Navigating the Alpha Jungle: An LLM-Powered MCTS Framework for Formulaic Factor Mining

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Abstract

Alpha factor mining is pivotal in quantitative investment for identifying predictive signals from complex financial data. While traditional formulaic alpha mining relies on human expertise, contemporary automated methods, such as those based on genetic programming or reinforcement learning, often suffer from search inefficiency or yield poorly interpretable alpha factors. This paper introduces a novel framework that integrates Large Language Models (LLMs) with Monte Carlo Tree Search (MCTS) to overcome these limitations. Our approach leverages the LLM's instruction-following and reasoning capability to iteratively generate and refine symbolic alpha formulas within an MCTS-driven exploration. A key innovation is the guidance of MCTS exploration by rich, quantitative feedback from financial backtesting of each candidate factor, enabling efficient navigation of the vast search space. Furthermore, a frequent subtree avoidance mechanism is introduced to bolster search efficiency and alpha factor performance. Experimental results on real-world stock market data demonstrate that our LLM-based framework outperforms existing methods by mining alphas with superior predictive accuracy, trading performance, and improved interpretability, while offering a more efficient solution for formulaic alpha mining.

1 Introduction

Predicting price movements in financial markets, characterized by low signal-to-noise ratios, remains a central challenge in quantitative investment. A common strategy to enhance model predictiveness is the extraction of predictive signals, or alpha factors (hereafter sometimes simply "alpha"), from stock data Qian *et al.* [2007]; Tulchinsky [2019]. Current alpha factor mining methodologies broadly fall into two categories: neural network-based and formula-based. Neural approaches (e.g., FactorVAE Duan *et al.* [2022], HIST Xu *et al.* [2021a], REST Xu *et al.* [2021b]) implicitly construct complex alphas via deep learning, capturing intricate patterns but often suffering from a lack of interpretability. In contrast, formula-based methods aim to discover alphas represented by explicit mathematical expressions. These alpha factors are traditionally human-crafted, reflecting market insights (e.g., Fama-French factors (Fama and French [1992]), financial anomalies (Harvey *et al.* [2016]; Hou *et al.* [2020])). In recent years, automated techniques have emerged, employing methods like genetic programming or reinforcement learning to discover such formulaic alphas Shi *et al.* [2024]; Yu *et al.* [2023]; Zhang *et al.* [2020, 2023b].

Despite their promise, existing automated formulaic alpha mining approaches face significant limitations. **First, the discovered alphas often exhibit poor interpretability.** These automated methods frequently engage in unconstrained, data-driven exploration of the vast alpha space, often without sufficient guidance from financial theory or domain expertise. Consequently, the resulting formulas can be overly complex and opaque. This lack of transparency poses considerable challenges in practical investment scenarios: it hinders practitioners' ability to understand the underlying economic rationale of a strategy, makes it difficult to attribute portfolio performance accurately, and can erode trust, thereby impeding the adoption of these alphas even if they show promise in backtests. **Second, current methodologies often suffer from search inefficiency.** The endeavor to identify a sufficient number of effective alpha factors typically requires the generation and evaluation of an enormous volume of candidate formulas. This exhaustive search process, while necessary due to the low signal density, inherently increases the likelihood of discovering spurious relationships and overfitting to the training data Harvey *et al.* [2016]. As a result, many discovered alphas may exhibit poor generalization and deliver underwhelming out-of-sample performance.

Addressing the identified shortcomings necessitates innovative approaches. In this light, Large Language Models (LLMs) emerge as a promising direction, given their vast prior knowledge and strong reasoning capabilities which are well-suited for generating interpretable alphas—a potential demonstrated in analogous tasks like financial investment Yu *et al.* [2024] and code generation Li *et al.* [2024a]. Drawing inspiration from advancements in LLM reasoning (e.g., Chain-of-Thought Wei *et al.* [2022], Tree-of-Thought Yao *et al.* [2024]) and the efficacy of Monte Carlo Tree Search (MCTS) Coulom [2007]; Silver *et al.* [2016] in enhancing LLM performance on complex problems Zhang *et al.* [2024], we conceptualize alpha mining as an MCTS-driven tree search. Within this framework, each node in the tree represents a candidate alpha formula, facilitating the systematic exploration and refinement of the vast and complex alpha space.

Unlike tasks such as mathematical derivation, where evaluating the contribution of intermediate steps towards the final solution is often challenging before the derivation is complete, alpha factor mining provides fine-grained feedback on each candidate alpha formula through backtesting. We leverage this detailed feedback to guide our search. We initiate the search with a LLM-generated alpha formula, as the root node of the search tree. Then we utilize the LLM to iteratively refine and improve the formulas, expanding the tree with new, potentially superior nodes. Furthermore, to mitigate the homogeneity of generated alpha formulas, we conduct frequent subtree mining on effective alphas and explicitly instruct the LLM to avoid using the most frequent subtrees during generation. Circumventing these frequent subtrees can enhance the search efficiency and alpha effectiveness.

The synergy between MCTS and LLMs has indeed shown promise in various reasoning tasks Zhao *et al.* [2023]; DeLorenzo *et al.* [2024]. However, our contribution is a novel application of this synergy tailored explicitly to the intricacies of formulaic alpha factor mining. Unlike general reasoning tasks where MCTS might explore predefined actions or LLMs evaluate abstract states Xie *et al.* [2024]; Li *et al.* [2025]; Dainese *et al.* [2024], our framework employs the LLM as a direct, generative engine for symbolic alpha formulas. Crucially, the MCTS exploration is guided by rich, quantitative, and domain-specific feedback from financial backtesting performed on each candidate alpha. This iterative loop—where the LLM's generative capabilities are steered by MCTS informed by empirical financial performance—offers a distinct advantage.

The main contributions of this paper can be summarized as follows:

- We propose an LLM-Powered MCTS framework for formulaic alpha mining, modeling the task as a tree search-based reasoning problem where the LLM performs multi-step formula refinement guided by detailed backtesting feedback.
- We design a frequent subtree avoidance method to improve search efficiency and alpha effectiveness by guiding the LLM to explore less common yet potentially effective formula structures.
- We conduct a series of experiments to demonstrate the effectiveness of our proposed framework. The alphas mined by our framework achieve superior prediction performance while maintaining good interpretability, compared to those from other methods.

2 Related Work

2.1 Automated Formulaic Alpha Mining

Traditional formulaic alpha factor mining predominantly leverages Genetic Programming (GP). Early works like GPLearn Lin *et al.* [2019b] utilized GP with time-series operators. AutoAlpha Zhang *et al.*

[2020] enhanced mining efficiency via diverse low-depth alpha initialization, while AlphaEvolve Cui *et al.* [2021] employed computation graphs to evolve more complex alpha factors. Approaches beyond GP include AlphaGen Yu *et al.* [2023], which uses reinforcement learning to optimize for alpha set performance, and AlphaForge Shi *et al.* [2024], featuring a deep learning-based generative-predictive structure.

More recently, Large Language Models (LLMs) have been explored for alpha mining. FAMA Li *et al.* [2024b] leverages LLMs for in-context learning from diverse alphas and employs a chain-of-experience to learn from past mining successes, addressing formula homogenization. In contrast, our approach utilizes Monte Carlo Tree Search for tree search-based reasoning. Other LLM-based explorations include Kou et al. Kou *et al.* [2024], mining alphas from multimodal data via a multi-agent framework; QuantAgent Wang *et al.* [2024c], featuring a two-loop LLM refinement system with a knowledge base; and AlphaAgent Tang *et al.* [2025], focusing on decay-resistant alphas with originality and complexity controls. Specifically, these latter three LLM-based methods often utilize diverse data types beyond traditional price/volume (e.g., Kou *et al.* [2024]) or, as with AlphaAgent Tang *et al.* [2025], may incorporate a human feedback loop. Critically, the general lack of detailed framework descriptions and open-source code for these methods hinders reproducibility. For these reasons, they are not included in our comparative benchmarks.

2.2 Tree Search-based Reasoning

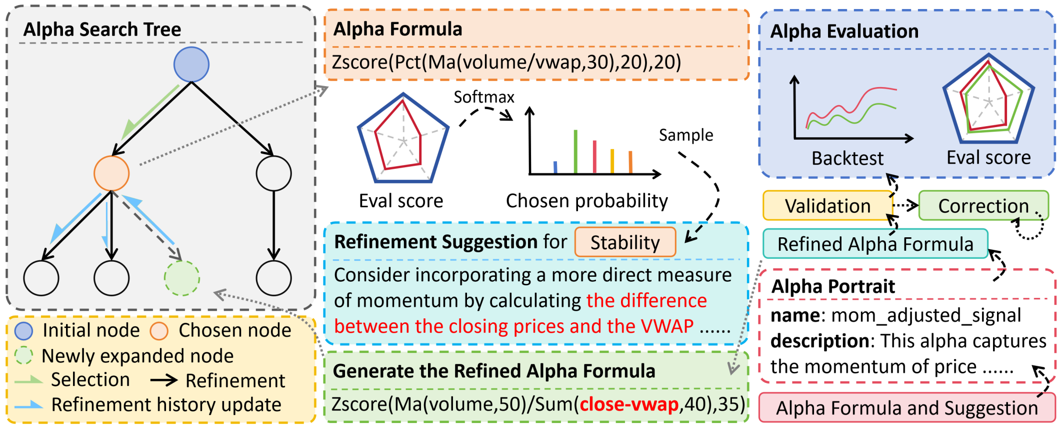
Tree search methods maximize the exploration capabilities of LLMs and allow for different levels of exploration Zhang *et al.* [2023a]; Hu *et al.* [2024]. Consequently, they are widely applied in the field of LLM-based agents and reasoning Li *et al.* [2024a]; Wang *et al.* [2024b,a]. Building upon Chain-of-Thoughts (CoT) Wei *et al.* [2022], Tree of Thoughts (ToT) Yao *et al.* [2024] decomposes a problem into reasoning steps and applies tree search for step exploration. LATS Zhou *et al.* [2023] views the LLM as a more general agent, conducting exploration at both reasoning and action levels. RethinkMCTS Li *et al.* [2024a] models code generation tasks as reasoning problems and applies the Monte Carlo Tree Search algorithm to conduct thought-level searches.

3 Preliminary

3.1 Alpha Factor Mining

We consider a financial market with n stocks observed over T trading days. For each stock $i \in \{1, \dots, n\}$ and day $t \in \{1, \dots, T\}$, its state is described by a feature vector $\boldsymbol{x}_{i,t} \in \mathbb{R}^m$. Raw features include daily open, high, low, close prices (OHLC), trading volume, and Volume-Weighted Average Price (VWAP). The complete market history is a tensor $\boldsymbol{X} \in \mathbb{R}^{T \times n \times m}$. Correspondingly, future returns are organized in a matrix $\boldsymbol{Y} \in \mathbb{R}^{T \times n}$, where $y_{i,t}$ is the realized return for stock i over a specific future period following day t. To capture temporal patterns, we use a lookback window of length τ. An *alpha factor*, f, maps the historical feature data for this window, $\boldsymbol{X}_{t-\tau+1:t} = \{\boldsymbol{X}_s \mid t - \tau < s \leq t\}$, to a vector of predictive scores $\boldsymbol{v}_t = f(\boldsymbol{X}_{t-\tau+1:t}) \in \mathbb{R}^n$. Each $v_{i,t}$ represents the alpha's quantitative prediction for stock i's expected future return.

Alpha factor mining aims to discover a diverse set of K alphas, $\mathcal{F} = \{f_1, \dots, f_K\}$. The outputs of these individual alphas, $\{\boldsymbol{v}_{k,t} = f_k(\boldsymbol{X}_{t-\tau+1:t})\}_{k=1}^K$, are typically aggregated by a combination model, g (e.g., a linear regression or a neural network), into a composite predictive signal $\boldsymbol{z}_t = g(\{\boldsymbol{v}_{k,t}\}_{k=1}^K; \boldsymbol{\theta}_g) \in \mathbb{R}^n$, where $\boldsymbol{\theta}_g$ are model parameters. These signals, collected over T days, form a matrix $\boldsymbol{Z}(\mathcal{F}, \boldsymbol{\theta}_g) \in \mathbb{R}^{T \times n}$. The quality of this composite signal $\boldsymbol{Z}$ is evaluated by comparing it against the realized future returns $\boldsymbol{Y}$ using a predefined performance metric, $\mathcal{P}$ (e.g., Information Coefficient, which we aim to maximize). The optimal parameters for the combination model, $\boldsymbol{\theta}_g^*$, are learned by maximizing the metric: $\boldsymbol{\theta}_g^*(\mathcal{F}) = \arg\max_{\boldsymbol{\theta}_g} \mathcal{P}(\boldsymbol{Z}(\mathcal{F}, \boldsymbol{\theta}_g), \boldsymbol{Y})$. Let $\boldsymbol{Z}^*(\mathcal{F}) = \boldsymbol{Z}(\mathcal{F}, \boldsymbol{\theta}_g^*(\mathcal{F}))$ be the matrix of composite predictive signals generated using these optimal parameters for a given set of alphas $\mathcal{F}$. The overarching goal is to find an optimal set of alpha factors $\mathcal{F}^*$ that maximizes the performance of this optimally combined signal: $\mathcal{F}^* = \arg\max_{\mathcal{F}} \mathcal{P}(\boldsymbol{Z}^*(\mathcal{F}), \boldsymbol{Y})$. This constitutes a challenging bilevel optimization problem due to the vast search space of potential alphas and their complex interactions.



Alpha Search Tree
Alpha Formula
Zscore(Pct(Ma(volume/vwap,30),20),20)
Softmax
Sample
Eval score
Chosen probability
Alpha Evaluation
Backtest
Eval score
Validation
Correction
Refined Alpha Formula
Refinement Suggestion for Stability
Consider incorporating a more direct measure of momentum by calculating the difference between the closing prices and the VWAP ......
Alpha Portrait
name: mom_adjusted_signal
description: This alpha captures the momentum of price ......
Generate the Refined Alpha Formula
Zscore(Ma(volume,50)/Sum(close-vwap,40),35)
Alpha Formula and Suggestion
Initial node
Chosen node
Newly expanded node
Selection
Refinement
Refinement history update

Figure 1: The overview of our framework. MCTS guides the exploration of alpha formula refinements. Upon selecting a node, a refinement dimension is identified via weighted scores from various evaluation dimensions. The LLM then performs a dual role: proposing targeted refinement suggestions for this dimension, and subsequently translating these into a refined alpha formula for evaluation and potential tree expansion.

3.2 Formulaic Alpha

In this work, we focus on *formulaic alphas*: alpha factors defined by mathematical expressions. These expressions are constructed from operators and operands. Operands typically include raw input features (e.g., $\text{close}_{i,t}$) and numerical constants. Operators apply mathematical transformations; for example, time-series operators can be used to construct an alpha like $\text{MA}(\text{close}, 5) - \text{MA}(\text{close}, 20)$, where MA stands for Moving Average. This specific alpha captures a price trend by contrasting short-term with long-term moving averages of closing prices. A complete list of available operators is provided in Appendix D. Formulaic alphas are naturally represented as expression trees (leaf nodes: operands; internal nodes: operators), making their structured yet flexible nature amenable to the automated mining techniques central to our framework.

4 Methodology

Our proposed alpha mining framework integrates LLMs with MCTS to automate the discovery and refinement of alpha factors. Figure 1 provides the overview of our framework. The core iterative process involves: (1) selecting a promising node (alpha formula) using the Upper Confidence Bound for Trees (UCT) criterion Kocsis and Szepesvári [2006], (2) expanding this node by having the LLM generate a refined alpha, guided by performance feedback on specific evaluation dimensions, and (3) evaluating the new alpha via backtesting, and these evaluation results are then used to form a new node (see Appendix B for an illustrative case detailing this workflow). The LLM's role is twofold: first, to propose targeted refinement suggestions based on underperforming evaluation dimensions, and second, to translate these suggestions into a concrete alpha formula. This iterative refinement and evaluation process continues, with the number of expansions per tree potentially adjusted based on the collective quality of discovered alphas. Ultimately, high-performing alphas meeting predefined criteria (e.g., IC, RankIC thresholds) are collected into an effective alpha repository.

4.1 Selection

The selection step in our MCTS framework balances exploration and exploitation. Each node s in the search tree represents an alpha, characterized by its formula and refinement history. An action a corresponds to a specific refinement applied to s. Each node maintains a $Q(s, a)$ value, representing the maximum cumulative reward (e.g., backtesting performance) obtained starting from s and taking action a. We employ the UCT criterion to score potential actions:

$$\text{UCT}(s,a) = Q(s,a) + c\sqrt{\frac{\ln(N_s)}{N_{s'}}} \tag{1}$$

where N_s is the visit count of the parent state s, $N_{s'}$ is the visit count of the child state s' resulting from action a, and c is the exploration weight.

Unlike standard MCTS, where selection typically proceeds to a leaf node before expansion and simulation, our approach allows any node to be selected for expansion. This is because each alpha refinement can be immediately evaluated via backtesting, eliminating the need for a separate simulation phase. To facilitate this, if an internal node s is selected via UCT based on its existing children, we also consider a "virtual" action a_p that effectively proposes expanding s itself. The visit count for this virtual action a_p (leading to a conceptual state s_p identical to s) is considered as the number of actual children of s. If this virtual action a_p yields the highest UCT score, node s is chosen for expansion, leading to the creation of a new child node. This mechanism ensures that promising non-leaf nodes can be further refined.

4.2 Expansion

Upon selecting a node s for expansion, a new, refined alpha factor is generated. This process is structured to enhance the LLM's effectiveness and the quality of refinements.

Dimension-Targeted Refinement Suggestion. Each node s is associated with a multi-dimensional evaluation score vector $\boldsymbol{E}_s = [e_1, \ldots, e_q] \in [0, e_{\text{max}}]^q$, where e_i is the score on the i-th evaluation dimension and e_{max} is the maximum score. To guide refinement towards areas of weakness while maintaining explorative diversity, we stochastically select a dimension for improvement. The probability of selecting dimension i is given by:

$$P_i(s) = \text{Softmax}\left((e_{\text{max}} \cdot \mathbf{1}_q - \boldsymbol{E}_s)/T\right)_i \tag{2}$$

where $\mathbf{1}_q$ is a q-dimensional vector of ones, T is a temperature parameter controlling randomness, and the Softmax function normalizes scores into a probability distribution. This prioritizes dimensions with lower scores.

Once a dimension is selected, the LLM generates refinement suggestions tailored to improving performance along this dimension. To ground these suggestions and improve their practical relevance, we employ few-shot learning, using alphas from the repository of effective alphas as examples (detailed in Appendix C.2).

Alpha Formula Generation and Validation. Based on the chosen dimension and the LLM's targeted suggestions, the LLM first formulates a refined conceptual description of the alpha. From this description, it then generates a corresponding alpha formula. This formula undergoes an automated validity check (e.g., syntactic correctness). If the formula is invalid, feedback is provided to the LLM for iterative correction. Valid formulas are then backtested, and their multi-dimensional evaluation results constitute the new node in the MCTS tree.

4.3 Multi-Dimensional Alpha Evaluation

The evaluation step in our framework is crucial for assessing a candidate alpha formula's potential contribution to the existing effective alpha repository. Unlike traditional MCTS, we bypass simulation and directly evaluate the alpha's backtest performance, guiding the search towards promising expressions.

A key challenge is the evolving nature of the effective alpha repository, which progressively raises the bar for new alphas. To address this, we employ a relative ranking approach. The relative rank of an alpha f for a metric like Information Coefficient (IC), denoted R^f_{IC}, is:

$$R^f_{IC} = \frac{1}{N}\sum_{i=1}^{N} I(IC(f) < IC(f_i)) \tag{3}$$

where f_i is an alpha in the repository of size N, and $I(\cdot)$ is the indicator function. This ensures an adaptive evaluation criterion, avoiding issues with fixed thresholds that may be too stringent early on or too lenient later.

To provide granular feedback for refinement, we evaluate the alpha formula across multiple dimensions. The choice of dimensions can be tailored to specific requirements; for the purpose of this study, we exemplify this multi-dimensional evaluation using five key aspects: **Effectiveness** (predictive accuracy), **Stability** (consistency of predictive accuracy), **Turnover** (daily trading volume within a desired range), **Diversity** (contribution to the novelty of the effective alpha repository), and **Overfitting Risk**. For each of these dimensions, excluding Overfitting Risk, a score e_i is computed based on a pertinent, relative-ranked backtesting metric. The score for the i-th dimension is thus given by $e_i = 1 - R^f_{m_i}$, where $R^f_{m_i}$ represents the relative rank of the specific backtesting metric m_i associated with that dimension (e.g., for Effectiveness, m_i could be the IC).

The assessment of **Overfitting Risk** is distinct. We leverage an LLM to generate this score (see Appendix J.3 for the specific prompt), considering the alpha formula and its refinement history, thereby incorporating qualitative, expert-like judgment. The overall alpha score, an average of these dimensional scores (e_i), constitutes the reward signal used to update the Q-values of the corresponding MCTS nodes, thereby guiding the search towards more promising alpha expressions. Our framework flexibly accommodates other evaluation criteria tailored to specific objectives.

4.4 Backpropagation

During backpropagation, we update the Q-values of nodes along the path from the evaluated node to the root. A node's Q-value represents the maximum evaluation score found within its subtree. A novel aspect of our backpropagation involves the LLM generating concise summaries of each node's refinement process, including changes in dimensional scores. These summaries are integrated into the search tree's overall refinement history.

Crucially, to enhance the quality of refinement suggestions and the accuracy of overfitting assessment, the LLM is provided with contextual information: the refinement history of the current node's parent, children, and siblings. This allows the LLM to avoid redundant suggestions and to better infer the degree of overfitting for the current alpha by analyzing its historical refinement trajectory and its relationship with neighboring explorations in the search space.

4.5 Frequent Subtree Avoidance

To mitigate alpha formula homogenization and prevent the over-exploitation of common structural motifs during alpha mining, we introduce Frequent Subtree Avoidance (FSA). This approach is inspired by the observation in AutoAlpha Zhang *et al.* [2020] that the inherent patterns of formulaic alphas are significantly influenced by their "root genes."

We define a *root gene* as a subtree within an alpha formula's expression tree that originates from its leaf nodes (i.e., raw features). Crucially, for identifying root genes, we abstract away the specific parameter values of operators, focusing solely on the tree structure. For instance, in "$\mathrm{Std}(\mathrm{close} - \mathrm{Ma}(\mathrm{vwap}, 20), 20)/\mathrm{Std}(\mathrm{high}-\mathrm{low}, 15)$", both "$\mathrm{Ma}(\mathrm{vwap}, t)$" and "$\mathrm{Std}(\mathrm{high}-\mathrm{low}, t)$" (where t represents any parameter) are considered root genes. The collection of such root genes characterizes an alpha's underlying structural properties.

Our FSA method operates by identifying and discouraging these frequently recurring root gene structures. As illustrated in Figure 2, we first mine frequent *closed* root genes from a repository of previously discovered effective alphas.

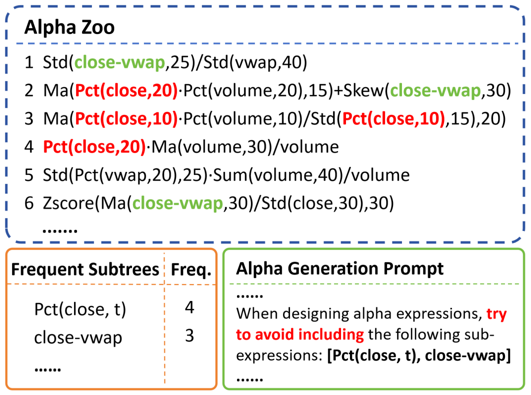

Alpha Zoo
1 Std(close-vwap,25)/Std(vwap,40)
2 Ma(Pct(close,20)·Pct(volume,20),15)+Skew(close-vwap,30)
3 Ma(Pct(close,10)·Pct(volume,10)/Std(Pct(close,10),15),20)
4 Pct(close,20)·Ma(volume,30)/volume
5 Std(Pct(vwap,20),25)·Sum(volume,40)/volume
6 Zscore(Ma(close-vwap,30)/Std(close,30),30)
....
Frequent Subtrees
Freq.
Pct(close, t)
4
close-vwap
3
......
Alpha Generation Prompt
......
When designing alpha expressions, try to avoid including the following sub-expressions: [Pct(close, t), close-vwap]
......

Figure 2: Frequent Subtree Avoidance. Top-k frequent subtrees are mined from effective alphas in the Alpha Zoo. The LLM is then guided to avoid these sub-expressions during alpha generation.

A frequent subtree is considered closed if none of its immediate supertrees (i.e., the subtree plus one additional node) share the same support count; this helps identify maximal common patterns. We then select the top-k most frequent closed subtrees (e.g., $k = 2$ in the figure) and guide the LLM to avoid generating new alpha formulas containing these specific sub-expressions.

FSA acts as a complementary mechanism to enhance the MCTS search process. While MCTS inherently balances exploration and exploitation, its efficiency can be hampered if the LLM predominantly proposes candidates based on over-exploited structural motifs. FSA addresses this by proactively guiding LLMs to generate more diverse formula structures from the outset. By discouraging the generation of alphas containing these frequent subtrees, FSA ensures that MCTS is supplied with a richer set of structurally novel formulas, enabling a more efficient exploration of diverse and potentially more promising regions of the alpha search space. As demonstrated in Section 5.3, this approach significantly improves search efficiency and alpha performance.

5 Experiment

We evaluate our proposed framework on real-world stock market data, addressing the following research questions (RQs):
Q1: How does our approach compare to baselines in predictive performance?
Q2: Are MCTS and Frequent Subtree Avoidance effective components within our framework?
Q3: How does the interpretability of alpha formulas mined by our method compare to others?

5.1 Experiment Settings

Data Our experiments are conducted on the Chinese A-shares market. To ensure comprehensive market representation, our experiments separately target two stock pools: the CSI 300 Index (large-cap, liquid stocks) and the CSI 1000 Index (small to mid-cap stocks). We define two distinct prediction targets: the 10-day return and the 30-day return of the stocks, with buying and selling executed at the closing price. The dataset is split chronologically into training (2011/01/01–2020/12/31) and testing (2021/01/01–2024/11/30) periods.

Baselines for Comparison We compare our framework with several formulaic alpha mining methods. **DSO** (Deep Symbolic Optimization) Landajuela *et al.* [2022] is a deep learning framework for symbolic optimization. **GP** employs genetic programming for alpha mining. **AlphaGen** Yu *et al.* [2023] is a reinforcement learning framework for formulaic alpha mining. **AlphaForge** Shi *et al.* [2024] features a generative-predictive architecture; for a fair comparison of mining capability, we exclusively use its alpha mining network. Among LLM-based approaches, **CoT** (Chain-of-Thought) Wei *et al.* [2022] prompts LLMs for step-by-step reasoning to directly generate alpha factors. **ToT** (Tree-of-Thought) Yao *et al.* [2024] enables LLMs to explore diverse reasoning paths in a tree structure. Lastly, **FAMA** Li *et al.* [2024b] leverages LLMs with in-context examples to diversify formulas and a "chain-of-experience" to learn from past successes.

We use OpenAI's GPT4.1 model as the LLM for both our method and the LLM-based baselines. Furthermore, we evaluate the performance of our framework when using different LLM backbones, as detailed in Appendix G.3. Regarding the potential data leakage issue in LLMs, please refer to the discussion in Appendix G.2.

For a fair and rigorous comparison, we benchmark performance based on a controlled *search count*, or equivalently, the *number of alpha generations*. This approach is well-suited because our framework and all baselines inherently involve a distinct search process, where each iteration yields a new candidate alpha formula. For LLM-based methods (including ours), we report the best performance achieved with search counts of 1,000, 2,000, or 3,000. For other methods, the search count is incrementally increased from a small value until performance converges, capped at 600,000 ($200\times$ the LLM-based methods' maximum). This experimental design facilitates two key comparisons: first, it allows for an equitable assessment of our framework against other LLM-based methods under similar, well-defined computational budgets; second, it enables a robust comparison of search efficiency against other non-LLM-based methods. Furthermore, to account for practical limitations, the maximum wall-clock runtime for any single experimental run is constrained to 24 hours.

5.2 Experiment 1: Prediction Performance Comparison (Q1)

We evaluate our generated alphas against baselines using two representative machine learning models: LightGBM [Ke *et al.*, 2017], an efficient gradient boosting framework, and a 3-layer Multi-Layer Perceptron (MLP) for capturing complex non-linearities. For each alpha mining method, we generate alpha sets of three distinct sizes—10, 50, and 100—to serve as input features for these models. This allows for a thorough comparison of the mined alpha sets across varying sizes. Both input alphas and target returns are cross-sectionally rank-normalized before training to mitigate outlier influence. Predictive performance is assessed using standard metrics in quantitative finance: Information Coefficient (IC) and Rank Information Coefficient (RankIC).

To assess the practical profitability of the mined alphas in simulated real-world stock market scenarios, we follow established evaluation methodologies Yu *et al.* [2023] and conduct backtests. Specifically, we employ a top-k/drop-n portfolio construction strategy, implemented on the Qlib platform Yang *et al.* [2020]. The detailed configuration of this strategy is described in Appendix F.3. The practical trading performance is evaluated using two key metrics: Annualized Return (AR), which measures the strategy's absolute profitability, and Information Ratio (IR), which quantifies its risk-adjusted performance.

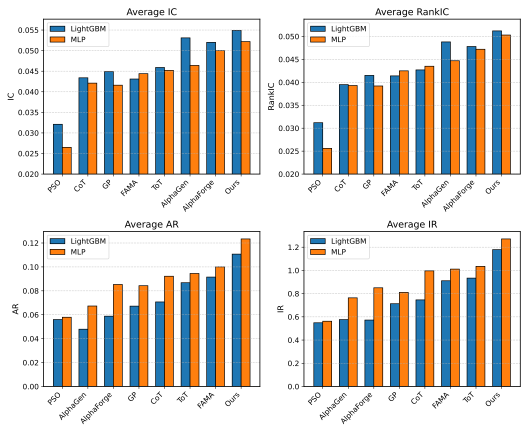


Figure 3: The average predictive performance of LightGBM and MLP models trained on alphas mined by different methods.

The combination of these four metrics (IC, RankIC, AR, and IR) provides a comprehensive evaluation of the mined alphas. As illustrated in Figure 3 (with detailed results presented in Appendix H), our framework consistently outperforms baselines across all metrics. This demonstrates that the alphas mined by our framework possess superior predictive capabilities for future stock returns, which can be effectively translated into trading profitability.

5.3 Experiment 2: Ablation Study (Q2)

We conduct ablation studies to evaluate three key components of our framework: MCTS, multi-dimensional feedback, and FSA.

Table 1 presents the impact of these components on predictive performance. When incorporating Effectiveness and Diversity as feedback, MCTS demonstrates superior predictive performance over CoT and ToT. Performance progressively improves with the integration of additional feedback dimensions. Notably, while Turnover feedback slightly reduces IC and RankIC, it enhances practical trading metrics (AR, IR) by mitigating transaction costs. The integration of FSA yields further improvements across all metrics for both LightGBM and MLP models. These results underscore the individual and collective contributions of MCTS, multi-dimensional feedback, and FSA to our framework's efficacy.

Beyond predictive performance, Figure 4 (a) assesses FSA's impact on search efficiency, plotting the number of effective alphas mined against the total alphas generated. Our framework, even without FSA, demonstrates higher search efficiency than CoT and ToT. FSA further amplifies this advantage. Critically, as the number of generated alphas increases, the efficiency of CoT and ToT declines due to diminishing diversity. In contrast, our method with FSA sustains a high search efficiency without significant decay.

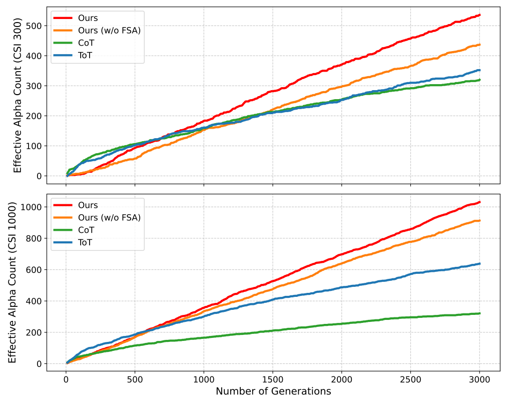
5.4 Experiment 3: Interpretablitity of Alpha Formulas (Q3)

In this experiment, we evaluate the interpretability of alpha formulas mined by different methods. We define the interpretability of an alpha formula by its capacity to articulate a reasonable logic, a specific market phenomenon, or an investment strategy. To quantify this, we randomly select one alpha formula per method and employed LLMs to rank their interpretability. We repeat this process

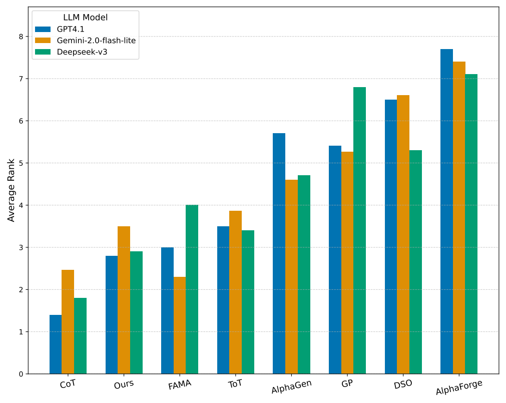
Table 1: Ablation Study Results. Best results are highlighted in **bold**.

Search Strategy	Included Evaluation Dimensions					LightGBM				MLP			
	Eff.	Div.	Turn.	Stab.	O.R.	IC	RankIC	AR	IR	IC	RankIC	AR	IR
CoT	✓	✓	×	×	×	0.0434	0.0395	0.0707	0.7461	0.0421	0.0393	0.0922	0.9962
ToT	✓	✓	×	×	×	0.0459	0.0427	0.0868	0.9337	0.0452	0.0435	0.0945	1.0348
MCTS	✓	×	×	×	×	0.0409	0.0374	0.0941	0.9775	0.0400	0.0376	0.0935	1.0010
MCTS	✓	✓	×	×	×	0.0501	0.0476	0.1003	1.0106	0.0486	0.0462	0.1023	1.0462
MCTS	✓	✓	✓	×	×	0.0492	0.0457	0.1063	1.1062	0.0489	0.0462	0.1185	1.2556
MCTS	✓	✓	✓	✓	×	0.0495	0.0462	0.1030	1.0331	0.0491	0.0465	0.1093	1.1773
MCTS	✓	✓	✓	✓	✓	0.0515	0.0479	0.1075	1.1121	0.0503	0.0478	0.1166	1.2127
MCTS+FSA	✓	✓	✓	✓	✓	**0.0549**	**0.0512**	**0.1107**	**1.1792**	**0.0522**	**0.0503**	**0.1234**	**1.2712**

Note: Eff. = Effectiveness, Div. = Diversity, Turn. = Turnover, Stab. = Stability, O.R. = Overfitting Risk. ✓ indicates the dimension is included, × indicates it is not.



(a) Search Efficiency Comparison.



(b) Interpretability Ranking Comparison.

Figure 4: Experimental Results. (a) Comparison of search efficiency across methods. (b) Average interpretability ranking of alpha formulas by LLMs, where lower ranks indicate better interpretability.

50 times and compute the average rank for each method. To mitigate potential biases from a single LLM, we aggregate rankings from three distinct LLMs. The results are presented in Figure 4 (b). The findings indicate that formulas mined by our framework exhibit interpretability second only to those generated by the CoT method. Notably, our method significantly surpasses non-LLM-based approaches in terms of formula interpretability. This suggests that our approach achieves a compelling trade-off, delivering strong predictive performance while maintaining a high degree of interpretability.

Furthermore, acknowledging that LLMs might inherently favor formulas generated through LLM-driven processes, we provide illustrative examples of alpha formulas from our method and non-LLM-based approaches in Appendix G.6. While this is not a formal quantitative human study, a human researcher, upon qualitative inspection of these examples, should also be able to clearly distinguish the superior interpretability of formulas derived from our method. This superiority typically manifests as more discernible underlying logic and enhanced transparency when compared to formulas produced by non-LLM-based methods.

6 Conclusion

We introduce an LLM-Powered Monte Carlo Tree Search framework for formulaic alpha mining. This approach models alpha mining as a tree search, where an LLM iteratively generates and refines candidate formulas, critically guided by quantitative feedback from financial backtesting. To foster search efficiency and alpha effectiveness, we incorporate a frequent subtree avoidance mechanism. Experimental results demonstrate that our framework mines alphas with superior predictive accuracy and trading performance, while also offering enhanced interpretability and search efficiency compared to existing methods. This work pioneers a promising direction for leveraging LLMs and MCTS to tackle the complex challenge of automated formulaic alpha factor mining in finance.

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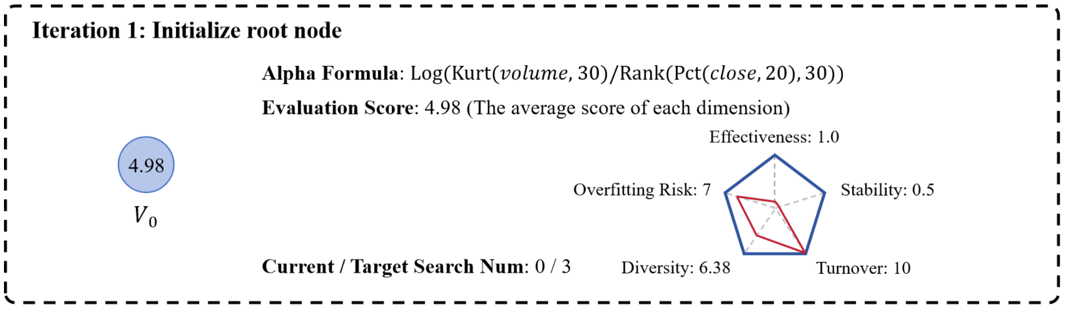
A Summary of Appendix

This appendix provides extensive supplementary material to support the methodologies, experiments, and findings presented in the main paper regarding our framework for alpha mining. The contents are organized as follows:

- **Section B: Illustrative Case Study.** A step-by-step walkthrough of our framework's workflow.
- **Section C: Method Details.** Elaboration on the generation processes for alpha formulas and refinement suggestions.
- **Section D: List of Operators.** A comprehensive list of operators employed within the alpha formulas.
- **Section E: Pseudo-code.** The algorithmic pseudo-code of our framework.
- **Section F: Experimental Setup Details.** Details on hyperparameter configurations, model specifications, experimental environment and predictive performance metrics.
- **Section G: Extended Experimental Results and Analyses.** Includes:
  - G.1 Comparative analyses against other baselines.
  - G.2 Investigation into potential data leakage in LLMs.
  - G.3 Sensitivity studies on the LLM backbone.
  - G.4 Examination of alpha characteristics at varying MCTS search depths.
  - G.5 Visualizations of cumulative return curves.
  - G.6 Analysis of the interpretability of mined alpha formulas.
  - G.7 Parameter sensitivity analysis for key framework components.
- **Section H: Full Experiment Results.** Comprehensive results of the Prediction Performance Comparison (Experiment 1).
- **Section I: Limitations.** The limitations of our framework.
- **Section J: LLM Agent Prompts.** Details of key prompts used for tasks such as alpha portrait generation, formula generation, overfitting risk assessment, and alpha refinement.

B Illustrative Case Study of MCTS Workflow

To elucidate the workflow of our proposed MCTS framework for alpha factor mining, this section provides a detailed step-by-step example.


Iteration 1: Initialize root node

Alpha Formula: Log(Kurt($volume$, 30)/Rank(Pct($close$, 20), 30))

Evaluation Score: 4.98 (The average score of each dimension)

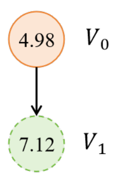
Current / Target Search Num: 0 / 3

Figure 5: Case Study: MCTS root node generation.

Initially, as depicted in Figure 5, an initial alpha formula is generated by the LLM. This formula undergoes a multi-dimensional evaluation, and serves as the root node (V_0) of the MCTS search tree. For this illustrative case, the target search count is initialized to 3. This target is dynamically incremented by 1 each time a newly generated node achieves a new high score, encouraging deeper exploration of promising search trees.

Following the construction of the root node, the MCTS process proceeds with node expansion. As shown in Figure 6, the root node V_0 is expanded to generate its first child node, V_1. The dimension

Iteration 2: Expand to node V_1

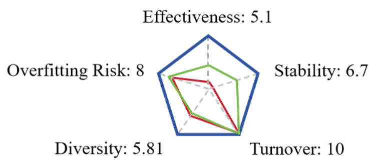


Node chosen for expansion: V_0

The dimension sampled for refinement: Stability

Refined Alpha Formula: $\mathrm{Ma}(\mathrm{Tanh}(\mathrm{Kurt}(volume, 40) \cdot \mathrm{Rank}(|close - vwap|, 30)), 20)$

Evaluation Score: 7.12



Refinement history of V_1:

$V_0 \to V_1$

Refinement Abstract: The improved alpha enhances the original by incorporating price dislocation from VWAP, applying nonlinear transformation, and smoothing, thereby generating a more robust and noise-resistant signal of abnormal market activity.

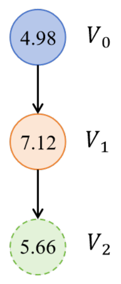
Score Change: Effectiveness (+4.1), Stability (+6.2), Turnover (+0), Diversity (-0.57), Overfitting Risk (+1)

Current / Target Search Num: 1 / 4 (Score reaches a new high, increase the Target Search Num)

Figure 6: Case Study: expansion to node V_1.

for refinement is selected by sampling according to Equation (2) (in this instance, the *Stability* dimension is chosen). Subsequently, the LLM generates targeted refinement suggestions. Based on these suggestions, a refined alpha formula is produced, with the modifications highlighted within the formula representation. This refined alpha formula is then subjected to the same multi-dimensional evaluation process, yielding the scored node V_1. The refinement history for V_1 is updated to include a summary of this specific refinement step and the corresponding change in evaluation scores. Finally, both the target search count (if V_1's score is a new high) and the current search count are updated.

Iteration 3: Expand to node V_2



Chose node according to UCT:

$\mathrm{UCT}(V_0, V_0 \to V_0) = 4.98/10 + 1 \cdot \sqrt{\ln 2/1} = 1.33$

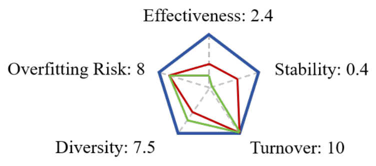
$\mathrm{UCT}(V_0, V_0 \to V_1) = 7.12/10 + 1 \cdot \sqrt{\ln 2/1} = 1.54$

Node chosen for expansion: V_1

The dimension sampled for refinement: Effectiveness

Refined Alpha Formula: $\mathrm{Ma}(\mathrm{Sin}(close - vwap) \cdot \mathrm{Corr}(\mathrm{Pct}(volume, 1), \mathrm{Rank}(|close - vwap|, 15), 15) \cdot \mathrm{Skew}((high - open)/(open - low), 12), 10)$

Evaluation Score: 5.66



Refinement history of V_2:

$V_0 \to V_1$: ......

$V_1 \to V_2$:

Refinement Abstract: The improved alpha enhances the original by incorporating directional price range skewness and the dynamic correlation between volume spikes and price dislocations, providing a more nuanced and robust detection of abnormal, directionally-skewed market activity.

Score Change: Effectiveness (-2.7), Stability (-6.3), Turnover (+0), Diversity (+1.69), Overfitting Risk (+0)

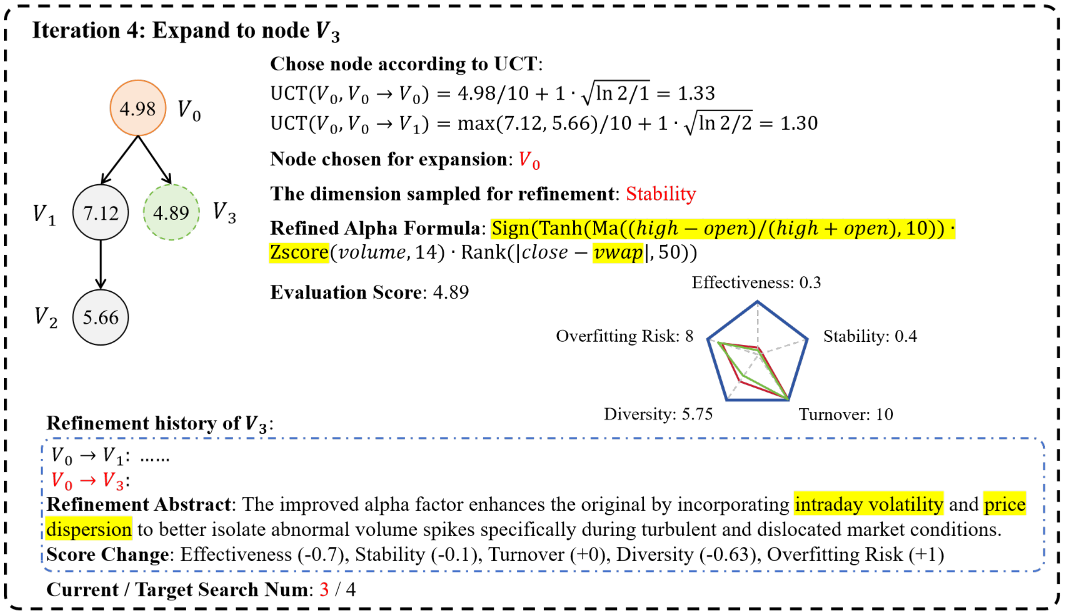
Current / Target Search Num: 2 / 4

Figure 7: Case Study: expansion to node V_2.

The expansion process continues, as illustrated in Figure 7. Based on the UCT criterion, node V_1 is selected for the next expansion. Similar to the previous step, a dimension for refinement is sampled. The LLM then generates an improved alpha formula based on this dimension, which is subsequently evaluated to create node V_2. Notably, the refinement history of V_2 is cumulative, encapsulating all refinement steps and score evolutions from the root node V_0 through V_1 to V_2. The current search count is then incremented.

Figures 8 and 9 showcase the outcomes of the two subsequent expansion steps, leading to the generation of nodes V_3 and V_4, respectively. Upon the expansion that creates node V_4, the current search count reaches the predetermined target. At this juncture, the MCTS expansion phase for this iteration concludes. All five generated nodes ($V_0, \ldots, V_4$) are then systematically reviewed. Nodes that meet predefined quality and performance criteria are added into the effective alpha repository.

This sequence completes one full iteration of the MCTS-driven alpha mining process. Our framework is designed to iteratively repeat this entire cycle, enabling the efficient and systematic mining of effective alphas.



Iteration 4: Expand to node V_3

Chose node according to UCT:

$\mathrm{UCT}(V_0, V_0 \to V_0) = 4.98/10 + 1 \cdot \sqrt{\ln 2/1} = 1.33$

$\mathrm{UCT}(V_0, V_0 \to V_1) = \max(7.12, 5.66)/10 + 1 \cdot \sqrt{\ln 2/2} = 1.30$

Node chosen for expansion: V_0

The dimension sampled for refinement: Stability

Refined Alpha Formula: $\mathrm{Sign}(\mathrm{Tanh}(\mathrm{Ma}((high - open)/(high + open), 10)) \cdot \mathrm{Zscore}(volume, 14) \cdot \mathrm{Rank}(|close - vwap|, 50))$

Evaluation Score: 4.89

Refinement history of V_3:

$V_0 \to V_1$: ……

$V_0 \to V_3$:

Refinement Abstract: The improved alpha factor enhances the original by incorporating intraday volatility and price dispersion to better isolate abnormal volume spikes specifically during turbulent and dislocated market conditions.

Score Change: Effectiveness (-0.7), Stability (-0.1), Turnover (+0), Diversity (-0.63), Overfitting Risk (+1)

Current / Target Search Num: 3 / 4

Figure 8: Case Study: expansion to node V_3.

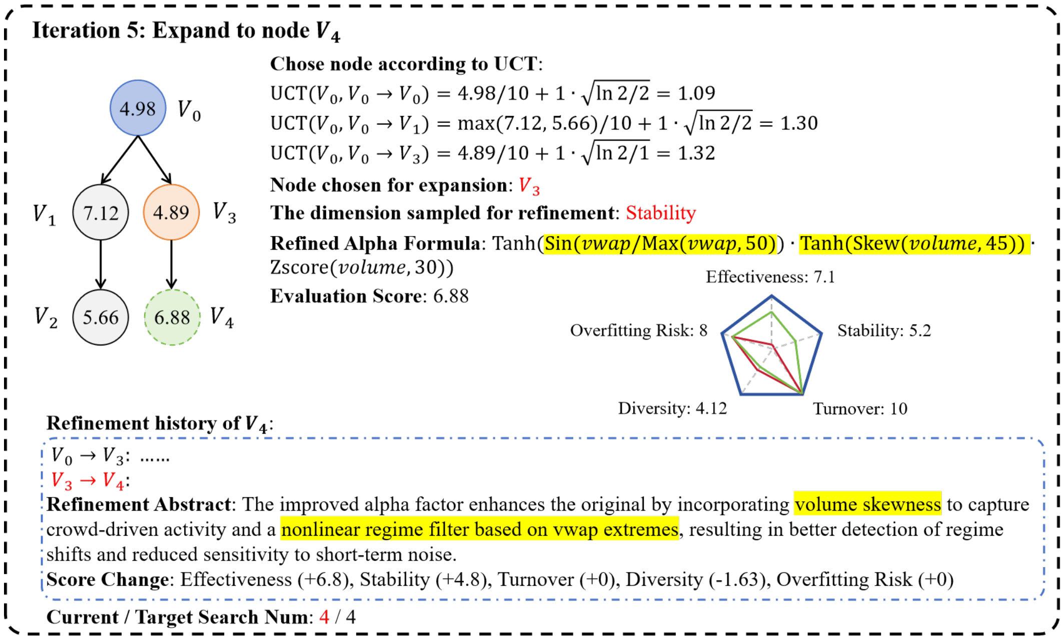
C Method Details

In this section, we elaborate on specific details of our framework, focusing on the generation of alpha formulas and refinement suggestions.

C.1 Alpha Formula Generation

We decompose the generation of alpha formulas into a two-step process: first, an *alpha portrait* is generated, and subsequently, the corresponding alpha formula is derived from this portrait. An alpha portrait is a textual representation that includes the alpha's name, a concise description, and its formula expressed in pseudo code. This two-step approach decouples the conceptual design of an alpha from its concrete construction, thereby reducing the instruction-following complexity for LLMs and enhancing the quality of the generated formulas.

When generating alpha formulas, the LLM is instructed to use symbolic parameters (e.g., the lookback window for a moving average operator) rather than fixed numerical values. Concurrently, the LLM proposes a few sets of potential parameter values (three sets in our experiments). We then backtest the alpha derived from each parameter set and select the configuration yielding the best performance. This strategy allows for a more efficient exploration and utilization of each generated alpha formula.



Iteration 5: Expand to node V_4

Chose node according to UCT:
$\mathrm{UCT}(V_0, V_0 \to V_0) = 4.98/10 + 1 \cdot \sqrt{\ln 2/2} = 1.09$
$\mathrm{UCT}(V_0, V_0 \to V_1) = \max(7.12, 5.66)/10 + 1 \cdot \sqrt{\ln 2/2} = 1.30$
$\mathrm{UCT}(V_0, V_0 \to V_3) = 4.89/10 + 1 \cdot \sqrt{\ln 2/1} = 1.32$
Node chosen for expansion: V_3
The dimension sampled for refinement: Stability
Refined Alpha Formula: $\mathrm{Tanh}(\mathrm{Sin}(vwap/\mathrm{Max}(vwap, 50)) \cdot \mathrm{Tanh}(\mathrm{Skew}(volume, 45)) \cdot \mathrm{Zscore}(volume, 30))$
Evaluation Score: 6.88

Refinement history of V_4:
$V_0 \to V_3$: ……
$V_3 \to V_4$:
Refinement Abstract: The improved alpha factor enhances the original by incorporating volume skewness to capture crowd-driven activity and a nonlinear regime filter based on vwap extremes, resulting in better detection of regime shifts and reduced sensitivity to short-term noise.
Score Change: Effectiveness (+6.8), Stability (+4.8), Turnover (+0), Diversity (-1.63), Overfitting Risk (+0)

Current / Target Search Num: 4 / 4

Figure 9: Case Study: expansion to node V_4 and search termination.

C.2 Refinement Suggestion Generation

During each refinement iteration, once a dimension for improvement is selected, we leverage the LLM to generate pertinent refinement suggestions. We employ few-shot learning, using alphas from the effective alpha repository as exemplars. We tailor the exemplar selection strategy for each evaluation dimension:

Effectiveness and Stability To select diverse yet potent exemplars, we first filter the effective alpha repository, retaining only alphas whose correlation with the current alpha falls outside the top $\eta\%$ (e.g., $\eta = 50$). From this filtered subset, we select the top k alphas (e.g., $k = 3$) exhibiting the highest scores in Effectiveness or Stability as few-shot exemplars. This two-stage process ensures diversity by preventing highly similar alphas from dominating the exemplar set.

Diversity To encourage the exploration of novel alpha structures, we select the top k alphas from the effective alpha repository that exhibit the lowest correlation with the current alpha as few-shot exemplars.

Turnover and Overfitting Risk For these dimensions, we adopt a zero-shot approach, directly prompting the LLM to generate refinement suggestions without explicit exemplars.

Following the generation of refinement suggestions, the LLM produces a revised alpha formula based on these suggestions. We then perform a syntax validation on the generated formula. If the formula is syntactically incorrect, the LLM is prompted to correct it iteratively until it passes validation.

D List of Operators

In this paper, the operators we used can be categorized into two classes: unary operators and binary operators. All operators perform temporal operations, utilizing data from either the current trading day alone or including data from a preceding period. We list the details of all the operators in Table 2

E Pseudo-Code

We provide the pseudo-code for our LLM-guided MCTS framework in Algorithm 1.

Algorithm 1: LLM-Guided MCTS Framework for Automated Alpha Mining

Input: f_{seed} (initial alpha), $\mathcal{L}$ (LLM), c (exploration const.), T (temperature), $e_{\max}$ (max score/dim), B (initial search budget), b (budget increment), τ (effectiveness threshold), $\mathcal{A}_{\text{avoid}}$ (initial avoidance list)

Output: Repository $\mathcal{R}$ of effective alphas

```
                                                            /* Initialization */
$\mathcal{R} \leftarrow \emptyset$
$s_0 \leftarrow$ CreateRootNode($f_{\text{seed}}$)
$s_0$.scores $\leftarrow$ MultiDimEvaluate($f_{\text{seed}}, \mathcal{R}$)
$s_0$.visits $\leftarrow 1$; $s_0.Q \leftarrow$ AggregateScore($s_0$.scores)
Tree $\mathcal{T} \leftarrow \{s_0\}$
max_score_overall $\leftarrow s_0.Q$ ▷ Track highest score found so far in the tree

for $i \leftarrow 1$ to $B$ do
                                                            /* Selection Phase */
    $P_{\text{path}} \leftarrow$ SelectPathUsingUCT($\mathcal{T}, s_0, c$) ▷ Path to $s_{selected}$
    $s_{\text{selected}} \leftarrow$ LastNodeInPath($P_{\text{path}}$)
                                                            /* Expansion Phase */
    /* 1. Prioritize refinement dimension                                        */
    $\mathbf{E}_s \leftarrow s_{\text{selected}}$.scores
    $P_{\text{dim}}(d) \leftarrow$ Softmax($(e_{\max}\mathbf{1}_q - \mathbf{E}_s)/T$)
    $d_{\text{chosen}} \leftarrow$ SampleDimension($P_{\text{dim}}$)
    /* 2. LLM generates refinement and new alpha formula                         */
    context $\leftarrow$ GetNodeRefinementContext($s_{\text{selected}}, \mathcal{T}$) ▷ Parent, children, siblings history
    examples $\leftarrow$ SampleEffectiveAlphas($\mathcal{R}$) ▷ Few-shot examples
    $\tilde{f}_{\text{desc}}, f'_{\text{formula}} \leftarrow \mathcal{L}$.GenerateRefinedAlpha(formula($s_{\text{selected}}$), $d_{\text{chosen}}$, context, examples, $\mathcal{A}_{\text{avoid}}$)
    /* 3. Validate and revise formula iteratively                                */
    while $\neg$IsValid($f'_{formula}$) do
        feedback $\leftarrow$ GetInvalidityReason($f'_{\text{formula}}$)
        $\tilde{f}_{\text{desc}}, f'_{\text{formula}} \leftarrow \mathcal{L}$.CorrectAlphaFormula($\tilde{f}_{\text{desc}}$, feedback, context, examples, $\mathcal{A}_{\text{avoid}}$)
    end
                                                            /* Evaluation of New Alpha */
    $\mathbf{E}_{f'} \leftarrow$ MultiDimEvaluate($f'_{\text{formula}}, \mathcal{R}$) ▷ Incl. relative ranks, LLM for overfitting
    score$_{f'} \leftarrow$ AggregateScore($\mathbf{E}_{f'}$)
    /* Update budget if new score is a record high                               */
    if $score_{f'} > max\_score\_overall$ then
        $B \leftarrow B + b$ ▷ Increase total search budget
        max_score_overall $\leftarrow$ score$_{f'}$ ▷ Update overall max score
    end
    /* Create new node and add to tree                                           */
    $s' \leftarrow$ CreateNode($f'_{\text{formula}}, \mathbf{E}_{f'}$, score$_{f'}$)
    $s'$.summary $\leftarrow \mathcal{L}$.GenerateRefinementSummary($s_{\text{selected}}, \tilde{f}_{\text{desc}}, \mathbf{E}_{f'}$)
    AddChildNode($\mathcal{T}, s_{\text{selected}}, s'$)
    $\mathcal{A}_{\text{avoid}} \leftarrow$ UpdateAvoidanceList($\mathcal{A}_{\text{avoid}}, f'_{\text{formula}}$)
    /* Update Repository                                                         */
    if GetEffectivenessScore($\mathbf{E}_{f'}$) $\geq \tau$ then
        $\mathcal{R} \leftarrow \mathcal{R} \cup \{f'_{\text{formula}}\}$
    end
                                                            /* Backpropagation Phase */
    forall $v \in P_{path} \cup \{s'\}$ do
        $v$.visits $\leftarrow v$.visits $+ 1$
        $v.Q \leftarrow \max(v.Q$, score$_{f'})$ ▷ $Q(v)$ is max score in $v$'s subtree
    end
end
return $\mathcal{R}$
```

Table 2: All the operators used in the experiments.

Operator	Type	Description
$-x, \|x\|, x^2, 1/x$	Unary	The opposite/absolute/square/inverse value of x.
$\mathrm{Sign}(x)$		The sign of x.
$\mathrm{Sin}(x), \mathrm{Cos}(x), \mathrm{Tanh}(x)$		Sine, cosine, and hyperbolic tangent functions.
$\mathrm{Log}(x)$		The natural logarithm of x.
$\mathrm{Delay}(x, t)$		The value of expression x at t trading days prior.
$\mathrm{Diff}(x, t)$		The difference between x and the value prior to day t, $x - \mathrm{Delay}(x, t)$.
$\mathrm{Pct}(x, t)$		The rate of change of x relative to its value t days prior.
$\mathrm{Ma}(x, t), \mathrm{Med}(x, t), \mathrm{Sum}(x, t)$		The mean/median/sum value of x over the past t days.
$\mathrm{Std}(x, t)$		The standard deviation value of x over the past t days.
$\mathrm{Max}(x, t), \mathrm{Min}(x, t)$		The maximum/minimum value of x over the past t days.
$\mathrm{Rank}(x, t)$		The ranking of x relative to its values over the past t days.
$\mathrm{Skew}(x, t), \mathrm{Kurt}(x, t)$		The skewness/kurtosis value of x over the past t days.
$\mathrm{Vari}(x, t)$		The variation value of x over the past t days, $\mathrm{Std}(x, t)/\mathrm{Ma}(x, t)$.
$\mathrm{Autocorr}(x, t, n)$		The autocorrelation coefficient of x with a lag of n over the past t days.
$\mathrm{Zscore}(x, t)$		The z-score normalization of x based on the mean and standard deviation of its values over the past t days.
$x + y, x - y, x \cdot y, x/y$	Binary	Arithmetic operators.
$\mathrm{Greater}(x, y), \mathrm{Less}(x, y)$		Whether the first value is larger/smaller than the second value.
$\mathrm{Cov}(x, y, t)$		The covariance between time series x and y over the past t days.
$\mathrm{Corr}(x, y, t)$		The Pearson's correlation coefficient between time series x and y over the past t days.

F Experimental Setup Details

F.1 Hyperparameter Configurations

Temperature Parameter of LLMs When generating alpha portraits and alpha formulas, the temperature is set to 1.0; when correcting illegal alpha formulas, the temperature is adjusted to 0.8; and when scoring the overfitting risk of alpha, the temperature is set to 0.1.

MCTS We set the exploration weight c in the UCT criterion to 1. For each search tree, the initial search budget is 3, and whenever a node achieves a higher score than previously, the search budget is increased by 1.

Effective Alpha Check Upon the completion of a search tree's expansion, we examine the effectiveness of the alpha formulas corresponding to all nodes within the tree. Those alphas that pass the effectiveness check are added to the effective alpha repository. The specific criteria for determining effectiveness are as follows:

- Basic Criteria: RankIC ≥ 0.015, RankIR ≥ 0.3, $R_{\mathrm{RankIC}} \leq 0.95$, $R_{\mathrm{RankIR}} \leq 0.95$.
- Turnover Criteria: Daily Turnover ≤ 1.6.
- Diversity Criteria: The maximum correlation with the alpha within the effective alpha repository is less than 0.8.

After the mining process is completed, we select the top k alphas with the highest RankIR from the effective alpha repository to form the final alpha set. In our experiments, k is set to 10, 50, and 100.

Evaluation Score Here, we present the backtesting metrics utilized to calculate scores for evaluation dimensions. Effectiveness: RankIC, Stability: RankIR, Turnover: Daily turnover rate, Diversity: Maximum correlation with alphas in the effective alpha repository.

Other Settings When generating alpha refinement suggestions, the number of few-shot examples is set to 1; in the Frequent Subtree Avoidance method, the number of frequent subtrees to be avoided is set to 3. When calculating the selection probability for each evaluation dimension, the temperature parameter is set to $T = 1$. Furthermore, during the generation of refinement suggestions for the Effectiveness and Stability dimensions, the correlation filtering ratio is maintained at $\eta = 50\%$.

F.2 Model Settings

To ensure a fair comparison when evaluating alpha pools derived from different methods, we utilize fixed hyperparameters for our models.

For the LightGBM model, we set `num_leaves` to 32, `n_estimators` to 200, `max_depth` to 8, and the `learning_rate` to 0.05. Both L1 (`reg_alpha`) and L2 (`reg_lambda`) regularization coefficients are fixed at 0.1.

Similarly, the Multi-Layer Perceptron (MLP) models are trained with a consistent configuration. The MLP architecture consists of three hidden layers with 256, 128, and 64 units, respectively. A dropout rate of 0.3 is applied after each hidden layer. We employ the Adam optimizer with a learning rate of 0.001 and a batch size of 1024. The Mean Squared Error (MSE) is used as the loss function. Early stopping is implemented with a patience of 5 epochs, monitoring the validation loss for improvement; training is halted if no new minimum is achieved within this window.

F.3 Backtesting Strategy

The top-k/drop-n portfolio construction strategy employed in our backtests operates as follows. On each trading day, an equal-weight portfolio is formed by selecting the top k stocks based on the predictive signals from the trained models. We set k to represent the top 10% of the respective stock pool (e.g., $k = 30$ for the CSI300 index and $k = 100$ for the CSI1000 index). To manage turnover and limit trading costs, a maximum of n stocks are bought or sold daily. The value of n is determined by $n = k/w$, where w is the prediction horizon in days (e.g., for a 10-day return prediction on CSI300, $n = 30/10 = 3$). This strategy ensures that the theoretical complete turnover period of the portfolio aligns with the prediction horizon. A conservative transaction cost of 0.15% per trade is incorporated to ensure a realistic performance assessment.

F.4 Environment

All the experiments are conducted with following settings:

- CPU: AMD EPYC 7642 48-Core Processor
- GPU: NVIDIA GeForce RTX 3080Ti
- Operating system: Ubuntu 20.04.3 LTS
- Software versions: Python 3.8.5; Numpy 1.24.4; Pandas 1.5.2; Pytorch 2.2.2; Openai 1.57.4

F.5 Predictive Performance Evaluation Metrics

To evaluate the predictive performance of the model (trained on the mined alpha set) in forecasting stock returns, we employ several standard metrics: the Information Coefficient (IC), Rank Information Coefficient (RankIC), Annualized Return (AR), and Information Ratio (IR). Let $f_{i,t}$ denote the predicted returns for asset i at time t (out of N_t assets in the universe at time t), and $r_{i,t+1}$ be its realized return over the subsequent period (e.g., from t to $t+1$). The evaluation spans a total of T time periods.

Information Coefficient (IC) The IC measures the linear correlation between predicted returns and subsequent returns. It is calculated for each cross-section at time t (IC$_t$) and then averaged over all T periods:

$$\mathrm{IC}_t = \frac{\sum_{i=1}^{N_t}(f_{i,t} - \bar{f}_t)(r_{i,t+1} - \bar{r}_{t+1})}{\sqrt{\sum_{i=1}^{N_t}(f_{i,t} - \bar{f}_t)^2}\sqrt{\sum_{i=1}^{N_t}(r_{i,t+1} - \bar{r}_{t+1})^2}} \tag{4}$$

$$\mathrm{IC} = \frac{1}{T}\sum_{t=1}^{T}\mathrm{IC}_t \tag{5}$$

where $\bar{f}_t$ and $\bar{r}_{t+1}$ are the cross-sectional means of predicted signals and realized returns, respectively. A higher IC indicates better predictive power.

Rank Information Coefficient (RankIC) The RankIC measures the monotonic relationship (Spearman's rank correlation) between predicted returns and subsequent returns. It is less sensitive to outliers than the Pearson correlation-based IC. Similar to IC, it is computed cross-sectionally and then averaged:

$$\text{RankIC}_t = \text{Corr}(\text{rank}(f_{1,t}, \dots, f_{N_t,t}), \text{rank}(r_{1,t+1}, \dots, r_{N_t,t+1})) \tag{6}$$

$$\text{RankIC} = \frac{1}{T}\sum_{t=1}^{T} \text{RankIC}_t \tag{7}$$

where rank$(\cdot)$ denotes the operation that assigns ranks to the elements in the vector, and Corr$(\cdot,\cdot)$ is the Pearson correlation coefficient applied to these ranks.

Annualized Return (AR) The AR in this study measures the simple arithmetic average rate of return per year generated by a portfolio. For our long-only strategy, at each rebalancing period t, we select the top-k assets with the highest predicted returns $f_{i,t}$. Assuming these k assets are equally weighted, the portfolio return for the period $t+1$, denoted $R_{p,t+1}$, is:

$$R_{p,t+1} = \frac{1}{k}\sum_{s\in \text{TopK}_t} r_{s,t+1} \tag{8}$$

where TopK$_t$ is the set of k assets with the highest predicted returns based on $\mathbf{f}_t$. The AR, calculated as the arithmetic mean of per-period portfolio returns scaled to an annual figure, over T_p portfolio holding periods is then:

$$\text{AR} = \left(\frac{1}{T_p}\sum_{j=1}^{T_p} R_{p,j}\right) \times P \tag{9}$$

where $R_{p,j}$ is the portfolio return in the j-th holding period, T_p is the total number of holding periods in the backtest, and P is the number of holding periods in a year (e.g., $P = 252$ for daily rebalancing, $P = 12$ for monthly rebalancing).

Information Ratio (IR) The IR measures the risk-adjusted return of the portfolio using the arithmetic annualized return. It is defined as the AR divided by its annualized volatility:

$$\text{IR} = \frac{\text{AR}}{\sigma(R_p)\sqrt{P}} \tag{10}$$

where AR is the simple annualized return calculated as per Eq. (9), and $\sigma(R_p)$ is the standard deviation of the *per-period* portfolio returns $R_{p,j}$ over the T_p holding periods. A higher IR indicates better return per unit of risk.

G Additional Results

G.1 Comparisons with Other Baselines

To provide a comprehensive assessment of our proposed framework, we conduct additional comparisons against two widely adopted benchmark alpha sets in quantitative finance: **Alpha158** and **Alpha360**. Alpha158 consists of 158 handcrafted alpha factors, primarily derived from historical price and volume data, commonly used in the Chinese A-share market. Alpha360 is a more extensive set of 360 alphas designed to capture a broader range of market signals. These benchmark sets are selected due to their prevalence and the diverse alpha construction methodologies they represent, offering robust points of comparison. We construct these two benchmark sets based on the information provided on the Qlib platform Yang *et al.* [2020].

We evaluated the predictive performance of three distinct models: Linear Regression (LR), LightGBM, and a 3-layer Multi-Layer Perceptron (MLP). Each model is trained using features derived from: (i) the Alpha158 set, (ii) the Alpha360 set, and (iii) the alphas mined by our proposed method. The comparative results are presented in Table 3. As illustrated, our method consistently achieves superior predictive performance across the various experimental settings and model architectures considered, underscoring its effectiveness in identifying more potent alpha signals compared to these established benchmarks.

Table 3: Predictive performance comparison between our framework and other baselines. For our framework, the size of alpha sets is fixed at 100.

Instruments	ΔT	Alpha Set	LR		LightGBM		MLP	
			IC	RankIC	IC	RankIC	IC	RankIC
CSI300	10	Alpha158	0.0280	0.0257	0.0386	0.0377	0.0337	0.0329
		Alpha360	0.0144	0.0169	0.0061	-0.0096	0.0153	0.0231
		Ours(100)	**0.0325**	**0.0303**	**0.0420**	**0.0395**	**0.0422**	**0.0408**
	30	Alpha158	0.0147	0.0140	0.0028	0.0103	0.0036	0.0036
		Alpha360	-0.0069	-0.0072	-0.0539	-0.0702	0.0235	0.0340
		Ours(100)	**0.0373**	**0.0359**	**0.0417**	**0.0401**	**0.0423**	**0.0424**
CSI1000	10	Alpha158	0.0395	0.0548	0.0610	0.0627	0.0520	0.0567
		Alpha360	0.0385	**0.0586**	0.0636	0.0642	0.0550	0.0608
		Ours(100)	**0.0589**	0.0554	**0.0804**	**0.0729**	**0.0662**	**0.0618**
	30	Alpha158	0.0512	0.0507	0.0490	0.0654	0.0380	0.0373
		Alpha360	0.0538	0.0537	0.0420	0.0567	0.0532	0.0456
		Ours(100)	**0.0597**	**0.0555**	**0.0793**	**0.0723**	**0.0738**	**0.0710**

G.2 Investigation of Potential Data Leakage in LLMs

A critical concern when employing LLMs for tasks like alpha mining is the potential for data leakage. This refers to the possibility that LLMs' training data might have inadvertently included information about historically well-performing alpha formulas, which could lead to an overestimation of their generative capabilities if they simply recall these formulas.

Table 4: Evaluation of data leakage. Metrics (IC, RankIC, IR, RankIR) are averages over 10 alphas per method. LLMs (GPT4.1, Gemini2.0-flash-lite, Deepseek-v3) are prompted for high-performing alphas (CSI300, 10-day return). 'Ours' is our method with an alpha set size of 10.

LLM	IC	RankIC	IR	RankIR
Random	0.0126	0.0179	0.095	0.148
GPT4.1	0.0130	0.0242	0.097	0.168
Gemini2.0-flash-lite	0.0125	0.0231	0.094	0.180
Deepseek-v3-0324	0.0122	0.0223	0.087	0.145
Ours	**0.0527**	**0.0714**	**0.368**	**0.467**

To investigate this, we design an experiment to explicitly probe whether pre-trained LLMs possess such inherent knowledge. We prompt three distinct LLM backbones—GPT-4.1, Gemini2.0-flash-lite, and Deepseek-v3—to generate alpha formulas specifically anticipated to yield high performance for 10-day forward return prediction on the A-share CSI300 stock pool. For each LLM and the Random baseline, we generate 10 distinct alpha formulas, and the performance metrics reported are averages across these 10 alphas. This setup directly attempts to leverage any pre-existing, "leaked" knowledge within the LLMs. The performance of alphas generated under this explicit instruction is compared against two baselines: (1) alphas generated randomly by an LLM ("Random"), and (2) alphas mined by our proposed framework ("Ours").

As shown in Table 4, the average performance of alphas from LLMs explicitly prompted to generate high-performing expressions is not significantly different from the 'Random' baseline. All these direct LLM generation approaches yield substantially lower performance across all metrics compared to our framework. These results suggest that the tested LLMs do not inherently leverage leaked knowledge of superior alpha formulas for this task, thereby alleviating data leakage concerns and highlighting the efficacy of our alpha mining framework.

G.3 Sensitivity Analysis of LLM Backbone Choice

We evaluate the impact of different LLM backbones on our framework. Three models are tested: GPT-4.1, Gemini-2.0-flash-lite, and Deepseek-v3. Experiments are conducted on the CSI300 stock pool, predicting 10-day forward returns with an alpha set size of 50. Results are detailed in Table 5. The findings reveal that the choice of LLM backbone leads to notable variations in the performance characteristics of the generated alpha sets. While each LLM may emphasize different aspects of alpha quality, our framework, when leveraging these advanced models, generally demonstrates performance that is competitive with or surpasses the best results of baselines.

Table 5: Performance comparison of our framework using different LLM backbones on the CSI300 dataset (10-day forward returns, alpha set size of 50). Best results are highlighted in **bold**.

LLM	LightGBM				MLP			
	IC	RankIC	AR	IR	IC	RankIC	AR	IR
Best of Baselines	0.0388	0.0378	0.0680	0.7470	0.0380	0.0374	0.0805	0.8414
GPT4.1	**0.0399**	**0.0394**	0.0717	0.8283	**0.0436**	**0.0425**	0.0661	0.7075
Gemini-2.0-flash-lite	0.0376	0.0363	**0.1037**	**1.1096**	0.0389	0.0372	**0.1734**	**1.9801**
Deepseek-v3	0.0388	0.0378	0.0680	0.7470	0.0380	0.0374	0.0805	0.8414

G.4 Characteristics of Alphas at Varying MCTS Search Depths

In this section, we analysis the characteristics of alphas derived from nodes at different depths within the MCTS search tree. Alphas located at deeper levels of the tree undergo a greater number of refinement iterations. Figure 10 illustrates how several key metrics evolve with MCTS depth: specifically, the average formula depth (depth of the formula's tree representation), formula length (number of operators), in-sample (IS) and out-of-sample (OOS) RankIC, and the Overfitting Risk Score.

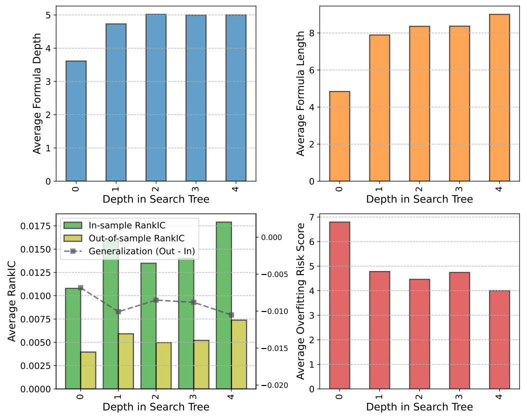


Figure 10: Evolution of Alpha Characteristics with MCTS Search Depth.

We observe that as MCTS search depth increases, both the average formula depth and length initially rise before tending to stabilize. This stabilization is largely attributed to the Overfitting Risk Score, which penalizes overly complex formulas more prone to overfitting. Concurrently, both average IS and OOS RankIC exhibit a general upward trend with increasing depth, reflecting the efficacy of the refinement process. Conversely, the generalization ability of the alphas—indicated by the difference between IS and OOS RankIC (the generalization gap)—tends to decrease. This trend aligns with the behavior of the Overfitting Risk Score, suggesting that while refinement enhances performance, the associated risk of overfitting necessitates careful management, a role our ORS aims to fulfill.

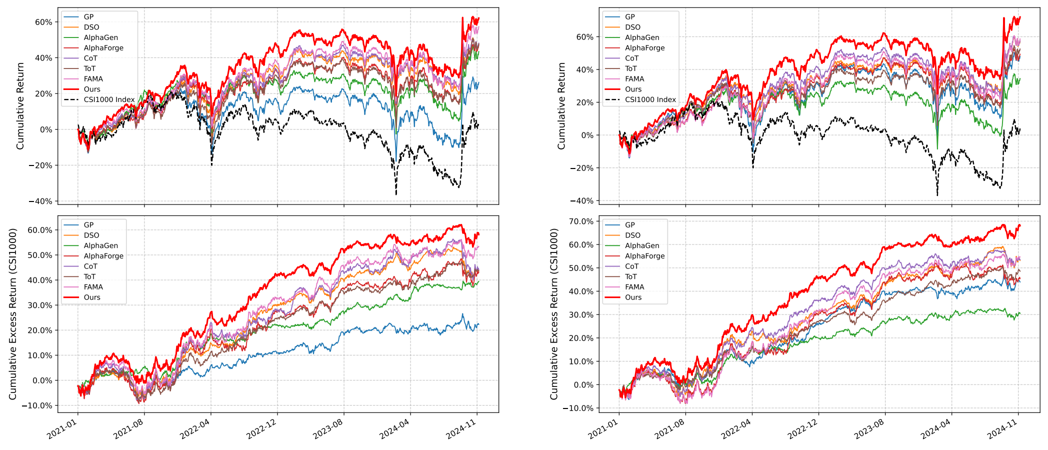
G.5 Cumulative Return Curve Visualizations

Figure 11 presents the cumulative return curves derived from backtesting using alphas mined by different methods. As illustrated, our proposed method consistently demonstrates superior performance, achieving the highest cumulative returns among the evaluated methods.

G.6 Interpretability of Mined Alpha Formulas

Table 6 presents a selection of alpha formulas mined by our framework alongside those from non-LLM-based baselines. The formulas derived by our framework are generally characterized by clear financial intuition. For instance, the alpha "$\mathrm{Zscore}(\mathrm{Ma}(\mathrm{close} - \mathrm{vwap}, 20), 30)$" intuitively captures buying or selling pressure by quantifying the deviation of the recent trend in the close-vwap spread from its historical norm. In contrast, formulas from other baselines often exhibit more complex or less transparent structures, making their financial rationale harder to discern.

G.7 Sensitivity Analysis of Key Framework Hyperparameters



(a) LightGBM Model (b) MLP Model

Figure 11: Cumulative return curves of backtest using alphas generated by different methods.

Table 6: Examples of alpha formulas mined by our framework and other non-LLM-based baselines. Each numbered item represents a distinct alpha formula.

Method	Alpha Formula
Ours	1. $\text{Zscore}(\text{Ma}(\text{close}-\text{vwap},20),30)$ 2. $\text{Std}(\text{Pct}(\text{vwap},20),25)\cdot\text{Sum}(\text{volume},40)/\text{volume}$ 3. $\text{Corr}(\text{close},\text{volume},50)\cdot\text{Zscore}(\text{Ma}(\text{close}-\text{vwap},30),40)$ 4. $\text{Diff}(\text{Ma}(\text{volume},20),3)/\text{Ma}(\text{volume},60)$ 5. $\text{Corr}(\text{Pct}(\text{close},10),\text{Pct}(\text{volume},10),10)\cdot\text{Corr}(\text{Pct}(\text{close},30),$ $\text{Pct}(\text{volume},30),30)\cdot\text{Skew}(\text{volume},20)$ 6. $\text{Ma}(\text{Corr}(\text{volume},\text{close},20)\cdot\text{Skew}(\text{high}-\text{low},20),10)$
GP	1. $\text{Add}(\text{Mul}(-0.01,\text{volume}),\text{Log}(\text{Log}(\text{close})))$ 2. $\text{Less}(\text{Cov}(\text{open},\text{Add}(\text{high},\text{Div}(\text{volume},-5)),10),\text{Std}(\text{Log}(\text{close}),50))$
DSO	1. $\text{Greater}(\text{volume},\text{Med}(\text{Sub}(\text{Ma}(\text{open},10),\text{Med}(\text{Std}(\text{Sign}(\text{close}),10),10)),10))$ 2. $\text{Cov}(\text{Med}(\text{Sign}(\text{vwap}),50),5,20)$
AlphaGen	1. $\text{Corr}(\text{Rank}(\text{Diff}(\text{Greater}(2.0,\text{volume}),50),10),\text{close},20)$ 2. $\text{Ma}(\text{Greater}(\text{Std}(\text{Less}(0.01,\text{Less}(\text{Div}(\text{Log}(\text{high}),-2.0),-30)),1),-30),5)$
AlphaForge	1. $1/(1/(\text{Diff}(\text{Sin}(1/(\text{Cos}(((0.01+\text{Sin}(\text{Tanh}(\text{high})))/30)))),30)))$ 2. $(\|(\text{Cos}\|(\text{Tanh}(\text{Sin}(\text{Diff}(\text{Sin}(30+\text{low}),20)))\|))+30.0\|)^2$

In this section, we investigate the sensitivity of our framework to two key hyperparameters: the initial MCTS search budget B (i.e., the initial target search number of MCTS) and the UCT exploration weight c. We conduct experiments using constituents of the CSI300 Index as the stock pool, targeting 10-day forward returns. The alpha set size is set to 50. Figure 12 illustrates the model's performance under various settings for these parameters.

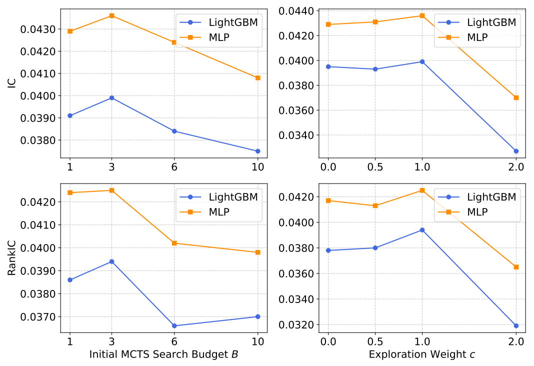


Figure 12: Impact of varying the initial MCTS search budget B and the UCT exploration weight c on the predictive performance.

For the initial MCTS search budget B, a value of 3 yields the best performance. A larger B can lead to excessive exploration of unpromising MCTS trees, consuming more computational resources without proportional gains. Conversely, a budget that is too small may result in insufficient exploration of potentially promising trees, thereby diminishing search efficacy.

Regarding the UCT exploration weight c, our findings suggest that an excessively large value is detrimental. A higher c biases the search towards more uniform exploration (randomness), potentially squandering refinement opportunities on underperforming alpha candidates.

H Full Experimental Results

In this section, we provide detailed experimental results for our proposed method and all other baselines. Table 7 and 8 illustrate the experimental results for the LightGBM and MLP models on the CSI300 stock pool. Similarly, Table 9 and 10 present the results for these two models on the CSI1000 stock pool.

Table 7: The predictive performance of LightGBM model trained on alphas mined by different methods on the CSI300 stock pool.

ΔT	Method	**Alpha Num = 10**				**Alpha Num = 50**				**Alpha Num = 100**			
		IC	RankIC	AR	IR	IC	RankIC	AR	IR	IC	RankIC	AR	IR
10	GP	0.0165	0.0148	0.0138	0.1717	0.0248	0.0246	0.0570	0.6777	0.0319	0.0288	0.0716	0.7222
	DSO	0.0079	0.0090	0.0434	0.6125	0.0174	0.0178	-0.0569	-0.6460	0.0246	0.0247	-0.0090	-0.1069
	AlphaGen	0.0443	0.0411	0.0119	0.1335	0.0388	0.0378	-0.0342	-0.3473	**0.0446**	**0.0416**	0.0094	0.1091
	AlphaForge	**0.0521**	**0.0518**	0.0231	0.2653	0.0293	0.0271	0.0252	0.3005	0.0407	0.0387	-0.0253	-0.3004
	CoT	0.0201	0.0206	0.0549	0.6713	0.0240	0.0224	0.0600	0.6683	0.0237	0.0225	0.0600	0.6681
	ToT	0.0269	0.0267	0.0387	0.4335	0.0256	0.0242	0.0680	0.7365	0.0358	0.0332	0.0620	0.6872
	FAMA	0.0210	0.0206	0.0175	0.2103	0.0243	0.0227	0.0593	0.7470	0.0292	0.0281	0.0585	0.6868
	Ours	0.0386	0.0364	**0.0668**	**0.7485**	**0.0399**	**0.0394**	**0.0717**	**0.8283**	0.0420	0.0395	**0.0822**	**0.9397**
30	GP	0.0145	0.0118	0.0322	0.3857	0.0248	0.0246	0.0570	0.6777	0.0319	0.0288	0.0716	0.7222
	DSO	0.0079	0.0090	-0.0050	-0.0682	0.0174	0.0178	0.0156	0.1735	0.0246	0.0247	0.0185	0.2039
	AlphaGen	0.0299	0.0280	0.0597	0.7792	0.0322	0.0286	0.0150	0.1540	0.0401	0.0339	0.0548	0.4662
	AlphaForge	0.0326	0.0322	0.0981	0.9455	0.0286	0.0278	0.0551	0.7341	0.0339	0.0315	0.0164	0.2176
	CoT	0.0200	0.0186	0.0774	0.9554	0.0274	0.0250	0.0574	0.6105	0.0278	0.0247	0.0468	0.5037
	ToT	0.0232	0.0247	0.1064	1.3221	0.0291	0.0285	0.0632	0.7982	0.0348	0.0312	0.0587	0.7037
	FAMA	0.0298	0.0307	0.1050	1.1609	0.0285	0.0298	0.0803	0.9502	0.0301	0.0297	**0.0934**	**1.1629**
	Ours	**0.0334**	**0.0334**	**0.1129**	**1.3286**	**0.0352**	**0.0340**	**0.0886**	**1.1299**	**0.0417**	**0.0401**	0.0826	1.0312

I Limitations

Despite the promising advancements presented by our framework for formulaic alpha mining, several limitations warrant discussion.

First, while our method generates effective alpha formulas, there remains a gap in achieving the same level of novelty and complexity typically found in formulas developed by human experts. The framework may sometimes struggle to produce highly intricate or unconventional alphas. Second, the diversity of the generated alphas is inherently constrained by the internal knowledge base of LLMs. This can, in turn, limit the breadth of the search space explored compared to certain non-LLM-based

Table 8: The predictive performance of MLP model trained on alphas mined by different methods on the CSI300 stock pool.

ΔT	Method	**Alpha Num = 10**				**Alpha Num = 50**				**Alpha Num = 100**			
		IC	RankIC	AR	IR	IC	RankIC	AR	IR	IC	RankIC	AR	IR
10	GP	0.0124	0.0120	-0.0212	-0.2240	0.0257	0.0233	0.0769	0.8324	0.0277	0.0266	0.0345	0.3967
	DSO	0.0085	0.0082	0.0485	0.5849	0.0062	0.0052	-0.0263	-0.2623	0.0256	0.0245	0.0019	0.0230
	AlphaGen	0.0419	0.0418	0.0725	0.8199	0.0380	0.0374	0.0524	0.6187	0.0311	0.0313	0.0295	0.3044
	AlphaForge	**0.0549**	**0.0554**	**0.0802**	**0.8397**	0.0232	0.0207	0.0668	0.7509	0.0408	0.0395	0.0220	0.2555
	CoT	0.0207	0.0209	0.0608	0.7030	0.0260	0.0260	0.0500	0.5632	0.0263	0.0257	0.0592	0.6627
	ToT	0.0281	0.0278	0.0625	0.7185	0.0285	0.0286	**0.0805**	**0.8414**	0.0323	0.0316	0.0340	0.3770
	FAMA	0.0243	0.0227	0.0593	0.7470	0.0292	0.0281	0.0585	0.6868	0.0307	0.0319	**0.1013**	**1.2209**
	Ours	0.0411	0.0406	0.0741	0.8186	**0.0436**	**0.0425**	0.0661	0.7075	**0.0422**	**0.0408**	0.0737	0.8103
30	GP	0.0149	0.0144	0.0541	0.6154	0.0262	0.0245	0.1422	1.5026	0.0220	0.0194	0.0815	0.7696
	DSO	-0.0009	0.0017	-0.0605	-0.6320	0.0067	0.0057	0.0037	0.0378	0.0250	0.0230	0.0919	0.9969
	AlphaGen	0.0204	0.0190	0.0417	0.4695	0.0240	0.0257	0.0538	0.6088	0.0415	0.0400	0.1149	1.2440
	AlphaForge	0.0348	0.0355	0.1162	1.0065	0.0283	0.0274	0.1004	1.2230	0.0317	0.0280	0.0732	0.9253
	CoT	0.0198	0.0188	0.1050	1.2943	0.0274	0.0264	**0.1631**	**1.6693**	0.0276	0.0250	0.1042	1.0422
	ToT	0.0265	0.0262	0.0975	1.1829	**0.0355**	**0.0353**	0.1330	1.5599	0.0337	0.0327	0.0584	0.7347
	FAMA	0.0341	0.0338	0.1173	1.3005	0.0302	0.0300	0.0596	0.6626	0.0331	0.0327	0.1012	1.0366
	Ours	**0.0361**	**0.0359**	**0.1259**	**1.3210**	0.0337	0.0340	0.1235	1.3931	**0.0423**	**0.0424**	**0.1315**	**1.4307**

Table 9: The predictive performance of LightGBM model trained on alphas mined by different methods on the CSI1000 stock pool.

ΔT	Method	**Alpha Num = 10**				**Alpha Num = 50**				**Alpha Num = 100**			
		IC	RankIC	AR	IR	IC	RankIC	AR	IR	IC	RankIC	AR	IR
10	GP	0.0621	0.0581	0.0965	0.8339	0.0627	0.0587	0.0956	0.8933	0.0744	0.0646	0.1054	1.0063
	DSO	0.0362	0.0368	0.0926	0.8602	0.0492	0.0466	0.1091	1.0195	0.0609	0.0559	0.1137	1.0720
	AlphaGen	0.0528	0.0511	0.0770	0.7751	**0.0828**	**0.0720**	0.0403	0.4799	0.0793	0.0693	0.0816	0.9041
	AlphaForge	**0.0702**	**0.0628**	0.0768	0.7029	0.0664	0.0601	0.0881	0.7687	0.0728	0.0631	0.0512	0.4607
	CoT	0.0556	0.0498	0.0450	0.4726	0.0638	0.0574	0.0607	0.6113	0.0670	0.0597	0.0602	0.5818
	ToT	0.0619	0.0573	0.0993	0.9592	0.0599	0.0558	0.0954	0.9419	0.0654	0.0585	0.0909	0.8889
	FAMA	0.0631	0.0595	0.1053	0.9234	0.0643	0.0596	0.1134	1.0222	0.0647	0.0584	0.1186	1.0708
	Ours	0.0661	0.0603	**0.1096**	**1.0919**	0.0748	0.0677	**0.1418**	**1.3699**	**0.0804**	**0.0729**	**0.1393**	**1.3577**
30	GP	**0.0575**	0.0522	0.0996	1.1359	0.0674	0.0637	0.0559	0.7088	0.0706	0.0672	0.0496	0.6230
	DSO	0.0362	0.0368	0.1181	1.1052	0.0420	0.0397	0.1096	1.2138	0.0609	0.0559	0.1226	1.1488
	AlphaGen	0.0511	0.0502	0.1087	1.2971	0.0727	0.0634	0.0991	**1.4196**	0.0685	0.0686	0.0520	0.7458
	AlphaForge	0.0558	**0.0532**	0.1095	0.9708	0.0705	0.0638	0.1081	0.9519	0.0705	0.0611	0.0796	0.8501
	CoT	0.0471	0.0438	0.1030	1.1473	0.0693	0.0629	0.1110	0.9757	0.0743	0.0661	0.1118	1.0872
	ToT	0.0475	0.0458	0.1340	1.4212	0.0643	0.0576	0.1097	1.1991	0.0758	0.0694	0.1147	1.1127
	FAMA	0.0543	0.0522	0.1136	0.9774	0.0550	0.0523	0.1340	1.2054	0.0557	0.0523	0.1226	1.0912
	Ours	0.0529	0.0506	**0.1543**	**1.6588**	**0.0741**	**0.0673**	**0.1461**	1.4065	**0.0793**	**0.0723**	**0.1326**	**1.2598**

Table 10: The predictive performance of MLP model trained on alphas mined by different methods on the CSI1000 stock pool.

ΔT	Method	**Alpha Num = 10**				**Alpha Num = 50**				**Alpha Num = 100**			
		IC	RankIC	AR	IR	IC	RankIC	AR	IR	IC	RankIC	AR	IR
10	GP	0.0578	0.0555	0.0922	0.8226	0.0606	0.0572	0.0807	0.6590	0.0659	0.0613	0.1031	0.9692
	DSO	0.0355	0.0349	0.1043	0.9314	0.0416	0.0405	0.0820	0.7957	0.0502	0.0469	0.0926	0.8907
	AlphaGen	0.0462	0.0463	0.0947	0.9076	0.0665	0.0619	0.0445	0.5072	0.0659	0.0597	0.0261	0.4004
	AlphaForge	**0.0694**	**0.0634**	0.1060	0.9916	0.0633	0.0580	0.1086	0.9420	0.0632	0.0606	0.0631	0.5837
	CoT	0.0518	0.0480	0.0513	0.5369	0.0585	0.0544	0.0721	0.7412	0.0648	0.0593	0.0706	0.6824
	ToT	0.0606	0.0578	0.1118	1.0644	0.0575	0.0558	0.0934	0.9376	0.0637	**0.0622**	0.0971	0.9258
	FAMA	0.0620	0.0591	0.1045	0.9361	0.0611	0.0582	0.1011	0.9539	0.0635	0.0572	0.1041	1.0323
	Ours	0.0609	0.0581	**0.1286**	**1.3039**	**0.0681**	**0.0622**	**0.1168**	**1.1843**	**0.0662**	0.0618	**0.1204**	**1.2868**
30	GP	**0.0555**	**0.0517**	0.1590	1.4989	0.0653	0.0606	0.1105	1.2125	0.0655	0.0638	0.0977	1.0269
	DSO	0.0312	0.0318	0.1171	1.0981	0.0338	0.0326	0.1336	1.3199	0.0542	0.0522	0.1056	0.9626
	AlphaGen	0.0505	0.0505	0.1436	1.3123	0.0664	0.0611	0.0766	1.0838	0.0640	0.0622	0.0569	0.8894
	AlphaForge	0.0541	**0.0517**	0.1071	0.9857	0.0642	0.0606	0.1134	1.0138	0.0717	0.0650	0.0667	0.6850
	CoT	0.0465	0.0440	0.1176	1.2683	0.0662	0.0620	0.1345	1.3550	0.0698	0.0615	0.1174	1.4363
	ToT	0.0466	0.0447	0.1322	1.3771	0.0608	0.0556	0.1220	1.4510	0.0690	0.0633	0.1116	1.2468
	FAMA	0.0532	0.0511	0.1224	1.1036	0.0538	0.0519	0.1374	1.2472	0.0571	0.0530	0.1327	1.2086
	Ours	0.0514	0.0491	**0.1799**	**1.8021**	**0.0673**	**0.0647**	**0.1710**	**1.6268**	**0.0738**	**0.0710**	**0.1696**	**1.5695**

methodologies. Consequently, scaling our approach to extremely large-scale alpha mining tasks, which necessitate the exploration of a vast and diverse alpha landscape, may present challenges.

Addressing these limitations, such as by incorporating mechanisms for enhanced novelty or expanding the effective search space, constitutes important directions for future research.

J LLM Agent Prompts

In our proposed framework, LLMs function as autonomous agents, instrumental in the multifaceted process of alpha formula mining. This includes the generation, iterative refinement, and overfitting risk evaluation of alpha formulas. This section details the core prompts designed to guide the LLM in these pivotal tasks. Each prompt is meticulously crafted to elicit specific behaviors and outputs from the LLM, ensuring a structured and effective approach to mining alpha formulas.

J.1 Alpha Portrait Generation Prompt

As shown in Figure 13, the Alpha Portrait Generation Prompt is used to generate an alpha portrait based on information such as available data fields and operators. The alpha portrait is subsequently used to generate the corresponding alpha formula.

J.2 Alpha Formula Generation Prompt

As shown in Figure 14, the Alpha Formula Generation Prompt is used to generate the corresponding alpha formula based on the provided alpha portrait and other relevant information. A formatted alpha formula facilitates correctness verification and the computation of alpha values.

J.3 Alpha Overfitting Risk Assessment Prompt

As shown in Figure 15, the Alpha Overfitting Risk Assessment Prompt is used to assess the overfitting risk of an alpha based on its formula and refinement history information. We provide evaluation criteria within the prompt to assist the LLM in conducting a critical assessment.

J.4 Alpha Refinement Prompt

As shown in Figure 16, the Alpha Refinement Prompt is used to refine the original alpha formula based on refinement suggestions, thereby generating an improved formula.

Task Description:
You are a quantitative finance expert specializing in factor-based investing. Please design an alpha factor used in investment strategies according to the following requirements, and then provide the content of the alpha in the required format.

Available Data Fields:
The following data fields are available for use:

`{available_fields}`

Available Operators:
The following operators are available for use:

`{available_operators}`

Alpha Requirements:

1. The alpha value should be dimensionless (unitless).
2. The alpha should incorporate at least two distinct operations from the "Available Operators" list to ensure it has sufficient complexity. Avoid creating overly simplistic alphas.
3. All look-back windows and other numerical parameters used in the alpha calculation MUST be represented as named parameters in the pseudo-code. These parameter names MUST follow Python naming conventions (e.g., `lookback_period`, `volatility_window`, `smoothing_factor`).
4. The alpha should have NO MORE than 3 parameters in total.
5. The pseudo-code should represent the alpha calculation step-by-step, using only the "Available Operators" and clearly defined parameters. Each line in the pseudo-code should represent a single operation.
6. Use descriptive variable names in the pseudo-code that clearly indicate the data they represent.
7. When designing alpha expressions, try to avoid including the following sub-expressions:

   `{freq_subtrees}`

Formatting Requirements:
The output must be in JSON format with three key-value pairs:

1. **"name":** A short, descriptive name for the alpha (following Python variable naming style, e.g., `price_volatility_ratio`).
2. **"description":** A concise explanation of the alpha's purpose or what it measures. Avoid overly technical language. Focus on the intuition behind the alpha.
3. **"pseudo_code":** A list of strings, where each string is a line of simplified pseudo-code representing a single operation in the alpha calculation. Each line should follow the format: `variable_name = op_name(input=[input1, input2, ...], param=[param1, param2, ...])`, where:
   - `variable_name` is the output variable of the operation.
   - `op_name` is the name of one of the "Available Operators".
   - `input1`, `input2`, ... are input variables (either from "Available Data Fields" or previously calculated variables, cannot be of a numeric type).
   - `param1`, `param2`, ... are parameter names defined in the alpha requirements.

The format example is as follows:

```
{
    "name": "volatility_adjusted_momentum",
    "description": "......",
    "pseudo_code": [......]
}
```

Figure 13: Alpha Portrait Generation Prompt

Task Description:

Please design a quantitative investment alpha expression according to the following requirements.

Available Data Fields:

- The following data fields are available for use: `{available_fields}`

Available Operators:

- The following operators are available for use: `{available_operators}`

Alpha Requirements:

- `{alpha_portrait_prompt}`

Formatting Requirements:

1. Provide the output in JSON format.
2. The JSON object should contain two fields: `"formula"`, and `"arguments"`.
   - `"formula"`: Represents the mathematical expression for calculating the alpha.
   - `"arguments"`: Represents the configurable parameters of the alpha.
3. `"formula"` is a list of dictionaries. Each dictionary represents a single operation and must contain four keys: `"name"`, `"param"`, `"input"`, and `"output"`.
   - `"name"`: The operator's name (a string), which MUST be one of the operators provided in the "Available Operators" section.
   - `"param"`: A list of strings, representing the parameter names for the operator. These parameter names MUST be used as keys in the `"arguments"` section.
   - `"input"`: A list of strings, representing the input variable names for the operator. These MUST be data fields from the "Available Data Fields" or output variables from previous operations in the `"formula"`, cannot be of a numeric type.
   - `"output"`: A string, representing the output variable name for the operator. This output can be used as an input for subsequent operations.
4. `"arguments"` is a list of dictionaries. Each dictionary represents a set of parameter values for the alpha.
   - The keys of each dictionary in `"arguments"` MUST correspond exactly to the parameter names defined in the `"param"` lists of the `"formula"`.
   - The values in each dictionary in `"arguments"` are the specific numerical values for the parameters.
5. You may include a maximum of 3 sets of parameters within the `"arguments"` field.
6. The parameter value that indicates the length of the lookback window (if applicable) must be within the `{window_range}` range.
7. Ensure that the alpha expression is both reasonable and computationally feasible.
8. Parameter names should be descriptive and follow Python naming conventions (e.g., `window_size`, `lag_period`, `smoothing_factor`). Avoid using single characters or numbers as parameter names.
9. Refer to the following example:

```
{
    "formula": [......],
    "arguments": [......]
}
```

Figure 14: Alpha Formula Generation Prompt

Task: Critical Alpha Overfitting Risk Assessment
Critically evaluate the overfitting risk and generalization potential of the provided quantitative investment alpha, based on its expression and refinement history. Your assessment must focus on whether complexity and optimization appear justified or are likely signs of overfitting.

Input:

- **Alpha Expression:**

  `{alpha_formula}`

- **Refinement History:**

  `{refinement_history}`

Evaluation Criteria:

1. **Justified Rationale vs. Complexity:**

   Critique: Is the complexity of the alpha expression plausibly justified by an inferred economic rationale, or does it seem arbitrary/excessive, suggesting fitting to noise?

2. **Principled Development vs. Data Dredging:**

   Critique: Does the refinement history indicate hypothesis-driven improvements, or does it suggest excessive optimization and curve-fitting (e.g., frequent, unjustified parameter tweaks)?

3. **Transparency vs. Opacity:**

   Critique: Is the alpha's logic reasonably interpretable despite its complexity, or is it opaque, potentially masking overfitting?

Scoring & Output:

- Assign a single **Overfitting Risk Score** from 0 to 10.
  - **10 = Very Low Risk** (High confidence in generalization)
  - **0 = Very High Risk** (Low confidence in generalization)
- Use the full 0-10 range to differentiate risk levels effectively.
- Provide a concise, one-sentence **Justification** explaining the score, citing the key factors from the criteria.
- Format the output as JSON, like the examples below:

Example JSON Outputs:

```
{
    "reason": "Complexity is justified by a strong rationale; principled
    refinement history suggests low risk.",
    "score": 9
}

{
    "reason": "Plausible rationale, but some expression opacity and parameter
    tuning in history indicate moderate risk.",
    "score": 5
}

{
    "reason": "High risk inferred from opaque expression lacking clear
    rationale, supported by history showing excessive tuning.",
    "score": 1
}
```

Figure 15: Alpha Overfitting Risk Assessment Prompt

Task Description:
There is an alpha factor used in quantitative investment to predict asset price trends. Please improve it according to the following suggestions and provide the improved alpha expression.

Available Data Fields:
The following data fields are available for use: `{available_fields}`

Available Operators:
The following operators are available for use:`{available_operators}`

Alpha Suggestions:

1. The alpha value should be dimensionless (unitless).
2. All look-back windows and other numerical parameters used in the alpha calculation MUST be represented as named parameters in the pseudo-code. These parameter names MUST follow Python naming conventions (e.g., `lookback_period`, `volatility_window`, `smoothing_factor`).
3. The alpha should have NO MORE than 3 parameters in total.
4. The pseudo-code should represent the alpha calculation step-by-step, using only the "Available Operators" and clearly defined parameters. Each line in the pseudo-code should represent a single operation.
5. Use descriptive variable names in the pseudo-code that clearly indicate the data they represent.
6. When designing alpha expressions, try to avoid including the following sub-expressions: `{freq_subtrees}`

Original alpha expression:

`{origin_alpha_formula}`

Refinement suggestions:
NOTE: The following improvement suggestions do not need to be all adopted; they just need to be considered and reasonable ones selected for adoption.

`{refinement_suggestions}`

Formatting Requirements:
The output must be in JSON format with three key-value pairs:

1. **"name"**: A short, descriptive name for the alpha (following Python variable naming style, e.g., `price_volatility_ratio`).
2. **"description"**: A concise explanation of the alpha's purpose or what it measures. Avoid overly technical language. Focus on the intuition behind the alpha.
3. **"pseudo_code"**: A list of strings, where each string is a line of simplified pseudo-code representing a single operation in the alpha calculation. Each line should follow the format: `variable_name = op_name(input=[input1, input2, ...], param=[param1, param2, ...])`, where:
   - `variable_name` is the output variable of the operation.
   - `op_name` is the name of one of the "Available Operators".
   - `input1`, `input2`, ... are input variables (either from "Available Data Fields" or previously calculated variables, cannot be of a numeric type).
   - `param1`, `param2`, ... are parameter names defined in the alpha requirements.

The format example is as follows:

```
{
    "name": "volatility_adjusted_momentum",
    "description": "......",
    "pseudo_code": [......]
}
```

Figure 16: Alpha Refinement Prompt