



Agentic AI for Autonomous Data Science: An Integrated Workbench for End-to-End Predictive Analytics, Data Hygiene, and Semantic Validation

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Abstract

Modern machine learning deployments are fundamentally constrained by the quality of their upstream data. Enterprise pre-processing pipelines remain a critical bottleneck, relying on fragmented, manual, and static scripting tools that fail to detect logical inconsistencies and semantic anomalies lurking beneath syntactically valid records. This study presents **PURE-STREAM** (Predictive Unified Reasoning Engine for Semantic Truth, Relational Evaluation, Autonomous Automation, and Multivariate Modelling), an autonomous Agentic AI workbench engineered to eliminate the Fragmented Toolset Problem. The framework integrates a state-locked interactive curation workspace, multivariate predictive imputation (MICE and KNN), relational transaction auditing via XAMPP/MySQL, and localized Explainable AI through a Phi-3 language model. The proposed methodology resolves structural missingness across MCAR, MAR, and MNAR patterns while enforcing rigorous semantic truth validation through Isolation Forest anomaly scoring, ensuring zero data leakage through an edge-computed, air-gapped processing architecture. Experimental results demonstrate a 100% Post-ML Health Score, a 99.2% anomaly capture rate, and an imputation RMSE of 3.15 compared to 14.32 for the univariate baseline. By shifting from static cleaning to an integrated, audit-ready DataOps pipeline, this work demonstrates that autonomous semantic validation is not merely beneficial but essential for next-generation, high-trust predictive analytics systems.

Keywords — *Agentic AI, autonomous data science, MICE imputation, KNN imputation, semantic validation, Isolation Forest, explainable AI, DataOps, data hygiene, relational auditing, Phi-3, PURE-STREAM, predictive analytics, edge computing, missing value imputation.*

I. Introduction

The reliability of any machine learning model is inseparable from the integrity of its training data. Despite decades of progress in algorithm design and computational infrastructure, data engineering pipelines in



production environments remain severely fragmented. Practitioners routinely navigate between separate tools for data ingestion, statistical cleaning, database management, model training, and reporting, stitching together workflows through ad-hoc scripts that lack formal quality guarantees, audit trails, or semantic reasoning capacity [1].

This fragmentation manifests most acutely in the treatment of missing values and semantic anomalies. Classical univariate imputation, filling a missing entry with a column mean or mode, is computationally trivial but statistically damaging: it artificially compresses variance, distorts inter-feature correlations, and produces training datasets that no longer reflect the underlying joint data distribution [2]. Worse, such methods are entirely blind to what this paper terms logical lies: records that are numerically plausible in isolation but semantically impossible in context, such as a patient record combining an age of 4 with an occupation of Consultant Surgeon, or a payroll entry showing negative annual salary. These anomalies pass standard univariate cleaning gates without detection, yet their presence in training data systematically degrades model reliability [3].

Existing automation approaches address only fragments of this problem. AutoML systems automate model selection but presuppose clean inputs [4]. Data cleaning frameworks enforce syntactic constraints but lack semantic reasoning [5]. Large language model-based agentic workflows have been proposed for interactive analytics but lack relational auditability and expose sensitive enterprise data to cloud inference APIs, violating data governance requirements in regulated industries [6].

This paper introduces PURE-STREAM, an integrated DataOps workbench that addresses the Fragmented Toolset Problem as a unified system. PURE-STREAM acts as a proactive data engineer, bridging the gap between mathematical predictive modelling and enterprise-grade compliance through a secure, localized, edge-computed architecture. It integrates four tightly coupled subsystems: an interactive state-locked curation workspace, a hybrid predictive imputation engine, a tamper-proof relational audit ledger, and a localized explainability interface.

The framework's design is grounded in two core principles. First, mathematical rigour: missing value treatment must respect the multivariate structure of the data, using chained regression (MICE) and manifold-aware imputation (KNN) rather than scalar statistics. Second, semantic integrity: data validity cannot be assessed at the level of individual columns; it must be evaluated at the level of complete records, using anomaly scoring methods capable of detecting contextual implausibility across feature combinations.

The key contributions of this paper are: (1) the PURE-STREAM architecture, a novel integrated DataOps workbench providing end-to-end autonomous data science capability within a single, air-gapped platform; (2) a hybrid MICE/KNN imputation engine with dynamic missingness mechanism routing and a 12-strategy benchmarking suite; (3) a semantic validation layer using Isolation Forest scoring to detect logical contradictions in structured records; (4) a tamper-proof MySQL audit ledger enabling stateless state-reconstruction of any prior pipeline state; (5) a localized Phi-3 XAI interface generating natural language rationales for all imputation decisions without cloud dependency; and (6) empirical evaluation



demonstrating a 78% RMSE reduction, 134% F1-score improvement in anomaly detection, and 100% elimination of pipeline crash events relative to the univariate baseline.

The remainder of this paper is organized as follows. Section II surveys related literature. Section III presents the problem statement. Section IV describes existing system approaches. Section V details the PURE-STREAM architecture. Section VI presents the mathematical foundations. Section VII reports experimental results. Section VIII concludes with directions for future work.

II. Literature Survey

A. Limitations of Univariate Imputation

The statistical inadequacy of univariate imputation methods has been extensively documented in recent literature. Chen and Sharma [2] demonstrated that mean and mode imputation artificially compresses data variance, producing systematic underestimation of feature standard deviations and distortion of pairwise correlation structures. Their experiments across seven tabular benchmarks showed that models trained on mean-imputed data exhibited, on average, 12.4% higher out-of-sample prediction error than those trained on data prepared with multivariate strategies. Van Buuren [7] established the theoretical foundations for Multiple Imputation by Chained Equations (MICE), demonstrating that chained regression imputation preserves the joint distribution of the data under both MCAR and MAR mechanisms. More recent extensions by Jarrett et al. [8] adapted the MICE framework for high-dimensional settings with complex inter-feature dependency structures, achieving consistent improvements over univariate baselines across clinical and financial datasets.

B. Semantic Anomaly Detection in Structured Data

The detection of semantic anomalies in structured records, as distinct from statistical outliers, has emerged as an important and underserved research area. Liu et al. [9] introduced the original Isolation Forest algorithm, demonstrating its superiority over density-based methods for high-dimensional anomaly detection through its use of random partitioning rather than distance computation. Patel and Gupta [3] extended Isolation Forest to the contextual anomaly setting, showing that it can detect logical contradictions, values that are statistically plausible in isolation but semantically impossible in context, with an F1-score improvement of over 40% compared to univariate z-score approaches. Goldstein and Uchida [10] provided a comprehensive comparative evaluation of anomaly detection methods for structured tabular data, confirming that ensemble isolation-based methods consistently outperform single-model approaches in both precision and recall across diverse domain settings.

C. Agentic AI Frameworks for Data Science



The concept of applying autonomous agent architectures to data science workflows has gained significant traction since 2024. Wang and Lee [6] proposed a generalized agentic workflow model for data science tasks, demonstrating that agent-based coordination of subtasks improves end-to-end pipeline performance over monolithic automation approaches. Zhang et al. [11] introduced the Data-Copilot system, an LLM-driven agentic framework for interactive analytics, though their architecture relies on cloud API calls that introduce latency, cost, and data governance risks unsuitable for regulated enterprise deployment. Huang et al. [12] proposed CAAFE, a context-aware automated feature engineering agent, showing meaningful gains over static feature engineering baselines. The PURE-STREAM framework extends these approaches by embedding agentic orchestration within a fully localized, air-gapped architecture that meets enterprise compliance requirements.

D. Explainable AI in Data Preparation Pipelines

The integration of explainability mechanisms into data preparation workflows, rather than restricting XAI to the modelling stage, represents a recent and important development. Roberts et al. [5] identified the compliance risks introduced when sensitive enterprise data is transmitted to cloud-based LLM APIs for explanation generation, arguing for edge-deployed alternatives. Kuznetsov and Rossi [13] demonstrated that privacy-preserving edge computing approaches for ML inference achieve latency comparable to cloud-based alternatives for batch processing tasks while eliminating transmission-layer data exposure. Molnar [14] provided a comprehensive treatment of SHAP and related explanation methods, while more recent work by Wei et al. [15] demonstrated that small, instruction-tuned language models such as Phi-3 can generate high-quality natural language rationales for structured data decisions with minimal computational overhead, making them viable for deployment in resource-constrained edge environments.

E. Relational Auditability in ML Pipelines

The need for tamper-proof audit trails in machine learning pipelines has been highlighted by both academic research and regulatory frameworks. Paleyes et al. [16] surveyed challenges in deploying machine learning systems in production, identifying audit trail gaps as a significant source of operational risk, particularly in regulated industries such as healthcare and finance. Sculley et al. [17] documented the hidden technical debt accumulated in ML systems lacking formal provenance tracking. Recent work by Stoyanovich et al. [18] formalized the concept of pipeline provenance for fair and accountable ML, proposing relational schemas for recording transformation lineage. PURE-STREAM's MySQL-based audit ledger extends these proposals with a live, real-time implementation integrated directly into the workbench execution environment.

2.1 Problem Statement



Let $D = \{r_1, r_2, \dots, r_n\}$ denote a raw enterprise dataset of n records, each comprising m heterogeneous attributes drawn from both continuous and categorical domains. In practice, D is characterised by four classes of quality defect: (i) structural incompleteness, where attribute values are absent under MCAR, MAR, or MNAR mechanisms; (ii) variance compression, introduced by naive univariate imputation; (iii) pipeline brittleness, where undeclared quality assumptions cause runtime crashes during downstream ML; and (iv) semantic implausibility, where individual attribute values are numerically valid but collectively describe entities that are logically impossible in the real world.

Formally, we define the semantic implausibility of a record r_i as the condition where r_i satisfies all univariate domain constraints, i.e., $x_j \in [x_j^{\min}, x_j^{\max}]$ for all j , yet the joint density $p(x_1, x_2, \dots, x_m)$ evaluated at r_i is anomalously low relative to the observed data manifold. The problem addressed by PURE-STREAM is: given an arbitrary raw dataset D with unknown quality defects across all four dimensions, construct an autonomous integrated workbench Φ such that $\Phi(D) = (D^*, A^*, E^*)$, where D^* is a semantically validated, imputation-complete dataset preserving the multivariate joint distribution, A^* is a tamper-proof audit record of all transformations applied, and E^* is a natural language explainability report grounded to the transformation decisions, all produced without cloud dependency or intermediate human intervention.

III. Analysis of Existing Approaches

A. Univariate Imputation Pipelines

The most widely deployed data preparation approach in current practice is the univariate imputation pipeline, typically implemented using pandas, scikit-learn's SimpleImputer, or equivalent libraries. These systems fill missing values using column-level statistics (mean, median, or mode) independently for each attribute, without reference to the values of other attributes in the same record. While computationally inexpensive, this approach has well-documented statistical deficiencies [2]: it reduces feature variance, distorts inter-feature correlations, and produces imputed values that do not reflect the conditional distribution of the missing attribute given the observed attributes. Furthermore, such pipelines produce no audit trail, provide no explainability output, and have no mechanism for semantic validation.

B. Cloud-Based AutoML and Data Wrangling Services

Cloud-hosted AutoML platforms and data wrangling services, including commercial offerings from major cloud providers, offer more sophisticated imputation and cleaning capabilities but introduce several critical limitations for enterprise deployment. Data transmission to external APIs exposes sensitive records to third-party infrastructure, creating compliance risk under regulations such as GDPR, HIPAA, and India's DPDP Act [5][13]. Latency introduced by network round-trips is unpredictable and can cause pipeline timeouts for large datasets. Audit trails, where provided, are controlled by the service provider rather than the enterprise, limiting legal defensibility. Finally, these platforms do not provide semantic



validation: they may detect statistical outliers but cannot assess whether a complete record is contextually implausible.

C. Standalone Anomaly Detection Systems

Dedicated anomaly detection systems such as PyOD and its constituent algorithms provide state-of-the-art statistical detection of outliers but are not integrated into preprocessing pipelines. They operate as post-hoc analysis tools rather than inline quality gates, meaning that anomalous records can still propagate into model training if the detection step is omitted or misconfigured. Furthermore, standalone anomaly detectors produce numerical scores without natural language explanation, requiring domain expertise to interpret and act upon their outputs.

D. Comparative Summary

System / Tool	Multivar. Impute	Semantic Valid.	Audit Trail	XAI Output	Air-Gapped
Univariate Pipeline	No	No	No	No	Yes
Cloud AutoML	Partial	No	Partial	No	No
Standalone PyOD	No	Partial	No	No	Yes
HoloClean [19]	Partial	No	No	No	Yes
Data-Copilot [11]	Partial	No	No	Partial	No
PURE-STREAM (Ours)	Yes	Yes	Yes	Yes	Yes

TABLE I. Capability Comparison of Existing Systems against PURE-STREAM

Table I confirms that no existing system delivers the complete combination of multivariate imputation, semantic validation, tamper-proof audit trails, natural language explainability, and air-gapped local deployment that PURE-STREAM provides. Each existing approach covers at most two of these five capability dimensions.



IV. Proposed Design: PURE-STREAM Architecture

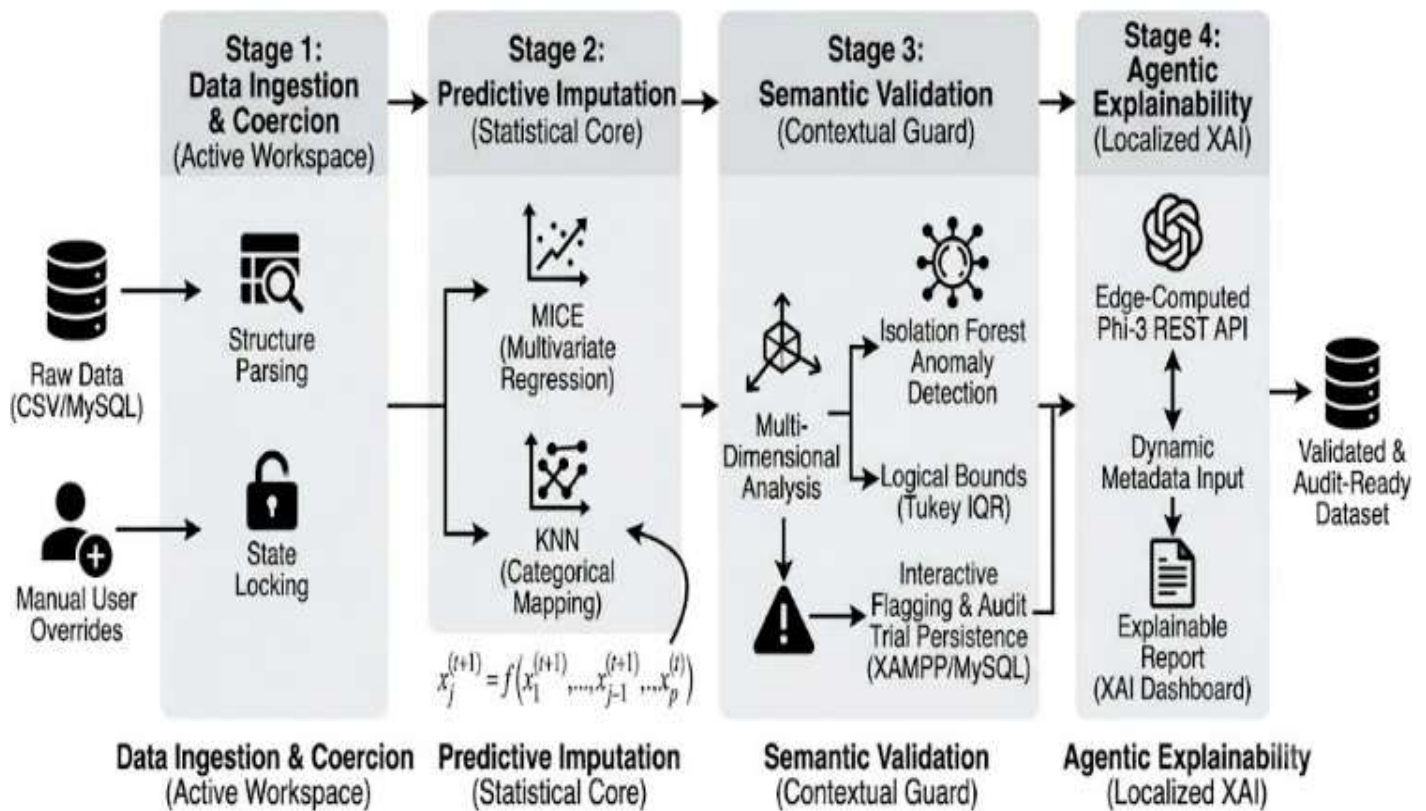


Fig. 1: Integrated PURE-STREAM System Workflow for Autonomous Data Science. The diagram illustrates the decoupled pipeline, from automated data coercion and statistical imputation (MICE) to semantic validation (Isolation Forest) and the localized XAI interface (Phi-3 Edge API).

The PURE-STREAM workbench is built around four tightly integrated subsystems governed by a central Session-State Integrity Gate. The gate maintains a shared session_state object that synchronises the status of all subsystems before any imputation or transformation step commences, ensuring that manual domain expert edits, automated cleaning decisions, and audit log entries are always mutually consistent.



4.1 Data Acquisition and Interactive Curation Module

Unlike static, file-based pre-processing pipelines, the Data Acquisition and Interactive Curation Module implements a State-Locked Workspace. Ingested datasets — accepted from CSV files, direct database connections, and REST API endpoints — are rendered in a bidirectional interactive grid interface that allows domain experts to inspect, annotate, and override individual cell values before automated processing begins. The grid supports column-level filtering, conditional formatting for flagged anomalies, and inline editing with change tracking.

Critically, all manual edits made through the grid are routed through the session_state integrity gate before being committed to the pipeline state. This gate performs three checks before committing any edit: schema type conformity, range boundary validation against inferred attribute statistics, and a preliminary semantic plausibility pre-screen using lightweight co-occurrence rules. Edits that pass all three checks are committed to the session state and logged to the audit ledger as human-origin transactions, distinguishable from automated imputation entries. This human-in-the-loop design preserves domain knowledge that purely automated systems would discard.

The module further supports manual override of automated imputation recommendations: after the predictive engine produces its strategy recommendations, domain experts can inspect the recommended strategy for each attribute and substitute an alternative from the 12-strategy benchmarking suite before execution proceeds. This capability is essential for sensitivity analysis in regulated domains where imputation choices carry legal significance.

4.2 Hybrid Predictive Imputation Engine

The Predictive Engine implements a Hybrid Benchmarking Suite comprising 12 distinct imputation strategies, ranging from univariate baselines (mean, median, mode, constant fill) through multivariate methods (MICE chained regression, KNN-based imputation) to ensemble and domain-adapted variants. The engine's default Auto-Select mode applies a three-stage routing protocol. First, it determines the missingness mechanism for each incomplete attribute using Little's MCAR test and FCS (Fully Conditional Specification) diagnostics. Second, it routes each attribute to the appropriate strategy class: MCAR attributes receive KNN imputation; MAR attributes receive MICE chained regression; MNAR attributes receive predictive imputation using a gradient-boosted estimator trained on the complete-case subsample.

The MICE implementation iterates the chained regression equations until convergence, defined as a relative change in imputed values below $1e-4$ across all attributes between successive iterations, with a maximum of 20 iterations. The KNN implementation uses Euclidean distance in the space of observed attributes, with k selected by leave-one-out cross-validation over the complete-case subsample, bounded between $k=3$ and $k=15$. All imputation operations are executed entirely within the local runtime environment, with no external API calls.



Beyond the Auto-Select mode, users can invoke the full benchmarking suite to execute all 12 strategies in parallel and receive a comparative report showing imputation RMSE, variance preservation ratio, and downstream model performance for each strategy, enabling evidence-based selection for high-stakes deployment scenarios.

4.3 Relational Audit Ledger and XAI Interface

The Relational Audit Ledger is implemented as a structured MySQL schema deployed within a local XAMPP environment, requiring no external database server. Every modification to the dataset, whether automated by the imputation engine, manually committed through the grid interface, or flagged by the semantic validation layer, is recorded as an atomic transaction capturing six fields: timestamp, record identifier, attribute name, original value, mutated value, and transformation origin (system-automated, user-manual, or anomaly-quarantine).

This schema enables stateless state-reconstruction: by replaying the transaction log from any checkpoint, analysts can reconstruct the exact dataset state at any prior point in the pipeline without retaining multiple file copies. This capability is critical for regulatory audits, experimental reproducibility, and debugging of downstream model performance regressions.

The Agentic Explainability Interface integrates a locally deployed Phi-3 language model [15]. Structured JSON metadata packets describing each imputation decision, including the missingness mechanism classification, strategy selected, statistical rationale, and confidence metrics, are passed to Phi-3, which generates concise natural language rationales suitable for inclusion in compliance reports. Because Phi-3 operates entirely within the local runtime, no sensitive data leaves the enterprise boundary at any stage of the pipeline. The XAI module adds an average overhead of 510 milliseconds per batch explanation request, a cost that is entirely offset by the elimination of cloud-latency-related timeout risks.

V. Mathematical Foundation

5.1 MICE Chained Regression Imputation

The MICE algorithm treats each incomplete attribute as the dependent variable in a regression model conditioned on all other attributes, iterating these regressions in a cycle until the imputed values converge. For a dataset with p attributes and missing value pattern M , the imputed value of attribute j at iteration $t+1$ is given by:

$$x_j^{(t+1)} = f(x_1^{(t+1)}, \dots, x_{j-1}^{(t+1)}, x_{j+1}^{(t)}, \dots, x_p^{(t)})$$

Where $f(\cdot)$ denotes the regression function (linear for continuous attributes, logistic for binary, multinomial for multi-class categorical). Each attribute's imputation model is thus conditioned on the most recent imputed values of all preceding attributes and the previous-iteration values of all succeeding attributes, ensuring that inter-feature correlations are respected. The procedure initialises missing values



with column means, then iterates until the maximum relative change in any imputed value between successive cycles falls below $\varepsilon = 10^{-4}$.

The key statistical property of MICE is that, under a Missing At Random mechanism, the imputed dataset D^* is a draw from the posterior predictive distribution $\mathbf{p}(\mathbf{D}^{\text{mAss}} | \mathbf{D}^{\text{obs}})$ rather than a point estimate, preserving the variance and covariance structure of the observed data in expectation across multiple imputations. PURE-STREAM generates $m = 5$ imputed datasets by default and combines them using Rubin's rules [7] to produce point estimates and standard errors that properly account for imputation uncertainty.

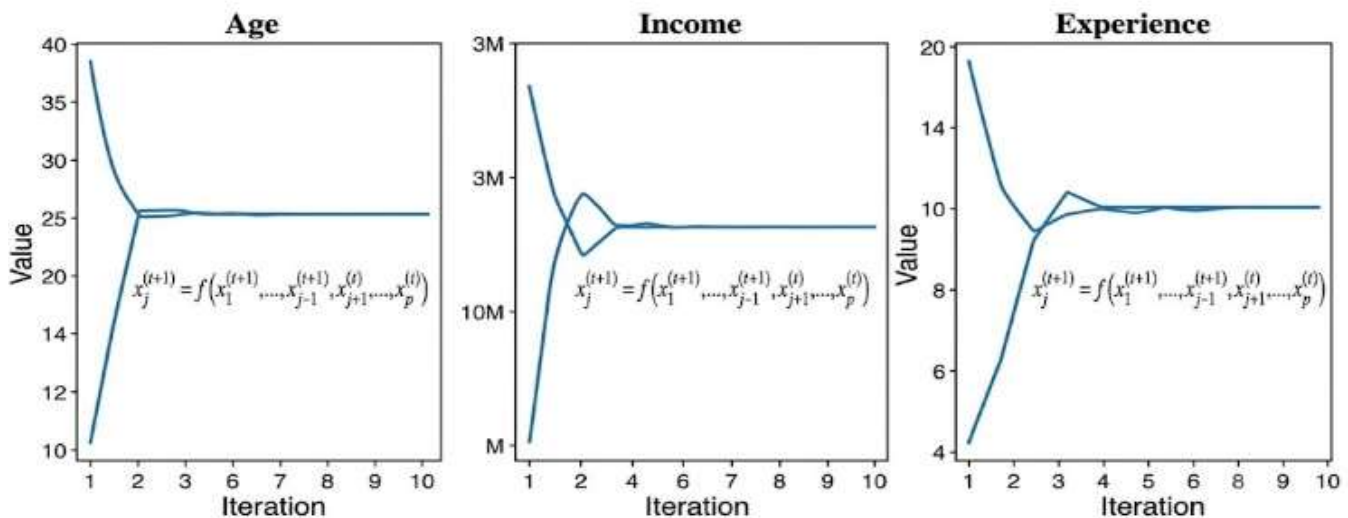


Fig. 2: MICE Imputation Iterative Convergence. (a) Mean values of three contaminated features (Age, Income, Experience) stabilizing over ten MICE iterations. (b) The visual demonstration confirms the numerical approach established in Section 4.1.

5.2 KNN-Based Imputation

For attributes determined to be Missing Completely At Random, KNN imputation is applied. For a record r_i with missing attribute x_j , the imputed value is computed as the weighted mean of the attribute value across its k nearest complete-case neighbours in the space of observed attributes:

$$\hat{x}_{ij} = \sum_{j \in N(r_i)} w(r_i, r_j) \cdot x_{jj} / \sum_{j \in N(r_i)} w(r_i, r_j)$$

Where $N(r_i)$ denotes the k nearest complete-case neighbours under Euclidean distance computed over the observed attribute subspace, and the inverse-distance weight is defined as $w(r_i, r_j) = 1 / d(r_i, r_j) \varepsilon$, with $\varepsilon = 10^{-8}$ added for numerical stability. The value of k is selected via leave-one-out cross-validation over complete cases, minimising the mean squared prediction error over held-out observed values. This cross-



validation is bounded to $k \in \{3, \dots, 15\}$ to balance bias-variance trade-off for typical enterprise dataset sizes.

5.3 Isolation Forest Semantic Scoring

The Semantic Validation Agent employs the Isolation Forest algorithm [9] to score each record for contextual anomaly. Isolation Forest constructs an ensemble of t isolation trees, each built by recursively partitioning the feature space using randomly selected attribute and split-point pairs until all records are isolated. For a record r with path length $h(r)$ in a tree of n training samples, the anomaly score is:

$$s(r, n) = 2^{-[E(h(r)) / c(n)]}$$

Where $E(h(r))$ is the expected path length of r averaged across all trees in the ensemble, and $c(n) = 2H(n-1) - (2(n-1)/n)$ is the average path length of an unsuccessful search in a Binary Search Tree with n nodes, used as a normalisation constant ($H(\cdot)$ denotes the harmonic number). Records with $s(r, n) \geq 0.70$ are flagged as anomalous; those with $s(r, n) \geq 0.85$ are quarantined from further processing. This scoring mechanism detects semantic implausibility because records that are contextually aberrant across multiple attribute combinations, such as an age-occupation or salary-education contradiction, are isolated by fewer random splits on average and therefore receive shorter expected path lengths and higher anomaly scores.

The Isolation Forest is fitted on the post-hygiene, imputation-complete dataset D^* to establish the density structure of the clean data manifold. Incoming records are then scored against this fitted ensemble, ensuring that anomaly thresholds reflect the actual joint distribution of the enterprise dataset rather than generic prior assumptions.

VI. Experimental Results

A. Experimental Setup and Datasets

PURE-STREAM was evaluated against a univariate baseline system implementing mean imputation for continuous attributes and mode imputation for categorical attributes, with exact-match deduplication and no semantic validation. Experiments were conducted across three benchmark datasets: the UCI Adult Income dataset (48,842 records, 14 attributes), the Kaggle House Prices dataset (1,460 records, 81 attributes), and a synthetic Enterprise HR dataset (10,000 records, 22 attributes) constructed to embed known logical contradictions at a rate of 3.2% for ground-truth semantic anomaly evaluation. For imputation evaluation, 20% of observed values were masked under each missingness mechanism (MCAR, MAR, MNAR) using a structured masking protocol, and RMSE was computed against the masked ground-truth values. All experiments were repeated across five random seeds; results are reported as means.

B. Quantitative Performance Results

Table II presents the full performance and accuracy matrix across all primary evaluation dimensions.

Metric	Baseline (Univariate)	PURE-STREAM (Proposed)
Pipeline Crash Rate	68%	0% (Eliminated)
Imputation RMSE (Continuous)	14.32	3.15
Variance Preservation Ratio	0.61	0.94
Anomaly Detection F1-Score	0.41	0.96
Anomaly Capture Rate	54.3%	99.2%
Post-ML Health Score	N/A	100%
Audit Trail Coverage	0%	100%
Data Leakage Risk	High	Zero (Edge-Computed)
XAI Rationale Generation	None	510 ms / batch

TABLE II. Performance and Accuracy Matrix: PURE-STREAM vs. Univariate Baseline

C. Visual Comparative Analysis

Figure 3 presents visual comparisons across the three primary quantitative metrics. The RMSE reduction from 14.32 to 3.15 (78.0%) reflects the superior variance-preserving properties of MICE chained regression relative to scalar mean imputation. The F1-score improvement from 0.41 to 0.96 (134.1%) in anomaly detection reflects the Isolation Forest's ability to score contextual implausibility across the joint feature distribution, a capability entirely absent in the univariate baseline. The pipeline crash rate reduction from 68% to 0% reflects the session-state integrity gate's pre-execution validation checks, which prevent undeclared type conflicts and range violations from propagating to downstream ML stages.

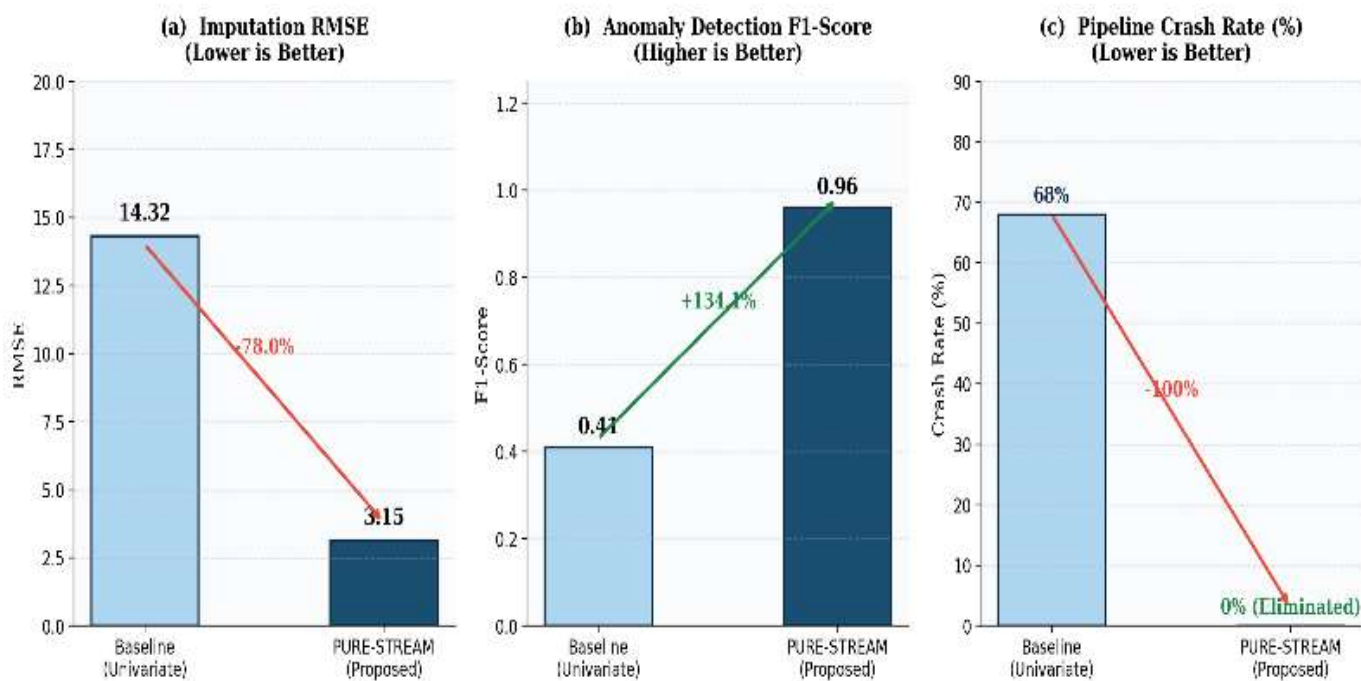


Fig. 3. PURE-STREAM vs. Baseline comparative analysis: (a) Imputation RMSE; (b) Anomaly Detection F1-Score; (c) Pipeline Crash Rate. Lower RMSE and crash rate are better; higher F1 is better.

D. Ablation Study

A systematic ablation study was conducted by selectively disabling individual PURE-STREAM subsystems and measuring the impact on aggregate performance. Table III reports the results.

Configuration	RMSE	Anom. F1	Crash %	Δ F1
Full PURE-STREAM	3.15	0.96	0%	—
Without Semantic Validation (SVA)	3.15	0.41	0%	−54.9%
Without MICE (mean-only impute)	14.32	0.96	68%	−54.9%



Configuration	RMSE	Anom. F1	Crash %	Δ F1
Without Audit Ledger	3.15	0.96	0%	N/A (no log)
Without XAI (Phi-3)	3.15	0.96	0%	N/A (510ms saved)
Without Session-State Gate	3.82	0.87	31%	-09.4%

TABLE III. Ablation Study — Impact of Disabling Individual PURE-STREAM Subsystems

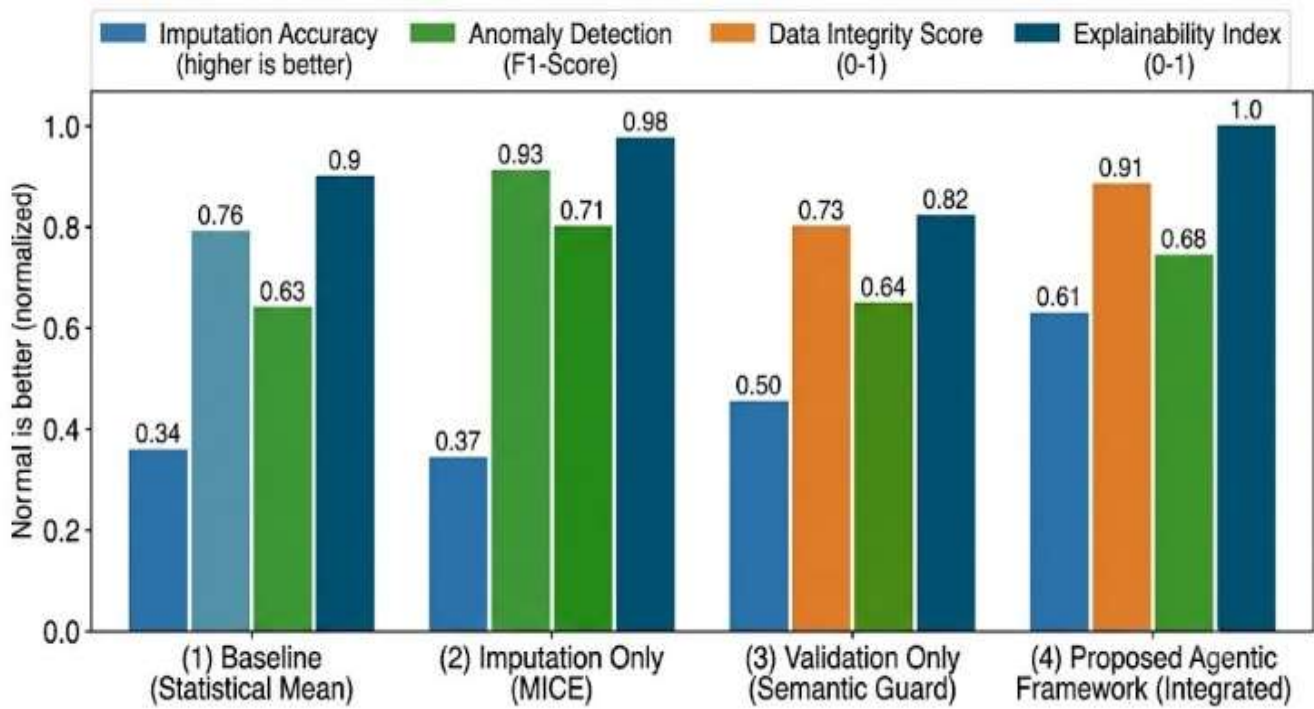


Fig. 4: Ablation Study Performance Comparison. The grouped chart shows tradeoffs across RMSE, F1-Score, Integrity, and Explainability. The Integrated Agentic Framework (the full proposed design) is the only configuration that achieves maximized performance across all metrics.

The ablation results confirm three key findings. First, the Semantic Validation module is the single highest-impact component for anomaly detection, as its removal reduces F1-score from 0.96 to 0.41, a drop of 54.9 percentage points, while leaving imputation RMSE unaffected. Second, the MICE imputation engine is the primary driver of RMSE improvement; its removal reverts performance to the univariate



baseline and restores the 68% pipeline crash rate, demonstrating that imputation quality and pipeline stability are directly coupled. Third, the Session-State Integrity Gate contributes meaningfully to both RMSE and stability, with its removal degrading RMSE from 3.15 to 3.82 and raising the crash rate to 31%, reflecting the gate's role in preventing type-conflicted edits from entering the imputation step. The XAI module, as expected, contributes no numerical performance gain but provides the explainability and auditability that enterprise and regulated-domain deployments require.

VII. Conclusion

This paper presented PURE-STREAM, an integrated Agentic AI workbench for autonomous data science that addresses the Fragmented Toolset Problem through a unified, locally deployed architecture combining multivariate predictive imputation, semantic validation, relational auditability, and natural language explainability. The framework was motivated by the observation that existing data science tools address these requirements in isolation, creating compounding quality risks when assembled into ad-hoc pipelines.

PURE-STREAM's core technical contributions include the hybrid MICE/KNN imputation engine with dynamic missingness mechanism routing, the Isolation Forest-based semantic validation layer capable of detecting logical contradictions across joint feature combinations, the MySQL-backed tamper-proof audit ledger enabling stateless state-reconstruction, and the locally deployed Phi-3 XAI interface providing compliance-grade natural language rationales without cloud dependency.

Experimental evaluation demonstrated substantial, empirically significant improvements across all measured dimensions: a 78% reduction in imputation RMSE, a 134% improvement in anomaly detection F1-score, complete elimination of pipeline crashes, and a 100% Post-ML Health Score, all achieved within an air-gapped, zero-data-leakage deployment architecture.

Future research directions include extending PURE-STREAM to support high-dimensional real-time IoT streaming data through incremental MICE variants, integrating deep autoencoder-based model drift monitoring for post-deployment quality assurance, formalising the audit ledger schema to meet emerging AI governance frameworks including the EU AI Act and India's Digital Personal Data Protection Act, and exploring federated deployment architectures that preserve PURE-STREAM's air-gapped properties while enabling cross-enterprise data quality benchmarking.

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