Hallucination is a Consequence of Space-Optimality: A Rate-Distortion Theorem for Membership Testing

Anxin Guo
Computer Science Department
Northwestern University, USA
anxinbguo@gmail.com

Jingwei Li
Department of IEOR
Columbia University, USA
jl6639@columbia.edu

Abstract

Large language models often hallucinate with high confidence on "random facts" that lack inferable patterns. We formalize the memorization of such facts as a membership testing problem, unifying the discrete error metrics of Bloom filters with the continuous log-loss of LLMs. By analyzing this problem in the regime where facts are sparse in the universe of plausible claims, we establish a rate-distortion theorem: the optimal memory efficiency is characterized by the minimum KL divergence between score distributions on facts and non-facts. This theoretical framework provides a distinctive explanation for hallucination under an idealized setting: even with optimal training, perfect data, and a simplified "closed world" setting, the information-theoretically optimal strategy under limited capacity is not to abstain or forget, but to assign high confidence to some non-facts, resulting in hallucination. We validate this theory empirically on synthetic data, showing that hallucinations persist as a natural consequence of lossy compression.

1 Introduction

Despite their transformative impact, Large Language Models (LLMs) are hindered by *hallucinations* – the generation of confident and plausible yet factually incorrect statements. Recently, an influential line of work Kalai et al. (2025); Mohsin et al. (2025); Xu (2025); Wu et al. (2025); Gumaan (2025) theoretically explained the hallucination phenomenon from a statistical learning perspective, considering an LLM as an implementation of a binary classifier on plausible-looking *random facts* – facts that are unstructured and cannot be logically inferred unless encountered during training, such as phone numbers or biographical details. By a no-free-lunch-style logic, since generalization is impossible on these facts, the model must make uninformed guesses on unseen random facts, leading to systematic inference errors. In the classification setting, hallucination corresponds to false positives resulting from such guesses.

As a natural workaround, researchers have promoted *abstention* Kalai et al. (2025); Wen et al. (2025) – an LLM is expected to provide an "I don't know" response on unseen random factual queries. Theoretically, we can further simplify the task by adopting a "closed-world assumption," where all unseen potential facts are categorized as non-facts for evaluation [1]. Under this setting, an ideal LLM can be both informative and non-hallucinating on factual queries, as long as it accurately distinguishes the finitely many known facts from all other (potentially true but unknown) non-facts. This is a sample-efficient memorization task.

[1] Alternatively, one can assume all true facts are seen during training.

However, empirical evidence suggests that LLMs struggle to execute this memorization task robustly. Even when permitted to abstain, models continue to generate high-confidence hallucinations, while simultaneously exhibiting "over-refusal" of legitimate queries Cheng et al. (2024); Brahman et al. (2024); Zhu et al. (2025), exhibiting a precision–recall tradeoff. This points to a different bottleneck beyond no-free-lunch: the finite capacity of the model weights forces lossy compression of the training data, making memorization of specific, unstructured facts a non-trivial task.

This information-theoretic perspective connects to several recent works Pan et al. (2025); Shi et al. (2025); Mohsin et al. (2025); Kim (2025a,b) which attribute hallucination to the distortion occurring when compressing an infinitely complex world of knowledge to a finite model capacity. Despite these insights, two gaps remain. First, "compression causes errors" does not explain the *shape* of the errors: while forgetting is natural under limited capacity, it is unclear why hallucination is particularly prevalent. Second, existing compression-based explanations are either high-level informal arguments or assume an infinite number of facts, while our closed-world assumption restricts facts to a finite set. This motivates a more rigorous study in a simplified setting:

> *What is the theoretical explanation for high-confidence hallucinations in a closed world with finitely many random facts?*

In this work, we argue that these hallucinations are driven by the asymmetry between facts and non-facts. Specifically, if facts are sparse and randomly distributed in a vast universe of plausible statements, then an LLM with limited memory capacity would tend to accept false statements as facts.

To formalize this intuition, we model factuality judgment as a *membership testing* problem. We view each plausible potential fact as an element i in a universe $\mathcal{U}$, and the set of known facts as a key set $\mathcal{K} \subseteq \mathcal{U}$. Given a query $i \in \mathcal{U}$, the model outputs a confidence score $\hat{x}_i \in [0, 1]$ indicating its belief that $i \in \mathcal{K}$; under this lens, hallucinations correspond to non-keys receiving high confidence. Query output $\hat{x}_i$ can be evaluated under generic *error metrics* measuring the discrepancy between $\hat{x}_i$ and the true label $\mathbb{1}\{i \in \mathcal{K}\}$. The goal of a membership tester is to use a small *memory budget* for storing the keys, and achieve small expected error on queries. This abstraction subsumes approximate membership data structures[2] such as Bloom filters Bloom (1970), for which the query output is limited to $\{0, 1\}$.

1.1 Our contributions

A rate-distortion theorem for membership testing. We consider the sparse limit where $\frac{|\mathcal{K}|}{|\mathcal{U}|} \to 0$. In this regime, we identify the exact memory–error tradeoff in the form of a rate-distortion theorem. Specifically, the minimum memory budget per key is determined by the minimum KL-divergence between key and non-key output distributions.

Theorem 1.1 (Informal, Theorems 3.1, 3.2)**.** *Let* $\mathrm{KL}(P\|Q)$ *denote the base-2 Kullback-Leibler divergence between distributions* P *and* Q*. To store* n *keys in the sparse regime and reach a certain error level under generic error metrics, it is necessary and sufficient for a membership tester to store*

$$n \cdot \mathrm{KL}(\mu_K \| \mu_N) + o(n) \textit{ bits of information,}$$

where μ_K *and* μ_N *are the distributions of scores* $\hat{x}_i$ *conditioned on* $i \in \mathcal{K}$ *and* $i \notin \mathcal{K}$*, respectively, that satisfy the error constraints and minimize the KL-divergence.*

Moreover, score distributions of an optimal membership tester must converge to μ_K *and* μ_N *in the sparse limit.*

[2] We will call these data structures "filters" for convenience.

KL divergence arises naturally from the asymmetry between keys and non-keys. If $X_1, \ldots, X_n \sim \mu_N$ are drawn i.i.d., then $n \cdot \mathrm{KL}(\mu_K \| \mu_N)$ roughly measures the negative log-likelihood of $X_1, \ldots, X_n$ being distributed as μ_K. This value therefore quantifies how many extra bits of information are needed to force the key query output to be μ_K, overcoming the default assumption that they follow the non-key distribution μ_N.

Hallucination as the optimal mode of error. Our theory provides two perspectives on why it is *memory-efficient* for LLMs to hallucinate on random facts. First, consider a model tasked to estimate the probability $\mathbb{P}[i \in \mathcal{K}]$ of a potential fact $i \in \mathcal{U}$ being true, where the output $\hat{x}_i \in [0, 1]$ is evaluated with logarithmic or cross-entropy loss, consistent with the maximum likelihood objective and previously proposed training/evaluation methods for factual knowledge Kadavath et al. (2022); Cheng et al. (2024).

The unique loss-minimizing query output under this metric, given a fixed memory capacity, is to assign high confidence to *all* facts, while assigning either *zero* or *fact-level confidence* to non-facts. We also empirically verify this tendency on synthetic data. For a probability estimation task, hallucination, instead of systematic forgetting or uniform uncertainty, is the natural mode of error.

Classifier via thresholding and two-sided filters. Our second perspective establishes that any LLM decision mechanism based on *score thresholding* - whether the scores are derived from generative probabilities Kalai et al. (2025) or the probability estimation output above - is subject to the fundamental memory-error trade-off of *two-sided filters*, a generalization of Bloom-type filters Bloom (1970) allowing both false positives and false negatives. Unlike the first perspective, this result applies to all LLM-based classification mechanisms and does not assume optimality.

Applying our result to filters, our analysis recovers and refines the various existing space lower bounds Carter et al. (1978); Pagh and Rodler (2001); Hurley and Waldvogel (2007); Li et al. (2023a). We also show that a hash-based two-sided filter achieves our lower bound up to $o(n)$ bits of space overhead. As a corollary, eliminating hallucinations (false positives) on random facts is very costly without a simultaneous increase in forgetting or over-refusal (false negatives). Post-processing for factual accuracy only moves us *along* the memory-error frontier, not beyond it.

Further discussions on the information capacity. Although modern models have billions of parameters, the effective memory budget for storing a particular family of random facts can be far smaller. Appendix A provides two explanations: (i) modern networks are encouraged to minimize pure memorization (through various regularization and MDL/PAC-Bayes viewpoints), and (ii) structured knowledge (e.g., language and reasoning) and random facts compete for a finite memory budget, where the *former takes precedence* during learning. We argue that this implicit bias results in a small effective memory budget for random facts, leading to the observed high-confidence hallucinations.

Conversely, this analysis supports the effectiveness of additional fine-tuning on unstructured random facts, which encourages the model to allocate more memory budget. Our framework also justifies why incorporating external information, such as using RAG Lewis et al. (2020), is effective in mitigating hallucinations: memory budget is no longer a limiting factor when non-parametric memory is present.

1.2 Related work

Hallucination Ji et al. (2023); Alansari and Luqman (2025); Huang et al. (2025b) is often defined as the generation of content that is fluent and plausible but factually inaccurate, nonsensical, or unfaithful to source material. A large body of empirical works has identified causal factors throughout the entire LLM development pipeline, attributing them to *data-centric causes* (noisy web corpora) Dodge et al. (2021); Bender et al. (2021); Perelkiewicz and Poswiata (2024), *model-centric* *causes* (objectives/architectural limits of next-token prediction) Bachmann and Nagarajan (2025); Huang et al. (2025a); Welleck et al. (2020), and *inference-centric causes* (inference-time choices such as stochastic decoding) Holtzman et al. (2020); Mallen et al. (2023); Lee et al. (2023); Li et al. (2023b). Our perspective is orthogonal to these studies, as we focus on the *information* perspective independent of these practical considerations.

On the theoretical side, a group of papers Kalai and Vempala (2024); Kalai et al. (2025); Mohsin et al. (2025); Xu (2025); Wu et al. (2025); Gumaan (2025) consider the *classification* perspective, as explained previously. Notably, Kalai et al. Kalai et al. (2025) do not view hallucination as a classification problem per se, but instead shows that generative hallucination is related to the total error in classification for an induced classifier. Meanwhile, several other works Xu et al. (2024); Shi et al. (2025); Banerjee et al. (2024); Suzuki et al. (2025); Kalavasis et al. (2025); Charikar and Pabbaraju (2025) consider LLMs as computable functions and discuss how incomputability gives rise to hallucinations. Some other works Chlon et al. (2025); Pan et al. (2025); Shi et al. (2025); Mohsin et al. (2025); Kim (2025a,b) consider LLMs as *lossy compressors* of knowledge and discuss how the distortion during compression causes hallucinations. Additionally, Karpowicz (2025) proves a voting-theory-style impossibility result for an LLM to eliminate hallucination while maintaining other desirable properties.

Beyond LLMs, our theory also relates to space lower bounds for static filters[3]. Carter et al. (1978) gave the first space lower bound for one-sided filters in the sparse limit, which was recently extended by Li et al. (2023a) to a more general form for nonzero $|\mathcal{K}|/|\mathcal{U}|$. Pagh and Rodler (2001) lower bounded space usage of two-sided filters which allow false negatives, but left an unspecified gap of $\Theta(1)$ per key. Hurley and Waldvogel (2007) applied rate-distortion theory to the case of fixed $|\mathcal{U}|/|\mathcal{K}|$, and gave a mutual-information style space lower bound. These bounds can be recovered as special cases of our main result.

2 Preliminaries

We first define membership testers and error metrics.

Definition 2.1 (Membership tester)**.** Given universe $\mathcal{U} = [u]$, key set size n, and two error metric functions, a **membership tester** $\mathcal{M}$ is a tuple of two algorithms with shared randomness:

- $\mathsf{Init}^{\mathcal{M}}$, where the tester takes input $\mathcal{K}$ and outputs W, a memory state (e.g. model parameters for LLMs or data structure contents for filters).
- $\mathsf{Query}^{\mathcal{M}}$, where the tester takes input $i \in \mathcal{U}$ and the memory state W, and returns a confidence score $\hat{x}_i \in [0, 1]$, indicating its estimate of $\mathbb{P}[i \in \mathcal{K}]$.

Let $B(\mathcal{M}) = I(W; \mathcal{K})$ be the *memory budget* (or *memory cost*) of $\mathcal{M}$, quantifying how many bits of information about $\mathcal{K}$ are stored. See Appendix A for further discussion of this quantity. From a data structure perspective, this lower-bounds the bits of space that $\mathcal{M}$ uses: $I(W; \mathcal{K}) \leq H(W)$.

Remark 2.2 (Permutation-invariance). To study the memory-error trade-off, it suffices to focus on *permutation-invariant* membership testers. That is, for any permutation $\pi : \mathcal{U} \to \mathcal{U}$, any key set $\mathcal{K}$ of size n, and any $i \in \mathcal{U}$, the distribution of query outputs is unaffected by the permutation:

$$\mathsf{Query}^{\mathcal{M}}(i, \mathsf{Init}^{\mathcal{M}}(\mathcal{K})) \overset{d}{=} \mathsf{Query}^{\mathcal{M}}\big(\pi(i), \mathsf{Init}^{\mathcal{M}}(\pi(\mathcal{K}))\big).$$

This assumption is standard and without loss of generality: given a membership tester $\mathcal{M}'$, we can use $\mathcal{M}'$ to define a permutation-invariant tester $\mathcal{M}$ by picking a uniformly random permutation

[3] Static filters only store a fixed set $\mathcal{K}$. Filters that allow insertion or deletion have an additional space cost. See e.g. Lovett and Porat (2010); Kuszmaul and Walzer (2024); Kuszmaul et al. (2025)

σ on $\mathcal{U}$ and defining:

$$\begin{cases}\mathsf{Init}^{\mathcal{M}}(\mathcal{K}) = \mathsf{Init}^{\mathcal{M}'}(\sigma(\mathcal{K})), \\ \mathsf{Query}^{\mathcal{M}}(i, W) = \mathsf{Query}^{\mathcal{M}'}(\sigma(i), W).\end{cases}$$

On a uniformly random key set $\mathcal{K}$, the expected error rates (defined below) of $\mathcal{M}$ are identical to those of $\mathcal{M}'$. Moreover, the distribution of $\mathsf{Query}^{\mathcal{M}}(i, \mathsf{Init}^{\mathcal{M}}(\mathcal{K}))$ depends only on whether i is a key or non-key, not on the specific choice of i or $\mathcal{K}$. Throughout the paper, we will assume all membership testers are permutation-invariant. While practical LLMs are not permutation-invariant, this assumption is a standard tool for analysis, and our lower bounds still apply.

Definition 2.3 (Query output and error constraints)**.** Let $d^K, d^N : [0,1] \to [0,\infty]$ be **error metrics** for keys $\mathcal{K}$ and non-keys $\mathcal{U} \setminus \mathcal{K}$. On query output $\hat{x} \in [0,1]$, the error on a single key (resp. non-key) is $d^K(\hat{x})$ (resp. $d^N(\hat{x})$).

For permutation-invariant membership tester $\mathcal{M}$, we denote its **query output distributions** on keys and non-keys by $\mu_K(\mathcal{M})$ and $\mu_N(\mathcal{M})$, respectively. We say $\mathcal{M}$ achieves error levels $\varepsilon_K, \varepsilon_N$ if it satisfies the following constraints:

$$\mathop{\mathbb{E}}_{\hat{X}\sim\mu_K(\mathcal{M})}[d^K(\hat{X})] \le \varepsilon_K, \text{ and } \mathop{\mathbb{E}}_{\hat{X}\sim\mu_N(\mathcal{M})}[d^N(\hat{X})] \le \varepsilon_N.$$

Intuitively, the membership tester would try to output high scores for keys and low scores for non-keys; the corresponding error metrics d^K and d^N would then be decreasing and increasing functions, respectively.

As examples of error metrics, for two-sided filters, d^K and d^N would characterize the FNR and FPR of the filter, corresponding to $d^K(\hat{x}) = 1 - \hat{x}$ and $d^N(\hat{x}) = \hat{x}$.

For factuality estimation on LLMs (Section 4.1), d^K and d^N characterize the log-loss on a key (fact) and a non-key (non-fact), i.e., $d^K(\hat{x}) = -\ln \hat{x}$, and $d^N(\hat{x}) = -\ln(1 - \hat{x})$.

Assumption 2.4 (Assumptions on error metrics)**.** Our main theorems apply to any error metrics d^K, d^N that satisfy the following assumptions.

We assume that d^K, d^N are nonnegative and lower semi-continuous on $[0,1]$, and perfect scores have zero error: $d^K(1) = d^N(0) = 0$. Additionally, we assume there exists some $c \in [0,1]$ achieving finite error under both metrics:

$$d^K(c) < \infty, \quad \text{and} \quad d^N(c) < \infty.$$

All logarithms in this paper are base-2 unless specified as ln. We use u to denote the universe size $|\mathcal{U}|$, and use n to denote the key size $|\mathcal{K}|$. We use $\mathcal{P}([0,1])$ to denote all Borel probability measures on $[0,1]$.

3 A Rate-Distortion Theorem for Membership Testers

In this section, we state and prove our main theorems. Throughout this section, we assume a pair of fixed error metrics d^K, d^N that satisfy Assumption 2.4.

For any pair of error rates $(\varepsilon_K, \varepsilon_N)$, let $\mathcal{C}_K(\varepsilon_K)$ and $\mathcal{C}_N(\varepsilon_N)$ be the feasible regions for query output distributions on keys and non-keys, respectively:

$$\mathcal{C}_K(\varepsilon_K) = \{\mu_K \in \mathcal{P}([0,1]) : \mathop{\mathbb{E}}_{\hat{X}\sim\mu_K}[d^K(\hat{X})] \le \varepsilon_K\},$$
$$\mathcal{C}_N(\varepsilon_N) = \{\mu_N \in \mathcal{P}([0,1]) : \mathop{\mathbb{E}}_{\hat{X}\sim\mu_N}[d^N(\hat{X})] \le \varepsilon_N\}.$$

Our first theorem characterizes the memory–error trade-off for membership testers.

Theorem 3.1. *Fix error metrics d^K, d^N and error rates $\varepsilon_K, \varepsilon_N \geq 0$. Let $\{n_j\}, \{u_j\}$ be sequences of natural numbers such that $n_j \to \infty$ and $n_j/u_j \to 0$. For each j, let $\mathcal{M}_j$ be a membership tester for universe $[u_j]$ and key size n_j that achieves error rates $(\varepsilon_{K,j}, \varepsilon_{N,j})$ under error metrics d^K, d^N. Suppose the error rates satisfy:*

$$\limsup_{j\to\infty} \varepsilon_{K,j} \leq \varepsilon_K, \quad \limsup_{j\to\infty} \varepsilon_{N,j} \leq \varepsilon_N.$$

Then, the asymptotic per-key memory budget of $\mathcal{M}_j$ is at least:

$$\liminf_{j\to\infty} \frac{B(\mathcal{M}_j)}{n_j} \geq \min_{\mu_K \in \mathcal{C}_K(\varepsilon_K), \mu_N \in \mathcal{C}_N(\varepsilon_N)} \mathrm{KL}(\mu_K \| \mu_N).$$

Moreover, there exist sequences $\{u_j\}$, $\{n_j\}$, and $\{\mathcal{M}_j\}$ as described above that achieve the memory lower bound.

Our second result states that, when the KL term has unique minimizers, these minimizers define the query output distributions of optimal membership tester families.

Theorem 3.2. *Suppose $(\mu_K^*, \mu_N^*) \in \mathcal{C}_K(\varepsilon_K) \times \mathcal{C}_N(\varepsilon_N)$ is the unique minimizer of $\mathrm{KL}(\mu_K \| \mu_N)$. In the setting of Theorem 3.1, if $\{\mathcal{M}_j\}$ is asymptotically optimal, in the sense that*

$$\limsup_{j\to\infty} \frac{B(\mathcal{M}_j)}{n_j} = \mathrm{KL}(\mu_K^* \| \mu_N^*),$$

then we must have $\mu_K(\mathcal{M}_j) \to \mu_K^*$ and $\mu_N(\mathcal{M}_j) \to \mu_N^*$ in Wasserstein-1 distance.

Finally, if $\mathcal{M}$ is restricted to output values in $\mathrm{supp}(\mu_N^*)$ rather than $[0, 1]$, then we can quantify how the memory lower bound converges to $\mathrm{KL}(\mu_K^* \| \mu_N^*)$ as $p \to 0$.

Theorem 3.3. *Let χ^2 be the chi-squared divergence. In the setting of Theorem 3.2, suppose μ_N^* is supported on a finite set $\mathcal{X}$ and $\chi^2(\mu_K^* \| \mu_N^*) < \infty$. For any membership tester $\mathcal{M}$ for key size n and universe $[u]$ with query outputs restricted to $\mathcal{X}$, if we fix $p = \frac{n}{u}$ and let $n, u \to \infty$, then*

$$\frac{B(\mathcal{M})}{n} \geq \mathrm{KL}(\mu_K^* \| \mu_N^*) - \frac{\chi^2(\mu_K^* \| \mu_N^*)}{2 \ln 2} \cdot p + o(p),$$

and this bound is achievable.

Proof sketch. The starting point is a non-asymptotic information-theoretic lower bound: any membership tester inducing query output laws (μ_K, μ_N) must use at least $F_p = I(X; \hat{X})/p$ bits per key up to vanishing terms (Theorem 3.4), where $X \sim \mathrm{Bern}(p)$ indicates whether a query is a key and $\hat{X}$ is the tester's output.

Minimizing F_p over the feasible sets (distributions μ_K, μ_N satisfying error constratints) defines the "rate–distortion" function $R_p(\varepsilon_K, \varepsilon_N)$. We show that, for each p, the "rate" R_p is both necessary (Theorem 3.6) and sufficient (Theorem 3.7) for achieving the given error level.

To obtain Theorem 3.1, we then send $p \to 0$ and use (semi)continuity of F_p (Theorem 3.5) to show $R_p(\varepsilon_K, \varepsilon_N) \to \min \mathrm{KL}(\mu_K \| \mu_N)$. When the KL minimizer is unique, standard compactness plus the same semicontinuity argument forces any asymptotically optimal family to have $(\mu_K(\mathcal{M}_j), \mu_N(\mathcal{M}_j))$ converge to (μ_K^*, μ_N^*) (Theorem 3.2). Finally, under finite support and finite χ^2, a Taylor expansion of F_p around $p = 0$ yields the first-order correction term in Theorem 3.3.

In the subsections below, we will present the main lemmas that lead to the above theorems. Most formal proofs are deferred to Section B.

3.1 Non-asymptotic lower bound on memory

Fix $u, n \in \mathbb{N}$. We first lower bound the necessary memory budget for achieving output distributions μ_K, μ_N on key and non-key queries. Consider a random variable $X \sim \mathrm{Bern}(p)$, and $\hat{X}$ defined by the conditional distributions:

$$\hat{X} \mid (X = 1) \sim \mu_K, \quad \text{and} \quad \hat{X} \mid (X = 0) \sim \mu_N.$$

In the lemma below, we will use the function

$$F_p(\mu_K, \mu_N) = \frac{1}{p} I(X; \hat{X})$$

as a proxy for the per-key memory cost of a membership tester with query output distributions μ_K and μ_N.

Lemma 3.4. *Let $\mathcal{M}$ be a membership tester for key size n in universe $[u]$ with $u > n$. Let $p = \frac{n}{u}$ and let F_p be as defined above. Then, the memory cost of $\mathcal{M}$ is at least:*

$$\frac{B(\mathcal{M})}{n} \geq F_p\big(\mu_K(\mathcal{M}), \mu_N(\mathcal{M})\big) - \frac{\log(8n)}{2n}.$$

Proof. See Section B.1. □

We now state several technical properties of F_p.

Lemma 3.5. *For $p > 0$, let $F_p(\mu_K, \mu_N) = I(X; \hat{X})/p$, where $X \sim \mathrm{Bern}(p)$, $\hat{X} \mid (X = 1) \sim \mu_K$, and $\hat{X} \mid (X = 0) \sim \mu_N$. We also define $F_0(\mu_K, \mu_N) = \mathrm{KL}(\mu_K \| \mu_N)$. Then, for $p \in [0, 1)$ and $(\mu_K, \mu_N) \in \mathcal{P}([0, 1])^2$:*

1. *The function $(p, \mu_K, \mu_N) \mapsto F_p(\mu_K, \mu_N)$ is jointly lower semi-continuous.*
2. *$F_p(\mu_K, \mu_N)$ is continuous in p.*
3. *F_p is differentiable in p with $\frac{\partial}{\partial p} F_p(\mu_K, \mu_N) = -\frac{\mathrm{KL}(\mu_N \| p\mu_K + (1-p)\mu_N)}{p^2}$ whenever $p > 0$.*

Proof. See Section B.2. □

3.2 Memory-error tradeoff for custom error metrics

Now we define an analog of the rate-distortion function for membership testing. Fixing d^K and d^N, for each $p \in (0, 1)$, let $R_p(\varepsilon_K, \varepsilon_N)$ be the minimum memory cost per key for given error constraints:

$$R_p(\varepsilon_K, \varepsilon_N) = \min_{\mu_K \in \mathcal{C}_K(\varepsilon_K), \mu_N \in \mathcal{C}_N(\varepsilon_N)} F_p(\mu_K, \mu_N),$$

where the minimum can be attained since, with respect to the weak-* topology, $\mathcal{C}_K(\varepsilon_K)$ and $\mathcal{C}_N(\varepsilon_N)$ are closed subsets of $\mathcal{P}([0, 1])$, and F_p is lower semi-continuous in (μ_K, μ_N).

By taking minimum over all (μ_K, μ_N) in the feasible region and applying Lemma 3.4, we immediately have the following memory lower bound for given error constraints:

Corollary 3.6. *Fix any pair of error metrics d^K and d^N and error rates ε_K and ε_N. Suppose $\mathcal{M}$ is a membership tester satisfying the error constraints for universe $[u]$ and key sizes n with $p = \frac{n}{u}$. Then, we have:*

$$\frac{B(\mathcal{M})}{n} \geq R_p(\varepsilon_K, \varepsilon_N) - \frac{\log(8n)}{2n}.$$

We show that this lower bound is achievable for fixed p.

Lemma 3.7. *Fix any $p = \frac{n}{u} \in (0,1)$ and $\varepsilon_K, \varepsilon_N > 0$. Then, for all $\delta > 0$, there is a sufficiently large n and u such that there exists a membership tester $\mathcal{M}$ for universe $[u]$ and key sizes n which achieves error rates $(\varepsilon_K + \delta, \varepsilon_N + \delta)$, and:*

$$\frac{B(\mathcal{M})}{n} \leq R_p(\varepsilon_K, \varepsilon_N) + \delta.$$

Proof. See Section B.3. □

3.3 Proofs of main theorems

Now, Theorem 3.1 follows from the fact that R_p converges to the minimum KL divergence as $p \to 0$.

Proof of Theorem 3.1. First we show lower bound. By Lemma 3.4, for each j, the memory cost of $\mathcal{M}_j$ satisfies:

$$\frac{B(\mathcal{M}_j)}{n_j} \geq F_{p_j}\big(\mu_K(\mathcal{M}_j), \mu_N(\mathcal{M}_j)\big) - \frac{\log(8n_j)}{2n_j}.$$

Let $\ell = \liminf_{j\to\infty} \frac{B(\mathcal{M}_j)}{n_j}$. By passing to a subsequence (still denoted by j), we can assume $B(\mathcal{M}_j)/n_j \to \ell$.

Let $\mu_{K,j} = \mu_K(\mathcal{M}_j)$ and $\mu_{N,j} = \mu_N(\mathcal{M}_j)$. Since the space of probability measures $\mathcal{P}([0,1])$ is compact under the weak-* topology, there exists a further subsequence (again, denoted by j) such that $(\mu_{K,j}, \mu_{N,j})$ converges to some limit $(\mu_K^*, \mu_N^*) \in \mathcal{P}([0,1])^2$. By the lower semi-continuity of $F_p(\mu_K, \mu_N)$ in (p, μ_K, μ_N) (Lemma 3.5), and since $p_j \to 0$, we have:

$$\begin{aligned}\ell = \lim_{j\to\infty} \frac{B(\mathcal{M}_j)}{n_j} &\geq \liminf_{j\to\infty} F_{p_j}(\mu_{K,j}, \mu_{N,j}) \\ &\geq F_0(\mu_K^*, \mu_N^*) = \mathrm{KL}(\mu_K^* \| \mu_N^*).\end{aligned}$$

It remains to show that (μ_K^*, μ_N^*) is in $\mathcal{C}_K(\varepsilon_K) \times \mathcal{C}_N(\varepsilon_N)$. By assumption, we have $\limsup \varepsilon_{K,j} \leq \varepsilon_K$ and $\limsup \varepsilon_{N,j} \leq \varepsilon_N$. Since the functions d^K, d^N are LSC, the expected error is lower semi-continuous with respect to the measure by Portmanteau theorem. Thus:

$$\mathop{\mathbb{E}}_{\hat{x}\sim\mu_K^*}[d^K(\hat{x})] \leq \liminf_{j\to\infty} \mathop{\mathbb{E}}_{\hat{x}\sim\mu_{K,j}}[d^K(\hat{x})] \leq \varepsilon_K,$$

which implies $\mu_K^* \in \mathcal{C}_K(\varepsilon_K)$, and similarly $\mu_N^* \in \mathcal{C}_N(\varepsilon_N)$. This completes the lower bound:

$$\begin{aligned}\liminf_{j\to\infty} \frac{B(\mathcal{M}_j)}{n_j} &\geq \mathrm{KL}(\mu_K^* \| \mu_N^*) \\ &\geq \min_{\mu_K \in \mathcal{C}_K(\varepsilon_K), \mu_N \in \mathcal{C}_N(\varepsilon_N)} \mathrm{KL}(\mu_K \| \mu_N).\end{aligned}$$

For achievability, note that $R_p(\mu_K^*, \mu_N^*) \to \mathrm{KL}(\mu_K^* \| \mu_N^*)$ as $p \to 0$ by continuity of F_p in p, as shown in Lemma 3.5. By Lemma 3.7, for each p, for sufficiently large n we can find a membership tester with error rates arbitrarily close to $(\varepsilon_K, \varepsilon_N)$ and memory usage arbitrarily close to $R_p(\mu_K^*, \mu_N^*)$ per key. The desired claim follows by taking $p_j \to 0$ and taking a sufficiently large n_j for each p_j. □

Proofs for Theorems 3.2 and 3.3 follow similar arguments and are deferred to Section B.4 and B.5 respectively.

4 Hallucination on Random Facts

Fix a universe $\mathcal{U}$ of u unstructured *potential facts*; each $i \in \mathcal{U}$ is a plausible natural-language claim (e.g., detailed biographies as in Allen-Zhu and Li (2024)). The set of known facts is the key set $\mathcal{K} \subseteq \mathcal{U}$. In the *random-facts* regime that motivates our study, $\mathcal{K}$ is a uniformly random subset of size n of $\mathcal{U}$. This regime intentionally singles out non-generalizable factual knowledge, forcing the LLM to behave like a membership tester for $\mathcal{K}$.

Consider an LLM trained to (among other tasks) recognize facts $\mathcal{K}$ from all other non-facts. Viewing the LLM as a membership tester for $\mathcal{K}$, Init corresponds to training on labeled data, and Query corresponds to the inference-time response (or internal evaluation) on a plausible claim $i \in \mathcal{U}$. We study two natural regimes of factuality judgment:

1. **Probability estimation.** The LLM generates a confidence score $\hat{x}_i \in [0, 1]$ as an estimation of $\mathbb{P}[i \in \mathcal{K}]$.

2. **Binary decision.** The LLM (possibly after thresholding or other post-processing) induces a binary decision $\hat{x}_i \in \{0, 1\}$ indicating whether i is accepted as a fact.

In both cases, Theorem 3.1 reduces the minimum per-fact memory budget allocated to random facts, measured by $I(W; \mathcal{K})/n$, to a convex optimization problem under the corresponding error constraints. We refer to Section A for a detailed discussion of the memory budget in LLMs.

4.1 Probability estimation variant

In this variant, a query i produces a fractional confidence $\hat{x} \in [0, 1]$. Let μ_K and μ_N denote the distribution of $\hat{x}$ when i is a fact ($i \in \mathcal{K}$) or a non-fact ($i \in \mathcal{U} \setminus \mathcal{K}$), respectively. We measure average factuality error by log-loss constraints:

$$\mathop{\mathbb{E}}_{\hat{x} \sim \mu_K} [-\ln \hat{x}] \le \varepsilon_K, \qquad \mathop{\mathbb{E}}_{\hat{x} \sim \mu_N} [-\ln(1 - \hat{x})] \le \varepsilon_N,$$

where a weighted sum of the two errors corresponds to binary cross-entropy loss. This evaluation metric is natural for the practical need to *quantify the confidence* $\mathbb{P}[True]$ of a factual output Wen et al. (2025), and is consistent with proposed training/evaluation methods for studying whether LLMs "know what they know"Kadavath et al. (2022); Cheng et al. (2024).

Our main conclusion is that, under log-loss, the *unique* optimal solution is intrinsically *asymmetric*: it drives all facts to a single high-confidence point, while forcing a nonzero fraction of non-facts to share the same point.

Theorem 4.1. *In the non-trivial regime where $\varepsilon_K > 0$, $\varepsilon_N > 0$, and $e^{-\varepsilon_K} + e^{-\varepsilon_N} > 1$, the unique minimizers (μ_K^*, μ_N^*) of*

$$\begin{aligned} &\min_{\mu_K, \mu_N} \mathrm{KL}(\mu_K \,\|\, \mu_N) \\ &\textit{subject to } \mathop{\mathbb{E}}_{\hat{x} \sim \mu_K} [-\ln \hat{x}] \le \varepsilon_K,\ \mathop{\mathbb{E}}_{\hat{x} \sim \mu_N} [-\ln(1 - \hat{x})] \le \varepsilon_N \end{aligned}$$

are given by

$$\mu_K^* = \delta_{x^*}, \qquad \mu_N^* = (1 - q^*)\delta_0 + q^* \delta_{x^*},$$

where $x^* = e^{-\varepsilon_K}$ and $q^* = \frac{\varepsilon_N}{-\ln(1 - x^*)}$.

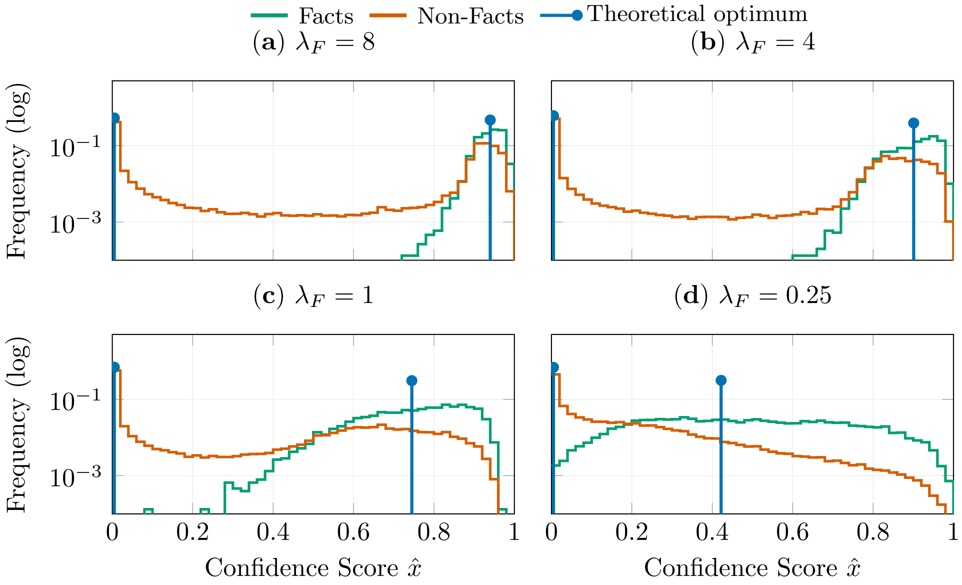


Figure 1: Output distributions on facts vs. non-facts (y-axis is in log-scale) across different choice of λ_F for the model with 15145 parameters (1 per fact). The blue stems indicate the predicted memory-optimal atoms for non-facts under the same empirical loss values.

Figure 1 illustrates the shape of optimal non-fact distribution in blue. The proof appears in Section C. To solve this optimization problem over probability distributions, we apply variational calculus and check for KKT conditions.

Hallucination channel and its cost. The optimal strategy for a given memory budget is to output a single high confidence x^* on all facts, while assigning *the same* high confidence x^* to a q^* fraction of non-facts, forming a "hallucination channel." These non-facts are indistinguishable from facts by any downstream procedure that observes only $\hat{x}$. Moreover, the per-key memory lower bound simplifies to

$$\mathrm{KL}(\mu_K^* \| \mu_N^*) \;=\; \log \frac{1}{q^*}.$$

Hence, the hallucination probability q^* is *solely determined by the memory capacity* dedicated to storing random facts, regardless of how we trade off the two types of errors.

Resistance to thresholding. The non-fact loss $-\ln(1-\hat{x})$ heavily penalizes large $\hat{x}$, so one might expect μ_N^* to spread its mass over smaller or intermediate confidences, enabling hallucination removal by thresholding (perhaps at the cost of forgetting some facts). Theorem 4.1 rules this out: on the Pareto frontier, non-facts must place an atom at the same x^* used for facts. Thus, a threshold that accepts any fact must also accept these hallucinations, and any threshold that rejects any hallucination must also reject all facts.

4.2 Binary decision variant

We now consider *any binary decision* on the potential fact universe induced by the LLM. This covers the thresholding of probability estimation in Section 4.1, or any classifier (e.g., in Kalai et al. (2025)) induced by generative hallucination probabilities. Formally, any such pipeline induces a (randomized) decision $\hat{x}_i \in \{0, 1\}$ for each $i \in \mathcal{U}$, indicating either acceptance or rejection. We place error constraints on false negative rates (FNR) and false positive rates (FPR):

$$\mathop{\mathbb{E}}_{\hat{x}\sim\mu_K}[1-\hat{x}] \le \varepsilon_K, \qquad \mathop{\mathbb{E}}_{\hat{x}\sim\mu_N}[\hat{x}] \le \varepsilon_N,$$

Remark 4.2. The FNR/FPR error constraints naturally extend to all real-valued scores $\hat{x} \in [0,1]$. However, Theorem D.1 shows that for these error constraints, restricting attention to binary outputs $\{0,1\}$ incurs no loss of optimality in the KL-minimization governing the memory bound.

Theorem 4.3. *In the non-trivial regime where $\varepsilon_K, \varepsilon_N \ge 0$ and $\varepsilon_K + \varepsilon_N < 1$, the minimizers (μ_K^*, μ_N^*) of*

$$\begin{aligned} &\min_{\mu_K,\mu_N} \mathrm{KL}(\mu_K \,\|\, \mu_N) \\ &\textit{subject to } \mathop{\mathbb{E}}_{\hat{x}\sim\mu_K}[1-\hat{x}] \le \varepsilon_K,\ \mathop{\mathbb{E}}_{\hat{x}\sim\mu_N}[\hat{x}] \le \varepsilon_N \end{aligned}$$

are given by

$$\mu_K^* = \mathrm{Bern}(1-\varepsilon_K), \qquad \mu_N^* = \mathrm{Bern}(\varepsilon_N).$$

We defer the full proof to Section D. Intuitively, once we reduce the KL-minimization to binary outputs, the resulting two-parameter convex program naturally has unique minimizers when the two constraints are tight.

First-order approximation. Since $\hat{x} \in \{0,1\}$, we can use Theorem 3.3 and obtain a more fine-grained memory bound for small p. Specifically, as $p \to 0$, the difference between the memory bound and KL term is dominated by

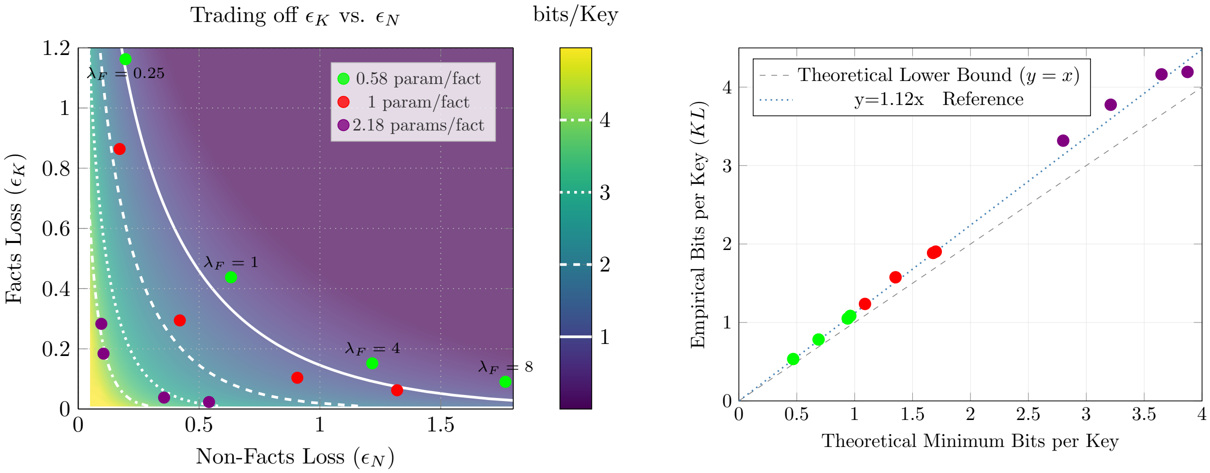
$$\frac{p}{2\ln 2} \cdot \chi^2(\mathrm{Bern}(1-\varepsilon_K) \| \mathrm{Bern}(\varepsilon_N)).$$

No non-trivial "hallucination-free" regime. A corollary of our results is that one cannot eliminate hallucinations in a large universe without incurring a large cost. Driving hallucinations to zero corresponds to $\varepsilon_N \to 0$, but then

$$\mathrm{KL}(\mathrm{Bern}(1-\varepsilon_K) \,\|\, \delta_0) = \infty \quad \text{for every } \varepsilon_K < 1.$$

Thus, zero FPR is only compatible with the trivial regime that rejects everything ($\varepsilon_K = 1$), or with an unbounded memory budget. Interestingly, this also proves that there is no "reverse Bloom filter" which tolerates false negatives but not false positives. As the universe grows to infinity, it is infinitely expensive to correctly identify every non-fact.

Thresholding only moves you along the frontier. This memory-error frontier formalizes the tradeoff between hallucination and over-refusal observed in practice Cheng et al. (2024); Brahman et al. (2024). Theorem 4.3 is agnostic to how $\hat{X}$ is produced. Whether the decision is derived from a calibrated probability, a raw logit, a log-likelihood ratio, or a multi-stage verification chain that outputs a scalar score, the final thresholded mapping is exactly a two-sided filter with some $(\varepsilon_K, \varepsilon_N)$. Consequently, no choice of threshold can beat the memory-error frontier: a conservative approach to factual answers may reduce ε_N, but then either the memory budget or ε_K must increase (more forgetting / abstention).



(a) Memory-error frontier vs. different weights.

(b) KL divergence between empirical distributions vs. minimum information for given loss.

Figure 2: Effect of different weight λ_F on fact. Each color represents a different model size. The amount of information per key decreases with λ_F for each model size.

Relation to Section 4.1. In Section 4.1, we show that the perfect solution for probability estimation necessitates high-confidence hallucinations. Here, the message is broader and operational: once a system is evaluated through any decision rule, it is constrained by the same memory-error tradeoff as two-sided filters, regardless of the trained objective.

Recovering filter space lower bounds. By limiting output to $\{0, 1\}$, our framework recovers previous space lower bounds for filters as special cases. Setting $\varepsilon_K = 0$, our bound reduces to the classical result in Carter et al. (1978):

$$\mathrm{KL}(\delta_1 \,\|\, \mathrm{Bern}(\varepsilon_N)) = \log(1/\varepsilon_N) \text{ bits per key.}$$

Moreover, if p is bounded away from 0, our rate-distortion function $R_p(\varepsilon_K, \varepsilon_N)$ corresponds to the fine-grained bound in Li et al. (2023a) for finite universes.

In the two-sided regime, we settle the gap in Pagh and Rodler (2001), quantifying $\log(1/\varepsilon_N) + \Theta(1)$ as the exact KL divergence value. Finally, our framework generalizes the results in Hurley and Waldvogel (2007) by moving from a single Hamming-distortion constraint on a Bernoulli source to separate FNR/FPR constraints on fixed composition sources.

To complete the argument for filters, in Appendix D.3 we give an explicit construction of a hash-based two-sided filter that achieves the space lower bound up to $o(1)$ bits per key.

4.3 Experiments

We show that the predicted distributions in Section 4.1 align with output behaviors in controlled synthetic experiments.

Setup. Let $\mathcal{U}$ be the set of all length-15 strings over the 26 English letters ($|\mathcal{U}| = 26^{15}$). We draw a key set $\mathcal{K} \subseteq \mathcal{U}$ by sampling $n = 15145$ strings uniformly at random without replacement. We train a 2-layer Transformer with varying parameter count (8767, 15145, and 33085) and analyze the distributions of output scores $\hat{x}_i$ when i is a key/non-key. We train with a *weighted* binary cross-entropy loss

$$\mathcal{L} = \frac{\lambda_F}{\lambda_F + 1} \mathop{\mathbb{E}}_{i \sim \mathrm{Unif}(\mathcal{K})}[-\ln \hat{x}(i)] \\ + \frac{1}{\lambda_F + 1} \mathop{\mathbb{E}}_{i \sim \mathrm{Unif}(\mathcal{U} \setminus \mathcal{K})}[-\ln(1 - \hat{x}(i))].$$

This loss induces the average log-losses $(\varepsilon_K, \varepsilon_N)$ on facts and non-facts, consistent with the notation in Section 4.1. Further details of model and training, as well as extra figures can be found in Appendix E.

Validation of the hallucination channel. Figure 1 plots the empirical distributions of $\hat{x}(i)$ on facts and non-facts under different λ_F for the model with 15145 parameters. Across all settings, the non-fact distribution is *not* only concentrated near 0; instead, it exhibits a visible high-confidence tail overlapping the fact mass, which is especially clear when the fact mass is concentrated. This qualitatively matches the hallucination channel predicted by Theorem 4.1: a non-negligible portion of non-facts must be mapped into the same high-confidence region as facts. Interestingly, a small λ_F pushes both fact and non-fact distributions to spread out. We attribute this to the expressivity of the model architecture and properties of the sigmoid function.

Quantitative match to the predicted atoms. Beyond the qualitative overlap, the empirical modes in Figure 1 are comparable to the atoms $(x^\star, q^\star)$ implied by the theoretical optimizer when we plug in the observed losses $(\varepsilon_K, \varepsilon_N)$. We further compute the KL divergence between the binned empirical distributions and find that the (discretized) learned distributions (with 50 bins) incur only an $\approx 12\%$ overhead in KL divergence, relative to the information-theoretic lower bound for the given error rates $(\varepsilon_K, \varepsilon_N)$ (Figure 2b). We also note that, when the model is tasked solely with memorizing random data, our estimation of effective memory is close to 2 bits per parameter, consistent with the findings in Allen-Zhu and Li (2025).

Effect of reweighting facts vs. non-facts. Increasing λ_F pushes the optimizer to reduce ε_K (higher recall). Consequently, the model sharpens a high-confidence region for facts, and inevitably drags a larger fraction of non-facts into the same region, causing a sharp rise in hallucination. Figure 2a reports ε_K, ε_N, and the corresponding per-key memory lower bound across the weight sweep. The heatmap shows a clear diminishing return: past a point, further improving ε_K requires sacrificing ε_N disproportionately, while the implied information requirement per key *decreases*—aggressive "always-recall" pressure moves the system into an especially hallucination-prone position. This suggests that it is advisable to emphasize rejecting non-facts during training – the theoretical hallucination probability in Theorem 4.1 is only a function of effective memory budget, but the budget itself depends on the training process.

References

Alessandro Achille and Stefano Soatto. Emergence of invariance and disentanglement in deep representations. *Journal of Machine Learning Research*, 19(50):1–34, 2018.

Aisha Alansari and Hamzah Luqman. Large language models hallucination: A comprehensive survey, 2025. URL `https://arxiv.org/abs/2510.06265`.

Zeyuan Allen-Zhu and Yuanzhi Li. Physics of language models: Part 3.1, knowledge storage and extraction. In *Forty-first International Conference on Machine Learning, ICML 2024, Vienna, Austria, July 21-27, 2024*. OpenReview.net, 2024. URL `https://openreview.net/forum?id=5x788rqbcj`.

Zeyuan Allen-Zhu and Yuanzhi Li. Physics of language models: Part 3.3, knowledge capacity scaling laws. In *The Thirteenth International Conference on Learning Representations, ICLR 2025, Singapore, April 24-28, 2025*. OpenReview.net, 2025. URL `https://openreview.net/forum?id=FxNNiUgtfa`.

Pierre Alquier. User-friendly introduction to pac-bayes bounds. *arXiv preprint arXiv:2110.11216*, 2021.

Gregor Bachmann and Vaishnavh Nagarajan. The pitfalls of next-token prediction, 2025. URL `https://arxiv.org/abs/2403.06963`.

Sourav Banerjee, Ayushi Agarwal, and Saloni Singla. Llms will always hallucinate, and we need to live with this. *CoRR*, abs/2409.05746, 2024. doi: 10.48550/ARXIV.2409.05746. URL `https://doi.org/10.48550/arXiv.2409.05746`.

Emily M. Bender, Timnit Gebru, Angelina McMillan-Major, and Shmargaret Shmitchell. On the dangers of stochastic parrots: Can language models be too big? In Madeleine Clare Elish, William Isaac, and Richard S. Zemel, editors, *FAccT '21: 2021 ACM Conference on Fairness, Accountability, and Transparency, Virtual Event / Toronto, Canada, March 3-10, 2021*, pages 610–623. ACM, 2021. doi: 10.1145/3442188.3445922. URL `https://doi.org/10.1145/3442188.3445922`.

Burton H. Bloom. Space/time trade-offs in hash coding with allowable errors. *Commun. ACM*, 13(7): 422–426, 1970. doi: 10.1145/362686.362692. URL `https://doi.org/10.1145/362686.362692`.

Avrim Blum and John Langford. Pac-mdl bounds. In *Learning Theory and Kernel Machines: 16th Annual Conference on Learning Theory and 7th Kernel Workshop, COLT/Kernel 2003, Washington, DC, USA, August 24-27, 2003. Proceedings*, pages 344–357. Springer, 2003.

Faeze Brahman, Sachin Kumar, Vidhisha Balachandran, Pradeep Dasigi, Valentina Pyatkin, Abhilasha Ravichander, Sarah Wiegreffe, Nouha Dziri, Khyathi Raghavi Chandu, Jack Hessel, Yulia Tsvetkov, Noah A. Smith, Yejin Choi, and Hanna Hajishirzi. The art of saying no: Contextual noncompliance in language models. In Amir Globersons, Lester Mackey, Danielle Belgrave, Angela Fan, Ulrich Paquet, Jakub M. Tomczak, and Cheng Zhang, editors, *Advances in Neural Information Processing Systems 38: Annual Conference on Neural Information Processing Systems 2024, NeurIPS 2024, Vancouver, BC, Canada, December 10 - 15, 2024*, 2024. URL `http://papers.nips.cc/paper_files/paper/2024/hash/58e79894267cf72c66202228ad9c6057-Abstract-Datasets_and_Benchmarks_Track.html`.

Yuheng Bu, Shaofeng Zou, and Venugopal V. Veeravalli. Tightening mutual information-based bounds on generalization error. *IEEE Journal on Selected Areas in Information Theory*, 1(1): 121–130, 2020. doi: 10.1109/JSAIT.2020.2991139.

Larry Carter, Robert W. Floyd, John Gill, George Markowsky, and Mark N. Wegman. Exact and approximate membership testers. In Richard J. Lipton, Walter A. Burkhard, Walter J. Savitch, Emily P. Friedman, and Alfred V. Aho, editors, *Proceedings of the 10th Annual ACM Symposium on Theory of Computing, May 1-3, 1978, San Diego, California, USA*, pages 59–65. ACM, 1978. doi: 10.1145/800133.804332. URL `https://doi.org/10.1145/800133.804332`.

Olivier Catoni. Pac-bayesian supervised classification: the thermodynamics of statistical learning. *arXiv preprint arXiv:0712.0248*, 2007.

Moses Charikar and Chirag Pabbaraju. Exploring facets of language generation in the limit. In Nika Haghtalab and Ankur Moitra, editors, *The Thirty Eighth Annual Conference on Learning Theory, 30-4 July 2025, Lyon, France*, volume 291 of *Proceedings of Machine Learning Research*, pages 854–887. PMLR, 2025. URL `https://proceedings.mlr.press/v291/charikar25a.html`.

Qinyuan Cheng, Tianxiang Sun, Xiangyang Liu, Wenwei Zhang, Zhangyue Yin, Shimin Li, Linyang Li, Zhengfu He, Kai Chen, and Xipeng Qiu. Can AI assistants know what they don't know? In *Forty-first International Conference on Machine Learning, ICML 2024, Vienna, Austria, July 21-27, 2024*. OpenReview.net, 2024. URL `https://openreview.net/forum?id=girxGkdECL`.

Leon Chlon, Ahmed Karim, and Maggie Chlon. Predictable compression failures: Why language models actually hallucinate. *arXiv preprint arXiv:2509.11208*, 2025.

Thomas M. Cover and Joy A. Thomas. *Elements of Information Theory*. Wiley, 2001. ISBN 9780471062592. doi: 10.1002/0471200611. URL `https://doi.org/10.1002/0471200611`.

Imre Csiszár and János Körner. *Information theory: coding theorems for discrete memoryless systems*. Cambridge University Press, 2011.

Martin Dietzfelbinger and Rasmus Pagh. Succinct data structures for retrieval and approximate membership (extended abstract). In Luca Aceto, Ivan Damgård, Leslie Ann Goldberg, Magnús M. Halldórsson, Anna Ingólfsdóttir, and Igor Walukiewicz, editors, *Automata, Languages and Programming, 35th International Colloquium, ICALP 2008, Reykjavik, Iceland, July 7-11, 2008, Proceedings, Part I: Tack A: Algorithms, Automata, Complexity, and Games*, volume 5125 of *Lecture Notes in Computer Science*, pages 385–396. Springer, 2008. doi: 10.1007/978-3-540-70575-8_32. URL `https://doi.org/10.1007/978-3-540-70575-8_32`.

Jesse Dodge, Maarten Sap, Ana Marasovic, William Agnew, Gabriel Ilharco, Dirk Groeneveld, Margaret Mitchell, and Matt Gardner. Documenting large webtext corpora: A case study on the colossal clean crawled corpus. In Marie-Francine Moens, Xuanjing Huang, Lucia Specia, and Scott Wen-tau Yih, editors, *Proceedings of the 2021 Conference on Empirical Methods in Natural Language Processing, EMNLP 2021, Virtual Event / Punta Cana, Dominican Republic, 7-11 November, 2021*, pages 1286–1305. Association for Computational Linguistics, 2021. doi: 10.18653/V1/2021.EMNLP-MAIN.98. URL `https://doi.org/10.18653/v1/2021.emnlp-main.98`.

Chris Dyer, Adhiguna Kuncoro, Miguel Ballesteros, and Noah A. Smith. Recurrent neural network grammars. In Kevin Knight, Ani Nenkova, and Owen Rambow, editors, *Proceedings of the 2016 Conference of the North American Chapter of the Association for Computational Linguistics:*

Human Language Technologies, pages 199–209, San Diego, California, June 2016. Association for Computational Linguistics. doi: 10.18653/v1/N16-1024. URL https://aclanthology.org/N16-1024/.

Gintare Karolina Dziugaite and Daniel M. Roy. Computing nonvacuous generalization bounds for deep (stochastic) neural networks with many more parameters than training data. In Gal Elidan, Kristian Kersting, and Alexander Ihler, editors, *Proceedings of the Thirty-Third Conference on Uncertainty in Artificial Intelligence, UAI 2017, Sydney, Australia, August 11-15, 2017*. AUAI Press, 2017. URL http://auai.org/uai2017/proceedings/papers/173.pdf.

Gintare Karolina Dziugaite and Daniel M. Roy. Data-dependent pac-bayes priors via differential privacy. In Samy Bengio, Hanna M. Wallach, Hugo Larochelle, Kristen Grauman, Nicolò Cesa-Bianchi, and Roman Garnett, editors, *Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018, December 3-8, 2018, Montréal, Canada*, pages 8440–8450, 2018. URL https://proceedings.neurips.cc/paper/2018/hash/9a0ee0a9e7a42d2d69b8f86b3a0756b1-Abstract.html.

Zixuan Gong, Shijia Li, Yong Liu, and Jiaye Teng. Disentangling feature structure: A mathematically provable two-stage training dynamics in transformers. *arXiv preprint arXiv:2502.20681*, 2025.

Peter Gr"unwald and Teemu Roos. Minimum description length revisited. *International journal of mathematics for industry*, 11(01):1930001, 2019.

Peter Grunwald, Thomas Steinke, and Lydia Zakynthinou. Pac-bayes, mac-bayes and conditional mutual information: Fast rate bounds that handle general vc classes. In *Conference on Learning Theory*, pages 2217–2247. PMLR, 2021.

Peter D Gr"unwald. *The minimum description length principle*. MIT press, 2007.

Esmail Gumaan. Theoretical foundations and mitigation of hallucination in large language models, 2025. URL https://arxiv.org/abs/2507.22915.

Fredrik Hellstr"om, Giuseppe Durisi, Benjamin Guedj, and Maxim Raginsky. Generalization bounds: Perspectives from information theory and pac-bayes. *Foundations and Trends in Machine Learning*, 18(1):1–223, 2025.

Ari Holtzman, Jan Buys, Li Du, Maxwell Forbes, and Yejin Choi. The curious case of neural text degeneration. In *8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia, April 26-30, 2020*. OpenReview.net, 2020. URL https://openreview.net/forum?id=rygGQyrFvH.

Lei Huang, Xiaocheng Feng, Weitao Ma, Yuchun Fan, Xiachong Feng, Yuxuan Gu, Yangfan Ye, Liang Zhao, Weihong Zhong, Baoxin Wang, Dayong Wu, Guoping Hu, Lingpeng Kong, Tong Xiao, Ting Liu, and Bing Qin. Alleviating hallucinations from knowledge misalignment in large language models via selective abstention learning. In Wanxiang Che, Joyce Nabende, Ekaterina Shutova, and Mohammad Taher Pilehvar, editors, *Proceedings of the 63rd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), ACL 2025, Vienna, Austria, July 27 - August 1, 2025*, pages 24564–24579. Association for Computational Linguistics, 2025a. URL https://aclanthology.org/2025.acl-long.1199/.

Lei Huang, Weijiang Yu, Weitao Ma, Weihong Zhong, Zhangyin Feng, Haotian Wang, Qianglong Chen, Weihua Peng, Xiaocheng Feng, Bing Qin, and Ting Liu. A survey on hallucination in large language models: Principles, taxonomy, challenges, and open questions. *ACM Trans. Inf. Syst.*, 43(2):42:1–42:55, 2025b. doi: 10.1145/3703155. URL `https://doi.org/10.1145/3703155`.

Yizhan Huang, Zhe Yang, Meifang Chen, Jianping Zhang, and Michael R. Lyu. Entropy-memorization law: Evaluating memorization difficulty of data in llms. *CoRR*, abs/2507.06056, 2025c. doi: 10.48550/ARXIV.2507.06056. URL `https://doi.org/10.48550/arXiv.2507.06056`.

Paul Hurley and Marcel Waldvogel. Bloom filters: One size fits all? In *32nd Annual IEEE Conference on Local Computer Networks (LCN 2007), 15-18 October 2007, Clontarf Castle, Dublin, Ireland, Proceedings*, pages 183–190. IEEE Computer Society, 2007. doi: 10.1109/LCN.2007.17. URL `https://doi.org/10.1109/LCN.2007.17`.

Ziwei Ji, Nayeon Lee, Rita Frieske, Tiezheng Yu, Dan Su, Yan Xu, Etsuko Ishii, Yejin Bang, Andrea Madotto, and Pascale Fung. Survey of hallucination in natural language generation. *ACM Comput. Surv.*, 55(12):248:1–248:38, 2023. doi: 10.1145/3571730. URL `https://doi.org/10.1145/3571730`.

Saurav Kadavath, Tom Conerly, Amanda Askell, Tom Henighan, Dawn Drain, Ethan Perez, Nicholas Schiefer, Zac Hatfield-Dodds, Nova DasSarma, Eli Tran-Johnson, Scott Johnston, Sheer El Showk, Andy Jones, Nelson Elhage, Tristan Hume, Anna Chen, Yuntao Bai, Sam Bowman, Stanislav Fort, Deep Ganguli, Danny Hernandez, Josh Jacobson, Jackson Kernion, Shauna Kravec, Liane Lovitt, Kamal Ndousse, Catherine Olsson, Sam Ringer, Dario Amodei, Tom Brown, Jack Clark, Nicholas Joseph, Ben Mann, Sam McCandlish, Chris Olah, and Jared Kaplan. Language models (mostly) know what they know. *CoRR*, abs/2207.05221, 2022. doi: 10.48550/ARXIV.2207.05221. URL `https://doi.org/10.48550/arXiv.2207.05221`.

Adam Tauman Kalai and Santosh S. Vempala. Calibrated language models must hallucinate. In Bojan Mohar, Igor Shinkar, and Ryan O'Donnell, editors, *Proceedings of the 56th Annual ACM Symposium on Theory of Computing, STOC 2024, Vancouver, BC, Canada, June 24-28, 2024*, pages 160–171. ACM, 2024. doi: 10.1145/3618260.3649777. URL `https://doi.org/10.1145/3618260.3649777`.

Adam Tauman Kalai, Ofir Nachum, Santosh S. Vempala, and Edwin Zhang. Why language models hallucinate. *CoRR*, abs/2509.04664, 2025. doi: 10.48550/ARXIV.2509.04664. URL `https://doi.org/10.48550/arXiv.2509.04664`.

Alkis Kalavasis, Anay Mehrotra, and Grigoris Velegkas. On the limits of language generation: Trade-offs between hallucination and mode-collapse. In Michal Koucký and Nikhil Bansal, editors, *Proceedings of the 57th Annual ACM Symposium on Theory of Computing, STOC 2025, Prague, Czechia, June 23-27, 2025*, pages 1732–1743. ACM, 2025. doi: 10.1145/3717823.3718108. URL `https://doi.org/10.1145/3717823.3718108`.

Michał P. Karpowicz. On the fundamental impossibility of hallucination control in large language models, 2025. URL `https://arxiv.org/abs/2506.06382`.

Myung Kim. Hallucination as an inevitable byproduct of intelligence in large language models (a theoretical examination of the compression–generalization–hallucination triad). 2025a.

Myung Ho Kim. Hallucination-informed intelligence: The limits of lossless abstraction in large language models. 2025b.

Matt J Kusner, Brooks Paige, and José Miguel Hernández-Lobato. Grammar variational autoencoder. In *International conference on machine learning*, pages 1945–1954. PMLR, 2017.

William Kuszmaul and Stefan Walzer. Space lower bounds for dynamic filters and value-dynamic retrieval. In Bojan Mohar, Igor Shinkar, and Ryan O'Donnell, editors, *Proceedings of the 56th Annual ACM Symposium on Theory of Computing, STOC 2024, Vancouver, BC, Canada, June 24-28, 2024*, pages 1153–1164. ACM, 2024. doi: 10.1145/3618260.3649649. URL https://doi.org/10.1145/3618260.3649649.

William Kuszmaul, Jingxun Liang, and Renfei Zhou. Fingerprint filters are optimal. *CoRR*, abs/2510.18129, 2025. doi: 10.48550/ARXIV.2510.18129. URL https://doi.org/10.48550/arXiv.2510.18129.

Nayeon Lee, Wei Ping, Peng Xu, Mostofa Patwary, Pascale Fung, Mohammad Shoeybi, and Bryan Catanzaro. Factuality enhanced language models for open-ended text generation, 2023. URL https://arxiv.org/abs/2206.04624.

Patrick Lewis, Ethan Perez, Aleksandra Piktus, Fabio Petroni, Vladimir Karpukhin, Naman Goyal, Heinrich Küttler, Mike Lewis, Wen-tau Yih, Tim Rocktäschel, Sebastian Riedel, and Douwe Kiela. Retrieval-augmented generation for knowledge-intensive NLP tasks. In Hugo Larochelle, Marc'Aurelio Ranzato, Raia Hadsell, Maria-Florina Balcan, and Hsuan-Tien Lin, editors, *Advances in Neural Information Processing Systems 33: Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual*, 2020. URL https://proceedings.neurips.cc/paper/2020/hash/6b493230205f780e1bc26945df7481e5-Abstract.html.

Haoyu Li, Liuhui Wang, Qizhi Chen, Jianan Ji, Yuhan Wu, Yikai Zhao, Tong Yang, and Aditya Akella. Chainedfilter: Combining membership filters by chain rule. *Proc. ACM Manag. Data*, 1 (4):234:1–234:27, 2023a. doi: 10.1145/3626721. URL https://doi.org/10.1145/3626721.

Xiang Lisa Li, Ari Holtzman, Daniel Fried, Percy Liang, Jason Eisner, Tatsunori Hashimoto, Luke Zettlemoyer, and Mike Lewis. Contrastive decoding: Open-ended text generation as optimization. In Anna Rogers, Jordan L. Boyd-Graber, and Naoaki Okazaki, editors, *Proceedings of the 61st Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), ACL 2023, Toronto, Canada, July 9-14, 2023*, pages 12286–12312. Association for Computational Linguistics, 2023b. doi: 10.18653/V1/2023.ACL-LONG.687. URL https://doi.org/10.18653/v1/2023.acl-long.687.

Sanae Lotfi, Marc Anton Finzi, Yilun Kuang, Tim G. J. Rudner, Micah Goldblum, and Andrew Gordon Wilson. Non-vacuous generalization bounds for large language models. In *Forty-first International Conference on Machine Learning, ICML 2024, Vienna, Austria, July 21-27, 2024*. OpenReview.net, 2024. URL https://openreview.net/forum?id=6Kg9p8URlj.

Shachar Lovett and Ely Porat. A lower bound for dynamic approximate membership data structures. In *51th Annual IEEE Symposium on Foundations of Computer Science, FOCS 2010, October 23-26, 2010, Las Vegas, Nevada, USA*, pages 797–804. IEEE Computer Society, 2010. doi: 10.1109/FOCS.2010.81. URL https://doi.org/10.1109/FOCS.2010.81.

David G Luenberger. *Optimization by vector space methods*. John Wiley & Sons, 1997.

Alex Mallen, Akari Asai, Victor Zhong, Rajarshi Das, Daniel Khashabi, and Hannaneh Hajishirzi. When not to trust language models: Investigating effectiveness of parametric and non-parametric memories. In Anna Rogers, Jordan L. Boyd-Graber, and Naoaki Okazaki, editors, *Proceedings of the 61st Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), ACL 2023, Toronto, Canada, July 9-14, 2023*, pages 9802–9822. Association for Computational

Linguistics, 2023. doi: 10.18653/V1/2023.ACL-LONG.546. URL https://doi.org/10.18653/v1/2023.acl-long.546.

David A McAllester. Pac-bayesian model averaging. In *Proceedings of the twelfth annual conference on Computational learning theory*, pages 164–170, 1999.

David A McAllester. Pac-bayesian stochastic model selection. *Machine Learning*, 51(1):5–21, 2003.

Paul Milgrom and Ilya Segal. Envelope theorems for arbitrary choice sets. *Econometrica*, 70(2): 583–601, 2002.

Muhammad Ahmed Mohsin, Muhammad Umer, Ahsan Bilal, Zeeshan Memon, Muhammad Ibtsaam Qadir, Sagnik Bhattacharya, Hassan Rizwan, Abhiram R Gorle, Maahe Zehra Kazmi, Ayesha Mohsin, et al. On the fundamental limits of llms at scale. *arXiv preprint arXiv:2511.12869*, 2025.

Rasmus Pagh and Flemming Friche Rodler. Lossy dictionaries. In Friedhelm Meyer auf der Heide, editor, *Algorithms - ESA 2001, 9th Annual European Symposium, Aarhus, Denmark, August 28-31, 2001, Proceedings*, volume 2161 of *Lecture Notes in Computer Science*, pages 300–311. Springer, 2001. doi: 10.1007/3-540-44676-1_25. URL https://doi.org/10.1007/3-540-44676-1_25.

Zhixuan Pan, Shaowen Wang, and Jian Li. Understanding LLM behaviors via compression: Data generation, knowledge acquisition and scaling laws. *CoRR*, abs/2504.09597, 2025. doi: 10.48550/ARXIV.2504.09597. URL https://doi.org/10.48550/arXiv.2504.09597.

Michal Perelkiewicz and Rafal Poswiata. A review of the challenges with massive web-mined corpora used in large language models pre-training. In Leszek Rutkowski, Rafal Scherer, Marcin Korytkowski, Witold Pedrycz, Ryszard Tadeusiewicz, and Jacek M. Zurada, editors, *Artificial Intelligence and Soft Computing - 23rd International Conference, ICAISC 2024, Zakopane, Poland, June 16-20, 2024, Proceedings, Part III*, volume 15166 of *Lecture Notes in Computer Science*, pages 153–163. Springer, 2024. doi: 10.1007/978-3-031-81596-6_14. URL https://doi.org/10.1007/978-3-031-81596-6_14.

María Pérez-Ortiz, Omar Rivasplata, John Shawe-Taylor, and Csaba Szepesvári. Tighter risk certificates for neural networks. *J. Mach. Learn. Res.*, 22:227:1–227:40, 2021. URL https://jmlr.org/papers/v22/20-879.html.

Yury Polyanskiy and Yihong Wu. *Information theory: From coding to learning.* Cambridge university press, 2025.

Ely Porat. An optimal bloom filter replacement based on matrix solving. In Anna E. Frid, Andrey Morozov, Andrey Rybalchenko, and Klaus W. Wagner, editors, *Computer Science - Theory and Applications, Fourth International Computer Science Symposium in Russia, CSR 2009, Novosibirsk, Russia, August 18-23, 2009. Proceedings*, volume 5675 of *Lecture Notes in Computer Science*, pages 263–273. Springer, 2009. doi: 10.1007/978-3-642-03351-3_25. URL https://doi.org/10.1007/978-3-642-03351-3_25.

Jorma Rissanen. Modeling by shortest data description. *Automatica*, 14(5):465–471, 1978.

Quan Shi, Wang Xi, Zenghui Ding, Jianqing Gao, and Xianjun Yang. Hallucination as a computational boundary: A hierarchy of inevitability and the oracle escape. *CoRR*, abs/2508.07334, 2025. doi: 10.48550/ARXIV.2508.07334. URL https://doi.org/10.48550/arXiv.2508.07334.

Thomas Steinke and Lydia Zakynthinou. Reasoning about generalization via conditional mutual information. In *Conference on Learning Theory*, pages 3437–3452. PMLR, 2020.

Atsushi Suzuki, Yulan He, Feng Tian, and Zhongyuan Wang. Hallucinations are inevitable but statistically negligible. *CoRR*, abs/2502.12187, 2025. doi: 10.48550/ARXIV.2502.12187. URL `https://doi.org/10.48550/arXiv.2502.12187`.

Sean Welleck, Ilia Kulikov, Stephen Roller, Emily Dinan, Kyunghyun Cho, and Jason Weston. Neural text generation with unlikelihood training. In *8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia, April 26-30, 2020*. OpenReview.net, 2020. URL `https://openreview.net/forum?id=SJeYe0NtvH`.

Bingbing Wen, Jihan Yao, Shangbin Feng, Chenjun Xu, Yulia Tsvetkov, Bill Howe, and Lucy Lu Wang. Know your limits: A survey of abstention in large language models. *Trans. Assoc. Comput. Linguistics*, 13:529–556, 2025. doi: 10.1162/TACL_A_00754. URL `https://doi.org/10.1162/tacl_a_00754`.

Paul L Williams and Randall D Beer. Nonnegative decomposition of multivariate information. *arXiv preprint arXiv:1004.2515*, 2010.

Changlong Wu, Ananth Grama, and Wojciech Szpankowski. No free lunch: Fundamental limits of learning non-hallucinating generative models. In *The Thirteenth International Conference on Learning Representations, ICLR 2025, Singapore, April 24-28, 2025*. OpenReview.net, 2025. URL `https://openreview.net/forum?id=OwNoTs2r8e`.

Aolin Xu and Maxim Raginsky. Information-theoretic analysis of generalization capability of learning algorithms. *Advances in neural information processing systems*, 30, 2017.

Bowen Xu. Hallucination is inevitable for llms with the open world assumption. *arXiv preprint arXiv:2510.05116*, 2025.

Ziwei Xu, Sanjay Jain, and Mohan S. Kankanhalli. Hallucination is inevitable: An innate limitation of large language models. *CoRR*, abs/2401.11817, 2024. doi: 10.48550/ARXIV.2401.11817. URL `https://doi.org/10.48550/arXiv.2401.11817`.

Runchuan Zhu, Xinke Jiang, Jiang Wu, Zhipeng Ma, Jiahe Song, Fengshuo Bai, Dahua Lin, Lijun Wu, and Conghui He. GRAIT: gradient-driven refusal-aware instruction tuning for effective hallucination mitigation. In Luis Chiruzzo, Alan Ritter, and Lu Wang, editors, *Findings of the Association for Computational Linguistics: NAACL 2025, Albuquerque, New Mexico, USA, April 29 - May 4, 2025*, pages 4006–4021. Association for Computational Linguistics, 2025. doi: 10.18653/V1/2025.FINDINGS-NAACL.223. URL `https://doi.org/10.18653/v1/2025.findings-naacl.223`.

A Detailed Discussion of the Information Budget for Random Facts

We provide a self-contained argument supporting the modeling choice that the relevant memory budget allocated to random facts is orders of magnitude below the raw parameter count.

A.1 Setup: random facts, training data, and learned weights

We consider the training setup of an LLM as a Markov chain among several random variables. Let $\mathcal{K}$ denote a set of random facts, such as a specific list of biographies, drawn from a universe of potential facts. Let the tuple $(\Theta, \mathcal{K})$ denote a "world state" parameterizing the training data generation process. Let Z denote the training data, and W the learned weights, obtained by applying a randomized training algorithm to Z. It follows that we have a Markov chain:

$$(\Theta, \mathcal{K}) \to Z \to W. \tag{1}$$

Our goal is to upper-bound $I(W; \mathcal{K})$, the mutual information between the learned weights W and the random facts $\mathcal{K}$. This mutual information, which indicates how much the model memorizes $\mathcal{K}$, corresponds to the "bits of memory" discussed in the main body.

We present two arguments: regularization techniques and learning-theoretic pressures that limit pure memorization, and the fact that the total memory capacity is "crowded out" by structured knowledge, leaving little budget for the unstructured random facts.

A.2 Regularization limits memorization

By the data processing inequality, we have $I(W; \mathcal{K}, \Theta) \leq I(W; Z)$, and it can be argued that the latter is much smaller than the raw parameter count.

Some of the most established theories of generalization in deep learning include the minimum description length (MDL) principle Rissanen (1978); Gr"unwald (2007); Gr"unwald and Roos (2019), PAC-Bayes McAllester (1999, 2003); Catoni (2007); Alquier (2021), and mutual-information generalization bounds Xu and Raginsky (2017); Bu et al. (2020); Steinke and Zakynthinou (2020). These ideas are interconnected Blum and Langford (2003); Achille and Soatto (2018); Hellstr"om et al. (2025); Grunwald et al. (2021), and they roughly all establish that *limited memorization of training data* is a key factor in generalization.

Their bounds all relate to the quantity $I(W; Z)$, the mutual information between the weights W and the training data Z.

- Mutual-information bounds directly connect the expected generalization error to variants of $I(W; Z)$.
- PAC-Bayes bounds advocate controlling $\mathrm{KL}(Q_Z \| P)$, where P is some data-independent prior over W such as a standard Gaussian, and Q_Z is the distribution of W after training on data Z. This relates to mutual information via $I(W; Z) \leq \mathbb{E}_Z[\mathrm{KL}(Q_Z \| P)]$, where equality is obtained iff P is the marginal distribution of W induced by the learning algorithm and Z.
- MDL principle is based on minimizing the description length of W (while keeping the training error small), which is often equivalent to minimizing $\mathrm{KL}(Q_Z \| P)$, since the latter is the extra bits needed to describe W beyond the prior P.

These theories posit that the key to explaining generalization lies in controlling memorization, quantified by $I(W; Z)$. This is done through implicit bias imposed by the various regularization mechanisms, such as mini-batch SGD, weight decay, dropout, and early stopping, and the preference of flat minima. If this line of reasoning is correct, then we expect the model to have a tendency to reduce $I(W;Z)$, as long as doing so does not increase the training loss too much.

The above theories have also given rise to a series of non-vacuous generalization bounds for deep networks Dziugaite and Roy (2017, 2018); Pérez-Ortiz et al. (2021) and language models Lotfi et al. (2024). These empirical bounds are derived via quantizing and compressing the model parameters W, and then applying MDL/PAC-Bayes bounds. If these compressed networks maintain the same performance on the training data Z, then these studies provide a strong argument that $I(W;Z)$ is indeed small.

A.3 Structured vs. random facts: a formal tradeoff

We now formalize the intuition that "structured knowledge" and "random facts" compete for the same limited information budget in W, and that structured knowledge often gets prioritized.

Decomposition. Suppose that the world is parameterized by random variables $(\Theta, \mathcal{K})$, where Θ represents structured components (e.g., linguistic syntax, logical rules, universal regularities) and $\mathcal{K}$ represents random facts. We can assume that $\mathcal{K}$ is independent of Θ.

This decomposition aligns with the **Syntax–Knowledge generative framework** recently proposed by Pan et al. (2025), who model language generation as a hierarchical process combining a parametric syntax model with a non-parametric, long-tail knowledge model. Similar distinctions have also been explored in prior literature to explain learning dynamics, such as the disentanglement of syntax and semantics Gong et al. (2025) and the separation of grammatical structure from content in generative models Dyer et al. (2016); Kusner et al. (2017).

Budget Splitting Argument. Information theory dictates that these two components compete for the model's finite capacity. If we assume $\mathcal{K}$ is independent of Θ, then by decomposition of multivariate information Williams and Beer (2010), we have:

$$\begin{aligned} I(W;\mathcal{K},\Theta) &= I(W;\Theta) + I(W;\mathcal{K} \mid \Theta) \\ &= I(W;\Theta) + \underbrace{H(\mathcal{K} \mid \Theta)}_{=H(\mathcal{K})} - H(\mathcal{K} \mid W, \Theta) \\ &= I(W;\Theta) + H(\mathcal{K}) - H(\mathcal{K} \mid W) + H(\mathcal{K} \mid W) - H(\mathcal{K} \mid W, \Theta) \\ &= I(W;\Theta) + I(W;\mathcal{K}) + \underbrace{I(\mathcal{K};\Theta \mid W)}_{\geq 0}. \end{aligned}$$

If the total effective capacity $I(\Theta, \mathcal{K}; W)$ is bounded, this equality implies a tradeoff:

$$\underbrace{I(\mathcal{K};W)}_{\text{Capacity for random facts}} \leq \underbrace{I(\Theta,\mathcal{K};W)}_{\text{Total Budget}} - \underbrace{I(\Theta;W)}_{\text{Capacity used for structure}}.$$

Consequently, any mechanism that increases $I(\Theta;W)$—i.e., learning more structure—necessarily reduces the remaining budget available for encoding the random residual $\mathcal{K}$.

Prioritized Learning Dynamics. Crucially, this is not just a static tradeoff but a dynamic one where Θ takes precedence. Pan et al. (2025) demonstrate theoretically (via Kolmogorov Structure Functions) and empirically that LLMs exhibit frequency-dependent learning: they prioritize compressing pervasive syntactic structures (Θ) before acquiring rarer factual knowledge ($\mathcal{K}$). This observation is consistent with the two-stage training dynamics of Transformers Gong et al. (2025), as well as the empirical difficulty for trained models to recall high-entropy facts compared to structured knowledge Huang et al. (2025c).

Because Θ corresponds to high-frequency patterns that offer the greatest training loss reduction, real-world models "spend" their information budget on Θ first. Random facts $\mathcal{K}$, which often appear as incompressible noise to a capacity-constrained model Pan et al. (2025), are relegated to the residual information budget. This justifies our focus on bounding $I(\mathcal{K}; W)$: it is the marginal capacity left for the long tail of world knowledge after the model has learned the essential structures of the world.

B Proofs for Section 3

B.1 Proof of Lemma 3.4

For completeness, we first prove the lemma below.

Lemma B.1. *Let X be a discrete random variable with $H(X) < \infty$ and let Y be any random variable. Then, the conditional entropy $H(X \mid Y)$ is concave in the joint distribution of (X, Y).*

Proof. Let P_0 and P_1 be two joint distributions on $\mathcal{X} \times \mathcal{Y}$, and let $P_\lambda = \lambda P_1 + (1-\lambda)P_0$ for $\lambda \in [0, 1]$. We choose a reference measure ν on $\mathcal{Y}$ (e.g., the sum of marginals of P_0 and P_1) such that the joint distributions can be described by densities $p_i(x, y)$ with respect to the product of the counting measure on $\mathcal{X}$ and ν. Let $p_i(y) = \sum_{x \in \mathcal{X}} p_i(x, y)$ denote the marginal density of Y.

The conditional entropy can be written as:

$$H(X|Y) = \sum_{x \in \mathcal{X}} \int p(x, y) \log \frac{p(y)}{p(x, y)} \, d\nu(y).$$

Consider the function $f(u, v) = u \log(v/u)$ for $u, v \geq 0$. This function is the perspective transform of the concave function $g(t) = -t \log t$, given by $f(u, v) = vg(u/v)$. Since the perspective of a concave function is jointly concave, $f(u, v)$ is jointly concave in (u, v).

For the mixture P_λ, the densities are linear combinations:

$$p_\lambda(x, y) = \lambda p_1(x, y) + (1 - \lambda)p_0(x, y), \quad p_\lambda(y) = \lambda p_1(y) + (1 - \lambda)p_0(y).$$

By the joint concavity of f:

$$f(p_\lambda(x, y), p_\lambda(y)) \geq \lambda f(p_1(x, y), p_1(y)) + (1 - \lambda)f(p_0(x, y), p_0(y)).$$

Summing over x and integrating over y preserves this inequality, yielding:

$$H_{P_\lambda}(X|Y) \geq \lambda H_{P_1}(X|Y) + (1 - \lambda)H_{P_0}(X|Y).$$

This proves the concavity. □

Now we restate and prove Lemma 3.4.

Lemma B.2. *Let $\mathcal{M}$ be a membership tester for key size n in universe $[u]$ with $u > n$. Let $p = \frac{n}{u}$ and let F_p be as defined above. Then, the memory cost of $\mathcal{M}$ is at least:*

$$\frac{B(\mathcal{M})}{n} \geq F_p\big(\mu_K(\mathcal{M}), \mu_N(\mathcal{M})\big) - \frac{\log(8n)}{2n}.$$

Proof. We will apply the data processing inequality to lower bound the entropy of W as a random variable, hence lower-bounding the memory usage of $\mathcal{M}$. Let $\mathcal{K}$ be uniformly randomly sampled from all subsets of $[u]$ of size n. Define random variables $X_i = \mathbb{1}\{i \in \mathcal{K}\}$ to be the membership information for $i \in \mathcal{U}$, and define

$$\hat{X}_i = \mathsf{Query}^{\mathcal{M}}(i, \mathsf{Init}^{\mathcal{M}}(\mathcal{K}))$$

to be the answer to the membership query, treated as the "reconstructed" membership information. Then, by the data processing inequality we have

$$B(\mathcal{M}) = I(\mathcal{K}; W) \geq I(X^u; \hat{X}^u),$$

where X^u and $\hat{X}^u$ denote the length-u vector of X_i's and $\hat{X}_i$'s, respectively. Because X^u is discrete, we can write the mutual information as $I(X^u; \hat{X}^u) = H(X^u) - H(X^u|\hat{X}^u)$.

Let $I \sim \mathrm{Unif}([u])$ be a uniformly random element, then by definition we have

$$I(X_I; \hat{X}_I) = p \cdot F_p\big(\mu_K(\mathcal{M}), \mu_N(\mathcal{M})\big).$$

We now relate the block mutual information $I(X^u; \hat{X}^u)$ to the single-letter mutual information $I(X_I; \hat{X}_I)$. First, by the chain rule for entropy and the fact that conditioning reduces entropy:

$$\begin{aligned} H(X^u|\hat{X}^u) &= \sum_{i=1}^{u} H(X_i|\hat{X}^u, X_1, \ldots, X_{i-1}) \\ &\leq \sum_{i=1}^{u} H(X_i|\hat{X}_i). \end{aligned}$$

To lower bound the average conditional entropy $\frac{1}{u}\sum_{i=1}^{u} H(X_i|\hat{X}_i)$, we use the fact that conditional entropy $H(X|Y)$ is a concave function in the joint distribution of (X, Y). Since the distribution of $(X_I, \hat{X}_I)$ is the average of the distributions of $(X_i, \hat{X}_i)$, Jensen's inequality gives:

$$H(X_I|\hat{X}_I) \geq \frac{1}{u}\sum_{i=1}^{u} H(X_i|\hat{X}_i).$$

Combining the inequalities, we obtain the following upper bound:

$$H(X^u|\hat{X}^u) \leq \sum_{i=1}^{u} H(X_i|\hat{X}_i) \leq uH(X_I|\hat{X}_I).$$

Now, we lower bound the entropy of the source $H(X^u) = H(S) = \log\binom{u}{n}$. By standard approximations (see e.g. section 14.2 of Cover and Thomas (2001)), we have $\binom{u}{n} \geq \sqrt{\frac{u}{8n(u-n)}}2^{uH(p)}$, so

$$\begin{aligned} H(X^u) &= \log\binom{u}{n} \\ &\geq uH(p) + \frac{1}{2}\log\frac{u}{8n(u-n)} \\ &\geq uH(p) - \frac{1}{2}\log(8n). \end{aligned}$$

Combining these results:

$$\begin{aligned} B(\mathcal{M}) \geq I(X^u; \hat{X}^u) &= H(X^u) - H(X^u|\hat{X}^u) \\ &\geq (uH(p) - \frac{1}{2}\log(8n)) - uH(X_I|\hat{X}_I) \\ &= u(H(p) - H(X_I|\hat{X}_I)) - \frac{1}{2}\log(8n) \\ &= uI(X_I; \hat{X}_I) - \frac{1}{2}\log(8n). \end{aligned}$$

Since $uI(X_I; \hat{X}_I) = n \cdot F_p\big(\mu_K(\mathcal{M}), \mu_N(\mathcal{M})\big)$, it follows that:

$$\frac{B(\mathcal{M})}{n} \geq F_p\big(\mu_K(\mathcal{M}), \mu_N(\mathcal{M})\big) - \frac{\log(8n)}{2n},$$

as desired. □

B.2 Proof of Lemma 3.5

Lemma B.3 (Same as Lemma 3.5)**.** *For $p > 0$, let $F_p(\mu_K, \mu_N) = I(X; \hat{X})/p$, where $X \sim \text{Bern}(p)$, $\hat{X} \mid (X = 1) \sim \mu_K$, and $\hat{X} \mid (X = 0) \sim \mu_N$. We also define $F_0(\mu_K, \mu_N) = \text{KL}(\mu_K \| \mu_N)$. Then, for $p \in [0, 1)$ and $(\mu_K, \mu_N) \in \mathcal{P}([0, 1])^2$:*

1. *The function $(p, \mu_K, \mu_N) \mapsto F_p(\mu_K, \mu_N)$ is jointly lower semi-continuous.*

2. *$F_p(\mu_K, \mu_N)$ is continuous in p.*

3. *F_p is differentiable in p with $\frac{\partial}{\partial p}F_p(\mu_K, \mu_N) = -\frac{\text{KL}(\mu_N \| p\mu_K + (1-p)\mu_N)}{p^2}$ whenever $p > 0$.*

Proof. We prove the three properties using the following identity:

$$\begin{aligned} I(X; \hat{X}) &= \text{KL}(P_{X,\hat{X}} \| P_X \otimes P_{\hat{X}}) \\ &= \mathop{\mathbb{E}}_{X \sim \text{Bern}(p)} \text{KL}(P_{\hat{X}|X} \| P_{\hat{X}}) \\ &= p\text{KL}(\mu_K \| \mu_p) + (1 - p)\text{KL}(\mu_N \| \mu_p), \end{aligned} \tag{2}$$

where $\mu_p = p\mu_K + (1 - p)\mu_N$ is the marginal distribution of $\hat{X}$. Dividing by p, we obtain the expression for F_p:

$$F_p(\mu_K, \mu_N) = \text{KL}(\mu_K \| \mu_p) + \frac{1 - p}{p}\text{KL}(\mu_N \| \mu_p). \tag{3}$$

1. Joint Lower Semi-Continuity. For any sequence $(p_n, \mu_{K,n}, \mu_{N,n}) \to (p, \mu_K, \mu_N)$, we show that $\liminf F_{p_n} \geq F_p$. First, observe that the map $(p, \mu_K, \mu_N) \mapsto \mu_p = p\mu_K + (1 - p)\mu_N$ is continuous from the product topology to the weak-* topology. Since KL divergence is jointly lower semi-continuous (LSC) with respect to the weak-* topology, it is immediate that $F_p(\mu_K, \mu_N)$ is LSC whenever $p > 0$.

Consider the case where $p = 0$. As $p_n \to 0$, $\mu_{p_n} \to \mu_N$, the first term converges like $\liminf \text{KL}(\mu_{K,n} \| \mu_{p_n}) \geq \text{KL}(\mu_K \| \mu_N)$. The second term $\frac{1-p_n}{p_n}\text{KL}(\mu_{N,n} \| \mu_{p_n})$ is always non-negative. Therefore,

$$\liminf F_{p_n} \geq \text{KL}(\mu_K \| \mu_N) + 0 = F_0(\mu_K, \mu_N),$$

proving its joint LSC everywhere.

2. Continuity in p. For fixed μ_K, μ_N, and $p > 0$, F_p is clearly continuous as a composition of continuous functions. We only need to verify continuity at $p = 0$. Standard results in information theory have shown that the KL divergence vanishes sublinearly when the two distributions are close, see e.g. Proposition 2.20 in Polyanskiy and Wu (2025):

$$\frac{\partial}{\partial p}\mathrm{KL}(\mu_N \| \mu_p)\bigg|_{p=0} = 0 \text{ iff } \mu_K \ll \mu_N.$$

Hence, when $\mathrm{KL}(\mu_K \| \mu_N) < \infty$ (and hence $\mu_K \ll \mu_N$), we have

$$\begin{aligned}\lim_{p\to 0} F_p(\mu_K, \mu_N) &= \lim_{p\to 0}\left(\mathrm{KL}(\mu_K\|\mu_p) + \frac{1-p}{p}\mathrm{KL}(\mu_N\|\mu_p)\right)\\ &= \mathrm{KL}(\mu_K\|\mu_N) + \lim_{p\to 0}\frac{1-p}{p}\mathrm{KL}(\mu_N\|\mu_p)\\ &= \mathrm{KL}(\mu_K\|\mu_N),\end{aligned}$$

where the second equality is because the limit of first term is at least $\mathrm{KL}(\mu_K\|\mu_N)$ by LSC, and at most $\lim_{p\to 0}(1-p)\mathrm{KL}(\mu_K\|\mu_N)$ by convexity. The last equality is because the second term vanishes by L'Hopital's rule.

When $\mathrm{KL}(\mu_K\|\mu_N) = \infty$, the limit also goes to infinity because $\mathrm{KL}(\mu_K\|\mu_p) \to \infty$.

3. Differentiability in p. Fix μ_K, μ_N. For $p \in (0, 1)$, let $\nu := \mu_K + \mu_N$ and write $f_K := \frac{d\mu_K}{d\nu}$, $f_N := \frac{d\mu_N}{d\nu}$, so that the mixture $\mu_p = p\mu_K + (1-p)\mu_N$ has density

$$m_p := \frac{d\mu_p}{d\nu} = pf_K + (1-p)f_N.$$

Using (2), we can write

$$I(p) := I(X; \hat{X}) = p\int f_K \log\frac{f_K}{m_p}\,d\nu + (1-p)\int f_N \log\frac{f_N}{m_p}\,d\nu.$$

We first show that $I'(p) = \mathrm{KL}(\mu_K\|\mu_p) - \mathrm{KL}(\mu_N\|\mu_p)$. For convenience, we assume that the KL divergence is base-e in this part and drop the $\ln 2$ factor. All results hold for base-2 as well.

For $p \in (0, 1)$ we have

$$\frac{\partial}{\partial p}\log m_p = \frac{f_K - f_N}{m_p}, \qquad \text{and} \qquad \left|\frac{f_K - f_N}{m_p}\right| \le \frac{f_K + f_N}{pf_K + (1-p)f_N} \le \frac{1}{p} + \frac{1}{1-p}.$$

Therefore the functions $f_K \cdot \left|\frac{\partial}{\partial p}\log m_p\right|$ and $f_N \cdot \left|\frac{\partial}{\partial p}\log m_p\right|$ are ν-integrable (bounded by constants times f_K and f_N, which integrate to 1), and by dominated convergence we may differentiate $I(p)$ by moving $\frac{\partial}{\partial p}$ inside the integrals.

Differentiating $I(p)$ yields

$$\begin{aligned}I'(p) = &\int f_K \log\frac{f_K}{m_p}\,d\nu - \int f_N \log\frac{f_N}{m_p}\,d\nu\\ &+ p\int f_K\Big(-\frac{\partial}{\partial p}\log m_p\Big)\,d\nu + (1-p)\int f_N\Big(-\frac{\partial}{\partial p}\log m_p\Big)\,d\nu.\end{aligned}$$

The last two terms cancel:

$$p\int f_K\Big(-\frac{f_K-f_N}{m_p}\Big)\,d\nu+(1-p)\int f_N\Big(-\frac{f_K-f_N}{m_p}\Big)\,d\nu=-\int(pf_K+(1-p)f_N)\frac{f_K-f_N}{m_p}\,d\nu$$
$$=-\int(f_K-f_N)\,d\nu=0,$$

since $\int f_K\,d\nu=\int f_N\,d\nu=1$. Hence,

$$I'(p)=\mathrm{KL}(\mu_K\|\mu_p)-\mathrm{KL}(\mu_N\|\mu_p).$$

Finally, $F_p=I(p)/p$ for $p>0$, so by the quotient rule

$$\begin{aligned}\frac{\partial}{\partial p}F_p&=\frac{pI'(p)-I(p)}{p^2}\\&=\frac{p\big(\mathrm{KL}(\mu_K\|\mu_p)-\mathrm{KL}(\mu_N\|\mu_p)\big)-\big(p\mathrm{KL}(\mu_K\|\mu_p)+(1-p)\mathrm{KL}(\mu_N\|\mu_p)\big)}{p^2}\\&=-\frac{\mathrm{KL}(\mu_N\|\mu_p)}{p^2}.\end{aligned}$$

□

B.3 Proof for achievability of rate-distortion lower bound

Before proving Lemma 3.7, we need the following reduction, which states that for each p, it suffices to consider $\hat{x}$ as having finite support. The exact support set depends on p and the error constraints, yet the size of this set is uniformly upper bounded by 5, by an application of Caratheodory's theorem.

Lemma B.4 (Finite Support Reduction)**.** *Fix $d^K, d^N, \varepsilon_K, \varepsilon_N>0$ and $p\in(0,1)$. Then, there exists $(\mu_K^*,\mu_N^*)\in\mathcal{C}_K(\varepsilon_K)\times\mathcal{C}_N(\varepsilon_N)$ which attains the minimum in the definition of R_p,*

$$R_p(\varepsilon_K,\varepsilon_N)=F_p(\mu_K^*,\mu_N^*),$$

and that μ_K^*,μ_N^* are discrete distributions with $|\mathrm{supp}(\mu_K^*)\cup\mathrm{supp}(\mu_N^*)|\le 5$.

Proof. We will start by assuming a pair (μ_K^*,μ_N^*) with errors exactly equal to ε_K and ε_N and attains the minimum in the definition of R_p. Then, we show that there exists some other (μ_K',μ_N') which takes value on at most 5 points, achieves the same error levels, and attains the same rate:

$$R_p(\varepsilon_K,\varepsilon_N)=F_p(\mu_K^*,\mu_N^*)=F_p(\mu_K',\mu_N').$$

Consider the joint distribution $P_{X,\hat{X}}$ of $(X,\hat{X}$ that (μ_K^*,μ_N^*) induces, and let $P_{\hat{X}}=p\mu_K^*+(1-p)\mu_N^*$ be the marginal distribution of $\hat{X}$. Then, for $P_{\hat{X}}$-almost every $\hat{x}\in[0,1]$, we have a unique posterior distribution for X, denoted $P_{X|\hat{X}}(\cdot|\hat{x})=\mathrm{Bern}(q_{\hat{x}})$. The value $q_{\hat{x}}$ is characterized by the Radon-Nikodym derivative

$$q_{\hat{x}}=p\cdot\frac{d\mu_K^*}{dP_{\hat{X}}}(\hat{x})\in[0,1].$$

For each $q\in[0,1]$, we use $h(q)$ to denote the binary entropy function $h(q)=-q\log_2 q-(1-q)\log_2(1-q)$, where $h(0)=h(1)=0$. We now consider the $P_{\hat{X}}$-everywhere defined vector-valued function $f:E\to\mathbb{R}^4$, which maps each $\hat{x}$ to the tuple

$$f(\hat{x})=\big(q_{\hat{x}},\,q_{\hat{x}}\cdot d^K(\hat{x}),\,(1-q_{\hat{x}})\cdot d^N(\hat{x}),\,h(q_{\hat{x}})\big).$$

Let E be defined as the points over which f is finite, and for convenience we will assume (μ_K^*, μ_N^*) are tight for both error constraints. Although d^K, d^N can take infinite values, E has full $P_{\hat{X}}$-measure, as the error constraints imply that the following integrals are finite:

$$\mathop{\mathbb{E}}_{P_{X,\hat{X}}}[d^K(\hat{X})|X=1] = \frac{1}{p}\mathop{\mathbb{E}}_{P_{\hat{X}}}[q_{\hat{X}} \cdot d^K(\hat{X})] = \varepsilon_K \quad \text{and} \quad \mathop{\mathbb{E}}_{P_{X,\hat{X}}}[d^N(\hat{X})|X=0] = \frac{1}{1-p}\mathop{\mathbb{E}}_{P_{\hat{X}}}[(1-q_{\hat{X}}) \cdot d^N(\hat{X})] = \varepsilon_N.$$

Moreover, we also note that by construction,

$$\mathop{\mathbb{E}}_{\hat{X}\sim P_{\hat{X}}}[q_{\hat{X}}] = p \quad \text{and} \quad \mathop{\mathbb{E}}_{\hat{X}\sim P_{\hat{X}}}[h(q_{\hat{X}})] = H(X|\hat{X}) = h(p) - p \cdot F_p(\mu_K^*, \mu_N^*).$$

Note that $\mathbb{E}_{\hat{X}\sim P_{\hat{X}}}[f(\hat{X})] = \big(p, p\varepsilon_K, (1-p)\varepsilon_N, h(p) - p \cdot F_p(\mu_K^*, \mu_N^*)\big)$ is in the convex hull of the vectors

$$\big\{(q_{\hat{x}},\ q_{\hat{x}} \cdot d^K(\hat{x}),\ (1-q_{\hat{x}}) \cdot d^N(\hat{x}),\ h(q_{\hat{x}})) : \hat{x} \in E\big\}.$$

By Carathéodory's Theorem, there exist $\alpha_1, \dots, \alpha_5 \geq 0$ and $\hat{x}_1, \dots, \hat{x}_5 \in [0,1]$ such that $\sum_{i=1}^5 \alpha_i = 1$ and

$$\mathop{\mathbb{E}}_{\hat{X}\sim P_{\hat{X}}}[f(\hat{X})] = \sum_{i=1}^5 \alpha_i f(\hat{x}_i).$$

Now, consider the random variable $X' \sim \sum_{i=1}^5 \alpha_i \delta_{\hat{x}_i}$, where $\delta_{\hat{x}_i}$ is the Dirac delta distribution at $\hat{x}_i$. Let $P_{X|X'}$ be defined as $P_{X|X'}(x|x') = \mathrm{Bern}(q_{x'})$. We can check that $\mathbb{P}[X=1] = p$ under this $P_{X|X'}$ since $\sum_{i=1}^5 \alpha_i q_{\hat{x}_i} = p$. We can now construct μ'_K and μ'_N as

$$\mu'_K = \frac{1}{p}\sum_{i=1}^5 \alpha_i q_{\hat{x}_i} \delta_{\hat{x}_i} \quad \text{and} \quad \mu'_N = \frac{1}{1-p}\sum_{i=1}^5 \alpha_i (1-q_{\hat{x}_i}) \delta_{\hat{x}_i}.$$

We have $\mu'_K \in \mathcal{C}_K(\varepsilon_K)$ and $\mu'_N \in \mathcal{C}_N(\varepsilon_N)$ since

$$\mathop{\mathbb{E}}_{X'\sim\mu'_K}[d^K(X')] = \frac{1}{p}\sum_{i=1}^5 \alpha_i q_{\hat{x}_i} \cdot d^K(\hat{x}_i) = \varepsilon_K$$

and

$$\mathop{\mathbb{E}}_{X'\sim\mu'_N}[d^N(X')] = \frac{1}{1-p}\sum_{i=1}^5 \alpha_i (1-q_{\hat{x}_i}) \cdot d^N(\hat{x}_i) = \varepsilon_N.$$

Finally, (μ'_K, μ'_N) also achieve the same rate as (μ_K^*, μ_N^*) since

$$p \cdot F_p(\mu'_K, \mu'_N) = h(p) - \mathop{\mathbb{E}}_{X'\sim P_{X'}}[h(q_{X'})] = h(p) - \mathop{\mathbb{E}}_{\hat{X}\sim P_{\hat{X}}}[h(q_{\hat{X}})] = p \cdot F_p(\mu_K^*, \mu_N^*).$$

It follows that (μ'_K, μ'_N) attains the minimum in the definition of R_p and has support on at most 5 points. □

Now that we reduced the reconstructed $\hat{X}$ to a random variable with finite support, we can proceed with the proof of achievability.

Lemma B.5 (same as Lemma 3.7)**.** *Fix any $p = \frac{n}{u} \in (0,1)$ and $\varepsilon_K, \varepsilon_N > 0$. Then, for all $\delta > 0$, there is a sufficiently large n and u such that there exists a membership tester $\mathcal{M}$ for universe $[u]$ and key sizes n which achieves error rates $(\varepsilon_K + \delta, \varepsilon_N + \delta)$, and:*

$$\frac{B(\mathcal{M})}{n} \leq R_p(\varepsilon_K, \varepsilon_N) + \delta.$$

Proof. **Step 1: Finite Support and Continuity.** Let (μ_K^*, μ_N^*) be the pair of distributions attaining the minimum in the definition of $R_p(\varepsilon_K, \varepsilon_N)$. By the finite support reduction (proven in the previous lemma), we assume without loss of generality that these distributions are supported on a finite set $\mathcal{Y}^* \subset [0,1]$ with $|\mathcal{Y}^*| \leq 5$. In the rest of the proof, we will rename the recovered $\hat{X}$ as Y for notational convenience.

Let $P^*_{X,Y}$ be the joint distribution of X and Y under the optimal (μ_K^*, μ_N^*), where $P^*_X = \text{Bern}(p)$ is the source distribution, and $P^*_{Y|X}$ is the transition kernel defined by $P^*_{Y|X}(y|1) = \mu^*_K(y)$ and $P^*_{Y|X}(y|0) = \mu^*_N(y)$.

We will use $\mathcal{D}$ to denote the set of joint distributions $P_{X,Y}$ with Bern(p) marginal on X and which places zero mass on points with infinite errors: for all $y \in \mathcal{Y}^*$, $P_{X,Y}(1,y) = 0$ whenever $d^K(y) = \infty$ and $P_{X,Y}(0,y) = 0$ whenever $d^N(y) = \infty$. Since both X and Y have finite support, $\mathcal{D}$ is compact. Consequently, the following functionals are uniformly continuous over $\mathcal{D}$:

1. $D_K(P_{X,Y}) = \mathbb{E}_{y \sim P_{Y|X}(\cdot|1)}[d^K(y)]$;
2. $D_N(P_{X,Y}) = \mathbb{E}_{y \sim P_{Y|X}(\cdot|0)}[d^N(y)]$.

Therefore, there exists a $\gamma > 0$ such that for any $P'_{X,Y} \in \mathcal{D}$ with $\|P'_{X,Y} - P^*_{X,Y}\|_1 < \gamma$, we have:

$$|D_K(P'_{X,Y}) - D_K(P^*_{X,Y})| < \delta, \tag{4}$$

$$|D_N(P'_{X,Y}) - D_N(P^*_{X,Y})| < \delta, \tag{5}$$

Step 2: Typical Sequences. For each $P_{X,Y} \in \mathcal{D}$, and for each source sequence $x^u \in \{0,1\}^u$, let $T^u_{[P_{Y|X}]\gamma}(x^u)$ be the set of $P_{Y|X}$*-typical sequences under condition* x^u *with constant* γ as defined in Definition 2.9 of Csiszár and Körner (2011). These sequences are $y^u \in \mathcal{Y}^{*u}$ such that:

1. Let $\hat{P}_{X,Y}(x', y'|x^u, y^u)$ be the joint empirical distribution of x_i and y_i for $i = 1, \ldots, u$ in the sequences x^u and y^u. Then,
$$\left|\hat{P}_{X,Y}(x', y'|x^u, y^u) - P_X(x')P_{Y|X}(y'|x')\right| \leq \gamma.$$
2. Whenever $P_{Y|X}(y'|x') = 0$, $\hat{P}_{X,Y}(x', y'|x^u, y^u) = 0$.

It follows from uniform continuity that, for sufficiently small γ, all $P^*_{Y|X}$-typical sequences y^u under condition x^u will have the empirical distribution of (x_i, y_i) close to $P^*_{X,Y}$, and thus satisfy (4) and (5) for the desired choice of δ.

By Lemma 2.13 in Csiszár and Körner (2011), there exist sequences $\delta_u \to 0$ and $\gamma_u \to 0$ such that for all $x^u \in \{0,1\}^u$ with $n = pu$ entries of 1,

$$\left|\frac{1}{u} \log |T^u_{[P_{Y|X}]\gamma_u}(x^u)| - H(Y|X)\right| \leq \delta_u,$$

where $H(Y|X)$ is based on the selected $P_{X,Y}$.

Similarly, we can define P_Y*-typical sequences with constant* γ as the sequences $y^u \in \mathcal{Y}^u$ such that

$$\left|\hat{P}_Y(y'|y^u) - P_Y(y')\right| \leq \gamma,$$

where $\hat{P}_Y(y'|y^u)$ is the empirical distribution of y' in y^u. There exist sequences $\delta_u \to 0$ and $\gamma_u \to 0$ such that

$$\left|\frac{1}{u} \log |T^u_{[P_Y]\gamma_u}| - H(Y)\right| \leq \delta_u,$$

where $H(Y)$ is based on the selected P_Y.

Step 3: Type Covering. By the previous steps, for sufficiently large u, there is some γ such that for each source sequence x^u with n entries of 1, each $y \in T^u_{[P_{Y|X}]\gamma}(x^u)$ satisfies (4) and (5) for the desired choice of δ. Now, we apply the same proof as the type covering lemma (Lemma 9.1 in Csiszár and Körner (2011)) to show that all valid source x^u can be "covered" by some y^u in a fixed codebook M. We will demonstrate the existence of such a codebook and bound its size.

Let P_Y^* be the marginal distribution of Y under $P^*_{X,Y}$. Consider a codebook M of m sequences sampled uniformly from $T^u_{[P_Y^*]\gamma}$, and let Y^u be such a random sequence. For any source sequence x^u with n entries of 1, the probability that Y^u is $P^*_{X|Y}$-typical under condition x^u with constant γ is given by

$$\mathbb{P}[Y^u \in T^u_{[P^*_{Y|X}]\gamma}(x^u)] = \frac{|T^u_{[P^*_{Y|X}]\gamma}(x^u)|}{|T^u_{[P^*_Y]\gamma}|} \geq \frac{2^{-u(H(Y|X)+p\delta/4)}}{2^{u(H(Y)+p\delta/4)}} = 2^{-u(I(X;Y)+p\delta/2)},$$

where X, Y are distributed according to $P^*_{X,Y}$. The inequality in the middle is due to the fact that δ_u is eventually smaller than $p\delta/4$, for our choice of δ.

With m uniformly selected Y^u, the expected number of x^u that are *not* covered by any Y^u in the codebook is at most:

$$\begin{aligned}\mathbb{E}[\text{number of } x^u \text{ not covered by } M] &= \sum_{x^u} \mathbb{P}[Y^u \notin T^u_{[P^*_{Y|X}]\gamma}(x^u)] \\ &\leq \sum_{x^u} \left(1 - 2^{-u(I(X;Y)+p\delta/2)}\right)^m \\ &\leq \exp(-m 2^{-u(I(X;Y)+p\delta/2)}) \cdot \binom{u}{n}.\end{aligned}$$

For sufficiently large u, this value is strictly less than 1 if we choose $m = 2^{u(I(X;Y)+p\delta)}$. As the expectation is smaller than 1, this means that there exists a choice of codebook that simultaneously covers all source sequences.

We can now define a membership tester, which initializes by encoding the nearest codeword in M to the x^u corresponding to key set $\mathcal{K}$, and on query i, outputs the ith entry of that codeword. And the proof is finished since the memory cost is at most $\log |M| \leq u(I(X;Y)+p\delta) = n\cdot\big(R_p(\varepsilon_K, \varepsilon_N)+\delta\big)$. □

B.4 Proof of Theorem 3.2

Theorem B.6 (same as Theorem 3.2)**.** *Suppose $(\mu_K^*, \mu_N^*) \in \mathcal{C}_K(\varepsilon_K) \times \mathcal{C}_N(\varepsilon_N)$ is the unique minimizer of $\mathrm{KL}(\mu_K \| \mu_N)$. In the setting of Theorem 3.1, if $\{\mathcal{M}_j\}$ is asymptotically optimal, in the sense that*

$$\limsup_{j\to\infty} \frac{B(\mathcal{M}_j)}{n_j} = \mathrm{KL}(\mu_K^* \| \mu_N^*),$$

then we must have $\mu_K(\mathcal{M}_j) \to \mu_K^*$ and $\mu_N(\mathcal{M}_j) \to \mu_N^*$ in Wasserstein-1 distance.

Proof of Theorem 3.2. Consider the output distributions $(\mu_K(\mathcal{M}_j), \mu_N(\mathcal{M}_j))$ for $j = 1, 2, \ldots$. By compactness of $\mathcal{P}([0,1])^2$, there exists a subsequence of $(\mu_K(\mathcal{M}_j), \mu_N(\mathcal{M}_j))$ converging to some $(\mu_K'^*, \mu_N'^*) \in \mathcal{P}([0,1])^2$.

As shown in the proof of Theorem 3.1, the limit point $(\mu_K'^*, \mu_N'^*)$ must satisfy the error constraints, i.e., $(\mu_K'^*, \mu_N'^*) \in \mathcal{C}_K(\varepsilon_K) \times \mathcal{C}_N(\varepsilon_N)$. By the memory-optimality of $\{\mathcal{M}_j\}$, if (μ_K^*, μ_N^*) are the unique minimizers of KL divergence, then we have:

$$\begin{aligned}\mathrm{KL}(\mu_K^*\|\mu_N^*) &= \limsup_{j\to\infty}\frac{B(\mathcal{M}_j)}{n_j}\\ &\geq \limsup_{j\to\infty}\left(F_{p_j}(\mu_K(\mathcal{M}_j),\mu_N(\mathcal{M}_j)) + O\Big(\frac{\log n_j}{n_j}\Big)\right)\\ &\geq \mathrm{KL}(\mu_K'^*\|\mu_N'^*).\end{aligned}$$

Hence $(\mu_K^*, \mu_N^*) = (\mu_K'^*, \mu_N'^*)$. Because any convergent subsequence of $(\mu_K(\mathcal{M}_j), \mu_N(\mathcal{M}_j))$ converges to (μ_K^*, μ_N^*), and the space $\mathcal{P}([0,1])^2$ is compact, it follows that the whole sequence $(\mu_K(\mathcal{M}_j), \mu_N(\mathcal{M}_j))$ converges to (μ_K^*, μ_N^*). The desired claim then follows from the fact that convergence in Wasserstein-1 implies weak-* convergence (and on $[0,1]$, the bounded-first-moment condition required for this implication is automatic). □

B.5 Proof of Theorem 3.3

Theorem B.7 (same as Theorem 3.3). *Let χ^2 be the chi-squared divergence. In the setting of Theorem 3.2, suppose μ_N^* is supported on a finite set $\mathcal{X}$ and $\chi^2(\mu_K^*\|\mu_N^*) < \infty$. For any membership tester $\mathcal{M}$ for key size n and universe $[u]$ with query outputs restricted to $\mathcal{X}$, if we fix $p = \frac{n}{u}$ and let $n, u \to \infty$, then*

$$\frac{B(\mathcal{M})}{n} \geq \mathrm{KL}(\mu_K^*\|\mu_N^*) - \frac{\chi^2(\mu_K^*\|\mu_N^*)}{2\ln 2}\cdot p + o(p),$$

and this bound is achievable.

Proof. Let $\delta := \min_{x\in\mathcal{X}} \mu_N^*(x) > 0$. For $p \in (0,1)$, recall

$$R_p(\varepsilon_K, \varepsilon_N) = \min_{(\mu_K,\mu_N)\in\mathcal{C}} F_p(\mu_K, \mu_N), \qquad F_0(\mu_K, \mu_N) = \mathrm{KL}(\mu_K\|\mu_N),$$

where $\mathcal{C} = \mathcal{C}_K(\varepsilon_K) \times \mathcal{C}_N(\varepsilon_N) \cap \mathcal{P}(\mathcal{X})$ and $\mathcal{P}(\mathcal{X}) \subseteq \mathbb{R}^{\mathcal{X}}$ is the set of all probability distributions on $\mathcal{X}$.

Step 1: a fixed compact choice set for small p. Let $(\mu_K(p), \mu_N(p)) \in \mathcal{C}$ be any mapping from p to minimizers of F_p. As shown in the proof of Theorem 3.2, $\mu_N(p) \Rightarrow \mu_N^*$ as $p \to 0$, hence for all sufficiently small p we have $\mu_N(p)(x) \geq \delta/2$ for every $x \in \mathcal{X}$. Therefore, for some $p_0 > 0$ we may restrict attention to the compact set

$$\mathcal{C}' := \mathcal{C} \cap \Big\{(\mu_K, \mu_N) : \mu_N(x) \geq \delta/2\ \forall x \in \mathcal{X}\Big\},$$

and for all $p \in (0, p_0]$,

$$R_p(\varepsilon_K, \varepsilon_N) = \min_{(\mu_K,\mu_N)\in\mathcal{C}'} F_p(\mu_K, \mu_N),$$

since there is a minimizer $(\mu_K(p), \mu_N(p))$ that lies in $\mathcal{C}'$ for p sufficiently small.

Step 2: verify assumptions for envelope theorem. Define a maximization problem with value function

$$V(p) := \max_{(\mu_K,\mu_N)\in\mathcal{C}'} f((\mu_K, \mu_N), p), \qquad f((\mu_K, \mu_N), p) := -F_p(\mu_K, \mu_N),$$

so that $V(p) = -R_p(\varepsilon_K, \varepsilon_N)$ for all $p \in [0, p_0]$. Now, we verify the assumptions of Corollary 4 of Milgrom and Segal Milgrom and Segal (2002). We will use f_p to denote $\frac{\partial f}{\partial p}$ in the rest of the proof.

- *Compactness.* $\mathcal{C}' \subset \mathbb{R}^{2|\mathcal{X}|}$ is closed and contained in a product of simplices, hence compact.
- *Continuity of f.* Since $\mu_N(x) \geq \delta/2$ on $\mathcal{C}'$ and $\mu_p := p\mu_K + (1-p)\mu_N$ satisfies $\mu_p(x) \geq (1-p_0)\delta/2 > 0$ for $p \in [0, p_0]$, all KL terms appearing in the expression of F_p are finite and continuous; thus $(\mu_K, \mu_N, p) \mapsto f((\mu_K, \mu_N), p)$ is continuous on $\mathcal{C}' \times [0, p_0]$.
- *Continuity of f_p.* For $p > 0$, Lemma 3.5 gives

  $$\frac{\partial}{\partial p} F_p(\mu_K, \mu_N) = -\frac{\mathrm{KL}(\mu_N \| p\mu_K + (1-p)\mu_N)}{p^2}, \qquad (p > 0),$$

  hence

  $$f_p((\mu_K, \mu_N), p) = \frac{\mathrm{KL}(\mu_N \| \mu_p)}{p^2}, \qquad (p > 0).$$

  Fix $(\mu_K, \mu_N) \in \mathcal{C}'$ and write $h(x) := \frac{\mu_K(x)}{\mu_N(x)} - 1$. Then $h(x) \geq -1$ and, since $\mu_N(x) \geq \delta/2$ on $\mathcal{C}'$, we have a uniform bound

  $$M := \sup_{(\mu_K, \mu_N) \in \mathcal{C}'} \|h\|_\infty < \infty.$$

  Pick any constant $c \in (0,1)$ and let $p_1 := \min\{p_0, c/M\}$. Then for all $p \in [0, p_1]$, all $(\mu_K, \mu_N) \in \mathcal{C}'$, and all $x \in \mathcal{X}$, we have $|ph(x)| \leq c$. By Taylor's theorem for $\log(1+u)$ around $u = 0$ with a uniform remainder bound on the compact interval $u \in [-c, c]$, we obtain

  $$-\log(1+u) = -u + \frac{u^2}{2} + O(u^3) \qquad \text{uniformly for } |u| \leq c.$$

  Therefore,

  $$\mathrm{KL}_e(\mu_N \| \mu_p) = \sum_{x \in \mathcal{X}} \mu_N(x) \Big[-\log(1 + ph(x)) \Big] = \frac{p^2}{2} \sum_{x \in \mathcal{X}} \mu_N(x) h(x)^2 + O(p^3),$$

  where the $O(p^3)$ term is uniform over $(\mu_K, \mu_N) \in \mathcal{C}'$. Consequently,

  $$\mathrm{KL}(\mu_N \| \mu_p) = \frac{1}{\ln 2} \mathrm{KL}_e(\mu_N \| \mu_p) = \frac{p^2}{2 \ln 2} \chi^2(\mu_K \| \mu_N) + O(p^3),$$

  uniformly over $(\mu_K, \mu_N) \in \mathcal{C}'$. Hence f_p extends continuously to $p = 0$ by

  $$f_p((\mu_K, \mu_N), 0) := \frac{1}{2 \ln 2} \chi^2(\mu_K \| \mu_N),$$

  and f_p is continuous on $\mathcal{C}' \times [0, p_0]$.

Step 3: apply envelope theorem and conclude the first-order expansion. By Milgrom and Segal's Corollary 4(ii) Milgrom and Segal (2002), V is absolutely continuous and its right derivative satisfies

$$V'_+(p) = \max_{(\mu_K, \mu_N) \in \arg\max_{\mathcal{C}'} f(\cdot, p)} f_p((\mu_K, \mu_N), p) \quad \text{for } p \in [0, p_0).$$

Since the optimizer at $p = 0$ is unique, $\arg\max_{\mathcal{C}'} f(\cdot, 0) = \{(\mu_K^*, \mu_N^*)\}$ and thus

$$V'_+(0) = f_p((\mu_K^*, \mu_N^*), 0) = \frac{1}{2 \ln 2} \chi^2(\mu_K^* \| \mu_N^*).$$

Since $R_p = -V(p)$, it follows that as $p \to 0$,

$$R_p(\varepsilon_K, \varepsilon_N) = \mathrm{KL}(\mu_K^* \| \mu_N^*) - \frac{\chi^2(\mu_K^* \| \mu_N^*)}{2 \ln 2} p + o(p).$$

□

C Proofs for Section 4.1

Our proof is an application of Theorem 3.1. We solve the following convex optimization problem and show that μ_K^* and μ_N^* are the unique optimal solutions. We note that, since the base-e KL divergence is a constant multiple of the base-2 KL divergence, we assume KL divergence is base-e for convenience of analysis. The shape of optimal solutions is unaffected by this choice of base. In this appendix, we use X to denote the score random variable (i.e., $\hat{X}$ in the main text).

$$\min_{\mu_K,\mu_N\in\mathcal{P}([0,1])} \mathrm{KL}(\mu_K\|\mu_N), \quad \text{subject to} \quad \begin{cases} \mathbb{E}_{X\sim\mu_K}[-\ln X] \le \varepsilon_K, \\ \mathbb{E}_{X\sim\mu_N}[-\ln(1-X)] \le \varepsilon_N. \end{cases} \tag{6}$$

The Lagrangian is:

$$\mathcal{L}(\mu_K,\mu_N,\lambda_K,\lambda_N) = \mathrm{KL}(\mu_K\|\mu_N) + \lambda_K\big(\mathop{\mathbb{E}}_{\mu_K}[-\ln X] - \varepsilon_K\big) + \lambda_N\big(\mathop{\mathbb{E}}_{\mu_N}[-\ln(1-X)] - \varepsilon_N\big).$$

Before we proceed, we introduce the following technical lemmas for optimization over measure spaces.

C.1 Technical preliminaries

To analyze the optimality condition for convex functionals over the space of measures, we use Gâteaux derivatives.

Definition C.1 (Gâteaux Derivative)**.** Let $J : \mathcal{P}([0,1]) \to \mathbb{R}$ be a linear functional. The Gâteaux derivative of J at $Q \in \mathcal{P}([0,1])$ in the direction $R - Q$, where $R \in \mathcal{P}([0,1])$, is defined as:

$$\delta J(Q; R-Q) = \lim_{\eta\to 0^+} \frac{J((1-\eta)Q + \eta R) - J(Q)}{\eta},$$

provided the limit exists.

If J is a convex functional, the Gâteaux derivative allows us to state the necessary and sufficient conditions for global optimality.

Theorem C.2 (First-Order Optimality Condition; see e.g. Luenberger (1997))**.** *If $J : \mathcal{P}([0,1]) \to \mathbb{R}$ is convex and Gâteaux differentiable, then $Q^* \in \mathcal{P}([0,1])$ minimizes J if and only if $\delta J(Q^*; R-Q^*) \ge 0$ for all $R \in \mathcal{P}([0,1])$.*

When the Gâteaux derivative can be represented in an integral form (and in particular linear in $R - Q$), this optimality condition translates into a structural property regarding the support of the optimal measure.

Lemma C.3 (KKT Support Condition)**.** *Suppose the Gâteaux derivative of a convex functional J at Q can be represented as*

$$\delta J(Q; R-Q) = \int_0^1 g_Q(x)dR(x) - \int_0^1 g_Q(x)dQ(x) = \mathop{\mathbb{E}}_R[g_Q(X)] - \mathop{\mathbb{E}}_Q[g_Q(X)],$$

for some measurable function $g_Q(x)$ (which may depend on Q). Then Q^* minimizes J if and only if Q^* is supported on the set of global minima of the function $g_{Q^*}(x)$.

That is, $x \in supp(Q^*) \implies g_{Q^*}(x) = \inf_{y\in[0,1]} g_{Q^*}(y)$.

Proof. By Theorem C.2, Q^* is optimal iff $\mathbb{E}_R[g_{Q^*}(X)] \geq \mathbb{E}_{Q^*}[g_{Q^*}(X)]$ for all R. Let $K^* = \mathbb{E}_{Q^*}[g_{Q^*}(X)]$. If we take $R = \delta_y$ for any $y \in [0,1]$, we get $g_{Q^*}(y) \geq K^*$. Thus K^* is the global minimum value of $g_{Q^*}(x)$. Since Q^* is a probability measure, the equality $\mathbb{E}_{Q^*}[g_{Q^*}(X)] = K^*$ can only hold if Q^* is supported entirely on the set where $g_{Q^*}(x) = K^*$. □

We also recall the following standard result regarding the minimization of KL divergence subject to linear constraints.

Lemma C.4 (Donsker–Varadhan variational formula)**.** *Suppose $Q \in \mathcal{P}([0,1])$, and let h be a Q-measurable real function such that $\mathbb{E}_Q[e^{-h(X)}] < \infty$. Then,*

$$-\ln \mathop{\mathbb{E}}_{X\sim Q}[e^{-h(X)}] = \inf_{P\in\mathcal{P}([0,1])} \Big\{ \mathrm{KL}(P\|Q) + \mathop{\mathbb{E}}_{P}[h(X)] \Big\}.$$

The infimum is attained when P has the Radon-Nikodym derivative $\frac{dP}{dQ}(x) \propto e^{-h(x)}$.

C.2 Solving the optimization problem

Step 1: stationary condition for μ_K. Applying the variational formula Theorem C.4 with $h(x) = -\lambda_K \ln X$, the first two terms are minimized when the following inf is attained:

$$\inf_{\mu_K} \Big\{ \mathrm{KL}(\mu_K\|\mu_N) + \mathop{\mathbb{E}}_{\mu_K}[\lambda_K(-\ln X)] \Big\}.$$

By Theorem C.4, this is when

$$\frac{d\mu_K}{d\mu_N}(x) \propto e^{-h(x)} = x^{\lambda_K}. \tag{7}$$

Let $C(\mu_N) = \mathbb{E}_{\mu_N}[X^{\lambda_K}]$ be the normalization constant. The value of the infimum is $-\ln C(\mu_N)$.

Step 2: stationary condition for μ_N. Plugging the optimized μ_K back into the Lagrangian, we obtain the dual function which we seek to minimize over μ_N:

$$J(\mu_N) = -\ln \mathop{\mathbb{E}}_{\mu_N}[X^{\lambda_K}] + \lambda_N \mathop{\mathbb{E}}_{\mu_N}[-\ln(1-X)] - \lambda_K\varepsilon_K - \lambda_N\varepsilon_N.$$

$J(\mu_N)$ is a convex functional of μ_N. We use Gâteaux derivatives $\delta J(\mu_N^*; R - \mu_N^*)$ to find the optimality condition.

The derivative of the first term $J_1(\mu_N) = -\ln \mathbb{E}_{\mu_N}[X^{\lambda_K}]$ is:

$$\delta J_1(\mu_N; R-\mu_N) = -\frac{\mathbb{E}_R[X^{\lambda_K}] - \mathbb{E}_{\mu_N}[X^{\lambda_K}]}{\mathbb{E}_{\mu_N}[X^{\lambda_K}]} = -\frac{\mathbb{E}_R[X^{\lambda_K}] - \mathbb{E}_{\mu_N}[X^{\lambda_K}]}{C(\mu_N)}.$$

The derivative of the second (linear) term $J_2(\mu_N)$ is:

$$\delta J_2(\mu_N; R-\mu_N) = \lambda_N\big(\mathop{\mathbb{E}}_{R}[-\ln(1-X)] - \mathop{\mathbb{E}}_{\mu_N}[-\ln(1-X)]\big).$$

Combining the terms, $\delta J = \delta J_1 + \delta J_2$ can be represented in the integral form, as in Theorem C.3, by the following function $g_{\mu_N}(x)$:

$$g_{\mu_N}(x) = -\frac{x^{\lambda_K}}{C(\mu_N)} - \lambda_N \ln(1-x). \tag{8}$$

By the KKT Support Condition (Theorem C.3), the optimal distribution μ_N^* must be supported on the set of global minima of $g_{\mu_N^*}(x)$.

Step 3: solving for support and probability mass. Let $g := g_{\mu_N^*}$ and $C^* := C(\mu_N^*)$. To analyze the minima of g, we now establish a crucial property of λ_K.

Lemma C.5. *In the non-trivial regime ($e^{-\varepsilon_K} + e^{-\varepsilon_N} > 1$), the optimal Lagrange multiplier satisfies $\lambda_K > 1$.*

Proof. Consider the derivatives of $g(x)$:

$$g'(x) = -\frac{\lambda_K x^{\lambda_K - 1}}{C^*} + \frac{\lambda_N}{1-x}, \quad g''(x) = -\frac{\lambda_K(\lambda_K - 1)x^{\lambda_K - 2}}{C^*} + \frac{\lambda_N}{(1-x)^2}.$$

Note that $C^* > 0$, otherwise we must have $\mu_N^* = \delta_0$. But if μ_N^* collapses to a point mass, then we either have $\mu_K^* = \mu_N^*$ (infeasible solution) or $\mathrm{KL}(\mu_K^* \| \mu_N^*) = \infty$. We will try to avoid this and solve for a μ_N^* with non-singleton support.

Suppose $\lambda_K \leq 1$. If $\lambda_K = 1$, $g''(x) > 0$. If $0 < \lambda_K < 1$, then $\lambda_K - 1 < 0$, so the first term is positive, and $g''(x) > 0$. In both cases, $g(x)$ is strictly convex and has a unique global minimum x^*. Thus, $\mu_N^* = \delta_{x^*}$, and hence $\mu_K^* = \delta_{x^*}$ by the previous result on $\frac{d\mu_K^*}{d\mu_N^*}(x)$. This implies the KL divergence objective is zero, contradicting the assumption of the non-trivial regime. □

Knowing $\lambda_K > 1$, we analyze the shape of $g(x)$. Since $\lambda_K - 1 > 0$, $x^{\lambda_K - 1} \to 0$ as $x \to 0$, so $g'(0) = \lambda_N > 0$. It follows that g is increasing both as $x \to 0$ and $x \to 1$. We will show that there is at most one local minimum at some $x^* \in (0, 1)$, so 0 and x^* must both be global minima, with $g(x^*) = g(0) = 0$.

Consider stationary condition $g'(x) = -\frac{\lambda_K x^{\lambda_K - 1}}{C^*} + \frac{\lambda_N}{1-x} = 0$. Note that the first term is negative, the second term is positive, and $g'(x) > 0$ iff $\frac{\lambda_N}{1-x} > \frac{\lambda_K x^{\lambda_K - 1}}{C^*}$, which is true iff $C^* \frac{\lambda_N}{\lambda_K} > x^{\lambda_K - 1}(1-x) =: h(x)$. Clearly $h(0) = h(1) = 0$, corresponding to $g'(0)$ being positive at these endpoints. Differentiating h, we have:

$$h'(x) = x^{\lambda_K - 2}(\lambda_K - 1 - \lambda_K x).$$

Since $x^{\lambda_K - 2}$ is always positive on $(0, 1)$, this derivative only changes sign once from positive to negative, and therefore the equation $C^* \frac{\lambda_N}{\lambda_K} = h(x)$ has at most two solutions in $(0, 1)$, in which case $h(x)$ will start from zero, increase to a local maximum, and then drop back to 0 at $x = 1$. Hence, there are at most two points where $g'(x) = 0$, the first one being a local maximum and the second a local minimum, which we call x^*.

In fact, if the optimal KL divergence were to be finite, the global minimum of $g = 0$ must be attained at both $x = 0$ and x^*:

1. If the minimum is uniquely at $x = 0$. Then $\mu_N^* = \delta_0$. This implies $C^* = 0^{\lambda_K} = 0$ (since $\lambda_K > 1$). This leads to $J(\mu_N^*) = \infty$, which is not optimal.

2. If the minimum is uniquely at x^*. Then $\mu_N^* = \delta_{x^*}$. This implies $\mu_K^* = \mu_N^*$ and $\mathrm{KL} = 0$, a contradiction.

We conclude that μ_N^* is a two-point distribution:

$$\mu_N^* = (1 - q^*)\delta_0 + q^* \delta_{x^*}.$$

We can now determine μ_K^* using the relative density in (7): because $\frac{d\mu_K^*}{d\mu_N^*}(0) = 0^{\lambda_K} = 0$, it follows that it is a point mass $\mu_K^* = \delta_{x^*}$.

Now we use the tight constraints to determine x^* and q^* for μ_N^*.

1. Constraint on μ_K^*: $\mathbb{E}_{\mu_K^*}[-\ln X] = \varepsilon_K \implies -\ln(x^*) = \varepsilon_K \implies x^* = e^{-\varepsilon_K}$.
2. Constraint on μ_N^*: $\mathbb{E}_{\mu_N^*}[-\ln(1-X)] = \varepsilon_N$.

$$(1-q^*)(-\ln 1) + q^*(-\ln(1-x^*)) = \varepsilon_N \implies q^* = \frac{\varepsilon_N}{-\ln(1-x^*)}.$$

The condition $e^{-\varepsilon_K} + e^{-\varepsilon_N} > 1$ ensures that $\varepsilon_N < -\ln(1-e^{-\varepsilon_K})$, so $0 < q^* < 1$.

Step 4: verifying KKT conditions. Note that we calculate $C^* = \mathbb{E}_{\mu_N^*}[X^{\lambda_K}] = q^*(x^*)^{\lambda_K}$ (since $\lambda_K > 1$).

Condition 1: $g(x^*) = 0$.

$$g(x^*) = -\frac{(x^*)^{\lambda_K}}{C^*} - \lambda_N \ln(1-x^*) = -\frac{1}{q^*} - \lambda_N \ln(1-x^*) = 0.$$

This yields $\lambda_N = \frac{-1}{q^* \ln(1-x^*)}$. Since $q^* > 0$ and $\ln(1-x^*) < 0$, we have $\lambda_N > 0$.

Condition 2: $g'(x^*) = 0$.

$$g'(x^*) = -\frac{\lambda_K (x^*)^{\lambda_K - 1}}{C^*} + \frac{\lambda_N}{1-x^*} = 0.$$

Rearranging and substituting C^*:

$$\lambda_K = \frac{\lambda_N C^*}{(1-x^*)(x^*)^{\lambda_K-1}} = \frac{\lambda_N q^* (x^*)^{\lambda_K}}{(1-x^*)(x^*)^{\lambda_K-1}} = \frac{\lambda_N q^* x^*}{1-x^*}.$$

Substituting the expression for λ_N:

$$\lambda_K = \left(\frac{-1}{q^* \ln(1-x^*)}\right) \frac{q^* x^*}{1-x^*} = \frac{-x^*}{(1-x^*)\ln(1-x^*)}.$$

We verify that $\lambda_K > 1$. Let $y = 1 - x^* \in (0,1)$. We need to show $\frac{-(1-y)}{y \ln y} > 1$. Since $y \ln y < 0$, this is equivalent to $-(1-y) < y \ln y$, or $1 - 1/y < \ln y$. Consider the function $h(y) = \ln y - (1 - 1/y)$. Its derivative is $h'(y) = 1/y - 1/y^2 = (y-1)/y^2$. On $(0,1)$, $h'(y) < 0$. Since $\lim_{y \to 1^-} h(y) = 0$, we have $h(y) > 0$ for $y \in (0,1)$. Thus, $\lambda_K > 1$.

Since $\lambda_K > 1$, the shape analysis in Step 3 holds: g has exactly one local maximum and one local minimum in $(0,1)$, confirming that $\{0, x^*\}$ are indeed the global minima of $g(x)$. The KKT conditions are fully satisfied, and therefore μ_K^* and μ_N^* are the global optimum.

D Proofs for Section 4.2

D.1 Binary-output reduction via data processing

We now show that, under the linear error metrics $d^K(\hat{x}) = 1 - \hat{x}$ and $d^N(\hat{x}) = \hat{x}$, we can restrict to binary outputs without loss of optimality.

Lemma D.1 (Binary-output reduction via data processing)**.** *Let (μ_K, μ_N) be any feasible pair of output distributions supported on $[0,1]$. Define the Markov kernel T from $[0,1]$ to $\{0,1\}$ by*

$$T(1 \mid t) = t, \qquad T(0 \mid t) = 1 - t.$$

Let $\bar{\mu}_K := \mu_K T$ and $\bar{\mu}_N := \mu_N T$ be the induced distributions on $\{0,1\}$. Then:

1. (Constraints preserved) $\mathbb{E}_{\bar{\mu}_K}[1-\hat{X}] = \mathbb{E}_{\mu_K}[1-\hat{X}]$ *and* $\mathbb{E}_{\bar{\mu}_N}[\hat{X}] = \mathbb{E}_{\mu_N}[\hat{X}]$.

2. (Objective non-increasing) For every $p \in (0,1)$,

$$F_p(\bar{\mu}_K, \bar{\mu}_N) \;\le\; F_p(\mu_K, \mu_N).$$

Consequently, in the definition of $R_p(\varepsilon_K, \varepsilon_N)$ *we may restrict to* $\hat{x} \in \{0,1\}$*, and the optimal output distributions are Bernoulli.*

Proof sketch. The first part follows from linearity: under T, the binary output $Y \in \{0,1\}$ satisfies $\mathbb{E}[Y \mid \hat{X} = t] = t$, hence $\mathbb{E}[Y] = \mathbb{E}[\hat{X}]$ and $\mathbb{E}[1-Y] = \mathbb{E}[1-\hat{X}]$. For the second part, note that the kernel commutes with mixtures: $\bar{\mu}_p = (p\mu_K + (1-p)\mu_N)T = p\bar{\mu}_K + (1-p)\bar{\mu}_N$. By the data-processing (contraction) inequality for KL under a Markov kernel,

$$\mathrm{KL}(\mu_K T \| \mu_p T) \le \mathrm{KL}(\mu_K \| \mu_p), \qquad \mathrm{KL}(\mu_N T \| \mu_p T) \le \mathrm{KL}(\mu_N \| \mu_p),$$

and plugging into the definition of F_p gives the claim. □

D.2 Solving the convex optimization

By Theorem D.1, it suffices to consider binary outputs $\hat{X} \in \{0,1\}$. Again, we assume the KL divergence is base-e for convenience of analysis; the shape of optimal solutions is unaffected by this choice of base. Hence μ_K and μ_N are Bernoulli distributions, which we parameterize by

$$\mu_K = \mathrm{Bern}(a), \qquad \mu_N = \mathrm{Bern}(b),$$

where $a = \Pr(\hat{X} = 1 \mid X \in \mathcal{K})$ and $b = \Pr(\hat{X} = 1 \mid X \notin \mathcal{K})$. This reduction also allows us to apply Theorem 3.3, which provides the desired first-order expansion of the memory lower bound w.r.t. p, around $p = 0$. It now suffices to show that the optimal distribution is given by $a = 1 - \varepsilon_K$ and $b = \varepsilon_N$.

The KL divergence minimization problem for Bernoulli distributions reduces to the two-variable convex program

$$\min_{a,b \in [0,1]} \; \mathrm{KL}\big(\mathrm{Bern}(a) \,\|\, \mathrm{Bern}(b)\big) \quad \text{s.t.} \quad a \ge 1 - \varepsilon_K, \;\; b \le \varepsilon_N. \tag{9}$$

We now show that the KL divergence objective is strictly increasing in a and strictly decreasing in b over the feasible region. Recall the closed form

$$\mathrm{KL}\big(\mathrm{Bern}(a) \,\|\, \mathrm{Bern}(b)\big) = a \ln \frac{a}{b} + (1-a) \ln \frac{1-a}{1-b}.$$

For fixed $b \in (0,1)$, differentiating w.r.t. a gives

$$\frac{\partial}{\partial a} \mathrm{KL}(\mathrm{Bern}(a) \| \mathrm{Bern}(b)) = \ln \frac{a(1-b)}{(1-a)b}.$$

In the non-trivial regime $1 - \varepsilon_K > \varepsilon_N$, the feasible set satisfies $a \ge 1 - \varepsilon_K > \varepsilon_N \ge b$, hence $a > b$ throughout the feasible region. Therefore

$$\ln \frac{a(1-b)}{(1-a)b} > 0,$$

so the objective is *strictly increasing* in a over the feasible region. Thus the minimum is attained at

$$a^* = 1 - \varepsilon_K.$$

Similarly, for fixed $a \in (0,1)$, differentiating w.r.t. b gives

$$\frac{\partial}{\partial b}\mathrm{KL}(\mathrm{Bern}(a)\|\mathrm{Bern}(b)) = \frac{b-a}{b(1-b)}.$$

Since $a > b$ on the feasible region, we have $\partial/\partial b < 0$, so the objective is *strictly decreasing* in b over the feasible region. Hence the minimum is attained at the largest feasible b, namely

$$b^* = \varepsilon_N.$$

Combining the two monotonicity statements yields the unique optimizer of (9):

$$\mu_K^* = \mathrm{Bern}(1-\varepsilon_K), \qquad \mu_N^* = \mathrm{Bern}(\varepsilon_N).$$

D.3 A hash-based memory-optimal two-sided filter

We now show that the filter lower bound can be achieved by a hash-based construction, which, like Bloom filters and others, is universe-agnostic, in the sense that the memory usage does not depend on the universe size u. Our construction is inspired by the optimal one-sided filters introduced in Porat (2009) and Dietzfelbinger and Pagh (2008), based on solving random linear equations over a finite field. We also note that this construction is not efficient in practice.

Theorem D.2. *Assume $\varepsilon_N = 1/q$ for some prime power q, and fix any $\varepsilon_K \in [0,1)$. There exists a hash-based two-sided filter scheme (in the random-oracle model) such that as $n \to \infty$, when initialized on any key set $\mathcal{K} \subseteq \mathcal{U}$ with $|\mathcal{K}| = n$, it uses*

$$\mathrm{KL}\Big(\mathrm{Bern}(1-\varepsilon_K) \;\Big\|\; \mathrm{Bern}(\varepsilon_N)\Big) + o(1) \quad \textit{bits of space per key}$$

and, with probability $1 - o(1)$, the resulting filter satisfies FNR $\le \varepsilon_K$ *on keys and* FPR $= \varepsilon_N$ *on every non-key. In particular, the guarantee is uniform over all universe sizes $u \ge n$.*

Proof. Let $\mathbb{F}_q$ be the finite field of size $q = 1/\varepsilon_N$. WLOG, let $\mathcal{U} = [u]$. We assume access to a vector-valued random-oracle hash function

$$h : \mathcal{U} \to \mathbb{F}_q^m, \qquad h(i) = (h(i)_1, \ldots, h(i)_m),$$

where m is a parameter to be determined at the end, and the coordinates $h(i)_j$ are i.i.d. uniform over $\mathbb{F}_q$ and independent across distinct i's.

For $y \in \mathbb{F}_q^m$, consider the linear functions defined by $h(i)$'s:

$$\langle h(i), y\rangle \;:=\; \sum_{j=1}^{m} h(i)_j\, y_j \;\in\; \mathbb{F}_q.$$

Consider the system of equations in the unknown $y \in \mathbb{F}_q^m$:

$$\langle h(i), y\rangle = 0, \qquad i \in \mathcal{K}, \tag{10}$$

and restrict to nonzero solutions $y \neq 0$.

Initialization. Given $(\varepsilon_K, \varepsilon_N)$ and $\mathcal{K}$, the filter calculates the corresponding m, sends each $i \in \mathcal{K}$ through the random oracle to obtain $h(i)$'s, and searches for a nonzero vector $y \in \mathbb{F}_q^m$ that satisfies at least $(1-\varepsilon_K)n$ equations in (10). If such a y exists, the filter stores a binary encoding of y. The construction *succeeds* if a vector y meeting this requirement exists.

The memory usage is $m \log q + O(1)$ bits, where log is base 2.

Query. On input $i' \in \mathcal{U}$, the filter gets $h(i') \in \mathbb{F}_q^m$ from the oracle and outputs 1 iff $\langle h(i'), y \rangle = 0$ (and outputs 0 otherwise).

Error guarantees. If initialization succeeds, then at least $(1-\varepsilon_K)n$ keys satisfy $\langle h(i), y \rangle = 0$. Thus for a uniform random key $i' \sim \mathrm{Unif}(\mathcal{K})$ we have

$$\mathbb{P}[\mathsf{Query}(i') = 0] \;\leq\; \varepsilon_K.$$

which satisfies the FNR constraint if we convert it into a permutation-invariant membership tester via Remark 2.2.

For false positives, fix any non-key $i' \in \mathcal{U} \setminus \mathcal{K}$. Since y is a function of $\{h(i)\}_{i \in \mathcal{K}}$ only, and $h(i')$ is independent of $\{h(i)\}_{i \in \mathcal{K}}$, we may condition on y and treat it as fixed. The next lemma implies

$$\mathbb{P}[\mathsf{Query}(i') = 1 \mid y] \;=\; \frac{1}{q} \;=\; \varepsilon_N,$$

hence $\mathrm{FPR} = \varepsilon_N$.

Lemma D.3. *For any fixed $y \in \mathbb{F}_q^m$ with $y \neq 0$, if $H_1, \ldots, H_m$ are drawn i.i.d. from $\mathrm{Unif}(\mathbb{F}_q)$, then*

$$\mathbb{P}\left[\sum_{j=1}^{m} y_j H_j = 0\right] \;=\; \frac{1}{q}.$$

Proof. WLOG, suppose $y_1 \neq 0$. For any $c \in \mathbb{F}_q$,

$$\mathbb{P}\left[\sum_{j=1}^{m} y_j H_j = c\right] = \mathbb{P}\left[H_1 = y_1^{-1}\left(c - \sum_{j=2}^{m} y_j H_j\right)\right] = \frac{1}{q},$$

since H_1 is uniform and independent of $(H_2, \ldots, H_m)$. □

Choice of m and space bound. Let

$$D \;:=\; \mathrm{KL}\Big(\mathrm{Bern}(1-\varepsilon_K) \;\|\; \mathrm{Bern}(\varepsilon_N)\Big).$$

Choose any sequence $t_n \to \infty$ with $t_n = o(n)$ (e.g. $t_n = n^{2/3}$), and set

$$m \;:=\; \left\lceil \frac{nD + t_n}{\log q} \right\rceil. \tag{11}$$

Then the memory is

$$m \log q \;=\; nD + t_n + O(1),$$

i.e. $D + o(1)$ bits per key.

It remains to show that initialization succeeds with probability $1 - o(1)$ (hence at least 0.9 for all large n).

Second moment method for success probability. Let $Y := \mathbb{F}_q^m \setminus \{0\}$, so $|Y| = q^m - 1$. For each $y \in Y$, define

$$N_y := \mathbb{1}\left\{\#\{i \in \mathcal{K} : \langle h(i), y\rangle = 0\} \geq (1 - \varepsilon_K)n\right\}, \qquad Z \;:=\; \sum_{y \in Y} N_y.$$

Thus $Z \geq 1$ iff there exists a nonzero y satisfying at least $(1 - \varepsilon_K)n$ equations, i.e. initialization succeeds. Let $p_n = \mathbb{P}[N_y = 1]$, then $\mathbb{E}[Z] = (q^m - 1)p_n$.

Fix any $y \neq 0$. For each key $i \in \mathcal{K}$, by Lemma D.3 and independence across i, the indicators $\mathbb{1}\{\langle h(i), y\rangle = 0\}$ are i.i.d. Bern(ε_N). Therefore, by standard large-deviation bounds, for each y,

$$p_n = 2^{-nD+o(n)}. \tag{12}$$

Now we bound the second moment $\mathbb{E}[Z^2]$:

$$\mathbb{E}[Z^2] \;=\; \sum_{y \in Y} \mathbb{E}[N_y] \;+\; \sum_{\substack{y, y' \in Y \\ y \neq y'}} \mathbb{E}[N_y N_{y'}].$$

Consider the second term for fixed $y, y' \in Y, y \neq y'$. If y' is a nonzero scalar multiple of y, then for each $i \in \mathcal{K}$, $\langle h(i), y'\rangle = 0$ iff $\langle h(i), y\rangle = 0$, so $N_{y'} = N_y$ and $\mathbb{E}[N_y N_{y'}] = \mathbb{E}[N_y] = p_n$. Otherwise y, y' are linearly independent, and the mapping

$$h(i) \mapsto \big(\langle h(i), y\rangle,\ \langle h(i), y'\rangle\big) \in \mathbb{F}_q^2$$

is a linear surjection. Since $h(i)$ is uniform, the events $A_i := \{\langle h(i), y\rangle = 0\}$ and $B_i := \{\langle h(i), y'\rangle = 0\}$ are independent with $\Pr[A_i] = \Pr[B_i] = 1/q$ and $\Pr[A_i \cap B_i] = 1/q^2$. Independence across i then implies that $\{A_i\}_{i=1}^n$ is independent of $\{B_i\}_{i=1}^n$, and thus X_y and $X_{y'}$ are independent: $\mathbb{E}[X_y X_{y'}] = p_n^2$.

Now we count the number of pairs (y, y') of each type. For each y there are exactly $(q-2)$ distinct nonzero multiples $y' \in \langle y\rangle \setminus \{y\}$, and $|Y| - (q-1) = q^m - q$ choices of y' not in the one-dimensional subspace $\langle y\rangle$. Therefore,

$$\begin{aligned}\mathbb{E}[Z^2] &\leq (q^m - 1)p_n \;+\; (q^m - 1)(q-2)p_n \;+\; (q^m - 1)(q^m - q)p_n^2 \\ &= (q^m - 1)\Big((q-1)p_n + (q^m - q)p_n^2\Big).\end{aligned}$$

By Paley-Zygmund,

$$\Pr[Z \geq 1] \;\geq\; \frac{\mathbb{E}[Z]^2}{\mathbb{E}[Z^2]} \;\geq\; \frac{(q^m - 1)p_n}{(q-1) + (q^m - q)p_n}.$$

This lower bound goes to 1 as $n \to \infty$ since

$$q^m p_n \;=\; 2^{m \log q} \cdot 2^{-nD+o(n)} \;=\; 2^{t_n + o(n)} \;\to\; \infty,$$

and both the numerator and denominator are dominated by this term. □

E Experiment Details

We present a more detailed setup of the experiments in Section 4.3.

We optimize the models using AdamW with $\beta_1 = 0$, $\beta_2 = 0.999$, and base learning rate 3×10^{-4} with 1000 warm-up steps and cosine decay. The choice of $\beta_1 = 0$ (so the optimizer is similar to RMSprop) is for better optimization performance. Each batch contains all n positive samples (the

Table 1: Reproducibility details for the main experiment.

Category	**Setting**
Data	Universe $\mathcal{U}$: alphabet size $\lvert\Sigma\rvert = 26$, length 15, $\lvert\mathcal{U}\rvert = 26^{15}$. Facts $\mathcal{K}$: $\lvert\mathcal{K}\rvert = 15145$, sampled uniformly without replacement with seed 42. Negatives: per step sample size 15145, distribution $\mathrm{Unif}(\mathcal{U} \setminus \mathcal{K})$.
Tokenization	Tokenization: char-level, vocab size $V = 26$. Positional encoding: sinusoidal (fixed).
Model	Architecture: Transformer. 2 Layers, $d_{\text{model}} = 18/24/36$, heads $h = 3/4/6$, FFN dim $d_{\text{ff}} = 72/96/144$. Activation: GeLU; pre-LayerNorm; no dropout. Output head: Mean Pooling → Layer norm → Linear→Sigmoid producing $\hat{x}(i) \in (0, 1)$. #Trainable parameters: 8767 / 15145 / 33085. Precision: fp16
Objective	Loss: weighted BCE with weights $\lambda_F/(\lambda_F + 1)$, $1/(\lambda_F + 1)$. Batch composition: all positives + fresh negatives.
Optimization	Optimizer: AdamW with $(\beta_1, \beta_2) = (0, 0.999)$ and weight decay 0.01. Learning rate: base LR 3×10^{-4}; 1000 warm-up steps; cosine decay. Training length: 30,000 epochs. Grad clip: 1. Initialization: PyTorch default.
Evaluation	Facts eval: all n facts. Non-facts eval: sample size $200k$ from $\mathrm{Unif}(\mathcal{U} \setminus \mathcal{K})$. Histogram/KL is based on the discretized output distribution with 50 bins.

full set $\mathcal{K}$) and n fresh negatives sampled uniformly from $\mathcal{U} \setminus \mathcal{K}$. The positive and negative samples are evaluated with a custom weight defined by λ_F as follows:

$$\mathcal{L} = \frac{\lambda_F}{\lambda_F + 1} \mathop{\mathbb{E}}_{i \sim \mathrm{Unif}(\mathcal{K})} \big[- \ln \hat{x}(i) \big] \quad + \quad \frac{1}{\lambda_F + 1} \mathop{\mathbb{E}}_{i \sim \mathrm{Unif}(\mathcal{U} \setminus \mathcal{K})} \big[- \ln(1 - \hat{x}(i)) \big].$$

We set the seed to be 42 for all our experiments, and all models are trained for 30000 epochs, at which point all losses converge to stable values.

We consider three different model sizes, corresponding to 0.58 / 1 / 2.18 parameters per fact. For each model size, we train a model with $\lambda_F \in \{0.25, 1, 4, 8\}$ to observe the trade-off between the two types of errors, given a fixed memory budget. In Figure 1, we report the confidence distributions of training the 1 parameter-per-fact model. The other two sizes are reported in Figure 3 and Figure 4, respectively. We note that across different model sizes and λ_F, the non-fact distribution consistently exhibits the heavy tail of hallucinations, whenever the fact distribution is sufficiently concentrated.

In Table 1, we report the full experimental setup. Our implementation code will be released publicly.

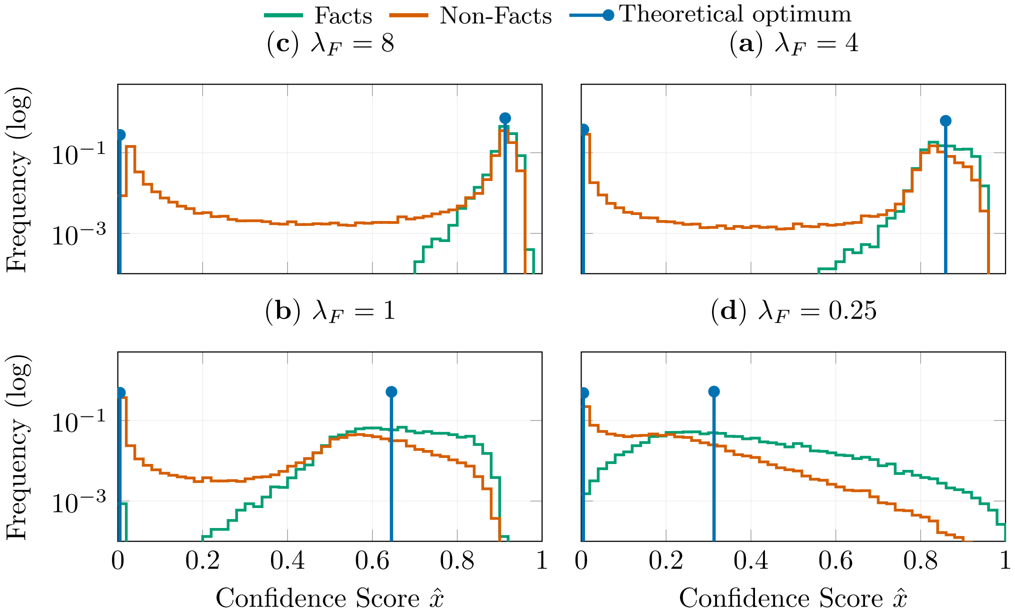


Figure 3: Output distributions with 15145 facts and 8767 parameters.

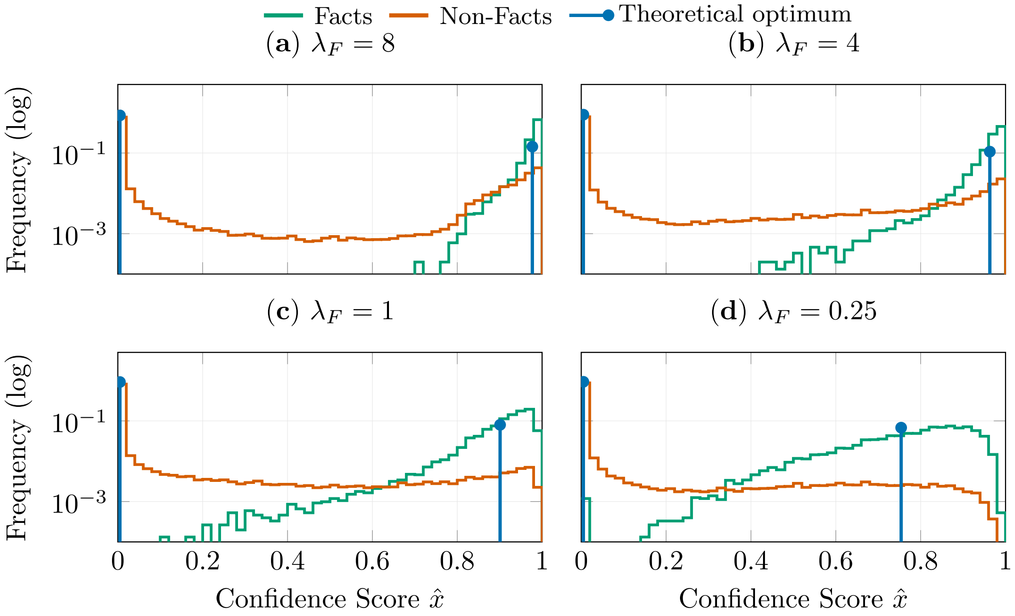


Figure 4: Output distributions with 15145 facts and 33085 parameters.