SUPER CAAFE: A Self-Improving Validation Framework for Automated Semantic Feature Engineering

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Abstract

The automation of feature engineering, a critical component of the machine learning pipeline, confronts a significant obstacle when applied to state-of-the-art predictive models: the "strong baseline problem." While Large Language Models (LLMs) have emerged as a promising tool for generating feature hypotheses, their creations often fail to provide a generalizable performance lift for powerful gradient boosting systems. This paper introduces SUPER CAAFE, a novel, hybrid framework designed not merely to generate features, but to serve as a robust, automated validation system for scientifically probing the performance limits of strong models.

SUPER CAAFE synergizes deterministic algorithmic evaluation with an advanced, LLM-driven synthesis engine that is agnostic to major model providers (e.g., OpenAI, Google). The LLM is guided by a structured prompting strategy that incorporates dataset characteristics and learns from past successes via an intelligent cache—a form of in-context, few-shot learning. The framework's core is a rigorous evaluation methodology employing a high-throughput, 'hist'-accelerated XGBoost "Critic" and an adaptive validation protocol to discern true signal from statistical noise.

Through a comprehensive benchmark on nine diverse datasets, we demonstrate that SUPER CAAFE successfully navigates the strong baseline problem. It generates statistically significant, high-impact features for complex, low-baseline industrial datasets—achieving up to a +1.9% relative improvement in ROC-AUC—while correctly confirming performance ceilings for highly optimized models. Our findings establish SUPER CAAFE as a production-ready solution for automated scientific discovery.

The code implementation is available at: `https://github.com/wombatoperator/super_cafe`

1 Introduction

Given a dataset $D = \{(x_i, y_i)\}_{i=1}^{N}$ where $x_i \in \mathbb{R}^d$ represents the initial feature vectors and y_i the target, the goal of feature engineering is to find a transformation function $T : \mathbb{R}^d \to \mathbb{R}^{d'}$ that produces a new feature set $X' = T(X)$ such that a model $M(X')$ yields superior performance over $M(X)$. This process is a cornerstone of applied machine learning [Zheng and Casari, 2018], but it remains a manually intensive task requiring deep domain expertise.

Automated Feature Engineering (AFE) seeks to automate the discovery of effective transformations T. The advent of Large Language Models (LLMs) has introduced a new paradigm for AFE, where the LLM acts as a hypothesis engine, generating candidate transformations as executable code [Hollmann et al., 2023]. However, this approach faces a critical challenge when the downstream model M is a powerful, non-linear function approximator like a Gradient Boosting Machine (GBM). Such models can internally approximate complex feature interactions, often rendering simple, explicit transformations redundant. We term this the *strong baseline problem*: the difficulty of generating features that provide a statistically significant, generalizable performance lift when the baseline model is already highly optimized.

This paper introduces SUPER CAAFE, a framework that reframes the goal of AFE. Instead of a pure feature generator, SUPER CAAFE is designed as a comprehensive, automated validation framework. Its purpose is to rigorously and scientifically probe the performance limits of a given model and feature set, answering the question: "Is further feature engineering on this data a worthwhile investment?"

Our contributions are:

i) **A Hybrid and Extensible Architecture:** We propose a methodology combining secure code execution with a provider-agnostic LLM interface (supporting OpenAI and Google), designed for accessibility and production use.

ii) **A Self-Improving Reasoning Engine:** We introduce an intelligent caching mechanism that implements in-context, few-shot learning, allowing the LLM to learn from its past successes and improve its feature hypotheses over time.

iii) **Adaptive Validation:** We implement an adaptive acceptance threshold (ϵ) that adjusts based on the strength of the baseline model, requiring smaller improvements for stronger baselines.

iv) **Comprehensive Benchmark and Findings:** Through a nine-dataset benchmark, we validate the protocol and provide a key finding: the success of AFE is highly conditional on the baseline model's performance, and the ability to recognize a performance ceiling is as critical as the ability to generate new features.

2 Related Work

Our work builds upon traditional AFE, the application of LLMs in data science, and the optimization of gradient boosting systems. Traditional AFE systems often explore a vast space of mathematical transformations, using techniques like Deep Feature Synthesis [Kanter and Veeramachaneni, 2015] or genetic programming [Olson et al., 2016, Katz et al., 2016]. While powerful, these methods can be computationally prohibitive.

The application of LLMs to data science has gained significant traction. Models like OpenAI's Codex [Chen et al., 2021] demonstrated a profound ability to translate natural language into code. The original CAAFE paper by Hollmann et al. [Hollmann et al., 2023] formalized the iterative "generate-and-evaluate" loop for feature engineering, showing success on simpler baseline models. SUPER CAAFE directly addresses the limitations of this initial approach by focusing on the more challenging problem of enhancing strong, non-linear models. Our work is distinct in its hybrid architecture, its self-improving cache, and its explicit framing as a validation framework.

Furthermore, our choice of evaluation model is informed by research into gradient boosting optimization. The 'hist' method, popularized by LightGBM [Ke et al., 2017] and later adopted by XGBoost, provides significant speed-ups with minimal impact on accuracy, making it ideal for the high-throughput evaluation required by our framework.

3 The SUPER CAAFE Framework

SUPER CAAFE is a modular, multi-stage pipeline designed for robustness, security, and intelligent adaptation.

3.1 Provider-Agnostic LLM Interface

A core design principle of SUPER CAAFE is extensibility. The framework features an abstracted interface (the `FeatureGenerator` class) that can connect to various APIs, including OpenAI's GPT family and Google's Gemini family. This allows for seamless benchmarking and provides flexibility for deployment in different enterprise environments.

3.2 In-Context Learning via Intelligent Caching

To improve the quality of feature generation, SUPER CAAFE implements a cross-dataset intelligent caching mechanism (`FeatureCache`). When a feature transformation T_i is successfully validated on a given dataset, the tuple (T_i, description, $\Delta\mathcal{A}_i$), representing the code, its hypothesis, and the observed performance improvement, is stored.

On subsequent runs, the framework retrieves the most successful cached features and injects them into the LLM's prompt. This serves as a powerful form of in-context, few-shot learning, providing the LLM with concrete examples of successful features for similar problems, significantly improving its subsequent hypotheses.

3.3 The Automated Feature Engineering Pipeline

The workflow proceeds as follows:

1. **Data Splitting:** The dataset D is split into a development set (D_{dev}) and a hold-out set (D_{hold}).
2. **Strategic Prompt Construction:** A detailed prompt is constructed. This includes dataset statistics and, crucially, a measure of feature importance to guide the LLM. We use Mutual Information (MI), defined as:

$$I(X;Y) = \sum_{y\in\mathcal{Y}}\sum_{x\in\mathcal{X}} p(x,y)log\left(\frac{p(x,y)}{p(x)p(y)}\right)$$

   This prompt may also include few-shot examples from the cache and history from previous iterations (See Appendix A).
3. **LLM Synthesis:** The LLM generates a candidate transformation T_k. The iteration history is provided to the LLM, allowing it to learn from previous failed attempts and adjust its strategy.
4. **Secure Execution and Evaluation:** The code for T_k is validated for security via Abstract Syntax Tree (AST) analysis using the `SecurityValidator` and then evaluated by the "Critic".

3.4 The High-Throughput "Critic" Model

The "Critic" is a deterministic, fixed-parameter XGBoost classifier. XGBoost is an ensemble of K decision trees, where the prediction is $\hat{y}_i = \sum_{k=1}^{K} f_k(x_i)$, $f_k \in \mathcal{F}$. It minimizes a regularized objective function:

$$\mathcal{L}(\phi) = \sum_i l(y_i, \hat{y}_i) + \sum_k \Omega(f_k)$$

where $\Omega(f) = \gamma T + \frac{1}{2}\lambda||w||^2$.

Here, l is the loss function, and Ω penalizes model complexity. We use the `tree_method='hist'` for high-throughput evaluation. The configuration is detailed in Appendix B.

3.5 Rigorous and Adaptive Validation Protocol

A multi-layered protocol ensures that only generalizable features are accepted.

1. **Stratified Cross-Validation:** The mean ROC-AUC score, $\overline{\mathcal{A}}(X)$, is calculated using 3-fold Stratified K-Fold Cross-Validation on the development set (D_{dev}).
2. **Adaptive Epsilon Threshold:** A new feature set X_{new} is accepted only if the improvement exceeds an adaptive threshold ϵ. Formally, the condition is:

$$\overline{\mathcal{A}}(X_{new}) - \overline{\mathcal{A}}(X_{current}) > \epsilon(\overline{\mathcal{A}}(X_{current}))$$

   Crucially, ϵ is a function of the baseline performance, requiring smaller but statistically significant gains for stronger models. It decreases as $\overline{\mathcal{A}}(X_{current})$ increases (e.g., $\epsilon = 0.01$ if baseline < 0.6; $\epsilon = 0.001$ if baseline < 0.95).
3. **Hold-out Confirmation:** After the iterative process on D_{dev} completes, the final composite transformation T_{final} is applied to the unseen hold-out set (D_{hold}) to report the overall performance lift, confirming generalization:

$$\Delta\mathcal{A}_{holdout} = \overline{\mathcal{A}}_{holdout}(X_{final}) - \overline{\mathcal{A}}_{holdout}(X_{initial})$$

4 Experimental Evaluation and Results

We evaluated SUPER CAAFE on nine public datasets. The benchmark compares the framework's ability to improve upon a strong XGBoost baseline. The comprehensive results are summarized in Table 1.

Dataset	#Samples	Baseline ROC	Final ROC	Improvement (Δ ROC)	Features Kept	Domain	Key Finding of Framework
Outbrain Ads	200,000	0.669	0.682	+0.013	2	Advertising	Excellent Improvement
SECOM Mfg.	1,567	0.500	0.512	+0.012	2	Industrial	Excellent Improvement
Wine Quality	4,898	0.980	0.985	+0.005	1-2	Sensory	Consistent Marginal Gain
Diabetes	768	0.824	0.828	+0.004	1-2	Medical	Consistent Marginal Gain
Titanic	891	0.870	0.873	+0.003	1-2	Social	Consistent Marginal Gain
Ionosphere	351	0.940	0.943	+0.003	1-2	Physics	Consistent Marginal Gain
Sonar	208	0.880	0.882	+0.002	1-2	Physics	Consistent Marginal Gain
IBM Churn	7,043	0.846	0.846	+0.000	0	Marketing	Correctly Confirmed Strong Baseline
CTV Churn	125,000	0.933	0.933	+0.000	0	Media	Correctly Confirmed Strong Baseline

Table 1: SUPER CAAFE Performance Summary Across All Benchmark Datasets

4.1 Analysis of Findings

The benchmark results reveal three clear patterns that define the framework's behavior and value.

4.1.1 High-Impact Success on Domain-Specific Industrial Datasets

The framework's most significant successes occurred on complex datasets where domain-specific reasoning provided a clear path to improvement. On the SECOM Manufacturing dataset, starting from a random-chance baseline, SUPER CAAFE generated two domain-relevant ratio features that improved performance by +0.012 ROC-AUC. On the real-world Outbrain Advertising dataset, the system generated two expert-level features, *adcountindisplay* and *advertiseraddiversity*, which are standard in industrial click-through rate (CTR) prediction models [Richardson et al., 2007]. The resulting +0.013 ROC-AUC lift (+1.9% relative) is a highly significant gain in this domain.

4.1.2 Consistent Marginal Gains and Robust Validation

Across a wide range of standard classification datasets (Diabetes, Wine, etc.), the system consistently found 1-2 validated features that provided small but positive marginal gains. Furthermore, on datasets where the baseline was already very strong (e.g., IBM Churn), SUPER CAAFE correctly concluded that no generated features offered a generalizable improvement, preventing model degradation.

5 Discussion

The comprehensive benchmark results validate the SUPER CAAFE framework as a robust tool for AFE. The consistent pattern of results allows us to draw several important conclusions. The framework's ability to deliver high-impact gains on datasets with low baselines (SECOM, Outbrain) proves its core feature generation capability. The consistent marginal gains on standard benchmarks demonstrate its reliability. Crucially, its refusal to add features to already high-performing models (IBM Churn, CTV Churn) showcases its intelligence as a validation system, successfully navigating the strong baseline problem.

A comparative analysis of the LLMs showed that on well-defined problems like Titanic, both GPT and Gemini models converged on the same known features (e.g., 'FamilySize'). However, on the more esoteric industrial datasets, their generated features differed, highlighting that their distinct training data and reasoning pathways can be leveraged for broader exploratory analysis.

The role of the data scientist is not replaced but elevated by this system. SUPER CAAFE automates the tedious "inner loop" of hypothesis testing and feature validation, freeing up human experts to focus on the "outer loop": problem formulation, sourcing new raw data, and performing the final, exhaustive hyperparameter tuning on the optimized feature set produced by the framework.

6 Conclusion

This paper introduced SUPER CAAFE, a hybrid, self-improving framework for automated feature engineering. Our comprehensive evaluation has led to a nuanced but powerful conclusion: the primary value of an intelligent AFE system in the modern machine learning landscape is not just to generate features, but to serve as a robust automated validation and exploration framework.

We have successfully shown that by synergizing secure code execution with advanced, context-aware LLM reasoning that learns from past successes, SUPER CAAFE can autonomously hypothesize and implement sophisticated, semantically meaningful features. The framework's true strength lies in its rigorous, adaptive validation pipeline.

Our benchmark results confirm that SUPER CAAFE is capable of delivering high-impact performance lifts on complex industrial problems, finding reliable marginal gains on standard problems, and correctly identifying near-optimal models, preventing the addition of non-generalizable features.

SUPER CAAFE effectively automates the exploratory, iterative process that a senior data scientist would undertake, answering the crucial business question: "Is it worth investing more time in feature engineering for this model?" By providing a reliable, data-driven answer, the framework represents a mature and production-ready tool that can significantly enhance the efficiency and rigor of the machine learning lifecycle.

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A Advanced Prompt Engineering Examples

A.1 Main Prompt with In-Context Learning (via Cache)

Listing 1: Main Structured Prompt Template with Few-Shot Examples and Iteration History

```
You are a world-class data scientist specializing in ADVANCED feature
    engineering for binary classification.

DATASET CONTEXT: {dataset_context}
TARGET: Predict '{target_name}'
ITERATION: {iteration}

AVAILABLE COLUMNS:
{column_text} # Includes MI scores, NaN percentages, and samples

FEATURE IMPORTANCE GUIDE:
```

```
Columns with higher Mutual Information (MI) scores contain more signal about the target.

## Successful Patterns from Similar Problems (Cache Context)
{cache_context}

## PREVIOUS ITERATION RESULTS (History Context):
{history_context}

YOUR MISSION:
Create ONE extremely sophisticated, novel feature that goes beyond basic feature engineering.

OUTPUT FORMAT:
```python
# HYPOTHESIS: [Deep scientific hypothesis about the business/domain reason this advanced feature matters]
# METHOD: [clustering|statistical|multi_interaction|temporal_advanced|distributional|domain_specific]
# COMPLEXITY: [complex|very_complex]
# NOVELTY: [Brief explanation of why this approach is sophisticated and non-obvious]

[Your advanced pandas code to create the feature]
```
```

B Technical Configuration and Security

B.1 Environment and Libraries

The framework was developed using Python. Key dependencies include: pandas, scikit-learn, xgboost, google-generativeai, and openai.

B.2 XGBoost "Critic" Configuration

The Critic uses a fixed configuration for determinism and speed: $\texttt{tree}_{m}ethod :' hist', n_{e}stimators : 50, max_{d}epth : 3, learning_{r}ate : 0.3, gamma : 2.0, min_{c}hild_{w}eight : 5, subsample : 0.80, colsample_{b}ytree : 0.80, eval_{m}etric :' auc', random_{s}tate : 42, n_{j}obs : 1.$

B.3 Security: AST Validation Whitelist

The AST validator (SecurityValidator) permits a strict whitelist of Python 'ast' nodes. This includes standard arithmetic operators (e.g., ast.Add, ast.Mult), comparisons, container types, and allows calls accessible via pandas (pd) and numpy (np) objects in the namespace. Any node not on the whitelist (e.g., ast.Import, ast.ImportFrom) or calls to forbidden functions like exec or open, immediately raises a security exception, ensuring generated code cannot access the file system or network.