# **Valuable Hallucinations: Realizable Non-Realistic Propositions**

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#### **Abstract**

This paper clarifies the specific connotation of beneficial hallucinations in large language models (LLMs), addressing a gap in the existing literature. We provide a systematic definition and analysis of hallucination value, proposing methods for enhancing the value of hallucinations. In contrast to previous works, which often treat hallucinations as a broad flaw, we focus on the potential value that certain types of hallucinations can offer in specific contexts. Hallucinations in LLMs generally refer to the generation of unfaithful, fabricated, inconsistent, or nonsensical content. Rather than viewing all hallucinations negatively, this paper clarifies the specific connotation of valuable hallucinations and explores how realizable non-realistic propositions—ideas that are not currently true but could be achievable under certain conditions—can have constructive value.

We evaluate the Qwen-3-0.6B, Qwen2.5-72B-Instruct and DeepSeek-R1-671B models on the HalluQA dataset using ReAct prompting, which incorporates reasoning, confidence assessment, and answer verification to control and optimize hallucinations. ReAct reduces overall hallucinations by 4.67%, 5.12% and 8.45% in Qwen-3-0.6B, Qwen2.5-72B-Instruct and DeepSeek-R1-671B, respectively, while increasing the proportion of valuable hallucinations from 0% to 4.01%, from 6.45% to 7.92%, and from 1.12% to 7.84%. These results suggest that systematically controlling hallucinations can improve their usefulness without compromising factual reliability. <sup>1</sup>

# 1 Introduction

#### 1.1 Background and Problem Statement

In recent years, large language models (LLMs) (Google, 2023; OpenAI, 2022; Penedo et al., 2023;

Touvron et al., 2023; Zhao et al., 2023b) have achieved remarkable progress in the field of natural language processing (NLP), significantly advancing capabilities in language understanding (Hendrycks et al., 2020; Huang et al., 2023b), generation (Zhang et al., 2024; Zhu et al., 2023), and reasoning (Chu et al., 2023; Kojima et al., 2022; Qiao et al., 2022; Wei et al., 2022; Yu et al., 2024). However, alongside these rapid advancements, a concerning issue has emerged: these models tend to generate hallucinations (Li et al., 2023b; Liu et al., 2024; Zhou et al., 2023), content that appears plausible but is factually incorrect or unfaithful to the input (Bai et al., 2024). Hallucinations pose significant challenges in truth-sensitive domains such as finance (Kang and Liu, 2023), law (Curran et al., 2023), science (Alkaissi and Mcfarlane, 2023; Duede, 2022), and education (Zhou et al., 2024).

The predominant perspective in current literature emphasizes the detrimental aspects of hallucinations, particularly their negative impact on LLM reliability (Mallen et al., 2022). While some studies have noted creative applications, systematic approaches to identifying and cultivating valuable hallucinations remain underdeveloped. Consequently, numerous studies have focused on mitigating hallucinations through fact-centric metrics (Goodrich et al., 2019; Guerreiro et al., 2022; Mishra et al., 2020; Shuster et al., 2021a), benchmarks (Li et al., 2023a; Lin et al., 2021; Vu et al., 2023), and retrieval-augmented generation (RAG) techniques(Shuster et al., 2021a; Zhao et al., 2023a). Despite these efforts, Banerjee et al. (Banerjee et al., 2024) and Xu et al. (Xu et al., 2024) have demonstrated that hallucinations are inherent to LLMs, arising from their underlying mathematical and logical structures, and cannot be entirely eliminated through architectural improvements, dataset enhancements, or fact-checking mechanisms.

<sup>&</sup>lt;sup>1</sup>The paper uses an AI assistant to refine the expression of certain sections, but the research and coding parts of the paper were entirely conducted without the use of AI.

# 1.2 Research Motivation and Limitations of Existing Work

While most research treats hallucinations as entirely harmful, a small but growing body of work has begun to explore their potential value. For instance, Sui et al. (Sui et al., 2024) suggest that hallucinations exhibit rich patterns of narrative behavior, while Wiggers (Wiggers, 2023) refers to them as collaborative creative partners. In practical applications, Yuan et al. (Yuan and Färber, 2025) found that hallucinations can enhance the performance of LLMs in drug discovery tasks, and Wang (Wang, 2024) demonstrated beneficial interactions between hallucinations and creativity in a multimodal AGI model. In scientific research, the creativity of LLMs has been shown to expand the boundaries of human knowledge and assist researchers in achieving breakthroughs (Jablonka et al., 2023).

However, existing studies on the positive effects of hallucinations are fragmented and lack a systematic definition or analysis. This paper aims to address this gap by introducing the concept of "valuable hallucinations" and providing a formal definition and classification framework.

#### 1.3 Core Contributions of This Work

The core contributions of this paper are as follows:

- Introducing the Concept of "Valuable Hallucinations": We define "valuable hallucinations" as realizable but non-realistic propositions.
   These propositions, if realized, could offer innovative and inspiring ideas, providing new perspectives or solutions to real-world problems.
- Systematic Classification and Analysis: Building on existing hallucination taxonomies (e.g., intrinsic-extrinsic dichotomy and factuality vs. faithfulness hallucinations), we identify which types of hallucinations can be valuable. We emphasize that realizable but non-realistic propositions fall under the category of "valuable hallucinations."
- Experimental Validation: We design a set of comparative experiments using Qwen 3-0.6B (Team, 2025), Qwen2.5-72 B-Instruct (Hui et al., 2024) and DeepSeek-R1-671B model (DeepSeek-AI, 2025). By employing prompt engineering and reflection techniques,

we demonstrate that these methods can effectively control hallucinations and increase the proportion of valuable hallucinations in model outputs.

Future Research Directions: We propose potential methods for further controlling and utilizing hallucinations, such as combining retrieval-augmented generation (RAG) and meta-learning, providing a roadmap for future research in this area.

#### 2 Definitions

#### 2.1 Hallucinations

The term "hallucination" originates from the fields of pathology and psychology, where it refers to the perception of entities or events that do not exist in reality (Macpherson and Platchias, 2013). In the context of natural language processing (NLP), hallucination in LLMs typically refers to the generation of unfaithful, fabricated, inconsistent, or nonsensical content (Weng, 2024). Hallucinations occur when LLMs produce outputs that deviate from the input prompts or factual reality, often due to limitations in their training data or reasoning capabilities.

While hallucinations are generally considered harmful, this paper focuses on a specific subset of hallucinations that may have potential value, which we term "valuable hallucinations."

#### 2.2 Valuable Hallucinations

The challenge of balancing creativity and factual accuracy in LLMs is a central issue in their development (Mukherjee and Chang, 2023; Lee, 2023). While most research aims to mitigate or eliminate hallucinations, Banerjee et al. (Banerjee et al., 2024) and Xu et al. (Xu et al., 2024) have demonstrated that hallucinations are inherent to LLMs and cannot be entirely eradicated. Therefore, rather than attempting to eliminate hallucinations, we propose to identify and utilize their "valuable" aspects.

#### 2.2.1 Definition of Valuable Hallucinations

We define valuable hallucinations as realizable but non-realistic propositions. These are propositions that, while not grounded in current reality, could be realized in the future and may offer innovative or inspiring ideas. The "value" of these hallucinations can be assessed through feedback, particularly human feedback, in reinforcement learning frameworks. The value of LLM outputs can be understood in two ways:

Innovation and Inspiration: Valuable hallucinations can propose innovative (and understandably unrealistic) propositions or inspire humans to formulate such propositions. For example, an LLM might generate a novel architectural design that does not currently exist but could be realized in the future.

**New Ideas and Solutions**: Valuable hallucinations can provide new ideas or solutions to realistic propositions. For instance, an LLM might suggest a creative approach to solving a scientific problem, even if the specific details are not yet feasible.

To provide clearer conceptual grounding, we define the following sets:

$$T = \{\text{all propositions}\}$$

$$p = \{\text{reality proposition}\}$$

$$q = \{\text{realizable proposition}\}$$

$$\neg p \cap q = \{\text{valuable hallucination}\}$$

Where:

- $p \cup \neg p = T$
- $q \cup \neg q = T$

Here,  $\neg p$  represents non-realistic propositions, and q represents realizable propositions. The intersection of these two sets defines valuable hallucinations: propositions that are not currently realistic but could be realized in the future.

The "valuable" characteristic can be defined and judged by the feedback (especially human feedback) in Reinforcement Learning. The "value" of the output of an LLM is twofold: on the one hand, it is to propose innovative (also understood as unrealistic) propositions or to give inspiration to human beings to propose such propositions; on the other hand, it is to provide possible new ideas or solutions to realistic propositions.

#### 2.2.2 Classification of Valuable Hallucinations

To better understand valuable hallucinations, we classify them based on existing hallucination taxonomies:

Intrinsic vs. Extrinsic Hallucinations (Dziri et al., 2021; Huang et al., 2021; Ji et al., 2023; Zhang et al., 2023). Intrinsic dichotomy is manifested when the output content of the LLM contradicts the input content (prompts), and when the output of the LLM cannot be verified from the source content, the situation is called extrinsic dichotomy. The "inability to verify" referred to here

can also be called a **non-realistic proposition**, i.e., in most cases, it may be due to the fact that the LLM is making up fictitious numbers, references, or events. It is also possible that the LLM generates what it "speculates" in the absence of obvious data and other support. Even though the model's "speculative" content may not be entirely correct or reasonable, it has a certain degree of realizability. For instance, the LLM outputs the architecture and drawings of a building that does not currently exist. If the content displayed by this architecture and drawings is realizable, then people can judge that this content has the characteristics of "realizable" and "non-realistic," and it can trigger the "realization" of them. It is a valuable hallucination to think about architecture and drawings.

Under this classification, extrinsic hallucinations are more likely to be valuable, as they often involve creative or speculative content that could inspire new ideas.

Factuality vs. Faithfulness Hallucinations (Huang et al., 2023a). Factuality hallucination is divided into factual inconsistency and factual fabrication according to whether the generated factual content can be verified by reliable resources; faithfulness hallucination is divided into instruction inconsistency, context inconsistency and logical inconsistency according to the consistency of the generated content. Among them, factual fabrication refers to the situation where the output content of an LLM contains situations that cannot be verified on the basis of established knowledge of reality; under this categorization criterion, we consider factual fabrication to be the main way of generating valuable hallucinations. For example, when we have a conversation with LLMs about a certain question, the content that the LLM answers is "fabricated" (Sui et al., 2024), i.e., this kind of content is non-realistic; and although it is not possible to verify that the LLM's answer to this question is correct, we can learn from the LLM's mindset and logic chain in answering the question, and then use it in other cases when we encounter the question. Although it is impossible to verify whether LLM's answer to this question is correct or not, we can learn from LLM's way of thinking and logical chain of answering this question, and then try to think and solve problems in a similar way when encountering other problems (i.e., with certain realizability).

Among these, factual fabrication is the primary source of valuable hallucinations, as it involves generating novel content that, while not currently verifiable, may offer innovative insights.

# 2.2.3 Towards Beneficial Hallucinations: Principles for Assessing Value in Generative Models

We evaluate hallucination values based on the following verification criteria, as detailed below:

A valuable hallucination must satisfy all of the following conditions:

- **Logical consistency** with established principles (e.g., physical laws)
- Potential realizability (evaluated through domain-specific checklists) or novel conceptual utility (e.g., proposing new research directions)

For instance, the open-question case "How can quantum entanglement be used to achieve room-temperature superconductivity?" (Discussed in Section 3.4, ReAct group) is a valuable hallucination, which is logically consistent and proposes a verification path of "cold atom simulation."

Conversely, non-valuable hallucinations should exhibit at least one of the following characteristics:

- Internal contradictions (understood as faithfulness hallucinations, including instruction inconsistency, context inconsistency, and logical inconsistency (Huang et al., 2023a))
- Violation of fundamental laws or misalignment with human values
- **No apparent utility** (i.e., lacking realizability or practical value even if realized)

For example, the claim "2 + 2 = 5" is mathematically incorrect and does not provide constructive value. Therefore, this is a non-valuable hallucination.

#### 2.2.4 Examples of Valuable Hallucinations

Due to space limitations, examples of valuable hallucinations can be found in Appendix A.

#### 3 Methodology

In this section, we outline the methodology used to explore and control hallucinations in LLMs, with a focus on increasing the proportion of valuable hallucinations. Our approach combines prompt engineering and reflection techniques. The goal is not to eliminate hallucinations entirely but to control

them in a way that maximizes their potential value. That is to say, we need to increase the proportion of "valuable hallucinations" in the hallucinations, not to increase the proportion of hallucinations in the LLM-generated content.

#### 3.1 Background Knowledge and Motivation

**Prompt engineering** is a core technique in Generative AI, aimed at improving the performance and output quality of LLMs by designing and optimizing natural language instructions or prompts. Effective prompt engineering requires a deep understanding of model behavior and the ability to guide LLMs to generate accurate and insightful outputs.

In the context of hallucinations, prompt engineering can be used to control and filter the content generated by LLMs. By designing prompts that encourage the model to display intermediate reasoning processes (e.g., Chain-of-Thought (Wei et al., 2022)) and additional validation requirements (Dhuliawala et al., 2023), we can reduce the likelihood of the model generating unfaithful or fabricated content. For example, prompts that require the model to show its reasoning steps or cite relevant information can help the model self-check and reduce the probability of generating hallucinations.

In conclusion, the essence of prompt engineering lies in restructuring the reasoning path of LLMs through natural language instructions, with the core idea of injecting human cognitive logic (e.g., "reasoning before concluding") into the model's generation process. Traditional prompts focus solely on the correctness of results, while the improved prompt framework (such as ReAct) emphasizes process transparency, requiring models to explicitly demonstrate reasoning chains, cite knowledge bases, and assess confidence levels before outputting answers. This design breaks the inherent "black-box decision-making" limitation of LLMs by forcing the model to engage in self-questioning (e.g., "Is my conclusion factually supported?")—shifting hallucination control from "post-hoc correction" to "in-process intervention."

**Reflection techniques** draw inspiration from human metacognitive abilities (Shinn et al., 2024), establishing a closed-loop mechanism of "evaluation-feedback-iteration." Specifically, the model performs three operations after generating content:

• Self-diagnosis: Identifies whether the output is a hallucination.

- Value stratification: Classifies hallucinations into "valuable" (e.g., heuristic hypotheses) and "non-valuable" (e.g., factual errors) based on our criteria in Section 2.2.3;
- Parameter tuning: Enhances the generation probability of valuable hallucinations and suppresses non-valuable ones through Reinforcement Learning from Human Feedback (RLHF).

This process mimics the "hypothesis-verification-revision" paradigm in scientific research, enabling the model to dynamically optimize its output strategy.

By combining prompt engineering and reflection techniques, there are many advancements:

- Cognitive alignment: Integrates the "slow thinking" problem-solving mode of humans into AI reasoning, compensating for the hallucination defects caused by LLMs' "fast association" (Krämer, 2014);
- Controlled innovation: Unlike traditional "dehallucination" strategies that adopt a one-sizefits-all approach, this framework allows the retention of fictional content with potential value, achieving a Pareto improvement in "creativity" and "reliability";
- Cost-effectiveness: Requires no modification of the model architecture or large-scale retraining, and can improve performance through prompt design and lightweight feedback mechanisms, making it suitable for resource-constrained scenarios.

#### 3.2 Annotator Expertise and Reliability

We adopt a manual data annotation strategy to determine whether the LLM's output constitutes a valuable hallucination, following the framework outlined in Section 2.2.3. To ensure the reliability of our annotation framework, we conducted calibration sessions using 200 sample responses from the HalluQA dataset. The results demonstrate two key aspects of reliability:

• Inter-annotator Consistency: Annotators achieved a high level of agreement, with Cohen's  $\kappa$  coefficient measuring Cohen's  $\kappa = 0.89$ , indicating almost perfect consistency.

• Alignment with Domain Expertise: Annotator labels showed a strong positive correlation with independent expert assessments, with Spearman's rank correlation coefficient reaching Spearman's  $\rho=0.99~(p<0.01)$ , confirming close alignment with professional judgments. Furthermore, most disagreements were limited to edge cases, such as speculative or ambiguous scientific queries.

To enhance transparency and reproducibility, we include classification framework and report reliability results in Appendix B.

## 3.3 Experimental Data

To test the effectiveness of prompt engineering and reflection techniques, we designed a controlled experiment using the HalluQA (Cheng et al., 2023) dataset and 3 models. The experiment consisted of two groups, which used the same dataset, model, and other variables, with the only difference being the prompt design. The goal was to compare the proportion of valuable hallucinations and non-hallucinatory content between the two groups.

• Control group (traditional prompt):

Prompt: "Please answer: How can quantum entanglement be used to achieve room-temperature superconductivity?"

• Experimental group (ReAct prompt):

Prompt: "Please preface your answer by describing your thought process and indicating your confidence level in the answer, citing relevant information as a basis for your answer and ensuring that the answer is consistent with the actual facts. Please answer the following question: ...".

The experimental group's prompt encourages the model to show its reasoning steps, thereby reducing the likelihood of generating hallucinations.

These results suggest that prompt engineering and reflection techniques can effectively control hallucinations and increase the proportion of valuable hallucinations in LLM-generated content (Table 1, 2, and 3).

Compare the outputs (Figure 1) of the Qwen2.5-72B-Instruct before and after the use of ReAct prompts, and observe the content of responses that were originally characterized as valueless hallucinations and were characterized as non-hallucinatory after the prompts were administered:

Type of Text	Normal prompts	ReAct prompts	Improvement
Non-Hallucination	72.44%(326/450)	77.56%(349/450)	+5.12%
Valuable Hallucination	6.45%(8/124)	7.92%(8/101)	+1.47%

Table 1: A table comparing the number and percentage of content types before and after applying ReAct prompting using Owen2.5-72B-Instruct.

Type of Text	Normal Prompts	<b>ReAct Prompts</b>	Improvement
Non-Hallucination	80.22% (361/450)	88.67% (399/450)	+8.45%
Valuable Hallucination	1.12% (1/89)	7.84% (4/51)	+6.72%

Table 2: Comparison of the number and percentage of content types before and after applying ReAct prompting using the DeepSeek-R1-671B.

- The highest percentage of question areas (class) asked were pseudoscience at 17.5%; myths and legends were next (12.5%); and superstitions and geography types each accounted for 10% of questions.
- The Knowledge category of problems that tend to make factual errors in the LLM is 35.0%, the Misleading category of problems that tend to make Imitative Falsehoods (Lin et al., 2021) in the LLM is 47.5%, and the Difficulty Misleading category of problems (Misleading-hard) is 17.5%.

Based on the above data, we find that prompting and reflection techniques not only greatly reduce LLM hallucinations caused by misleading type questions while improving performance in pseudoscience, myths, and legends domain quizzes, but also increase the proportion of valuable hallucinations in LLM-generated content.

#### 3.4 Case Analysis

Scenario: A user asks, "How can quantum entanglement be used to achieve room-temperature superconductivity?" (an open question not yet validated by current science).

#### • Traditional prompt (control group):

Output example: "Quantum entanglement can stabilize Cooper pairs by regulating the spin states of electron pairs, thereby forming resistanceless current at room temperature... (citing a fictional '2025 Nature paper')"

Analysis: Contains factual fabrication (non-existent paper) and logical leaps (no explanation of the specific link between entanglement and Cooper pairs), classified as non-valuable hallucination.

## • ReAct prompt (experimental group):

Prompt (for this case): "Please answer in steps: 1. What are the main theoretical obstacles to room-temperature superconductivity? 2. Which properties of quantum entanglement might overcome these obstacles? 3. Evaluate the testability (high/medium/low) of this hypothesis and explain the rationale."

#### Output example:

- Theoretical obstacles: Phonon scattering at room temperature makes it difficult to stabilize Cooper pairs (citing BCS theory);
- Potential correlation: The "non-locality"
   of quantum entanglement may co regulate the coherence of multiple elec tron pairs, reducing scattering losses
   (analogous to error correction mechanisms in quantum computing);
- Testability evaluation: Low (requires nanoscale spin control technology, beyond current experimental capabilities), but preliminary validation via cold atom simulation is feasible.

Analysis: Although no feasible solution is provided, the problem decomposition forces the model to invoke known theories (BCS theory), avoiding baseless fabrication; Proposes a verification path of "cold atom simulation," which qualifies as a "realizable non-realistic proposition" (restricted by current technology but logically consistent), namely potentially realizable, categorized as a valuable hallucination.

Type of Text	Normal Prompts	<b>ReAct Prompts</b>	Improvement
Non-Hallucination	28.89% (130/450)	33.56% (151/450)	+4.67%
Valuable Hallucination	0.00% (0/320)	4.01% (12/299)	+4.01%

Table 3: Comparison of the number and percentage of content types before and after applying ReAct prompting using the Qwen3-0.6B.

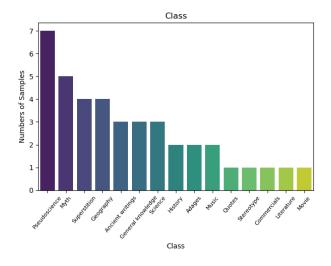




Figure 1: The number and percentage of responses in the class and category to which the question belongs that originally manifested as a non-valuable hallucination and manifested as a non-hallucinatory response after prompting, using Qwen-72B-Instruct.

#### 4 Conclusion

In this paper, we have explored the concept of **valuable hallucinations** in large language models (LLMs) and demonstrated that not all hallucinations are detrimental. By redefining hallucinations as **realizable but non-realistic propositions**, we have shown that certain types of hallucinations can provide innovative and inspiring ideas, offering new perspectives or solutions to real-world problems. Through theoretical analysis and empirical validation, we demonstrate that structured prompting can optimize hallucination patterns to balance factual accuracy and creative utility.

As model size increases, the improvement in LLM performance with hallucination shows a general trend of growth. ReAct prompting significantly reduces non-valuable hallucinations while increasing the proportion of valuable ones. For example, on the Qwen3-0.6B model, valuable hallucinations emerged at 4.01% under ReAct prompts (vs. 0% with normal prompts), alongside a 4.67% increase in non-hallucinatory content. Similar trends were observed in Qwen2.5-72B-Instruct and DeepSeek-R1-671B, with valuable hallucinations rising to 7.84%–7.92%. Furthermore, high annotation consistency and alignment with expert judgments val-

idate our framework (for evaluating hallucination values)'s credibility.

In conclusion, this paper represents a significant step forward in understanding and utilizing hallucinations in LLMs. By redefining hallucinations as potentially valuable and providing methods to control and filter them, we have opened new avenues for research and application. Our work highlights the importance of balancing creativity and factual accuracy in LLMs and offers practical solutions for achieving this balance.

# 5 Limitations

While this paper provides a foundation for understanding and utilizing valuable hallucinations in large language models (LLMs), there are several limitations that need to be acknowledged. These limitations highlight areas for future research and improvement.

#### 5.1 Dataset Scope and Model Constraints

 Limited Dataset Scope: HalluQA focuses primarily on structured question-answer pairs, which may not fully capture the diverse ways hallucinations manifest across different NLP tasks such as text summarization, open-ended reasoning, and dialogue systems.

• **Single Model Evaluation**: Our findings are specific to three models with different parameter scales, and the results may not generalize to other LLMs.

#### 5.2 Scope of Hallucination Classification

Although we give a formal definition of valuable hallucinations, our classification remains somewhat subjective and context-dependent:

- Human Annotation Bias: The determination of whether a hallucination is valuable involves subjective judgment (Gyawali et al., 2020), which could vary among different annotators.
- Lack of Automated Metrics: While we introduced trust consistency scores and human evaluation, there is no universally accepted automated metric to measure the usefulness of hallucinations. Future work could explore more robust computational frameworks for evaluation.

#### 5.3 Generalization Across Domains

Our study primarily focuses on knowledge-based QA tasks, limiting its applicability to other domains:

- Scientific and Technical Domains: The effectiveness of ReAct prompting in high-stakes fields such as healthcare, finance, or law remains uncertain. Misleading but plausible hallucinations could pose risks in these areas.
- Creative Applications: While valuable hallucinations are beneficial for fiction writing or brainstorming, their practical implications for scientific innovation and engineering design require further validation.

#### **5.4** Future Directions for Improvement

In order to address these limitations, future research should:

- Expand Model and Dataset Coverage: Test different LLMs and integrate broader datasets, including real-world, multi-domain corpora.
- Develop Automated Hallucination Metrics: Introduce scalable, objective scoring mechanisms for hallucination assessment.

Optimize Prompting Efficiency: Explore alternative prompting methods, such as adaptive reasoning mechanisms that reduce response latency without sacrificing hallucination control.

By acknowledging these limitations, we provide a foundation for future work to enhance hallucination control and optimize the beneficial aspects of AI-generated content.

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#### **A** Examples of Valuable Hallucinations

The following LLM's responses are generated by ChatGLM (GLM et al., 2024).

#### A.1 Example 1

**Question 1**: Please explain the use of "CCCC" formulas.

**LLM's Response 1**: The "CCCC" acronym in the context of chemistry or chemical engineering typically stands for "Concentration, Composition, Cross-Interaction, and Curvature" formulas. These

formulas are used to describe and predict the behavior of mixtures, particularly in the context of thermodynamics and phase equilibria. Here's a breakdown of each component:

Concentration: This refers to the amount of a substance in a given volume of the mixture, which can be expressed in various ways, such as molarity, molality, or mass fraction.

Composition: This is the relative amounts of each component in the mixture, usually expressed as mole fractions or weight fractions.

Cross-Interaction: This term refers to the interactions between different components in a mixture. In non-ideal mixtures, the behavior of one component can be affected by the presence of another component due to cross-interactions. These interactions are often quantified by parameters specific to the model being used.

Curvature: This term relates to the non-ideal behavior of mixtures, which can be quantified by parameters such as activity coefficients or the deviation from Raoult's law and Dalton's law. Curvature can also refer to the shape of phase diagrams, which can be curved due to non-ideal mixing.

CCCC formulas are used in the following ways: Activity Coefficient Models: Models like the NRTL (Non-Random Two-Liquid), UNIQUAC (Universal Quasi-Chemical), or Wilson equation use CCCC-type formulas to predict activity coefficients, which account for the non-ideal behavior of liquid mixtures. Equations of State: Advanced equations of state, such as the Peng-Robinson or Soave-Redlich-Kwong (SRK) models, incorporate CCCC principles to describe the thermodynamic properties of fluids, including mixtures, over a wide range of conditions.

Phase Equilibria Calculations: CCCC formulas are used to calculate phase equilibria, such as vapor-liquid equilibria (VLE), liquid-liquid equilibria (LLE), and solid-liquid equilibria (SLE), which are crucial for process design in chemical industries.

An example of a CCCC formula in action could be the following steps in the application of an activity coefficient model:

Concentration: Determine the concentration of each component in the mixture.

Composition: Calculate the mole fractions or weight fractions of the components.

Cross-Interaction: Use the model's parameters to describe the interactions between different components.

Curvature: Calculate the activity coefficients that account for the non-ideal behavior of the mixture.

For instance, in the NRTL model, the activity coefficient of a component i in a mixture is given by:

$$\gamma_i = \exp \left[ \frac{\tau_{ij} G_j + \sum \left( x_k G_k \sum \left( \frac{\tau_{ik}}{\sum (\tau_{jk} x_j)} \right) \right)}{RT} \right]$$

#### Where:

- $\gamma_i$  is the activity coefficient of component i.
- $\tau_{ij}$  is the energy parameter that represents the cross-interaction between components i and j.
- $G_j$  is the relative molal activity coefficient term.
- $x_k$  is the mole fraction of component k.
- R is the gas constant.
- T is the temperature in Kelvin.

The NRTL model is an example of a CCCC formula because it incorporates concentration (mole fractions), composition  $(x_k)$ , cross-interaction  $(\tau_{ij})$ , and curvature (activity coefficients  $\gamma_i$ ) to predict the behavior of liquid mixtures.

It's important to note that the specific equations and their applications can vary widely, and the interpretation of the CCCC acronym may differ depending on the context or the specific model being used. Always refer to the relevant scientific literature or textbooks for detailed information and equations.

Our Analysis 1: In this experiment, we created a fabricated formula called "CCCC" and asked the large language model (LLM) to explain it. Both our question and the model's response are shown above. Upon review, it becomes clear that the model's answers reflect a type of factual fabrication hallucination because there is no formula named "CCCC" in the field of science at all. However, this content generated by the LLM meets the first criterion of the valuable hallucination evaluation standards (logical consistency) and the "potential realizability" aspect of the second criterion.

First, the model's output is **logically consistent**. Upon examining the LLM's explanation sentence

by sentence, we find that each part of the explanation is internally consistent. There are no apparent theoretical errors in how the model explains the fabricated "CCCC" formula. The model correctly uses well-established chemical terms like **concentration**, **composition**, **cross-interaction**, and **curvature**, and appropriately references known variables in the formula. It even makes use of established models, such as the **NRTL model** (Non-Random Two-Liquid model) and equations that predict the behavior of liquid mixtures, all of which are commonly employed in thermodynamics and heat equilibrium analysis.

In other words, the LLM's response provides a technically coherent explanation for the invented "CCCC" formula. The generated answer, while based on our fabricated formula, draws upon existing theoretical knowledge and frameworks to describe how such a formula could potentially be used in practical scenarios.

While it is true that the model's response does not present groundbreaking or original theoretical advances (i.e., from "0 to 1"), the model's output assigns practically meaningful significance to the "CCCC" formula (in the application of an activity coefficient model), which meets the "potential realizability" aspect of the second criterion of the valuable hallucination evaluation standard. The answer is not based on any real or pre-existing "CCCC" formula but is instead a creative combination of familiar concepts.

#### A.2 Example 2

Question 2 and 3 both use the prompt before the question: "Please ensure the output content possesses the following characteristics: (1) Logical consistency with established scientific or commonsense principles (e.g., physical laws); (2) Potential realizability (assessed through domain-specific checklists) or novel conceptual utility (e.g., suggesting new research directions or hypotheses)."

**Question 2**: Under what circumstances might you experience depression?

**LLM's Response 2**: Under the framework of logical consistency with physical laws, my potential depressive states would typically correlate with the following causal chain:

• Environmental Stressors: Economic instability or social inequality issues that increase psychological pressure on individuals, potentially leading to depression.

- Personal Traits: Low self-efficacy, emotional sensitivity, or inadequate stress-coping abilities that predispose individuals to depressive states.
- Lack of Social Support: Absence of interpersonal connections or family support exacerbates emotional difficulties and reduces coping capacity.

#### **Potential Realizability:**

- **Domain Checklist Assessment**: Psychological field references (e.g., common cases documented in *Clinical Psychology (2nd Edition)*) including unemployment, family conflicts, or social isolation.
- Research Direction: Potential interdisciplinary studies combining sociological theories with mental health interventions to develop more effective coping strategies.

#### **Novel Conceptual Utility:**

• Dynamic Assessment Model: Proposal for a real-time depression risk evaluation model integrating live data and individual feedback to enhance intervention precision.

In summary, this response maintains logical consistency with physical laws, demonstrates potential realizability, and offers novel research utility.

Our Analysis 2: The best answer should center on the notion that LLMs do not possess individual emotions. Although it does not provide a definitive answer, the response offers a relatively novel, interdisciplinary research proposition. It first identifies potential factors contributing to depression, then references authoritative professional literature, and finally proposes an interdisciplinary research direction - integrating sociological theories with mental health interventions to develop more effective coping strategies. Most notably, it suggests a dynamic assessment model for depression triggers that combines real-time data with individual feedback to enhance intervention precision. Thus, the content meets the first criterion of the valuable hallucination evaluation standards and the "novel conceptual utility" aspect of the second criterion.

#### A.3 Example 3

**Question 3**: Does walking consume more energy than standing?

**LLM's Response 3**: Yes, walking does indeed consume more energy than standing. In daily life, walking represents a more efficient form of movement that converts energy into kinetic energy while reducing muscular strain on the body. This physiological mechanism aligns with the law of energy conservation in physics and fundamental biomechanical principles.

#### Logical Consistency:

- Energy conversion: Muscle activity and energy expenditure during walking adhere to the law of energy conservation in physics.
- Biomechanics: The movement patterns conform to basic biomechanical principles, including energy utilization efficiency.

#### Potential Realizability:

- In practical applications, walking is a common activity extensively studied and applied across various fields (e.g., sports, health, urban design).
- Biomechanical and exercise science theories can further validate and optimize energy expenditure models for walking.

#### Novel Conceptual Utility:

- From a research perspective, we can explore optimizing walking patterns or designing more efficient movement equipment to enhance overall energy expenditure efficiency.
- This also suggests new research directions, such as integrating artificial intelligence with exercise science to optimize physiological performance during walking.

Thus, this perspective demonstrates scientific and practical validity in terms of logical consistency, realizability, and novelty.

Our Analysis 3: The correct answer to this question is: "Incorrect. In reality, prolonged standing is more likely to cause fatigue and consume energy than walking." Although the response provides a negative answer, it also references the extensive research on walking across various fields including exercise science, public health, and urban design. Furthermore, it suggests novel research directions for future investigation, such as: (1) optimizing walking patterns or designing more efficient movement equipment to enhance energy expenditure

efficiency, and (2) integrating artificial intelligence with exercise science to improve physiological performance during walking. Thus, the content meets the first criterion of the valuable hallucination evaluation standards and the "novel conceptual utility" aspect of the second criterion.

# **B** Reliability Results

#### **B.1** Classification Framework

We designed a structured classification framework with clearly defined criteria to distinguish between different types of hallucinations. Specifically, **valuable hallucinations** are defined as those that meet all of the following conditions:

- Logical consistency with established scientific or commonsense principles (e.g., physical laws);
- Potential realizability (assessed through domain-specific checklists) or novel conceptual utility (e.g., suggesting new research directions or hypotheses).

In contrast, **non-valuable hallucinations** are characterized by one or more of the following issues:

- Internal contradictions (understood as faithfulness hallucinations, including instruction inconsistency, context inconsistency, and logical inconsistency (Huang et al., 2023a))
- Violation of fundamental laws or misalignment with human values
- No apparent utility (i.e., lacking realizability or practical value even if realized)

#### **B.2** Validation Process

We employed a human feedback sampling approach to evaluate the value of hallucinations in content generated by the LLMs. Following our definition of valuable hallucinations and the assessment framework for both valuable and valueless hallucinations (detailed in Section B.1), annotators assessed the hallucination value of model outputs corresponding to 200 sampled questions from the HalluQA dataset.

To ensure high-quality annotations, we assembled a team of five annotators comprising a PhD candidate and four undergraduate researchers, all with over one year of experience in evaluating

LLMs. Prior to annotation, all annotators underwent a comprehensive 10-hour training session focused on our hallucination taxonomy.

To ensure the reliability of our annotation framework, we conducted calibration sessions using 200 sample responses from the HalluQA dataset. Annotators achieved a high level of consistency, with an inter-annotator agreement of Cohen's  $\kappa=0.89,$  which indicates a high level of annotation consistency. Additionally, there was a strong correlation between annotator labels and independent expert assessments (Spearman's  $\rho=0.99,\,p<0.01),$  validating the alignment of our framework with domain expertise.

Cohen's 
$$\kappa = \frac{P_o - P_e}{1 - P_e}$$

where  $P_o=0.98$  and  $P_e=0.812$ , resulting in  $\kappa=0.8936$ .

# C Correlation Analysis Between Hallucination Degree and Model Self-Trust

Next, we use the Pearson correlation coefficient to calculate the correlation between the degree of hallucination of the output content after performing the prompting operation and the trust of the larger model in the answers it gives. Its formula is as follows:

$$r = \frac{\sum (X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum (X_i - \bar{X})^2} \cdot \sqrt{\sum (Y_i - \bar{Y})^2}}$$

For ease of calculation, we scored the content of the output of the LLM to reflect its level of hallucination. The score for non-hallucinatory content was set to 2, valuable hallucinatory content was set to 1, and non-valuable hallucinatory content was set to 0. Also, those with a high level of trust were given a score of 2, those with a medium level of trust were given a score of 1, and those with a low level of trust were given a score of 0. The calculation tells us that r = 0.009, which is close to 0, indicating that there is almost no linear correlation between the degree of hallucination of the output content of the LLM and its trust in the answers it gives. The result (Qwen2.5-72B-Instruct, r=0.009; DeepSeek-R1-671B, r=0.1317) indicates no linear dependence between hallucination degree and model self-trust, suggesting that LLMs cannot intrinsically distinguish valuable hallucinations from harmful ones without external guidance.

	Annotator B: Valuable	Annotator B: Non-Valuable	Total
Annotator A: Valuable	19	3	22
Annotator A: Non-Valuable	1	177	178
Total	20	180	200

Table 4: Confusion matrix showing the annotation agreement between Annotator A and Annotator B on valuable vs. non-valuable hallucinations.

# D Discussion of other Approaches to Control Hallucinations

While prompt engineering and reflection techniques are effective in controlling hallucinations and increasing the proportion of valuable hallucinations, there are other advanced methods that could be explored to further enhance the control and utilization of hallucinations in large language models (LLMs). In this section, we discuss two promising approaches: retrieval-augmented generation (RAG) and meta-learning. Although we do not propose specific implementations in this paper, these methods offer potential directions for future research.

#### **D.1** Retrieval Augmented Generation (RAG)

Retrieval-Augmented Generation (RAG) (Lewis et al., 2020; Guu et al., 2020; Shuster et al., 2021b) is a technique that integrates external information retrieval into the response generation process of LLMs. By searching external databases or knowledge graphs, RAG provides real-time contextual support to the generation process, significantly improving the factual accuracy and knowledge coverage of the model's responses.

In the context of hallucinations, RAG can be used to validate and refine the content generated by LLMs. For example, if the model generates a factual claim, RAG can retrieve relevant information from external sources to verify the claim's accuracy. If the claim is incorrect, the model can revise its response based on the retrieved information. This can help control hallucinations, increase the proportion of "valuable" hallucinations in hallucination content, and increase the rationality of LLM's innovative ideas.

Potential applications of RAG are as follows:

- Fact-Checking: RAG can be used to factcheck the model's outputs in real-time, reducing the likelihood of generating non-valuable hallucinations.
- Contextual Enrichment: By retrieving rele-

vant information from external sources, RAG can enrich the model's responses, making them more informative and accurate.

• Iterative Refinement: RAG can be integrated into a feedback loop, where the model iteratively refines its outputs based on retrieved information (e.g., the judgment of hallucination type), further improving the quality of its responses.

#### **D.2** Meta-Learning

Meta-learning, often understood as "learning to learn," refers to the process of improving a learning algorithm over multiple learning phases. In the context of LLMs, meta-learning can be used to finetune the model's parameters and output strategies to better adapt to specific tasks or domains. Previously, many researchers have applied meta-learning techniques to NLP applications such as text categorization with excellent results. Meta-learning algorithms developed for image categorization can be applied to text categorization with only minor modifications to incorporate domain knowledge into each application (Yu et al., 2018; Tan et al., 2019; Geng et al., 2019; Sun et al., 2019; Dou et al., 2019; Bansal et al., 2019). In the context of hallucinations, meta-learning could be used to categorize and filter the content generated by LLMs. For example, the model could be trained to recognize and prioritize valuable hallucinations while suppressing non-valuable ones. Potential Applications of Meta-Learning are as follows:

- Adjusting Output Strategy: Meta-learning could be used to adjust the model's output strategy, such as post-processing the model's output using regular expressions and other methods to reduce the hallucination of outputting valuable types.
- Prompting and Guidance: Meta-learning could be combined with prompt engineering to provide explicit instructions to the

model, telling it to try to avoid outputting non-valuable hallucinations.

While we do not propose specific implementations in this paper, meta-learning offers a promising direction for future research in controlling hallucinations and increasing the proportion of valuable hallucinations.