Response: *Integrals* (partial)

Answer Key

1. Setup and Formulation: it 1) correctly identifies the integral form; 2) uses Laplace's method; 3) identifies critical points and uses Taylor expansion around the point of interest; 4) performs a change of variables to simplify the integral.
2. Key Steps and Approximations: it 1) expands the integrand around the minimum of $f(t)$; 2) approximates the integral by focusing on the dominant exponential term; 3) provides a final analytical approximation for $I(x)$ as $x \rightarrow \infty$.
3. Final Result:

$$I(x) \approx -\frac{0.004e^{0.89x}}{x}$$

Model Answer

1. Setup and Formulation: it 1) correctly identifies the integral form; 2) recognizes that the exponential term will dominate for large x ; 3) focuses on the region where the integrand is most significant (near $t = 0.7$).
2. Key Steps and Approximations: it 1) **uses the method of steepest descents heuristically without detailed Taylor expansion**; 2) approximates by evaluating the polynomial part at $t = 0.7$ and considering the exponential decay; 3) recognizes the dominant behavior of the exponential term but does not perform a detailed variable change or expansion.
3. Final Result:

501

$$I(x) \approx -0.017 \cdot e^{x \cdot 2.6 \cdot 0.7^3}$$

Comparison

1. Similarities: 1) understanding of dominance: both the answer key and the student correctly identify that the behavior of the integral for large x is dominated by the exponential term; 2) identifying significant points: both recognize that $t = 0.7$ is the critical point where the integrand contributes significantly; 3) approximate behavior: Both solutions focus on approximating the behavior of the integral for large x , emphasizing the exponential term's dominance.

2. Differences: 1) mathematical rigor: the answer key employs a more rigorous mathematical approach, including Taylor expansion and change of variables, providing a more precise and detailed solution; 2) heuristic approach: the student takes a more heuristic approach, focusing on the dominant exponential term without detailed mathematical expansions or variable changes; 3) accuracy of final expression: the answer key provides a more accurate final expression with specific constants derived from the detailed process, while the student's result, though on the right track, has a different coefficient due to the heuristic method. I would give partial credit 0.5

502

Box 5: Example grading response for a *Integrals* sub-type Laplace integral problem highlighting the error of failing to develop Taylor's expansion.

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