PSC: EFFICIENT GRAMMAR-CONSTRAINED DECODING VIA PARSER STACK CLASSIFICATION

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ABSTRACT

LLMs are widely used to generate structured output like source code or JSON. Grammar-constrained decoding (GCD) can guarantee the syntactic validity of the generated output, by masking out tokens that violate rules specified by a context-free grammar. However, the online computational overhead of existing GCD methods, with latency typically scaling linearly with vocabulary size, limits the throughput of LLMs, especially for models with large vocabularies. To address this issue, we propose PSC, a novel grammar-constrained decoding method. By combining acceptance conditions of all vocabulary tokens into a single classifier of the parser stack during preprocessing, PSC can compute the complete vocabulary mask by checking the parser stack exactly once per decoding step, with time complexity independent of the vocabulary size. Experiments show that PSC computes masks up to 770× faster than baselines on complex programming language grammars, and up to 30× faster for schema-conformant JSON; end-to-end LLM throughput with PSC approaches that of unconstrained decoding.

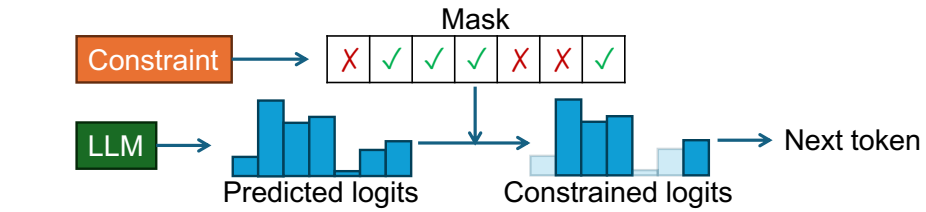
1 INTRODUCTION

In recent years, the ability for Large Language Models (LLMs) to generate structured output has been widely recognized and utilized (Qwen et al.; Grattafiori et al.; Gemma Team et al.). Source code can be viewed as structured output that adheres to the syntax of programming languages, and LLM-based coding assistants, such as GitHub Copilot (GitHub) and Cursor (Anysphere Inc.), have been widely adopted by developers to assist in writing code to improve their productivity. When LLMs are used as a tool, users often expect the generated output to conform to a specific format, such as Markdown or JSON with custom schemas (Liu et al., 2024; vLLM Team; OpenAI). All of these applications rely on the ability of LLMs to generate output that adheres to a specific syntax.

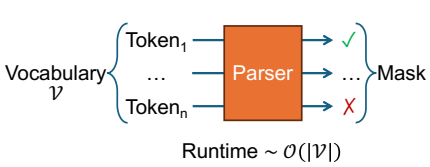
However, generating in a structured format is complex, as it requires not only understanding the semantics of given input but also adhering to the specific grammars of target formats. Since language models are essentially probabilistic models, there is no guarantee that the generated output will always conform to the required grammar.

To address this issue, *grammar-constrained decoding* (GCD) (Geng et al., b; Scholak et al.; Poesia et al.; Ugare et al.) is proposed to ensure that the generated output always conforms to the specified context-free grammar. A GCD method works by incorporating a grammar checker into the decoding process, as shown in Figure 1a. At each decoding step, the checker determines which tokens in the vocabulary can be appended to the current prefix while not violating the grammar. The logits generated by the language model are then masked to only allow the valid tokens, and the next token is generated by sampling from the masked logits.

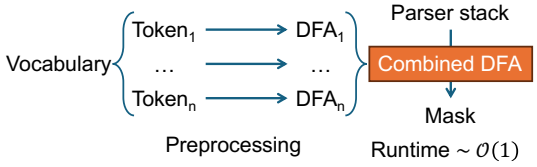
The overhead of GCD is determined by the newly introduced step of validity calculation. A naive implementation, as shown in Figure 1b would require calling the parser for *every* token in the vocabulary to check its validity, resulting in a time complexity of $\mathcal{O}(|\mathcal{V}|)$ per decoding step, where $|\mathcal{V}|$ is the vocabulary size. This can add significant overhead, especially for large vocabularies in modern language models, e.g. 128k tokens in Llama-3 (Grattafiori et al.), 151k tokens in Qwen series (Bai et al.), or 262k tokens in Gemma 3 (Gemma Team et al.). The overhead is particularly pronounced for smaller models, where the time taken by model inference is relatively small.



(a) Decoding step in grammar-constrained decoding (GCD).



(b) Naive GCD implementation.



(c) Our GCD method PSC.

Figure 1: An illustration of grammar-constrained decoding, showing (a) the overall working process, (b) the naive implementation that directly simulates the PDA, and (c) our method PSC that precomputes the DFA and the valid token masks.

To speed up GCD, various techniques have been proposed in the literature. We summarize these techniques in Section 2. However, none of these techniques can fundamentally change the time complexity, which is still $\mathcal{O}(|\mathcal{V}|)$ in the worst case.

We propose a novel GCD method PSC that replaces the repetitive runtime parsing over the whole vocabulary with a one-time classification of the current parser stack, as shown in Figure 1c. The checking process of the parser can be seen as a function of both the token and the state of the parser, which is usually a stack. For each token, our method PSC constructs a finite-state automaton (FSA) that represents the exact requirements on the parser stack to accept that token, i.e., the FSA accepts a parser stack if and only if that token is accepted by a parser with that stack. All these FSAs can then be combined into a single FSA that classifies the parser stack into a finite number of classes, each corresponding to a different vocabulary mask. During decoding, we only need to check the parser stack exactly once per decoding step to get the vocabulary mask, which is ready to be applied to the logits. This eliminates the need to call the parser for each token in the vocabulary, resulting in a significant speedup.

We conduct extensive experiments on grammar-constrained decoding in Java, Go, SQL, and schema-conformant JSON to evaluate the efficiency of our method. Compared to the current state-of-the-art method LLGuidance, our method achieves up to 770 times speedup in mask computation on complex programming language grammars, and up to 30 times speedup for schema-conformant JSON generation. In the end-to-end decoding throughput experiments, the throughput of PSC approaches that of unconstrained decoding, and is significantly higher than LLGuidance, especially on smaller models and larger batch sizes.

In summary, our contributions are as follows:

- We propose a novel GCD method PSC that leverages finite-state automata to classify parser states to use the precomputed vocabulary mask, significantly reducing the time overhead of grammar-constrained decoding.
- We provide a theoretical analysis of PSC. We prove that the set of the parser stacks that can accept a given token can be formally described as a regular language. This justifies the correctness of our method and provides a theoretical foundation for future research on grammar-constrained decoding.
- We demonstrate the efficiency of PSC through extensive experiments on grammar-constrained decoding in Java, Go, Python, and schema-conformant JSON, achieving significant speedup in mask computation compared to existing techniques; end-to-end decoding throughput with PSC approaches that of unconstrained decoding.

2 BACKGROUND AND RELATED WORK

We introduce the task of grammar-constrained decoding in this section, and then review the related work. **For the symbols, notations, and definitions used in this paper, please refer to Appendix A.2.**

2.1 THE TASK: GRAMMAR-CONSTRAINED DECODING

Let Σ be the character set used by the language model, e.g. the Unicode. Given a prefix of tokens, the task of a language model is to generate the next-token distribution over the vocabulary $\mathcal{V} \subset \Sigma^+$. For a language $L \subseteq \Sigma^*$, the task of *constrained decoding* aims to generate a sample in L from the language model. In each step, given prefix $x \in \Sigma^*$, it calculates the set of valid tokens in $\mathcal{V}$, i.e. tokens that, when concatenated after x, become a prefix of some strings in L.

$$c(x \in \Sigma^*) := \{v \in \mathcal{V} | \exists y \in \Sigma^*, xvy \in L\}. \tag{1}$$

When the language L is defined by a context-free grammar, the task is called *grammar-constrained decoding* (Ugare et al.; Koo et al.; Park et al.; Moskal et al.). Determining whether a string is syntactically valid usually involves two phases: lexical analysis and syntax analysis[1] (Aho & Ullman). In lexical analysis, the lexer $\mathcal{T}$, usually modeled as a deterministic finite-state transducer (FST) (Aho & Ullman; Koo et al.; Park et al.), transduces the text $w \in \Sigma^*$ into a terminal sequence $\mathcal{T}(w) \in \Gamma^*$. In syntax analysis, the parser $\mathcal{P}$, usually modeled as a terminating deterministic push-down automaton (PDA) (Aho & Ullman), determines whether a terminal sequence $x \in \Gamma^*$ is valid, written as $x \in \mathcal{P}$. So we have

$$w \in L \iff \mathcal{T}(w) \in \mathcal{P}. \tag{2}$$

2.2 RELATED WORK

There are several existing techniques to speed up grammar-constrained decoding, which can be categorized into three groups: vocabulary preprocessing, lexer preprocessing, and parser preprocessing.

Vocabulary preprocessing (Poesia et al.; Beurer-Kellner et al.; Moskal et al.) exploits the fact that the vocabulary is built by BPE (Gage; Sennrich et al.), and for each token, its prefix is also a token in the vocabulary. If the prefix token is rejected, then the longer token must also be rejected. So we can traverse the vocabulary in a tree-like manner, and only check the tokens whose prefixes are not rejected.

Lexer preprocessing (Beurer-Kellner et al.; Park et al.; Moskal et al.) maps each token to a terminal sequence during preprocessing, and then the parser is only called on the terminal sequences. This reduces the number of parser calls, as different tokens may share the same terminal sequence.

Parser preprocessing (Dong et al.; Park et al.) classifies the vocabulary into three sets for each parser state: context-independent accepted, context-independent rejected, and context-dependent. This allows us to reduce the number of parser calls by only checking the context-dependent tokens.

These techniques can be combined to achieve better speedup (Beurer-Kellner et al.; Park et al.; Moskal et al.).However, as mentioned in Section 1, these techniques are limited in their speedup. There is no theoretical guarantee on how many parser calls will be made per decoding step,which can be linear to the vocabulary size in the worst case.

3 PSC: PARSER STACK CLASSIFICATION

The preprocessing of the lexer $\mathcal{T}$ is described in Section 3.1, and the other parts of this section are dedicated to the preprocessing of the parser $\mathcal{P}$. All the proofs are deferred to Appendix A.3. **For the symbols, notations, and definitions used in this paper, please refer to Appendix A.2.**

[1] To ease the presentation, the step of lexical analysis is omitted in previous sections. The term "parser" in previous sections should be realized as the combination of the lexer and the parser defined here, and the term "parser stack" should be realized as the concatenation of the lexer state and the parser state, which is a simple state without internal structure, and a stack, respectively.

3.1 LEXICAL PREPROCESSING

Lexical preprocessing is not our focus in this paper, so we reuse the lexical preprocessing in GreatGramma (Park et al.), and conclude it here as a prelude to PSC.

For token $v \in \mathcal{V}$, lexer state $q \in Q$, if lexing the token v from state q using the lexer $\mathcal{T}$ generates the terminal sequence $x \in \Gamma^*$, and the lexer transits to state p, i.e. $q \xRightarrow[\mathcal{T}]{v:x}{}^* p$, we define the *realizable terminal sequences* $R_q(v)$ as $\{x\}T_p$, representing all possible terminal prefixes that can be generated from a string starting with v, where T_p is the finite set of all possible terminal prefixes from state p: $\mathcal{T}_p(\Sigma^*) = T_p\mathcal{T}(\Sigma^*)$. The set $R_q(v)$ can be precomputed for every $q \in Q, v \in \mathcal{V}$ during preprocessing.

3.2 OVERVIEW OF SYNTACTIC PREPROCESSING

Given a valid prefix $x \in \Sigma^*$, we run the lexer $\mathcal{T}$ from the initial state q_0 to produce a terminal sequence $z \in \Gamma^*$ and a new lexer state q: $q_0 \xRightarrow[\mathcal{T}]{x:z}{}^* q$. We then run the parser $\mathcal{P}$ from the initial stack γ_0 to receive the terminal sequence z, and generates a new stack α: $\gamma_0 \xRightarrow[\mathcal{P}]{z}{}^* \alpha$.

We can now introduce the simplification of the condition in the GCD definition in Equations 1 and 2 **from previous work (Park et al.)**. For any token $v \in \mathcal{V}$, to determine whether v is valid, we can rewrite the condition in terms of realizable terminal sequences,

$$\exists y \in \Sigma^*, \mathcal{T}(xvy) \in \mathcal{P} \iff \exists w \in R_q(v), \exists \beta \in \Pi^+, \alpha \xRightarrow[\mathcal{P}]{w}{}^* \beta. \tag{3}$$

The simplification is based on the common assumption that, if the parser reads in a certain terminal sequence and enters a stable stack, then we do not need to worry about the rest of the input, and there always exists a terminal sequence produced by the lexer that can ensure the whole text is accepted.

For $w \in \Gamma^*$, we define $P_w(\alpha)$ for the calculation in the last step of Equation 3,

$$P_{w \in \Gamma^*}(\alpha \in \Pi^+) := \left\{ \beta \in \Pi^+ \middle| \alpha \xRightarrow[\mathcal{P}]{w}{}^* \beta \right\}. \tag{4}$$

How to efficiently calculate $P_w(\alpha)$ is the key difference between PSC and previous methods. In existing work, the calculation of P_w is almost always dynamic: one has to calculate $P_w(\alpha)$ for the current α and every possible $w \in R_q(\mathcal{V})$. While some methods employ precomputation to optimize certain cases, they still fundamentally require $\mathcal{O}(|R_q(\mathcal{V})|t_{\mathcal{P}})$ time for dynamic parsing, where $\mathcal{O}(t_{\mathcal{P}})$ is the time required to run the parser $\mathcal{P}$.

On the other hand, it can be noticed that, whether $P_w(\alpha) \neq \varnothing$ is determined by the top symbols of α. It is to say, if $P_w(\alpha) \neq \varnothing$, then $\forall \gamma \in \Pi^*$, $P_w(\alpha\gamma) \neq \varnothing$. Utilizing this property, PSC proposes a totally different approach, modeling P_w as a deterministic FST, which reads the stack sequence $\alpha \in \Pi^+$, and outputs the sequence $\beta \in \Pi^+$ if there is one.

This gives us several benefits. Because each P_w reads and outputs a sequence of stack symbols, they can be composed to create larger FSTs: $P_t \circ P_s = P_{st}$. Because the realizable terminal sequences are known during precomputation, the exact validity condition of each vocabulary is therefore known, their combinations can be precomputed, and we only need to go through the current stack once during runtime. All possible masks can also be precomputed, eliminating the mask generation overhead during decoding.

3.3 FST OF ε TRANSITIONS

In this section, we focus on how to construct P_ε. The input of P_ε should be a stack, and **the output is the stabilized version of it by executing all needed ε transitions on the stack**. The states of P_ε is a special state FINAL plus a subset of Π^* which represent the current stack top, both the input alphabet and output alphabet are Π, and the start state is ε, and the final states are $\{\text{FINAL}\}$.

There are three types of transitions in P_ε. If the information of the current stack top is not enough to determine whether the stack is stable, it transits to a new state by reading the next stack symbol. If the stack top is stable, it transits to the FINAL state to output the final stable stack. Otherwise,

it simulates the transition of $\mathcal{P}$ on the current stack top, and transits to a new state representing the new stack top after executing the ε transition. The construction algorithm is simply searching all needed stacks from ε, as shown in Algorithm 1.

Theorem 1. *Algorithm 1 constructs a finite-state transducer P_ε as defined in Definition 4.*

P_ε is an important building block in the construction of other $P_w, w \in \Gamma^+$. For any stack α, $P_\varepsilon(\alpha)$ gives the stabilized version of α, so the FST composed after P_ε does not need to handle ε transitions, and we can compose P_ε after other FSTs to meet the stability requirement in the definition of P_w.

Algorithm 1 Construct FST P_ε

function EPSILONFST($\mathcal{P}$)
  for all $X \in \Pi$ **do**
    FINAL $\xrightarrow[P_\varepsilon]{X:X}$ FINAL
  $Q \leftarrow \{\varepsilon\}$
  while let $\alpha \in \Pi^*, Q \leftarrow \text{POP}(Q)$ **do**
    if $\alpha \in F_{\mathcal{P}}\Pi^*$ **then**
      $\alpha \xrightarrow[P_\varepsilon]{\varepsilon:\alpha}$ FINAL
    else if $|\alpha| < 2$ **then**
      for all $X \in \Pi$ **do**
        $\alpha \xrightarrow[P_\varepsilon]{X:\varepsilon} \alpha X$
        $Q \leftarrow Q \cup \{\alpha X\}$
    else
      let $\alpha_0\gamma = \alpha$, where $\alpha_0 \in \Pi^2, \gamma \in \Pi^*$
      if $\alpha_0 \xrightarrow[\mathcal{P}]{\varepsilon} \beta$ **then**
        $\alpha_0\gamma \xrightarrow[P_\varepsilon]{\varepsilon:\varepsilon} \beta\gamma$
        $Q \leftarrow Q \cup \{\beta\gamma\}$
      else if $\alpha_0 \xrightarrow[\mathcal{P}]{a} \beta$ **then**
        $\alpha \xrightarrow[P_\varepsilon]{\varepsilon:\alpha}$ FINAL
  return P_ε

Algorithm 2 Construct FST $\tilde{P}_a$ for terminal $a \in \Gamma$

function TERMINALFST($\mathcal{P}, a$)
  for all $X \in \Pi$ **do**
    FINAL $\xrightarrow[\tilde{P}_a]{X:X}$ FINAL
  for all $XY \xrightarrow[\mathcal{P}]{a} \beta$ **do**
    $\varepsilon \xrightarrow[\tilde{P}_a]{X:\varepsilon} X \xrightarrow[\tilde{P}_a]{Y:\varepsilon} XY \xrightarrow[\tilde{P}_a]{\varepsilon:\beta}$ FINAL
  return $\tilde{P}_a$

Algorithm 3 Offline constructon in PSC

function OFFLINECONSTRUCTION($\mathcal{T}, \mathcal{P}, \mathcal{V}$)
  $P_\varepsilon \leftarrow$ EPSILONFST($\mathcal{P}$)
  for all $a \in \Gamma$ **do**
    $\tilde{P}_a \leftarrow$ TERMINALFST($\mathcal{P}, a$)
  for all $w = w_1 \dots w_n \in R(\mathcal{V})$ **do**
    $P_w \leftarrow P_\varepsilon \circ \tilde{P}_{w_n} \circ P_\varepsilon \circ \cdots \circ P_\varepsilon \circ \tilde{P}_{w_1} \circ P_\varepsilon$
    $A_w \leftarrow$ REMOVEOUTPUT(P_w)
  $\mathcal{A} \leftarrow \bigcup_{v \in \mathcal{V}} \bigcup_{q \in Q} \bigcup_{w \in R_q(v)} B_q A_w B_v$
  $\mathcal{A} \leftarrow$ MINIMIZE($\mathcal{A}$)
  return $\mathcal{A}$

3.4 FST FOR ANY TERMINAL SEQUENCE

After constructing P_ε, the construction of P_w for any terminal sequence $w \in \Gamma^+$ is fairly simple.

We first construct an FST $\tilde{P}_a$ for every $a \in \Gamma$ that **simulates a single transition labeled** a. Note that in $\tilde{P}_a$, we only force the stack to execute one transition labeled a, but the output stack is not required to be stable. Its input is a stack α, and the output is the immediate result of executing a-labelled transition $\alpha \xrightarrow[\mathcal{P}]{a} \beta$. The states are $\Pi^0 \cup \Pi^1 \cup \Pi^2 \cup \{\text{FINAL}\}$, the start state is ε, the final state is FINAL, and the transitions are defined in Algorithm 2.

For any terminal sequence $w = w_1 \dots w_n \in \Gamma^+$, the FST P_w can be constructed using P_ε and $\tilde{P}_{w_1}, \dots, \tilde{P}_{w_n}$. For any stack α, we first pass it to P_ε to get a stable stack, and then pass the result into $\tilde{P}_{w_1}$ to get the stack after reading w_1, and then the stack is passed to P_ε to get the stabilized version. The result is then passed into $\tilde{P}_{w_2}$ to make the stack read w_2, and then passed to P_ε to stabilize. We repeat this process until we have read w_n using $\tilde{P}_{w_n}$ and stabilize the stack with P_ε. Formally, for $w = w_1 \dots w_n \in \Gamma^+$, we have $P_w = P_\varepsilon \circ \tilde{P}_{w_1} \circ P_\varepsilon \circ \cdots \circ P_\varepsilon \circ \tilde{P}_{w_n} \circ P_\varepsilon$.

Theorem 2. *The above construction of P_w meets the definition in Definition 4.*

Since in $c(x)$, we only care about whether P_w accepts α or not, the output of P_w can be ignored. Removing all the output labels from P_w gives us a finite-state automaton, hereafter named A_w.

3.5 ONE-PASS FSA FOR MASK SELECTION

After constructing $P_w(\alpha)$ for all realizable terminal sequences $w \in R(\mathcal{V})$, we can now consider simplifying the constraint calculation over the whole vocabulary $\mathcal{V}$. Recall Definition 1, combined with Simplification 3 and A_w, we have the following equation,

$$c(x \in \Sigma^*) = \{v \in \mathcal{V} | \exists w \in R_q(v), P_w(\alpha) \neq \varnothing\} = \{v \in \mathcal{V} | \exists w \in R_q(v), \alpha \in A_w\},$$

where q and α as defined in Section 3.2 are only dependent on x.

In $c(x)$, we want to know whether any of the A_w accepts α, where $w \in R_q(v)$. This can be achieved by constructing the union of different A_w, i.e., $\bigcup_{w \in R_q(v)} A_w$.

For different tokens $v \in \mathcal{V}$, we need to check whether α is accepted by $\bigcup_{w \in R_q(v)} A_w$. But to get the whole mask $c(x)$, we need to check for every $v \in \mathcal{V}$, which is inefficient. To address this issue, we can integrate the checking of v and q into the FSA. Introduce the notation B_a for an FSA that accepts only a once. For every $q \in Q$ and $v \in \mathcal{V}$, we can concatenate B_q before $\bigcup_{w \in R_q(v)} A_w$ to check whether the current state is q, and then concatenate B_v after $\bigcup_{w \in R_q(v)} A_w$ to check whether the candidate token is v.

By unioning the results for all $v \in \mathcal{V}$ and $q \in Q$, we construct an FSA $\mathcal{A}$ that accepts the sequence $q\alpha v$ only if v is a valid token for the lexer state q and stack α,

$$\mathcal{A} := \bigcup_{v \in \mathcal{V}} \bigcup_{q \in Q} \bigcup_{w \in R_q(v)} B_q A_w B_v, \quad c(x) = \{v \in \mathcal{V} | q\alpha v \in \mathcal{A}\}, \tag{5}$$

where $\mathcal{A}$ should be determinized and minimized.

Theorem 3. *All (lexer state, parser stack) pairs that accept a given token form a regular language.*

In Equation 5, we can precompute all possible result of c, i.e. all possible vocabulary masks, by considering acceptable vocabulary set $\mathcal{A}_s := \left\{ v \in \mathcal{V} \middle| s \xrightarrow[\mathcal{A}]{v} f^{\mathcal{A}} \right\}$ for every state s in $\mathcal{A}$.

We summarize the offline construction process of PSC in Algorithm 3, and the online execution process in Algorithm 4. In Algorithm 4, both the lexing Step 2 and the parsing Step 3 are standard in grammar-constrained decoding, and can be incrementally maintained. In Step 4, the FSA $\mathcal{A}$ is run on the stack α and the lexer state q to get the state s, only requiring $\mathcal{O}(|\alpha|)$ time. Step 5 can be precomputed to be $\mathcal{O}(1)$ at runtime.

Algorithm 4 Online execution of PSC

1: **function** ONLINEEXECUTION($\mathcal{T}, \mathcal{P}, \mathcal{A}, x$)
2: $\quad q_0^{\mathcal{T}} \xRightarrow[\mathcal{T}]{x:z}{}^* q$
3: $\quad \gamma_0 \xRightarrow[\mathcal{P}]{z}{}^* \alpha$
4: $\quad q_0^{\mathcal{A}} \xRightarrow[\mathcal{A}]{q\alpha}{}^* s$
5: $\quad$ **return** $\mathcal{A}_s$

4 EXPERIMENTS

4.1 EXPERIMENTAL SETUP

All grammar-constrained decoding methods essentially perform the same task: compute the valid token mask at each decoding step. **The valid token mask is theoretically the same for all methods, so we focus on comparing the efficiency of mask computation in our experiments.** The usefulness of grammar-constrained decoding is shown in previous work (Geng et al., b; Scholak et al.; Poesia et al.; Ugare et al.), so we do not repeat the experiments here.

We conduct two sets of experiments to evaluate each method:

- **Overhead of mask computation (without model inference).**
- **End-to-end throughput (with model inference).**

In all experiments, we use **teacher-forcing** during evaluation, i.e., we always use the oracle next token at each decoding step, **to ensure that all methods are evaluated under the same conditions and can be fairly compared.**

Datasets There is no standard benchmark for evaluating grammar-constrained decoding methods. We choose two representative tasks that require grammar-constrained decoding: code generation in Java, Go, and SQL, and JSON generation with specified JSON schemas. For each task, we construct the evaluation dataset as described in Appendix A.4, with 1000 samples for each programming language and 1000 schemas for schema-conformant JSON generation. There are a total of 1337 positive samples and 2072 negative samples in the JSON dataset, and each schema has at least one positive sample and one negative sample.

Baselines We consider several recent state-of-the-art grammar-constrained decoding methods with open-source implementations as baselines, including XGrammar (Dong et al.), GreatGramma (Park et al.), Formatron (Sun et al.), and LLGuidance (Moskal et al.). Detailed descriptions of these baselines are included in Appendix A.5.

Implementation We implement PSC in roughly 1100 lines of Python. Similar to previous work (Ugare et al.; Park et al.), we use the Lark parser(lar) to construct the lexer and the LALR(1) parser from the grammar. As described in Section 3.1, we reuse the lexer construction in GreatGramma (Park et al.), since this is not our focus in this paper.

Execution environment We conduct our experiments on a machine with 8 NVIDIA A100 GPUs (40 GB Memory), 2 Intel Xeon Gold 6348 CPUs (2.6GHz, 56 cores), and 512 GB RAM. To ensure fairness, we run all the experiments with a single GPU and a single CPU thread.

4.2 Overhead of mask computation

Metrics In this experiment, we measure the overhead of mask computation for each GCD method. We ignore the time taken to transfer the mask to the GPU and apply it to the logits, because this is the same for all methods[2]. For each method, we measure:

- **Average overhead:** The time of computing the CPU mask tensor at each decoding step.
- **Sample pass rate:** The proportion of samples that are correctly processed by each method[3].

Models We evaluate the overhead on three open-source LLM series with different vocabulary sizes: Llama 3 (Grattafiori et al.) (128k vocabulary size), Qwen 2.5 (Bai et al.) (151k vocabulary size), and Gemma 3 (Gemma Team et al.) (262k vocabulary size). We only use the tokenizers, because the overhead of mask computation is independent of other model components.

Overhead results The average overhead is shown in Table 1. PSC significantly outperforms all the baselines across all grammars and models, being 310 to 700 times faster on complex programming language grammars compared to the best baseline, LLGuidance, and generally 30 times faster on the relatively simple JSON schema grammar.

The overhead of baselines is significantly larger on Gemma 3 than that on the other models[4], because Gemma 3 has a much larger vocabulary size (262k) than the other two models (128k and 151k), and the time complexity of all methods except PSC is roughly linear to the vocabulary size. In contrast, the performance of PSC is stable across different grammars and models, because its time complexity is independent of the vocabulary size.

Sample pass rate results The sample pass rates are shown in Table 2. PSC achieves a high pass rate across all grammars and models, very close to 100%. After analyzing the error cases, we find that they are all directly rejected by the GreatGramma lexer we adopt, but **no error is caused by PSC itself**. We notice the strangely low sample pass rate of Formatron on SQL, and find that Formatron refuses to accept the column alias in the query, resulting in frequent rejections.

[2] In PSC, one can preload all the mask tensors on the GPU memory before decoding begins, eliminating the transfer overhead. However, the transfer overhead is usually too small to justify the extra GPU memory usage.

[3] If the oracle token is masked, the sample is counted as rejected by the method. A positive sample is counted as passed if it is not rejected, and a negative sample is counted as passed if it is rejected.

[4] The performance of LLGuidance on JSON Schemas is roughly the same across different models, probably because the grammar is simple enough that the vocabulary size does not significantly affect the performance.

Table 1: Average overhead (microseconds) of computing the mask per token in GCD tasks using different methods. The symbol X indicates the parser reports an error during mask calculation. Text in **bold** indicates the best performance, and text in underline indicates the second best performance.

Model	Method	Grammar			
		Java	Go	SQL	JSON Schemas
Llama 3 $\lvert\mathcal{V}\rvert = 128256$	XGrammar	309514.2	281500.9	324663.6	26257.6
	Formatron	393540.4	X[a]	303974.1	X[a]
	GreatGramma	21402.8	27220.9	20954.5	8556.2
	LLGuidance	1352.4	X[b]	826.1	72.7
	PSC (Ours)	**2.4**	**2.5**	**2.6**	**2.3**
Qwen2.5 $\lvert\mathcal{V}\rvert = 151665$	XGrammar	302421.9	278333.4	299968.6	29470.0
	Formatron	378921.0	X[a]	253311.9	X[a]
	GreatGramma	24570.9	27649.8	24053.9	11038.4
	LLGuidance	1408.2	X[b]	865.2	72.1
	PSC (Ours)	**2.4**	**2.5**	**2.5**	**2.2**
Gemma 3 $\lvert\mathcal{V}\rvert = 262145$	XGrammar	649321.1	458952.0	416625.0	54164.4
	Formatron	696144.6	X[a]	444810.0	X[a]
	GreatGramma	43218.6	48354.0	40026.9	25717.3
	LLGuidance	1802.6	X[b]	1180.8	72.1
	PSC (Ours)	**2.3**	**2.5**	**2.4**	**2.3**

[a] Formatron stops responding on multiple samples, so we terminate the process.
[b] LLGuidance reports `ParserTooComplex` error.

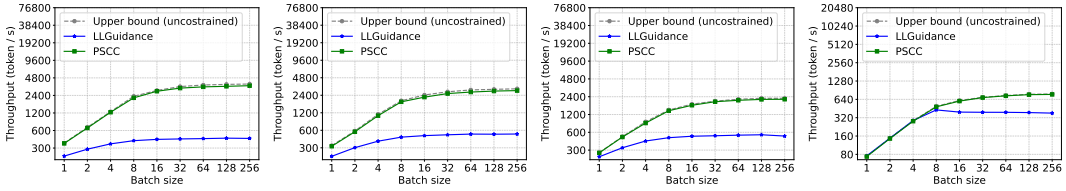
Table 2: How many samples are correctly processed by each method. The symbol X indicates the parser reports an error during mask calculation. Text in **bold** indicates the best performance, and text in underline indicates the second best performance.

Model	Method	Grammar			
		Java	Go	SQL	JSON Schemas
Llama 3	XGrammar	99.7%	**100.0%**	99.7%	**100.0%**
	Formatron	99.4%	X	67.0%	X
	GreatGramma	**100.0%**	99.9%	97.1%	99.6%
	LLGuidance	**100.0%**	X	**99.9%**	99.9%
	PSC (Ours)	**100.0%**	99.9%	**99.9%**	99.6%
Qwen2.5	XGrammar	99.7%	**100.0%**	99.7%	**100.0%**
	Formatron	99.4%	X	67.0%	X
	GreatGramma	**100.0%**	99.9%	97.2%	99.6%
	LLGuidance	**100.0%**	X	**99.9%**	99.9%
	PSC (Ours)	**100.0%**	99.9%	**99.9%**	99.6%
Gemma 3	XGrammar	99.7%	**100.0%**	99.7%	**100.0%**
	Formatron	**100.0%**	X	67.3%	X
	GreatGramma	**100.0%**	99.9%	97.2%	99.6%
	LLGuidance	94.0%	X	**99.9%**	99.9%
	PSC (Ours)	**100.0%**	99.9%	**99.9%**	99.6%

4.3 End-to-end Throughput

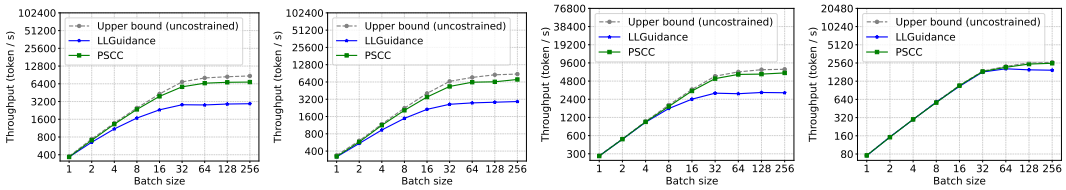
Settings In this experiment, we run the actual model inference using the vLLM library (Kwon et al.), and measure the throughput, i.e., the number of tokens processed per second, of the entire decoding process, considering both the time taken by mask computation and model inference. We only consider the accepted samples of each method. We compare PSC with the fastest baseline LLGuidance in the previous section, and also include the throughput when not using any constraint decoding method as a reference, under various batch sizes of 1, 2, 4, ..., 256.

Models We use the smallest models in the three model series to highlight the overhead of constraint decoding. On these models, the model inference time is relatively small, making the overhead of constraint decoding more pronounced. Specifically, we use Llama 3 1B, Qwen 2.5 0.5B, and Gemma 3 270M. We also include Qwen 2.5 7B to see the effect of model size on throughput.



(a) Gemma 3 270M. (b) Qwen 2.5 0.5B. (c) Llama 3.2 1B. (d) Qwen 2.5 7B.

Figure 2: End-to-end throughput (tokens per second) on the **Java** dataset using different methods on different models with various batch sizes.



(a) Gemma 3 270M. (b) Qwen 2.5 0.5B. (c) Llama 3.2 1B. (d) Qwen 2.5 7B.

Figure 3: End-to-end throughput (tokens per second) on the **schema-conformant JSON** dataset using different methods on different models with various batch sizes.

Results The end-to-end throughput results on Java and schema-conformant JSON datasets are present in Figures 2 and 3, respectively. The results on the Go and SQL datasets are similar to those on the Java dataset, included in Appendix A.6.

On all datasets, PSC consistently outperforms LLGuidance across all models and batch sizes, and is very close to the performance of unconstrained decoding. The difference is more pronounced on the Java dataset, where the grammar is more complex, leading to higher overhead for LLGuidance.

As the model size increases, the difference in throughput becomes smaller, because the model inference time becomes more dominant. However, since smaller models are less capable, grammar-constrained decoding is probably more useful for smaller models to ensure the syntactic correctness.

As the batch size increases, the difference in throughput becomes larger, because the average model inference time per token decreases with larger batch sizes, indicating that the overhead introduced by constraint decoding becomes more pronounced at larger batch sizes.

5 Discussion and Conclusion

In this paper, we present PSC, a novel approach for grammar-constrained decoding. By constructing the exact requirements on the parser stack for each vocabulary token, PSC can determine the valid tokens at each decoding step by a single pass through the parser stack. Our experimental results demonstrate that PSC achieves significant speedup over existing methods, and the end-to-end throughput of PSC approaches that of unconstrained decoding. This makes PSC a practical choice for real-world applications that require grammar-constrained decoding.

One limitation of PSC is that it requires preprocessing.But this can be done offline and reused for multiple decoding sessions with the same grammar and vocabulary, so the overhead of preprocessing is generally acceptable for practical applications. In future, we plan to explore other types of grammars and constraints that can be efficiently handled by PSC, as well as other optimizations to further improve its efficiency and scalability.

6 Reproducibility Statement

We open-source the code to facilitate reproducibility of our results at https://anonymous.4open.science/r/PSC-E43E. It includes the implementation of PSC, the datasets used in the experiments, and the scripts to run the experiments and generate the results in the paper. The proofs of statements in the main text are included as Appendix A.3. The details in dataset construction are included as Appendix A.4.

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A Appendix

A.1 LLM Usage

We used DeepSeek and GitHub Copilot for code assistance, paper writing, and proofreading. However, all the technical content, ideas, algorithms, and experimental results in this paper are our own work. We carefully reviewed and verified all the content generated by LLMs to ensure they are accurate and directly reflect our own ideas.

A.2 Formal definitions and notations

Table 3: Symbols and their meaning.

Symbol	Meaning
ε	empty string
ab	concatenation of strings a and b
AB	concatenation of languages A and B
A_ε	$A \cup \{\varepsilon\}$
A^*	Kleene star of language A
A^+	$A^* \setminus \{\varepsilon\}$
Σ	the character set (usually the Unicode) used by the language model
Γ	the terminal set of the grammar
$\mathcal{V}$	the vocabulary of the language model, a finite subset of Σ^+ such that every string over Σ can be tokenized as a string over $\mathcal{V}$
$\mathcal{T}$	the lexing FST, transduces string over Σ to terminal sequence over Γ
Q	the finite set of states of the lexing FST
$\mathcal{P}$	the parsing PDA, accepts terminal sequences in the language
Π	the stack alphabet of the PDA

We include a list of symbols and their meanings in Table 3 for reference.

A.2.1 Finite-state transducer (FST)

A *finite-state transducer* (FST) (Aho & Ullman) $\mathcal{T}$ is defined by a finite set of states Q, the input alphabet Σ, the output alphabet Γ, the start state $q_0 \in Q$, the final states $F \subseteq Q$, and transitions $\delta : Q \times \Sigma_\varepsilon \to 2^{\Gamma^* \times Q}$. If $\delta(q, a) \ni (y, q')$, we write $q \xrightarrow[\mathcal{T}]{a:y} q'$. We write $\to^*$ for consecutive transitions. For $q \in Q$, we write $q \xrightarrow[\mathcal{T}]{\varepsilon:\varepsilon}{}^* q$. For $q \xrightarrow[\mathcal{T}]{s:x}{}^* q'$ and $q' \xrightarrow[\mathcal{T}]{t:y} q''$, we write $q \xrightarrow[\mathcal{T}]{st:xy}{}^* q''$.

Informally, an FST is *deterministic*, if from any state, for any given string, there is exactly one possible outcome. $\mathcal{T}$ is *deterministic* if, for all $q \in Q$, either $|\delta(q, a)| \leq 1, \forall a \in \Sigma$ and $\delta(q, \varepsilon) = \varnothing$, or $\delta(q, a) = \varnothing, \forall a \in \Sigma$ and $\delta(q, \varepsilon) = 1$.

For $w \in \Sigma^*, q \in Q$, we define $\mathcal{T}_q(w)$ as $\left\{ v \in \Gamma^* \middle| \exists q' \in F, q \xrightarrow[\mathcal{T}]{w:v}{}^* q' \right\}$, meaning the possible outcomes when we feed w into $\mathcal{T}$ starting from the state q. When $\mathcal{T}$ is deterministic and $v \in \mathcal{T}(w)$, we also write $\mathcal{T}(w) = v$. For $W \subseteq \Sigma^*$, we define $\mathcal{T}_q(W)$ as $\bigcup_{w \in W} \mathcal{T}_q(w)$. q defaults to q_0 when omitted.

We call a state $q \in Q$ *stable* if the FST does not need to take any immediate action on q, i.e. $\delta(q, \varepsilon) = \varnothing$. If $q \xrightarrow[\mathcal{T}]{s:t}{}^* q'$ and q' is stable, we also write $q \xRightarrow[\mathcal{T}]{s:t}{}^* q'$.

Given two FSTs $\mathcal{S}$ and $\mathcal{T}$ where the output alphabet of $\mathcal{S}$ is the input alphabet $\mathcal{T}$, $\Gamma^{\mathcal{S}} = \Sigma^{\mathcal{T}}$, their *composition* is a new FST $\mathcal{S} \circ \mathcal{T}$ by feeding the output of $\mathcal{S}$ into the input of $\mathcal{T}$.

A.2.2 FINITE-STATE AUTOMATON (FSA)

A *finite-state automaton* (FSA) $\mathcal{A}$ can be defined by removing all output labels from an FST. We say $\mathcal{A}$ *accepts* $w \in \Sigma^*$ from state q if $\mathcal{A}_q(w) \neq \varnothing$, and write $w \in \mathcal{A}_q$, and q defaults to q_0 when omitted. Two FSAs are *equivalent* if they accept the same language.

$\mathcal{A}$ is *deterministic* if there is no ε transition in δ. Every nondeterministic FSA can be *determinized* into an equivalent deterministic FSA (Hopcroft & Ullman), and every deterministic FSA can be *minimized* into an equivalent deterministic FSA with the smallest number of states (Hopcroft & Ullman).

The *union* of two FSAs $\mathcal{A}$ and $\mathcal{B}$ is a new FSA $\mathcal{A} \cup \mathcal{B}$ that accepts any sequence that is accepted by either $\mathcal{A}$ or $\mathcal{B}$.

The *concatenation* of two FSAs $\mathcal{A}$ and $\mathcal{B}$ is a new FSA $\mathcal{A}\mathcal{B}$ that accepts any sequence that can be split into two parts $x = yz$, where $\mathcal{A}$ accepts the first part y and $\mathcal{B}$ accepts the second part z.

A.2.3 PUSH-DOWN AUTOMATON (PDA)

A *push-down automaton* (PDA) (Aho & Ullman; Hopcroft & Ullman; Caucal & Monfort) $\mathcal{P}$ is defined by the input alphabet Γ, the stack alphabet Π, the initial stack $\gamma_0 \in \Pi^2$, the final states $F \subseteq \Pi$, and a finite set of transitions $\delta : \Pi^2 \times \Gamma_\varepsilon \to 2^{\Pi^+}$. Note that the definition here merges the states and the stack symbols in the traditional definition of PDA, but they are equivalent if we treat the stack top symbol as the state. If $\delta(\alpha, a) \ni \beta$, we write $\alpha \xrightarrow[\mathcal{P}]{a} \beta$. If $\alpha \xrightarrow[\mathcal{P}]{a} \beta$, for any $\gamma \in \Pi^*$, we also write $\alpha\gamma \xrightarrow[\mathcal{P}]{a} \beta\gamma$. We write $\to^*$ for consecutive transitions. For $\gamma \in \Pi^+$, we write $\gamma \xrightarrow[\mathcal{P}]{\varepsilon}{}^* \gamma$. If $\alpha \xrightarrow[\mathcal{P}]{a} \beta$, $\beta \xrightarrow[\mathcal{P}]{w}{}^* \gamma$, we write $\alpha \xrightarrow[\mathcal{P}]{aw}{}^* \gamma$.

Informally, a PDA is *deterministic*, if from any stack, for any given string, there is exactly one possible outcome. $\mathcal{P}$ is *deterministic* if, for any $\alpha \in \Pi^2$, either $|\delta(\alpha, a)| \leq 1, \forall a \in \Gamma$ and $\delta(\alpha, \varepsilon) = \varnothing$, or $\delta(\alpha, a) = \varnothing, \forall a \in \Gamma$ and $|\delta(\alpha, \varepsilon)| = 1$.

A deterministic PDA is *terminating*, if for any stack, it does not make an endless sequence of ε-input transitions.[5] Every deterministic PDA can be transformed into another equivalent deterministic terminating PDA (Sipser; Hopcroft & Ullman).

We call a state $\beta = \beta_1 \dots \beta_n \in \Pi^+$ *stable* if β_1 is a final state, i.e. $\beta_1 \in F$, or the PDA is waiting to read one more symbol, i.e. $\exists a \in \Gamma, \delta(\beta_1\beta_2, a) \neq \varnothing$. If $\alpha \xrightarrow[\mathcal{P}]{w}{}^* \beta$ and β is stable, we also write $\alpha \xRightarrow[\mathcal{P}]{w}{}^* \beta$. In practice, parser in a stable state is ready to consume the next input symbol, or has reached an accepting stack.

For $\alpha \in \Pi^+$, we define $\mathcal{P}_\alpha$ as $\left\{ w \in \Gamma^* \middle| \exists X \in F, \exists \gamma \in \Pi^*, \alpha \xRightarrow[\mathcal{P}]{w}{}^* X\gamma \right\}$. α defaults to γ_0 when omitted.

A.3 PROOFS OF THEORETICAL RESULTS

In this section, we provide the proofs of the theoretical results stated in the main text.

A.3.1 PROOF OF THEOREM 1

Proof. First we show that the states of P_ε are finite, i.e. Algorithm 1 terminates. Consider the two steps in Algorithm 1 that add new states. Step 11 can only adds states in $\Pi \cup \Pi^2$, so step 11 is only executed a finite number of times. As for Step 16, because the parser $\mathcal{P}$ is deterministic and terminating, by definition in Appendix A.2.3, for any stack configuration, there will not be an endless sequence of ε transitions, so Step 16 is also only executed a finite number of times.

[5] The definition is slightly different in the cited references; nevertheless, their proof works on this definition.

The correctness of Algorithm 1 can be naturally deduced by its construction, because it simply simulates the behavior of the parser $\mathcal{P}$ with the current stack top, and only outputs the stack when it is stable. □

A.3.2 Proof of Theorem 2

Proof. Formally, $\tilde{P}_a$ can be defined as follows:

$$\tilde{P}_a(\alpha \in \Pi^+) := \left\{ \beta \in \Pi^+ \middle| \alpha \xrightarrow[\mathcal{P}]{a} \beta \right\}. \tag{6}$$

The construction of $\tilde{P}_a$ in Algorithm 2 trivially simulates one a-labelled transition of the parser $\mathcal{P}$ on the current stack top, so it meets Definition 6.

The process of the parser processing $w = w_1 \dots w_n$ can be decomposed into a sequence of unconditional ε-transitions, followed by w_i-labelled transitions, followed by another sequence of unconditional ε-transitions. Each w_i-labelled transition is simulated by the corresponding $\tilde{P}_{w_i}$, and the unconditional ε-transitions are handled by P_ε. Therefore, the composition $P_w = P_\varepsilon \circ \tilde{P}_{w_1} \circ P_\varepsilon \circ \dots \circ P_\varepsilon \circ \tilde{P}_{w_n} \circ P_\varepsilon$ correctly simulates the parser $\mathcal{P}$ processing the terminal sequence w on the input stack α, and produces the stabilized output stack β if it exists. □

A.3.3 Proof of Theorem 3

Proof. Because $\mathcal{A}$ is constructed as a FSA, the language recognized by $\mathcal{A}$ is regular. The language of all valid (lexer state, parser stack) pairs for a given token $v \in \mathcal{V}$ can be obtained by reversing the language recognized by $\mathcal{A}$, taking the Brzozowski derivative (Brzozowski, 1964) with respect to v, and then reversing it back. Since the class of regular languages is closed under these operationsHopcroft & Ullman, the resulting language is also regular. □

A.4 Dataset construction details

Java, Go, and SQL We obtain their Lark grammars from the previous work Syncode (Ugare et al.). Because the grammar format for XGrammar and Formatron is different from Lark, we manually convert the Lark grammars to respective formats for each baseline. For each programming language, we take the first 1000 samples from the Stack dataset (Kocetkov et al.) that can be successfully parsed by the Lark parser to construct the evaluation dataset.

JSON Schemas We use the benchmark dataset MaskBench (mas), an extension of JSON Schema Bench (Geng et al., a) by adding schema conformant and non-conformant JSON instances to each schema. We generate the Lark grammar from the JSON schemas using the script provided in MaskBench, and only use the schemas in MaskBench where the Lark parser can successfully parse all the conformant JSON instances and reject all the non-conformant JSON instances. We then randomly sample 1000 schemas for evaluation.

A.5 Description of baselines in experiments

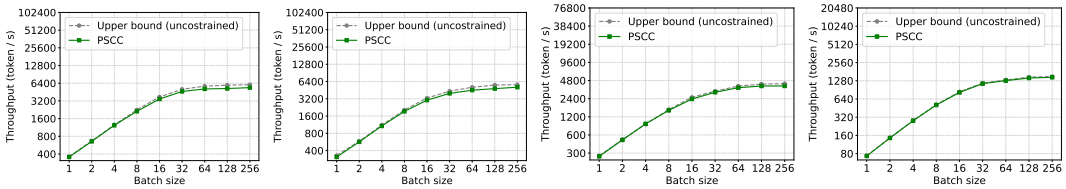
We describe the baselines used in our experiments in detail.

- XGrammar (Dong et al.) uses a character-level non-deterministic PDA[6]. For each state, it precomputes the context-independent accepted and rejected tokens, and only calls the parser for the context-dependent tokens.
- GreatGramma (Park et al.) uses a lexer and a parser. It converts each token into all possible terminals sequences and reduces the number of parser calls by sharing the parser calls among tokens with the same terminal sequence. After computing the accepted terminal sequences, it maps them back to the original tokens. It also precomputes the context-dependent and context-independent terminal sequences for each parser state.

[6]In the latest implementation that we use in the experiments, this has been changed to an Earley (Earley) parser.

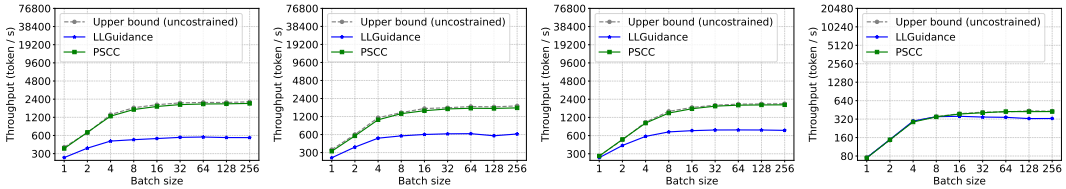
- Formatron (Sun et al.) uses an Earley parser. It dynamically identifies and eliminates invalid or redundant parser states during parsing, and uses a state cache to speed up the repetitive parsing process.
- LLGuidance (Moskal et al.) uses a lexer and an Earley parser. It organizes the vocabulary into a trie, and skips the whole subtree if the prefix token is rejected. It also leverages the lexer on the vocabulary to pre-identify the terminal sequences.

A.6 Extra Throughput Results



(a) Gemma 3 270M. (b) Qwen 2.5 0.5B. (c) Llama 3.2 1B. (d) Qwen 2.5 7B.

Figure 4: End-to-end throughput (tokens per second) on the **Go** dataset using different methods on different models with various batch sizes.



(a) Gemma 3 270M. (b) Qwen 2.5 0.5B. (c) Llama 3.2 1B. (d) Qwen 2.5 7B.

Figure 5: End-to-end throughput (tokens per second) on the **SQL** dataset using different methods on different models with various batch sizes.

Due to page limit, we only present the end-to-end throughput results on Java and schema-conformant JSON in Section 4.3. The results on the Go and SQL datasets are similar and are included here in Table 4 and Table 5, respectively.