d^{2}Cache: Accelerating Diffusion-Based LLMs via Dual Adaptive Caching

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Core message: Diffusion LLMs cannot use standard KV cache because bidirectional attention makes one token update change the whole sequence context. d^{2}Cache solves this with a training-free, token-level adaptive cache that refreshes only the KV states that matter at each step.

Method:
Dual Adaptive Cache

Stage 1 selects masked tokens that are likely to change soon. Stage 2 keeps the prompt and decoded tokens with the highest attention influence.

3.5×
Average speedup
Across LLaDA-Inst and Dream-Inst over six benchmarks.

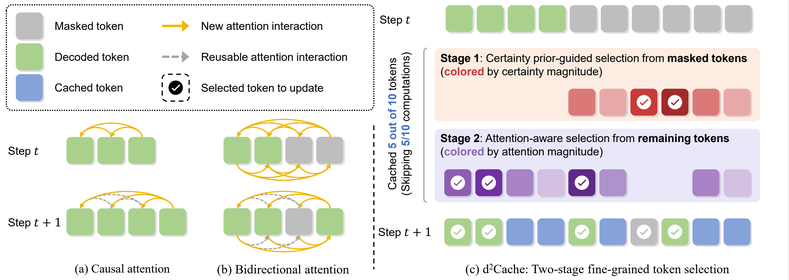
4.7×
Best-case speedup
Dream-Inst on GSM8K improves from 2.62 to 12.25 tok/s.

+2.0 pts
Quality gain
Average score rises from 51.4 to 53.4 on Dream-Inst.

Why dLLMs Are Hard to Cache

- Autoregressive models can reuse KV states because new tokens are appended under causal attention.
- Diffusion LLMs iteratively replace masked tokens inside a fixed-length sequence with **bidirectional attention**.
- Updating one token changes the context seen by all others, so naive KV reuse is invalid and full recomputation becomes expensive.
- Existing cache methods rely on coarse refresh windows or static/dynamic segments, which miss token-level dynamics.

From Full Recompute to Adaptive Refresh

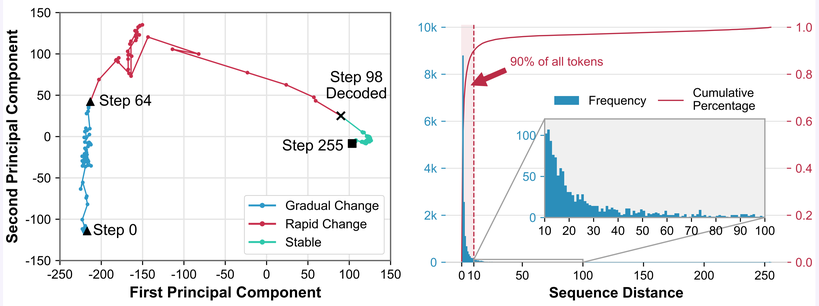


d^{2}Cache replaces coarse segment rules with token-level selection: refresh the small subset of tokens whose KV states are most valuable, and reuse the rest.

Three Empirical Observations

- **Masked tokens follow three phases:** gradual change → rapid change → stable. Only the rapid-change phase needs active refresh.
- **Decoding is local:** 90% of newly decoded tokens appear within distance 10 of the most recently decoded token.
- **Attention is sparse:** prompt and decoded tokens receive most of the attention, while masked tokens receive little.

Token Dynamics



Left: masked-token KV states change sharply only right before decoding. Right: consecutive decoded positions are usually close to each other, which motivates a local certainty prior.

d^{2}Cache Overview

d^{2}Cache splits tokens into **prompt**, **masked**, and **decoded** groups, then refreshes KV states with a two-stage strategy:

- **Stage 1:** select masked tokens that are likely to be decoded soon.
- **Stage 2:** among the remaining tokens, keep only those with the largest attention influence.
- Refresh KV states for the selected tokens and reuse cached KV states for everything else.

Stage 1: Certainty Prior-Guided Selection

For each masked token at position i, estimate how likely it is to be decoded soon from the density of nearby known tokens:

$$D(i) = \sum_{j=0}^{L-1} \exp\left(-\frac{|i-j|^2}{2\sigma^2}\right) \mathbb{I}_{\{j \notin M\}}$$

Combine this structural prior with the model confidence s^i and select the top-k masked tokens:

$$M^* = \underset{i \in M}{\arg\operatorname{top_k}} D(i) \cdot s^i$$

- Higher $D(i)$ means stronger local support from prompt or already decoded tokens.
- This also yields a more reliable **quasi left-to-right decoding order**.

Stage 2: Attention-Aware Selection

For prompt and decoded tokens, d^{2}Cache computes attention rollout and derives an influence score

$$c_j = \sum_{i=1}^{L} C_{ij}^{(N)}$$

Then it selects the smallest set of tokens whose cumulative influence exceeds threshold p.

- High-influence prompt/decoded tokens are refreshed.
- Low-influence tokens safely keep their cached KV states.

Why Selective Updates Win

- More computation is not always better for dLLMs.
- Updating masked tokens during the gradual-change phase wastes compute without helping quality.
- d^{2}Cache refreshes KV states only when token dynamics or attention concentration justify it.
- The method is **training-free** and does not change model parameters.

What Changes in Decoding

- Confidence-only NAR decoding tends to show unstable ordering and premature end-of-sequence overconfidence.
- Certainty prior-guided decoding is more stable because it prefers tokens supported by nearby known context.
- This makes d^{2}Cache not only a cache mechanism, but also a more reliable decoding strategy.

Experimental Setup

- Models: LLaDA-Inst and Dream-Inst
- Tasks: GSM8K, MBPP, HumanEval, Math-500, GPQA, MMLU-Pro
- Baselines: Vanilla, dLLM-Cache, Fast-dLLM
- Default settings: $\sigma = 10$, top-$k = 32$, $p = 0.1$

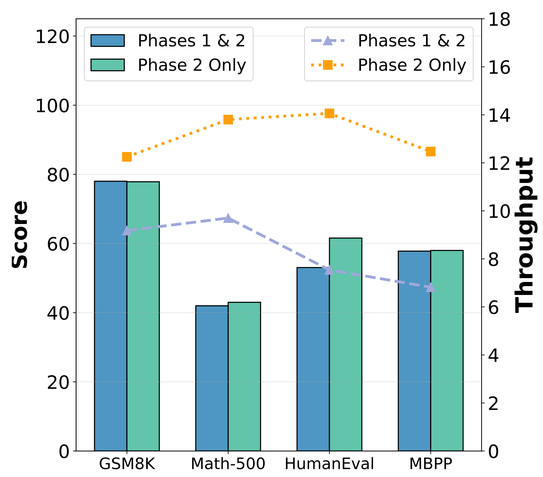
Main Results

Method	LLaDA Thr.	LLaDA Score	Dream Thr.	Dream Score
Vanilla	3.54	43.6	3.64	51.4
dLLM-Cache	8.16	43.8	7.64	50.9
Fast-dLLM	9.38	43.4	9.59	51.7
d^{2}Cache	**12.24**	**44.4**	**12.89**	**53.4**

d^{2}Cache delivers the best overall balance of **throughput**, **latency**, and **quality**.

- **Dream-Inst on GSM8K:** 2.62 → 12.25 tok/s, a **4.7**× speedup, while score improves from 76.7 to 78.2.
- **Against Fast-dLLM:** d^{2}Cache is usually both faster and more accurate.

Ablation: Update Only the Important Phase



Phase-2-only updates are faster than updating both phases, while keeping comparable or better quality.

Takeaways

- Diffusion LLM caching should be treated as a **fine-grained token selection problem**: d^{2}Cache uses **certainty prior** for masked tokens and **attention influence** for prompt/decoded tokens, reducing redundant computation while often improving decoding quality.