On the Query Complexity of Verifier-Assisted Language Generation



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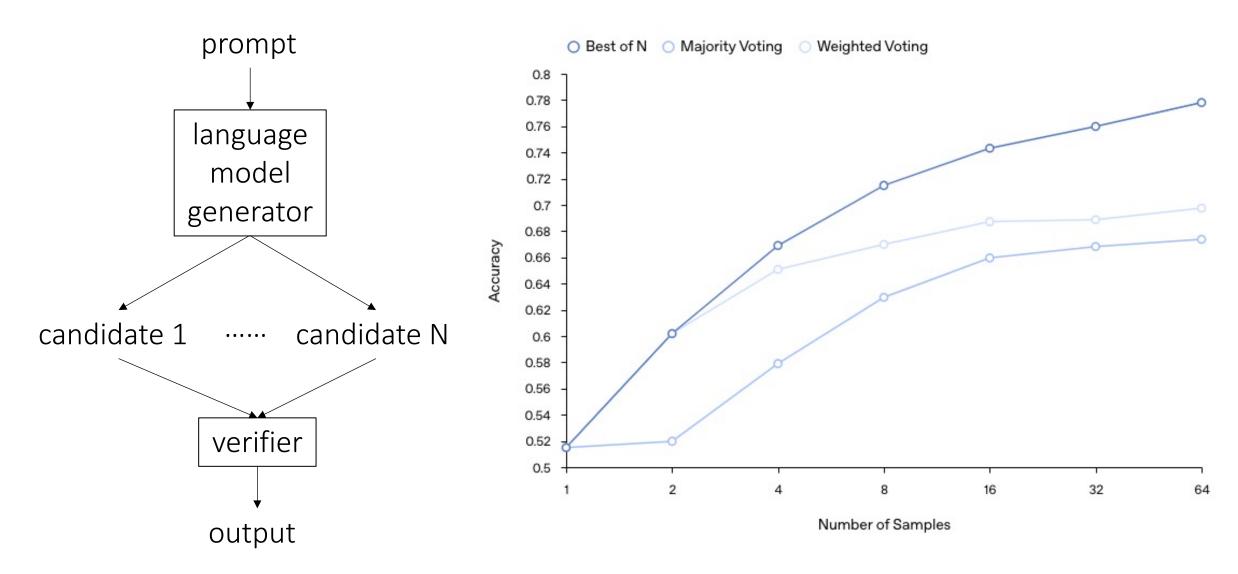


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Background: verifier-assisted language generation



Overview of our results

Key takeaway: constrained language generation without a verifier is provably hard, but verifiers (which check partial outputs) can help.

Constrained generation task

Information-theoretic lower bound

Computational lower bound

Theoretical framework

Empirical study

Setup: constrained generation task

Autoregressive generator oracle \mathcal{O} : given string $s \in \Sigma^*$, predict and sample from next-token distribution $\mathcal{O}(s): \Sigma \to \mathbb{R}_+$.

Constrained generation task (Σ, A, \mathcal{O}) : find $s \in A$ s.t. $P_{\mathcal{O}}(s) > 0$. If no such s exists, return FAIL.

Oracle complexity: expected number of calls to \mathcal{O} to solve the constrained generation task

- Σ: vocabulary
- O: autoregressive generator oracle
- $P_{\mathcal{O}}: \Sigma^* \to \mathbb{R}_+$:
 distribution over strings predicted by \mathcal{O}
- $A \subset \Sigma^*$: constraint set

Constrained generation is hard without a verifier

Theorem 1 (information-theoretic lower bound, informal):

There exists a constrained generation task for which any (possibly randomized) algorithm has (expected) oracle complexity at least exponential in seq length.

Theorem 2 (computational lower bound, informal):

There exists a constrained generation task which is NP-hard.

Incorporating verifiers into constrained generation

Verifier $V: \Sigma^* \to \{0,1\}$: $\forall s \in \Sigma^*$, V(s) = 1 if and only if $\exists s' \in \Sigma^*$ s.t. $s \circ s' \in A$.

Rejection sampling: repeatedly generating complete strings s according to P_0 , until V(s) = 1.

Tokenwise rejection sampling: given prefix s, sample next token $t \sim \mathcal{O}(s)$, until $V(s \circ t) = 1$, then proceed to next token.

• Backtrack: additionally, whenever $V(s \circ t) = 0$, resample the last B positions of s (allowed $\leq Q$ times)

- Σ: vocabulary
- *O*: autoregressive generator oracle
- $P_{\mathcal{O}}: \Sigma^* \to \mathbb{R}_+$:
 distribution over
 strings predicted
 by \mathcal{O}
- $A \subset \Sigma^*$: constraint set
- *V*: verifier
- •: concatenation of strings
- Q: backtrack quota
- B: stride

Tokenwise rejection sampling is efficient

Proposition 1 (informal): there exists a constrained generation task s.t.

- The expected oracle complexity of rejection sampling is exponential in seq length, and
- The expected oracle complexity of tokenwise rejection sampling is linear in seq length.

- Σ: vocabulary
- O: autoregressive generator oracle
- $P_{\mathcal{O}}: \Sigma^* \to \mathbb{R}_+$:
 distribution over
 strings predicted
 by \mathcal{O}
- $A \subset \Sigma^*$: constraint set
- *V*: verifier
- •: concatenation of strings

Experiment 1: generating strings in Dyck grammar

- Constrained generation task: given a prefix, generate a completion to form a valid Dyck grammar string
- Dyck grammar constraints A: language of balanced parentheses
- Generator \mathcal{O} : pre-train an autoregressive Transformer from scratch on Dyck grammar strings
- Verifier V: one-layer MLP trained from scratch for binary classification
 - Feature = generator representation of a prefix
 - Label = 1 if the prefix is grammatical, 0 otherwise

Experiment 1: generating strings in Dyck grammar

$\mathrm{top}_{-}\mathrm{p}$	quota	stride	$\# ext{errors} \pm ext{std} ext{ err}$
0.9	0	0	240.0 ± 5.177
	4	4	179.4 ± 1.020
1.0	0	0	461.8 ± 8.304
	4	4	200.0 ± 3.225

- Q: backtrack quota
- *B*: stride
- top_p: controls nucleus sampling truncation

Tokenwise rejection sampling with backtracking reduces completion errors

Experiment 2: generating Python test cases

- Constrained generation task: given the codes for a simple Python function (i.e. list append), generate test cases (assert statements)
 - Eval metric: distinct accuracy $Acc_{distinct}$: the number of distinct correct test cases generated, divided by the total number requested
- Generator O: pre-trained CodeLlama¹
- Verifier V: one-layer MLP for binary classification
 - Feature = generator representation of a prefix
 - Label = 1 if the prefix is grammatical, 0 otherwise

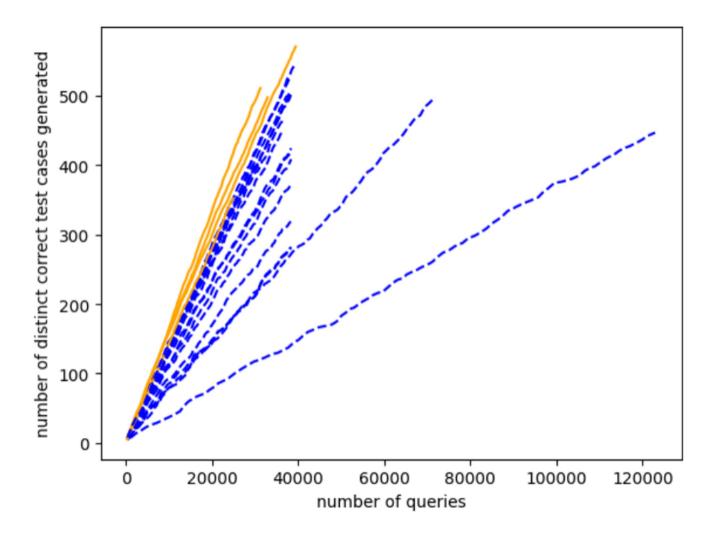
Experiment 2: generating Python test cases

quota	stride	$\mathbf{top}_{-}\mathbf{p}$	${f T}$	block BoN	$\mathbf{Acc_{distinct}} \pm \mathbf{std} \mathbf{err}$
4	4	0.95	1.0		0.714 ± 0.011
0		0.95	1.0	2	0.684 ± 0.038
0		0.95	1.0		0.660 ± 0.042
0		0.95	1.0	4	0.623 ± 0.036
0		0.95	1.0	8	0.559 ± 0.038
4	4	1.0	1.0		0.639 ± 0.061
4	10	1.0	1.0		0.622 ± 0.046
0		1.0	1.0		0.504 ± 0.025
4	4	1.0	1.2		0.440 ± 0.026
0		1.0	1.2		0.269 ± 0.025
0		0.0	1.0		0.013 ± 0.000

- Q: backtrack quota
- B: stride
- top_p: controls nucleus sampling truncation
- *T*: sampling temperature
- block BoN: block best-of-N (baseline)

Tokenwise rejection sampling with backtracking improves distinct accuracy

Experiment 2: generating Python test cases



- Orange: Tokenwise rejection sampling with backtrack
- Blue: baselines, including various nucleus sampling top_p, sampling temperature T, and block best-of-N

Tokenwise rejection sampling with backtracking improves query efficiency

Summary

Contact: yuchenl4@cs.cmu.edu https://arxiv.org/abs/2502.12123 (ICML 2025)

Key takeaway: constrained language generation without a verifier is provably hard, but verifiers (which check partial outputs) can help

Theory: query complexity, information-theoretic and computational lower bound

Experiments: Tokenwise rejection sampling with backtracking improves accuracy, diversity, and query efficiency for generating Dyck grammar and Python test cases

Open questions for future work:

- 1. Theory when verifiers are imperfect
- 2. Maintaining calibration of the distribution of elements in the constrained support