
DynaTree: Dynamic Tree-based Speculative Decoding with Adaptive Pruning

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Abstract

Autoregressive generation in large language models (LLMs) suffers from inherent sequential bottlenecks that severely underutilize modern GPU parallelism. Speculative decoding accelerates inference by using a smaller draft model to propose candidate tokens for parallel verification by the target model. However, existing linear approaches explore only a single token sequence per iteration, leading to substantial computational waste when early predictions fail. We propose **DynaTree**, a tree-based speculative decoding framework that generates multiple candidate paths through top- k branching at each tree level and verifies them simultaneously via specialized tree attention mechanisms. To manage the exponential growth of tree size, we introduce an adaptive pruning strategy that dynamically eliminates low-probability branches based on learned probability thresholds. Experiments on Pythia models demonstrate that DynaTree achieves $1.62\times$ speedup over standard autoregressive decoding, substantially outperforming both existing assisted generation methods and linear speculative decoding baselines. Comprehensive analysis reveals critical trade-offs between tree depth, branching factor, and pruning aggressiveness, with consistent improvements observed across varying generation lengths.

1 Introduction

The remarkable capabilities of large language models (LLMs) have transformed natural language processing, yet their deployment faces a fundamental bottleneck: the sequential nature of autoregressive token generation. During the decode phase, each new token must be generated conditioned on all previously generated tokens, forcing the model to perform a full forward pass for every single token (2). This step-by-step dependency severely underutilizes modern GPU parallelism, as powerful compute units remain idle while awaiting the next token, creating what is fundamentally a *memory-bound* rather than compute-bound process (3; 4).

Speculative decoding has emerged as a promising solution to this bottleneck (1). The core insight is elegant: use a smaller, faster *draft model* to rapidly propose multiple candidate tokens, then leverage the target model’s parallel processing capability to verify all candidates in a single forward pass. If the target model agrees with the draft predictions, multiple tokens are accepted simultaneously, effectively amortizing the cost of the expensive target model inference. Critically, this acceleration comes with a mathematical guarantee: the output distribution remains *identical* to standard autoregressive generation through careful rejection sampling (5).

However, existing speculative decoding methods predominantly employ *linear* drafting strategies, where the draft model proposes a single sequential chain of K tokens (e.g., $t_1 \rightarrow t_2 \rightarrow t_3 \rightarrow \dots \rightarrow t_K$). This single-path exploration suffers from a critical inefficiency: if any token t_i in the sequence

** Equal contribution.

is rejected during verification, *all subsequent tokens* t_{i+1} through t_K are discarded, wasting both the draft generation effort and verification computation. When the draft model’s predictions diverge from the target model’s distribution—which is common, especially for smaller draft models—this leads to poor acceptance rates and limits the achievable speedup (6).

This observation motivates a natural question: why restrict speculation to a single path? If the uncertainty lies in which token will be correct, exploring multiple candidate paths in parallel should increase the probability that at least one path aligns with the target model’s preferences. This insight motivates a shift from linear chains to tree-based speculation structures, where the draft model generates the top- B candidate tokens at each depth level, creating multiple parallel exploration paths. For instance, with branch factor $B=3$ and depth $D=3$, the tree can explore up to 27 distinct token sequences simultaneously, dramatically increasing the likelihood of finding an acceptable path.

However, this approach introduces two critical challenges. First, verifying all tree nodes efficiently requires a specialized tree attention mechanism with causality-preserving masks, enabling the target model to process the entire tree structure in a single forward pass. Second, naively expanding a full tree leads to exponential growth (B^D nodes), quickly overwhelming computational budgets. To address this, we introduce an adaptive pruning strategy that dynamically eliminates low-probability branches based on a probability threshold τ and enforces a maximum node budget, balancing exploration breadth with computational efficiency.

We present **DynaTree**, a tree-based speculative decoding framework that instantiates these ideas.

We conduct comprehensive experiments on Pythia-2.8B (target) and Pythia-70M (draft) models, demonstrating that DynaTree achieves $1.62\times$ speedup over standard autoregressive decoding—significantly outperforming both HuggingFace’s assisted generation ($1.36\times$) and linear speculative decoding with $K=6$ ($1.11\times$). Through systematic hyperparameter analysis across 450 configurations, we identify optimal settings ($D=8$, $B=3$, $\tau=0.03$ for 500-token generation) and reveal critical trade-offs between tree depth, branching factor, and pruning aggressiveness. Ablation studies confirm that dynamic pruning contributes a 25.4% relative improvement by reducing tree size while maintaining acceptance quality. Our main contributions are: we propose DynaTree, a tree-based speculative decoding framework with adaptive pruning that achieves superior speedup over linear baselines; we provide comprehensive empirical analysis of the depth-breadth-threshold parameter space, establishing best practices for tree configuration; and we demonstrate consistent performance gains across varying generation lengths, providing insights into when tree-based exploration offers the greatest advantage.

2 Related Work

2.1 Speculative Decoding

Speculative decoding was introduced by **(author?)** (1) to accelerate LLM inference through a draft-verify paradigm. Linear implementations propose sequential token chains for parallel verification, but suffer from single-path inefficiency where early rejections waste all subsequent computation (6). Recent work has explored draft model selection trade-offs (13) and theoretical speedup bounds, but the fundamental limitation of linear exploration persists.

2.2 Tree-Based and Parallel Decoding

Tree-based speculation has been explored in SpecInfer (7) and OPT-Tree (8), which construct adaptive draft trees to maximize expected acceptance length. Our work differs by introducing probability-threshold-based adaptive pruning and providing systematic empirical analysis of the tree parameter space. Medusa (9) achieves parallel prediction through multiple decoding heads but requires model-specific fine-tuning, whereas DynaTree operates as a training-free inference-time technique.

2.3 Dynamic Pruning Strategies

ProPD (10) introduces early pruning based on top- k prediction heads, while CAST (11) develops cost-aware tree construction. DySpec (12) employs greedy dynamic expansion guided by draft model confidence. Our adaptive pruning strategy combines probability thresholds with node budgets, offering a simpler yet effective approach that balances exploration with computational efficiency.

3 Placeholder for Method Section

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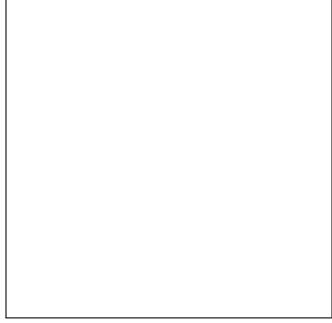


Figure 1: Sample figure caption.

Table 1: Sample table title

| Part | | |
|----------|-----------------|------------------------|
| Name | Description | Size (μm) |
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```

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```
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Acknowledgments and Disclosure of Funding

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