JoinBoost: Grow Trees Over Normalized Data Using Only SQL

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ABSTRACT

Although dominant for tabular data, ML libraries that train tree models over normalized databases (e.g., LightGBM, XGBoost) require the data to be denormalized as a single table, materialized, and exported. This process is not scalable, slow, and poses security risks. In-DB ML aims to train models within DBMSes to avoid data movement and provide data governance. Rather than modify a DBMS to support In-DB ML, is it possible to offer competitive tree training performance to specialized ML libraries...with only SQL?

We present JoinBoost, a Python library that rewrites tree training algorithms over normalized databases into pure SQL queries. It is portable to any DBMS, offers competitive performance on fast DBMSes, and is scalable to the capabilities of the underlying DBMS. JoinBoost extends prior work on factorized learning techniques from both algorithmic and systems perspectives. Prior work was limited to training individual decision trees, and performed work sharing when evaluating a single node split. We first show that there are considerable work-sharing opportunities between nodes as well, and then extend support to gradient boosting, which trains a sequence of trees over residuals. The key challenge is to update the Y variables to the new residual *without materializing the join result.* Although this view update problem is generally ambiguous, we identify conditions for tree models where this is correct. On the systems side, residual updates are the major performance bottleneck, and so we study support in existing DBMSes. We find that copy-on-write semantics are sufficient for fast updates, and validate this with two implementations using DuckDB. Our experiment shows that JoinBoost is 3× (1.1×) faster for random forests (gradient boosting) compared to LightGBM, and over an order magnitude faster than state-of-the-art In-DB ML systems. Further, JoinBoost scales well beyond LightGBM in terms of the # features, DB size, and join graph complexity (galaxy schemas).

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1 INTRODUCTION

Tree-based models—ranging from decision trees, random forests, and gradient boosting—are recursive space-partitioning algorithms used for classification and regression [50]. In contrast to the popular neural network models, tree models remain the most effective [32] and popular models for tabular datasets. For instance, random forests and gradient boosting were rated the most popular ML model from 2019 to 2021 on Kaggle [7]. In response, the ML community has developed optimized tree-training libraries, such as LightGBM [42] and XGBoost [21], that offer easy-to-use API, excellent single-node performance, and can run on distributed frameworks like Spark [73] or Dask [63].

In practice, however, almost all tabular datasets are normalized and stored in a DBMS. Using ML libraries introduces performance, usability, and privacy drawbacks. First, the libraries expect a single (typically CSV) training dataset. Thus, the developer must denormalize the database into a “wide table” $R_{\bowtie}$, materialize and export $R_{\bowtie}$, and load it into the library. The join materialization cost is prohibitive for all but the simplest schemas and smallest databases—the $1.2GB$ IMDB dataset (Figure 4) is well over $1TB$ when fully materialized due to N-to-N relationships. Second, managing the exported data as well as the separate execution frameworks adds considerable operational complexity and is error-prone [67, 69]. Third, exporting sensitive data can raise privacy concerns [2].

Ideally, we would “move compute to the data” and train tree-based models directly within the DBMS. This would let developers manage the entire data lifecycle—preparation, cleaning, analysis, and modeling—within a single DBMS, and benefit from the DBMSes’ excellent security, performance, and scalability. To be broadly useful, we believe an initial In-DB solution should meet three criteria: (C1) be easily portable to any DBMS by translating ML algorithms into vanilla SQL queries, (C2) offer training performance comparable with the SOTA ML libraries (e.g., LightGBM), and (C3) scale to massive data warehouse sizes and complexity. Unfortunately, these criteria are often in tension. Common wisdom and prior results suggest that training tree models via SQL queries is portable but notoriously slow [33, 71, 73] as DBMSes do not employ model-specific optimizations. However, specialized optimizations [21, 42] or GPU acceleration [15, 34, 56] achieve competitive performance at the expense of portability to general DBMSes.

To optimize training over normalized schemas common in DBMSes, recent works in factorized ML [43, 44, 53, 64] avoid materializing joins by treating ML as semi-ring aggregation queries over the join graph; the aggregations can then be pushed through the joins. This approach potentially provides DBMSes with an edge over conventional ML libraries that face significant expenses for join materialization and export during training. Thus, it is intriguing to investigate the potential of training tree models in DBMSes using vanilla SQL, with the factorized ML optimizations.

Nevertheless, the current applicability of factorized ML to tree-based models is restricted due to both algorithmic and system-related limitations. LMFAO [64] describes a factorized algorithm that is limited to decision trees, and does not support the widely used gradient boosting models. It rewrites the tree node split algorithm into a batch of group-by aggregations, and uses multi-query optimization to share work between the aggregations. Unfortunately, it does not support the residual updates needed for gradient boosting models. Even for single decision tree training, LMFAO fails to exploit considerable work-sharing between parent-child tree nodes. Finally, LMFAO lacks portability because its performance is tied to a compilation engine specially designed for their batch-wise query execution. In our experiments, despite using an off-the-shelf DBMS (DuckDB [61]), we train decision trees 1.9× faster than LMFAO.

To this end, we present JoinBoost[1], the first In-DB ML system for tree-models that meets criteria C1-3. JoinBoost is a Python library that supports decision trees, random forests, and gradient boosting. JoinBoost mirrors LightGBM's training API, trains and returns identical models to LightGBM, and is portable to any DBMS or data frame library[2]. **On a single node, JoinBoost trains a gradient boosting model with 100 trees** 1.1× **faster than LightGBM, and is** 3× **faster for random forests. Moreover, JoinBoost easily scales in the # of features, join graph complexity, and dataset size (TPC-DS SF=1000 in Section 6.2), whereas LightGBM runs out of memory.**

There are two major challenges towards training gradient boosting models over normalized databases. The first is to design the algorithms for factorized gradient boosting. Each boosting iteration trains a decision tree on the *residuals* from the previous tree, so it needs to update the target Y attribute to the residual in the denormalized table $R_{\bowtie}$; however, $R_{\bowtie}$ *is not materialized in factorized ML*, and such view update are in general ambiguous [22]. To address this, we logically rewrite residual updates over $R_{\bowtie}$ into a join between $R_{\bowtie}$ and an *update relation* U, which contains an attribute for the residual and all the attributes referenced in the decision tree. This can be achieved by leveraging the unique characteristics of tree-based models, where the leaves form a non-overlapping partition of the training data.

The second is the system optimizations. We reveal residual updates as the main bottleneck for gradient boosting in current DBMSes: Residual updates require sequential writes to all values in a column. However, we find this operator is not efficient in existing DBMSes due to a combination of columnar compression, write-ahead-log, and concurrency control; these are fundamental to DBMSes but not necessary for gradient boosting. To match the performance of LightGBM, update performance needs to be similar to a parallelized write to an in-memory byte array. Columnar DBMSes can in theory already do this: by simply creating a new column of residual values and adding it as a projection [70], or by using copy-on-write semantics. We emulate this using DuckDB Pandas API [8]: DuckDB performs joins and aggregations, and Pandas updates residual (as a dataframe column). This improves updates by ∼15×, and makes gradient boosting competitive (within 2× to LightGBM). One drawback is that aggregations are slowed by ∼1.6× due to DuckDB-Pandas interop overhead. To study the full potential, we further modify DuckDB internals (<100 LOC) to support a schema update that swaps the existing residual column with the newly created one; with this, JoinBoost is 1.1× faster than LightGBM.

To summarize, our contributions are as follows:

- We improve prior batch optimization [64] by sharing intermediates (materialized as tables in DBMSes) across batches (tree nodes); this improves decision trees and random forests by 3×.
- We extend factorized ML to gradient boosting by enabling residual updates (for boosting) on non-materialized joins.
- We reveal residual updates as the bottleneck for current DBMSes. We optimize this both logically and physically, without and with minor DBMS modifications, to achieve competitive performance.
- We conduct extensive experiments of JoinBoost on different DBMS backends (local and cloud), using datasets with varying feature numbers, sizes (TPC-DS with SF 10⟶1000), and join graph complexity (galaxy schemas), against SOTA ML libraries (LightGBM,XGBoost,Sklearn) and In-DB systems (LMFAO,MADLib).

Note: The paper is self-contained and references to appendices can be skipped, or can be found in the technical report [9].

2 RELATED WORK

Tree-based ML Libraries. Random forest [17] and gradient boosting [29] are the de-facto ensemble models supported by almost all standard ML libraries including Sklearn [58], TensorFlow [11] and Keras [23]. The state-of-the-art Tree-based ML libraries are LightGBM [42] and XGBoost [21]. Both specialize in only Tree-based models, are heavily optimized and outperform the rest according to previous benchmarks [14]. According to Kaggle 2021 surveys [7], among all the commonly used ML libraries, XGBoost and LightGBM are ranked 4th and 6th respectively for popularity (while all the top 3 also support Tree-based ML). However, none of them apply factorized ML for normalized datasets.

Tree-based models are well-studied, backed by theoretic guarantees [48, 59], and have a large number of variants. To better handle categorical attributes, CatBoost [60] proposes novel permutation-based statistics to encode categorical attributes. To support uncertainty estimation, NGBoost [26] proposes gradient boosting algorithms for probabilistic predictions. These works are complementary and JoinBoost could be extended to support these algorithms.

In-DB ML systems. Most in-DB ML works [27, 33, 71] focus on extending DBMSes (e.g., PostgreSQL for MADLib) to support linear algebra using UDFs and user-defined types. However, these are not needed for tree-based models that only rely on simple aggregations.

Other work optimizes ML training by leveraging specialized features (distributed execution [16, 38, 39, 45, 73] or GPU acceleration [15, 34, 47, 56]) of a specific DBMS. Although we focus on optimizing the single-node CPU setting via SQL rewrites, JoinBoost can run on any DBMS and benefit from its optimizer and executor. For instance, Section 6.2 scales decision tree training on TPC-DS SF=1000 using a cloud DBMS. We leave further DBMS-, data-, and model-specific optimizations to future work.

[1]Open-sourced at https://anonymous.4open.science/r/JoinBoost-FBC4
[2]Currently supports DuckDB, MariaDB, MonetDB, MySQL, Oracle, PostgreSQL, Spark-SQL, SQLite, SQLServer, Redshift, Azure Synapse Analytics, BigQuery, and Pandas.

In practice, cloud vendors (Azure [1], Redshift [4], BigQuery [49], Snowflake [3]) offer SQL syntax to train tree models. Under the covers, however, they still materialize and export join results to an external library (`LightGBM` or `XGBoost`). Thus, we do not consider them in-DB ML from a performance or portability standpoint.

Factorized ML systems. Factorized ML is optimized to train models over normalized databases. There are two classes. The first class translates ML models as aggregations over an appropriately designed semi-ring, and pushes aggregations through joins to achieve asymptotically lower time complexity. They support many popular models (ridge regression [64], SVM [43], factorization machine [64]), and approximate others (k-means [25], GLM [36]). Of these, only `LMFAO` [64] supports decision trees, albeit in a limited way (see Section 6.5). Further, most factorized ML works build specialized query optimizers and executors from scratch, which hinders portability (of the systems and performance wins) to existing DBMSes. `JoinBoost` extends factorized ML to tree models via vanilla SQL queries, and shows competitive performance with `LightGBM`.

The second class factorizes linear algebra operations over joins [20, 46, 74] by carefully iterating over the tables, caching intermediates, and combining their results. Compared to the first class, these works support any model that can be formulated as linear algebra statements, such as K-means and GLM (without approximation). However, they only reduce space and not time complexity, and are worse than naive denormlization when the data fits in memory [46].

3 BACKGROUND

In this section, we provide the background of factorized query execution, and tree-based models.

3.1 Annotated Relations and Message Passing

This section provides an overview of annotated relations and message passing fundamental to factorized query execution [13, 54].

Data Model. We use the traditional relational data model with the following notations: Given relation R, let uppercase A be an attribute, $dom(A)$ be its domain, $S_R = [A_1, \cdots, A_n]$ be its schema, $t \in R$ as a tuple of R, and $t[A]$ be tuple t's value of attribute A. Throughout examples, we also include the schema in the square bracket followed by the relation $R[A_1, \cdots, A_n]$ to help understanding. The domain of R is then the Cartesian product of attribute domains $dom(R) = dom(A_1) \times \cdots \times dom(A_n)$.

Annotated Relations. The annotated relational model [31, 40, 52] maps each $t \in R$ to a commutative semi-ring $(D, +, \times, 0, 1)$, where D is a set, $+$ and $\times$ are commutative binary operators closed over D, and $0/1$ are the zero/unit elements. These annotations form the basis of provenance semi-rings [31], and are amenable query optimizations based on algebraic manipulation. Different semi-ring definitions support different aggregation functions, ranging from standard statistical functions to ML models. For instance, the natural numbers semi-ring $(\mathbb{N}, +, \times, 0, 1)$ allows for integer addition and multiplication, and supports the *COUNT* aggregate. For an annotated relation R, let $R(t)$ denote tuple t's annotation.

Semi-ring Aggregation Query. Semi-ring aggregation queries can now be re-expressed over annotated relations by translating group-by (general projection) and join operations respectively into $+$ and $\times$ operations over the semi-ring annotations:

$$(\gamma_{\mathbf{A}} R)(t) = \sum \{R(t_1) | \; t_1 \in R, t = \pi_{\mathbf{A}}(t_1)\} \tag{1}$$

$$(R \bowtie T)(t) = R(\pi_{S_R}(t)) \times T(\pi_{S_T}(t)) \tag{2}$$

(1) The annotation for each group-by result in $\gamma_{\mathbf{A}} R$ sums the annotations of all tuples in its input group. (2) The annotation of each join result in $R \bowtie T$ is the product of semi-ring annotations from its contributing tuples in R and T.

Aggregation Pushdown. The key optimization in factorized query execution [13, 65] is to distribute aggregations (additions) through joins (multiplications).

Consider $\gamma_D(R[A, B] \bowtie S[B, C] \bowtie T[C, D])$. The naive execution first materializes the join result and then computes the aggregation. This costs $O(n^3)$ where n is each relation's cardinality. An alternative evaluation could apply aggregation (addition) to R before joining (multiplication) with S, aggregate again before joining with T, and then apply a final aggregation. The largest intermediate result, and thus the join complexity, is now $O(n)$.

$$\gamma_D(\gamma_C((\gamma_B R[A, B]) \bowtie S[B, C]) \bowtie T[C, D])$$

Message Passing. Given a join graph, the above optimization can be viewed as *Message Passing* [57]. While *Message Passing* supports general SPJA queries [35], it is sufficient for tree models to restrict ourselves to SPJA queries with zero (γ) or one (γ_A) group-by attribute. Message passing works as follows:

Message passing operates over a tree that spans the join graph. For the root, we can pick any relation (taking cost models into account) that contains the grouping attribute. Then we direct all the edges of the join graph toward the root to form a tree[3].

Starting from the leaf, we send messages along its path to the root. Each message is computed as: (1) Join the relation with all incoming messages from children relations, if any. This blocks until all children have emitted messages. Then (2) let $\mathbb{A}$ be the attributes in the current relation that are also contained in the remaining relations in the path to the root. Compute $\gamma_{\mathbb{A}}$ over the previous join result, and emit the result to the parent relation.

Consider again $\gamma_D(R[A, B] \bowtie S[B, C] \bowtie T[C, D])$ along the join graph: $R - S - T$. If we choose T as the root, then the directed join graph is $R \longrightarrow S \longrightarrow T$ and the messages are:

$$m_{R \to S} = \gamma_B R[A, B], \qquad m_{S \to T} = \gamma_C(m_{R \to S} \bowtie S[B, C])$$

Once the root receives and joins with all messages, it performs **absorption**, which simply applies the final group-by: $\gamma_D(m_{S \to T} \bowtie T[C, D])$. In some cases, the aggregate result is already part of the semi-ring (e.g., *COUNT* and the natural numbers semi-ring); in other cases, such as tree-based models, the semi-ring decomposes the training metric into their constituent statistics, so we combine them in the final annotation to restore the metric (see next section).

3.2 Tree-based Models

In this section, we describe the traditional tree-based models. The algorithms are based on CART [18], and its extensions (e.g., bagging and boosting) follow standard ML textbooks [50].

[3]The algorithm applies to acyclic join graphs. Cyclic join graphs can be pre-joined into acyclic join graphs using standard hypertree decomposition [13, 41].

Semi-ring	Zero/One	Operator	Lift
Variance $(\mathbf{Z}, \mathbf{R}, \mathbf{R})$	**0:** $(0, 0, 0)$ **1:** $(1, 0, 0)$	$(c_1, s_1, q_1) + (c_2, s_2, q_2) = (c_1 + c_2, s_1 + s_2, q_1 + q_2)$ $(c_1, s_1, q_1) \times (c_2, s_2, q_2) = (c_1c_2, s_1c_2 + s_2c_1, q_1c_2 + q_2c_1 + 2s_1s_2)$	$(1, y, y^2)$
Class Count $(\mathbf{Z}, \mathbf{Z}, ..., \mathbf{Z})$	**0:** $(0, ..., 0)$ **1:** $(1, ..., 0)$	$(c_1, c_1^1, ..., c_1^k) + (c_2, c_2^1, ..., c_2^k) = (c_1 + c_2, c_1^1 + c_2^1, ..., c_1^k + c_2^k)$ $(c_1, c_1^1, ..., c_1^k) \times (c_2, c_2^1, ..., c_2^k) = (c_1c_2, c_1^1c_2 + c_1c_2^1, ..., c_1^kc_2 + c_1c_2^k)$	$(1, 0, ..., c^y = 1, ..., 0)$

Table 1: Example commutative semi-rings for decision trees. Variance semi-ring supports regression criteria like Reduction in Variance; Class Count semi-ring supports classification criteria like Gini Impurity, Information Gain, and Chi-Square.

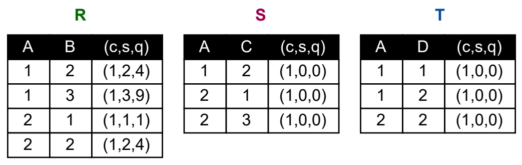
Decision Tree. Decision Tree is a function that maps (predicts) target variable Y from a set of features $\mathbf{X}$. Internally, decision tree stores a tree structure where each edge is associated with a predicate σ over single attribute $X \in \mathbf{X}$, and each leaf is associated with some prediction value $p \in dom(Y)$. Decision Tree makes prediction for $t \in Dom(\mathbf{X})$ by traversing the tree edges where t satisfies the edge predicate till the leaf and outputting the leaf prediction. We represent decision tree as a set of selection prediction pairs $\{(l.\sigma, l.p)\}$ for each tree leaf l, where $l.\sigma$ is the conjunction of predicates along the path from the root to l and $l.p$ is leaf prediction. The set of $l.\sigma$ in decision tree are mutually exclusive and collectively exhaustive in $Dom(\mathbf{X})$.

Given relation R with a set of features $\mathbf{X}$ and target variable Y where $\mathbf{X} \cup \{Y\} \subseteq S_R$, the training process of decision tree over R recursively splits R to minimize some criterion $c(\cdot)$. Particularly, the most popular criteria are *Variance* for regression, and *Gini Impurity, Entropy and Chi-Square* for classification. The splits for numerical attribute $A \in \mathbf{X}$ is inequality-based $(\sigma_{A>v}, \bar{\sigma}_{A \leq v})$, while the splits for categorical attribute A could be equality-based $(\sigma_{A=v}, \bar{\sigma}_{A \neq v})$ or set-based $(\sigma_{A \in V}, \bar{\sigma}_{A \notin V})$ using greedy algorithm [28]. Given the criteria $c(\cdot)$ and split σ, the reduction of criteria after the split is $c(R) - (c(\sigma(R)) + c(\bar{\sigma}(R)))$. Tree growth could be depth-wise or best-first [68]. Depth-wise growth splits the tree node with the least depth, and best-first growth splits the tree node greedily with the largest criteria reduction. Finally, each leaf prediction is the average Y for regression or mode Y for classification.

Bagging and Boosting. Large deep decision trees easily overfit, so ensemble techniques like bagging and boosting combine many weak learners (e.g., decision trees with smaller depth or leaves) to produce a more robust model. The most popular tree-based ensemble models are random forest [17] (bagging) and gradient boosting [29] (boosting). Random forest trains multiple decision trees over samples of R independently in parallel and aggregates their predictions (e.g., average) for the final prediction; Gradient boosting sequentially trains the next decision tree based on gradients of the criterion function with respect to the prediction from the previous decision trees.

3.3 Factorized Learning for Tree-Stumps

We now introduce tree models over joins, and how factorized execution can accelerate their training. We consider a database with a set of relations $\mathcal{R} = \{R_1, R_2, ..., R_n\}$, we want to train a tree-based model over $R_{\bowtie} = R_1 \bowtie R_2 ... \bowtie R_n$ with a set of features $\mathbf{X}$ and target variable Y. Let R_Y be the relation that contains Y (or pick one if Y is in many relations as a join key). To keep the text simple, we will assume natural join, set semantics, and the Variance split criteria; Appendix B describes extensions to theta and outer joins, bag semantics, and formula for classification semi-rings.



R

A	B	(c,s,q)
1	2	(1,2,4)
1	3	(1,3,9)
2	1	(1,1,1)
2	2	(1,2,4)

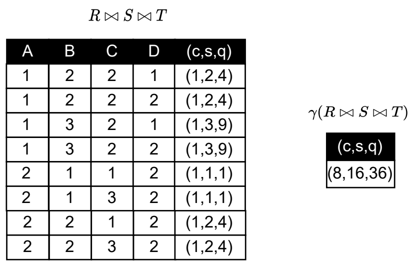
S

A	C	(c,s,q)
1	2	(1,0,0)
2	1	(1,0,0)
2	3	(1,0,0)

T

A	D	(c,s,q)
1	1	(1,0,0)
1	2	(1,0,0)
2	2	(1,0,0)

(a) Relations annotated with variance semi-ring, join graph $R - S - T$, target variable B and features C,D.



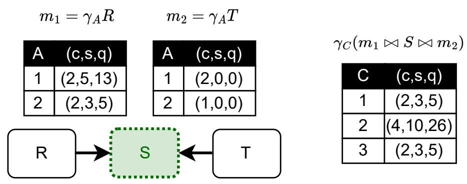
$R \bowtie S \bowtie T$

A	B	C	D	(c,s,q)
1	2	2	1	(1,2,4)
1	2	2	2	(1,2,4)
1	3	2	1	(1,3,9)
1	3	2	2	(1,3,9)
2	1	1	2	(1,1,1)
2	1	3	2	(1,1,1)
2	2	1	2	(1,2,4)
2	2	3	2	(1,2,4)

$\gamma(R \bowtie S \bowtie T)$

(c,s,q)
(8,16,36)

(b) Naive join $R_{\bowtie}$ and aggregation query $\gamma(R_{\bowtie})$.



$m_1 = \gamma_A R$

A	(c,s,q)
1	(2,5,13)
2	(2,3,5)

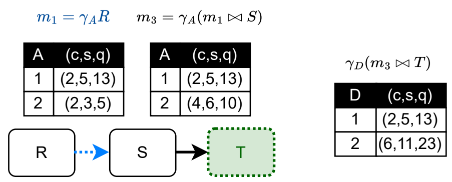
$m_2 = \gamma_A T$

A	(c,s,q)
1	(2,0,0)
2	(1,0,0)

$\gamma_C(m_1 \bowtie S \bowtie m_2)$

C	(c,s,q)
1	(2,3,5)
2	(4,10,26)
3	(2,3,5)

(c) Message passing for aggregation query $\gamma_C(R_{\bowtie})$. The root node is dotted in green.



$m_1 = \gamma_A R$

A	(c,s,q)
1	(2,5,13)
2	(2,3,5)

$m_3 = \gamma_A(m_1 \bowtie S)$

A	(c,s,q)
1	(2,5,13)
2	(4,6,10)

$\gamma_D(m_3 \bowtie T)$

D	(c,s,q)
1	(2,5,13)
2	(6,11,23)

(d) Message sharing between aggregation queries $\gamma_D(R_{\bowtie})$ and $\gamma_C(R_{\bowtie})$. The reusable message is dotted in blue.

Figure 1: Factorized decision stump training.

Factorized learning avoids materializing $R_{\bowtie}$ by expressing learning algorithms as semi-ring aggregation queries, and applying aggregation pushdown over join. Let us first describe semi-ring annotations for trees and then the training algorithms.

Tree Semi-rings. We now illustrate how to use variance semi-ring (Table 1) to compute the Variance criterion for regression trees.

Each semi-ring defines a $lift(\cdot)$ function [52] that annotates a base tuple with its appropriate semi-ring element. Variance semi-ring initially annotates each tuple $t \in R_Y$ with $R_Y(t) = (1, t[Y], t[Y]^2)$, and tuples from the remaining relations with the 1 element $(1, 0, 0)$. During message passing, the annotations are combined via + and

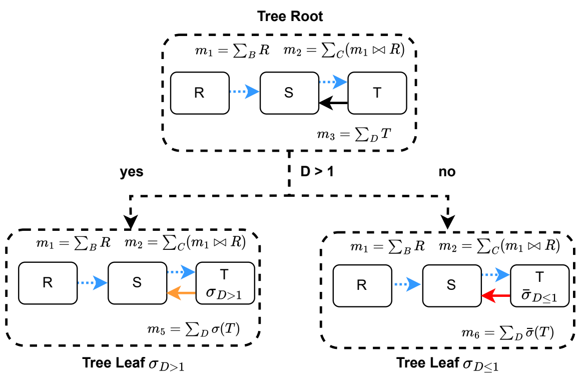

Tree Root
$m_1 = \sum_B R$ $m_2 = \sum_C (m_1 \bowtie R)$
R
S
T
$m_3 = \sum_D T$
yes
D > 1
no
$m_1 = \sum_B R$ $m_2 = \sum_C (m_1 \bowtie R)$
R
S
T $\sigma_{D>1}$
$m_5 = \sum_D \sigma(T)$
Tree Leaf $\sigma_{D>1}$
$m_1 = \sum_B R$ $m_2 = \sum_C (m_1 \bowtie R)$
R
S
T $\bar{\sigma}_{D\leq 1}$
$m_6 = \sum_D \bar{\sigma}(T)$
Tree Leaf $\sigma_{D\leq 1}$

Figure 2: Share computations between the parent node and children nodes after the split. Dotted messages are shared.

$\times$ as defined in Table 1. The aggregated semi-ring $\gamma(R_{\bowtie})$ is then a 3-tuple (C, S, Q) that represents the count, sum of Y, and the sum of squares of Y. The variance statistic is easily derivable from this aggregated semi-ring as $variance = Q - S^2/C$. In this way, any filter aggregation query over the join graph is expressible via message passing and lightweight post-processing.

Example 1. *Consider the database $\mathcal{R} = \{R, S, T\}$ in Figure 1a annotated with variance semi-ring, join graph $R - S - T$, and target variable $Y = B$. To compute the variance over $R_{\bowtie}$, the naive solution is to materialize $R_{\bowtie}$ (Figure 1b), then compute the variance $= 4$ over column B. We can compute $(C, S, Q) = \gamma(R \bowtie S \bowtie T) = (8, 16, 36)$ and variance $= Q - S^2/C = 36 - 16 \times 16/8 = 4$*

Factorized Decision Stump and Message Caching. Factorized learning relies on semi-ring aggregations to avoid materializing $R_{\bowtie}$. Training a decision stump requires computing the set of aggregation queries grouped by each feature: $\{\gamma_X(R_{\bowtie}) | X \in \mathbf{X}\}$. Executing each query via message passing one by one is wasteful because messages could be reused across queries. Consider the example in Figure 1:

Example 2. *Let $\mathbf{X} = \{C, D\}$, and suppose we first aggregate on C (Figure 1c). We choose S as the message passing root because it contains C; we then pass messages m_1 from R to S and m_2 from T to S, and absorb the messages into S. We then aggregate on D (Figure 1d). We choose T as the message passing root, pass m_1 from R to S, m_3 from S to T, and absorb into T. The two queries can reuse m_1.*

Recent work [35] shows that a simple caching scheme that materializes all messages between relations in the join graph (in both directions) is very effective in a range of analytical workloads. The factorized learning system `LMFAO` [64] also performs batch query optimization for splitting a single decision tree node. In the special case of decision trees, where each query groups by at most one feature, its optimizations are equivalent to this simple caching scheme. However, `LMFAO` focuses on optimizing the batch of queries for a single decision tree node at a time and misses work sharing opportunities across tree nodes. It also does not support residual updates necessary for gradient boosting.

4 FACTORIZED TREE-BASED MODELS

This section discusses the algorithms of factorized tree-based models. The key novelties are (1) for the decision tree, we share the computations to evaluate the split criteria for not only expanding a single tree node, but also *across levels in the tree*; (2) we study the problem of updating residuals, which opens up a new class of boosting models like gradient boosting.

4.1 Factorized Decision Tree

Previous factorized learning algorithms [44, 64] are based on batch optimization of aggregation queries, which is sufficient for models with closed-form solutions (e.g., ridge regression [64] or factorization machine [64]). However, the training process of tree-based models is iterative: the aggregation queries for the children nodes depend on the split (query results) from the parent node and can't batch ahead. As a result, previous algorithms have to either forgo the work-sharing opportunities between tree nodes, or batch the aggregation queries for all possible splits (which is impractical as the number of possible splits grows exponentially in tree depth).

Our key observation is that messages as intermediate results can not only be shared by the batch of aggregation queries within the tree node, but also among tree nodes. Consider the example:

Example 3. *Following Example 2, suppose the best split for the tree root is $\sigma_{D>1}$. The split applies $\sigma_{D>1}$ and $\bar{\sigma}_{D\leq 1}$ to relation T as it contains attribute D. After the split, there are two leaf nodes with relations: $\sigma(R_{\bowtie}) = R \bowtie S \bowtie \sigma(T)$ and $\bar{\sigma}(R_{\bowtie}) = R \bowtie S \bowtie \bar{\sigma}(T)$. Then, for each leaf node, we need to recursively compute the batch of aggregation queries and identify the next split through Message Passing. As illustrated in Figure 2, for both leaf nodes, all messages (in blue) along the path $R \rightarrow S \rightarrow T$ are the same as those from the tree root. We only need to recompute message $m_{T\rightarrow S}$ in each tree leaf. Note that the message $m_{S\rightarrow R}$ is skipped because R's attributes are not used as features in this model.*

In general, after a split over an attribute in relation R_i, all messages along the path from leaves to R_i can be re-used. The proof is as follows: all messages from the leaf relations (excluding R_i) are unchanged, and recursively, if a relation's (excluding R_i) incoming messages are unchanged, its outgoing message is also unchanged. This is orthogonal to prior batch optimization work [64] because we can cache and reuse the messages after batching for future nodes. This further improves batch optimization by >3× (Section 6.5).

4.2 Factorized Random Forest Models

A random forest model simply trains multiple decision trees over random samples of the training data, and aggregates (e.g., averages) their predictions during inference. The main challenge is to efficiently draw a uniform sample over non-materialized $R_{\bowtie}$. We use ancestral sampling [19]: starting from a root relation in the join graph, we draw a sample s, filter the child relations by tuples that join with s, and recurse through the join graph. To ensure uniformity over $R_{\bowtie}$, the sampling is weighted. Given the current sample s, tuple t from the next relation R is weighted by $P(t|s) = P(t, s)/P(s)$. The probability $P(t)$ for $t \in R$ is proportional to the number of tuples $t_{\bowtie}$ in $R_{\bowtie}$ with $\pi_{S_R}(t_{\bowtie}) = t$ [66, 75]. This is efficiently computed with message passing and caching [35, 66].

Minor Optimizations. First, we coalesce the messages for *COUNT* query with those for the tree criterion. For instance, the c element in Variance Semi-ring captures the *COUNT* statistics. Second, for snowflake schemas where the fact table has N-to-1 relationships with the rest of the tables, we sample the fact table directly [72].

4.3 Factorized Boosted Tree-based Models

Boosted tree-based Models like gradient boosting [29] iteratively train the next tree to predict the residuals from the previous trees. In each iteration, we need to update the target variable to be the residual $\mathcal{E} = Y - P$, where P is the current prediction. In other words, for each leaf node l in the last decision tree, we logically want to update the subset of $R_{\bowtie}$ matching $l.\sigma$ to the difference between y and $l.p$. The fundamental challenge is: how to apply these updates without materializing $R_{\bowtie}$?

A tempting approach is to treat this as a view update problem: we wish to update the attributes in the view of $R_{\bowtie}$ and translate it into updates over the base relations. However, the general problem is well known to be non-deterministic [22]. A related approach is factorized IVM [37, 52], but that updates $R_{\bowtie}$ given changes to the base relations, which is the reverse of our problem.

Update Relation U: While view updates are hard in general, residual updates are a special case because the UPDATEs are guaranteed to be non-overlapping, so we can rewrite the set of UPDATEs into a join with an *Update Relation* U. The benefit is that we can apply factorized learning over join.

To construct U, recall from Section 3.2 that a decision tree is modeled as a set of (predicate, prediction) pairs. In addition, each tuple in $R_{\bowtie}$ corresponds to exactly one leaf node. Let $\mathbf{A}$ be the set of attributes referenced by the predicate in the decision tree. U contains the projection of $\mathbf{A}$ over $R_{\bowtie}$, as well as its leaf's prediction.

The next boosting iteration requires computing $\mathcal{E} = Y - P$ over $R_{\bowtie} \bowtie U$, and lifting the resulting relation based on $\mathcal{E}$: $lift_{\mathcal{E}}(U \bowtie R_{\bowtie})$ in order to correctly annotate each tuple[4]. In general, $lift_{\mathcal{E}}$ cannot be pushed before the join, so $R_{\bowtie} \bowtie U$ would need to be materialized. The challenge is to *annotate* U with semi-ring annotations such that: $Annotate(U) \bowtie R_{\bowtie} = lift_{\mathcal{E}}(U \bowtie R_{\bowtie})$

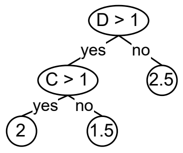
Variance Semi-ring. The primary semi-ring for gradient boosting is the variance semi-ring, which is amenable to construction. We define $Annotate(U) = lift_{-P}(U)$—given a tuple $u \in U$ with prediction $u[P] = p$, its annotation is $(1, -p, p^2)$. Note that defining $Annotate(U)$ for an arbitrary semi-ring structure is non-trivial, and we leave this exploration to future work.

Proposition 4.1. *For any tuple* $t \in (U \bowtie R_{\bowtie})$, $lift_{\mathcal{E}}(U \bowtie R_{\bowtie})(t) = (lift_{-P}(U) \bowtie R_{\bowtie})(t)$.

Proof. Let $y = t[Y]$ and $p = t[P]$. Consider the materialized result of $U \bowtie R_{\bowtie}$. It contains target variable Y and prediction P, so t's residual is $t[\mathcal{E}] = y - p$. Thus, $lift_{\mathcal{E}}(U \bowtie R_{\bowtie})(t) = (1, y - p, (y-p)^2)$. We also know that $Annotate(U)(t) = lift_{-P}(U)(t) = (1, -p, p^2)$. Since $R_{\bowtie}(\pi_{S_{R_{\bowtie}}}(t)) = (1, y, y^2)$, the annotation for $(Annotate(U) \bowtie R_{\bowtie})(t)$ is then $(1, -p, p^2) \times (1, y, y^2) = (1, y - p, p^2 + y^2 - 2py) = (1, y - p, (y-p)^2)$. □

Example 4. *The decision tree in Figure 3a has 3 leaf nodes whose predicates and predictions are:* $(\sigma_{D\leq 1}, p = 2.5)$, $(\sigma_{D>1 \wedge C\leq 1}, p = 1.5)$, *and* $(\sigma_{D>1 \wedge C>1}, p = 2)$. *The set of attributes involved with predicates is* $\mathbf{A} = \{C, D\}$. *The update relation is shown in Figure 3b. The semi-ring of residuals over join* $U \bowtie R_{\bowtie}$ *(with additional residual* $E = Y - P$ *column to help understanding) is shown in Figure 3d. It is easy to verify that the annotations in* R_{ϵ} *are the same as those in* $R \bowtie S \bowtie T \bowtie U$.

[4]Because we lift relations based on different target variable Y, we add the target variable as a subscript $lift_Y$ to disambiguate.

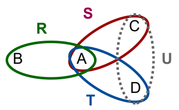


(a) Decision Tree.

U

C	D	P	(c,s,q)
1	1	2.5	(1,-2.5,6.25)
1	2	1.5	(1,-1.5,2.25)
2	1	2.5	(1,-2.5,6.25)
2	2	2	(1,-2,4)
3	2	2	(1,-2,4)

(b) Update Relation U.



(c) Join Graph.

A	B	C	D	P	$\mathcal{E}$	(c,s,q)
1	2	2	1	2.5	-0.5	(1,-0.5,0.25)
1	2	2	2	2	0	(1,0,0)
1	3	2	1	2.5	0.5	(1,0.5,0.25)
1	3	2	2	2	1	(1,1,1)
2	1	1	2	1.5	-0.5	(1,-0.5,0.25)
2	1	3	2	2	-1	(1,-1,1)
2	2	1	2	1.5	0.5	(1,0.5,0.25)
2	2	3	2	2	0	(1,0,0)

(d) Materialized $R_{\bowtie}$ with prediction P, residual $\mathcal{E} = Y - P$ and annotation $(1, \epsilon, \epsilon^2)$ lifted on $\mathcal{E}$ for the next tree.

Figure 3: Update Relation U for decision tree residual updates over the non-materialized $R_{\bowtie}$. Each tuple in $U \bowtie R_{\bowtie}$ has the same annotation as the materialized $R_{\bowtie}$ lifted on $\mathcal{E}$. Therefore, the materialization of $R_{\bowtie}$ can be avoided.

Challenges: The update relation can introduce cycles to the join graph; however *Message Passing* only applies to acyclic join graphs (e.g., Figure 3c shows cycle $A \rightarrow C \rightarrow D$). Standard hypertree decomposition [13, 41] removes cycles by joining the relations in a cycle and materializing their join result R' (e.g., $S[A, C] \bowtie T[A, D] \bowtie U[C, D]$), and replacing these relations in the join graph with R'. However, this is not scalable for gradient boosting, because the cluster grows in size as update relations are added in each iteration. As the trees split using different attributes, we eventually converge to materializing the full join $R_{\bowtie}$.

We introduce two solutions that are sufficient for scalable factorized boosting in practical scenarios. The first exploits the N-to-1 relationships in snowflake schemas along the paths through the dimension tables: it rewrites decision tree leaf node predicates as a semi-join over the fact table rather than over $R_{\bowtie}$. The second extends the first solution to support galaxy schemas with multiple fact tables using a technique we call Clustered Predicate Trees.

4.3.1 Semi-join Selection for Fact Table: Snowflake schemas have a single tall fact table F and N-to-1 foreign key relationships along the path towards the dimension tables. In that case, we can rewrite predicates over dimension tables as semi-joins (predicates[5]) over the fact table. Consider a path $F - D_1 - ... - D_k$, and selection σ over D_i. Since D_{i-1} has a N-to-1 relationship with D_i,

$$D_{i-1} \bowtie \sigma(D_i) = (D_{i-1} \ltimes \sigma(D_i)) \bowtie D_i = \sigma'(D_{i-1}) \bowtie D_i$$

where σ' is predicate $D_{i-1}.\mathcal{X} \in \pi_{\mathcal{X}}(\sigma(D_i))$ and $\mathcal{X}$ is the join keys between D_{i-1} and D_i. Therefore, predicates over the dimension tables can be recursively rewritten as semi-joins over the fact table.

[5]We treat left semi-joins as filters over the left relation so its annotations don't change.

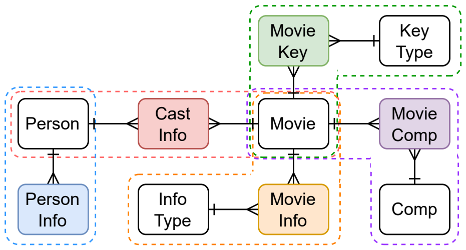


Figure 4: Clusters for IMDB dataset. Each cluster is enclosed by dotted lines and its fact table is filled.

In these cases, F contains the attributes $\mathbf{A}$ in the update relation, and will not create any cycle [13].

To avoid accumulating more update relations in each boosting iteration, we replace F with $F \bowtie U$ in each iteration.

4.3.2 Clustered Predicate Tree: Rewriting selection as semi-join is not possible through a 1-to-N relationship. These are common in galaxy schema, which contains multiple fact tables. *Clustered Predicate Tree* (CPT) restricts each boosted tree to split on features that can be pushed to the same fact table. To do so, we cluster relations such that in each cluster, a single (fact) table F has N-to-1 relationships along the path to all other relations in the cluster. During training, the root decision tree node can be split on any feature, but the remaining splits are restricted to attributes in the same cluster. Although this can impact model accuracy, this lets us efficiently update residuals over join graphs that would otherwise be infeasible to train using existing techniques.

Example 5. *Figure 4 shows the IMDB [5] join graph. The five clusters are enclosed by dotted lines and the cluster's fact table is highlighted. If the current tree initially splits on Person's age, then the rest of the tree can only split on attributes in Person or Person Info.*

5 `JOINBOOST` OVERVIEW AND OPTIMIZATIONS

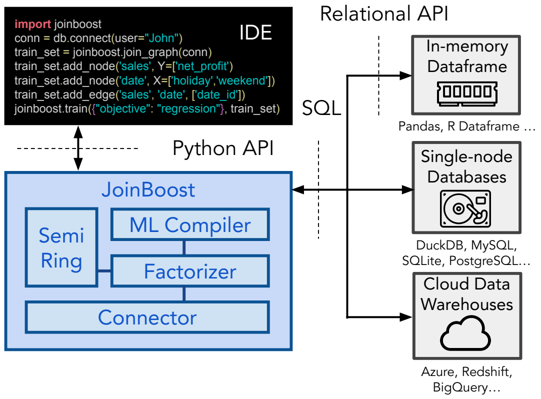
We now present the system overview and optimizations.

5.1 `JoinBoost` Developer Interface

As described in Section 1, our design goals are portability, API compatibility, and performance. We evaluate performance in the experiments, so focus on portability and compatibility below.

Portability: Our design deviates from prior factorized query execution works [21, 42, 44, 64], which build (fast) custom execution engines. In contrast, `JoinBoost` is implemented as a Python-based ML library that transparently generates SQL queries to the user's desired DBMS backend (Figure 5).

API Compatibility: `JoinBoost` exposes a similar Python API as `LightGBM` and `XGBoost`. In these libraries, the user first defines a training dataset, and passes it, along with training parameters (e.g., objective, metric, number of leaves), to a `train()` method. The `JoinBoost` user similarly defines the training dataset by initializing a join graph (the relations and join conditions between the relations), providing a database connection, and specifying the features and target variable. If the user only specifies the relations, `JoinBoost` will infer the join graph that covers those relations from the database schema, and raise an error if the graph is ambiguous (e.g., multiple foreign key references between relations) or it requires a cross-product. The user can freely define data transformation/pre-processing views and build the join graph atop those views. Finally, the user passes the training dataset and optional training parameters to `train()`. For consistency, `JoinBoost` also accepts the same training parameters as `LightGBM`.



```
import joinboost
conn = db.connect(user="John")
train_set = joinboost.join_graph(conn)
train_set.add_node('sales', Y=['net_profit')
train_set.add_node('date', X=['holiday','weekend'])
train_set.add_edge('sales', 'date', ['date_id'])
joinboost.train({"objective": "regression"}, train_set)
```

Figure 5: `JoinBoost` Architecture. `JoinBoost` translates its Python API calls into message passing algorithms that are executed as SQL queries on backend DBMSes and dataframes.

Example 6. *Figure 5 illustrates a simple example inspired by TPC-DS. The user creates a database connection, and initializes the training dataset as a join graph with relations* [`sales`, `date`], *join attribute* `date_id`, *features* $\mathbf{X}$ = [`holiday`, `weekend`] *and target variable* Y = `net_profit`. *Finally, the user chooses model parameters* ($\{objective = regression\}$) *and runs* `train` *over the training dataset.*

`JoinBoost` internally translates the ML algorithms into a series of `CREATE TABLE` and `SELECT` SQL queries. Compared to in-DB systems like `MADLib` [33], `JoinBoost` generates pure SQL and does not require user-defined types or functions. This enables portability (criteria C2): `JoinBoost` runs on embedded databases, single-node databases, cloud data warehouses, and even `Pandas` and `R` dataframes using `DuckDB`'s relational API [8].

The compiler fully supports decision trees, random forests, and gradient Boosting with all learning parameters that `LightGBM` supports. Currently, regression with *RMSE* objective supports galaxy schema with Clustered Predicate Trees; other objectives (e.g., *MAE*, *huber*, *softmax*...) require snowflake schema. We are actively extending capabilities to support pruning, dropout and early stopping, which build on the techniques in the preceding sections.

Safety and Provenance: Training never modifies user data. To achieve that, `JoinBoost` creates and modifies temporary tables in a specified namespace or with a unique prefix. By default, `JoinBoost` deletes all temporary tables after training, but users can keep them for provenance or debugging.

5.2 Architecture Overview

The *ML Compiler* translates the training algorithms for the desired model into semi-ring aggregation queries over the join graph, and returns a reference to the trained model. For instance, it issues queries to evaluate all possible splits for a given node, and chooses the best split. At this stage, the compiler treats the join graph as a large "wide" table; factorization is applied in a later step.

The *Semi-ring Library* stores semi-ring definitions and translates math expressions in the compiler-generated queries ($\times, +, lift$) into SQL aggregation functions. $lift(R)$ creates a copy of a base relation R that contains an additional attribute for each component in the semi-ring (e.g., c, s, q in the variance semi-ring). This also ensures that any update in-place will not modify user data. In addition to the variance (for regression) and the class count (for classification) semi-rings, JoinBoost implements semi-rings for a wide range of popular objectives; it supports *RMSE* for snowflake and galaxy schemas, and *MAE, huber loss, fair loss, log loss, softmax* and more for snowflake schemas (see Appendix B for full list).

The *Factorizer* decomposes each aggregation query into message passing and absorption queries. It also materializes each message as a database table, and re-uses them when possible. After choosing a node split, the factorizer keeps messages that can be reused in descendent nodes (Section 4.1) and drops the rest.

Finally, the *Connector* takes our internal SQL representation, and translates them into the appropriate SQL string or dataframe API calls. Although DBMSes are notorious for incompatible SQL variants, JoinBoost only uses a subset of SQL that is generally consistent across vendors. For instance, it generates standard non-nested SPJA queries with simple algebra expressions.

5.3 Residual Updates Logical Optimization

Although correct, the residual update technique in Section 4.3 is still expensive to implement naively. For simplicity, if we assume a single join attribute A between the fact table F and update table U, and the variance semiring, the SQL query would be:

```
CREATE TABLE F_updated AS
    SELECT F.c*U.c AS c,
           F.s*U.c+U.s*F.c AS s,
           F.q*U.c+U.q*F.c+2*F.s*U.s AS q, ...
      FROM F JOIN U ON A
```

where c, s, q are the components of the semiring, and the remaining columns in F are copied over (shown as ...). Unfortunately, this is >50× slower than LightGBM's residual update procedure (see experiments below), because U can potentially be as large as the materialized $R_{\bowtie}$. To this end, we present an optimization for snowflake and galaxy schemas that completely avoids materializing U as well as $F \bowtie U$.

5.3.1 Semi-join Update Optimization. We will directly UPDATE the fact table's semi-ring annotations. Let us start with a snowflake schema. Recall that each decision tree leaf node l logically corresponds to a separate join graph containing a set of messages (Figure 2), and let $l.\sigma$ be its predicate and $l.p$ be its prediction.

Also, the semi-join optimization in Section 4.3 translates predicates over $R_{\bowtie}$ (e.g., $l.\sigma$) into semi-joins between F and the relevant incoming messages $\mathcal{M}$. A message $m_i \in \mathcal{M}$ is relevant if it is along a join path from a relation containing an attribute in $l.\sigma$ and F. For each leaf node l, we execute the following query, where $F.a_i$ is the join attribute with its relevant incoming message m_i:

```
UPDATE F SET c * 1 AS c,     s - l.p*c AS s,
             q + l.p*l.p*c - 2*s*l.p AS q
       WHERE F.ai IN (SELECT ai IN mi) AND ...
```

In some databases, updates in-place can be very slow. Thus an alternative is to create a new fact table with the updated semi-ring annotations. Let l_j be the j^{th} leaf in the decision tree, and $m_{i,j}$, $a_{i,j}$ be the i^{th} message and its join attribute with F in l_j's join graph:

```
CREATE TABLE F_updated AS
  SELECT
   CASE WHEN F.a_ij IN (SELECT a_ij FROM m_ij) AND ... THEN s - l_j.p*c
        WHEN ... // Other leaves
    END AS s,
    ...  // other semi-ring components
    ...  // copy other attributes in F
  FROM F
```

The same ideas apply to galaxy schemas, where F corresponds to the fact table of the current tree's cluster. Further, we show in the technical report [9] that c and q are not necessary to materialize, thus only s is needed for the variance semi-ring.

5.3.2 Pilot Study. When should we perform in-place updates as compared to creating new tables? On which DBMSes? We now report a microbenchmark to understand the performance trade-offs, and use them to motivate a new optimization. We used an Azure VM, with Ubuntu 20.04.4, Intel(R) Xeon(R) Platinum 8370C CPU @ 2.80GHz, 16 cores, 128 GB memory, and an SSD.

Workloads. We create a synthetic fact table $F(s, d, c_1, ..., c_k)$ with $100M$ rows to simulate residual updates in a decision tree with 8 leaves. s is the semi-ring column to update, $d \in [1, 10K]$ is the join key, and c_k are simply extra columns that would need to be duplicated in a new table. For the i^{th} leaf node, its prediction is a random float, and we construct its semi-join message $m_i(d)$ to contain all values in $(1250 \times (i-1), 1250 \times i]$.

Methods. We evaluate three approaches. Naive materializes Update Relation U, then re-create fact table: $F' = F \bowtie_{\text{A}} U$ as discussed in Section 4.3. SET and CREATE use the update-in-place and create table optimizations in the preceding subsubsection. CREATE-k denotes the number of extra columns in F, where $k \in \{0, 5, 10\}$; we set $k = 0$ for Naive, and k does not affect SET.

DBMSes. We evaluate two systems. DBMS-X is a popular commercial RDBMS that supports both column-oriented (X-col) and row-oriented (X-row) storage and query processing. DBMS-X is disk-based only, and we set the isolation and recovery to the lowest level (read uncommitted and minimum logging). DuckDB [61] is a popular embedded column-oriented OLAP DBMS and is highly performant [10]. DuckDB has disk-based (D-disk) and memory-based (D-mem) modes. As a reference, we also use LightGBM to train 1 iteration of gradient Boosting with the same training settings, and report residual update time.

Experiment Results. Figure 6 shows that Naive incurs high materialization and join costs. CREATE is ∼ 2× faster for DBMS-X and ∼ 4× faster for DuckDB, but its cost grows linearly with k. SET mainly depends on the DBMS—it is prohibitive for DBMS-X, but more efficient than CREATE when $k > 5$ for DuckDB. All DBMS approaches take >3s for updating residuals. In contrast, LightGBM stores the target variable in a C++ array and performs parallel writes; its residual update takes ∼0.2s. These poor results are due to four main factors.

- **Compression:** CREATE in X-col incurs high compression costs: the database is 1GB in X-col as compared to 2.6GB for DuckDB. This also penalizes SET due to decompression.
- **Write-ahead Log (WAL)** introduces costly disk writes.

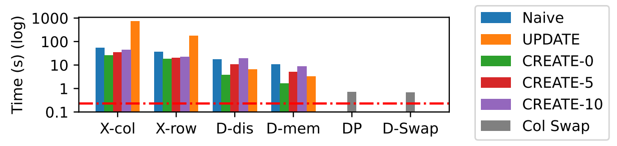


Figure 6: Residual update time (log) for different DBMSes. `Naive` materializes the update relation and joins it with the fact table. `Update` updates the fact table in place with semi-join. `CREATE-k` creates a new fact table, with k extra columns besides s and d. `Col Swap` creates a column of new s and swaps it with the old s in the fact table. `X-col/row` are column/row-based backends of `DBMS-X`. `D-disk/mem` are disk/memory-based `DuckDB`. `DP` (Section 5.4) uses `Pandas` dataframe for the Column Swap. `D-Swap` (Section 5.4) modifies `DuckDB` internals to natively support Column Swap. The red horizontal line is the residual update time for `LightGBM`.

- **Concurrency Control (CC):** In-memory `DuckDB` doesn't use WAL, but incurs MVCC [51] overheads, including versioning, and logging for undo and validation.
- **Implementation:** `DuckDB`'s update is currently single threaded.

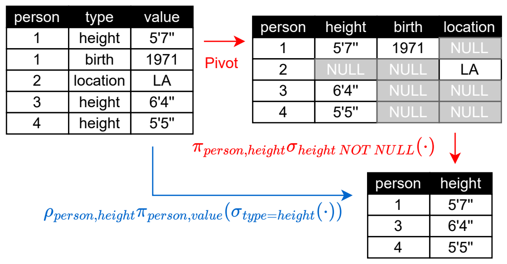
5.4 Residual Updates Physical Optimization

Logical rewrites are effective but still much slower than `LightGBM`'s residual updates, even when existing CC mechanisms are lowered. We observe that `JoinBoost` does not need durability and concurrency control, since it writes to private tables, performs application-level concurrency control (Section 5.5), and can simply re-run upon failure. Compression is also unnecessary for the heavily updated columns. Therefore, we wish to evaluate residual updates when WAL, CC, and compression are turned off.

We present two solutions. The first solution, which we call `DP` (`DuckDB` + `Pandas`), uses the `DuckDB` Relational API [8] *without* modifying `DuckDB` internals. `DuckDB` supports direct access to `Pandas` dataframes [55], an in-memory data structure that stores columns in contiguous uncompressed C arrays. We store the fact table F as a dataframe, and use the relational API to join F with the rest of the `DuckDB` tables for training. To update residuals, we found that creating a new column for the residuals avoids duplicating the other columns in F and yields the best performance. Thus we first use `DuckDB` relational operators to compute (in multi-threads) the semi-ring annotations for updated residuals, whose result is stored in a NumPy array. We then replace the old column with it using the `Pandas` API (by swapping the column pointers). `DP` reduces residual updates to $0.72s$–competitive with `LightGBM` (Figure 6).

While `DP` reduces the update bottleneck, joining `DuckDB` tables with `Pandas` dataframes does degrade aggregations due to `DuckDB`-`Pandas` interop overhead, and thus training time, by ~1.6× (Section 6.4). Ideally, columnar DBMSes can natively support this form of batch column-wise update at near-memory-bandwidth rates based on copy-on-write semantics.

To verify this, our second solution, `D-Swap`, modifies the internals of `DuckDB` (<100LOC) to support column swaps between two `DuckDB` tables. `DuckDB` stores tables in row groups, with each group containing pointers to the column data. `D-Swap` iterates through the row groups of the two relations and swaps the column pointers. This operation is lightweight ($< 1ms$), and has a similar residual update



person	type	value
1	height	5'7"
1	birth	1971
2	location	LA
3	height	6'4"
4	height	5'5"

person	height	birth	location
1	5'7"	1971	NULL
2	NULL	NULL	LA
3	6'4"	NULL	NULL
4	5'5"	NULL	NULL

person	height
1	5'7"
3	6'4"
4	5'5"

Pivot
$\pi_{person,height}\sigma_{height\ NOT\ NULL}(\cdot)$
$\rho_{person,height}\pi_{person,value}(\sigma_{type=height}(\cdot))$

Figure 7: Pivot Transformation Optimizations over *Person_Info* in IMDB. Naively, the sparse pivot result is materialized, then each feature (e.g., height) is selected to evaluate the split criteria (red). The query could be rewritten as a selection over type column by feature name, thus avoiding the materialization of a sparse pivot table (blue).

performance to `DP` (Figure 6), but does not degrade aggregations (Section 6.4). In our experiments, we emulate this optimization's effect if applied to columnar DBMS (`DBMS-X`). We suggest columnar DBMS developers incorporate this operation to support efficient In-DB gradient boosting.

5.5 Additional Optimizations and Features

We apply a variety of optimizations to `JoinBoost` to improve performance and increase usability.

5.5.1 Inter-query Parallelism. Parallelism has been widely exploited by ML libraries. `LightGBM` implements parallelized sort, aggregation, and residual updates, and across split candidates. Similarly, `Sklearn` parallelizes across trees. For `JoinBoost`, most DBMSes provide intra-query parallelism. However, there are diminishing returns for any individual query or operation. Thus, `JoinBoost` aggressively parallelizes across queries as well. There are many parallelization opportunities across e.g., trees in a random forest, leaf nodes in a decision tree, candidates splits for a decision tree node, and messages to evaluate a candidate split. Of course, there are also dependencies between these queries: a message's query depends on its upstream messages, absorption depends on its incoming messages, tree nodes depend on queries from its ancestor nodes, and a gradient boosting tree depends on its preceding trees.

To this end, `JoinBoost` uses a simple scheduler. Each query Q tracks its dependent queries. When Q completes, it sets the ready bit for its dependent queries. If all of a query's dependencies are set, then it is added to a FIFO run queue. Empirically, 4 threads worked best for intra-query parallelism; the rest are used for inter-query parallelism. This reduces the gradient boosting training time by 28% and random forest by 35% (Appendix C).

5.5.2 Data Transformations. Prior factorized learning work [44] introduced techniques that use functional dependencies to prune attributes prior to training, and to avoid materializing one-hot encodings for categorical attributes. A benefit of a middle-ware approach to in-DB ML is that we can leverage existing query optimizations to support other data transformations. In addition to the prior techniques above, `JoinBoost` introduces an optimization to support "pivot" transformations.

ML algorithms traditionally expect a dense matrix representation of the features. In contrast, DBMSes store sparse representations that need to be pivoted for ML libraries. Figure 7 illustrates IMDB data containing attribute-value pairs (e.g., birth, 1971) that encode information about a person.

If type were used as a feature, we first need to pivot the attribute into a sparse table with one column for each type value (e.g., height, birth). This matrix is then aggregated to compute statistics during training. To avoid this, Cunningham et al. [24] describe an optimization that rewrites aggregations over pivots as selections over the original table. JoinBoost easily supports such optimizations simply by adding an additional rewriting step. For the IMDB dataset, this optimization speeds up node splits by 3.8× for the $Person\_Info$ table, compared to naive pivoting.

5.5.3 Histogram-based Cuboid. A popular technique implemented in LightGBM and XGBoost is histogram-based gradient boosting. It computes histograms over each feature, and replaces each feature's value with its bin id (the cardinality is the same). Varying the number of bins trades off accuracy for lower training time.

A natural optimization is to leverage data cubes [30] when the number of bins is small and the data is sparse. We evaluate a naive approach that materializes the full dimensional cuboid—GROUP BY all feature attributes—and uses it instead of factorized learning to execute the aggregation queries for training. On the Favorita dataset, 5 bins result in a cuboid with $3M$ rows, as compared to 80M for the full join result. Since training is based on semi-ring annotations, the rest of the algorithms remain the same.

5.5.4 Missing Join Keys. ML libraries like LightGBM and XGBoost provide native support for missing values because they are ubiquitous in real-world datasets. They evaluate losses by allocating missing values to either side of a candidate split and choosing the best one. JoinBoost efficiently supports this: candidate splits are already computed using a group-by, so the missing values will be aggregated in a group. We simply add the missing value's annotation to each split candidate and choose the best. The overhead is negligible compared to the aggregation itself.

What if the join key is missing values, as this affects the join's output cardinality? Semi-ring annotations naturally support this: message passing simply uses full outer joins instead of inner joins, and then applies the procedure above.

6 EXPERIMENTS

We focus attention on the fastest alternative: ML libraries (XGBoost, LightGBM, Sklearn). We start with a single-node setting, and then evaluate scalability to the number of features, the types of joins, database size, and multiple nodes. We then evaluate our optimizations. Finally, we compare with factorized (LMFAO) and non-factorized (MADLib) in-DB ML techniques.

Main Takeaways: JoinBoost is well suited for decision tree and random forest training in existing columnar engines. Adding the simple column swap feature further makes columnar DBMSes competitive for gradient boosting models. When combined with the scalability, operational, and security benefits, JoinBoost makes SQL-based In-DB tree training a practical option.

Datasets. We primarily report results using the Favorita [6] dataset used in prior factorized ML work [64, 65] (Figure 8). Sales is the fact table and largest relation (2.7GB CSV, 80M rows), and has N-to-1

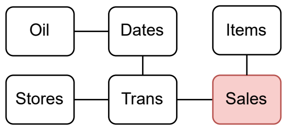


Figure 8: Favorita schema. Sales is the fact table.

relationships with the other dimensions ($< 2MB$ each). There are 13 features. We report TPC-DS results for scalability experiments and use IMDB for galaxy schema experiments; additional TPC-H/DS results are in the Appendix C.

Preprocess. Although Favorita and TPC-H/DS are standard benchmarks in prior factorized learning evaluations [64], their features are non-predictive and lead to highly unbalanced trees. This artificially favors JoinBoost since all but one leaf node in the decision tree would contain very few records, and thus take negligible training time—the performance differences with other systems are fully dominated by join materialization. To ensure balanced trees and fair comparison, we impute one feature attribute in each of the 5 dimension tables with random integers drawn from $[1, 1000]$. Then we impute the target variable as sum of transformed features[6]. Finally, we dictionary encode strings into 32-bit unsigned integers [12, 62] to avoid parsing errors in ML libraries like LightGBM.

Models. We evaluate decision tree, random forest, and gradient boosting. JoinBoost is intended to complement other DBMS workloads, so all experiments start with data persistent on disk but not in memory. We assume by default that data are already persisted in the disk-based DBMSes (DBMS-X and disk-based DuckDB). We report the end-to-end training time for decision tree of max depth 10, and vary the number of trees (iterations) in the random forest and gradient boosting. For JoinBoost, the main cost is from DBMSes, and the Python codes introduce negligible ($<0.1s$) overhead.

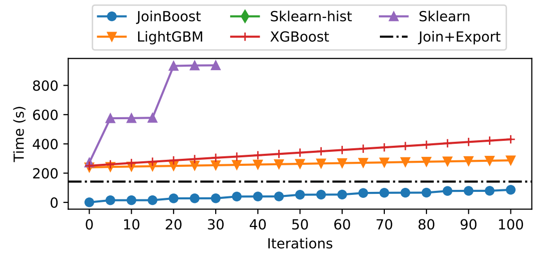
Methods. We evaluate JoinBoost with different database backends. DBMS-X (X-col and X-row for column and row-oriented storage and execution engines) and DuckDB-disk (D-disk) are disk-based and can directly execute queries on the base database, whereas memory-based DuckDB (D-mem) first loads the database from disk. DP refers to the disk-based DuckDB backend using Pandas updates through the DuckDB's relational API, and D-Swap refers to the modified memory-based DuckDB for efficient residual updates (Section 5.4). By default, we use D-Swap as the backend as it has the best performance (Section 6.4). The ML libraries[7] (LightGBM, XGBoost, Sklearn) expect a single CSV as input, so incur the cost to materialize and export the join result (~$7GB$ for Favorita), load the CSV, and train the model. DuckDB joins and exports the data faster than DBMS-X, so we report its numbers.

Hardware: All experiments are conducted on an Azure VM, with Ubuntu 20.04.4, Intel(R) Xeon(R) Platinum 8370C CPU@2.80GHz, 16 cores, 128 GB memory, and an SSD.

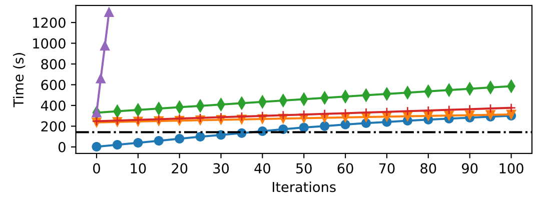
6.1 Comparison With ML Libraries

We compare with state-of-the-art ML libraries for training tree-based models (LightGBM [42], XGBoost [21]) and the popular Sklearn [58]

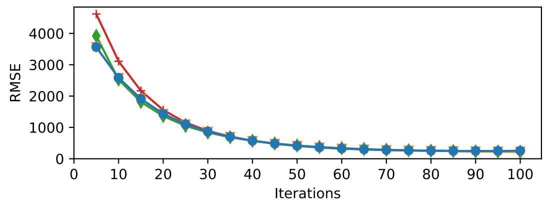
[6]Favorita applies: $y = f_{item} log(f_{items}) + log(f_{oil}) - 10f_{dates} - 10f_{stores} + f_{trans}^2$
[7]For LightGBM and XGBoost, while their python APIs are widely used, it has memory issues (https://github.com/microsoft/LightGBM/issues/1032) so we use the CLI version.



(a) Random Forest Training time. JoinBoost is ∼3× faster than LightGBM.



(b) Gradient Boosting Training time. JoinBoost is ∼1.1× faster.



(c) Gradient Boosting Accuracy. The final *RMSE* is nearly identical.

Figure 9: Gradient Boosting and Random Forest training time and accuracy on Favorita compared to ML libraries. The dotted black line is join materialization and export costs.

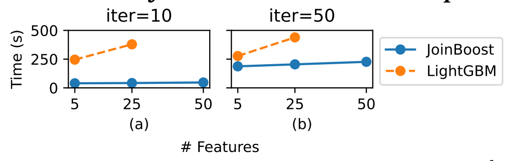


Figure 10: Gradient Boosting Training Time of 10th (a) and 50th (b) iteration when varying # of imputed features (x-axis). LightGBM runs out of memory when imputed 50 features.

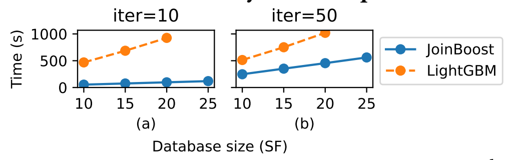


Figure 11: Gradient Boosting Training Time of 10th (a) and 50th (b) iteration. The X-axis varies TPC-DS SF (database size). LightGBM runs out of memory when $SF = 25$.

Python ML library. Sklearn implements standard and histogram-based gradient boosting with algorithms similar to LightGBM, so we report both implementations. We set the number of bins to 1000 for LightGBM and XGBoost, and 255 for Sklearn (its limit). By default, we train gradient boosting and random forest with best-first growth and 8 max leaves per tree. The gradient boosting learning rate is 0.1 and the random forest sampling rate without replacement is 10%. We report up to 100 iterations. The 0th iteration reports the join materialization, export, and load costs.

Figure 9a shows random forest results. JoinBoost is ∼3× faster than LightGBM by avoiding materialization and export costs (dotted black line), and loading costs; it also parallelizes across trees. In fact, JoinBoost finishes 100 iterations before the export is done. Sklearn also parallelizes across trees, but is so slow that we terminate after 32 iterations. The final model error (*RMSE*) is nearly identical (∼2500) for JoinBoost, LightGBM and XGBoost.

Figure 9b shows gradient boosting results. JoinBoost is ∼1.1× faster than LightGBM, and is ∼1.2× faster than XGBoost by avoiding materialization and export costs. Figure 9c shows the model *RMSE*. JoinBoost and LightGBM have equivalent *RMSE* across iterations as both employ the same algorithm, while the final *RMSE* is similar across all. Note that the models begin to converge around 60 iterations; JoinBoost converges by the time LightGBM and XGBoost have loaded their data. As LightGBM dominates the other ML libraries, we primarily compare with it below.

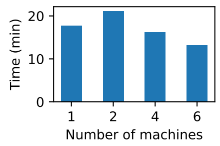


Figure 12: Decision Tree Training Time over TPC-DS (SF=1000) in Data Warehouse. Increasing the number of machines to 4 (6) reduces the training time by 10% (25%).

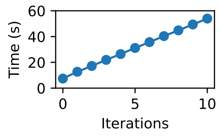


Figure 13: Gradient Boosting Training over IMDB dataset with a galaxy schema. Each tree takes ∼5*s*. ML libraries do not run because the join is too large to materialize.

6.2 Scalability

We now study scalability to # features, DB size, and join complexity.

# Features. We train gradient boosting using Favorita and vary the number of features from 5 to 50, and report training time at the 10th and 50th iterations. Figure 10 shows that LightGBM slows by >1.5× with 25 features, and runs out of memory (125GB) at 50 features. XGBoost supports out-of-core training, but took∼4000s to train 50 features for 10 iterations, and wrote ∼80*GB* of intermediate results to disk (not plotted). JoinBoost scales linearly with >10× lower slope, and scales to out-of-core execution thanks to the DBMS.

Single-node Scalability. Favorita is a fixed dataset, so we use TPC-DS (145 features) to scale the database ($SF \in [10, 25]$). Figure 11 shows that both systems scale linearly, but JoinBoost has a lower slope (∼10× lower at 10th iteration, and ∼2× lower at 50th). LightGBM runs out of memory at $SF = 25$.

Cloud-warehouse Scalability. We use a cloud data warehouse DW-X to train a decision tree with max depth 3 over TPC-DS SF=1000, and study multi-machine scalability. Each machine has 74 cores, 300GB of memory, and SSDs. We replicate dimensional tables across the machines, and hash-partition the fact table. Figure 12 shows that 2 machines introduce a shuffle stage that slows training, and increasing to 4 (6) machines reduces training by 10% (25%).

Galaxy Schemas. Galaxy schemas have N-to-N relationships that are prohibitive to materialize. We use clustered predicate trees (Section 4.3.2) to train gradient boosting on the IMDB dataset (Figure 4).

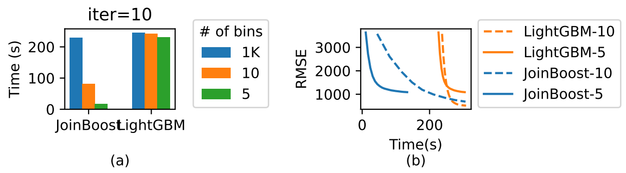


Figure 14: Histogram-based Gradient Boosting. (a) `JoinBoost` is much faster with fewer bins due to the smaller cuboid sizes. (b) Training time-accuracy trade-off. `JoinBoost` with $\#bin = 5$ pushes the Pareto frontier and reaches $RMSE = 1500$ in $20s$.

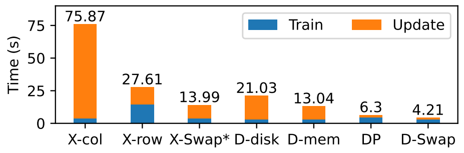


Figure 15: Training and residual update time for one decision tree on Favorita for different DBMSes. `X-Swap*` is the theoretical runtime by simulating column swaps.

`Cast_Info` is $\sim 1GB$ and the total DB is $1.2GB$. `JoinBoost` scales linearly with the number of iterations (Figure 13); it trains one tree and updates residuals in each cluster's fact table within $\sim 5s$. `LightGBM` cannot run because the join result is $>1TB$.

6.3 Histogram-based Gradient Boosting

We vary the number of histogram bins to study when using the cuboid optimization (Section 5.5.3) is effective. For bin=5, 10, $1K$, the cuboid contains $\sim 3M$, $\sim 25M$, and $\sim 80M$ rows respectively.

Figure 14(a) shows that at iteration 10 and $bin = 5$, `JoinBoost` speeds up by >100× the smaller cuboid size and faster aggregation queries, whereas `LightGBM` only slightly improves. As we run more boosting iterations (Figure 14(b)) `JoinBoost-5` quickly converges ($\sim 20s$); `JoinBoost-10` takes longer to converge because the cuboid is larger but is still competitive to `LightGBM`. In theory, we could gradually increase the number of bins throughout training to further improve model accuracy, but leave this to future work.

6.4 Effect of DBMSes

We now use Favorita to train 1 iteration of gradient boosting, and compare train and update costs for different DBMSes (`DBMS-X` and `DuckDB`). To study the potential benefits of column swapping (Section 5.4) in commercial systems, `X-Swap*` reports the theoretical cost using the time to create the updated column as a new table (since column swapping is then "free").

Figure 15 breaks down train and update costs. Decision trees and random forests only require training (blue bar), which is dominated by columnar execution: `X-col` and `DuckDB` take $3.2 - 3.9s$ versus $14.5s$ for `X-row`. Gradient boosting introduces high update costs across all of the baseline DBMSes. We see that using Pandas to perform the update (`DP`) reduces residual updates by ~15× ($17.8s \rightarrow 1.2s$), but slows training by 60% ($3.2s \rightarrow 5.1s$) due to DuckDB-Pandas interop overhead. `D-opt` implements column swapping inside `DuckDB` and improves training. We also see that adding column swapping to `DBMS-X` (`X-Swap*`) leads to respectable gradient boosting performance (~3× of `D-Swap`) but can benefit from its out-of-memory and multi-node scalability features.

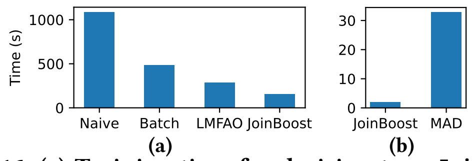


Figure 16: (a) Training time for decision tree. `JoinBoost`'s caching and work sharing improve over `LMFAO`, naive materialization and query batching variants. (c) Training time for decision tree. `JoinBoost` is ∼16× faster than `MADLib`.

6.5 Comparison With In-DB ML Techniques

We first compare with the dominant factorized approach (`LMFAO` [64]), followed by the non-factorized approach (`MADLib`).

Factorized ML. We first compare with `LMFAO` [64], which supports decision trees (but not gradient boosting or random forests). We train a decision tree (max depth=10) with best-first growth; the trained tree is balanced and has 1024 leaves. Via correspondence, the `LMFAO` authors shared a version that compiles a program for the queries used to split the root tree node, and reuses it for growing the rest of the tree. We set the highest optimization level for `LMFAO`, and exclude the time for query compilation ($\sim 15s$) and data loading. To separate algorithmic vs implementation differences, we implement two variations of `JoinBoost`. `Naive` materializes the join result and does not use factorized ML. `Batch` implements `LMFAO`'s core logical optimizations (Multi Root, Aggregate Push-down and Merge View) for decision tree; this corresponds to message passing with message re-use within, but not between tree nodes.

Figure 16a reports the training time. Even with the custom engine and specialized optimizations, `LMFAO` is still ∼1.9× slower than `JoinBoost` due to the lack of message caching (Section 4.1). By eliminating the implementation differences, `Batch` demonstrates that message caching improves training by ∼3×. The improvement is because half the messages across tree nodes are cached, and the sizes of the cached messages tend to be much larger; the intuition is that the messages outgoing from the relation containing the split attribute will be smaller, since the split predicate has been applied. In theory, two-pass semi-join reduction [13, 54] could reduce message sizes, but the high overheads outweigh benefits [12]. `Batch` is ∼2× faster than `Naive` due to factorization and shared work.

Non-Factorized ML. `MADLib` [33] is a PostgreSQL extension that supports ML using user-defined types and functions. `MADLib` doesn't apply factorized ML, so the join has to be materialized. `MADLib` times out after 1 hour when training a decision tree model (max depth=10) on the full Favorita dataset, so we reduced the training data size to 10k rows; for `JoinBoost`, we reduced the fact table to 10k rows. Figure 16b shows that `JoinBoost` is ∼16× faster than `MADLib`. This reproduces prior findings [64], and is likely due to the lack of factorized ML and an inefficient implementation.

7 CONCLUSION

`JoinBoost` is the first In-DB factorized ML system for tree models (decision trees, random forests, and gradient boosting) with only SQL. `JoinBoost` is comparable or faster than the SOTA `LightGBM` ML library on in-memory datasets, but scales well beyond `LightGBM`'s capabilities in terms of # of features, database size, and join graph complexity. `JoinBoost` exposes a Python API that mimics `LightGBM`'s API and is portable to any DBMS and dataframe library.

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A DECISION TREE FROM SEMI-RING

In this section, we present the algorithms to express the criteria of reduction in variance for regression, information gain, gini impurity and chi-square for classifications based on the semi-ring in Table 1. Computing these criteria is at the heart of decision tree training. Our algorithm here is based on `Sklearn`[8].

Aggregated Semi-ring: It has been shown that [13, 64], for variance semi-ring, the aggregated semi-ring $\gamma(R_{\bowtie})$ is a 3-tuple (C, S, Q) that represents the count $C = \sum_{t \in R_{\bowtie}} 1$, sum of target variable $S = \sum_{t \in R_{\bowtie}} t[Y]$, and the sum of squares of target variable $Q = \sum_{t \in R_{\bowtie}} t[Y]^2$. For classification with k classes, the aggregated semi-ring $\gamma(R_{\bowtie})$ is a $(k+1)$-tuple $(C, C^1, ..., C^k)$ that represents the total count $C = \sum_{t \in R_{\bowtie}} 1$ and count of each class $C^i = \sum_{t \in R_{\bowtie}} \mathbf{1}_{t[Y]=i}$.

Reduction in variance for regression: In the scope of variance semi-ring and given $R_{\bowtie} = R_1 \bowtie R_2 \ldots \bowtie R_n$ and schema $S_1, \ldots, S_n$, let the average of $R_{\bowtie}[y]$ be $\hat{y}$. The total variance of the target variable in $R_{\bowtie}$ can be computed as

$$\begin{aligned} var(R_{\bowtie}) &= \sum_{t \in R_{\bowtie}} (t[y] - \hat{y})^2 \\ &= \sum_{t \in R_{\bowtie}} t[y]^2 - 2 \sum_{t \in R_{\bowtie}} t[y] \cdot \hat{y} + \sum_{t \in R_{\bowtie}} \hat{y}^2 \\ &= \sum_{t \in R_{\bowtie}} t[y]^2 - \sum_{t \in R_{\bowtie}} \hat{y}^2 = Q - S^2/C \end{aligned}$$

The third equation holds because $\sum_{t \in R_{\bowtie}} t[y] = \sum_{t \in R_{\bowtie}} \hat{y}$. Consider a selection predicate σ where the attributes in σ, which splits $R_{\bowtie}$ into $\sigma(R_{\bowtie})$ and $\bar{\sigma}(R_{\bowtie})$, and let the average of y in $\sigma(R_{\bowtie})$ and $\bar{\sigma}(R_{\bowtie})$ be $\hat{y}_\sigma$ and $\hat{y}_{\bar{\sigma}}$, respectively. Let their aggregated semi-ring be $\gamma(\sigma(R_{\bowtie})) = (C_\sigma, S_\sigma, Q_\sigma)$ and $\gamma(\bar{\sigma}(R_{\bowtie})) = (C - C_\sigma, S - S_\sigma, Q - Q_\sigma)$. Thus, the new variance of $\sigma(R_{\bowtie})$ and $\bar{\sigma}(R_{\bowtie})$ can be similarly computed as

$$\begin{aligned} var(\sigma(R_{\bowtie})) &= \sum_{t \in \sigma(R_{\bowtie})} t[y]^2 - \sum_{t \in \sigma(R_{\bowtie})} \hat{y}_\sigma^2 = Q_\sigma - S_\sigma^2/C_\sigma \\ var(\bar{\sigma}(R_{\bowtie})) &= \sum_{t \in \bar{\sigma}(R_{\bowtie})} t[y]^2 - \sum_{t \in \bar{\sigma}(R_{\bowtie})} \hat{y}_{\bar{\sigma}}^2 \\ &= (Q - Q_\sigma) - (S - S_\sigma)^2/(C - C_\sigma) \end{aligned}$$

Thus, the reduction in variance can be expressed as computations using variance semi-ring

$$\begin{aligned} & var(R_{\bowtie}) - (var(\sigma(R_{\bowtie})) + var(\bar{\sigma}(R_{\bowtie}))) \\ &= -S^2/C + S_\sigma^2/C_\sigma + (S - S_\sigma)^2/(C - C_\sigma) \end{aligned}$$

As an optimization, we note Q term is canceled out for the reduction in variance. Therefore, we don't include Q during training.

To parse it into SQL for each feature A, we can compute its best split in one query using the window function. Note that, to avoid overflow, we need to compute s_t^2/c_t as $(s_t/c_t) \times s_t$.

```
SELECT A,-(stotal/ctotal)*stotal+(s/c)*s+(stotal-s)/(ctotal-c)*(stotal-s)
FROM (SELECT A, SUM(c) OVER(ORDER BY A) as c, SUM(s) OVER(ORDER BY A) as s
    FROM (  SELECT A, s, c
            FROM R
            GROUP BY A
         ))
ORDER BY criteria DESC
LIMIT 1;
```

[8]https://scikit-learn.org/stable/modules/tree.html#tree-mathematical-formulation

Classification: In the scope of class count semi-ring and given $R_{\bowtie}$, we will show that the criteria for classification (information gain, Gini impurity, Chi-square) can be computed given the aggregated class count semi-ring structures. Then it follows the same logic that we do not have to materialize the full $R_{\bowtie}$. Classification criteria are based on the probability of each class, which could be computed as $p^k = C^k/C$. The different criteria can be computed as:

$$entropy(R_{\bowtie}) = -\sum_{k=1}^{K} p^k \log p^k = -\sum_{k=1}^{K} (C^k/C) log(C^k/C)$$

$$gini(R_{\bowtie}) = 1 - \sum_{i=1}^{K} (p^k)^2 = 1 - \sum_{i=1}^{K} (C^k/C)^2$$

Consider a selection predicate σ where the attributes in σ, which splits $R_{\bowtie}$ into $\sigma(R_{\bowtie})$ and $\bar{\sigma}(R_{\bowtie})$. Let their aggregated semi-ring be $\gamma(\sigma(R_{\bowtie})) = (C_\sigma, C_\sigma^1, ..., C_\sigma^k)$ and $\gamma(\bar{\sigma}(R_{\bowtie})) = (C_{\bar{\sigma}}, C_{\bar{\sigma}}^1, ..., C_{\bar{\sigma}}^k) = (C - C_\sigma, C - C_\sigma^1, ..., C - C_\sigma^k)$. We can compute the reduction after the split in a way similar to regression.

Chi-square of the split is computed as:

$$\chi^2 = \sum_{i=1}^{K} \left(\frac{(C_\sigma^i - C^i C_\sigma/C)^2}{C^i C_\sigma/C} + \frac{(C_{\bar{\sigma}}^i - C^i C_{\bar{\sigma}}/C)^2}{C^i C_{\bar{\sigma}}/C} \right)$$

B BOOSTED TREES FROM SEMI-RING

In this section, we discuss the details of building Gradient Boosting from Semi-ring. We use the semi-rings as defined in Table 2.

B.1 Semi-ring Extension

Extension to bag semantics and weighted relations. Tuples in relations could be weighted. For relation R_i, let w be the function that maps tuple $t \in R_i$ to the weight as a real number. We modify the definition of semi-ring such that their count is a real number, then annotate relations as before, but their annotations are further multiplied by $(w(t), 0, 0)$ for weighting.

Extension to theta joins and outer joins. The support for theta joins over annotated relations is straightforward:

$$(R \bowtie_\theta T)(t) = \begin{cases} R(\pi_{S_R}(t)) \times T(\pi_{S_T}(t)), \theta(t) \\ Zero\ Element, \neg\theta(t) \end{cases}$$

To support outer-join, note that the semantic of annotated relation is that tuples not in the relation are annotated with zero-element [13]. This is undesirable as zero-element annihilates other elements when multiplied. Therefore for outer-join, we define the non-existed tuples to be annotated with one-element. Let $J = S_R \cap S_T$ be the join key between R and S:

$$(R \supset\!\!\bowtie T)(t) = \begin{cases} R(\pi_{S_R}(t)) \times T(\pi_{S_T}(t)), \pi_{S_T}(t) \in T \\ R(\pi_{S_R}(t)), \pi_J(t) \notin \pi_J(T) \wedge \pi_{S_T - J}(t)\ ALL\ NULL \end{cases}$$

B.2 Boosted Trees Preliminary

We provide the background of Boosted Tree based on [21, 42, 50].

Objective. We consider ML model f that maps tuple $t \in R_{\bowtie}$ to the prediction. The prediction is a real number for regression, and a set of real numbers corresponding to the probabilities of classes

Semi-ring	**Zero/One**	**Operator**	**Lift**
Regression $(\mathbf{R}, \mathbf{R})$	**0:** $(0,0)$ **1:** $(1,0)$	$(h_1, g_1) + (h_2, g_2) = (h_1 + h_2, g_1 + g_2)$ $(h_1, g_1) \times (h_2, g_2) = (h_1 h_2, g_1 h_2 + g_2 h_1)$	$(h(t), g(t))$
Classification $((\mathbf{R}, \mathbf{R}), ..., (\mathbf{R}, \mathbf{R}))$	**0:** $((0,0), ..., (0,0))$ **1:** $((1,0), ..., (1,0))$	$((h_1^1, g_1^1), ..., (h_1^k, g_1^k)) + ((h_2^1, g_2^1), ..., (h_2^k, g_2^k))$ $= ((h_1^1 + h_2^1, g_1^1 + g_2^1), ..., (h_1^k + h_2^k, g_1^k + g_2^k))$ $((h_1^1, g_1^1), ..., (h_1^k, g_1^k)) \times ((h_2^1, g_2^1), ..., (h_2^k, g_2^k))$ $= ((h_1^1 h_2^1, g_1^1 h_2^1 + g_2^1 h_1^1), ..., (h_1^k h_2^k, g_1^k h_2^k + g_2^k h_1^k))$	$((h^1(t), g^1(t)), ..., (h^k(t), g^k(t)))$

Table 2: Gradient Semi-rings for gradient boosting.

Task	Loss function	Gradient $g(\cdot)$	Hessian $h(\cdot)$	Prediction P
Regression	L2/rmse: $(\epsilon)^2$	ϵ	1	$mean(\mathcal{E})$
	L1/mae: $\lvert\epsilon\rvert$	$sign(\epsilon)$	1	$median(\mathcal{E})$
	Huber Loss: $\begin{cases} 0.5\epsilon^2, \lvert\epsilon\rvert \le \delta \\ \delta(\lvert\epsilon\rvert - 0.5\delta), else \end{cases}$	$\begin{cases} \epsilon, \lvert\epsilon\rvert \le \delta \\ \delta \cdot sign(\epsilon), else \end{cases}$	1	p^*
	Fair Loss: $c\lvert\epsilon\rvert - c^2 log(\lvert\epsilon\rvert/c + 1)$	$c\epsilon/(\lvert\epsilon\rvert + c)$	$c^2/(\lvert\epsilon\rvert + c)^2$	p^*
	Poisson Loss: $e^p - yp$	$e^p - y$	e^p	p^*
	Quantile Loss: $\begin{cases} (\alpha - 1)\epsilon, \epsilon < 0 \\ \alpha\epsilon, \epsilon \ge 0 \end{cases}$	$\begin{cases} \alpha - 1, \epsilon < 0 \\ \alpha, \epsilon \ge 0 \end{cases}$	1	$pctl_\alpha(\mathcal{E})$
	mape: $\lvert y - p\rvert / max(1, \lvert y\rvert)$	$\frac{sign(y-p)}{max(1,\lvert y\rvert)}$	1	$median(\mathcal{E})$
	Gamma Loss: $\frac{\frac{y}{p} - log(\frac{y}{p\psi})}{\psi} + log(y)$	$1 - ye^{-p}$	ye^{-p}	p^*
	Tweedie Loss: $-\frac{ye^{(1-\rho)log(p)}}{1-\rho} + \frac{e^{(2-\rho)log(p)}}{2-\rho}$	$-ye^{(1-\rho)p} + e^{(2-\rho)p}$	$-(1-\rho)ye^{(1-\rho)p} + (2-\rho)e^{(2-\rho)p}$	p^*
Classification	Softmax: $-y^k log(p^k)$	$p^k - y^k$	$\frac{K}{K-1}p^k(1 - p^k)$	p^*

Table 3: Summary of Gradient and Hessian implemented in the source codes from `LightGBM`. We note that Gradients and Hessians are not mathematically rigorous; they have been normalized and approximated for practical concerns. The residual $\epsilon = y - p$. $\mathcal{E}$ is the residual column. $pctl_\alpha$ is α percentile function.

for classification. We want to train a model f that minimizes the following objective:

$$L(f) = \sum_{t \in R_{\bowtie}} l(f(t), t[Y]) + \Omega(f)$$

Here, l is the loss function and Ω is the regularization function.

Regularization. For boosted tree of K iterations, f uses K additive functions $f_1, ..., f_K$ for predictions:

$$f(t) = \sum_{k=1}^{K} f_k(t)$$

The regularization term prefers tree models with smaller number of leaves and variance. For each tree f_i, let T_i be its number of leaves and p_i be a vector of leaf predictions. Then:

$$\Omega(f) = \alpha \sum_{k=1}^{K} T_k + 0.5\beta \sum_{k=1}^{K} ||p_i||^2$$

Optimization. Boosted Trees iteratively train decision trees to optimize the objective based on the predictions from previous trees. For ith tree f_k, it is optimizing:

$$L^i(f_i) = \sum_{t \in R_{\bowtie}} l(\sum_{k=1}^{i-1} f_k(t) + f_i(t), t[Y]) + \Omega(f_i)$$

After applying second optimization and removing constant terms:

$$\tilde{L}^i(f_i) = \sum_{t \in R_{\bowtie}} (g_t f_i(t) + 0.5 h_t f_i^2(t)) + \Omega(f_i)$$

where g_t and h_t are the gradients and hessians on the loss $l(\sum_{k=1}^{i-1} f_k(t), t[Y])$ for tuple t with respect to the predictions from previous trees $\sum_{k=1}^{i-1} f_k(t)$.

Next, we study the optimal prediction for leaf node. Consider a leaf node of decision tree f_i with number of leaves T_i, selection predicate σ and prediction p as a variable. The optimization objective (after removing constant terms) for this leaf node is then:

$$\tilde{L}^i_\sigma(p) = \sum_{t \in \sigma(R_{\bowtie})} (g_t p + 0.5 h_t p^2) + 0.5\beta p^2$$

The optimal prediction is then:

$$p^* = -\frac{\sum_{t \in \sigma(R_{\bowtie})} g_t}{\sum_{t \in \sigma(R_{\bowtie})} h_t + \beta}$$

And the objective becomes:

$$\tilde{L}^i_\sigma(p^*) = -0.5\frac{(\sum_{t\in\sigma(R_\bowtie)} g_t)^2}{\sum_{t\in\sigma(R_\bowtie)} h_t + \beta}$$

Finally, we study the problem of evaluating a split. Consider the selection predicate σ that splits $R_\bowtie$ into $\sigma(R_\bowtie)$ and $\bar{\sigma}(R_\bowtie)$. The initial loss before split is:

$$\tilde{L} = -0.5\frac{(\sum_{t\in R_\bowtie} g_t)^2}{\sum_{t\in R_\bowtie} h_t + \beta}$$

The loss after split is:

$$\tilde{L}_\sigma + \tilde{L}_{\bar{\sigma}} + \alpha = -0.5[\frac{(\sum_{t\in\sigma(R_\bowtie)} g_t)^2}{\sum_{t\in\sigma(R_\bowtie)} h_t + \beta} + \frac{(\sum_{t\in\bar{\sigma}(R_\bowtie)} g_t)^2}{\sum_{t\in\bar{\sigma}(R_\bowtie)} h_t + \beta}] + \alpha$$

The α term is because spliting increases the number of leaves. Finally, the reduction of loss from the split is:

$$\tilde{L} - (\tilde{L}_\sigma + \tilde{L}_{\bar{\sigma}} + \alpha)$$

The training process of Boosted Trees evaluates the reduction of loss for all candidate splits and chooses the best one.

B.3 Boosted Trees from Semi-ring

From the last section, we find that the core statistics over relational tables are the sum of gradients and hessians on the loss. Therefore, we build gradient semi-ring and lift relation based on the gradient and hessian for different objective functions, thus avoiding the materialization of $R_\bowtie$.

The definition of gradient semi-ring is in Table 2 and the formula of gradients and hessians for different objective functions based on LightGBM are in Table 3. We note that the gradients and hessians are not mathematical rigourious, and some losses are approximated. For example, mean absolute error has hessian undefined when error = 0, and 0 for the rest. Hessian can't be zero, and thus the loss is approximated without second order gradient (so hessian all 1) [9].

C OTHER EXPERIMENTS

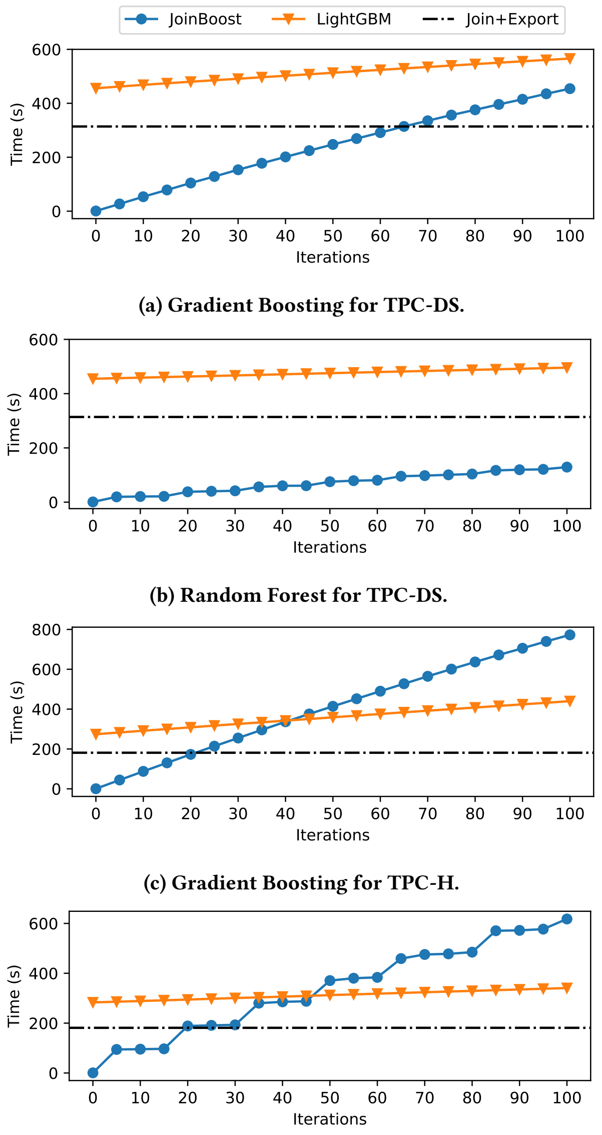
C.1 Comparison with LightGBM

Figure 17 shows the experiment results for TPC-DS with SF=10. JoinBoost is ∼ 3× faster than LightGBM for random forests, and ∼ 1.3× faster than LightGBM for gradient boosting. For TPC-H, JoinBoost is slowed because of the large dimension tables (Orders and PartSupp). The messages between the fact table and these two dimension tables are large but expensive. To address this, the junction hypertree could be redesigned to reduce message sizes [35] as future works.

C.2 Parallelization

We use JoinBoost with (para) and without (w/o) inter-query parallelism, but always with intra-query optimization (4 threads per query for para and 16 threads per query for w/o), to train a tree of 8 leaves. Figure 18 shows the result.

[9]https://github.com/microsoft/LightGBM/pull/175



(a) Gradient Boosting for TPC-DS.

(b) Random Forest for TPC-DS.

(c) Gradient Boosting for TPC-H.

(d) Random Forest for TPC-H.

Figure 17: Gradient Boosting and Random Forest training time and model performance compared to the SOTA ML Frameworks. Dotted black line is the overhead of materializing the join and export join by DuckDB.

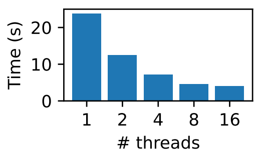


Figure 18: (a) Training time of 1 tree of 8 leaves for intra-query parallelism with a varying number of threads.

D OTHER OPTIMIZATIONS

Identity and Semi-join Message Optimizations. Snowflake schemas often exhibit a property that allows us to drop messages (and skip the associated joins) along *Identity Paths* during message passing. An identity path starts from a leaf relation (usually a dimension table), and flows along 1-to-N relationship edges, as long as each relation is not R_Y and no join key is missing. The key property is that semi-ring addition (aggregation) does not apply along the identity path due to the 1-to-N join relationships.

Let $L \rightarrow P$ connects leaf relation L to P. Each tuple $\in L$ is annotated with the 1 semi-ring element, and each tuple in P joins with exactly one tuple in L. $m_{L \rightarrow P}$ is an *Identity Message* because it doesn't change P's annotations, and thus can be dropped. Relations along the identity path are all initially annotated with 1, so this applies recursively. This optimization is used when splitting the root decision tree node.

Now suppose the best split was on attribute l in L, so the edge is now $\sigma_l(L) \rightarrow P$. Although L does not emit an identity message, we know that each tuple in the message is annotated with 1. Thus, we don't materialize the semi-ring elements as columns and can rewrite the join with P as a semi-join, and simply filter P by the join values in $\sigma_l(L)$.