# On the Query Complexity of Verifier-Assisted Language Generation



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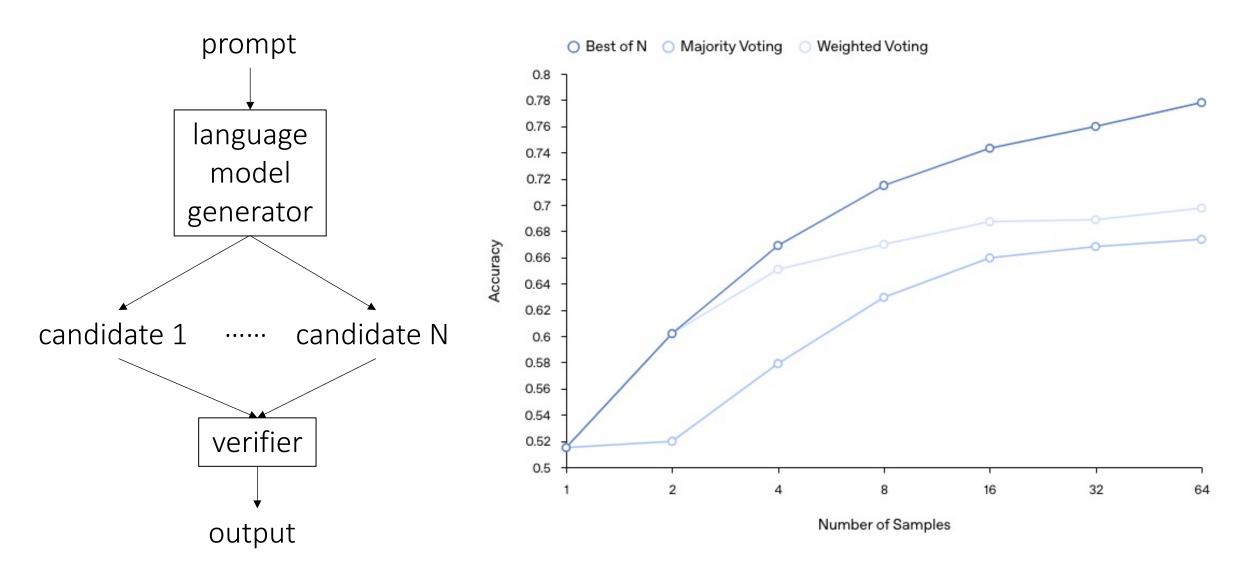


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# Background: verifier-assisted language generation



#### 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  $(\Sigma, A, \mathcal{O})$ : 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	$\operatorname{stride}$	$\# ext{errors} \pm  ext{std}  ext{ err}$
0.9	0	0	$240.0 \pm 5.177$
	4	4	$179.4 \pm 1.020$
1.0	0	0	$461.8 \pm 8.304$
	4	4	$200.0 \pm 3.225$

- 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

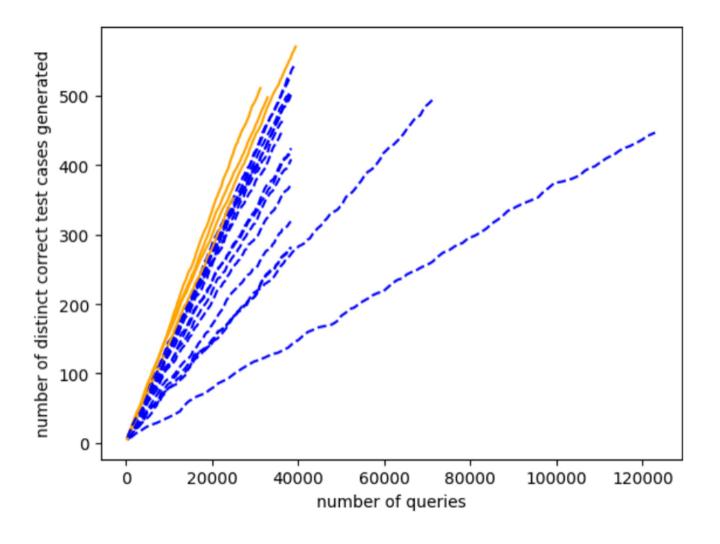
#### Experiment 2: generating Python test cases

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

- 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