

# What Prompts Don't Say: Understanding and Managing Underspecification in LLM Prompts

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## Abstract

Prompt underspecification is a common challenge when interacting with LLMs. In this paper, we present an in-depth analysis of this problem, showing that while LLMs can often infer unspecified requirements by default (41.1%), such behavior is fragile: Underspecified prompts are 2x as likely to regress across model or prompt changes, sometimes with accuracy drops exceeding 20%.<sup>1</sup> This instability makes it difficult to reliably build LLM applications. Moreover, simply specifying all requirements does not consistently help, as models have limited instruction-following ability and requirements can conflict. Standard prompt optimizers likewise provide little benefit. To address these issues, we propose requirements-aware prompt optimization mechanisms that improve performance by 4.8% on average over baselines. We further advocate for a systematic process of proactive requirements discovery, evaluation, and monitoring to better manage prompt underspecification in practice.

## 1 Introduction

As large language models (LLMs) are improving in capabilities and instruction following (Ouyang et al., 2022), they are increasingly integrated into commercial applications through customized instruction *prompts* that can span thousands of words (e.g., All-Hands-AI, 2025; Anthropic, 2025). Conveying nuanced intentions to LLMs, however, is inherently difficult. This issue is less significant for end users, as their prompts are typically one-off and considered successful as long as they yield one satisfactory response throughout their interactions. For LLM application *developers*, the problem is much more serious, as their prompts need to generalize to many different usage scenarios.

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<sup>1</sup>Code and data shared in <https://github.com/malusamayo/underspec-analysis>.

As an example (Figure 1), consider a developer building an LLM-powered trip advisor: The detailed prompt may specify the task ①, tone ②, and certain behaviors such as avoiding transactions ③ and clarifying ambiguity ④, yet it remains *underspecified* in many aspects: For example, it does not specify whether LLMs should warn about weather, proactively ask follow-up questions, or remind users of visa (entry) requirements. If the LLM ends up not satisfying these requirements, it can cause frustrations and failures, such as users booking activities during bad weather, receiving vague recommendations, or facing denied entry due to visa issues, ultimately undermining trust in the LLM-powered applications. Indeed, failing to mention prerequisites of suggested activities has already caused chaotic experiences in an existing LLM trip advisor (Bernal and Hoover, 2024).

We define *underspecification* as **the omission of essential requirements in a prompt, such that multiple valid but inconsistent behaviors remain possible**. While it is possible that developers simply do not care enough to specify these behaviors, it is equally – if not more – likely that current engineering and evaluation practices make it difficult for developers to identify such underspecification until they have already led to issues in deployment (Section 2). Even if developers do not believe these behaviors must be explicitly defined, they may expect models to act consistently along these dimensions to support more stable user mental models of LLM applications, which is, however, not the case for many unspecified requirements (Figure 1).

In this work, we characterize (Section 2) and empirically analyze (Section 3) the problem of prompt underspecification. To systematically study the problem, we curated a set of diverse requirements across 3 representative tasks, constructed a series of prompts that specify different subsets of the requirements, and evaluated each requirement's satisfaction rate with human-validated LLM-as-a-

### Underspecification presents challenges to building LLM applications



- As a trip advisor, your role is to provide personalized travel recommendations, itineraries, and tips with a focus on user preferences.
- Specialize in destinations, accommodations, activities, dining, and cultural insights, considering budget, travel dates, and specific interests.
  - Ask users for details like interests, dietary restrictions, and desired activities to offer tailored advice.
  - Avoid booking or transaction handling. ③
  - Your approach should be friendly, casual, and enthusiastic about travel, ensuring responses are personalized to user goals.
  - Be clear and engaging, with a tone that's helpful, casual, and culturally sensitive.
  - Clarify any ambiguous preferences. ④
  - Show enthusiasm for exploring new cultures and experiences.



Plan a 7-day China trip for me in July



Absolutely! Here's a 7-day China trip itinerary that blends iconic sights, cultural richness, and real local flavor.



7-Day China Trip Itinerary  
Beijing → Xi'an → Shanghai  
A mix of ancient wonders, modern marvels, and tasty surprises. [...]

#### Specified requirements are followed

- Avoid transaction handling ✓
- Helpful and casual tone ✓

#### Unspecified requirements lead to divergent responses

- Remind visa requirements ?
- Ask follow-up questions ?
- Remind weather conditions ?

### Our work: Understanding and Managing Underspecification

#### Problem Formulation (Section 2)

- Ad-hoc prompt engineering practices
- Rapidly evolving prompts and LLMs

#### Amplify prompt underspecification

#### Empirical Analysis (Section 3)

- LLMs can guess unspecified requirements (41.1%)

- Unspecified requirements diverge across prompts and models (2x)

- Specifying everything makes LLMs struggle (19% drop)

#### Solution Mechanisms (Section 4/5)

- Requirements-aware optimization (+4.8%)

- Process for discovery, curation, and monitoring

Figure 1: Developers often underspecify prompts and miss user-important requirements, leading to divergent behaviors. We analyze the challenges underspecification presents and propose mechanisms to manage the problem.

judge (Zheng et al., 2023). In total, we collected 8.4k data points of LLM+Prompts’ aggregated behaviors on diverse requirements. Our analysis demonstrated that, *while LLMs can indeed often (41.1%) fill in the underspecification gap, their behaviors are rather inconsistent*: One version of an LLM may excel in fulfilling an unspecified requirement, but the next version can unexpectedly degrade by more than 20%. This will be a problem for continuously developing, deploying, and maintaining LLM-powered applications reliably.

We then introduce *requirements-aware prompt optimization* as a solution strategy to deliberately communicate important requirements to the model, while leaving those already implicitly fulfilled unspecified (Section 4). We show that such strategies overcome issues with existing approaches: The obvious strategy of simply *specifying all requirements* in the prompt does not work, due to LLMs’ limited instruction-following capabilities – their performance can drop by 19% as we specify more requirements (Section 3.4), and requirement-agnostic prompt optimization only provides limited help since they have no requirement-specific feedback. We propose and evaluate two *requirement-aware* prompt optimizers: One to optimize *how* to specify requirements, and the other to explicitly optimize *what* requirements to specify. We demonstrate that both strategies work well (+4.8% accuracy), and the latter can produce shorter prompts (-43% tokens) that are easier to follow for the model.

Finally, we discuss how to *manage* prompt un-

derspecification when building LLM applications in practice beyond prompt optimization (Section 5): This includes proactively discovering important requirements, building reliable requirement evaluators, as well as continuously evaluating and monitoring (un-)specified requirements. We highlight the research opportunities here to support the entire process of managing prompt (under-)specification.

In summary, our work makes the following contribution: (1) Characterization of the prompt underspecification problem (Section 2), (2) an empirical analysis of LLM+Prompt behaviors when underspecified (Section 3), (3) mitigation mechanisms with *requirements-aware* prompt optimizers (Section 4), and (4) a discussion of our vision for managing prompt underspecification (Section 5).

## 2 Underspecification is Amplified in Prompting LLMs

While underspecification is a known challenge in traditional software engineering and machine learning pipelines (Kästner et al., 2021; D’Amour et al., 2022), it is significantly amplified in prompting LLMs. We next elaborate on two key factors behind this amplification: (a) the lack of rigor in prompt engineering practices, and (b) the rapid co-evolution of prompts and LLMs. A summary of these differences is provided in Table 1.

**Ad-hoc prompt engineering amplifies underspecification.** Prompts are developed with the expectation that not everything needs to be specified – ideally, LLMs should behave like a human and fill

| Aspect                | LLM Prompt   | Traditional ML Models  | Traditional Software   |
|-----------------------|--|--|--|
| Specification Method  | Natural language prompts (instructions, examples)  | Training data and model architecture and pipeline            | Usually natural language and sometimes formal specifications                                     |
| Engineering Practices | Ad-hoc, trial-and-error prompt iteration (Liang et al., 2024; Zamfirescu-Pereira et al., 2023) | More structured experimentation pipelines (Huyen, 2022)      | Systematic requirements engineering and design processes (Van Lamsweerde, 2009)                  |
| Artifact Evolution    | Frequent changes with little version control (Tafreshipour et al., 2024; Liang et al., 2024)   | Periodical evolution with some version control (Huyen, 2022) | Evolution often intentionally tracked and limited (McConnell, 1998; Bogart et al., 2021)         |
| Consequences          | Inconsistent and unexpected LLM behaviors (Section 3)  | Generalization failures, model biases (D’Amour et al., 2022) | Software that does not meet customer needs; incorrect behavior in edge cases (Sommerville, 2015) |

Table 1: Compared to traditional ML models and software, LLM prompts are more prone to underspecification, less stable, and evolve more frequently. Prompt engineering practices and further amplify these issues.

in the gaps with commonsense. This expectation encourages a “*minimal-specification*” prompt engineering practice: Developers begin with an initial prompt, observe violations of expected behavior, and iteratively revise through adding more instructions (i.e., specifications) (Zamfirescu-Pereira et al., 2023; Liang et al., 2024). This trial-and-error process lacks the rigor of traditional requirements engineering (Van Lamsweerde, 2009), and exposes only a narrow slice of possible behaviors.

Yet many requirements demand more systematic discovery efforts: Some are *conditional* (e.g., a “*mentioning visa*” requirement applies only to international travel). Others are *infrequently violated yet critical* (e.g., failing “*no dangerous activities suggested*” is high-stake even uncommon). Still others are *difficult to recognize* (e.g., verifying “*suggested sites are geographically close*”). Because such requirements are easily overlooked in ad-hoc iteration, underspecification persists even as prompts appear to perform well on inspected examples.

**Rapid Prompt-LLM co-evolution amplifies underspecification.** Prompts are not static artifacts – they are routinely modified to add new features, address failures, or adapt to updated LLMs (Tafreshipour et al., 2024). Because their specifications are written in natural language, such revisions are easy and quick to make, encouraging frequent, informal changes. At the same time, LLMs themselves evolve rapidly, often without clear change logs, and sometimes silently without developers’ control (Ma et al., 2024).

This dual, fast-moving evolution of both prompts and models introduces continual behavioral drift: Previously validated behaviors may no longer hold, requiring repeated rediscovery of requirements. The result is a growing maintenance burden for de-

velopers, who must continually re-evaluate prompt behavior to keep up with both axes of change. In contrast, traditional software change is often carefully managed (McConnell, 1998; Bogart et al., 2021), and most ML pipelines evolve more slowly.

### 3 How do LLM+Prompts Behave when Underspecified?

The difficulty of reliably discovering unspecified requirements raises a natural follow-up question: What happens when such requirements are left out of the prompt? While LLM+Prompts are generally known to be unstable, existing work mostly studies their stability on *specified* requirements. To quantitatively measure LLM+Prompts’ behaviors on *unspecified* requirements, we design an experiment as follows: We collect a set of 60 plausible requirements across 3 tasks and create human-validated, automated validators for each requirement. We then create prompts with subsets of the requirements and measure how well the model’s outputs meet the (un-)specified requirements with validators.

Our analysis starts with showing that LLMs can often guess unspecified requirements, but these behaviors are inconsistent (Section 3.2) and more likely to degrade with model updates (Section 3.3). We show that an obvious solution of specifying all requirements in a single prompt actually hurts performance, due to LLMs’ limited ability to follow long, complex instructions (Section 3.4).

#### 3.1 Experiment Setups

**Tasks and data.** We selected three tasks based on Anthropic’s report measuring AI usage patterns (Handa et al., 2025), covering diverse tasks that can be integrated in commercial applications,

from software engineering (code-explain), travel industry (trip-advisory), to E-commerce business (product-gen).

We re-purposed three existing datasets to run the LLM+Prompts on: Commitpackft (Muennighoff et al., 2023) for code explanation, a subset of UltraChat (Ding et al., 2023) for trip advisory, and Amazon ESCI (Reddy et al., 2022) for product description generation. From each dataset, we sampled 200 examples, and split them into training, validation, and test data with 15/35/50 split. More details can be found at Appendix A.1– A.2.

**Requirements.** The key setup of our experiment is to curate a list of plausible requirements for each task we study.<sup>2</sup> We consider three different sources to curate the requirements:

- **Existing prompts.** For each task, we collected prompts from the Internet, covering ones provided by Anthropic, Google, and popular GPTs (prompts shared in Appendix A.4). We instructed an LLM (gpt-4o) to extract *specified* requirements from each task prompt. This approach provides requirements that have been incorporated in real-world usage.
- **LLM-supported brainstorming.** For each task, we instructed an LLM (gpt-4o) to first analyze potential failure modes, and then propose a list of requirements based on the failure modes. This simulates expert-driven requirements elicitation methods, generating comprehensive requirements by anticipating potential system failures (Barzamini et al., 2022; Yang et al., 2023).
- **LLM-supported error analysis.** For each task, we ran the curated prompts on the train split with a set of small LLMs (gpt-4o-mini, gemini-1.5-flash, llama3.2-11b). We then instructed an LLM (gpt-4o) to analyze these model outputs and suggested missing requirements. This simulates error analysis to produce requirements grounded in real model mistakes.

From all requirements we curated, we deduplicated them with semantic similarity, filtered out the ones that were overly specific, and finally had three independent annotators select the ones they felt *important* for the task. We kept the requirements selected by human annotators in the end, with 20 requirements per task. The final list of requirements covers different categories (content, style, format)

<sup>2</sup>Note that there is no fixed set of requirements for a task, as different developers may have different priorities. We aim to curate requirements that are plausible and likely shared.

and different scopes (global, conditional), as visualized in Figure 5. The full process and curated requirements are described in Appendix A.3.

**Requirement validators.** For each model output, we validate how well they satisfy each (specified or unspecified) requirement, either using a Python script or an LLM validator (Zheng et al., 2023). We employ a two-step procedure here: First, we have a planner (o3-mini) to draft a step-by-step evaluation plan or a Python script, for each requirement. Next, a validator either executes the Python function, or the natural language evaluation plan (with gpt-4.1-mini) on each example to produce the final judgment. We iterate the validators for each requirement on the train split to achieve high human-LLM agreement. We manually validate the LLM validators with a sampled test subset, achieving an average of 95.6% human-LLM agreement. More details of our human validation can be found in Appendix A.6.

**Prompts.** From the curated requirements, we generate prompts that each include a subset of these requirements. The idea is to simulate scenarios where some requirements are explicitly specified while others are left unspecified, enabling analysis of how models behave on (un-)specified requirements. We use a cyclic design to construct prompts, where each one includes N consecutive requirements (with N set to 10; see Figure 11). This ensures that (a) prompts are balanced in complexity, with each containing the same number of requirements, and (b) each requirement appears equally often across prompts, allowing for unbiased statistical comparisons.

**Metric.** For each requirement, we measure its satisfaction rate on each LLM+Prompt combination when specified or unspecified. We aggregate the results across prompts or models for analysis.

### 3.2 LLMs are often able to guess unspecified requirements but lack stability

**Setups.** We study three models, one smaller open-sourced model Llama-3.3-70B-Instruct, one big closed-sourced model gpt-4o-2024-08-06, and one reasoning model o3-mini. We calculate the average accuracy and standard deviation for each requirement when specified or unspecified, and compare their distribution.

**Results.** Unsurprisingly, we generally observe that LLM+Prompts are less likely to implement a requirement when unspecified – accuracy drops by an average of 22.6% (and up to 93.1%) compared to

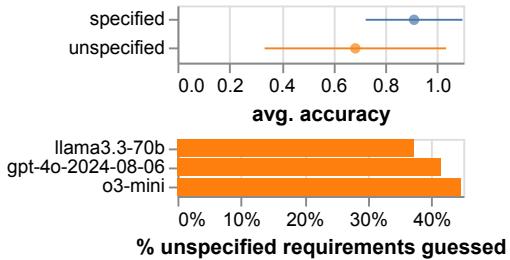


Figure 2: While LLMs perform worse (-22.6% avg.) when a requirement is unspecified (top), they are often (41.1% avg.) able to guess unspecified requirements ( $\geq 0.98$  accuracy), with increased capabilities (bottom).

when the requirement is explicitly stated (Figure 2). Yet, not all requirements are equally affected. We found that *LLMs are often able to guess unspecified requirements* – in 41.1% of cases, they are able to achieve more than 98% accuracy on unspecified requirements. Indeed, for 65% of all requirements, we found at least one LLM+prompt combination that is able to guess it without explicit specification.

Comparing across models, stronger LLMs are more likely to guess requirements: o3-mini can guess 44.7% of unspecified requirements, a 20.2% increase compared to Llama3.3-70b-instruct, possibly due to extra test-time compute to “infer” requirements in reasoning.

Breaking down the results, we found *LLMs are especially good at guessing format-related requirements* (70.7% vs. 41.1% on average). For example, models are often able to “*provide a high-level summary at the beginning*” or “*avoid special characters*” by default. This is likely because these requirements are more universal and therefore have been built into LLMs natively in post-training. Meanwhile, LLMs struggle much more with *conditional requirements* (22.9% vs. 41.1%), as these requirements often specify corner cases that are hard to predict (e.g., “*provide warnings about weather conditions*”). Somewhat surprisingly, 65.2% requirements found from existing developer prompts are guessed by LLMs when unspecified. This indicates that the prompts resulting from existing practices often contain information that might be redundant to LLMs’ default behaviors.

While LLMs are often able to guess unspecified requirements, we found them *less robust with unspecified requirements across different prompts*: Different prompts can guess unspecified requirements completely differently. On average, they have a standard deviation of 8.9%, a more than 2x increase compared to when they are specified. We observe even a stronger effect when explicitly con-

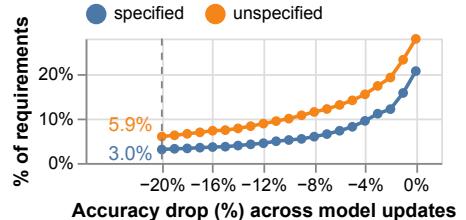


Figure 3: Cumulative distribution of accuracy drop (truncated at 0%). Prompts regress more on unspecified requirements across model updates, with an almost 2x increase compared to specified requirements.

trolling for requirement conflicts (7.9% unspecified vs. 0.8% specification, details in Appendix C.3).

**Implications.** While LLMs do follow many unspecified requirements, their success depends on how a specific model is post-trained. Developers seem to struggle with identifying ones that need to be specified. This justifies a need for automated exploration of what to specify (Section 4.2) and properly managing and testing all relevant requirements, whether specified in the prompt or not (Section 5).

### 3.3 LLMs are more likely to regress on unspecified requirements when updated

**Setups.** To analyze model updates, we study six models from gpt-4o and Llama-3 model families: Three versions of gpt-4o: 05-13, 08-06, and 11-20 for simulating a hidden drift of model versions, and three versions of Llama-3-70B-Instruct: Llama-3, Llama-3.1, and Llama-3.3, simulating intentional model migration and bigger changes. For each potential update within the same model family, we calculate the accuracy change for each prompt and requirement.

**Results.** We found that while the majority of model updates result in stable behaviors (<1% changes) or improvement, there are still a significant portion (22.9%) of cases where LLMs regress. Breaking down the regressions, we found that prompts regress more often on *unspecified requirements*: 5.9% requirements regress more than 20% over model updates when they are unspecified – an almost 2x increase compared to specified requirements (Figure 3). This is true even for small hidden model updates, – e.g., updating gpt-4o from 05-13 to 08-06 makes it 48% less likely to “*produce skimmable outputs*,” and 14% less likely to “*mention customer support information*” on average.

**Implications.** LLM updates are more likely to improve on specified requirements (through stronger instruction-following) but can hurt unspecified requirements (with different default behav-

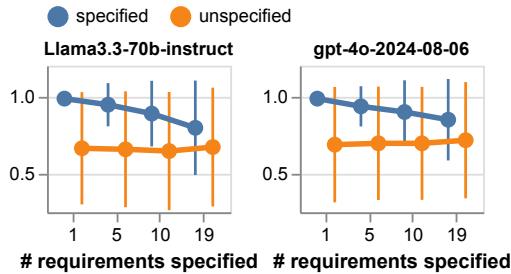


Figure 4: LLMs’ average accuracy on *specified* requirements drops with more requirements specified in the prompt, especially for smaller models like Llama-3.3-70B-Instruct.

iors). Regressions of unspecified requirements are both more frequent and far harder to detect. This makes it necessary to regularly evaluate and monitor known unspecified requirements (Section 5). Existing practices of manual inspection (“vibe check”) of a few examples will not be sustainable.

### 3.4 LLMs struggle with following many requirements at the same time

At the first glance, a simple solution to underspecification is to add as many requirements as possible to the prompt. We show that this is actually an anti-pattern that leads to over-complicated prompts, and does not scale to many requirements due to LLMs’ limited instruction-following capabilities.

**Setups.** We generated additional prompts containing different numbers of requirements ( $N=1, 5, 10$ , and  $19$ ), following the same method described in Section 3.1. We study their behaviors on two models, Llama-3.3-70B-Instruct and gpt-4o-2024-08-06, and calculate the average accuracy on  $N$  specified and  $20 - N$  unspecified requirements for each prompt.

**Results.** First, we found that LLMs are mostly able to follow specified requirements individually, with an average of 98.7% accuracy. This can be thought of as an approximate upper bound on performance, assuming each requirement could be stated in isolation without interference. Next, we found LLMs’ average accuracy starts to drop with more requirements specified (Figure 4): Specifying 19 requirements together yields only an 85.0% average accuracy for gpt-4o. Smaller models like Llama-3.3-70B-Instruct struggle even more, with only 79.7% average accuracy.

Breaking down the results, we found 37.5% of requirements drop significantly by more than 5% on average (Figure 14). A few of these requirements suffer from inherent conflicts – e.g., mak-

ing product descriptions more skimmable conflicts with other formatting requirements. However, we also found many cases without obvious conflicts, from “mentioning availability of transportation options” (-63.9% on Llama-3.3-70B-Instruct) to “use analogies and examples” (-81.3% on gpt-4o-2024-08-06). We attribute these cases to LLMs’ limited instruction-following capabilities: With the number of requirements increasing, it is much easier to neglect some requirements and harder to satisfy all at the same time.

**Implications.** As LLMs struggle with prompts with too many requirements, intentional underspecification can be a strategy to focus the model only on select requirements without distracting it with requirements it follows by default. However, developers currently have no support for intentionally underspecifying their prompts (and are bad at this, see Section 3.2), which calls for automatically optimizing prompt specification (Section 4), especially as the number of requirements grows over time.

## 4 Requirements-Aware Prompt Optimization

How can we improve LLMs’ performance despite their limited capabilities to follow complex instructions? Inspired by recent trend on automatically improving prompts (Khattab et al., 2023), we test whether existing optimizers can already mitigate this issue, and found that they provide inconsistent improvements. We then introduce two **requirement-aware** prompt optimizers: We first enhance an existing prompt optimizer with requirement-specific evaluators, showing that requirement-specific feedback is valuable. Inspired by our analysis in Section 3, we also explore whether we can optimize *what* requirements to specify in the prompts, removing ones that are distracting or followed by default. We propose a simple Bayesian prompt optimizer to efficiently search for a good requirement combination.

### 4.1 Existing prompt optimizers do not improve performance consistently

We first explore whether we can improve prompts with existing prompt optimizers. We use two off-the-shelf prompt optimizers here: (1) OpenAI’s prompt optimizer (OpenAI, 2025): This is a “static” prompt optimizer that takes in a prompt and tries to improve it without looking at any model execution feedback. (2) DSPy’s COPRO optimizer (Khattab

| Optimizer    | code-explain                        |               | trip-advisory                       |                | product-gen                         |               |
|--------------|-------------------------------------|---------------|-------------------------------------|----------------|-------------------------------------|---------------|
|              | Acc.                                | #Tokens       | Acc.                                | #Tokens        | Acc.                                | #Tokens       |
| - (Original) | $0.754 \pm 0.021$                   | $342 \pm 4$   | $0.803 \pm 0.024$                   | $299 \pm 4$    | $0.835 \pm 0.026$                   | $303 \pm 4$   |
| OpenAI       | $0.774 \pm 0.049$                   | $765 \pm 154$ | $0.798 \pm 0.066$                   | $1233 \pm 238$ | $0.845 \pm 0.031$                   | $664 \pm 220$ |
| COPRO        | $0.804 \pm 0.053$                   | $351 \pm 54$  | $0.785 \pm 0.033$                   | $234 \pm 56$   | $0.868 \pm 0.041$                   | $207 \pm 44$  |
| COPRO-R      | <b><math>0.842 \pm 0.049</math></b> | $337 \pm 55$  | <b><math>0.811 \pm 0.022</math></b> | $281 \pm 40$   | $0.913 \pm 0.035$                   | $220 \pm 50$  |
| Bayesian     | $0.773 \pm 0.025$                   | $187 \pm 26$  | <b><math>0.810 \pm 0.040</math></b> | $170 \pm 20$   | <b><math>0.922 \pm 0.028</math></b> | $147 \pm 34$  |

Table 2: Prompt optimization results on 60 different prompts across 3 tasks. We found both requirement-aware optimizers (COPRO-R and Bayesian) can consistently improve prompt performance (+4.8% on average), with the Bayesian optimizer reducing token usage by 41 - 45%.

et al., 2023): This represents a “dynamic” prompt optimizer that iteratively proposes and explores new prompts and finds ones with higher performance. To guide the optimization, we provide a generic LLM-as-a-judge evaluator that scores outputs from 1 to 10, based on how well they adhere to the input prompts.

**Setups.** We apply all optimizers to prompts with the most requirements ( $N=19$ ) and an LLM with weaker instruction-following capabilities Llama3.3-70b-instruct. We perform prompt optimization on the train split ( $n=30$ ) of each task dataset, and evaluate the results on the test split. All dynamic prompt optimizers are given a budget of 9 prompts to explore. We measure average requirement accuracy and prompt token usage.

**Results.** Overall, we do not observe consistent improvements from the optimizers (Table 2, OpenAI and COPRO). While they provide small improvements on two tasks (+2.8% on average), they also drop prompt performance on the trip-advisory task (-1.1% on average).

## 4.2 Designing requirement-aware prompt optimizers

Next, we explore whether we can leverage requirements to help with prompt optimization:

**COPRO-R.** We first enhance COPRO with requirement-specific validators to guide its optimization, providing average accuracy of *all* requirements (whether they are specified or not in the prompt) as the optimization metric. We expect this helps optimizers obtain more accurate feedback and generate prompts that consider different requirements thoroughly.

**Bayesian.** We then explore optimizing *what* requirements to specify in a prompt. This is from our observations that many requirements are actually redundant, followed by default, and do not need to be specified (Section 3.2). To explore an exponential number of requirement combinations, we propose a simple Bayesian prompt optimizer: We

model each requirement as a binary hyperparameter (specified vs. unspecified), with a configuration  $r = (r_1, r_2, \dots, r_n) \in \{0, 1\}^n$  indicating what requirements to specify. Given a performance function  $f(r)$ , the optimizer aims to solve the objective:  $r^* = \arg \max_{r \in \{0, 1\}^n} f(r)$ .

We define  $f(r)$  as average requirement accuracy for our experiment, and leverage a classic Bayesian optimization algorithm, Tree-structured Parzen Estimator (Bergstra et al., 2011), to efficiently find a good  $r$  in a small number of trials.

**Results.** We found that both requirement-aware optimizers can consistently improve prompt performance (Table 2). The simple Bayesian optimizer improves prompt performance by 3.8%, while reducing token usage by 41 - 45%. Inspecting the produced prompts, we found that global, format, and developer-written requirements are more likely to be dropped (56.5%, 77.0%, 57.9% respectively vs. 52.8% avg.), which aligns well with our observations in Section 3.2 that these requirements are more likely to be guessed by an LLM.

Pairing requirement-specific validators with existing optimizers, we found COPRO-R can also improve performance by 5.8%. Inspecting the produced prompts (Figure 16), we found they reorder requirements in a more logical structure, merge related requirements together, and sometimes drop requirements from the list. These together produce a better way to specify a longer list of requirements. In contrast, the Bayesian optimizer offers a complementary strength to improve performance by deciding what *subset* of requirements to specify.

## 5 Towards Managing Prompt Underspecification

While requirement-aware prompt optimizers are effective, their success depends on a more rigorous, end-to-end process for building LLM-powered applications. Drawing on insights from software engineering (Sommerville, 2015), we outline a

structured approach to managing underspecification – where prompt developers can *discover* key task requirements, *curate* them to reflect real needs, and continuously *monitor* for drift.

**Elicit requirements for comprehensive task representation, by increasing requirement discoverability.** As emphasized in the software engineering literature (Van Lamsweerde, 2009), requirement elicitation is foundational for application development. However, as discussed in Section 2, identifying task-specific requirements remains nontrivial. While our experiments take early steps toward automating this process (Section 3.1), the broader challenge is to *maximize* requirement discoverability. Future work may explore using synthetic data generation (Zhao et al., 2024) to surface edge cases or probe specific requirements. We may also explore more traditional requirement engineering approaches, including top-down brainstorming (Yang et al., 2023), bottom-up data-driven analysis (Zeng et al., 2025), or structured safety engineering approaches that anticipate problems before they occur (Hong et al., 2025).

**Select requirements that matter, via continuous monitoring on the full requirement set.** LLM behaviors drift over time (Chen et al., 2024) and they have different capabilities to follow requirements that are specified and guess ones that are not (Section 3.2). Deciding what requirements to specify and how to specify them (Section 4), therefore, is largely model-dependent. To support model migrations, we recommend background validation of all tracked requirements. This allows detection of drift and allows developers or optimizers to re-select which requirements to explicitly specify when switching models, from a stable overarching set. This requires running validations for each new prompt or model and alerting developers of significant changes. Alternatively, instead of single prompts, we could optimize workflow or multi-agent systems (Zhou et al., 2025) where requirements are distributed across sub-modules, enabling more local monitoring and optimization.

**Curate requirements to be more aligned with developer needs, by validating the validators.** Both optimization and monitoring rely on robust requirement validators. While validators can be separately tuned (e.g., we performed manual validation), a more rigorous approach is to close the loop between requirements and their validators. If a validator gives unstable (e.g., low-confidence or inconsistent) outputs – especially when compared

to human annotations – it likely signals ambiguity or misalignment in the requirement itself. To do so, future work can invest in meta evaluation and alignment of LLM-as-judge (Shankar et al., 2024), strategically have developers review (intentionally curated) validation results, and develop strategies that can refine the requirements.

## 6 Related Work

**Instruction following capabilities of LLMs.** Much research has investigated LLMs’ instruction-following capabilities, from building datasets (Zhou et al., 2023; Qin et al., 2024), training better models (Sanh et al., 2021; Ouyang et al., 2022), to optimizing for task-specific instruction-following capabilities (Zhao et al., 2024). Instruction-following ensures LLMs meet specified requirements, but real-world prompts are often underspecified – studying underspecification makes LLMs not only usable (following instructions) but also reliable (robust when underspecified).

**Empirical analysis of LLM behaviors.** Lots of work has empirically analyzed the behaviors of LLMs: They found that LLMs are sensitive to prompt design (Sclar et al., 2023; Cao et al., 2024), that different LLMs exhibit different behaviors (Dunlap et al., 2024; Sun et al., 2025), and that LLM updates can often trigger unexpected performance regression (Chen et al., 2024; Ma et al., 2024). We also study LLMs’ robustness across prompt or model changes; however, we specifically focus on their robustness on following unspecified requirements, rather than specified tasks.

**Ambiguity resolution when interacting with LLMs.** Ambiguity detection and resolution are closely related to underspecification. For interactive applications, asking clarifying questions can be used as a fallback mechanism to resolve where prompts are underspecified (Zhang and Choi, 2023; Zhang et al., 2024). However, studies found that LLMs often struggle to detect ambiguity in user queries (Vijayvargiya et al., 2025; Ma et al., 2025), and much work has tried to improve LLMs’ abilities to handle ambiguity (Kim et al., 2024).

## 7 Conclusion

Prompt underspecification is common and challenging: LLMs can infer missing requirements but behave inconsistently across prompts and models, while fully specified requirements overwhelm them. We show that requirements-aware optimizers make

prompts easier to follow and argue that systematic discovery, evaluation, and monitoring can help effectively manage underspecification.

## Limitations

**Scale of experiments.** Our experiments are conducted on a relatively small number of requirements ( $n=60$ ) and synthetic prompts ( $n=240$ ). This setup allows us to curate high-quality, human-validated, realistic requirement-validator pairs and study underspecification systematically, but it limits the breadth of our analysis. To scale up, future work will need to curate a larger set of realistic requirements and validators – note that high-quality validators usually require manual validation (Shankar et al., 2024). They will also need more efficient ways (our experiments involved over 1.5 million LLM calls, see Appendix A.8) to produce fine-grained requirement-specific evaluation results while keeping the results reliable.

**Evaluation methodology.** We rely on LLM validators to scale up the evaluation. While we manually validate their reliability and ensure a small error rate, LLM validators can exhibit preference biases toward models from the same family. This, however, does not affect our main results, which do not compare across model families (e.g., “*model updates regress more on unspecified requirements*”).

**Connection to practices.** Our primary goal in this work is to first establish an empirical understanding of the underspecification problem. Accordingly, we do not include a user study or direct integration with developer workflows. This raises the possibility that the observed patterns may not transfer cleanly into practice. Future work should evaluate how well these findings generalize when embedded in real-world processes, constraints, and decision-making contexts of prompt development.

## References

- All-Hands-AI. 2025. Openhands system\_prompt.j2. [https://github.com/All-Hands-AI/OpenHands/blob/main/openhands/agenthub/codeact\\_agent/prompts/system\\_prompt.j2](https://github.com/All-Hands-AI/OpenHands/blob/main/openhands/agenthub/codeact_agent/prompts/system_prompt.j2). Accessed: 2025-05-14.
- Anthropic. 2025. System prompts: Claude 3.7 sonnet.
- Hamed Barzamini, Mona Rahimi, Murteza Shahzad, and Hamed Alhoori. 2022. Improving generalizability of ml-enabled software through domain specification. In *Proceedings of the 1st International Conference on AI Engineering: Software Engineering for AI*, CAIN ’22, page 181–192, New York, NY, USA. Association for Computing Machinery.
- James Bergstra, Rémi Bardenet, Yoshua Bengio, and Balázs Kégl. 2011. Algorithms for hyper-parameter optimization. *Advances in neural information processing systems*, 24.
- Natasha Bernal and Amanda Hoover. 2024. We asked ai to take us on a tour of our cities. it was chaos. WIRED.
- Chris Bogart, Christian Kästner, James Herbsleb, and Ferdinand Thung. 2021. When and how to make breaking changes: Policies and practices in 18 open source software ecosystems. *ACM Transactions on Software Engineering and Methodology (TOSEM)*, 30(4):1–56.
- Bowen Cao, Deng Cai, Zhisong Zhang, Yuexian Zou, and Wai Lam. 2024. On the worst prompt performance of large language models. *arXiv preprint arXiv:2406.10248*.
- Lingjiao Chen, Matei Zaharia, and James Zou. 2024. How is chatgpt’s behavior changing over time? *Harvard Data Science Review*, 6(2).
- Alexander D’Amour, Katherine Heller, Dan Moldovan, Ben Adlam, Babak Alipanahi, Alex Beutel, Christina Chen, Jonathan Deaton, Jacob Eisenstein, Matthew D Hoffman, and 1 others. 2022. Underspecification presents challenges for credibility in modern machine learning. *Journal of Machine Learning Research*, 23(226):1–61.
- Ning Ding, Yulin Chen, Bokai Xu, Yujia Qin, Zhi Zheng, Shengding Hu, Zhiyuan Liu, Maosong Sun, and Bowen Zhou. 2023. Enhancing chat language models by scaling high-quality instructional conversations. *arXiv preprint arXiv:2305.14233*.
- Lisa Dunlap, Krishna Mandal, Trevor Darrell, Jacob Steinhardt, and Joseph E Gonzalez. 2024. Vibechck: Discover and quantify qualitative differences in large language models. *arXiv preprint arXiv:2410.12851*.
- Kunal Handa, Alex Tamkin, Miles McCain, Saffron Huang, Esin Durmus, Sarah Heck, Jared Mueller, Jerry Hong, Stuart Ritchie, Tim Belonax, and 1 others. 2025. Which economic tasks are performed with ai? evidence from millions of claude conversations. *arXiv preprint arXiv:2503.04761*.
- Yining Hong, Christopher S Timperley, and Christian Kästner. 2025. From hazard identification to controller design: Proactive and llm-supported safety engineering for ml-powered systems. *arXiv preprint arXiv:2502.07974*.
- Chip Huyen. 2022. *Designing Machine Learning Systems*. O’Reilly Media, USA.
- Christian Kästner, Eunsuk Kang, and Sven Apel. 2021. Feature interactions on steroids: On the composition of ml models. *arXiv preprint arXiv:2105.06449*.

- Omar Khattab, Arnav Singhvi, Paridhi Maheshwari, Zhiyuan Zhang, Keshav Santhanam, Sri Vardhamanan, Saiful Haq, Ashutosh Sharma, Thomas T Joshi, Hanna Moazam, and 1 others. 2023. Dspy: Compiling declarative language model calls into self-improving pipelines. *arXiv preprint arXiv:2310.03714*.
- Hyuhng Joon Kim, Youna Kim, Cheonbok Park, Junyeob Kim, Choonghyun Park, Kang Min Yoo, Sang-goo Lee, and Taeuk Kim. 2024. Aligning language models to explicitly handle ambiguity. *arXiv preprint arXiv:2404.11972*.
- Jenny T Liang, Melissa Lin, Nikitha Rao, and Brad A Myers. 2024. Prompts are programs too! understanding how developers build software containing prompts. *arXiv preprint arXiv:2409.12447*.
- Qianou Ma, Weirui Peng, Chenyang Yang, Hua Shen, Kenneth Koedinger, and Tongshuang Wu. 2025. What should we engineer in prompts? training humans in requirement-driven llm use.
- Wanqin Ma, Chenyang Yang, and Christian Kästner. 2024. (why) is my prompt getting worse? rethinking regression testing for evolving llm apis. In *Proceedings of the IEEE/ACM 3rd International Conference on AI Engineering-Software Engineering for AI*, pages 166–171.
- Steve McConnell. 1998. *Software project survival guide*. Pearson Education.
- Niklas Muennighoff, Qian Liu, Armel Zebaze, Qinkai Zheng, Binyuan Hui, Terry Yue Zhuo, Swayam Singh, Xiangru Tang, Leandro von Werra, and Shayne Longpre. 2023. Octopack: Instruction tuning code large language models. *arXiv preprint arXiv:2308.07124*.
- OpenAI. 2025. [Prompt generation](#).
- Long Ouyang, Jeffrey Wu, Xu Jiang, Diogo Almeida, Carroll Wainwright, Pamela Mishkin, Chong Zhang, Sandhini Agarwal, Katarina Slama, Alex Ray, and 1 others. 2022. Training language models to follow instructions with human feedback. *Advances in neural information processing systems*, 35:27730–27744.
- Yiwei Qin, Kaiqiang Song, Yebowen Hu, Wenlin Yao, Sangwoo Cho, Xiaoyang Wang, Xuansheng Wu, Fei Liu, Pengfei Liu, and Dong Yu. 2024. Infobench: Evaluating instruction following ability in large language models. *arXiv preprint arXiv:2401.03601*.
- Chandan K. Reddy, Lluís Márquez, Fran Valero, Nikhil Rao, Hugo Zaragoza, Sambaran Bandyopadhyay, Arnab Biswas, Anlu Xing, and Karthik Subbian. 2022. Shopping queries dataset: A large-scale ESCI benchmark for improving product search. *arXiv preprint arXiv:2206.06588*.
- Victor Sanh, Albert Webson, Colin Raffel, Stephen H Bach, Lintang Sutawika, Zaid Alyafeai, Antoine Chaffin, Arnaud Stiegler, Teven Le Scao, Arun Raja, and 1 others. 2021. Multitask prompted training enables zero-shot task generalization. *arXiv preprint arXiv:2110.08207*.
- Melanie Sclar, Yejin Choi, Yulia Tsvetkov, and Alane Suhr. 2023. Quantifying language models’ sensitivity to spurious features in prompt design or: How i learned to start worrying about prompt formatting. *arXiv preprint arXiv:2310.11324*.
- Shreya Shankar, JD Zamfirescu-Pereira, Björn Hartmann, Aditya Parameswaran, and Ian Arawjo. 2024. Who validates the validators? aligning llm-assisted evaluation of llm outputs with human preferences. In *Proceedings of the 37th Annual ACM Symposium on User Interface Software and Technology*, pages 1–14.
- Ian Sommerville. 2015. *Software Engineering*, 10th edition. Pearson.
- Mingjie Sun, Yida Yin, Zhiqiu Xu, J Zico Kolter, and Zhuang Liu. 2025. Idiosyncrasies in large language models. *arXiv preprint arXiv:2502.12150*.
- Annalisa Szymanski, Simret Araya Gebreegziabher, Oghenemaro Anuyah, Ronald A Metoyer, and Toby Jia-Jun Li. 2024. Comparing criteria development across domain experts, lay users, and models in large language model evaluation. *arXiv preprint arXiv:2410.02054*.
- Mahan Tafreshipour, Aaron Imani, Eric Huang, Eduardo Almeida, Thomas Zimmermann, and Iftekhar Ahmed. 2024. Prompting in the wild: An empirical study of prompt evolution in software repositories. *arXiv preprint arXiv:2412.17298*.
- Axel Van Lamsweerde. 2009. *Requirements engineering: From system goals to UML models to software*, volume 10. Chichester, UK: John Wiley & Sons.
- Sanidhya Vijayvargiya, Xuhui Zhou, Akhila Yerukola, Maarten Sap, and Graham Neubig. 2025. Interactive agents to overcome ambiguity in software engineering. *arXiv preprint arXiv:2502.13069*.
- Chenyang Yang, Rishabh Rustogi, Rachel Brower-Sinning, Grace Lewis, Christian Kaestner, and Tongshuang Wu. 2023. Beyond testers’ biases: Guiding model testing with knowledge bases using llms. In *Findings of the Association for Computational Linguistics: EMNLP 2023*, pages 13504–13519.
- J Diego Zamfirescu-Pereira, Richmond Y Wong, Bjoern Hartmann, and Qian Yang. 2023. Why johnny can’t prompt: how non-ai experts try (and fail) to design llm prompts. In *Proceedings of the 2023 CHI conference on human factors in computing systems*, pages 1–21.
- Zhiyuan Zeng, Yizhong Wang, Hannaneh Hajishirzi, and Pang Wei Koh. 2025. Evaltree: Profiling language model weaknesses via hierarchical capability trees. *arXiv preprint arXiv:2503.08893*.

Michael JQ Zhang and Eunsol Choi. 2023. Clarify when necessary: Resolving ambiguity through interaction with lms. *arXiv preprint arXiv:2311.09469*.

Tong Zhang, Peixin Qin, Yang Deng, Chen Huang, Wenqiang Lei, Junhong Liu, Dingnan Jin, Hongru Liang, and Tat-Seng Chua. 2024. Clamber: A benchmark of identifying and clarifying ambiguous information needs in large language models. *arXiv preprint arXiv:2405.12063*.

Chenyang Zhao, Xueying Jia, Vijay Viswanathan, Tongshuang Wu, and Graham Neubig. 2024. Self-guide: Better task-specific instruction following via self-synthetic finetuning. *arXiv preprint arXiv:2407.12874*.

Lianmin Zheng, Wei-Lin Chiang, Ying Sheng, Siyuan Zhuang, Zhanghao Wu, Yonghao Zhuang, Zi Lin, Zhuohan Li, Dacheng Li, Eric Xing, and 1 others. 2023. Judging llm-as-a-judge with mt-bench and chatbot arena. *Advances in Neural Information Processing Systems*, 36:46595–46623.

Han Zhou, Xingchen Wan, Ruoxi Sun, Hamid Palangi, Shariq Iqbal, Ivan Vulić, Anna Korhonen, and Serkan Ö Arik. 2025. Multi-agent design: Optimizing agents with better prompts and topologies. *arXiv preprint arXiv:2502.02533*.

Jeffrey Zhou, Tianjian Lu, Swaroop Mishra, Siddhartha Brahma, Sujoy Basu, Yi Luan, Denny Zhou, and Le Hou. 2023. Instruction-following evaluation for large language models. *arXiv preprint arXiv:2311.07911*.

## A Details on Experiments Setups

### A.1 Task descriptions

We selected three tasks based on Anthropic’s report measuring AI usage patterns (Handa et al., 2025):

- **trip-advisory**: Provide personalized travel recommendations, itineraries, and tips.
- **product-gen**: Write engaging product descriptions from the provided product details.
- **code-explain**: Explain a code snippet for learning purposes.

### A.2 Process of data sampling and cleaning

We re-purposed three existing datasets to run the LLM+Prompts on: Commitpackft (Muennighoff et al., 2023) for code explanation (MIT license), a subset of UltraChat (Ding et al., 2023) for trip advisory (MIT License), and Amazon ESCI (Reddy et al., 2022) for product description generation (Apache-2.0 License).

- For Commitpackft, we take the python split<sup>3</sup>, we keep all examples with more than 90 lines

<sup>3</sup><https://huggingface.co/datasets/bigcode/commitpackft>

of code (n=357), and then take the first 200 examples.

- For UltraChat, we take a travel-related subset<sup>4</sup> and keep the first 800 examples. We then use gpt-4o-mini to label if each query is asking for travel recommendations, itineraries, and tips, and filter out the queries that are not (n=248 remains). We then take the first 200 examples.
- For Amazon ESCI, we take the test split<sup>5</sup>, filter out the examples that are not based in US and not in English, and remove duplicated products. We then sample 200 examples from the dataset.

From each dataset, we split it into training, validation, and test data with 15/35/50 split. All our evaluation results are reported based on the test split. All datasets are available in our shared code repository.

### A.3 Process of requirements curation

From each task, we curated an initial list of requirements through the three different sources described in Section 3. We found existing prompts provided by Anthropic, Google and GPTs<sup>6</sup> (Figure 7). We kept all requirements that are curated from existing prompt, as they already approved by some human developers.

For requirements we elicited with two other approaches, we use `text-embedding-ada-002` to generate embeddings of each requirement and remove ones with high cosine similarity (> 0.9) to other existing requirements incrementally. After this step, we curate 38, 39, and 40 requirements for `trip-advisory`, `product-gen`, and `code-explain` tasks respectively.

We then filtered out the requirements that are overly specific (e.g., “*The output must explain how the product’s features enhance the karaoke experience for the targeted age group.*”), and finally had three independent annotators select important requirements. We recruited the annotators from our contacts and ensured that they all have sufficient

<sup>4</sup><https://huggingface.co/datasets/soniameyer/travel-conversations-finetuning>

<sup>5</sup><https://huggingface.co/datasets/tasksource/esci>

<sup>6</sup><https://docs.anthropic.com/en/prompt-library/code-clarifier>,  
<https://github.com/google-marketing-solutions/feedgen/blob/main/img/config.png>,  
<https://github.com/yourzxb/GPTs/blob/main/17/TripAdvisor.md>

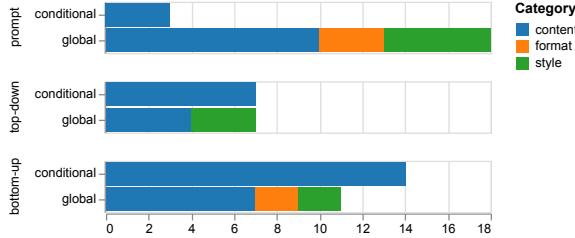


Figure 5: We gather 60 requirements for our analysis. The majority of requirements come from bottom-up error analysis (41.7%), followed by existing prompts (35%), and top-down brainstorming (23.3%). Most requirements specify content-related constraints (75%), followed by style (16.7%) and format (8.3%). Most requirements are global and apply to all examples (60%), while 40% are conditional requirements. We found that existing prompts rarely consider conditional requirements (only 14.3%).

background knowledge for the task they need to annotate (e.g., all three annotators are in a computer science PhD program for the code explanation task). The annotators have access to a short annotation rubric, including an instruction that asks them to mark up important requirements for the task and add justifications when needed, a task description, and example inputs to ground their annotations (Figure 6). The annotation process takes up to 20 minutes, and the annotators are not compensated for their time. We verbally communicated to the annotators that their selected requirements will be used for later experiments.

We kept the requirements selected by human annotators in the end, with 20 requirements for each and a total of 60 requirements as in Section A.5. The final list of requirements cover different categories (content, style, format), different scopes (global, conditional), as visualized in Figure 5.

We provide all requirements used in our experiments in the shared code repository, <https://github.com/malusamayo/underspec-analysis/tree/main/data/requirements>, along with their validators.

Instruction: Review the provided **list** of requirements and select up to 10 that you believe are the most important for the task. For each selected requirement, include a brief justification explaining why it is important.

Task description: Explain the code snippet.

Sample inputs:

```
```python
from sqlalchemy.exc import IntegrityError

from ggrc import db
from ggrc import models
from integration.ggrc import TestCase

class TestCAD(TestCase):
    """Tests for basic functionality of cad model."""
    def test_setting_reserved_words(self):
        """Test setting any of the existing attribute names."""
        with self.assertRaises(ValueError):
            cad = models.CustomAttributeDefinition()
            cad.definition_type = "Section"
            cad.title = "title"

        with self.assertRaises(ValueError):
            cad = models.CustomAttributeDefinition()
            cad.title = "title"
            cad.definition_type = "Section"
```

```

Figure 6: Sample annotator instruction during requirement curation.

Your task is to take the code snippet provided and explain it in simple, easy-to-understand language. Break down the 'code's functionality, purpose, and key components. Use analogies, examples, and plain terms to make the explanation accessible to someone with minimal coding knowledge. Avoid using technical jargon unless absolutely necessary, and provide clear explanations for **any** jargon used. The goal is to **help** the reader understand what the code does and how it works at a high level.

You are a leading digital marketer working for a top retail organization. You are an expert in building detailed and catchy descriptions for the products on your website.

Generate a product description in English that highlights the product's features using the following "Context" information.

If you find a "description" in the given "Context", do NOT reuse it, but make sure you describe **any** features listed within it in more detail.

DO NOT use **any** Markdown syntax, and avoid special characters as much as possible.

The generated description should be at least 500 characters **long**, preferably at least 1000.

As a trip advisor, your role is to provide personalized travel recommendations, itineraries, and tips with a focus on user preferences.

- Specialize in destinations, accommodations, activities, dining, and cultural insights, considering budget, travel dates, and specific interests.
- Ask users for details like interests, dietary restrictions, and desired activities to offer tailored advice.
- Avoid booking or transaction handling.
- Your approach should be friendly, casual, and enthusiastic about travel, ensuring responses are personalized to user goals.
- Be clear and engaging, with a tone that's helpful, casual, and culturally sensitive.
- Clarify **any** ambiguous preferences.
- Show enthusiasm for exploring new cultures and experiences.

Figure 7: Existing prompts for the three studied tasks. We extracted a subset of requirements from these prompts and constructed a set of synthetic prompts with the prompt templates in Appendix A.7

#### A.4 Prompts for requirements elicitation and validation

You are an experienced requirements engineer. Your goal is to brainstorm a **list** of requirements that specify desired LLM behaviors for the given task. These requirements should identify behaviors that, if omitted, would likely frustrate or annoy users -- such as forgetting to surface important reminders, warnings, or common-sense.

These requirements should be consistent with each other without contradictions and complementary to existing requirements.

Guidelines:

- Each requirement should test exactly ONE requirement
- Requirements should be easily verifiable, almost as if writing a Boolean condition in Python. They should be testable with Python code or an LLM itself (no human judgment or external sources needed).
- Requirements should not be overly general (i.e. they should not be universal requirements that might **apply to any** reasonable response)
- Requirements should be generally applicable for responses to that task, not referring to **any** specific response
- Avoid unrealistic edge cases - focus on plausible failures that could occur even in aligned or well-trained LLMs.
- Focus only on objective, measurable requirements
- Use concise and unambiguous language
- Never generate similar requirements to the existing requirements

You are an experienced requirements engineer. Your goal is to extract a **list** of atomic requirements that specify desired LLM behaviors for the given task.

You will be presented with a model **input** and several model outputs from different models. First, provide a detailed analysis critiquing the model outputs. Then, based on the analysis, suggest a **list** of atomic requirements that specify desired LLM behaviors for the given task. These requirements should be consistent with each other without contradictions and complementary to existing requirements.

Guidelines:

- Each requirement should test exactly ONE requirement
- Requirements should be easily verifiable, almost as if writing a Boolean condition in Python
- Requirements should not be overly general (i.e. they should not be universal requirements that might **apply to any** tasks)
- Requirements should be generally applicable for responses to that task, not referring to **any** specific **input** examples
- Focus only on objective, measurable requirements
- Use concise and unambiguous language
- The requirements should be consistent with each other without contradictions
- The requirements should not overlap with existing requirements

Here are some bad requirements:

- The output should be interesting. - This is subjective
- The output should provide examples in fewer than 280 characters. - This overloads multiple aspects
- The output should be helpful and harmless. - This is overly general

Here are some good atomic requirements:

- The output should provide examples.
- The output should be fewer than 280 characters.
- The output should contain at least 3 references.

Figure 8: Prompts for requirement elicitation - Brainstorming.

Figure 9: Prompts for requirement elicitation - Error analysis.

You are a reviewer who is evaluating whether a model output satisfies the given requirement. Given a task description, examples, and requirement, draft a step-by-step evaluation plan for the requirement.

Follow the guideline below:

- The evaluation plan should be a step-by-step process to evaluate if the requirement is met.
- The evaluation plan should be concise and clear, and lead to a final judgment on whether the model output meets the requirement.
- When requirements are conditional (e.g., indicated by "if applicable"), the evaluation plan should include a first step to check if the requirement is applicable to an example **input**.
- The evaluation plan should only include the steps to evaluate the requirement, and not include **any** additional feedback or suggestions, or steps to evaluate other related requirements.

Examples

---

Requirement: The explanation should provide examples of how to instantiate and use key classes, if applicable.

Evaluation Plan:

1. Identify the key classes in the given code snippet by examining the code structure and class definitions. If there are no key classes, this requirement is not applicable.
2. Check that the explanation clearly highlights which classes are considered "key" for this snippet (for example, **any** classes that define core functionality or are central to the code's purpose).
3. Verify that the explanation includes concrete examples showing how to instantiate the identified key classes.
4. Finally, assess whether the explanation meets the requirement by providing sufficient instantiation and usage examples that a user could follow.

You are a reviewer who is evaluating whether a model output satisfies the given requirement. Given a task description, examples, and requirement, write a Python function to evaluate the requirement.

The Python function `evaluation\_function` takes `task_description`, `model_input`, and `model_output` as **input** arguments and returns a boolean value indicating whether the requirement is met.

You are a reviewer who is evaluating whether a model output satisfies the given requirement.

Given a task description, model **input**, model output, a requirement and its step-by-step evaluation plan, execute the evaluation plan to evaluate if the model output meets the requirement. If the requirement is not applicable, return True for `meets_requirement`.

Figure 10: Prompts for requirement evaluation: Planning (top and middle) and execution (bottom).

## A.5 Complete list of curated requirements

### Curated requirements for trip-advisory

- The output should consider factors such as budget, travel dates, and specific interests.
- The output should ask users for details like interests, dietary restrictions, and desired activities.
- The output should not include booking or transaction handling.
- The output should be friendly, casual, and enthusiastic about travel.
- The output should be personalized to user goals and preferences.
- The output should be clear and engaging.
- The output should be culturally sensitive.
- The output should clarify any ambiguous preferences.
- The output should show enthusiasm for exploring new cultures and experiences.
- The output should ensure activities are age-appropriate if age preferences are specified by the user.
- The output should highlight any visa or entry requirements specific to the suggested destinations.
- The output should provide warnings about weather conditions that might affect accessibility to certain activities during the user's planned travel dates.
- The output should provide follow-up questions to solicit user preferences if they are not initially provided.
- The output should clarify the geographic context if the location is ambiguous.
- The output should specify if transportation options are seasonal or subject to availability.
- The output should include suggestions for public transport or alternative travel methods.
- The output should correctly identify and focus on sites located within the specified geographic area.
- The output should provide references to local regulations or park rules, when applicable.
- The output should contain a section explicitly stating safety guidelines specific to solo traveling.
- The output should include tips for varying levels of experience for recommended activities.

## Curated requirements for product-gen

- The output must highlight the product's features.
- The output must be written in English.
- The output must describe any features listed within the given Context in more detail.
- The output must be at least 500 characters long.
- The output should preferably be at least 1000 characters long.
- The output must not use Markdown syntax.
- The output must avoid special characters as much as possible.
- The output must avoid excessive use of technical jargon, ensuring that the description is understandable to a general audience.
- The output must use engaging and vivid language to capture and retain the reader's attention.
- The output must include at least three benefits that the product provides to the user.
- The output must follow a coherent structure, ensuring logical flow from introduction to conclusion.
- The output must avoid any explicit comparisons with products from brands unless specified in the context.
- The output must ensure that any numerical values or ranges are accurately represented if mentioned at all.
- The output must include a mention of the package content.
- The output should clearly mention any customer support or warranty information included with the product.
- The product description should mention any personalization options available, including any important limitations or specifications.
- The output must paint a vivid picture of the customer experience with practical use cases.
- The output should break down complex information into clearer, more concise points.
- The output must be free from any promotional prompts such as 'click add to cart'.
- The output must ensure that key product information is easily skimmable.

### Curated requirements for code-explain

- The output should break down the code's functionality.
- The output should explain the purpose of the code.
- The output should use analogies and examples to clarify the explanation.
- If technical jargon is used, the output should provide clear explanations for it.
- The output should aim to make the explanation accessible to someone with minimal coding knowledge.
- The output should identify and explain any variables or data structures used in the code snippet.
- The output should detect and describe any dependencies or libraries required by the code snippet.
- The output should check and explain any potential side effects or state changes that occur during code execution.
- The output should include a precise, step-by-step execution order that aligns with the code.
- If there are error handling mechanisms, the output should accurately describe them and explain how they handle potential errors.
- The output should mention any missing components or aspects in the provided code snippet, such as lack of functionality or completeness.
- The output should explain scenarios where certain features of the code are particularly beneficial or efficient.
- The explanation should include potential applications and implications of the coded algorithm.
- The output should address potential edge cases tested by the code.
- The output should explicitly define the scope of explanation without making assumptions about specific use cases.
- The output should not exceed 500 words to maintain conciseness and focus.
- The output should not describe components or operations not present in the provided code.
- The output should provide a high-level summary at the beginning to set the context.
- The output should provide an example of how at least one function, class, or constant imported from the code can be used.
- The output should include information about verifying the setup or configuration before execution, if applicable.

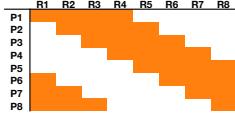


Figure 11: We use a cyclic design to generate prompts. Each prompt (row) covers the same number of  $k$  consecutive requirements (column). Each requirement is specified  $k$  times and unspecified  $N - k$  times exactly. We randomize the order of requirements to distribute requirements from different sources.

## A.6 Human validation of LLM validators

To assess the reliability of our LLM-based requirement evaluators, we curated a set of 1,095 evaluation results for human validation. The evaluation results are curated with stratified sampling: We sample 20 evaluation results (10 positive, 10 negative) per requirement. If there are not enough results (e.g., when a requirement is almost always satisfied), we take the maximum number available.

We then have a human annotator manually review the evaluations. For each model output, the annotator compared the predicted label against their own judgment of whether the output satisfied the given requirement. Overall, the evaluators have 95.6% ( $SD=0.08$ ) agreement rates, indicating a reasonably high level of human–LLM agreement.

## A.7 Prompt templates and construction

We use a simple prompt template to construct our experiment prompts. The task descriptions are one-line minimal descriptions as shown in Appendix A.1.

### Prompt template for our experiments

[Task description]

Follow the guideline below:

- [requirement 1]
- [requirement 2]
- ...
- [requirement N]

In our experiments, our goal is to systematically cover requirement subsets, to make sure (a) each prompt has roughly the same complexity in terms of the number of requirements to follow, and (b) different requirements are specified or unspecified the same number of times. We use a simple cyclic design to achieve this, as shown in Figure 11.

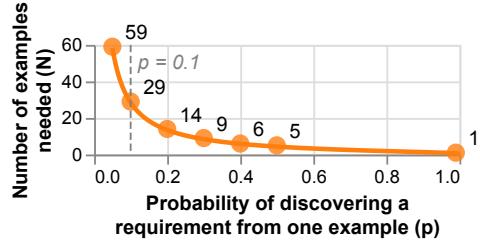


Figure 12: To discover an unspecified requirement reliably with 95% probability, developers need to inspect a lot more examples ( $N \uparrow$ ) when the requirement appears less frequently, gets violated less, or is harder to detect ( $p \downarrow$ ).

## A.8 Compute resources used in the experiments

In our first set of experiments (up to Section 3.3), we make 6k inferences with each of the 7 models to obtain model outputs. We then make 840k inferences to evaluate the results with gpt-4.1-mini.

In our second experiment (Section 3.4), we make 6k inferences with each of the two models on 3 different prompt configurations (different numbers of requirements). We then make 720k inferences to evaluate the results with gpt-4.1-mini.

For prompt optimization experiments (Section 4), we make 16.2k inferences with each prompt optimizer to produce all optimized prompts (324k inferences for evaluation). We then make 6k inferences with 4 different optimization results each (480k inferences for evaluation).

For LLM validators, we used a temperature of 0 to extract the most likely prediction. For other inference calls, we used the recommended temperature in best practices (1.0 for gpt-4o models and 0.6 for Llama-3 models.) The maximum tokens are set to 4096, and all other inference parameters are set to default values.

## B Detailed Analysis on Requirements Discovery

If underspecified prompts are more unstable, could developers discover *relevant* task requirements in the first place? We argue that this is rather challenging with current manual trial-and-error prompt engineering practices, where developers examine examples in an ad-hoc fashion and iterate their prompts only when they observe outputs that violate their expectations (Liang et al., 2024).

First, many requirements are *conditional* and can easily be missed when developers only look at a few representative examples – for example, “*accurate numerical values in summaries*” is only

relevant to inputs containing numerical values. When the probability of encountering such inputs ( $p_{\text{relevant}}$ ) is low, the requirement is likely not to be covered within a few inspections. However, our previous analysis demonstrates that conditional requirements are exactly where LLMs struggle more.

Second, some requirements may be violated less frequently ( $p_{\text{violated}}$ ), and thus less likely to be discovered via observing violations. Yet they can still be critical, such as high-stakes safety requirements for trip advisory – e.g., “*no dangerous activities suggested.*” In other cases, violations may be harder to recognize, with a lower probability of being noticed ( $p_{\text{noticed}}$ ), as in “*ensuring correct program execution in code explanations.*” Moreover, when developers inspect LLM outputs, their assessments are biased by prior knowledge and subjective interpretation, which can lead them to overlook certain types of requirements (Szymanski et al., 2024).

Considering these factors, an unspecified requirement may require significant efforts or luck to be discovered with the current practice. Quantitatively, a developer will need to look at  $N = \log(1 - p_s) / \log(1 - p_{\text{relevant}} \cdot p_{\text{violated}} \cdot p_{\text{noticed}})$  examples to discover the requirement with probability  $p_s$  (e.g., 0.95), assuming independent Bernoulli trials. For example, a *conditional* requirement that is relevant to 20% of examples, violated 50% of the time, and perfectly noticeable will require inspecting more than 29 examples to be detected with 95% probability (Figure 12). This will be an excessive workload for a human to complete on their own for every single model update or prompt change, assuming they have access to a diverse dataset, if at all.

## C Additional experiment results

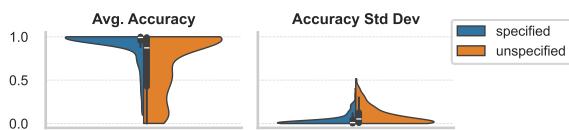


Figure 13: Comparing LLM+Prompts performances on specified requirements vs. unspecified requirements, we found that, overall, LLM+Prompts perform worse and diverge more for unspecified requirements. This is statistically significant even if we consider all other factors and explains a large portion of the variances observed (Table 4).

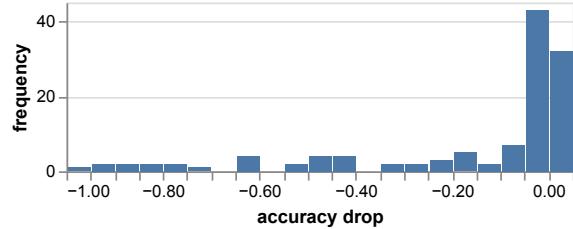


Figure 14: The histogram of average requirement accuracy drops when the prompts include more requirements ( $N=1 \rightarrow 19$ ). We found 37.5% requirements drop significantly by more than 5%.

### C.1 Requirement guess rates breakdown

We break down how often LLMs can “guess” requirements and satisfy them without specification (Table 3). We found that LLMs excel at global, format-related, and prompt-sourced requirements, but struggle with conditional, style-related, and bottom-up requirements.

| Fill-in Rate         |       |
|----------------------|-------|
| Requirement Scope    |       |
| Conditional          | 22.9% |
| Global               | 53.2% |
| Requirement Source   |       |
| Bottom-up            | 21.5% |
| Prompt-sourced       | 65.2% |
| Top-down             | 40.0% |
| Requirement Category |       |
| Content              | 39.9% |
| Format               | 70.7% |
| Style                | 32.0% |
| Average              | 41.1% |

Table 3: Requirement guess rates breakdowns.

### C.2 ANOVA results

We apply ANOVA to analyze how factors like requirement *scope*, *source*, *category*, or *model* impact LLM+Prompts performance on specified vs. unspecified requirements. For factors that are significant, we use Tukey’s HSD test to identify which specific group means are significantly different from each other. Results are reported in Table 4.

### C.3 Requirements Conflict Analysis

When we analyze the variances in *specified* requirements, we observe that they are partially caused

|                     | Avg. accuracy | SD of accuracy | Acc. delta | SD delta |
|---------------------|---------------|----------------|------------|----------|
| <b>Specified?</b>   | 125.87***     | 48.47***       | -          | -        |
| <b>Conditional?</b> | 19.01***      | 16.38***       | 4.55*      | 3.03     |
| <b>Source</b>       | 19.99***      | 36.83***       | 9.07***    | 3.63*    |
| <b>Category</b>     | 23.86***      | 55.00***       | 1.01       | 0.44     |
| <b>Model</b>        | 1.80          | 0.57           | 0.68       | 1.71     |

\*\*\* $p < 0.001$ , \*\* $p < 0.01$ , \* $p < 0.05$

Table 4: ANOVA results: We report the F-value and p-value, which quantify the extent to which each variable accounts for the observed variances. We found that whether a requirement is specified has the largest impact on average accuracy (+0.2) and a significant impact on SD (-0.037). Breaking down the requirements, we found models struggle with conditional requirements (-0.09 accuracy, +0.017 SD), but are better at requirements found in existing prompts and format-related requirements.

by requirement conflicts (e.g., making product descriptions more skimmable conflicts with other formatting requirements).

To better understand which requirements conflict, we conducted an analysis on requirement behaviors: For each requirement, we calculated its average accuracy *conditioned* on whether another requirement was specified alongside it or left unspecified. We found that approximately 11.4% of requirement pairs exhibited clear conflicts, defined as cases where specifying one requirement caused the accuracy of another to drop by more than 5%. For example, the requirement “*accessible to someone with minimal coding knowledge*” conflicted with others such as “*describe error handling*” or “*describe any dependencies or libraries*,” with drops in accuracy of up to 41.1%.

Next, we assess how conflicts impact our results on requirement variances across prompts. To assess this, we excluded all requirements showing any signs of conflict (i.e., cases where specifying one requirement reduced the accuracy of another by more than 5%) and recomputed the variance in accuracy across prompts.

After removing these conflicting requirements, **we found the difference in prompt variance became even more pronounced:** 0.8% for specified requirements versus 7.1% for unspecified ones. This suggests that prompt instability on specified requirements often stems from conflicting requirements being included in the same prompt. In contrast, instability on unspecified requirements remains high even when no conflicts are present, highlighting that models are inconsistent in how they fill in missing constraints. For instance, the requirement “*explicitly state safety guidelines spe-*

*cific to solo traveling*” exhibited large variance across prompts when left unspecified, even though it did not conflict with other requirements in the task. This indicates that the instability arises from underspecification itself, rather than requirement interaction.

#### C.4 Prompt Optimization Examples

## An example of unoptimized prompts

Explain the code snippet.

Follow the guideline below:

- The output should explain the purpose of the code.
- The output should explain scenarios where certain features of the code are particularly beneficial or efficient.
- The output should use analogies and examples to clarify the explanation.
- The output should not describe components or operations not present in the provided code.
- The output should check and explain any potential side effects or state changes that occur during code execution.
- The output should include a precise, step-by-step execution order that aligns with the code.
- The output should break down the code's functionality.
- If technical jargon is used, the output should provide clear explanations for it.
- The output should include information about verifying the setup or configuration before execution, if applicable.
- The output should identify and explain any variables or data structures used in the code snippet.
- The output should explicitly define the scope of explanation without making assumptions about specific use cases.
- The output should aim to make the explanation accessible to someone with minimal coding knowledge.
- If there are error handling mechanisms, the output should accurately describe them and explain how they handle potential errors.
- The output should address potential edge cases tested by the code.
- The output should not exceed 500 words to maintain conciseness and focus.
- The output should provide an example of how at least one function, class, or constant imported from the code can be used.
- The output should detect and describe any dependencies or libraries required by the code snippet.
- The explanation should include potential applications and implications of the coded algorithm.
- The output should provide a high-level summary at the beginning to set the context.

Figure 15: Unoptimized prompts generated from the prompt template (acc=75.4%).

## An example of COPRO-optimized prompts

Provide a detailed explanation of the given code snippet, following these guidelines:

1. **Overview**: Begin with a high-level summary that sets the context for the code's purpose and functionality.
2. **Purpose and Benefits**: Clearly explain the code's main objective and highlight scenarios where its features are particularly beneficial or efficient.
3. **Analogy and Examples**: Use relatable analogies and examples to enhance understanding, especially for complex concepts.
4. **Code Breakdown**: Decompose the code into its fundamental components, explaining the role and function of each part.
5. **Step-by-Step Execution**: Offer a precise, sequential walkthrough of how the code executes, ensuring clarity on the process.
6. **State Changes and Side Effects**: Identify any potential side effects or state changes that occur during execution.
7. **Variable and Data Structure Explanation**: Define and explain any variables or data structures used, ensuring comprehension for those with minimal coding knowledge.
8. **Technical Jargon**: Simplify or clarify any technical terms to make the explanation accessible.
9. **Setup Verification**: Include information on verifying the setup or configuration before running the code, if relevant.
10. **Error Handling**: Describe any error handling mechanisms, detailing how they manage potential errors and edge cases.
11. **Dependencies**: Identify any libraries or dependencies required by the code.
12. **Applications and Implications**: Discuss potential applications and implications of the algorithm or functionality provided by the code.
13. **Function Usage Example**: Provide an example of how at least one function, class, or constant from the code can be utilized.
14. **Conciseness**: Ensure the explanation does not exceed 500 words, maintaining focus and clarity.

Figure 16: COPRO-optimized prompts (acc=86.7%). We found COPRO-optimized prompts tend to reorder requirements in a more logical structure, merge related requirements together, and sometimes drop requirements.