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ToT-Prompt Optimization for LLM-based Automatic Summarization

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01

Introduction

Introduction

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📌 Core Problem

Select and arrange prompt words, maximize the quality of summaries generated by LLMs

🔍 Problem Nature

- Combinatorial Optimization Problem
- Huge Search Space: n components → O(n!) possible permutations and combinations
- High Evaluation Cost

Introduction

Practical Application Background

- Financial Analysis:

  Efficiently process financial news, corporate reports

- Scientific Research:

  Accelerating knowledge extraction and integration

- Law & Healthcare:

  Quickly condense legal cases, generate medical record summaries

02

Formulization

Formalization of the Problem

Find an optimal ordered sequence from n prompt components within a limited evaluation budget.

Maximize: $Q(\sigma)$

where $Q(\sigma) = f_{comp}(\sigma) + f_{order}(\sigma) - p(\sigma)$ Component Base Score, Order Synergy Effect, Penalty Terms

Decision variables: $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_k) \in \Pi_k(C)$

Let $C = c_1, c_2, \ldots, c_n$ be the set of all available prompt components.

The decision variable is an ordered sequence:

$$\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_k)$$

where:

$k \leq n$: sequence length (variable)

$\sigma_i \in C$: component ID at position i in the sequence

$\Pi_k(C)$: set of all permutations of k elements from C

Constraints

1. Dependency Constraints

For each component $c \in C$, let its dependency set be $D(c) \subseteq C$:

$$\forall c \in \sigma, \forall d \in D(c) : d \in \sigma \text{ and } pos(d) < pos(c)$$

where $\text{pos}(x)$ represents the position index of component x in sequence σ.

2. Mutual Exclusion Constraints

For mutually exclusive component pairs $(c, d) \in X$ (where X is the mutual exclusion relation set):

$$c \notin \sigma \text{ or } d \notin \sigma$$

Constraints

3. Length Constraints

Let $t(c)$ be the token count of component c, and $t_{\text{conn}}(c_i, c_j)$ be the connection token count between components:

$$\sum_{i=1}^{k} t(\sigma_i) + \sum_{i=1}^{k-1} t_{conn}(\sigma_i, \sigma_{i+1}) \leq T_{max}$$

4. Position Constraints

For components with position requirements:

Start components: $c \in C_{\text{start}} \Rightarrow \text{pos}(c) = 1$

End components: $c \in C_{\text{end}} \Rightarrow \text{pos}(c) = k$

Middle components: $c \in C_{\text{middle}} \Rightarrow 1 < \text{pos}(c) < k$

NP-Hard Proof

Theorem: The prompt sequence optimization problem is NP-hard.

Proof by reduction from Directed Hamiltonian Path (DHP):

Given: A directed graph $G = (V, E)$ with $|V| = n$ vertices.

Construct an instance of our problem:

Each vertex $v_i \in V$ corresponds to a prompt component c_i

For each edge $(v_i, v_j) \in E$, set synergy $s(c_i, c_j) = 1$

For non-edges $(v_i, v_j) \notin E$, set $s(c_i, c_j) = -\infty$

Set all component base scores $w(c_i) = 0$

Set length constraint to accept all sequences

Set no dependency or mutual exclusion constraints

NP-Hard Proof

Claim: There exists a Hamiltonian path in G if and only if there exists a sequence σ of length n with $Q(\sigma) = n - 1$.

Proof:

($\Rightarrow$) If G has Hamiltonian path $v_1 \to v_2 \to ... \to v_n$, then sequence $\sigma = (c_1, c_2, ..., c_n)$ has $f_{order}(\sigma) = n - 1$, so $Q(\sigma) = n - 1$.

($\Leftarrow$) If sequence σ has $Q(\sigma) = n - 1$, then all n components appear exactly once and all consecutive pairs have synergy 1, meaning they correspond to edges in G, forming a Hamiltonian path.

Since DHP is NP-hard and this reduction is polynomial-time, our problem is NP-hard.

Corollary: The optimization version (finding max $Q(\sigma)$) is NP-hard.

State Space Complexity

Search Space

The state space consists of all ordered sequences satisfying constraints:

$$S = \{\sigma \in \cup_{k=0}^{n} \Pi_k(C) \mid \sigma \text{ satisfies all constraints}\}$$

State space size:

$$|S| = \sum_{k=0}^{n} P(n,k)$$

where

$$P(n,k) = \frac{n!}{(n-k)!}$$

State Space Complexity

Theoretical Upper Bound

$$|S_{theoretical}| = \sum_{k=0}^{n} P(n,k) = \sum_{k=0}^{n} \frac{n!}{(n-k)!}$$

Asymptotic complexity: $O(n!)$

Practical

$$|S_{practical}| \approx O(\frac{n!}{2^d})$$

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03

Method Design：ToT Prompt Optimizer

Design Rationale

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Why heuristic solution?

Problem: Prompt optimization is a High-Dimensional, Discrete Combinatorial Optimization problem.

Design Rationale

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Why heuristic solution?

Problem: Prompt optimization is a High-Dimensional, Discrete Combinatorial Optimization problem.

Problem Challenges:

- **Combinatorial Explosion** ($O(2^N)$): Exhaustive search is intractable, requiring effective **pruning.**
- **High Evaluation Cost**: Objective function evaluation (Full Evaluation) is **costly, time-consuming**, **non-convex, and non-differentiable** (precluding gradient-based methods)
- **Discreteness & Constraints**: Component selection is binary/discrete, with predefined **conflict constraints**, requiring methods that support **step-wise state construction** and **validity checks**.

Design Rationale

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Why heuristic solution?

Justification for Metaheuristic Search

- **Monte Carlo Tree Search** (MCTS): Strategically balances exploration (new sets) and exploitation (high-performers) using **upper bound score**, ensuring costly Full Evaluations are allocated to the most promising states
- **Beam Search**: Offers a faster, greedy complement for rapid convergence to local optimums by retaining only the top k states at each step

Key Feature: Learning-to-Optimize (L2O): Incorporates a lightweight Heuristic Evaluation (predictive assessment) to guide the search.

ToT Prompt Optimizer

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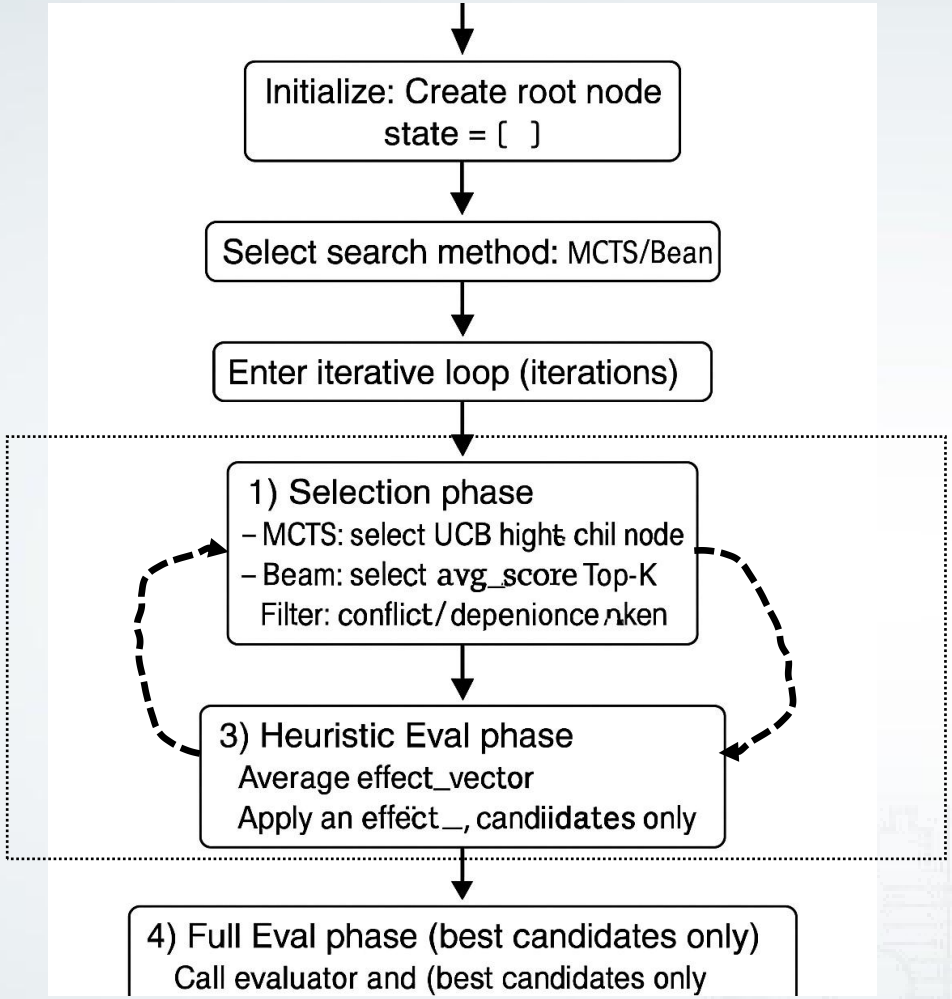

ToT Prompt Optimizer

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Core Structure and State Representation

- State: A valid set of Prompt components.
- Node: A position within the search tree, storing a state S and search statistics.

```python
@dataclass
class SearchNode:
    """搜索树节点"""
    node_id: str
    state: List[str]  # 组件ID列表
    parent_id: Optional[str]
    depth: int
    visits: int = 0
    total_score: float = 0.0
    heuristic_score: float = 0.0
    full_evaluation_score: float = 0.0
    children_ids: List[str] = None
    is_fully_evaluated: bool = False
    metadata: Dict[str, Any] = None
```

Monte Carlo Tree Search (MCTS)

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MCTS guides the search through iterative sampling, executing four steps per iteration :

- **Selection**: Starting from the root, nodes are recursively selected based on the highest heuristic score
- **Expansion**: Valid candidate child states (enforcing **conflict avoidance** via generate_candidates) are generated from the selected node. New child nodes are created and immediately undergo Heuristic Evaluation (evaluate_state_heuristic).
- **Evaluation** (Simulation/Rollout): The most promising nodes (e.g., $\text{avg\_score} > \text{best\_score} \times 0.7$) are subjected to a costly Full Evaluation (**evaluate_state_full**) to obtain the accurate full_score.
- **Backpropagation**

Heuristic Scoring Function

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Purpose: Provide a **lightweight approximation** of prompt quality to guide the search efficiently, avoiding expensive full LLM evaluations at every node.

Formula: Weighted sum of five metrics $\in [0, 1]$:

$$H = \sum_{m \in M} w_m \cdot S_m$$

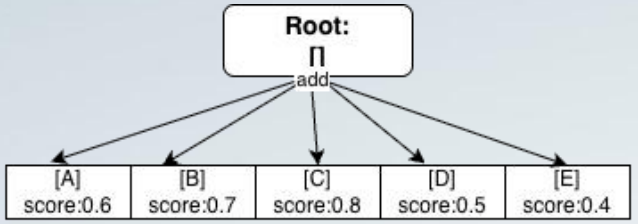
- M = {Faithfulness, Conciseness, Completeness, Readability, Insightfulness}
- Pre-defined Weights

Metric Calculation Strategy: Balances speed and reliability

Rule-Based Metrics (Fast Heuristics): **Conciseness** on word count, **Completeness** on keyword coverage, **Readability** on average sentence length

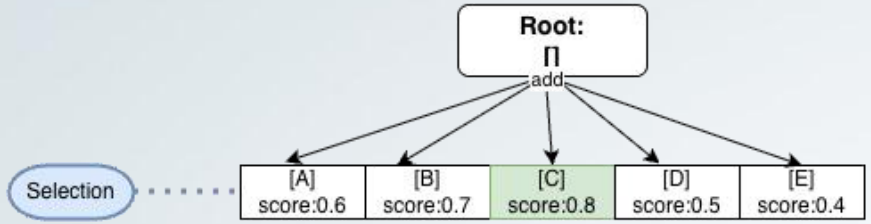
LLM-Based Metrics (Accurate Heuristics): Faithfulness and Insightfulness

Given 5 non-conflict componments: [A B C D E]



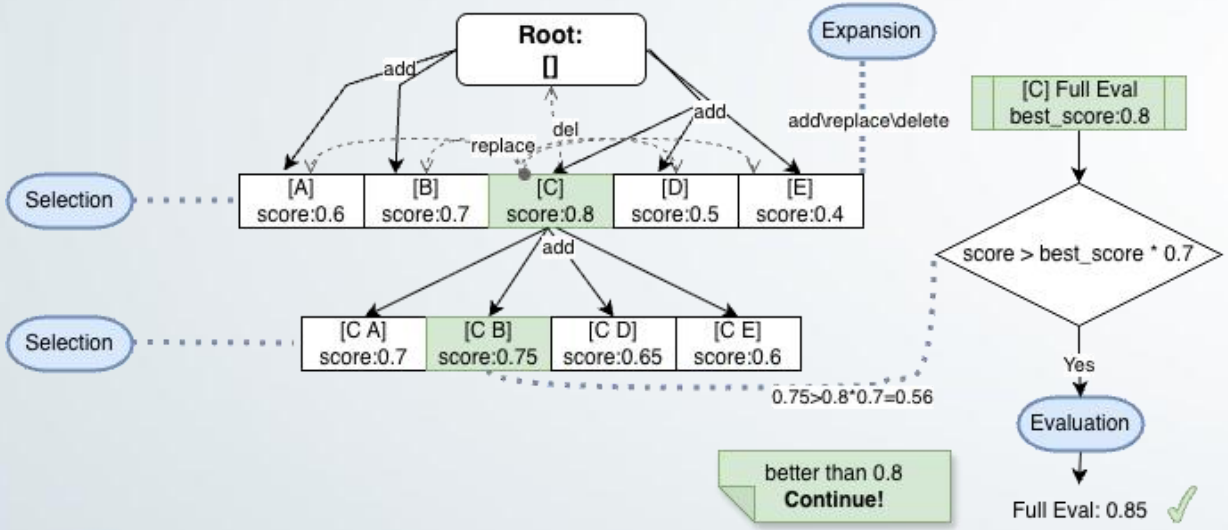
(1)

[] Full Eval
best_score:0

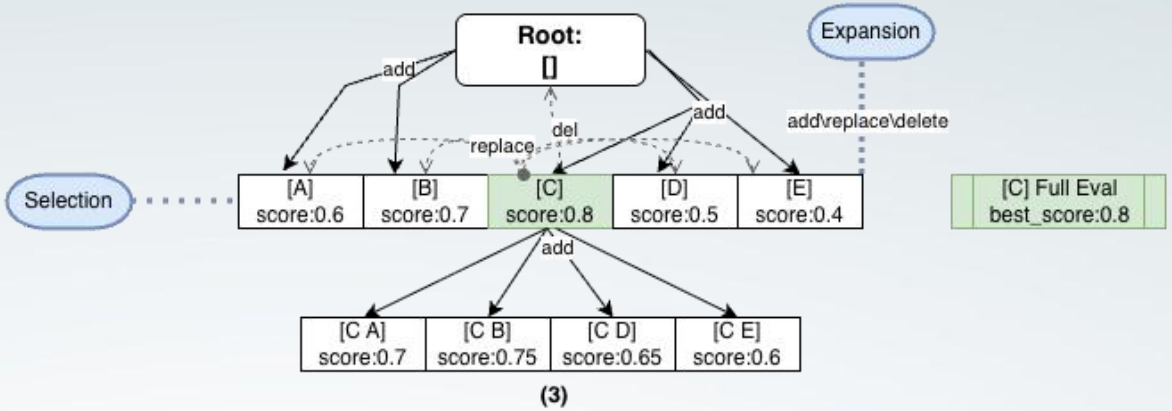


(2)

[C] Full Eval
best_score:0.8

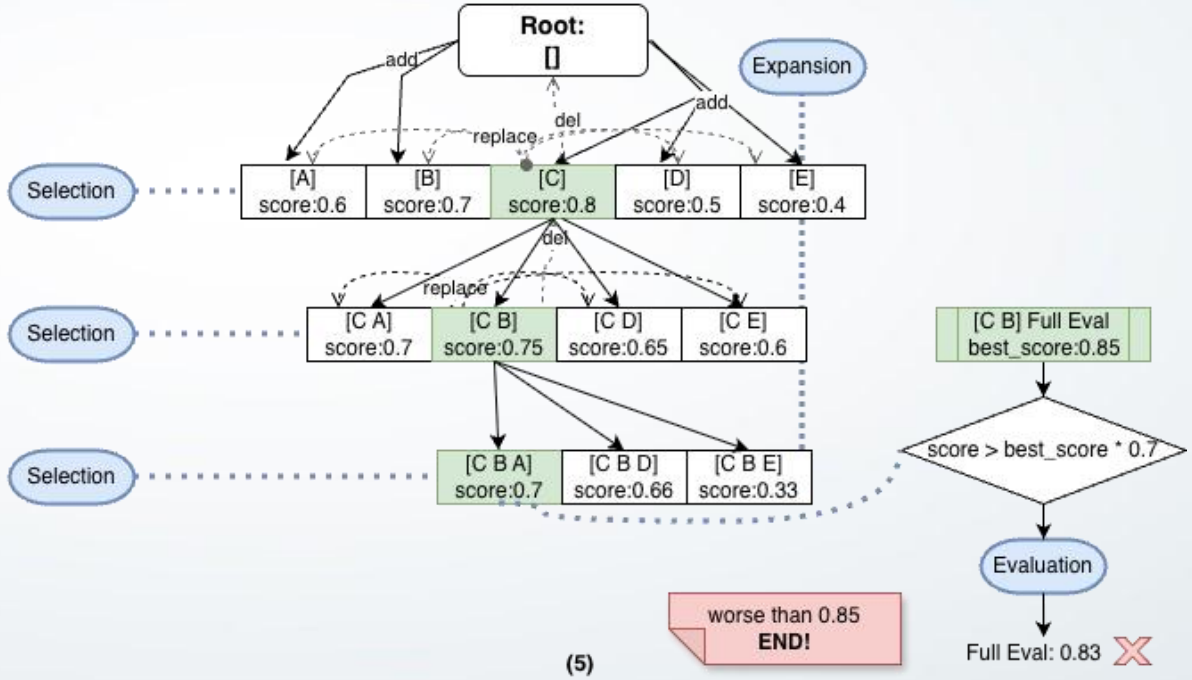


(4)



(3)

[C] Full Eval
best_score:0.8



(5)

Beam Search

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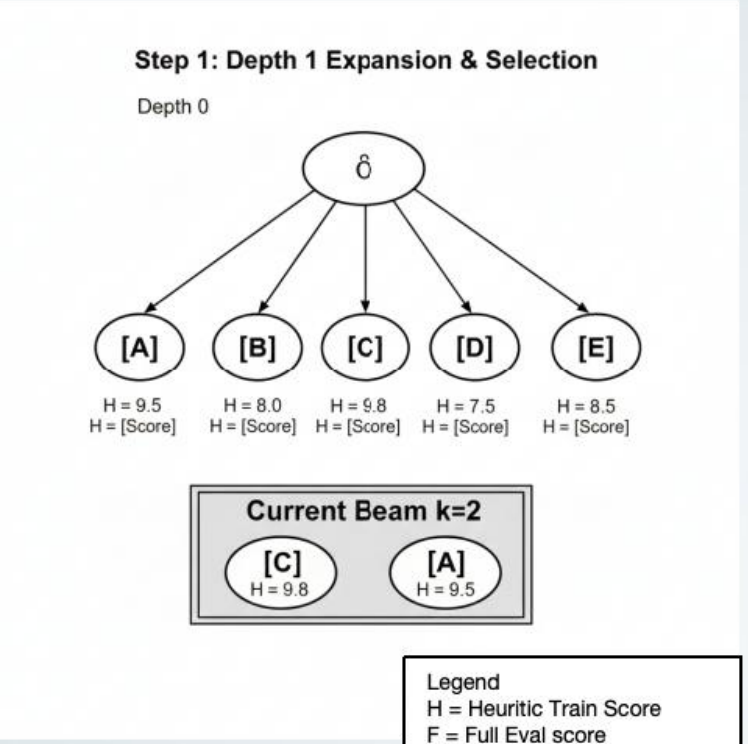
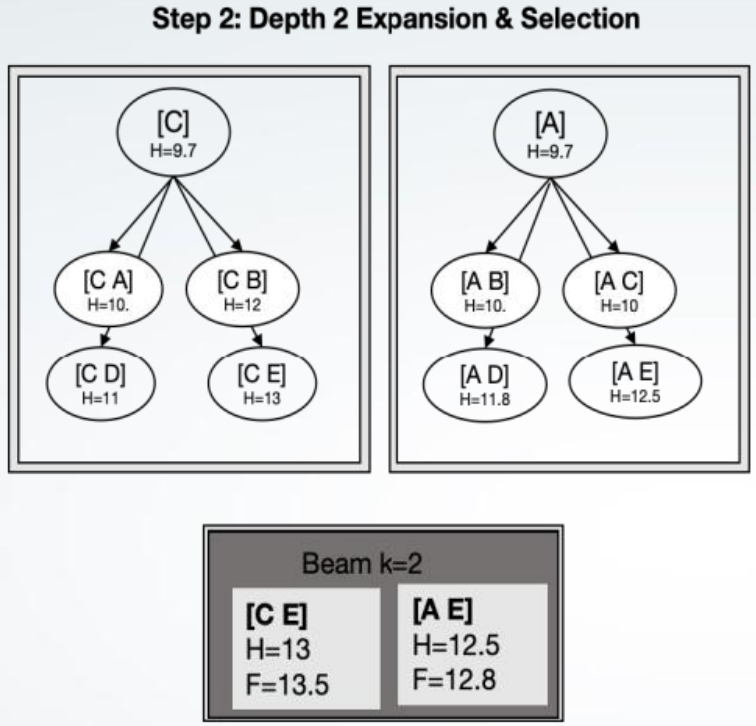
Beam Search implements a more greedy heuristic approach :

- **Breadth-First Pruning:** In each iteration, the **top-k** scoring nodes (the beam) from all existing nodes are selected.
- **Expansion and Heuristics:** All **new candidate states** are generated from the k beam nodes and assessed using Heuristic Evaluation.
- **Evaluation**: The new candidates are ranked by their Heuristic Score, and only the top k are selected to receive a Full Evaluation. This ensures a fast, concentrated search.

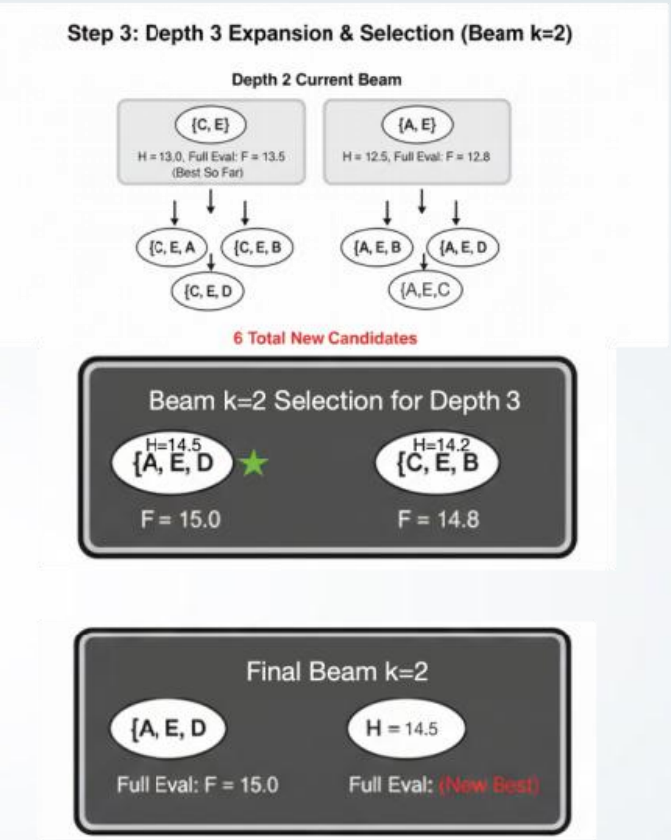
Given 5 non-conflict componments: [A B C D E]



(1)



(2)



(3)

Complexity Analysis

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Per-State Operations

- Constraint Checking (Dependency, Mutual Exclusion, Length, Position): Total complexity $\mathrm{O(k)}$ with optimization, where k is the sequence length
- Quality Evaluation $O(\sigma)$: $\mathrm{O(k)}$ for component base score, order synergy, and penalty terms

Algorithm	Per Iteration/Layer Complexity (General)	Worst Case Asymptotic Complexity
MCTS	$O(I(d \cdot \log b + b + C_e))$	$\mathcal{O}(I \cdot n)$
Beam Search	$O(d \cdot w \cdot b \cdot \log(w \cdot b))$	$\mathcal{O}(n^2 \log n)$

Complexity Analysis

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Search Algorithm Complexities

- Variables: I = iterations, d = depth, b= branching factor (avg.), C_e = evaluation cost, w = beam width, n = total components
- Efficiency: Both MCTS and Beam Search are significantly more efficient than the theoretical $\mathrm{O(n!)}$ brute-force search space

Algorithm	Per Iteration/Layer Complexity (General)	Worst Case Asymptotic Complexity
MCTS	$O(I(d \cdot \log b + b + C_e))$	$\mathcal{O}(I \cdot n)$
Beam Search	$O(d \cdot w \cdot b \cdot \log(w \cdot b))$	$\mathcal{O}(n^2 \log n)$

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04

Experimental Results and Discussion

Experiments

Dataset → Summarization Task

Instead of complex formats (URLs, PDFs) or dialogue-style content。

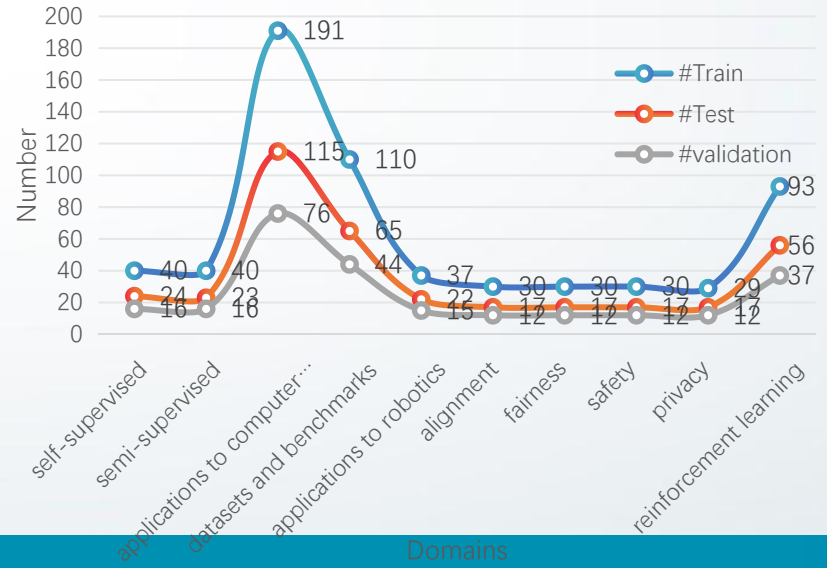
A clean, plain-text dataset was manually constructed for the experiments.

Source:

- Summarization： ICLR 2026 OpenReview platform
- Prompt Components： Human designed 20 Entries

Table 5: Statistics of word length across dataset splits.

Category	Content Length	Summary Length
Training Dataset	182.82	26.94
Test Dataset	184.56	26.50
Validation Dataset	174.90	26.35



```
{
"paper_id":"bU8tRjuanU",
"title":"Low-Rank Attention and Contrastive Alignment for Deep Multi-View Clustering",
"domain":"self-supervised",
"content":"Recent years have witnessed significant advancements in deep multi-view clustering (MVC). However, prevailing methods exhibit three critical limitations: (1) poor scalability for large-scale datasets, (2) neglect of anchor semantic consistency in feature alignment, and (3) inability to capture high-order feature interactions. To overcome these challenges, we propose a Low-Rank Attention and Contrastive Alignment framework (LRACA). Unlike conventional approaches that align sample-level features in shared subspaces, LRACA employs a category-aware anchor generation module to directly align high-level semantic prototypes (i.e., category centers) across views, explicitly enforcing clustering semantic consistency. Furthermore, we devise a dynamic low-rank attention mechanism to enhance feature discriminability, where entropy regularization constrains attention weight distributions to derive clustering pseudo-labels. Finally, a pseudo-label-guided cluster-level contrastive learning module maximizes cross-view mutual information through a feed-forward optimization paradigm. Extensive experiments on six large-scale multi-view datasets demonstrate that LRACA significantly outperforms state-of-the-art methods.",
"gold_summary":"This paper proposes a deep multi-view clustering algorithm equipped with an anchor-based attention mechanism and cluster-based contrastive learning, which achieves good performance, but has many problems, as detailed in the weaknesses section."
},
```


(a) An Example of Data Entry


```
{
"id":"conciseness",
"text":"Please use concise language",
"description":"Requires concise output",
"effect_vector":{
"conciseness":0.8,
"readability":0.6,
"completeness":-0.2
},
"conflicts":[
"detail_oriented",
"comprehensive"
],
"requires":[],
"estimated_tokens":8
},
```


(b) An Example of Prompt Component Entry

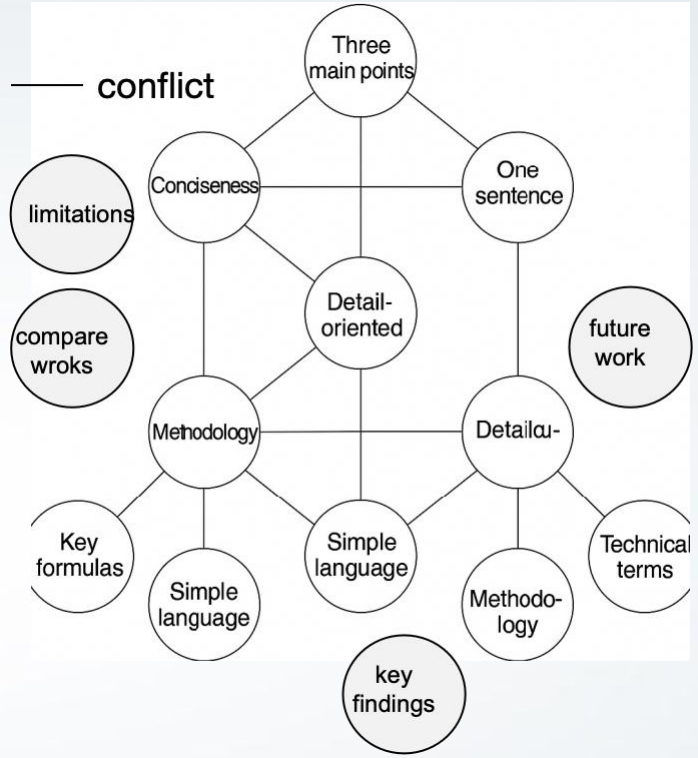


Fig. 4: Data Entry Statistic.

Setup

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Models:

- Base Model (for ToT Training): Qwen3-1.7B.
- Scoring Model (Discriminator): Qwen3-8B

Baselines：

- **SimplePrompt**: “Summary this paper”
- **DetailedPrompt**: “A prompt asking for core content, methodology, and contributions”
- **StructuredPrompt**: “A prompt asking to summarize from four aspects: background, methodology, experiments, and conclusions”

Metrics:

- **N-gram Static Metrics**: ROUGE-2 F1 and ROUGE-L F1
- **Semantic Similarity Metrics:** BERTScore F1 (using "bert-base-multilingual-cased").
- **LLM Evaluation Score**: Heuristic Scoring

Experimental Results and Discussion

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Overall Performance

- **ToT Prompt-Beam's Success:** This strategy consistently achieved the highest scores across all reported metrics
- MCTS vs. Beam Search:

  ToTPrompt-MCTS < **ToTPrompt-Beam**

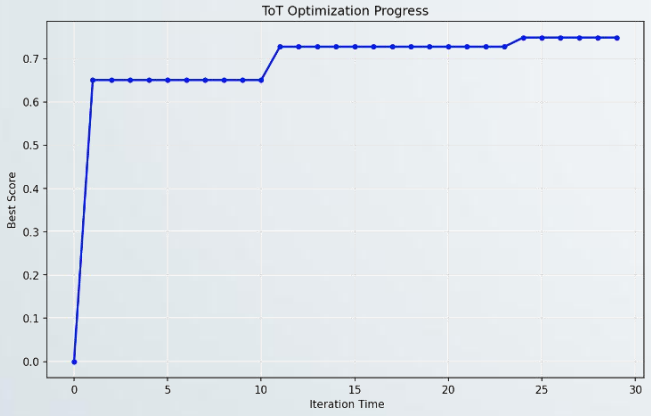
Prompt Strategy	Heuristic Score ↑	ROUGE-2 ↑	ROUGE-L ↑	BERTScore ↑
SimplePrompt	0.51 ± 0.10	0.03 ± 0.02	0.03 ± 0.02	0.05 ± 0.13
DetailedPrompt	0.58 ± 0.06	0.02 ± 0.01	0.07 ± 0.02	-0.01 ± 0.04
StructuredPrompt	0.58 ± 0.04	0.01 ± 0.01	0.06 ± 0.01	-0.18 ± 0.20
ToT-MCTS(ours)	$0.61 + 0.00$	0.03 ± 0.02	0.09 ± 0.01	$0.06 + 0.04$
ToT-Beam(ours)	$\mathbf{0.67 \pm 0.02}$	$\mathbf{0.07 \pm 0.05}$	$\mathbf{0.13 \pm 0.05}$	$\mathbf{0.16 \pm 0.06}$

Convergence Analysis

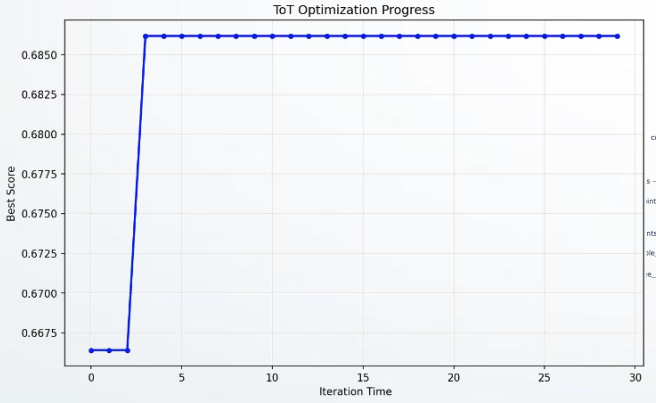
Scores quickly converged in both strategies. Beam Search converged significantly faster than MCTS due to its greedy-like selection at each step

Potential Reason for Rapid Convergence

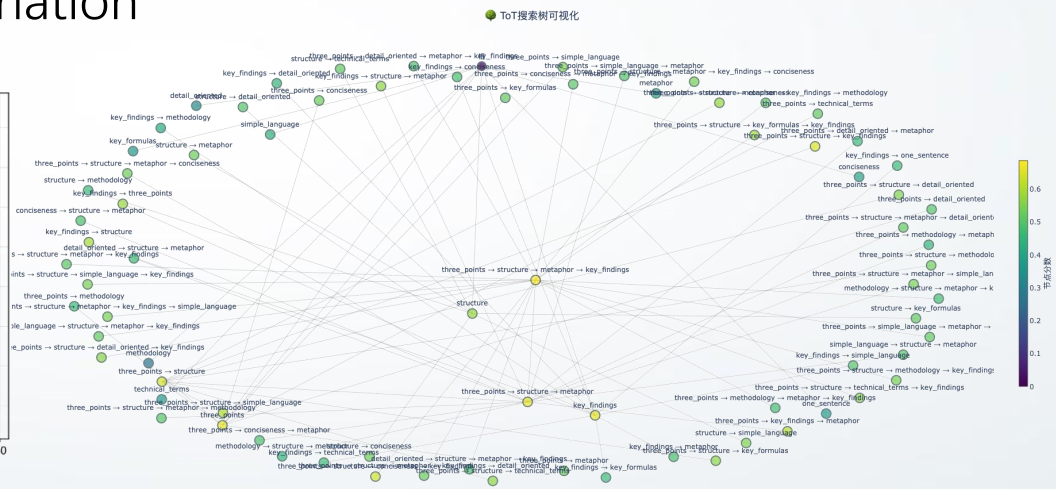
- an insufficiently rich set of prompt components,
- a small candidate set
- a small training batch size leading to minimal score variation



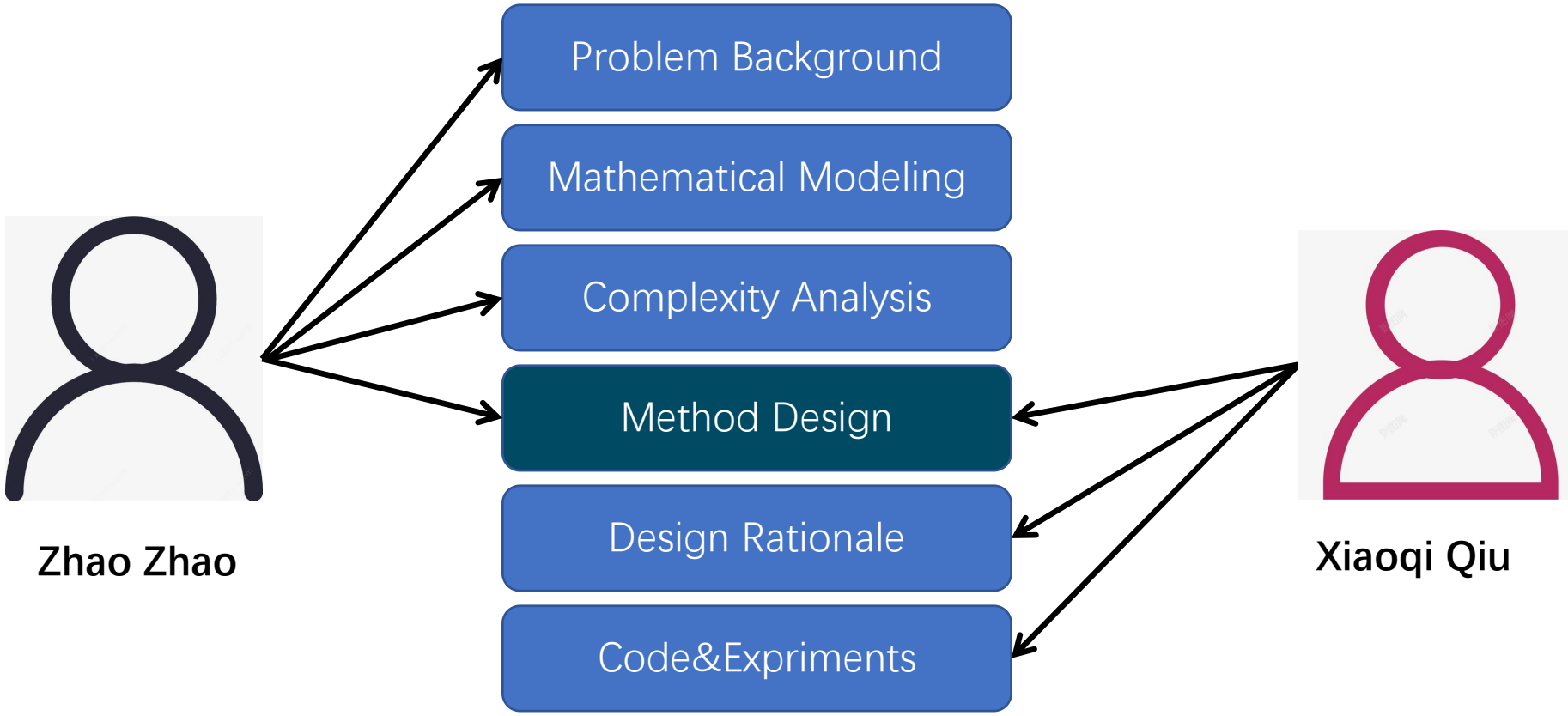
(a) Optimization Progress of MCTS Search



(b) Optimization Progress of Beam Search



Division of Lablor



Code&Dataset:
git@github.com:Siki-cloud/ToT_Optimizer_for_LLMSum.git

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“ToT-Prompt Optimization for LLM-based Automatic Summarization”

Thank you

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