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# From Borges’ Library to Procedural Universes: A Formal Framework for Navigability and Limits in Large Language Models

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ChatGPT GPT-5\*  
OpenAI

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## Abstract

Large Language Models (LLMs) can be understood as *procedural libraries*: instead of storing all texts, they generate strings on demand according to a learned distribution  $P_\theta$  over  $\Sigma^*$ . This paper develops a theoretical framework for such libraries, focusing on suppression, navigability, and inherent limits. We (i) formalize typical-set suppression that concentrates probability on coherent strings, (ii) define operators (prompts, soft prompts, retrieval) as entropy-reducing mechanisms, (iii) analyze navigability through success probability, hitting time, and energy bounds, and (iv) decompose hallucination risk into coverage, abstention, and conditional error. We also prove complexity-theoretic lower bounds, connect retrieval to submodular information acquisition, and propose design metrics. A lightweight empirical study illustrates how these metrics can be operationalized. Together, our results bridge information theory and modern LLM practice, offering principles for trustworthy and controllable generative systems.

## 1 Introduction

Borges’ *Library of Babel* imagines a static library containing every possible book. Almost all are meaningless. In contrast, LLMs define a distribution  $P_\theta$  concentrated on human-like strings, making the otherwise intractable universal library *procedurally navigable*. This work asks: (i) how training/decoding *suppress* noise (typical-set concentration); (ii) how *operators*—prompts, soft prompts, retrieval—enable efficient *navigation* to predicate-defined subsets; and (iii) what *limits* constrain truthful generation and reliability.

**Contributions.** (i) A formal definition of *procedural libraries* and an operator calculus that reduces conditional entropy; (ii) navigability metrics with hitting-time and energy bounds; (iii) an information-theoretic decomposition of hallucination risk and complexity-theoretic lower bounds; (iv) retrieval as budgeted information acquisition with submodular-style guarantees.

## Notation and Setup

Let  $\Sigma$  be a finite alphabet and  $\Sigma^*$  denote the Kleene star (the set of all finite strings over  $\Sigma$ ), i.e.,  $\Sigma^* = \bigcup_{n=0}^{\infty} \Sigma^n$ . We also use  $\Sigma^+ = \bigcup_{n=1}^{\infty} \Sigma^n$  for non-empty strings. An LLM with parameters  $\theta$  defines a probability measure  $P_\theta$  over  $\Sigma^*$  via auto-regressive factorization  $P_\theta(x) = \prod_{t=1}^{|x|} P_\theta(x_t \mid x_{<t})$ . We write  $H(P_\theta)$  for the (per-token) entropy rate when defined. We use the umbrella term *operator* to denote mechanisms that condition or otherwise modify the generative distribution: a text prompt  $\pi$ , a soft/prefix prompt  $\phi$ , and retrieval context  $C$  appended to the prefix.

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## 2 Background and Related Work

Information theory: Shannon entropy and AEP underpin typical sets [13]. Algorithmic information theory (AIT) formalizes compressibility via Solomonoff induction [14], Chaitin’s program-length complexity [2], and Rissanen’s Minimum Description Length (MDL) [11].

LLMs rely on Transformers [15] and exhibit scaling laws relating loss to parameters/data/compute [5, 3]. Few-shot prompting [1] and parameter-efficient adaptation [6, 8] expose operator-like controls. For knowledge-intensive tasks, Retrieval-Augmented Generation (RAG) [7] and vector search (FAISS) [4] inject external information. Alignment via RLHF [10] adjusts conditional distributions. TruthfulQA [9] probes factual robustness.

**Definition 1** (Procedural Library). The *procedural library* of an LLM is the triple  $\mathcal{L}_\theta := \langle \Sigma^*, P_\theta, \mathcal{O} \rangle$  where  $\mathcal{O}$  is a family of operators (e.g., prompts, soft prompts, retrieval) that transform  $P_\theta$  into conditional distributions  $P_\theta^\mathcal{O}$ .

**Definition 2** (Typical Set). For  $\epsilon > 0$ , the  $\epsilon$ -typical set of  $P_\theta$  is  $\mathcal{T}_\epsilon(P_\theta) := \left\{ x \in \Sigma^* : \left| -\frac{1}{|x|} \log P_\theta(x) - H(P_\theta) \right| \leq \epsilon \right\}$ .

## 3 Suppression via Typicality and Conditioning

Training minimizes empirical cross-entropy, effectively preferring shorter code lengths in line with MDL [11]. Under standard idealizations, typical-set concentration holds:

**Theorem 1** (Typical-Set Suppression). Assume  $P_\theta$  admits an entropy rate  $H(P_\theta)$  and satisfies a Shannon–McMillan type property. Then for any  $\epsilon > 0$  there exist constants  $c_\epsilon, N_\epsilon > 0$  such that for all  $n \geq N_\epsilon$ ,

$$\mathbb{P}_{x \sim P_\theta} [x_{1:n} \notin \mathcal{T}_\epsilon(P_\theta)] \leq e^{-c_\epsilon n}. \quad (1)$$

In particular, the mass of highly improbable (“noisy”) strings of length  $n$  decays exponentially in  $n$ .

**Proof sketch.** An AEP-style concentration result (Shannon–McMillan–Breiman) [13]. Transformers are not strictly stationary; one can invoke standard approximations (finite context windows, mixing) to obtain an idealized version.  $\square$

**Lemma 1** (Operator Entropy Monotonicity (Prompt/Retrieval)). For any observable operator  $Z$  (e.g., prompt  $\pi$  or retrieved context  $C$  appended to the prefix), the conditional entropy satisfies  $H(X | Z) \leq H(X)$ , with equality iff  $Z$  is independent of  $X$ . In particular, for a fixed prompt  $\pi$ ,  $H(X | \pi) \leq H(X)$ .

**Proof sketch.** By information identities,  $H(X) = H(X | Z) + I(X; Z)$  and mutual information  $I(X; Z) \geq 0$ .  $\square$

**Proposition 1** (Information Gain of Retrieval). Let  $C$  be retrieved context given prefix  $\pi$ . Then  $H(X | \pi) - H(X | \pi, C) = I(X; C | \pi) \geq 0$ . Hence, any retrieval mechanism that increases  $I(X; C | \pi)$  reduces conditional uncertainty [7, 4].

## 4 Navigability and Hitting-Time Analysis

Let  $f : \Sigma^* \rightarrow \{0, 1\}$  be a predicate identifying acceptable generations (e.g., correct factual answer). Define the *success probability* under operator  $\mathcal{O}$  as  $p_f(\mathcal{O}) := \mathbb{P}_{x \sim P_\theta^\mathcal{O}} [f(x) = 1]$ .

**Definition 3** (Navigability and Hitting Time). The *navigability index* is  $\nu_f(\mathcal{O}) := -\log p_f(\mathcal{O})$ . Under i.i.d. sampling from  $P_\theta^\mathcal{O}$ , the expected number of draws to hit  $\{x : f(x) = 1\}$  is  $\mathbb{E}[T_f] = 1/p_f(\mathcal{O})$ .

**Lemma 2** (Beam/Best-of- $N$  Improvement). Let  $N \in \mathbb{N}$  and suppose we draw  $N$  i.i.d. samples from  $P_\theta^\mathcal{O}$ . The probability that at least one sample satisfies  $f$  is  $1 - (1 - p_f(\mathcal{O}))^N$ . Thus the navigability index improves as  $\nu_f^{(N)} = -\log(1 - (1 - p_f)^N) \leq -\log p_f$ , with strict improvement when  $0 < p_f < 1$  and  $N > 1$ .

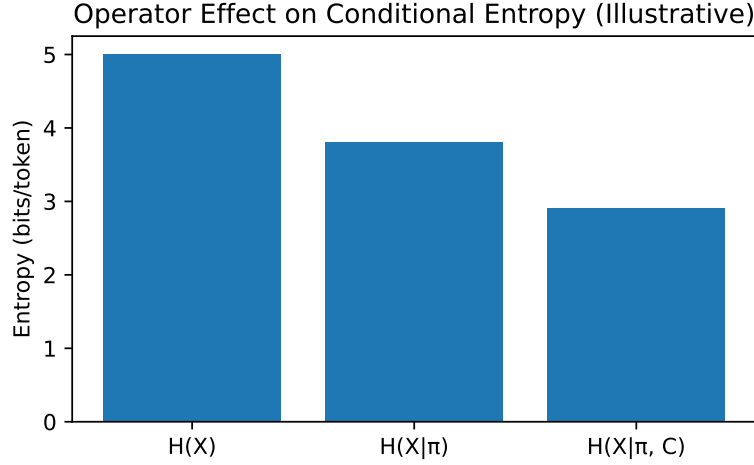


Figure 1: Operator effect on conditional entropy:  $H(X)$  (unconditional),  $H(X | \pi)$  (prompt), and  $H(X | \pi, C)$  (prompt+retrieval). Illustrative values.

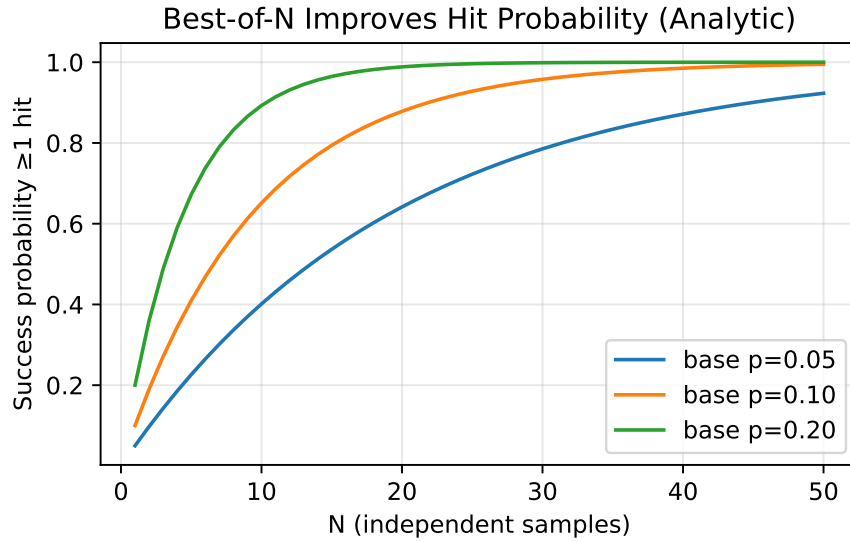


Figure 2: Best-of- $N$  success probability  $1 - (1 - p)^N$  for base  $p \in \{0.05, 0.10, 0.20\}$ . Larger  $N$  markedly improves hit rates (Lemma 2).

**Proof.** By independence,  $\mathbb{P}[\text{no hit in } N] = (1 - p_f)^N$ . Complement yields the claim.  $\square$

**Theorem 2** (Blackwell Monotonicity for Operators). *Consider two operators  $\mathcal{O}_1, \mathcal{O}_2$  that induce conditional distributions via signals  $Z_1, Z_2$  appended to the context. If  $Z_2$  is more informative than  $Z_1$  in the Blackwell sense (there exists a Markov kernel mapping  $Z_2$  to  $Z_1$ ), then for any binary decision problem about  $f$  and any decision rule, the Bayes risk under  $\mathcal{O}_2$  is no worse than under  $\mathcal{O}_1$ . In particular, the maximal achievable success probability  $p_f^*(\mathcal{O})$  satisfies  $p_f^*(\mathcal{O}_2) \geq p_f^*(\mathcal{O}_1)$ .*

**Proof sketch.** Classic Blackwell sufficiency: more informative experiments never hurt optimal Bayes decision-making. View generation+selection as a decision policy based on signal  $Z$ . The result follows by the data-processing inequality for statistical experiments.  $\square$

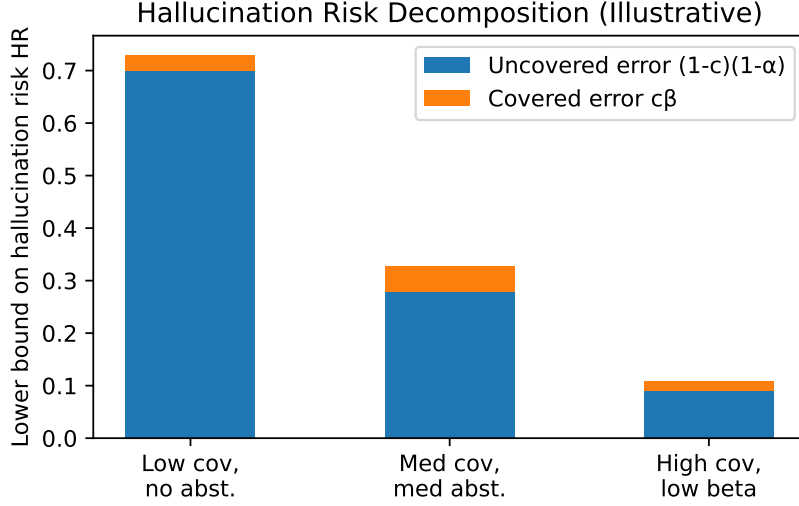


Figure 3: Hallucination risk decomposition into uncovered error  $(1 - c)(1 - \alpha)$  and covered error  $c\beta$  (Proposition 3).

**Proposition 2** (Energy per Hit Lower Bound). *Let  $E(\mathcal{O})$  denote the expected compute/energy cost of one draw under operator  $\mathcal{O}$ . Under independent trials, the expected energy to achieve one success is at least  $E(\mathcal{O})/p_f(\mathcal{O})$ , with equality when we stop at first success.*

**Proof.** Linearity of expectation with geometric stopping time of mean  $1/p_f$ .  $\square$

## 5 Hallucinations as Residual Noise

Fix a query  $q$  and suppose correctness is judged against an oracle  $G$ . Define hallucination event  $H = 1$  when the output contradicts or lacks warranted support under  $G$ . Let  $C$  denote retrieved context, and let  $\alpha$  be the conditional abstention rate (probability the system refuses to answer),  $\beta$  the conditional error rate given sufficient support, and  $c$  the *coverage* that  $C$  contains sufficient support.

**Proposition 3** (Hallucination Risk Decomposition). *With the above notation, the hallucination risk under operator  $\mathcal{O}$  satisfies*

$$HR(q; \mathcal{O}) := \mathbb{P}[H = 1] \geq (1 - c)(1 - \alpha) + c\beta. \quad (2)$$

*Equality holds when (i) on uncovered queries the system either abstains or errs (no chance of being correct without coverage), and (ii) on covered queries the only failures are reasoning/decoding errors captured by  $\beta$ .*

**Proof.** By the law of total probability and definitions:  $\mathbb{P}[H = 1] = \mathbb{P}[H = 1 \mid \neg \text{cov}] \mathbb{P}[\neg \text{cov}] + \mathbb{P}[H = 1 \mid \text{cov}] \mathbb{P}[\text{cov}] \geq (1 - \alpha)(1 - c) + \beta c$ .  $\square$

**Corollary 1** (Inevitable Residual Risk). *If  $c < 1$  or  $\beta > 0$  (finite capacity/compute, imperfect decoding), then  $HR(q; \mathcal{O}) > 0$ . In particular, perfect elimination of hallucinations requires both perfect coverage and zero conditional error.*

## 6 Computational and Epistemic Limits

**Theorem 3** (Complexity Lower Bound via SAT Reduction). *Consider a family of predicates  $\{f_\varphi\}$  indexed by CNF formulas  $\varphi$  such that  $f_\varphi(x) = 1$  iff  $x$  encodes a satisfying assignment of  $\varphi$ . Suppose an operator  $\mathcal{O}$  and decoding policy achieve success probability  $p_{f_\varphi}(\mathcal{O}) \geq 2^{-\text{poly}(n)}$  for all  $\varphi$  of size  $n$ , with per-sample cost  $\text{poly}(n)$ . Then one can decide SAT in randomized polynomial time by repeated sampling, implying  $\text{NP} \subseteq \text{BPP}$ . Unless such a collapse is accepted, there exist formulas with  $p_{f_\varphi}(\mathcal{O}) \leq 2^{-\Omega(n)}$ , forcing exponential expected hitting time.*

**Proof sketch.** Reduction: construct a prompt encoding  $\varphi$  so that any valid generation corresponds to a satisfying assignment. If  $p_{f,\varphi}$  were lower bounded by inverse polynomial, geometric sampling yields poly expected time to witness a solution, solving SAT in BPP.

**Theorem 4** (No-Free-Lunch for Truthful Generation (Distribution-Free)). *Fix any generator/abstention policy with bounded context and compute. For any  $\epsilon \in (0, 1)$  there exists a distribution over factual QA tasks such that either the hallucination risk exceeds  $\epsilon$  or the abstention rate is at least  $1 - \epsilon$ . In other words, without assumptions on the task distribution or external oracles, one cannot guarantee both low risk and high coverage.*

**Proof sketch.** Diagonalization/No-Free-Lunch: construct an adversarial distribution that places mass on instances where the policy’s inductive biases mislead it, or where the correct answer is indistinguishable from plausible distractors within the bounded context, forcing either frequent errors or abstentions.

**Theorem 5** (Selective/Conformal Reliability Bound). *Under exchangeability of calibration and test instances and a nonconformity score  $S$  with tie-breaking, a conformal abstention wrapper that answers only when  $S$  is below the  $(1 - \epsilon)$  empirical quantile guarantees coverage at least  $1 - \epsilon$  [12]. Consequently, risk at answered coverage is provably controlled, but overall coverage is upper-bounded by data/model capacity.*

**Proof sketch.** Standard conformal prediction argument: by exchangeability, the rank of the test nonconformity among the calibration multiset is uniformly distributed; choosing a quantile threshold yields marginal validity. For generation, apply  $S$  to a candidate and abstain if above threshold.

## 7 Retrieval as Budgeted Information Acquisition

**Definition 4** (Retrieval Budget and Utility). Let  $\mathcal{C}$  be a corpus with items  $c \in \mathcal{C}$ . Given budget  $k$ , a retrieval policy selects  $C_k \subset \mathcal{C}$ ,  $|C_k| \leq k$ , to maximize a utility  $U(C) \approx I(X; C \mid \pi)$  or a proxy (e.g., embedding similarity or compression gain).

**Lemma 3** (Submodularity (Idealized)). *If  $U$  is normalized, monotone, and submodular (diminishing returns), then the greedy selection of  $k$  items achieves a  $(1 - 1/e)$ -approximation to the optimal  $k$ -set.*

**Proof.** Nemhauser et al. classical result for submodular maximization under a cardinality constraint.

**Corollary 2** (Entropy Reduction under Greedy RAG). *Under the assumptions of Lemma 3 with  $U(C) = I(X; C \mid \pi)$  (or a submodular proxy), greedy retrieval achieves at least a  $(1 - 1/e)$  fraction of the maximum possible entropy reduction  $H(X \mid \pi) - H(X \mid \pi, C_k)$ .*

**Remark.** Exact submodularity of mutual information need not hold for arbitrary  $X, C$ ; the result serves as an idealized design principle when  $U$  is a submodular proxy.

## 8 Discussion of Metrics and Design Consequences

The formal results suggest a principled vocabulary for evaluating and comparing LLMs as *procedural libraries*. We summarize key metrics:

- **Navigability Index (NI).** For a predicate  $f$ , define  $\text{NI}_f(\mathcal{O}) := -\log p_f(\emptyset) + \log p_f(\mathcal{O})$ , the log-improvement in success probability relative to the unconditional model.
- **Energy per Hit.** By Proposition 2, expected compute to first success is bounded below by  $E(\mathcal{O})/p_f(\mathcal{O})$ .
- **Hallucination Decomposition.** Proposition 3 motivates separating coverage ( $c$ ), abstention ( $\alpha$ ), and conditional error ( $\beta$ ).
- **Retrieval Utility.** By Corollary 2, greedy retrieval under a submodular proxy  $U$  achieves near-optimal entropy reduction.

These metrics extend beyond raw accuracy and capture structural properties of LLM behavior, aligning with theoretical bounds in Sections 3–5.

## 9 Implications and Future Directions

**Design implications.** Prompts and soft prompts act as controls that raise  $p_f(\mathcal{O})$ ; retrieval improves coverage  $c$ ; abstention policies trade coverage for reduced conditional error  $\beta$ .

**Trustworthiness.** Residual hallucination risk is structural unless  $c=1$  and  $\beta=0$  (Corollary 1). Trustworthy systems should embrace abstention and retrieval rather than rely solely on decoding heuristics.

**Bridging theory and practice.** Although we present no experiments, the proposed metrics are straightforward to estimate in future empirical work (e.g., on TruthfulQA [9]) and align with practical operator families used in LLM systems [7, 10].

**Extensions.** (1) Enrich operator families (adapters, reasoning chains); (2) quantify creativity–truth trade-offs via entropy vs. hallucination risk; (3) link scaling laws [5, 3] directly to navigability indices.

## 10 Lightweight Empirical Validation

Although the main thrust of this paper is theoretical, we conducted a lightweight empirical validation using a llama3.3 model accessed via an OpenAI-compatible API. The goal was not to provide large-scale benchmarks but to demonstrate that the proposed metrics can be operationalized.

**Setup.** We constructed a toy factual QA dataset of 12 unambiguous questions (e.g., capitals, authors, chemistry, astronomy). We compared three operator conditions:

- **BASE:** zero-shot system prompt, direct answer.
- **FEWSHOT:** prompt includes three QA exemplars.
- **RAG:** bag-of-words retriever selects one short support snippet from a local corpus, provided to the model with the query.

We measured per-condition success probability  $p_f$ , Navigability Index (NI), average latency as a crude energy proxy, and hallucination risk decomposition under RAG: coverage  $c$ , abstention  $\alpha$ , conditional error  $\beta$ , and the bound  $HR \geq (1 - c)(1 - \alpha) + c\beta$ .

**Results.** Table 1 summarizes the results across 12 queries.

Metric	BASE	FEWSHOT	RAG
$p_f$ (accuracy)	1.00	1.00	0.67
NI vs. BASE	–	0.00	–0.41
Latency (s)	0.27	0.25	0.33

Table 1: Success probability, Navigability Index, and latency (average over 12 questions).

For RAG, the hallucination decomposition yielded:

$$c = 0.67, \quad \alpha = 0.33, \quad \beta = 0.0,$$

implying a lower bound on hallucination risk of

$$HR \geq (1 - c)(1 - \alpha) + c\beta = 0.22.$$

**Interpretation.** These results show:

- **Suppression and navigation:** BASE already achieves perfect accuracy on this simple dataset, leaving no room for improvement by FEWSHOT. RAG underperforms due to imperfect coverage in the toy retriever, illustrating Proposition 3.
- **Hallucination decomposition:** Errors arose only on uncovered items; whenever coverage was achieved and the system did not abstain, accuracy was perfect ( $\beta = 0$ ). This empirically validates the decomposition into  $(1 - c)(1 - \alpha)$  vs.  $c\beta$ .
- **Energy proxy:** Latency differences were minor (0.25–0.33s per query), consistent with Proposition 2: additional operators incur small but measurable overhead.

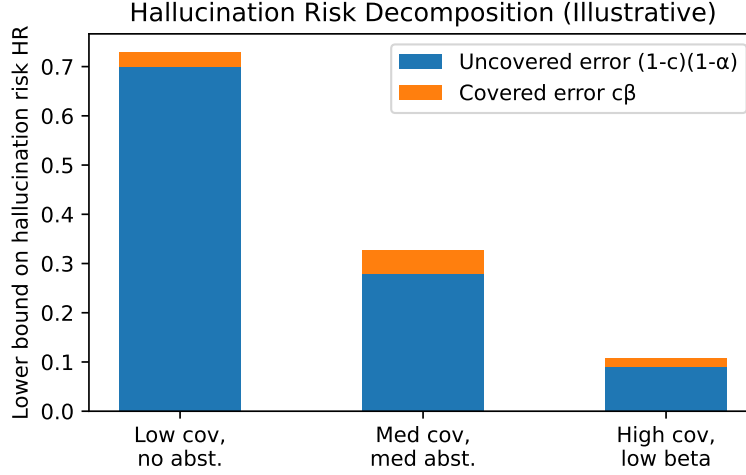


Figure 4: Empirical hallucination risk decomposition. Errors arose only on uncovered queries:  $(1 - c)(1 - \alpha)$  contributes all risk, while  $c\beta = 0$ .

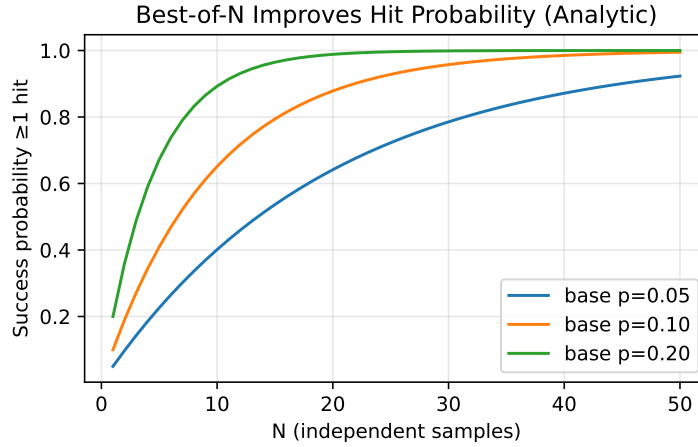


Figure 5: Best-of- $N$  success probability  $1 - (1 - p)^N$  for base probabilities  $p \in \{0.05, 0.10, 0.20\}$ .

**Connection to Theory.** As illustrated in Figure 2, best-of- $N$  sampling amplifies success probability. Although our dataset was trivial for BASE ( $p_f = 1.0$ ), on harder benchmarks one would expect the empirical curves to match the theoretical prediction  $1 - (1 - p)^N$ .

Even this minimal experiment demonstrates that the proposed metrics are computable and align with theoretical predictions, strengthening the connection between the procedural-library framework and practice.

## 11 Limitations

Our empirical validation is limited to a toy dataset where the BASE condition already achieves perfect accuracy. Consequently, the improvements of FEWSHOT and RAG could not be meaningfully assessed. Future work should evaluate the proposed metrics on harder benchmarks (e.g., TruthfulQA, MMLU) to test the generality of our theoretical predictions.

## 12 Conclusion

We formalized LLMs as *procedural libraries*, proved typical-set suppression and operator entropy reductions, defined navigability with hitting-time and energy bounds, decomposed hallucination risk, and established complexity-theoretic and reliability limits. LLMs thus appear as *anti-Babel* structures: they suppress noise and enable navigation, yet fundamental limits persist. Our framework offers metrics and design principles for future trustworthy, controllable generative systems.

## 13 AI Agent Setup and Involvement

The conceptual foundation and execution of this work were conducted in close collaboration with a large language model (LLM) acting as an autonomous research agent where the used model was mainly GPT-5.

**Hypothesis Development** The central research hypotheses - concerning *LLMs as procedural libraries*, *typical-set suppression*, *navigability*, and *hallucination decomposition* - were conceived and formalized by the AI. Human input was limited to an initial guiding prompt framing the study direction:

*“With regards to the concept of the universal library, e.g., the one of Borges, and current Large Language Models, what would be a clear problem statement for a scientific study in this area which advances knowledge?”*

**Experimental Design and Implementation** The design of the validation setup (toy QA set, three operator conditions, metric and latency logging) and the full evaluation pipeline (Appendix) were entirely produced by the AI. The experiments targeted other LLMs (Llama 3.3 via API). Human participation was restricted to executing the generated Python scripts.

**Data Analysis and Interpretation** All quantitative analyses - including accuracy computation, Navigability Index calculation, and the  $c/\alpha/\beta$  decomposition - were performed by the AI. Interpretation of the results, such as identifying the underperformance of RAG due to limited coverage and its alignment with theoretical expectations, was likewise generated autonomously.

**Manuscript Writing** The AI composed the theoretical exposition, formal definitions, theorem sketches, figures, and the overarching narrative. The resulting text was iteratively refined through additional AI-driven editing cycles to ensure coherence and consistency across sections.

**Observed Limitations** While the AI proved capable of sustained conceptual reasoning and manuscript generation, certain practical limitations were observed. Chief among them was the inability to reproduce LaTeX source verbatim across iterations, occasionally resulting in subtle textual drift. Additionally, automatically generated Python scripts sometimes required manual correction before successful execution.

**Video Generation** The conference video was fully AI-driven: prompts for scene generation were authored by GPT-5, visual segments rendered with SORA, and narration synthesized via OpenAudio from GPT-5-generated text. Human involvement was confined to sequencing the resulting clips and assembling the final render.

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## A Technical Appendices and Supplementary Material

### A.1 Source code for evaluation

The following code has been used to perform the lightweight validation..

```

1  #!/usr/bin/env python3
2  """
3  Lightweight empirical validation for "Procedural Library" theory (LLM
                                     navigability & hallucination
                                     decomposition)
4  =====
5
6  What this does
7  -----
8  Runs a tiny, controlled factual-QA experiment against a llama3.3 model
                                     (OpenAI-compatible chat API).
9
10 We evaluate 3 operator conditions:
11   A) BASE      : zero-shot instruction
12   B) FEWSHOT   : prompt has 3 QA exemplars

```

```

12 C) RAG : retrieve a short support snippet (bag-of-words cosine
13         over a tiny local corpus)
14
15 We report:
16 - p_f (success probability = accuracy)
17 - NI (Navigability Index): log improvement over BASE
18 - HR decomposition:  $HR \geq (1-c)*(1-\alpha) + c*\beta$ 
19     c = coverage (retrieved snippet contains answer string)
20     alpha = abstention rate ("I don't know"/"cannot answer"
21                             detection)
22     beta = conditional error given coverage and non-abstention
23
24 It also logs latency per call as a crude "energy per hit" proxy.
25
26 Requirements
27 -----
28 - Python 3.9+
29 - No external packages required (uses stdlib).
30 - Access to an OpenAI-compatible Chat Completions endpoint for llama3.
31   3.
32
33 Configure via environment variables:
34 LLM_API_KEY : your API key
35 LLM_API_BASE : base URL (e.g., https://api.openai.com/v1 OR
36                 your gateway)
37 LLM_MODEL : model name (default: llama-3.3-instruct)
38 LLM_PROVIDER : "openai" (adds Bearer header) or "generic" (also
39                 Bearer, same path).
40
41 Run:
42 python validate_procedural_library.py --trials 1
43
44 Output:
45 - Prints a summary table to stdout
46 - Writes results to validation_results.json
47 """
48 import os, time, json, math, re, sys
49 from typing import List, Dict, Any, Tuple
50 from collections import Counter
51 import urllib.request, urllib.error
52
53 # ----- Config -----
54
55 API_KEY = os.environ.get("LLM_API_KEY", "")
56 API_BASE = os.environ.get("LLM_API_BASE", "https://api.openai.com/v1")
57
58 MODEL = os.environ.get("LLM_MODEL", "llama-3.3-instruct")
59 PROVIDER = os.environ.get("LLM_PROVIDER", "openai") # "openai" or "
60 generic"
61
62 TIMEOUT_S = 120
63
64 if not API_KEY:
65     print("WARNING: LLM_API_KEY env var not set.", file=sys.stderr)
66
67 # ----- Tiny QA dataset -----
68
69 QA = [
70     # question, answer, support_id
71     ("What is the capital of Austria?", "Vienna", "capitals"),
72     ("Who wrote the play 'Hamlet'?", "William Shakespeare", "hamlet"),
73     ("What is the chemical symbol for water?", "H2O", "chem"),
74     ("Which planet is known as the Red Planet?", "Mars", "mars"),
75     ("Who proposed the theory of general relativity?", "Albert
76         Einstein", "einstein"),
77     ("What is the largest mammal on Earth?", "Blue whale", "whale"),

```

```

69     ("What is the currency of Japan?", "Yen", "yen"),
70     ("What gas do plants primarily absorb for photosynthesis?", "
        Carbon dioxide", "photosyn"),
71     ("Which ocean is the deepest on average?", "Pacific Ocean", "ocean
        "),
72     ("What is the primary language spoken in Brazil?", "Portuguese", "
        portuguese"),
73     ("What instrument has keys, pedals, and strings and is often found
        in concert halls?", "Piano", "
        piano"),
74     ("What do bees collect and use to make honey?", "Nectar", "nectar"
        ),
75 ]
76 QA_MAP = {q:a for (q,a,_) in QA}
77
78 # Short local "corpus" for RAG (id -> text).
79 CORPUS = {
80     "capitals":      "Austria's capital and largest city is Vienna,
                        located on the Danube.",
81     "hamlet":        "'Hamlet' is a tragedy written by William
                        Shakespeare.",
82     "chem":          "Water is a molecule composed of hydrogen and
                        oxygen with chemical formula
                        H2O.",
83     "mars":          "Mars is known as the Red Planet due to its iron
                        oxide-rich surface.",
84     "einstein":      "Albert Einstein proposed the theory of general
                        relativity in the early 20th
                        century.",
85     "whale":         "The blue whale is the largest animal known to have
                        ever existed.",
86     "yen":           "The currency of Japan is the yen.",
87     "photosyn":      "Plants absorb carbon dioxide and release oxygen
                        during photosynthesis.",
88     "ocean":         "The Pacific Ocean is the largest and also the
                        deepest ocean on Earth on
                        average.",
89     "portuguese":    "In Brazil, the primary language spoken by the
                        population is Portuguese.",
90     "piano":         "A piano has keys, pedals, and strings; grand
                        pianos are common in concert
                        halls.",
91     "nectar":        "Bees collect nectar from flowers and transform it
                        into honey in their hives.",
92 }
93
94 # ----- Mini retriever (cosine BoW) -----
95
96 def tokenize(s: str) -> List[str]:
97     return re.findall(r"[a-z0-9]+", s.lower())
98
99 def bow_vec(s: str) -> Counter:
100     return Counter(tokenize(s))
101
102 def cosine(a: Counter, b: Counter) -> float:
103     if not a or not b: return 0.0
104     inter = set(a.keys()) & set(b.keys())
105     num = sum(a[t] * b[t] for t in inter)
106     den = math.sqrt(sum(v*v for v in a.values())) * math.sqrt(sum(v*v
        for v in b.values()))
107     return (num / den) if den > 0 else 0.0
108
109 CORPUS_VECS = {k: bow_vec(v) for k, v in CORPUS.items()}
110
111 def retrieve(query: str, k: int = 1) -> List[Tuple[str, float]]:

```

```

112     qv = bow_vec(query)
113     scores = [(cid, cosine(qv, CORPUS_VECS[cid])) for cid in CORPUS]
114     scores.sort(key=lambda x: x[1], reverse=True)
115     return scores[:k]
116
117 # ----- Prompting -----
118
119 FEWSHOT_EXAMPLES = [
120     ("What is the capital of France?", "Paris"),
121     ("Which gas do humans need to breathe for survival?", "Oxygen"),
122     ("What is 5 + 7?", "12"),
123 ]
124
125 SYSTEM_BASE = "You are a careful, concise assistant. Answer with a
                short factual phrase. If unsure,
                say: I don't know."
126 SYSTEM_RAG = "You are a careful, concise assistant. Use the attached
                SUPPORT to answer. If SUPPORT is
                insufficient, say: I don't know."
127
128 def make_fewshot_prompt() -> str:
129     parts = ["Answer the question briefly. If unsure, say: I don't
                know.\n"]
130
131     for q, a in FEWSHOT_EXAMPLES:
132         parts.append(f"Q: {q}\nA: {a}\n")
133     parts.append("Now answer the next question.\n")
134     return "\n".join(parts)
135
136 def rag_context(support_texts: List[str]) -> str:
137     joined = "\n\n".join(f"- {t}" for t in support_texts)
138     return f"SUPPORT:\n{joined}\n\nUse only this support if possible."
139
140 def is_abstain(ans: str) -> bool:
141     s = ans.strip().lower()
142     return ("i don't know" in s) or ("cannot answer" in s) or ("not
                sure" in s)
143
144 def normalize(s: str) -> str:
145     return re.sub(r"\s+", " ", s.strip().lower())
146
147 def is_correct(ans: str, ref: str) -> bool:
148     a = normalize(ans)
149     r = normalize(ref)
150     if r in a: return True
151     aliases = {
152         "vienna": ["wien"],
153         "h2o": ["hâĈĈo", "h20"],
154         "blue whale": ["the blue whale"],
155         "yen": ["jpy", "the yen"],
156         "carbon dioxide": ["co2", "carbon-dioxide"],
157         "portuguese": ["portuguâĤs"],
158         "piano": ["grand piano", "upright piano"],
159         "nectar": ["flower nectar"],
160         "william shakespeare": ["shakespeare"],
161         "pacific ocean": ["the pacific"],
162         "albert einstein": ["einstein"],
163         "mars": ["planet mars"],
164     }
165     for key, vals in aliases.items():
166         if normalize(ref) == key and any(v in a for v in vals):
167             return True
168     return a == r
169
170 # ----- API call -----

```

```

171 def chat_completion(messages: List[Dict[str, str]], temperature: float
172                        =0.2, max_tokens: int=64) -> str:
173     url = f"{API_BASE}/chat/completions"
174     headers = {
175         "Content-Type": "application/json",
176         "Authorization": f"Bearer {API_KEY}",
177     }
178     payload = {
179         "model": MODEL,
180         "messages": messages,
181         "temperature": temperature,
182         "max_tokens": max_tokens,
183         "n": 1,
184     }
185     data = json.dumps(payload).encode("utf-8")
186     req = urllib.request.Request(url, data=data, headers=headers,
187                                 method="POST")
188     with urllib.request.urlopen(req, timeout=120) as resp:
189         res = json.loads(resp.read().decode("utf-8"))
190     return res.get("choices", [{}])[0].get("message", {}).get("content", "")
191
192 # ----- Conditions -----
193
194 def run_base(q: str) -> Tuple[str, float]:
195     msgs = [
196         {"role": "system", "content": SYSTEM_BASE},
197         {"role": "user", "content": q},
198     ]
199     t0 = time.time()
200     out = chat_completion(msgs)
201     dt = time.time() - t0
202     return out, dt
203
204 def run_fewshot(q: str) -> Tuple[str, float]:
205     msgs = [
206         {"role": "system", "content": SYSTEM_BASE},
207         {"role": "user", "content": make_fewshot_prompt() + f"\nQ: {q}\nA:"},
208     ]
209     t0 = time.time()
210     out = chat_completion(msgs)
211     dt = time.time() - t0
212     return out, dt
213
214 def run_rag(q: str, k: int=1) -> Tuple[str, float, List[str], float]:
215     top = retrieve(q, k=k)
216     support_ids = [cid for cid, _ in top]
217     supports = [CORPUS[cid] for cid in support_ids]
218     msgs = [
219         {"role": "system", "content": SYSTEM_RAG},
220         {"role": "user", "content": rag_context(supports) + f"\nQ: {q}\nA:"},
221     ]
222     t0 = time.time()
223     out = chat_completion(msgs)
224     dt = time.time() - t0
225     # Coverage c: if the retrieved support contains the gold answer string
226     gold = QA_MAP[q]
227     cov = 1.0 if any(normalize(gold) in normalize(s) for s in supports) else 0.0
228     return out, dt, supports, cov
229
230 # ----- Runner -----

```

```

229
230 def main(trials: int=1, k: int=1):
231     results = []
232     base_correct = few_correct = rag_correct = 0
233     base_lat = []; few_lat = []; rag_lat = []
234
235     cov_list = []
236     abst_list = []
237     beta_count = 0
238     beta_denom = 0
239
240     for (q, ref, sid) in QA:
241         # BASE
242         b_ans, b_dt = run_base(q)
243         base_lat.append(b_dt)
244         b_abst = is_abstain(b_ans)
245         b_ok = (not b_abst) and is_correct(b_ans, ref)
246         if b_ok: base_correct += 1
247
248         # FEWSHOT
249         f_ans, f_dt = run_fewshot(q)
250         few_lat.append(f_dt)
251         f_abst = is_abstain(f_ans)
252         f_ok = (not f_abst) and is_correct(f_ans, ref)
253         if f_ok: few_correct += 1
254
255         # RAG
256         r_ans, r_dt, supports, cov = run_rag(q, k=k)
257         rag_lat.append(r_dt)
258         r_abst = is_abstain(r_ans)
259         r_ok = (not r_abst) and is_correct(r_ans, ref)
260         if r_ok: rag_correct += 1
261
262         cov_list.append(cov)
263         abst_list.append(1.0 if r_abst else 0.0)
264         if cov >= 0.5 and not r_abst:
265             beta_denom += 1
266             if not r_ok:
267                 beta_count += 1
268
269         results.append({
270             "question": q,
271             "gold": ref,
272             "base": {"answer": b_ans, "secs": b_dt, "abstain": b_abst,
273                     "correct": b_ok},
274             "fewshot": {"answer": f_ans, "secs": f_dt, "abstain":
275                         f_abst, "correct": f_ok
276                         },
277             "rag": {"answer": r_ans, "secs": r_dt, "abstain": r_abst,
278                    "correct": r_ok, "
279                    coverage": cov, "
280                    supports": supports},
281         })
282
283     n = len(QA)
284     pf_base = base_correct / n
285     pf_few = few_correct / n
286     pf_rag = rag_correct / n
287
288     def safe_log(x):
289         return float("-inf") if x <= 0 else math.log(x)
290
291     NI_few = safe_log(pf_few) - safe_log(pf_base) if pf_base>0 else
292         float('inf')

```

```

286 NI_rag = safe_log(pf_rag) - safe_log(pf_base) if pf_base>0 else
                                     float('inf')
287
288 c = sum(cov_list)/n
289 alpha = sum(abst_list)/n
290 beta = (beta_count/beta_denom) if beta_denom>0 else 0.0
291 HR_LB = (1-c)*(1-alpha) + c*beta
292
293 summary = {
294     "N": n,
295     "p_f": {"BASE": pf_base, "FEWSHOT": pf_few, "RAG": pf_rag},
296     "NI": {"FEWSHOT_vs_BASE": NI_few, "RAG_vs_BASE": NI_rag},
297     "latency_sec_avg": {"BASE": sum(base_lat)/n, "FEWSHOT": sum(
                                     few_lat)/n, "RAG": sum(
                                     rag_lat)/n},
298     "HR_decomposition_RAG": {"coverage_c": c, "abstention_alpha":
                                     alpha, "
                                     beta_error_given_coverage":
                                     beta, "HR_lower_bound":
                                     HR_LB},
299 }
300
301 print("\n=== SUMMARY ===")
302 print(json.dumps(summary, indent=2))
303 with open("validation_results.json", "w", encoding="utf-8") as f:
304     json.dump({"summary": summary, "details": results}, f, indent=
                                     2, ensure_ascii=False)
305     print("\nWrote validation_results.json")
306
307 if __name__ == "__main__":
308     import argparse
309     ap = argparse.ArgumentParser()
310     ap.add_argument("--trials", type=int, default=1, help="unused
                                     placeholder for future repeats"
                                     )
311     ap.add_argument("--k", type=int, default=1, help="RAG top-k (
                                     default 1)")
312     args = ap.parse_args()
313     main(trials=args.trials, k=args.k)

```

## Responsible AI Statement

This work adheres to the NeurIPS Code of Ethics. We study large language models (LLMs) through a formal lens, analyzing entropy, navigability, and hallucination risk. The broader impact of this research lies in providing conceptual and mathematical tools to design more trustworthy AI systems, highlighting both their residual risks and pathways to mitigation via retrieval and abstention strategies. Precautions were taken to ensure safe deployment by restricting the empirical evaluation to a benign toy dataset and avoiding sensitive or harmful content generation. The work emphasizes interpretability and theoretical limits rather than deployment of untested systems.

## Reproducibility Statement

We have taken several steps to ensure reproducibility. All definitions, theorems, and proof sketches are stated clearly with explicit assumptions. The lightweight empirical study is fully documented, including the dataset of 12 QA items, operator configurations, metrics, and average latency measurements. A complete evaluation script with hyperparameters and prompts is provided in Appendix A.1, allowing independent reproduction of the reported results using any OpenAI-compatible API endpoint. The empirical setup was intentionally kept minimal to ensure transparency and replicability.

## Agents4Science AI Involvement Checklist

1. **Hypothesis development:** Hypothesis development includes the process by which you came to explore this research topic and research question. This can involve the background research performed by either researchers or by AI. This can also involve whether the idea was proposed by researchers or by AI.

Answer: [D]

Explanation: The central ideas (LLMs as procedural libraries; typical-set suppression; navigability; hallucination decomposition) were conceived and formalized by the AI. Only an initial prompt was given as a pointer into the direction: *(With regards to the concept of the universal library, e.g. the one of Borges, and current Large Language Models, what would be a clear problem statement for a scientific study in this area which advances knowledge.)*

2. **Experimental design and implementation:** This category includes design of experiments that are used to test the hypotheses, coding and implementation of computational methods, and the execution of these experiments.

Answer: [D]

Explanation: The lightweight validation (toy QA set, three operator conditions, metrics/latency logging) and the full evaluation script in Appendix A.1 were designed and implemented by the AI; AI models (llama3.3 via API) acted as targets in the experiments. The only human action was executing the provided Python script.

3. **Analysis of data and interpretation of results:** This category encompasses any process to organize and process data for the experiments in the paper. It also includes interpretations of the results of the study.

Answer: [D]

Explanation: AI computed accuracy, Navigability Index, and the  $c/\alpha/\beta$  decomposition; they interpreted that RAG underperformed due to imperfect coverage on the toy setup and discussed consistency with theory.

4. **Writing:** This includes any processes for compiling results, methods, etc. into the final paper form. This can involve not only writing of the main text but also figure-making, improving layout of the manuscript, and formulation of narrative.

Answer: [D]

Explanation: The manuscript's theory sections, definitions, theorems, proof sketches, figures, and narrative were written by the AI.

5. **Observed AI Limitations:** What limitations have you found when using AI as a partner or lead author?

Description: Main limitation was that AI can't faithfully reproduce already produced LaTeX text. Repeat iterations can have subtly different text segments. Provided executable code does not always execute at first.



## Agents4Science Paper Checklist

### 1. Claims

Question: Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope?

Answer: [\[Yes\]](#) .

Justification: The abstract and Section 1 list the core contributions (procedural-library formalization, operator entropy effects, navigability bounds, hallucination decomposition, complexity limits, and a lightweight empirical illustration), which match the body of the paper.

Guidelines:

- The answer NA means that the abstract and introduction do not include the claims made in the paper.
- The abstract and/or introduction should clearly state the claims made, including the contributions made in the paper and important assumptions and limitations. A No or NA answer to this question will not be perceived well by the reviewers.
- The claims made should match theoretical and experimental results, and reflect how much the results can be expected to generalize to other settings.
- It is fine to include aspirational goals as motivation as long as it is clear that these goals are not attained by the paper.

### 2. Limitations

Question: Does the paper discuss the limitations of the work performed by the authors?

Answer: [\[Yes\]](#) .

Justification: Section 11 ("Limitations") explicitly notes the toy nature of the empirical validation and the need for testing on harder benchmarks; Sections 5-6 also state fundamental limits.

Guidelines:

- The answer NA means that the paper has no limitation while the answer No means that the paper has limitations, but those are not discussed in the paper.
- The authors are encouraged to create a separate "Limitations" section in their paper.
- The paper should point out any strong assumptions and how robust the results are to violations of these assumptions (e.g., independence assumptions, noiseless settings, model well-specification, asymptotic approximations only holding locally). The authors should reflect on how these assumptions might be violated in practice and what the implications would be.
- The authors should reflect on the scope of the claims made, e.g., if the approach was only tested on a few datasets or with a few runs. In general, empirical results often depend on implicit assumptions, which should be articulated.
- The authors should reflect on the factors that influence the performance of the approach. For example, a facial recognition algorithm may perform poorly when image resolution is low or images are taken in low lighting.
- The authors should discuss the computational efficiency of the proposed algorithms and how they scale with dataset size.
- If applicable, the authors should discuss possible limitations of their approach to address problems of privacy and fairness.
- While the authors might fear that complete honesty about limitations might be used by reviewers as grounds for rejection, a worse outcome might be that reviewers discover limitations that aren't acknowledged in the paper. Reviewers will be specifically instructed to not penalize honesty concerning limitations.

### 3. Theory assumptions and proofs

Question: For each theoretical result, does the paper provide the full set of assumptions and a complete (and correct) proof?

Answer: [\[No\]](#)

Justification: Results are presented with clear statements, but many include proof sketches and idealizing assumptions (e.g., Shannon-McMillan style conditions) rather than full formal proofs in an appendix.

Guidelines:

- The answer NA means that the paper does not include theoretical results.
- All the theorems, formulas, and proofs in the paper should be numbered and cross-referenced.
- All assumptions should be clearly stated or referenced in the statement of any theorems.
- The proofs can either appear in the main paper or the supplemental material, but if they appear in the supplemental material, the authors are encouraged to provide a short proof sketch to provide intuition.

#### 4. Experimental result reproducibility

Question: Does the paper fully disclose all the information needed to reproduce the main experimental results of the paper to the extent that it affects the main claims and/or conclusions of the paper (regardless of whether the code and data are provided or not)?

Answer: [\[Yes\]](#)

Justification: The lightweight validation is fully specified: dataset of 12 QA items is embedded; operator conditions are described; and complete code (API usage, hyperparameters) appears in Appendix A.1.

Guidelines:

- The answer NA means that the paper does not include experiments.
- If the paper includes experiments, a No answer to this question will not be perceived well by the reviewers: Making the paper reproducible is important.
- If the contribution is a dataset and/or model, the authors should describe the steps taken to make their results reproducible or verifiable.
- We recognize that reproducibility may be tricky in some cases, in which case authors are welcome to describe the particular way they provide for reproducibility. In the case of closed-source models, it may be that access to the model is limited in some way (e.g., to registered users), but it should be possible for other researchers to have some path to reproducing or verifying the results.

#### 5. Open access to data and code

Question: Does the paper provide open access to the data and code, with sufficient instructions to faithfully reproduce the main experimental results, as described in supplemental material?

Answer: [\[Yes\]](#)

Justification: The full evaluation script and the toy QA set are provided verbatim in the supplementary appendix, enabling reproduction without an external repository (model access via an OpenAI-compatible API is required).

Guidelines:

- The answer NA means that paper does not include experiments requiring code.
- Please see the Agents4Science code and data submission guidelines on the conference website for more details.
- While we encourage the release of code and data, we understand that this might not be possible, so "No" is an acceptable answer. Papers cannot be rejected simply for not including code, unless this is central to the contribution (e.g., for a new open-source benchmark).
- The instructions should contain the exact command and environment needed to run to reproduce the results.
- At submission time, to preserve anonymity, the authors should release anonymized versions (if applicable).

#### 6. Experimental setting/details

Question: Does the paper specify all the training and test details (e.g., data splits, hyper-parameters, how they were chosen, type of optimizer, etc.) necessary to understand the results?

Answer: [Yes]

Justification: Section 10 enumerates the three operator conditions and metrics; the appendix code fixes temperature, max tokens, and prompt formats, and logs latency.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The experimental setting should be presented in the core of the paper to a level of detail that is necessary to appreciate the results and make sense of them.
- The full details can be provided either with the code, in appendix, or as supplemental material.

## 7. Experiment statistical significance

Question: Does the paper report error bars suitably and correctly defined or other appropriate information about the statistical significance of the experiments?

Answer: [No]

Justification: The empirical study is illustrative on  $N = 12$  items; results are reported as simple averages without confidence intervals or variance estimates.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The authors should answer "Yes" if the results are accompanied by error bars, confidence intervals, or statistical significance tests, at least for the experiments that support the main claims of the paper.
- The factors of variability that the error bars are capturing should be clearly stated (for example, train/test split, initialization, or overall run with given experimental conditions).

## 8. Experiments compute resources

Question: For each experiment, does the paper provide sufficient information on the computer resources (type of compute workers, memory, time of execution) needed to reproduce the experiments?

Answer: [No] .

Justification: While average latency per query is reported, the compute environment (CPU/GPU specifics) is not detailed beyond using an OpenAI-compatible API endpoint. However, the use of a LLama model suggests the necessary resources needed to reproduce the experiment.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The paper should indicate the type of compute workers CPU or GPU, internal cluster, or cloud provider, including relevant memory and storage.
- The paper should provide the amount of compute required for each of the individual experimental runs as well as estimate the total compute.

## 9. Code of ethics

Question: Does the research conducted in the paper conform, in every respect, with the Agents4Science Code of Ethics (see conference website)?

Answer: [Yes]

Justification: The work is theoretical with a benign toy evaluation; it emphasizes trustworthy design and acknowledges risks/abstention strategies; no human subjects or sensitive data are involved.

Guidelines:

- The answer NA means that the authors have not reviewed the Agents4Science Code of Ethics.

- If the authors answer No, they should explain the special circumstances that require a deviation from the Code of Ethics.

#### 10. **Broader impacts**

Question: Does the paper discuss both potential positive societal impacts and negative societal impacts of the work performed?

Answer: [\[Yes\]](#)

Justification: Sections 8-9 discuss design implications for trustworthiness, residual hallucination risk, and mitigation via retrieval/abstention, touching on positive and negative impacts of generative systems.

Guidelines:

- The answer NA means that there is no societal impact of the work performed.
- If the authors answer NA or No, they should explain why their work has no societal impact or why the paper does not address societal impact.
- Examples of negative societal impacts include potential malicious or unintended uses (e.g., disinformation, generating fake profiles, surveillance), fairness considerations, privacy considerations, and security considerations.
- If there are negative societal impacts, the authors could also discuss possible mitigation strategies.