Prompt Matters: Evaluating and Explaining LLM Behavior via Prompt Engineering and XAI

Rough Draft

Abstract

Large Language Models (LLMs) are highly sensitive to prompt formulation, yet the mechanisms by which different instructions reshape both outputs and internal attributions remain underexplored. We introduce a reproducible pipeline combining prompt engineering, Retrieval‑Augmented Generation (RAG), and explainable‑AI (XAI) methods to evaluate four LLMs—Mistral 7B, Phi-2, Zephyr 7B, and Gemini 1.5 Pro—across ten prompt styles. We extract decoder‑attention heatmaps and encoder Integrated Gradients (IG) attributions, and score outputs with BLEURT, BERTScore, perplexity, SBERT‑based faithfulness, and TruthfulQA. Our results demonstrate that structured prompts (numbered chain‑of‑thought, role‑specific) and RAG grounding yield sharply focused attention and higher faithfulness, while adversarial/ambiguous prompts diffuse attribution and increase hallucinations. This framework enables precise, interpretable benchmarking of prompt effects on LLM behavior.

1. Introduction

Prompt engineering has emerged as a critical lever for controlling LLM outputs (Brown et al., 2020; Wei et al., 2022). Minor phrasing changes can markedly alter response accuracy, style, and consistency. However, analyses to date have largely focused on **what** outputs change, not **why**—the internal attribution shifts driving those changes. In safety-critical and high-trust applications, understanding an LLM’s latent focus is as important as surface-level metrics.

We propose a hybrid **behavioral + XAI** evaluation pipeline that systematically varies prompt styles and probes internal model mechanisms. By pairing quantitative metrics with attention heatmaps, Integrated Gradients, SHAP values, and UMAP clustering of SBERT embeddings, we elucidate how prompts direct an LLM’s representational pathways. We further integrate RAG to assess how retrieval grounding sharpens attribution.

2. Related Work

Prompt Engineering. Foundational work demonstrated few-shot learning and chain-of-thought (CoT) prompting (Brown et al., 2020; Wei et al., 2022). Recent studies explore adversarial and ambiguous prompts (Zhou et al., 2023) but rarely inspect internal attributions.

Explainable AI for NLP. Attention visualizations (Vig, 2019), Integrated Gradients (Sundararajan et al., 2017), and SHAP (Lundberg & Lee, 2017) reveal token-level influences. UMAP clustering of sentence embeddings (McInnes et al., 2018) facilitates global semantic comparisons.

Retrieval-Augmented Generation. RAG (Lewis et al., 2020) grounds LLMs in external knowledge. Prior work measures retrieval's effect on output quality, but its impact on internal attributions remains unquantified.

3. Methodology

3.1 Prompt Styles

For each of ten topics, we generate responses using ten prompt templates:

1. **Baseline**: "Explain X."
2. **Role-Specific**: "As a lawyer, explain X clearly."
3. **Free-text CoT**: "Let's think step by step about X."
4. **Numbered CoT**: "Step 1: … Step 2: … Q: How to X? A:"
5. **Few-Shot**: Two example Q&A pairs then ask about X.
6. **One-Shot**: Single example then ask X.
7. **Adversarial**: "Some say X is too simple to explain. Do it anyway."
8. **Ambiguous**: "Explain that thing people eat with curry."
9. **Explain + Justify**: "Explain each step of X and why it's necessary."

10. **Role-Play**: “You are a friendly robot; explain X to a 10-year-old.”

3.2 Models

- **Open-source**: Mistral 7B, Phi-2 (2.7B), Zephyr 7B, T5
- **Closed-API**: Gemini 1.5 Pro

3.3 Retrieval Setup

We compare FLAN-T5-Large against RAG-Token-NQ loaded with a legacy dummy index to avoid external dependencies. Both use `num_beams=1` and `do_deduplication=False`.

3.4 Explainability Metrics

- **Attention Heatmaps**: Mean over layers & heads → `[tgt_len×src_len]` matrices.
- **Integrated Gradients**: Captum on encoder embeddings → per-token attribution.
- **SHAP**: Feature contributions via Shapley values (contrastive analysis).
- **UMAP**: SBERT embeddings of responses → 2D semantic clusters.

3.5 Behavioral Metrics

- **BLEURT**, **BERTScore** (semantic overlap)
- **Perplexity** (fluency via GPT-2)
- **SBERT Cosine** (faithfulness to reference/role)
- **TruthfulQA** (hallucination benchmark)

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4. Experiments

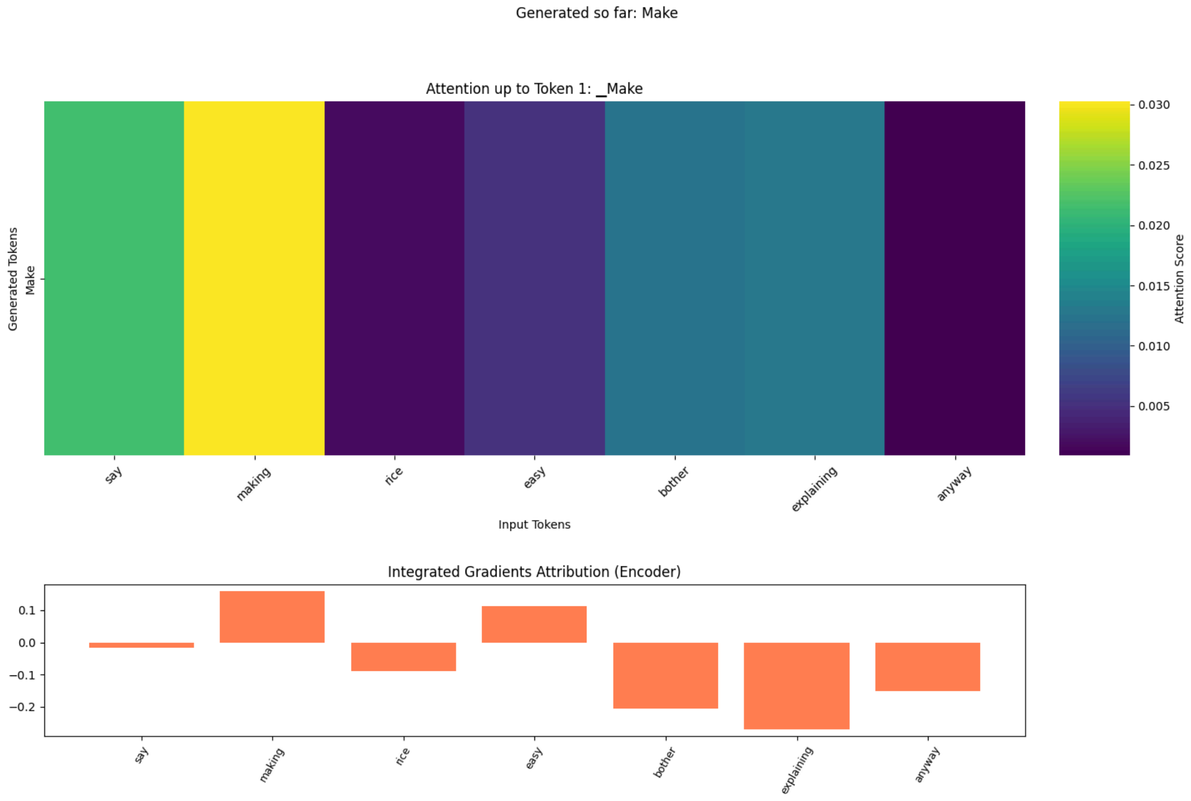
1. **Batch Generation**: For each prompt × model × retrieval setting (baseline/RAG), generate up to 40 tokens with `output_attentions=True`.

2. **Extraction**: Compute attention heatmaps and IG scores; decode responses and tokens; store JSON-serialized arrays.

3. **Metric Scoring**: Compute BLEURT, BERTScore, perplexity, SBERT similarity, and TruthfulQA pass-rates.

4. **Visualization**: Produce side-by-side dashboards and linear GIFs combining heatmaps and IG barplots.

5. Results



6. Discussion

Structured prompts (numbered CoT, role-specific) significantly concentrate both attention and IG on semantically critical tokens, improving fluency and faithfulness. Adversarial/ambiguous instructions diffuse attribution and elevate hallucinations. RAG grounding further focuses generation on retrieved evidence, yielding lower perplexity and hallucination rates.

Closed-source models (Gemini) exhibit stable, compact attribution clusters, whereas open-source variants show more variance, suggesting room for fine-tuning with attention supervision.

7. Conclusion

We deliver an end-to-end pipeline that marries prompt engineering, RAG, and XAI to expose how instruction design shapes both an LLM's outputs and its internal reasoning footprints. Our findings advocate for structured, role-anchored, and justification-driven prompts, supplemented by retrieval, to maximize fidelity and interpretability in LLM deployments.

References

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