AUTOMATED FEATURE ENGINEERING BY PROMPTING

Anonymous authors
Paper under double-blind review

ABSTRACT

Automated feature engineering (AutoFE) liberates data scientists from the burden of manual feature construction, a critical step for tabular data prediction. While the semantic information of datasets provides valuable context for feature engineering, it has been underutilized in most existing works. In this paper, we introduce AutoFE by Prompting (FEBP), a novel AutoFE algorithm that leverages large language models (LLMs) to process dataset descriptions and automatically generate features. Incorporating domain knowledge, the LLM iteratively refines feature construction through in-context learning of top-performing example features and provides semantic explanations. Our experiments on real-world datasets demonstrate the superior performance of FEBP over state-of-the-art AuoFE methods. We also conduct ablation study to verify the impact of dataset semantic information and examine the behavior of our LLM-based feature search process.

1 INTRODUCTION

Tabular data, a form of structured data comprising instances and attributes, have extensive use in vast domains, e.g., credit assessment, market prediction, and quality control. Traditional machine learning models, especially tree-based models (Breiman, 2001; Ke et al., 2017), have strong performance on tabular datasets of small and medium sizes (Grinsztajn et al., 2022) and good interpretability. Feature engineering is the process of computing new features from feature attributes of a dataset to enhance downstream model performance, which is crucial for traditional ML models as the new features extract useful information for target prediction by capturing complex non-linear relationships. Feature engineering by hand requires domain expertise to alleviate the significant human labor.

Automated feature engineering (AutoFE) uses high-level algorithms and models to automate the FE process such that the performance is comparable to domain experts. Existing AutoFE methods, such as (Zhu et al., 2022a;b; Zhang et al., 2023), compute and evaluate a large number of features in a trial-and-error manner. While some learn to optimize the feature utility during the FE process, these methods do not utilize domain knowledge to guide the feature search. The need to start from scratch for new datasets or downstream models hampers their effectiveness and efficiency. Besides, these methods do not offer explanation of the computed features, impairing the interpretability.

The descriptions contained in tabular datasets provide rich context for feature engineering. Domain experts consult attribute descriptions to select relevant feature attributes and compute new features useful for predicting the target. For example, the *square footage* of a house times the *average housing price per square foot* in the neighborhood can be a good predictor of the *market value* of the house. Large language models (LLMs) (Radford et al., 2019; Brown et al., 2020; OpenAI, 2023; Touvron et al., 2023a;b), pretrained on large volumes of text data, handle general natural language processing tasks and encapsulate extensive domain knowledge. Under proper prompt instructions, the LLM may process the dataset semantic information and utilize its knowledge to automatically compute features in a manner similar to domain

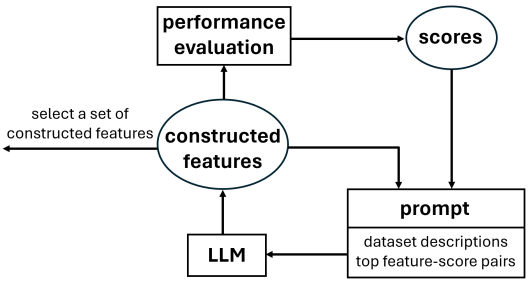


Figure 1: Overview of FEBP: (1) prompting the LLM to construct new features by providing dataset descriptions and example features; (2) evaluating the constructed features; (3) updating the prompt with top-performing features and scores; and (4) selecting a set of features and adding them to the dataset.

experts. The work by Hollmann et al. (2023) demonstrates the potential of applying LLMs for AutoFE, but it is not sufficiently effective in terms of feature search.

We propose AutoFE by Prompting (FEBP), a novel AutoFE algorithm that leverages LLMs for effective, efficient, and interpretable feature engineering, as illustrated in Figure 1. By providing dataset descriptions and example features in canonical Reverse Polish Notation (cRPN), we prompt the LLM to generate new features. After evaluating the features, we update the prompt with top-performing features and their evaluation scores and instruct the LLM to construct further features. Through this iterative process, the LLM explores the feature space and improves solutions through in-context learning of successful examples. The semantic information of data not only guides the feature search, but helps the LLM understand and learn from the patterns in example features. Applying domain knowledge, the LLM generates semantically meaningful features and explains their usefulness. Experiments on seven real-world datasets demonstrate that FEBP significantly outperforms state-of-the-art baselines, achieving over 5% performance gain on average across three downstream models. Additionally, our ablation study shows that incorporating dataset semantic context improves the performance. We also analyze the behavior of the LLM-based feature search process and examine the effects of hyperparameters.

Our main contributions are: (1) We introduce a novel LLM-based AutoFE algorithm that utilizes dataset semantic information for automated feature search. This is the first method capable of generating features in string representations while providing semantic explanations. (2) We benchmark the performance of our approach against state-of-the-art baselines using both GPT-3.5 and GPT-4. (3) We investigate the impact of semantic context on our approach, analyze the behavior of the LLM-based feature search process, and examine hyperparameter effects.

2 Related Work

Large Language Models. LLMs are large-scale general-purpose neural networks pretrained on large corpora of raw text data for natural language processing, typically built with transformer-based architectures (Vaswani et al., 2017). Generative LLMs, such as the GPT family (Radford et al., 2019; Brown et al., 2020; OpenAI, 2023) and the LLaMA family (Touvron et al., 2023a;b), are pretrained to successively predict the next token given the input text and can be finetuned using reinforcement learning from human feedback (Ziegler et al., 2019; Ouyang et al., 2022). By this means, they acquire the knowledge about syntax and semantics of human languages and are able to achieve state-of-the-art performance on various tasks like text generation, summarization, and question answering. LLMs can be adapted to specific tasks without changing model parameters through prompt engineering. Few-shot learning (Brown et al., 2020) includes examples in the prompt for the language model to learn in-context. Leveraging such capability, the LLM may function as a problem solver (Yang et al., 2024) that iteratively improves candidate solutions according to the task description and feedback. Chain-of-though (Wei et al., 2022; Kojima et al., 2022) enables complex reasoning capabilities of LLMs through intermediate reasoning steps.

Automated Feature Engineering. AutoFE computes new features for the input data and augments or replaces portions of the existing features, to enhance the performance of downstream models. Common AutoFE approaches include expansion-reduction (Kanter & Veeramachaneni, 2015; Horn et al., 2020; Zhang et al., 2023), evolutionary algorithms (Smith & Bull, 2005; Zhu et al., 2022a), and reinforcement learning (Khurana et al., 2018; Li et al., 2023; Wang et al., 2023). DIFER (Zhu et al., 2022b) utilizes neural networks to learn the utility of constructed features and optimize features in the embedding space. OpenFE (Zhang et al., 2023) introduces a feature boost algorithm to speedup feature evaluation. Nonetheless, these approaches do not utilize the semantic information of data, which impedes the performance and interpretability of engineered features.

AutoFE with Domain Knowledge. The benefits of incorporating domain knowledge in AutoFE include: (1) improving the effectiveness; and (2) reducing the cost of learning an AutoFE model, especially the feature evaluation overhead. Prior works take different directions. One direction is to transfer the knowledge through pretraining. LFE (Nargesian et al., 2017) represents features with quantile sketches transferable across datasets and inputs them to a feature transformation recommendation model. FETCH (Li et al., 2023) is an RL-based AutoFE framework taking tabular data as the state and generalizable to new data. E-AFE (Wang et al., 2023) pretrains a feature evaluator

to efficiently learn the RL-based AutoFE model. The other direction is to leverage the semantic information of datasets. KAFE (Galhotra et al., 2019) leverages knowledge graphs to identify semantically informative features relevant to the prediction task. CAAFE (Hollmann et al., 2023) manipulates Pandas data frames using the code generated from the LLM based on dataset descriptions. In our work, we adopt a compact form of feature representation in strings with pre-defined transformation operators. Our approach reduces the search space and helps the LLM learn the patterns of useful features, leading to stronger and more robust performance. We further discuss the differences between our approach and CAAFE in Appendix G.

3 NOTATIONS

We denote a tabular dataset as $D = \langle \mathbb{X}, \boldsymbol{y} \rangle$, where $\mathbb{X} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_d\}$ is the set of raw features with $\boldsymbol{x}_i \in \mathbb{R}^n$ for $i = 1, \ldots, d$ and $\boldsymbol{y} \in \mathbb{R}^n$ is the target. We construct a new feature $\tilde{\boldsymbol{x}} = t(\boldsymbol{x}_{j_1}, \ldots, \boldsymbol{x}_{j_o})$ by transforming existing features $\boldsymbol{x}_{j_1}, \ldots, \boldsymbol{x}_{j_o}$ via some operator $t \in \mathbb{R}^n \times \ldots \times \mathbb{R}^n \to \mathbb{R}^n$ of arity o. Given a set of transformation operators $\mathbb{T}$, we define the feature space $\mathbb{X}_\mathbb{T}$ recursively as: for any $\tilde{\boldsymbol{x}} \in \mathbb{X}_\mathbb{T}$, either $\tilde{\boldsymbol{x}} \in \mathbb{X}$; or $\exists t \in \mathbb{T}$, s.t., $\tilde{\boldsymbol{x}} = t(\tilde{\boldsymbol{x}}_{j_1}, \ldots, \tilde{\boldsymbol{x}}_{j_o})$, where $\tilde{\boldsymbol{x}}_{j_1}, \ldots, \tilde{\boldsymbol{x}}_{j_o} \in \mathbb{X}_\mathbb{T}$. To measure feature complexity, we compute the order of a feature $\tilde{\boldsymbol{x}} \in \mathbb{X}_\mathbb{T}$ as:

$$\alpha(\tilde{\boldsymbol{x}}) = \begin{cases} 0 & \text{if } \tilde{\boldsymbol{x}} \in \mathbb{X}, \\ 1 + \max_j \alpha(\tilde{\boldsymbol{x}}_j) & \text{if } \tilde{\boldsymbol{x}} = t(\tilde{\boldsymbol{x}}_{j_1}, \ldots, \tilde{\boldsymbol{x}}_{j_o}) \text{ for some } t \in \mathbb{T}. \end{cases} \tag{1}$$

The constrained feature space with the order upper bounded by k is denoted as $\mathbb{X}_\mathbb{T}^{(k)} = \{\tilde{\boldsymbol{x}} \in \mathbb{X}_\mathbb{T} \mid \alpha(\tilde{\boldsymbol{x}}) \leq k\}$.

We denote the performance of a downstream machine learning model algorithm M on the dataset as $\mathcal{E}_M(\mathbb{X}, \boldsymbol{y})$. Our objective of AutoFE is to construct a set of features $\tilde{\mathbb{X}}^*$ to optimize the model performance by adding them to the dataset, specifically:

$$\tilde{\mathbb{X}}^* = \underset{\tilde{\mathbb{X}} \subset \mathbb{X}_\mathbb{T}}{\arg\max}\ \mathcal{E}_M(\mathbb{X} \cup \tilde{\mathbb{X}}, \boldsymbol{y}). \tag{2}$$

4 METHODOLOGY

In this section, we present AutoFE by Prompting (FEBP), a novel AutoFE algorithm leveraging the power of LLMs, particularly, the GPT models (Radford et al., 2019; Brown et al., 2020; OpenAI, 2023). The high-level idea is to provide the LLM with descriptive information of the dataset in the prompt and guide it to search for effective features using examples.

We represent features in a compact form in our prompt. A feature $\tilde{\boldsymbol{x}} \in \mathbb{X}_\mathbb{T}$ is expressible as a tree, where the leaf nodes are raw features and the internal nodes are operators. However, the expression trees of features containing commutative operators (like addition and multiplication) are not unique since the child nodes of these operators are unordered. We introduce a canonicalization scheme: arranging operator nodes before feature nodes for left skewness and lexicographically sorting the nodes within each group. We then serialize the canonical expression tree into the postorder depth-first traversal string, i.e., canonical reverse Polish notation (cRPN), ensuring the one-to-one mapping between features and string representations. We denote the feature corresponding to an RPN string f as $\tilde{\boldsymbol{x}}_f$ and the set of features corresponding to a set of RPN strings $\mathbb{F}$ as $\tilde{\mathbb{X}}_\mathbb{F}$. We refer to Appendix A for further discussion.

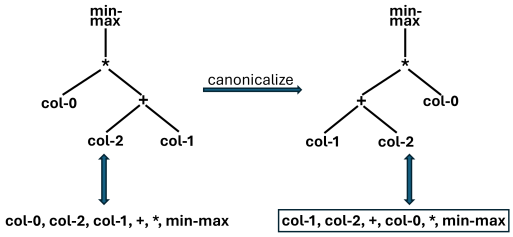


Figure 2: We obtain the canonical RPN (cRPN) by reordering nodes of the expression tree.

Our prompt contains: (1) a meta description of the dataset (optional); (2) an indexed list of the dataset attributes, with attribute types, value ranges, and descriptions; (3) lists of transformation operators with descriptions, grouped by the arity; (4) a ranked list of example features with performance evaluation scores; and (5) an output template for new features and explanations. Figure 3 outlines the structure of our prompt. The descriptions of the dataset and attributes provide contextual information for the LLM to understand the data and apply domain knowledge. The value ranges of attributes

(1) Dataset description:
This dataset contains information on default payments, demographic factors, credit data, and history of payment of credit card clients ...
(2) Dataset contains the following columns:
col-0 (int) [10000, 800000]: LIMIT_BAL: Amount of given credit in NT dollars (includes individual and family/supplementary credit
col-1 (category) {1, 2}: SEX: Gender (1=male, 2=female) . . .
col-23 (category) {0, 1}: default.payment.next.month: Default payment (1=yes, 0=no)
(3) We have the following unary operators:
sqrt_abs: taking the square root of the absolute value . . .
We have the following binary operators:
+: summing two columns . . .
Feature strings are reverse Polish notation (RPN) expressions that operate on the columns of our dataset. Each feature string constructs an extra column that is useful for the downstream model Random Forests to predict the target col-23. The model will be trained on the dataset with the constructed columns and evaluated on a holdout set. The best columns will be selected.
(4) Below are feature strings arranged in ascending order based on their performance scores. Higher scores are better.
Feature
col-17,col-21,*,col-20,+,sqrt_abs
Score
0.0011 . . .
Feature
col-4,col-6,*,col-12,col-16,-,sqrt_abs,*
Score
0.0014
Give me a new feature string that is different from all strings above and has a higher score. Use no more than five operators. Make sure all columns and operators exist and do not include the target column. Follow the syntax of RPN.
(5) Output format:
Feature
(Feature name and description)
Usefulness
(Explanation why this adds useful real world knowledge to predict the target col-23 according to dataset description)

Figure 3: Prompt template. Sections requiring dataset information are highlighted in blue. The ranked list of feature examples and scores that gets updated in our feature search algorithm is highlighted in orange.

Feature
col-11,col-11,col-12,-,log,*
This feature calculates the log of the difference between the September bill statement (col-11) and the August bill statement (col-12), then multiplies it by the September bill amount.

Usefulness
This feature captures the change in the bill amount from August to September in a logarithmic scale, which can effectively highlight significant changes in spending patterns. Large fluctuations in credit card bills could be indicative of financial distress, which may impact the likelihood of defaulting on payments, while the logarithmic transformation allows for handling potential skewness in the data distribution. By incorporating this feature, the model can better understand how temporal changes in spending behavior relate to the probability of default, providing richer contextual information beyond static features.

Figure 4: The LLM constructs a new feature in RPN and explains its usefulness from the semantic perspective.

are useful for selecting appropriate feature transformations, e.g., min-max normalization when the scale is too large. We include the descriptions of transformation operators as they help the LLM parse example features in RPN syntax and construct syntactically valid feature strings. The output template not only structures the output but instructs the LLM to reason about the usefulness of the proposed features and offer semantic explanations, utilizing the chain-of-thought technique (Wei et al., 2022; Kojima et al., 2022). We additionally add a constraint instruction to use no more than a certain number of operators, which reduces the search space and regularizes the solutions. Figure 4 shows an example LLM output. The prompt can further include attribute statistics like mean, standard deviation, and skewness, and we leave that for future work.

We initialize the prompt with k random features from the constrained feature space $\tilde{\boldsymbol{x}}_1, \ldots, \tilde{\boldsymbol{x}}_k \in \mathbb{X}_{\mathbb{T}}^{(2)}$ represented in cRPN for demonstration. This lets the LLM start search from a small feature space where it is easier to identify the basic patterns of promising features. Optionally, we can import external example features. We prompt the LLM to construct a fixed number of m new feature in an iteration. For each constructed feature string f, we first try to obtain the cRPN expression f^c to check whether f^c is syntactically valid and not a duplicate of existing features. If both criteria are met, we evaluate the performance score of adding the single feature to the dataset $s = \mathcal{E}_M(\mathbb{X} \cup \{\tilde{\boldsymbol{x}}_{f^c}\}, \boldsymbol{y})$ through cross validation on the training data and add $\langle f^c, s\rangle$ to the candidate set $\mathbb{F}_{cand}$. When f^c is among the top-k candidate features in terms of the score s, we update prompt examples with the top-k pairs $\langle f', s'\rangle \in \mathbb{F}_{cand}$ ranked in the ascending order, taking score increment $s' - \mathcal{E}_M(\mathbb{X}, \boldsymbol{y})$ from the baseline. We then instruct the LLM to construct additional features using the updated prompt. To select candidate features, we successively add candidate features to the dataset from the best to the worst and determine the optimal number of features to add based on validation performance, which is evaluated over sets of candidate features and thus takes feature interactions into account. Algorithm 1 summarizes our methodology. The size of the prompt scales linearly with the number of features in the dataset d and the number of example features k and stays roughly constant across feature construction iterations. Thus, the cost of an LLM generation step in line 3 is almost constant.

Algorithm 1: AutoFE by Prompting

Input : Dataset $D = \langle \mathbb{X}, \boldsymbol{y} \rangle$, downstream model M, large language model LLM, and optionally an external set of features with evaluation scores $\mathbb{F}_{ext}$

Output: A set of engineered features $\mathbb{F}$

1 Initialize prompt P with dataset descriptions and example features; $\mathbb{F}_{cand} \leftarrow \mathbb{F}_{ext}$ if $\mathbb{F}_{ext}$ is available, otherwise $\mathbb{F}_{cand} \leftarrow \emptyset$; $\mathbb{F}_{set} \leftarrow \emptyset$
2 **repeat**
3 $\quad \mathbb{F}_{LLM} = \{f_1, \ldots, f_m\} \leftarrow LLM(P)$ ▷ `Feature generation`
4 $\quad$ **for** each $f \in \mathbb{F}_{LLM}$ **do**
5 $\quad\quad f^c \leftarrow$ Canonicalize f
6 $\quad\quad$ **if** f^c is valid and $f^c \notin \mathbb{F}_{cand}$ **then** ▷ `Feature evaluation`
7 $\quad\quad\quad$ Evaluate cross validation performance score $s \leftarrow \mathcal{E}_M(\mathbb{X} \cup \{\boldsymbol{x}_{f^c}\}, \boldsymbol{y})$ on training data
8 $\quad\quad\quad \mathbb{F}_{cand} \leftarrow \mathbb{F}_{cand} \cup \{\langle f^c, s \rangle\}$
9 $\quad\quad$ **end**
10 $\quad$ **end**
11 $\quad$ Update P such that P contains the top-k $\langle f', s' \rangle \in \mathbb{F}_{cand}$ as ordered by s'
12 $\quad$ **if** feature selection **then**
13 $\quad\quad$ **for** $n \leftarrow 1$ **to** $|\mathbb{F}_{cand}|$ **do** ▷ `Feature selection`
14 $\quad\quad\quad \mathbb{F}_n \leftarrow$ The top-n features in $\mathbb{F}_{cand}$ as ordered by s
15 $\quad\quad\quad$ Evaluate performance score $s_n \leftarrow \mathcal{E}_M(\mathbb{X} \cup \tilde{\mathbb{X}}_{\mathbb{F}_n}, \boldsymbol{y})$ on validation data
16 $\quad\quad$ **end**
17 $\quad\quad \mathbb{F}_{set} \leftarrow \mathbb{F}_{set} \cup \{\langle \mathbb{F}_{n^*}, s_{n^*} \rangle\}$, where $n^* \leftarrow \text{argmax}_n s_n$
18 $\quad$ **end**
19 **until** stopping criteria are met
20 **return** $\mathbb{F}$ in $\mathbb{F}_{set}$ with the maximum validation score

The computation cost of feature evaluation in line 7 is also constant, preserving the efficiency and scalability of our algorithm. The evaluations in line 7 and at lines 13-16 are parallelizable.

Methodologically, we instruct the LLM to act as a problem solver (Yang et al., 2024) within our algorithm. Similar to evolutionary algorithms (Smith & Bull, 2005; Zhu et al., 2022a; Morris et al., 2024) that generate new solutions through crossover and mutations on high-fitness candidates, we maintain a pool of top-performing candidate features as examples. By learning examples and scores in-context (Brown et al., 2020), the LLM can recognize patterns of promising features and propose new features that are likely to be effective. For instance, it may make analogies to, modify, or combine example features (Appendix F.2). Early in the search, we expect greater exploration due to the diversity of initial examples. As iterations progress, the LLM focuses more on exploiting promising feature spaces, gradually refining the search until convergence. The dataset semantic information serves as a prior that guides the selection of feature attributes and operators to enhance the effectiveness of feature search. The sampling temperature of the LLM can be adjusted to balance exploration and exploitation, with higher temperatures encouraging more diverse solutions and lower temperatures favoring incremental changes to existing examples.

We adopt the same set of transformation operators $\mathbb{T}$ as those in (Zhu et al., 2022b), including:

- Unary transformations: logarithm, reciprocal, square root, and min-max normalization;
- Binary transformations: addition, subtraction, multiplication, division, and modulo.

When computing min-max normalization, we take the minimum and maximum from the training data. Other transformations require only the information of an individual example. Hence, all our transformation operations can be performed instance by instance on each individual test example without leaking the information of other test examples. As discussed by Overman et al. (2024), data leakage is an issue that has not been properly addressed in many existing AutoFE works.

5 Experiments

5.1 Experimental Setup

We benchmark performance on seven public real-world datasets from Kaggle and UCI repositories covering different domains. The descriptive information of datasets and attributes is retrieved

Table 1: Dataset statistics. The selected datasets cover different domains and vary in size. Four of them are for regression tasks and three for classification tasks.

Name	Task	# Samples	# Features	# Numerical	# Categorical
Airfoil (AF)	Regression	1,503	5	5	0
Boston Housing (BH)	Regression	506	13	12	1
Bikeshare (BS)	Regression	731	10	6	4
Wine Quality Red (WQR)	Regression	1,599	11	11	0
AIDS Clinical Trials (ACT)	Classification	2,139	23	9	14
Credit Default (CD)	Classification	30,000	23	14	9
German Credit (GC)	Classification	1,000	20	10	10

from the sources without further processing. The downstream models we evaluate include linear models (LASSO for regression tasks and logistic regression for classification tasks), Random Forests (Breiman, 2001), and LightGBM (Ke et al., 2017). For linear models, we target-encode categorical features and min-max scale all features. We tune downstream model parameters by randomized search prior to and post AutoFE, because the model algorithm may need reconfiguration to accommodate the added features. Data are randomly split into training (64%), validation (16%), and test (20%) sets. We evaluate regression performance with $1 - (relative\, absolute\, error)$[1] and classification performance with accuracy. A higher evaluation score indicates better performance.

We compare our FEBP with the following state-of-the-art AutoFE methods:

- DIFER (Zhu et al., 2022b): A neural network-based method that optimizes features in the embedding space utilizing LSTMs to encode and decode features;
- OpenFE (Zhang et al., 2023): An expansion-reduction method that evaluates and ranks features up to a certain order using a feature boost algorithm;
- CAAFE (Hollmann et al., 2023): An LLM-based method that produces Python code based on dataset descriptions to manipulate Pandas data frames.

We employ *gpt-3.5-turbo-0125*[2] and *gpt-4-0613*[2] as the LLMs in our experiments. For FEBP, we include $k = 10$ example features in the prompt and set the temperature of GPT models to 1 based on validation performance. We prompt the LLM to construct $m = 1$ feature in each generation step for more accurate control of feature generation. We perform feature selection each time 10 new candidate features are constructed and terminate the algorithm once we have 200 candidate features. Parameters of the baseline AutoFE methods are initialized per the corresponding papers. For CAAFE (Hollmann et al., 2023), we raise the number of iterations from 10 to 20. Drastically increasing this limit causes failures due to the context window size of GPT models. We report results from five repeated runs unless stated otherwise.

5.2 Performance Comparison

Table 2 compares the performance between FEBP and baseline methods. While there is no single method that dominates all test cases, FEBP achieves the best mean performance score and the lowest mean rank. FEBP yields over 5% average performance gain over downstream models using raw features, with over 15% gain for linear models and around 2% gain for Random Forests and LightGBM. Greater performance gain is observed using linear models because Random Forests and LightGBM can model complex non-linear relationships themselves. The Friedman-Nemenyi test shows that the performance difference between FEBP and baseline methods other than DIFER is statistically significant at the $p = 0.01$ level. We note that the post-AutoFE parameter tuning improves the performance of DIFER the most, as DIFER adds many more features to the datasets (Appendix D.7). FEBP is considerably more efficient as it evaluates only 200 candidate features during feature search, whereas DIFER evaluates over 2000 candidate features (Appendix D.8).

Additionally, we observe that the performance of FEBP or CAAFE with GPT-4 is not significantly different from that with GPT-3.5. On FEBP, GPT-4 yields better performance for linear models but slightly worse performance for Random Forests. We speculate that the stronger in-context learning capability of GPT-4 increases the likelihood of overfitting to the training samples.

[1] $1 - \frac{\sum_i |y_i - \hat{y}_i|}{\sum_i |y_i - \bar{y}|}$, where y is the target and $\hat{y}$ is the prediction.

[2] `https://platform.openai.com/docs/models`

Table 2: Summary of experimental results. For each compared method, the left and right columns show the results without and with parameter tuning of the downstream model algorithm post AutoFE, respectively. The best results are highlighted in boldface, and the second best results are underlined.

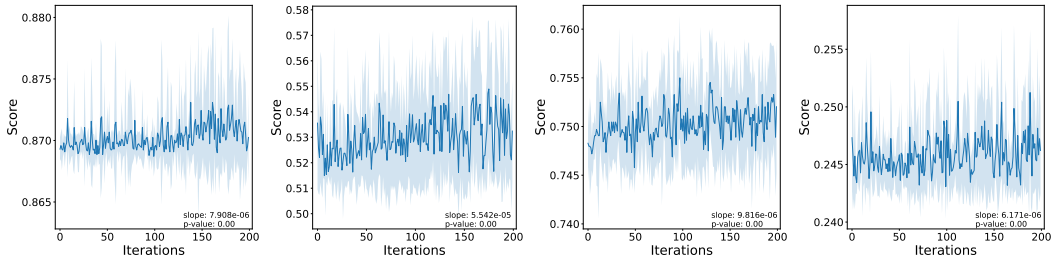
Model	Dataset	Raw	DIFER		OpenFE		CAAFE				FEBP (ours)			
							GPT-3.5		GPT-4		GPT-3.5		GPT-4	
Linear Model	AF	0.3474	0.5870	0.6090	0.4300	0.4303	0.4011	0.4016	0.4376	0.4378	0.6612	0.6616	**0.6649**	0.6647
	BH	0.3776	0.5013	0.4994	0.3900	0.3880	0.4788	0.4765	0.4503	0.4506	0.4995	0.5025	0.5184	**0.5289**
	WQR	0.2696	0.2475	0.2630	0.2713	0.2736	0.2742	0.2757	**0.2776**	0.2776	0.2722	0.2745	0.2713	0.2748
	ACT	0.8505	0.8715	**0.8799**	0.8729	0.8729	0.8519	0.8514	0.8565	0.8570	0.8729	0.8794	0.8766	0.8762
	CD	0.8267	0.8273	0.8280	0.8265	0.8268	0.8265	0.8267	0.8238	0.8238	0.8282	0.8282	0.8288	**0.8288**
	GC	0.7100	0.7140	0.7420	0.7320	0.7280	0.7350	0.7330	0.7210	0.7210	0.7570	0.7460	**0.7590**	0.7420
Mean		0.5636	0.6248	0.6369	0.5871	0.5866	0.5946	0.5941	0.5945	0.5946	0.6485	0.6487	**0.6532**	0.6526
Mean Rank		12.00	8.17	5.50	9.25	8.50	8.67	8.17	8.83	8.17	4.75	3.17	3.00	**2.83**
Random Forests	AF	0.7677	0.7650	0.7786	0.7579	0.7682	0.7711	0.7693	0.7696	0.7720	0.7709	**0.7787**	0.7681	0.7749
	BH	0.5426	**0.5718**	0.5701	0.5658	0.5620	0.5556	0.5556	0.5512	0.5492	0.5549	0.5533	0.5543	0.5522
	BS	0.9446	0.9865	0.9871	0.9901	0.9901	**0.9916**	**0.9916**	0.9818	0.9816	0.9873	0.9881	0.9845	0.9848
	WQR	0.3662	0.3838	0.3832	0.3753	0.3729	0.3718	0.3718	0.3693	0.3693	**0.3862**	0.3845	0.3810	0.3810
	ACT	0.8808	0.8897	0.8897	0.8832	0.8841	0.8827	0.8855	0.8827	0.8827	**0.8925**	0.8921	0.8893	0.8864
	CD	0.8293	0.8285	0.8291	0.8287	0.8285	0.8291	0.8289	0.8294	0.8287	0.8295	0.8294	**0.8295**	0.8276
	GC	0.7450	0.7550	0.7500	0.7650	0.7570	**0.7690**	0.7620	0.7660	0.7630	0.7640	0.7620	0.7680	0.7680
Mean		0.7252	0.7400	0.7411	0.7380	0.7376	0.7387	0.7378	0.7357	0.7352	0.7408	**0.7412**	0.7392	0.7393
Mean Rank		11.57	7.29	5.14	7.07	7.64	5.71	6.93	8.43	9.79	**4.14**	4.29	6.00	7.00
Light-GBM	AF	0.8375	0.8285	0.8411	0.8188	0.8244	0.8364	0.8348	**0.8430**	0.8426	0.8311	0.8392	0.8366	0.8395
	BH	0.5537	0.5607	0.5636	**0.5693**	0.5618	0.5540	0.5571	0.5478	0.5501	0.5619	0.5644	0.5642	0.5595
	BS	0.9429	0.9763	0.9786	0.9751	0.9797	0.9555	0.9565	0.9449	0.9487	0.9737	0.9754	0.9801	**0.9813**
	WQR	0.3825	0.4145	**0.4182**	0.3898	0.3884	0.4131	0.4035	0.3902	0.3952	0.4118	0.4171	0.4021	0.4042
	ACT	0.8832	0.8794	0.8827	0.8808	0.8799	0.8822	0.8860	0.8827	0.8818	0.8888	**0.8925**	0.8902	**0.8925**
	CD	0.8300	0.8283	0.8277	0.8293	0.8287	0.8296	0.8298	0.8301	0.8294	0.8301	0.8297	**0.8303**	0.8294
	GC	0.7250	0.7650	0.7600	0.7550	0.7700	0.7490	0.7550	0.7450	0.7720	0.7680	0.7720	**0.7760**	0.7700
Mean		0.7364	0.7504	0.7531	0.7454	0.7476	0.7457	0.7461	0.7405	0.7457	0.7522	**0.7558**	0.7542	0.7538
Mean Rank		9.43	8.29	5.86	8.86	8.57	8.43	7.71	8.29	7.93	5.71	**3.57**	**3.57**	4.79
Mean		0.6806	0.7091	0.7140	0.6953	0.6958	0.6979	0.6976	0.6950	0.6967	0.7171	0.7185	**0.7187**	0.7183
Mean Rank		10.95	7.90	5.50	8.35	8.23	7.55	7.58	8.50	8.65	4.88	**3.70**	4.25	4.98

Table 3: Performance comparison of FEBP with and without semantic blinding. For each compared version, the left and middle columns show the results without and with parameter tuning of the downstream model algorithm post AutoFE, respectively, and the right column shows the number of LLM responses. The results where the full version outperforms the blinded version are highlighted in boldface.

Model	Dataset	Raw	GPT-3.5						GPT-4					
			Blinded			Full			Blinded			Full		
Linear Model	AF	0.3474	0.6613	0.6602	450.0	0.6612	**0.6616**	**339.8**	0.6678	0.6672	275.0	0.6649	0.6647	371.4
	BH	0.3776	0.4678	0.4794	438.0	**0.4995**	**0.5025**	**378.6**	0.4869	0.4996	295.6	**0.5184**	**0.5289**	335.4
	WQR	0.2696	0.2643	0.2733	442.8	**0.2722**	**0.2745**	**328.4**	0.2645	0.2702	244.6	**0.2713**	**0.2748**	312.6
	ACT	0.8505	0.8790	0.8799	442.8	0.8729	0.8794	**372.2**	0.8720	0.8729	238.8	**0.8766**	**0.8762**	377.4
	CD	0.8267	0.8283	0.8283	454.8	0.8282	0.8282	**342.0**	0.8282	0.8289	238.2	**0.8288**	0.8288	250.4
	GC	0.7100	0.7460	0.7390	432.2	**0.7570**	**0.7460**	**379.0**	0.7430	0.7410	231.2	**0.7590**	**0.7420**	310.6
Mean		0.5636	0.6411	0.6433	443.4	**0.6485**	**0.6487**	**356.7**	0.6437	0.6461	253.9	**0.6532**	**0.6526**	326.3
Random Forests	AF	0.7677	0.7644	0.7743	425.2	**0.7709**	**0.7787**	**393.2**	0.7610	0.7690	274.2	**0.7681**	**0.7749**	314.2
	BH	0.5426	0.5483	0.5483	479.2	**0.5549**	**0.5533**	**374.4**	0.5507	0.5491	238.4	**0.5543**	**0.5522**	278.6
	BS	0.9446	0.9628	0.9628	510.0	**0.9873**	**0.9881**	**386.8**	0.9535	0.9543	247.4	**0.9845**	**0.9848**	255.0
	WQR	0.3662	0.3749	0.3738	461.4	**0.3862**	**0.3845**	**362.6**	0.3666	0.3674	253.0	**0.3810**	**0.3810**	283.2
	ACT	0.8808	0.8864	0.8841	475.8	**0.8925**	**0.8921**	**357.6**	0.8874	0.8841	222.4	**0.8893**	**0.8864**	424.0
	CD	0.8293	0.8283	0.8282	497.0	**0.8295**	**0.8294**	**349.8**	0.8291	0.8286	375.2	**0.8295**	0.8276	**304.0**
	GC	0.7450	0.7630	0.7580	459.2	**0.7640**	**0.7620**	**368.2**	0.7510	0.7490	229.6	**0.7680**	**0.7680**	471.8
Mean		0.6806	0.7326	0.7328	472.5	**0.7408**	**0.7412**	**370.4**	0.7285	0.7288	262.9	**0.7392**	**0.7393**	333.0
Light-GBM	AF	0.8375	0.8304	0.8356	479.6	**0.8311**	**0.8392**	**380.2**	0.8185	0.8266	284.6	**0.8366**	**0.8395**	360.6
	BH	0.5537	0.5503	0.5467	490.8	**0.5619**	**0.5644**	**342.0**	0.5500	0.5609	238.4	**0.5642**	0.5595	345.6
	BS	0.9429	0.9693	0.9691	480.2	**0.9737**	**0.9754**	**380.0**	0.9539	0.9536	312.6	**0.9801**	**0.9813**	**236.8**
	WQR	0.3825	0.4087	0.4151	493.0	**0.4118**	**0.4171**	**322.8**	0.4057	0.4050	246.8	0.4021	0.4042	293.6
	ACT	0.8832	0.8864	0.8883	513.0	**0.8888**	**0.8925**	**367.4**	0.8813	0.8748	229.0	**0.8902**	**0.8925**	359.6
	CD	0.8300	0.8284	0.8292	490.8	**0.8301**	**0.8297**	**352.2**	0.8295	0.8299	218.6	**0.8303**	0.8294	371.2
	GC	0.7250	0.7620	0.7620	482.4	**0.7680**	**0.7720**	**376.6**	0.7550	0.7550	225.0	**0.7760**	**0.7700**	382.2
Mean		0.6806	0.7479	0.7494	490.0	**0.7522**	**0.7558**	**360.2**	0.7420	0.7437	250.7	**0.7542**	**0.7538**	335.7
Mean		0.6806	0.7105	0.7118	469.9	**0.7171**	**0.7185**	**362.7**	0.7078	0.7092	255.9	**0.7187**	**0.7183**	331.9

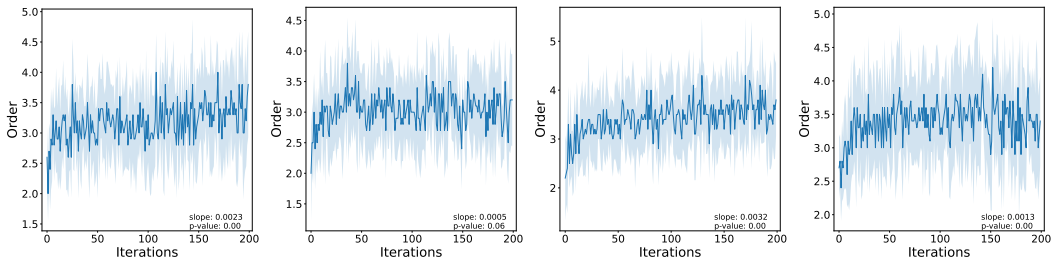
5.3 Effect of Semantic Context

To examine the impact of dataset semantic context, we compare the full version of FEBP with the semantically blinded version where the descriptions of datasets are removed (Appendix C.2). From Table 3, the full version outperforms the blinded version in terms of the mean performance score using all three downstream models. The Friedman-Nemenyi test shows that the performance difference is statistically significant at the $p = 0.01$ level. The performance difference is more pronounced for Random Forests and LightGBM, likely because the inclusion of non-semantically meaningful features consumes model capacity and causes greater overfitting to the training data.



(a) ACT **(b)** BH **(c)** GC **(d)** WQR

Figure 5: The cross validation score of candidate features on training data across iterations.



(a) ACT **(b)** BH **(c)** GC **(d)** WQR

Figure 6: The order of candidate features across iterations.

We also report the number of LLM responses to help assess feature construction efficiency. As shown in Table 3, GPT-4 constructs features more efficiently than GPT-3.5 due to its broader knowledge. While incorporating dataset semantic information improves the feature construction efficiency of GPT-3.5, it reduces that of GPT-4. This is because the semantic information introduces bias, leading GPT-4 to generate more similar responses.

5.4 Performance Analysis

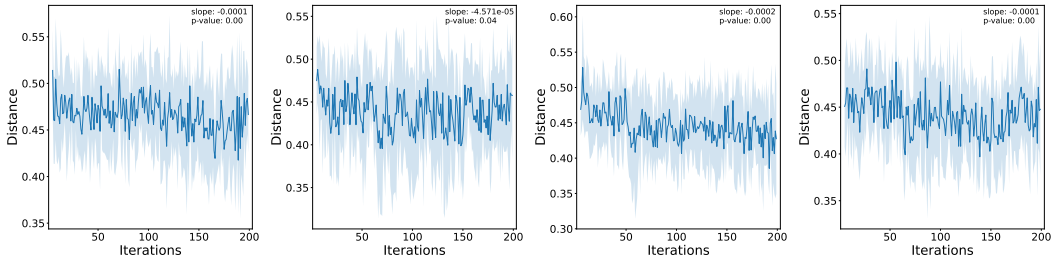
We analyze our LLM-based feature search process for deeper insights. Here, we present experimental results on the ACT, BH, GC, and WQR datasets using linear models from ten repeated runs with *gpt-3.5-turbo-0125*. The plots display the slope and p-value from one-tailed t-tests in OLS regressions, with the shaded area representing one standard deviation above and below the mean.

Feature Learning. We examine the cross validation score of candidate features on the training data across feature construction iterations. Figure 5 shows a general upward trend in the score as the number of iterations increases. This demonstrates that FEBP effectively improves the quality of constructed features through in-context learning of top-performing examples during feature search.

Feature Complexity. We analyze the order of candidate features across feature construction iterations. Figure 6 shows that the feature order increases more rapidly in the early iterations and stabilizes over time. On the one hand, FEBP effectively explores more complex features within promising feature spaces. On the other hand, our constraint instruction regularizes the process, preventing the generation of overly complex features.

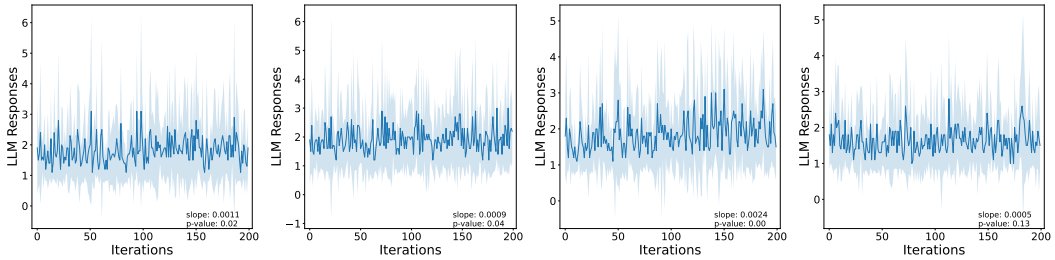
Feature Divergence. We analyze the divergence of a new candidate features from previous ones during feature search. To measure this, we compute the edit distance between canonical feature expression trees using the algorithm from (Zhang & Shasha, 1989), normalizing the distance by the total number of nodes in both trees. Figure 7 displays the mean normalized tree edit distance between the current feature and the previous five features across iterations. The observed downward trend indicates that the feature search is converging.

Feature Construction Efficiency. We examine the number of LLM responses required to construct new candidate features. Figure 8 shows an upward trend over iterations, indicating that more responses are discarded. This is due to the increasing difficulty of constructing non-duplicate features



(a) ACT **(b)** BH **(c)** GC **(d)** WQR

Figure 7: The mean normalized tree edit distance between a new candidate feature and previous five features.



(a) ACT **(b)** BH **(c)** GC **(d)** WQR

Figure 8: The number of LLM responses to construct a new candidate feature across iterations.

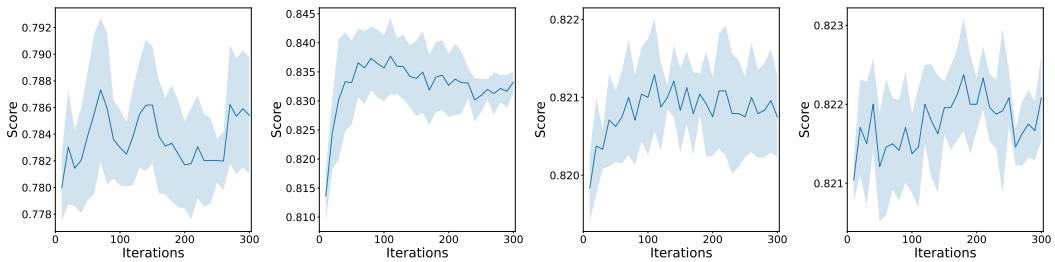
and the higher likelihood of syntactical errors as features become more complex. However, since the increase is small, FEBP remains scalable across a large number of iterations.

5.5 Hyperparameter Effect

Number of Iterations. Figure 9 shows the validation scores on the AF and CD datasets, which contain the smallest and largest numbers of features, respectively, using Random Forests and LightGBM. The validation score is evaluated after adding the selected set of candidate features to the dataset, as indicated by s_{n^*} in line 17 of Algorithm 1. We terminate our algorithm once we have 200 candidate features, as constructing additional features does not substantially enhance the performance, but constructing fewer features degrades the performance in some cases.

Temperature. Table 4 reports the maximum validation score across iterations along with the number of LLM responses, under different temperature settings. We observe that the best performance and feature construction efficiency are achieved when the temperature is set to 1. Lower temperatures increase the likelihood of the LLM repeating existing features, while higher temperatures make the LLM more prone to generating errors in responses, both reducing feature construction efficiency.

Number of Examples in Prompt. Table 5 reports the maximum validation score across iterations along with the number of LLM responses, using varying numbers of example features in the prompt.



(a) RF on AF **(b)** LGBM on AF **(c)** RF on CD **(d)** LGBM on CD

Figure 9: The validation score across iterations using Random Forests and LightGBM.

Table 4: Effect of the LLM temperature. For each compared setting, the left column shows the validation score, and the right column shows the number of LLM responses.

Model	Dataset	Temperature 0.5		1		1.5	
RF	AF	0.7875	794.4	0.7914	393.2	0.7916	609.2
	CD	0.8211	823.2	0.8219	349.8	0.8218	672.6
LGBM	AF	0.8365	1313.2	0.8430	380.2	0.8418	627.6
	CD	0.8225	519.8	0.8226	352.2	0.8223	662.6
Mean		0.8169	862.7	0.8197	368.9	0.8194	643.0

Table 5: Effect of the number of example features in the prompt. For each compared setting, the left column shows the validation score, and the right column shows the number of LLM responses.

Model	Dataset	Number of Examples 1		5		10		20	
RF	AF	0.7910	464.0	0.7930	409.2	0.7914	393.2	0.7860	372.8
	WQR	0.3897	339.4	0.3937	329.8	0.3948	362.6	0.3940	330.0
	CD	0.8215	429.6	0.8213	371.2	0.8219	349.8	0.8218	343.2
LGBM	AF	0.8421	440.4	0.8433	404.6	0.8430	380.2	0.8420	384.2
	WQR	0.4265	336.6	0.4294	334.8	0.4301	322.8	0.4333	330.4
	CD	0.8228	449.4	0.8224	361.2	0.8226	352.2	0.8228	321.2
Mean		0.6823	409.9	0.6839	368.5	0.6840	360.1	0.6833	347.0

We observe that the best performance is achieved with 10 examples. Additionally, we observe that feature construction efficiency improves as the number of examples increases, as this helps the LLM reduce errors and generate more diverse responses. However, providing too many examples can hinder the in-context learning of optimal feature patterns, as shown by the performance decline.

6 Conclusion

We propose a novel LLM-based AutoFE algorithm for effective, efficient, and interpretable feature engineering that leverages the semantic information of datasets. Our approach provides the LLM with dataset descriptions and example features represented in canonical RPN, prompting it to construct new features. The LLM iteratively explores the feature space and improves feature construction by learning from top-performing examples. Experimental results demonstrate that our approach significantly outperforms state-of-the-art AutoFE methods and the inclusion of semantic context from dataset descriptions enhances performance. We also analyze the behavior of our LLM-based feature search process. Our work paves the way for further LLM-driven applications on automated machine learning pipelines and underscores the potential of utilizing semantic information. In the future, we plan to incorporate adaptive techniques for prompt design.

Ethical Statement

All datasets used in this work are publicly available, free of personal information, and intended for research purposes only. Our use of GPT models complies with the terms and conditions of OpenAI.

Reproducibility Statement

The anonymized source code of this work can be accessed at `https://anonymous.4open.science/r/FEBP`.

References

Leo Breiman. Random forests. *Machine learning*, 45:5–32, 2001.

Tom Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared D Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, et al. Language models

are few-shot learners. In *Proceedings of Advances in neural information processing systems*, volume 33, pp. 1877–1901, 2020.

Milton Friedman. The use of ranks to avoid the assumption of normality implicit in the analysis of variance. *Journal of the american statistical association*, 32(200):675–701, 1937.

Sainyam Galhotra, Udayan Khurana, Oktie Hassanzadeh, Kavitha Srinivas, and Horst Samulowitz. Kafe: Automated feature enhancement for predictive modeling using external knowledge. In *Proceedings of NeurIPS 2019 Workshop: Knowledge Representation & Reasoning Meets Machine Learning*, 2019. URL https://kr2ml.github.io/2019/papers/KR2ML_2019_paper_17.pdf.

Leo Grinsztajn, Edouard Oyallon, and Gael Varoquaux. Why do tree-based models still outperform deep learning on typical tabular data? In *Proceedings of the thirty-sixth Conference on Neural Information Processing Systems Datasets and Benchmarks Track*, 2022.

Noah Hollmann, Samuel Müller, and Frank Hutter. Large language models for automated data science: Introducing CAAFE for context-aware automated feature engineering. In *Proceedings of the thirty-seventh Conference on Neural Information Processing Systems*, 2023. URL https://openreview.net/forum?id=9WSxQZ9mG7.

Franziska Horn, Robert Pack, and Michael Rieger. The autofeat python library for automated feature engineering and selection. In *Proceedings of Machine Learning and Knowledge Discovery in Databases*, pp. 111–120. Springer, 2020.

James Max Kanter and Kalyan Veeramachaneni. Deep feature synthesis: Towards automating data science endeavors. In *Proceedings of 2015 IEEE international conference on data science and advanced analytics (DSAA)*, pp. 1–10. IEEE, 2015.

Guolin Ke, Qi Meng, Thomas Finley, Taifeng Wang, Wei Chen, Weidong Ma, Qiwei Ye, and Tie-Yan Liu. Lightgbm: A highly efficient gradient boosting decision tree. In *Proceedings of Advances in Neural Information Processing Systems*, volume 30, 2017. URL https://proceedings.neurips.cc/paper_files/paper/2017/file/6449f44a102fde848669bdd9eb6b76fa-Paper.pdf.

Udayan Khurana, Horst Samulowitz, and Deepak Turaga. Feature engineering for predictive modeling using reinforcement learning. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 32, 2018.

Takeshi Kojima, Shixiang Shane Gu, Machel Reid, Yutaka Matsuo, and Yusuke Iwasawa. Large language models are zero-shot reasoners. In *Advances in Neural Information Processing Systems*, 2022. URL https://openreview.net/forum?id=e2TBb5y0yFf.

Liyao Li, Haobo Wang, Liangyu Zha, Qingyi Huang, Sai Wu, Gang Chen, and Junbo Zhao. Learning a data-driven policy network for pre-training automated feature engineering. In *Proceedings of the eleventh International Conference on Learning Representations*, 2023.

Clint Morris, Michael Jurado, and Jason Zutty. Llm guided evolution - the automation of models advancing models. In *Proceedings of the Genetic and Evolutionary Computation Conference*, GECCO '24, pp. 377–384, New York, NY, USA, 2024. Association for Computing Machinery. URL https://doi.org/10.1145/3638529.3654178.

Fatemeh Nargesian, Horst Samulowitz, Udayan Khurana, Elias B Khalil, and Deepak S Turaga. Learning feature engineering for classification. In *Proceedings of International Joint Conference on Artificial Intelligence*, volume 17, pp. 2529–2535, 2017.

Peter Bjorn Nemenyi. *Distribution-free multiple comparisons.* Princeton University, 1963.

OpenAI. Gpt-4 technical report, 2023. URL https://cdn.openai.com/papers/gpt-4.pdf.

Long Ouyang, Jeffrey Wu, Xu Jiang, Diogo Almeida, Carroll Wainwright, Pamela Mishkin, Chong Zhang, Sandhini Agarwal, Katarina Slama, Alex Ray, et al. Training language models to follow instructions with human feedback. In *Proceedings of Advances in Neural Information Processing Systems*, volume 35, pp. 27730–27744. Curran Associates, Inc., 2022. URL https://proceedings.neurips.cc/paper_files/paper/2022/file/b1efde53be364a73914f58805a001731-Paper-Conference.pdf.

Tom Overman, Diego Klabjan, and Jean Utke. Iife: Interaction information based automated feature engineering, 2024. URL https://arxiv.org/abs/2409.04665.

Alec Radford, Jeff Wu, Rewon Child, David Luan, Dario Amodei, and Ilya Sutskever. Language models are unsupervised multitask learners, 2019. URL https://d4mucfpksywv.cloudfront.net/better-language-models/language-models.pdf.

Matthew G Smith and Larry Bull. Genetic programming with a genetic algorithm for feature construction and selection. *Genetic Programming and Evolvable Machines*, 6:265–281, 2005.

Hugo Touvron, Thibaut Lavril, Gautier Izacard, Xavier Martinet, Marie-Anne Lachaux, Timothée Lacroix, Baptiste Rozière, Naman Goyal, Eric Hambro, Faisal Azhar, Aurelien Rodriguez, Armand Joulin, Edouard Grave, and Guillaume Lample. Llama: Open and efficient foundation language models, 2023a. URL https://arxiv.org/abs/2302.13971.

Hugo Touvron, Louis Martin, Kevin Stone, Peter Albert, Amjad Almahairi, Yasmine Babaei, Nikolay Bashlykov, Soumya Batra, Prajjwal Bhargava, Shruti Bhosale, et al. Llama 2: Open foundation and fine-tuned chat models, 2023b. URL https://arxiv.org/abs/2307.09288.

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Lukasz Kaiser, and Illia Polosukhin. Attention is all you need. In *Proceedings of Advances in Neural Information Processing Systems*, volume 30, 2017. URL https://proceedings.neurips.cc/paper_files/paper/2017/file/3f5ee243547dee91fbd053c1c4a845aa-Paper.pdf.

Kafeng Wang, Pengyang Wang, and Chengzhong Xu. Toward efficient automated feature engineering. In *Proceedings of 2023 IEEE 39th International Conference on Data Engineering (ICDE)*, pp. 1625–1637, 2023. doi: 10.1109/ICDE55515.2023.00128.

Jason Wei, Xuezhi Wang, Dale Schuurmans, Maarten Bosma, brian ichter, Fei Xia, Ed H. Chi, Quoc V Le, and Denny Zhou. Chain of thought prompting elicits reasoning in large language models. In *Advances in Neural Information Processing Systems*, 2022. URL https://openreview.net/forum?id=_VjQlMeSB_J.

Chengrun Yang, Xuezhi Wang, Yifeng Lu, Hanxiao Liu, Quoc V Le, Denny Zhou, and Xinyun Chen. Large language models as optimizers. In *Proceedings of the twelfth International Conference on Learning Representations*, 2024. URL https://openreview.net/forum?id=Bb4VGOWELI.

Kaizhong Zhang and Dennis Shasha. Simple fast algorithms for the editing distance between trees and related problems. *SIAM J. Comput.*, 18:1245–1262, 12 1989. doi: 10.1137/0218082.

Tianping Zhang, Zheyu Zhang, Zhiyuan Fan, Haoyan Luo, Fengyuan Liu, Qian Liu, Wei Cao, and Jian Li. Openfe: automated feature generation with expert-level performance. In *Proceedings of the 40th International Conference on Machine Learning*, ICML'23, 2023.

Guanghui Zhu, Shen Jiang, Xu Guo, Chunfeng Yuan, and Yihua Huang. Evolutionary automated feature engineering. In *Proceedings of Pacific Rim International Conference on Artificial Intelligence*, pp. 574–586. Springer, 2022a.

Guanghui Zhu, Zhuoer Xu, Chunfeng Yuan, and Yihua Huang. Difer: Differentiable automated feature engineering. In *Proceedings of the first International Conference on Automated Machine Learning*, volume 188 of *Proceedings of Machine Learning Research*, pp. 17/1–17. PMLR, 25–27 Jul 2022b. URL https://proceedings.mlr.press/v188/zhu22a.html.

Daniel M Ziegler, Nisan Stiennon, Jeffrey Wu, Tom B Brown, Alec Radford, Dario Amodei, Paul Christiano, and Geoffrey Irving. Fine-tuning language models from human preferences, 2019. URL https://arxiv.org/abs/1909.08593.

A Discussion on Canonical RPN Feature Representation

A.1 Why RPN

RPN provides a compact and unambiguous form of feature representation. In contrast, infix expression requires extra information such as brackets to determine operator precedence. Without brackets, the feature in infix expression col-0 $-$ (col-1 $+$ col-2) would be indistinguishable from the feature (col-0 $-$ col-1) $+$ col-2, while both features are distinctively encoded in RPN. Such compactness and unambiguity of RPN facilitate sequential modeling since there is no need to model the extra information, e.g., the positions of brackets.

Compared with other forms of feature representation such as prefix expression of depth-first traversal or breadth-first traversal, RPN better encodes the recursive structure of the expression tree. The bottom-up enumeration of tree nodes makes it easy for the LLM to evaluate the feature expression by scanning the sequence from left to right, for instance, ((col-0 col-1 $-$) col-2 $+$) (parentheses denote recursion). Using the prefix expression ($+$ ($-$ col-0 col-1) col-2) or breadth-first expression ($+$ ($-$ [col-2] col-0 col-1)), however, the LLM always needs to look back to find the operator, which undermines sequential modeling. We find in our experiments that when using prefix expression, the LLM encounters difficulty in generating syntactically valid feature expressions.

A.2 Why Canonicalization

While there is one-to-one mapping between feature expression trees and RPN expressions, a feature that contains commutative operators (like addition and multiplication) can be represented by different RPN expressions, since the child nodes of these operators are unordered. We introduce a canonicalization scheme: arranging operator nodes before feature nodes and lexicographically sorting the nodes within each group. Through canonicalization, we create one-to-one mapping between features and cRPN expressions. This ensures the consistency of our feature representation and facilitates the in-context learning of feature patterns.

By arranging operator nodes before feature nodes, we also introduce left skewness to the expression tree that enhances the clarity of the recursive structure in cRPN. As illustrated in Figure 10, the original feature expression (col-2 (col-1 col-0 $+$) $*$) becomes ((col-0 col-1 $+$) col-2 $*$) after canonicalization, so that the LLM does not need to look back for col-2 when evaluating the expression. We refer to Appendix E for additional experiments.

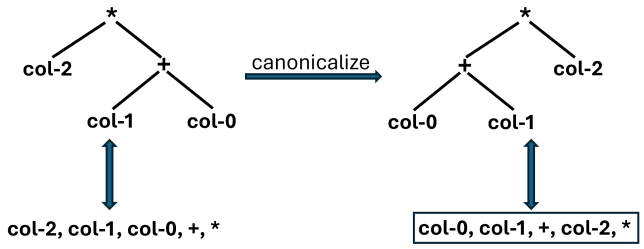


Figure 10: Our canonicalization scheme introduces left skewness to the expression tree.

B CONVERSION BETWEEN FEATURE EXPRESSION TREE AND RPN

Algorithms 2 and 3 detail the process of conversion between a feature expression tree and an RPN feature string. We check the RPN syntactical validity of a feature string in Algorithm 3 by checking whether there is enough child node in the stack in line 6 and the size of the stack is exactly one (the root) in line 13 returning the output.

Algorithm 2: Feature Expression Tree to RPN

Input : A feature expression tree T
Output: An RPN feature string f

```
1  r ← the root of T
2  Initialize string f ← ϵ, stack S ← [r], and visited ← ∅
3  repeat
4      u ← S.peek()
5      if u ∈ visited then
6          f.append(u)
7          S.pop()
8      end
9      else
10         for each child v of u in the reverse order do
11             S.push(v)
12         end
13         visited ← visited ∪ {u}
14     end
15 until S is empty
16 return f
```

Algorithm 3: RPN to Feature Expression Tree

Input : An RPN feature string f
Output: The root of a feature expression tree T

```
1  Initialize stack S ← []
2  for i ← 1 to |f| do
3      u ← the i-th element of f
4      if u is an operator then
5          o ← the arity of u
6          for j ← 1 to o do
7              v ← S.pop()
8              Prepend v to the list of children of u
9          end
10     end
11     S.push(u)
12 end
13 return S.pop()
```

C EXAMPLE PROMPTS

C.1 FULL PROMPT

Figure 11 shows an example of full prompts used in our main experiments.

Figure 11: Example full prompt on the Credit Default dataset.

Dataset description:
This dataset contains information on default payments, demographic factors, credit data, history of payment, and bill statements of credit card clients in Taiwan from April 2005 to September 2005.
Dataset contains the following columns:
col-0 (int) [10000, 800000]: LIMIT_BAL: Amount of given credit in NT dollars (includes individual and family/supplementary credit
col-1 (category) {1, 2}: SEX: Gender (1=male, 2=female)
col-2 (category) {0, 1, 2, 3, 4, 5, 6}: EDUCATION: (1=graduate school, 2=university, 3=high school, 4=others, 5=unknown, 6=unknown)
col-3 (category) {0, 1, 2, 3}: MARRIAGE: Marital status (1=married, 2=single, 3=others)
col-4 (int) [21, 79]: AGE: Age in years
col-5 (category) {-2, -1, 0, 1, 2, 3, 4, 5, 6, 7, 8}: PAY_0: Repayment status in September, 2005 (-1=pay duly, 1=payment delay for one month, 2=payment delay for two months, ... 8=payment delay for eight months, 9=payment delay for nine months and above)
...
col-23 (category) {0, 1}: default.payment.next.month: Default payment (1=yes, 0=no)
We have the following unary operators:
log: taking the log of the absolute value
sqrt_abs: taking the square root of the absolute value
min_max: min-max normalization
reciprocal: taking the reciprocal
We have the following binary operators:
+: summing two columns
−: subtracting two columns
∗: multiplying two columns
/: taking the division of two columns
mod_column: taking the modulo of two columns
Feature strings are reverse Polish notation (RPN) expressions that operate on the columns of our dataset. Each feature string constructs an extra column that is useful for the downstream model Random Forests to predict the target col-23. The model will be trained on the dataset with the constructed columns and evaluated on a holdout set. The best columns will be selected.
Below are feature strings arranged in ascending order based on their performance scores. Higher scores are better.

Feature
col-17,col-21,*,col-20,+,sqrt_abs
Score
0.0011
...
Feature
col-4,col-6,*,col-12,col-16,-,sqrt_abs,*
Score
0.0014

Give me a new feature string that is different from all strings above and has a higher score. Use no more than five operators. Make sure all columns and operators exist and do not include the target column. Follow the syntax of RPN.

Output format:
Feature

(Feature name and description)

Usefulness
(Explanation why this adds useful real world knowledge to predict the target col-23 according to dataset description)

C.2 SEMANTICALLY BLINDED PROMPT

Figure 12 shows an example of semantically blinded prompts used in our experiments in Section 5.3.

Figure 12: Example semantically blinded prompt on the Credit Default dataset.

Dataset contains the following columns:
col-0
col-1
col-2
col-3
col-4
col-5
...
col-23
We have the following unary operators:
log: taking the log of the absolute value
sqrt_abs: taking the square root of the absolute value
min_max: min-max normalization
reciprocal: taking the reciprocal
We have the following binary operators:
+: summing two columns
−: subtracting two columns
∗: multiplying two columns
/: taking the division of two columns
mod_column: taking the modulo of two columns
Feature strings are reverse Polish notation (RPN) expressions that operate on the columns of our dataset. Each feature string constructs an extra column that is useful for the downstream model Random Forests to predict the target col-23. The model will be trained on the dataset with the constructed columns and evaluated on a holdout set. The best columns will be selected.
Below are feature strings arranged in ascending order based on their performance scores. Higher scores are better.

Feature
col-17,col-21,*,col-20,+,sqrt_abs
Score
0.0011
...
Feature
col-4,col-6,*,col-12,col-16,-,sqrt_abs,*
Score
0.0014

Give me a new feature string that is different from all strings above and has a higher score. Use no more than five operators. Make sure all columns and operators exist and do not include the target column. Follow the syntax of RPN.

Output format:
Feature

(Feature name and description)

Usefulness
(Explanation why this adds useful real world knowledge to predict the target col-23 according to dataset description)

D EXPERIMENTAL DETAILS

D.1 DATA SOURCES

Table 6 summarizes the sources of datasets used in our experiments. Datasets are selected such that they cover different domains and both regression and classification tasks. Most of them have been used in previous works (Zhu et al., 2022a;b; Zhang et al., 2023; Hollmann et al., 2023).

Table 6: Sources of datasets.

Name	Source
Airfoil (AF)	https://archive.ics.uci.edu/dataset/291/airfoil+self+noise
Boston Housing (BH)	https://www.kaggle.com/datasets/arunjangir245/boston-housing-dataset
Bikeshare (BS)	https://www.kaggle.com/datasets/marklvl/bike-sharing-dataset
Wine Quality Red (WQR)	https://archive.ics.uci.edu/dataset/186/wine+quality
AIDS Clinical Trials (ACT)	https://archive.ics.uci.edu/dataset/890/aids+clinical+trials+group+study+175
Credit Default (CD)	https://www.kaggle.com/datasets/uciml/default-of-credit-card-clients-dataset
German Credit (GC)	https://archive.ics.uci.edu/dataset/573/south+german+credit+update

D.2 EXPERIMENTAL PLATFORM

All experiments are conducted on the Ubuntu 22.04.4 LTS operating system, 16 Intel(R) Core(TM) i7-7820X CPUs, and 4 NVIDIA GeForce RTX 2080 Ti GPUs, with the framework of Python 3.11.9 and PyTorch 1.12.1.

D.3 FEATURE TRANSFORMATION OPERATORS

We list the details of all feature transformation operators below.

Unary transformations:

- Logarithm: Element-wise logarithm of the absolute value;
- Reciprocal: Element-wise reciprocal;
- Square root: Element-wise square root of the absolute value;
- Min-max normalization: Element-wise min-max normalization, with the min and max values from the training data.

Binary transformations:

- Addition: Element-wise addition;
- Subtraction: Element-wise subtraction;
- Multiplication: Element-wise multiplication;
- Division: Element-wise division;
- Modulo: Element-wise modulo.

D.4 Parameter Tuning of Downstream Models

We tune the parameters of downstream models prior to and post AutoFE using randomized search implemented in an Sklearn package[3]. Table 7 lists the configurations of parameter tuning for each downstream model. We set the number of randomized search iterations to 100.

Table 7: Hyperparameter search space for downstream models.

Model	Parameter	Search Space
Linear Model	regularization	loguniform(0.00001, 100)
Random Forests	num estimators	randint(5, 250)
	max depth	randint(1, 250)
	max features	uniform(0.01, 0.99)
	max samples	uniform(0.1, 0.9)
LightGBM	num estimators	randint(10, 1000)
	num leaves	randint(8, 64)
	learning rate	loguniform(0.001, 1)
	bagging fraction	uniform(0.1, 0.9)
	feature fraction	uniform(0.1, 0.9)
	reg lambda	loguniform(0.001, 100)

D.5 Standard Deviations

Tables 8-11 report the sample standard deviations corresponding to the experimental results in Tables 2-5, respectively.

D.6 Statistical Tests

We perform the Friedman test (Friedman, 1937) to determine whether there is statistically significant difference among the compared AutoFE methods. The Friedman test p-values for the results in Tables 2 and 3 are 1.16×10^{-47} and 3.95×10^{-34}, respectively. Hence, we can reject the null hypothesis that the performance is the same for all methods. We perform the Nemenyi post-hoc test (Nemenyi, 1963) to further determine which AutoFE methods have different performance. Tables 12 and 13 summarize the p-values for the pairwise comparisons in Tables 2 and 3, respectively. From Table 12, the performance difference between our method FEBP and baseline methods other than DIFER (Zhu et al., 2022b) is statistically significant at the $p = 0.01$ level. From Table 13, the performance difference between the full version of FEBP and the semantically blinded version is statistically significant at the $p = 0.01$ level.

To highlight the performance difference when using Random Forests and LightGBM, we perform additional statistical tests for the results in Table 2 excluding the linear model results. The Friedman test p-value is 6.14×10^{-23}. Table 14 summarizes the p-values from the Nemenyi post-hoc test for pairwise comparison. We observe that FEBP with GPT-3.5 and post-AutoFE parameter tuning significantly outperforms all baselines except DIFER at the $p = 0.05$ level. With GPT-4, the performance difference between FEBP and CAAFE (Hollmann et al., 2023) is still statistically significant at the $p = 0.05$ level.

[3] https://scikit-learn.org/1.5/modules/generated/sklearn.model_selection.RandomizedSearchCV.html

Table 8: Standard deviations of Table 2, summary of experimental results.

Model	Dataset	Raw	DIFER		OpenFE		CAAFE				FEBP (ours)			
							GPT-3.5		GPT-4		GPT-3.5		GPT-4	
Linear Model	AF	–	0.2559	0.2012	0.0015	0.0014	0.0099	0.0102	0.0511	0.0513	0.0101	0.0100	0.0267	0.0268
	BH	–	0.0092	0.0153	0.0169	0.0188	0.0196	0.0184	0.0408	0.0419	0.0111	0.0149	0.0254	0.0184
	WQR	–	0.0305	0.0223	0.0058	0.0055	0.0046	0.0038	0.0060	0.0060	0.0135	0.0112	0.0068	0.0044
	ACT	–	0.0179	0.0073	0.0140	0.0105	0.0035	0.0021	0.0054	0.0053	0.0085	0.0051	0.0040	0.0062
	CD	–	0.0014	0.0006	0.0006	0.0002	0.0006	0.0007	0.0057	0.0051	0.0013	0.0007	0.0006	0.0009
	GC	–	0.0272	0.0104	0.0097	0.0076	0.0100	0.0125	0.0134	0.0108	0.0120	0.0213	0.0108	0.0152
Random Forests	AF	–	0.0054	0.0044	0.0032	0.0036	0.0032	0.0034	0.0108	0.0084	0.0090	0.0086	0.0059	0.0095
	BH	–	0.0142	0.0131	0.0034	0.0068	0.0050	0.0050	0.0084	0.0113	0.0057	0.0077	0.0059	0.0046
	BS	–	0.0128	0.0113	0.0003	0.0003	0.0003	0.0003	0.0208	0.0207	0.0088	0.0070	0.0157	0.0154
	WQR	–	0.0108	0.0109	0.0030	0.0076	0.0022	0.0022	0.0051	0.0051	0.0034	0.0069	0.0022	0.0026
	ACT	–	0.0048	0.0058	0.0037	0.0087	0.0030	0.0055	0.0020	0.0030	0.0055	0.0051	0.0043	0.0054
	CD	–	0.0010	0.0011	0.0003	0.0004	0.0005	0.0004	0.0008	0.0001	0.0011	0.0010	0.0009	0.0017
	GC	–	0.0184	0.0177	0.0154	0.0110	0.0082	0.0076	0.0065	0.0164	0.0114	0.0067	0.0097	0.0097
Light-GBM	AF	–	0.0029	0.0029	0.0058	0.0036	0.0067	0.0027	0.0072	0.0077	0.0129	0.0054	0.0061	0.0041
	BH	–	0.0147	0.0260	0.0128	0.0150	0.0114	0.0111	0.0145	0.0188	0.0169	0.0076	0.0134	0.0073
	BS	–	0.0092	0.0070	0.0007	0.0004	0.0159	0.0198	0.0056	0.0139	0.0151	0.0139	0.0033	0.0034
	WQR	–	0.0134	0.0164	0.0072	0.0133	0.0084	0.0080	0.0116	0.0134	0.0123	0.0085	0.0097	0.0092
	ACT	–	0.0048	0.0042	0.0068	0.0094	0.0061	0.0045	0.0045	0.0027	0.0027	0.0017	0.0050	0.0077
	CD	–	0.0009	0.0013	0.0004	0.0010	0.0008	0.0005	0.0010	0.0007	0.0004	0.0004	0.0004	0.0008
	GC	–	0.0141	0.0184	0.0184	0.0184	0.0222	0.0166	0.0079	0.0199	0.0076	0.0045	0.0096	0.0146

Table 9: Standard deviations of Table 3, performance comparison of FEBP with and without semantic blinding.

Model	Dataset	Raw	GPT-3.5						GPT-4					
			Blinded			Full			Blinded			Full		
Linear Model	AF	–	0.0147	0.0156	36.1	0.0101	0.0100	28.8	0.0162	0.0161	25.8	0.0267	0.0268	92.3
	BH	–	0.0444	0.0519	39.0	0.0111	0.0149	42.2	0.0161	0.0131	66.7	0.0254	0.0184	58.6
	WQR	–	0.0133	0.0032	48.9	0.0135	0.0112	15.3	0.0128	0.0046	23.5	0.0068	0.0044	80.6
	ACT	–	0.0088	0.0107	15.4	0.0085	0.0051	17.5	0.0056	0.0085	15.5	0.0040	0.0062	54.8
	CD	–	0.0014	0.0003	27.6	0.0013	0.0007	13.1	0.0021	0.0011	13.2	0.0006	0.0009	14.8
	GC	–	0.0114	0.0042	32.3	0.0120	0.0213	14.3	0.0125	0.0114	11.0	0.0108	0.0152	36.4
Random Forests	AF	–	0.0086	0.0058	60.3	0.0090	0.0086	47.3	0.0092	0.0079	27.9	0.0059	0.0095	93.6
	BH	–	0.0068	0.0068	45.3	0.0057	0.0077	14.5	0.0142	0.0132	24.7	0.0059	0.0046	23.0
	BS	–	0.0186	0.0181	112.1	0.0088	0.0070	47.8	0.0103	0.0088	38.8	0.0157	0.0154	39.2
	WQR	–	0.0078	0.0081	40.5	0.0034	0.0069	18.5	0.0092	0.0075	19.1	0.0022	0.0026	45.2
	ACT	–	0.0099	0.0035	33.7	0.0055	0.0051	13.1	0.0100	0.0093	16.6	0.0043	0.0054	85.7
	CD	–	0.0015	0.0008	53.3	0.0011	0.0010	14.5	0.0005	0.0008	83.4	0.0009	0.0017	56.9
	GC	–	0.0067	0.0057	28.9	0.0114	0.0067	17.3	0.0210	0.0143	12.8	0.0097	0.0097	113.1
Light-GBM	AF	–	0.0104	0.0060	66.8	0.0129	0.0054	21.7	0.0142	0.0155	39.6	0.0061	0.0041	73.1
	BH	–	0.0131	0.0170	60.7	0.0169	0.0076	20.7	0.0119	0.0121	25.7	0.0134	0.0073	36.1
	BS	–	0.0152	0.0178	76.3	0.0151	0.0139	31.8	0.0048	0.0049	74.5	0.0033	0.0034	32.1
	WQR	–	0.0151	0.0028	36.9	0.0123	0.0085	17.3	0.0195	0.0190	21.1	0.0097	0.0092	46.3
	ACT	–	0.0021	0.0030	44.2	0.0027	0.0017	28.5	0.0042	0.0128	15.7	0.0050	0.0077	49.6
	CD	–	0.0011	0.0011	59.4	0.0004	0.0004	15.7	0.0007	0.0010	5.6	0.0004	0.0008	85.7
	GC	–	0.0130	0.0148	41.7	0.0076	0.0045	23.0	0.0117	0.0094	13.7	0.0096	0.0146	46.9

Table 10: Standard deviations of Table 4, effect of temperature.

Model	Dataset	Temperature					
		0.5		1		1.5	
RF	AF	0.0071	160.9	0.0042	47.3	0.0040	34.7
	CD	0.0005	324.3	0.0004	14.5	0.0005	64.1
LGBM	AF	0.0042	523.3	0.0044	21.7	0.0022	59.8
	CD	0.0008	174.7	0.0007	15.7	0.0005	73.0

Table 11: Standard deviations of Table 5, effect of the number of example features in the prompt.

Model	Dataset	Number of Examples							
		1		5		10		20	
RF	AF	0.0054	55.8	0.0035	45.0	0.0042	47.3	0.0056	24.0
	WQR	0.0088	19.6	0.0038	11.4	0.0027	18.5	0.0096	29.6
	CD	0.0005	46.5	0.0007	19.1	0.0004	14.5	0.0006	17.8
LGBM	AF	0.0065	103.2	0.0031	21.6	0.0044	21.7	0.0044	56.4
	WQR	0.0048	16.9	0.0057	32.4	0.0064	17.3	0.0064	26.5
	CD	0.0003	71.2	0.0002	39.0	0.0007	15.7	0.0005	17.5

Table 12: The Nemenyi post-hoc test p-values for pairwise comparison of the methods in Table 2. Results that are significant at the $p = 0.05$ confidence level are highlighted in boldface.

		Raw	DIFER		OpenFE		CAAFE				FEBP (ours)			
							GPT-3.5		GPT-4		GPT-3.5		GPT-4	
Raw		1.0000	**0.0010**	**0.0010**	**0.0203**	**0.0086**	**0.0010**	**0.0010**	**0.0409**	**0.0179**	**0.0010**	**0.0010**	**0.0010**	**0.0010**
DIFER		**0.0010**	1.0000	0.3235	0.4051	0.5626	0.9000	0.9000	0.2697	0.4310	**0.0397**	**0.0010**	**0.0028**	0.1535
		0.0010	0.3235	1.0000	**0.0010**	**0.0010**	**0.0343**	**0.0397**	**0.0010**	**0.0010**	0.9000	0.7526	0.9000	0.9000
OpenFE		**0.0203**	0.4051	**0.0010**	1.0000	0.9000	0.9000	0.9000	0.9000	0.9000	**0.0010**	**0.0010**	**0.0010**	**0.0010**
		0.0086	0.5626	**0.0010**	0.9000	1.0000	0.9000	0.9000	0.9000	0.9000	**0.0010**	**0.0010**	**0.0010**	**0.0010**
CAAFE	GPT-3.5	**0.0010**	0.9000	**0.0343**	0.9000	0.9000	1.0000	0.9000	0.8216	0.9000	**0.0016**	**0.0010**	**0.0010**	**0.0105**
		0.0010	0.9000	**0.0397**	0.9000	0.9000	0.9000	1.0000	0.7929	0.9000	**0.0019**	**0.0010**	**0.0010**	**0.0125**
	GPT-4	**0.0409**	0.2697	**0.0010**	0.9000	0.9000	0.8216	0.7929	1.0000	0.9000	**0.0010**	**0.0010**	**0.0010**	**0.0010**
		0.0179	0.4310	**0.0010**	0.9000	0.9000	0.9000	0.9000	0.9000	1.0000	**0.0010**	**0.0010**	**0.0010**	**0.0010**
FEBP	GPT-3.5	**0.0010**	**0.0397**	0.9000	**0.0010**	**0.0010**	**0.0016**	**0.0019**	**0.0010**	**0.0010**	1.0000	0.9000	0.9000	0.9000
		0.0010	**0.0010**	0.7526	**0.0010**	**0.0010**	**0.0010**	**0.0010**	**0.0010**	**0.0010**	0.9000	1.0000	0.9000	0.9000
	GPT-4	**0.0010**	**0.0028**	0.9000	**0.0010**	**0.0010**	**0.0010**	**0.0010**	**0.0010**	**0.0010**	0.9000	0.9000	1.0000	0.9000
		0.0010	0.1535	0.9000	**0.0010**	**0.0010**	**0.0105**	**0.0125**	**0.0010**	**0.0010**	0.9000	0.9000	0.9000	1.0000

Table 13: The Nemenyi post-hoc test p-values for pairwise comparison of the methods in Table 3. Results that are significant at the $p = 0.05$ confidence level are highlighted in boldface.

		Raw	GPT-3.5				GPT-4			
			Blinded		Full		Blinded		Full	
Raw		1.0000	**0.0010**	**0.0010**	**0.0010**	**0.0010**	**0.0017**	**0.0010**	**0.0010**	**0.0010**
GPT-3.5	Blinded	**0.0010**	1.0000	0.9000	**0.0062**	**0.0010**	0.9000	0.9000	**0.0010**	**0.0057**
		0.0010	0.9000	1.0000	0.1775	**0.0066**	0.3858	0.9000	**0.0105**	0.1677
	Full	**0.0010**	**0.0062**	0.1775	1.0000	0.9000	**0.0010**	**0.0069**	0.9000	0.9000
		0.0010	**0.0010**	**0.0066**	0.9000	1.0000	**0.0010**	**0.0010**	0.9000	0.9000
GPT-4	Blinded	**0.0017**	0.9000	0.3858	**0.0010**	**0.0010**	1.0000	0.9000	**0.0010**	**0.0010**
		0.0010	0.9000	0.9000	**0.0069**	**0.0010**	0.9000	1.0000	**0.0010**	**0.0062**
	Full	**0.0010**	**0.0010**	**0.0105**	0.9000	0.9000	**0.0010**	**0.0010**	1.0000	0.9000
		0.0010	**0.0057**	0.1677	0.9000	0.9000	**0.0010**	**0.0062**	0.9000	1.0000

Table 14: The Nemenyi post-hoc test p-values for pairwise comparison of the methods in Table 2, excluding linear model results. Results that are significant at the $p = 0.05$ confidence level are highlighted in boldface.

		Raw	DIFER		OpenFE		CAAFE				FEBP (ours)			
							GPT-3.5		GPT-4		GPT-3.5		GPT-4	
Raw		1.0000	**0.0010**	**0.0010**	0.5006	0.3953	**0.0010**	**0.0012**	0.3875	0.2344	**0.0010**	**0.0010**	**0.0010**	**0.0010**
DIFER		**0.0010**	1.0000	0.9000	0.6382	0.7345	0.9000	0.9000	0.7414	0.8996	0.4263	**0.0299**	0.1392	0.9000
		0.0010	0.9000	1.0000	**0.0098**	**0.0171**	0.9000	0.8308	**0.0178**	**0.0412**	0.9000	0.8377	0.9000	0.9000
OpenFE		0.5006	0.6382	**0.0098**	1.0000	0.9000	0.6175	0.7138	0.9000	0.9000	**0.0010**	**0.0010**	**0.0010**	**0.0171**
		0.3953	0.7345	**0.0171**	0.9000	1.0000	0.7138	0.8102	0.9000	0.9000	**0.0010**	**0.0010**	**0.0010**	**0.0289**
CAAFE	GPT-3.5	**0.0010**	0.9000	0.9000	0.6175	0.7138	1.0000	0.9000	0.7207	0.8790	0.4493	**0.0334**	0.1516	0.9000
		0.0012	0.9000	0.8308	0.7138	0.8102	0.9000	1.0000	0.8170	0.9000	0.3422	**0.0199**	0.1017	0.9000
	GPT-4	0.3875	0.7414	**0.0178**	0.9000	0.9000	0.7207	0.8170	1.0000	0.9000	**0.0010**	**0.0010**	**0.0010**	**0.0299**
		0.2344	0.8996	**0.0412**	0.9000	0.9000	0.8790	0.9000	0.9000	1.0000	**0.0026**	**0.0010**	**0.0010**	0.0661
FEBP	GPT-3.5	**0.0010**	0.4263	0.9000	**0.0010**	**0.0010**	0.4493	0.3422	**0.0010**	**0.0026**	1.0000	0.9000	0.9000	0.9000
		0.0010	**0.0299**	0.8377	**0.0010**	**0.0010**	**0.0334**	**0.0199**	**0.0010**	**0.0010**	0.9000	1.0000	0.9000	0.7414
	GPT-4	**0.0010**	0.1392	0.9000	**0.0010**	**0.0010**	0.1516	0.1017	**0.0010**	**0.0010**	0.9000	0.9000	1.0000	0.9000
		0.0010	0.9000	0.9000	**0.0171**	**0.0289**	0.9000	0.9000	**0.0299**	0.0661	0.9000	0.7414	0.9000	1.0000

D.7 Number of Selected Features

Table 15 compares the number of features added to the datasets. Our method FEBP adaptively determines the number of features and selects fewer features than DIFER (Zhu et al., 2022b), demonstrating the effectiveness of the features generated by our method.

Table 15: The number of selected features.

Model	Dataset	DIFER	OpenFE	FEBP Blinded		FEBP	
				GPT-3.5	GPT-4	GPT-3.5	GPT-4
Linear Model	AF	310	10	167	165	162	183
	BH	156	10	104	141	144	90
	WQR	109	10	57	80	43	55
	ACT	113	10	84	49	85	14
	CD	157	10	92	68	74	74
	GC	105	10	75	97	120	51
Random Forests	AF	387	10	39	19	15	34
	BH	186	10	4	6	19	77
	BS	46	10	9	7	9	65
	WQR	63	10	9	44	39	45
	ACT	339	10	55	35	69	61
	CD	178	10	97	74	94	89
	GC	92	10	68	84	31	59
Light-GBM	AF	325	10	30	55	42	24
	BH	118	10	15	17	16	25
	BS	287	10	119	48	68	116
	WQR	454	10	64	29	129	128
	ACT	132	10	54	46	16	51
	CD	409	10	68	53	12	50
	GC	501	10	61	86	16	35
Mean		223	10	64	60	60	66

D.8 Computation Cost

Table 16 compares the number of features evaluated during the feature search process. Guided by domain knowledge, our method FEBP evaluates much fewer features than DIFER (Zhu et al., 2022b) and OpenFE (Zhang et al., 2023).

Tables 17 and 18 summarize the computation time, using *gpt-3.5-turbo-0125* as the LLM. For FEBP, the computation time of LLM generation and feature evaluation is relatively stable across datasets of varying sizes. We note that the LLM generation time can be substantially reduced by instructing the LLM to generate multiple features in a generation step.

Table 16: The number of evaluated features.

Model	Dataset	DIFER	OpenFE	FEBP
Linear Model	AF	2083	224	200
	BH	2081	1167	200
	WQR	2083	929	200
	ACT	2077	4310	200
	CD	2088	3385	200
	GC	2076	4169	200
Random Forests	AF	2085	224	200
	BH	2079	1051	200
	BS	2082	310	200
	WQR	2085	929	200
	ACT	2079	1636	200
	CD	2086	1801	200
	GC	2078	2139	200
Light-GBM	AF	2084	224	200
	BH	2080	1051	200
	BS	2083	310	200
	WQR	2084	929	200
	ACT	2079	1636	200
	CD	2087	1801	200
	GC	2078	2139	200
Mean		2082	1518	200

Table 17: Comparison of computation time, in minutes.

Model	Dataset	DIFER	OpenFE	CAAFE	FEBP
Linear Model	AF	33.49	0.21	1.73	42.80
	BH	41.17	0.21	1.18	41.28
	WQR	34.94	0.25	1.21	42.33
	ACT	44.18	0.40	1.25	43.60
	CD	433.94	1.49	3.17	57.82
	GC	29.30	0.37	1.68	43.71
Random Forests	AF	178.50	0.23	4.22	63.30
	BH	89.07	0.24	5.52	51.70
	BS	98.50	0.23	4.05	51.13
	WQR	298.46	0.29	9.35	63.12
	ACT	78.44	0.28	3.82	44.66
	CD	571.33	1.12	14.05	94.08
	GC	60.41	0.28	3.24	45.06
Light-GBM	AF	301.56	0.25	5.81	63.06
	BH	62.30	0.24	3.01	44.84
	BS	74.59	0.24	2.55	45.23
	WQR	361.19	0.29	5.68	58.97
	ACT	36.39	0.28	1.73	42.71
	CD	102.04	1.07	2.49	46.34
	GC	48.63	0.28	2.97	43.03
Mean		148.92	0.41	3.94	51.44

Table 18: Computation time of different components of FEBP, in minutes.

Model	Dataset	LLM Generation	Feature Evaluation	Feature Selection
Linear Model	AF	16.73	22.98	3.08
	BH	18.50	20.18	2.60
	WQR	19.07	20.24	3.02
	ACT	18.92	20.97	3.71
	CD	16.73	25.14	15.95
	GC	17.01	23.24	3.47
Random Forests	AF	15.34	25.32	22.64
	BH	18.60	23.69	9.41
	BS	15.12	25.16	10.87
	WQR	12.75	23.81	26.56
	ACT	13.79	21.67	9.20
	CD	12.48	25.89	55.71
	GC	14.80	21.91	8.35
Light-GBM	AF	17.37	21.06	24.63
	BH	19.70	20.40	4.74
	BS	17.03	22.18	6.02
	WQR	16.27	21.19	21.51
	ACT	19.18	20.24	3.29
	CD	16.53	21.68	8.13
	GC	17.00	20.40	5.63
Mean		16.65	22.37	12.43

E ADDITIONAL ABLATION STUDY

To examine the impact of our canonicalization scheme, we compare the full version of FEBP with the reduced version without RPN canonicalization. From Table 19, the full version outperforms the reduced version in terms of the mean performance score using all three downstream models. The Friedman test p-value is 1.29×10^{-28}. Table 20 summarizes the p-values from the Nemenyi post-hoc test for pairwise comparison, which shows that the performance difference is statistically significant at the $p = 0.05$ level for the cases with GPT-3.5 and post-AutoFE parameter tuning as well as GPT-4 without post-AutoFE parameter tuning. We also observe a decrease in the number of LLM responses without canonicalization. This is because the expression becomes more flexible, reducing the likelihood of duplication with existing features during feature generation.

Additionally, we find that when switching to prefix feature expressions, the LLM encounters difficulty generating syntactically valid feature expressions, leading to a failure to complete one single run in our experiments.

Table 19: Performance comparison of FEBP with and without RPN canonicalization. For each compared version, the left and middle columns show the results without and with parameter tuning of the downstream model algorithm post AutoFE, respectively, and the right column shows the number of LLM responses. The results where the full version outperforms the reduced version are highlighted in boldface.

Model	Dataset	Raw	GPT-3.5						GPT-4					
			w/o Canonicalization			Full			w/o Canonicalization			Full		
Linear Model	AF	0.3474	0.6679	0.6688	338.6	0.6612	0.6616	339.8	0.6538	0.6529	321.2	**0.6649**	**0.6647**	371.4
	BH	0.3776	0.5048	0.5076	351.2	0.4995	0.5025	378.6	0.4987	0.5030	310.8	**0.5184**	**0.5289**	335.4
	WQR	0.2696	0.2702	0.2735	336.2	**0.2722**	**0.2745**	**328.4**	0.2690	0.2706	279.0	**0.2713**	**0.2748**	312.6
	ACT	0.8505	0.8748	0.8794	366.4	0.8729	0.8794	372.2	0.8738	0.8752	298.0	**0.8766**	**0.8762**	377.4
	CD	0.8267	0.8280	0.8290	350.4	**0.8282**	0.8282	**342.0**	0.8270	0.8271	285.4	**0.8288**	**0.8288**	**250.4**
	GC	0.7100	0.7370	0.7330	352.0	**0.7570**	**0.7460**	379.0	0.7550	0.7490	447.2	**0.7590**	0.7420	**310.6**
Mean		0.5636	0.6471	0.6486	349.1	**0.6485**	**0.6487**	356.7	0.6462	0.6463	323.6	**0.6532**	**0.6526**	326.3
Random Forests	AF	0.7677	0.7628	0.7762	358.0	**0.7709**	**0.7787**	393.2	0.7743	0.7843	340.2	0.7681	0.7749	**314.2**
	BH	0.5426	0.5573	0.5573	364.0	0.5549	0.5533	374.4	0.5491	0.5460	322.4	**0.5543**	**0.5522**	**278.6**
	BS	0.9446	0.9804	0.9807	372.2	**0.9873**	**0.9881**	386.8	0.9778	0.9777	284.4	**0.9845**	**0.9848**	**255.0**
	WQR	0.3662	0.3776	0.3726	334.6	**0.3862**	**0.3845**	362.6	0.3739	0.3719	269.8	**0.3810**	**0.3810**	283.2
	ACT	0.8808	0.8879	0.8841	353.4	**0.8925**	**0.8921**	357.6	0.8841	0.8864	327.6	**0.8893**	0.8864	424.0
	CD	0.8293	0.8283	0.8285	381.6	**0.8295**	**0.8294**	**349.8**	0.8290	0.8287	297.2	**0.8295**	0.8276	304.0
	GC	0.7450	0.7660	0.7620	342.2	0.7640	0.7620	368.2	0.7680	0.7610	368.2	0.7680	**0.7680**	471.8
Mean		0.6806	0.7372	0.7373	358.0	**0.7408**	**0.7412**	370.4	0.7366	0.7366	315.7	**0.7392**	**0.7393**	333.0
Light-GBM	AF	0.8375	0.8322	0.8365	343.6	0.8311	**0.8392**	380.2	0.8280	0.8350	376.0	**0.8366**	**0.8395**	**360.6**
	BH	0.5537	0.5599	0.5556	339.2	**0.5619**	**0.5644**	342.0	0.5577	0.5548	315.2	**0.5642**	**0.5595**	345.6
	BS	0.9429	0.9643	0.9664	368.8	**0.9737**	**0.9754**	380.0	0.9597	0.9609	276.2	**0.9801**	**0.9813**	**236.8**
	WQR	0.3825	0.4075	0.4042	346.4	**0.4118**	**0.4171**	**322.8**	0.4036	0.4032	288.2	0.4021	**0.4042**	293.6
	ACT	0.8832	0.8813	0.8860	342.4	**0.8888**	**0.8925**	367.4	0.8822	0.8879	313.2	**0.8902**	**0.8925**	359.6
	CD	0.8300	0.8302	0.8291	355.8	0.8301	**0.8297**	**352.2**	0.8295	0.8291	301.6	**0.8303**	**0.8294**	371.2
	GC	0.7250	0.7640	0.7650	346.2	**0.7680**	**0.7720**	376.6	0.7620	0.7650	428.8	**0.7760**	**0.7700**	**382.2**
Mean		0.6806	0.7485	0.7490	348.9	**0.7522**	**0.7558**	360.2	0.7461	0.7480	328.5	**0.7542**	**0.7538**	335.7
Mean		0.6806	0.7141	0.7148	352.2	**0.7171**	**0.7185**	362.7	0.7128	0.7135	322.5	**0.7187**	**0.7183**	331.9

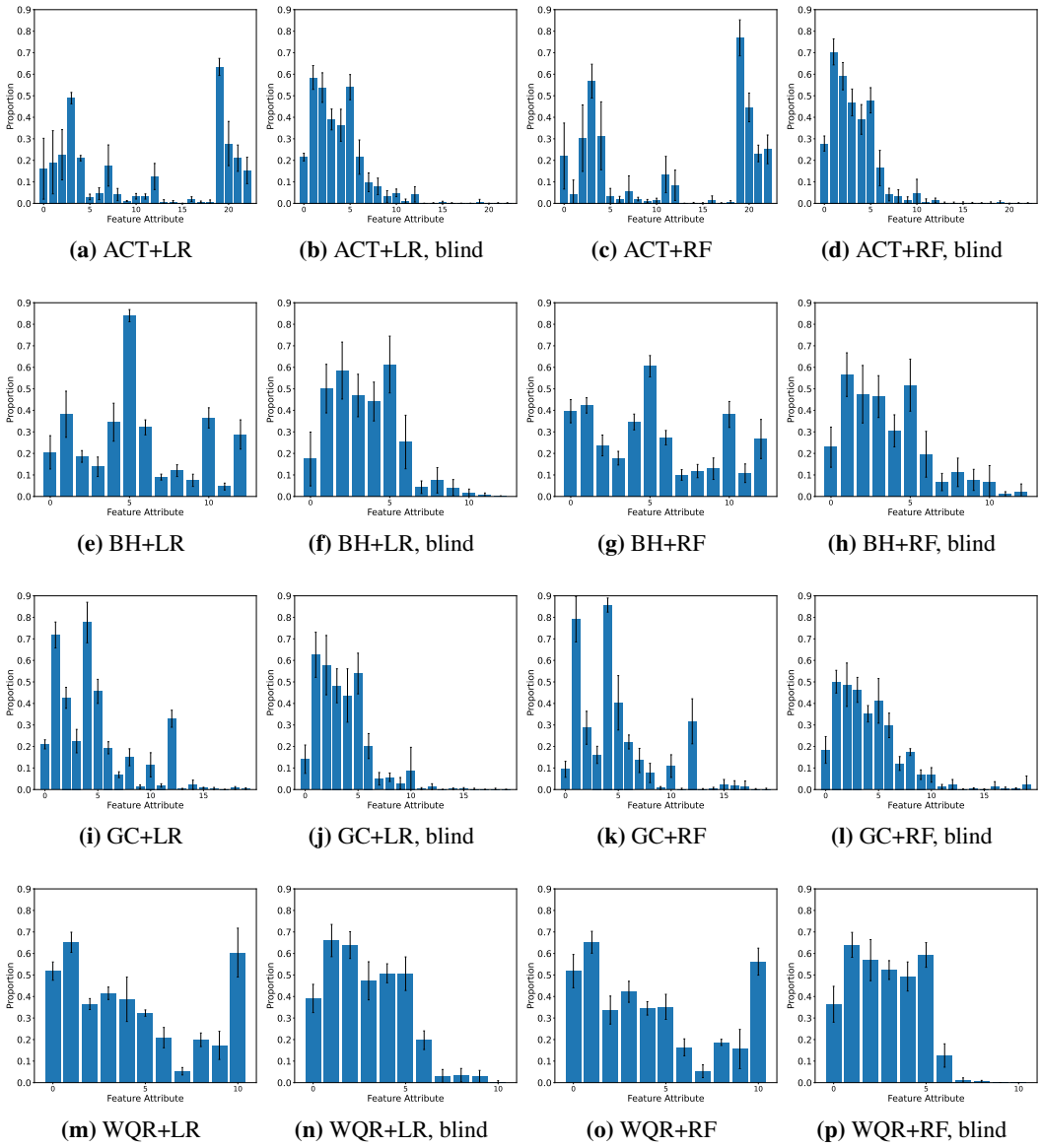
Table 20: The Nemenyi post-hoc test p-values for pairwise comparison of the methods in Table 19. Results that are significant at the $p = 0.05$ confidence level are highlighted in boldface.

		Raw	GPT-3.5				GPT-4			
			w/o		Full		w/o		Full	
Raw		1.0000	**0.0010**	**0.0010**	**0.0010**	**0.0010**	**0.0010**	**0.0010**	**0.0010**	**0.0010**
GPT-3.5	w/o	**0.0010**	1.0000	0.9000	0.2977	**0.0060**	0.9000	0.9000	**0.0224**	0.4293
		0.0010	0.9000	1.0000	0.6618	**0.0433**	0.8811	0.8889	0.1230	0.7871
	Full	**0.0010**	0.2977	0.6618	1.0000	0.9000	**0.0341**	**0.0355**	0.9000	0.9000
		0.0010	**0.0060**	**0.0433**	0.9000	1.0000	**0.0010**	**0.0010**	0.9000	0.8028
GPT-4	w/o	**0.0010**	0.9000	0.8811	**0.0341**	**0.0010**	1.0000	0.9000	**0.0010**	0.0635
		0.0010	0.9000	0.8889	**0.0355**	**0.0010**	0.9000	1.0000	**0.0010**	0.0659
	Full	**0.0010**	**0.0224**	0.1230	0.9000	0.9000	**0.0010**	**0.0010**	1.0000	0.9000
		0.0010	0.4293	0.7871	0.9000	0.8028	0.0635	0.0659	0.9000	1.0000

F Additional Analysis

F.1 Feature Analysis

Figure 13 shows the proportion of constructed features containing each feature attribute across different datasets and downstream models, for both the full and semantically blinded versions of FEBP. In the blinded version, we observe that the LLM tends to prioritize earlier feature attributes in the dataset while paying less attention to later ones, reflecting an inherent bias of the language model. In contrast, in the full version, the selection of feature attributes is guided by the semantic information of the dataset rather than the positional order of the attributes. This highlights the role of dataset semantic information in our feature construction process.



(a) ACT+LR **(b)** ACT+LR, blind **(c)** ACT+RF **(d)** ACT+RF, blind

(e) BH+LR **(f)** BH+LR, blind **(g)** BH+RF **(h)** BH+RF, blind

(i) GC+LR **(j)** GC+LR, blind **(k)** GC+RF **(l)** GC+RF, blind

(m) WQR+LR **(n)** WQR+LR, blind **(o)** WQR+RF **(p)** WQR+RF, blind

Figure 13: The proportions of constructed features containing each feature attribute.

F.2 FEATURE SEARCH EXAMPLE

Figure 14 shows examples of the LLM-based feature search process from a single run. In iteration 155, the generated feature is a combination of three examples. In iteration 158, the generated feature is a combination of two examples and columns are modified. Iteration 160 shows a modification of the example feature. Iteration 161 shows an analogy of the example feature.

Figure 14: Examples of feature search.

Iteration 155
Feature:
6, 12, division, 18, *, min_max
Prompt examples:
4, log, 13, *, 17, min_max, sqrt_abs, +
6, 12, *, 21, sqrt_abs, +
4, 14, +, 18, *, min_max
11, 21, +, 6, *, sqrt_abs
2, 4, +, 6, division, log
4, 6, +, 16, *, 17, +, min_max
6, 21, division, 17, log, *
12, min_max, 18, *, 5, mod_column
2, 6, mod_column, 17, +, sqrt_abs
2, 3, +, 4, sqrt_abs, *
4, 12, division, 16, *, min_max, sqrt_abs

Iteration 158
Feature:
5, log, 19, *, 15, +, min_max
Prompt examples:
4, log, 13, *, 17, min_max, sqrt_abs, +
6, 12, *, 21, sqrt_abs, +
4, 14, +, 18, *, min_max
11, 21, +, 6, *, sqrt_abs
2, 4, +, 6, division, log
4, 6, +, 16, *, 17, +, min_max
6, 21, division, 17, log, *
12, min_max, 18, *, 5, mod_column
2, 6, mod_column, 17, +, sqrt_abs
2, 3, +, 4, sqrt_abs, *
4, 12, division, 16, *, min_max, sqrt_abs

Iteration 160
Feature:
11, 21, *, 4, +, 14, mod_column
Prompt examples:
4, log, 13, *, 17, min_max, sqrt_abs, +
6, 12, *, 21, sqrt_abs, +
4, 14, +, 18, *, min_max
11, 21, +, 6, *, sqrt_abs
2, 4, +, 6, division, log
4, 6, +, 16, *, 17, +, min_max
6, 21, division, 17, log, *
12, min_max, 18, *, 5, mod_column
2, 6, mod_column, 17, +, sqrt_abs
2, 3, +, 4, sqrt_abs, *
4, 12, division, 16, *, min_max, sqrt_abs

Iteration 161
Feature:
6, 12, +, 17, *, min_max
Prompt examples:
6, 12, *, 21, sqrt_abs, +
4, 14, +, 18, *, min_max
11, 21, *, 4, +, 14, mod_column

11, 21, +, 6, *, sqrt_abs
2, 4, +, 6, division, log
4, 6, +, 16, *, 17, +, min_max
6, 21, division, 17, log, *
12, min_max, 18, *, 5, mod_column
2, 6, mod_column, 17, +, sqrt_abs
2, 3, +, 4, sqrt_abs, *
4, 12, division, 16, *, min_max, sqrt_abs

G DIFFERENCES TO CAAFE

While our work FEBP and CAAFE (Hollmann et al., 2023) both utilize LLMs to construct new features incorporating dataset semantic information, they differ in several key aspects. We design FEBP such that it taps into the in-context learning capability of LLMs and performs effective feature search. In FEBP, we provide top-performing constructed features in the prompt as learning examples, label them with performance scores, and rank them by score. We demonstrate that the LLM learns to optimize feature construction over the course of algorithm. CAAFE instead stores all previous instructions and code snippets in the conversation history, which hinders the in-context learning of optimal feature patterns. It quickly consumes the LLM's context as the algorithm iterates, incurring more and more LLM generation costs. In comparison, the LLM generation cost of FEBP stays constant across iterations, without a maximum limit on the number of iterations it can perform. Therefore, our method FEBP has stronger capability of feature search in large search spaces requiring more iterations, such as datasets with numerous feature attributes.

We also represent features in a different form in FEBP, i.e., canonical RPN (cRPN). We refer to Appendix A for further discussion. Compared with the Python code representation in CAAFE, cRPN is more compact, which not only reduces LLM generation costs but also makes the in-context learning of feature patterns easier, and more human interpretable. The use of pre-defined operators reduces the search space and simplifies the learning process for optimizing feature construction. Together, our approach gives better control than code representation and helps avoid undesirable or unexpected LLM outputs. Another benefit of cRPN is that it is convenient to import external features (as outlined in Algorithm 1) and export the results as individual features, providing compatibility with other feature engineering methods.

More fundamentally, we demonstrate in this work that general-purpose LLMs like GPTs can effectively model recursive tree structures in the form of cRPN feature expressions and reason the structures in the context of semantic information, paving the way for further LLM-driven applications. We hereby underscore the importance of adopting proper representation for the downstream task to tap into LLMs' potential.