Towards Scalable Dataframe Systems

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ABSTRACT

Dataframes are a popular and convenient abstraction to represent, structure, clean, and analyze data during exploratory data analysis. Despite the success of dataframe libraries in R and Python (pandas), dataframes face performance issues even on moderately large datasets. In this paper, we take the first steps towards formally defining dataframes, characterizing their properties, and outlining a research agenda towards making dataframes more interactive at scale. We draw on tools and techniques from the database community, and describe ways they may be adapted to serve dataframe systems, as well as the new challenges therein. We also describe our current progress toward a scalable dataframe system, MODIN, which is already up to 30× faster than pandas in preliminary case studies, while enabling unmodified pandas code to run as-is. In its first 18 months, MODIN is already used by over 60 downstream projects, has over 250 forks, and 3,900 stars on GitHub, indicating the pressing need for pursuing this agenda.

1. INTRODUCTION

For all of their commercial successes, relational databases have notable limitations when it comes to “quick-and-dirty” exploratory data analysis (EDA)—data needs to be defined schema-first before it can be examined, data that is not well-structured is difficult to query, and any query beyond SELECT * requires an intimate familiarity with the schema, which is particularly problematic for wide tables. For more complex analyses, the declarative nature of SQL makes it awkward to develop and debug queries in a piecewise, modular fashion, conflicting with best practices for software development. Due to these limitations, programming languages such as Python and R support the so-called dataframe abstraction, which provides a functional interface that is more tolerant of unknown data structure and well-suited to developers and data scientists, as well as their workflows, including REPL-style imperative interfaces and data science notebooks [54].

Dataframes have several characteristics that make them an appealing choice for data exploration:
- an intuitive data model that embraces an implicit ordering on both rows and columns and treats them symmetrically;
- a query language that bridges a variety of data analysis modalities including relational (e.g., filter, join), linear algebra (e.g., transpose), and spreadsheet-like (e.g., pivot) operators;
- an incrementally composable query syntax that encourages easy and rapid validation of simple expressions, and their iterative refinement and composition into complex queries; and
- native embedding in a host language such as Python with familiar imperative semantics.

Characteristics such as these have helped dataframes become incredibly popular for EDA; for instance, the dataframe abstraction provided by pandas within Python (pandas.pydata.org), has, as of 2019, been downloaded over 200 million times, served as a dependency for over 160,000 repositories in GitHub, and starred on GitHub more 22,000 times. Python’s own popularity has been attributed to the success of pandas for data exploration and data science [79]. Due to its ubiquity, we focus on pandas for concreteness.

Pandas has been developed from the ground up via open-source contributions; pandas DataFrame API operators and their implementations have been provided by dozens of contributors to satisfy immediate or ad-hoc needs, spanning capabilities that mimic relational algebra, linear algebra, and spreadsheet formula computation. To date, the pandas DataFrame API has ballooned to over 200 distinct operators [13]. R, which is both more mature and more carefully curated than pandas, has only 70 operators—but this is still far more than, say, relational and linear algebra combined [15].

While this rich API is sometimes cited as a reason for pandas’ attractiveness, the set of operators has significant redundancies, often with different performance implications. These redundancies place a considerable burden on users to select the optimal way of expressing their goal. For example, one blog post cites five different ways to express the same goal, with performance varying from 0.3ms to 600ms (a 1700× increase) [6]; meanwhile, the pandas documentation itself offers multiple recommendations for how to enhance performance [11]. As a result, many users eschew the bulk of the API, relying only on a small subset of operators [13]. The complexity of the API and evaluation semantics also make it difficult to apply traditional query optimization techniques. Indeed, each operator within a pandas “query plan” is executed completely before subsequent operators are executed, with limited optimization, and no reordering of operators or pipelining (unless explicitly done so by the user using .pipe). Moreover, the performance of the pandas DataFrame API breaks down when processing even moderate volumes of data that do not fit in memory, as we will see subsequently—this is especially problematic due to pandas’ eager evaluation semantics, wherein intermediate data items often surpass main memory limits and must be paged to disk.

In this paper, we (i) provide a candidate formalism for dataframes and enumerate their capabilities with a new algebra, and define a research agenda that builds on our formalism to make dataframes faster and more scalable, by leveraging tools and techniques from the database community; and (ii) describe our first steps toward this goal with our prototype, MODIN. MODIN (github.com/modin-project/modin) is an accelerated implementation of the pandas dataframe API, enabling unmodified pandas code to run with more efficiency and scalability; MODIN is already used by over 60 downstream projects, and has over 250 forks and 3,900 stars on
From a representational viewpoint, how do current dataframe systems evaluate each expression in its entirety after it is composed, forcing the user to wait until the result is computed; other data systems \([21]\) opt for entirely lazy evaluation, deferring computation until the user requests to inspect the result, forcing them to wait then. Instead, can we perform background computation to compute the results of query sub-expressions in the background, while still prioritizing the results that the user actively requests, giving us the best of both worlds? In doing background computation of this form, we may have many query sub-expressions concurrently being executed. How do we execute all of them while sharing computation as much as possible, prioritizing those whose results the user might examine? Then, when the user actually examines a result, the user typically previews the first or last \(k\) result rows; how do we prioritize returning these rows over the rest, especially with an ordered data model and a new algebra? We can return a response even faster by recognizing that users typically inspect intermediate results for debugging. So how do we allow users to view an approximate version of each intermediate result quickly, so that they can move on to the next step of analysis? Finally, given that users often iteratively compose queries many times over the course of a session, building on top of previously composed sub-expression results, how do we leverage materialization and reuse to accelerate computation?

In describing the aforementioned challenges, we focus on the pandas dataframe system \([14]\) for concreteness. Pandas is much more popular than other dataframe implementations, and is therefore well worth our effort to study and optimize. We will discuss other dataframe implementations and related work in Section 7. We also provide a bit of history into dataframe origins in Section 3.1. We begin our paper with an example dataframe workflow that will serve as a running example for the paper.

2. DATAFRAME EXAMPLE

Consider an analyst exploring the relationship between price, rating, and product features across different iPhone models. Figure 1 illustrates the steps taken and the results in the context of a Jupyter Notebook (https://jupyter.org). With this example, we aim to illustrate key aspects of a typical dataframe workflow.

Data ingest and cleaning. Initially, the analyst reads in the iPhone comparison chart from an e-commerce webpage, as shown in In[1] in Figure 1. The analyst prints out the first few lines of the dataframe to verify that the pandas data loading function call resulted in the expected dataframe. They do so by simply calling products. We omit this call and all subsequent calls to display dataframes to save space, and instead depict the call alongside the corresponding output. Based on this preview of the dataframe, the analyst identifies a sequence of actions for cleaning their dataset:

- **C1 [Ordered point updates]:** The front camera description for the iPhone 11 Pro has an anomalous value of 120 MP (indicated in Figure 1 in bold for emphasis), far exceeding that of other models—likely a data entry error. To fix this, the analyst performs spreadsheet-like point updates, by setting a new value for the entry at row 2 column 0 via an iloc command, as in In[2], and then verifies the output in Out[2].

- **C2 [Matrix-like transpose]:** To make it easier to compare across different products, the rows and columns should be switched, so that the rows correspond to products and the attributes correspond to features. The analyst makes this switch by transposing the data via .T in In[3] and then inspects the results in Out[3].
Ordered point updates

Matrix-like transpose

Column transformation

Read Excel

One-to-many column mapping

Joins

Matrix Covariance

Figure 1: Example of an end-to-end data science workflow, from data ingestion, cleaning, wrangling, to analysis. The variable names of the dataframes being printed are indicated on the left, and the Cleaning or Analysis phase (denoted by C or A, respectively) are indicated on the right.

Analysis. With the data cleaned and prepared, the analyst performs the following operations to analyze the data:

One-to-many column mapping: The analyst encodes categorical features as binary indicators (0/1) across multiple columns via the one-hot encoding scheme. As shown in line 1 of In[6], this encoding is invoked via the `get_dummies` function, with the results in `one_hot_df`.

Joins: To combine the information in prices with the product features in `one_hot_df`, the analyst performs a left inner join via `.merge()` on the column corresponding to iPhone model names in line 2 of In[6], and inspects the results in Out[6].

Matrix Covariance: With all the relevant numerical data in the same dataframe, the analyst now computes the covariance between all of the features via a call to `df.cov()` in In[7], with the results in Out[7].

This example demonstrated only a sample of the capabilities of dataframes. Nevertheless, it serves to illustrate the common use cases for dataframes: immediate visual inspection after most operations, each incrementally building on the results of previous ones, point and batch updates via user-defined functions, and a diverse set of operators for wrangling, cleaning, and analyzing data. Next, we formally defines the dataframe data model, and query language.

3. DATAFRAME FUNDAMENTALS

There are many competing open-source and commercial implementations of dataframes, but there is no formal definition or an enumeration of dataframe properties in literature to date. In this section, we start with a brief history (Section 3.1), and provide a reference data model (Section 3.2) and algebra (Section 3.3) to ground discussion. We then demonstrate the expressiveness of the algebra via examples (Section 3.4), and discuss extensions (Section 3.5). We finally provide some quantitative statistics into dataframe usage in Section 3.6.

3.1 A Brief History of Dataframes

The S programming language was developed at Bell Laboratories in 1976 to support statistical computation. Dataframes were first introduced to S in 1990, and presented by Chambers, Hastie, and Pregibon at the Computational Statistics conference [25]. The authors state: “We have introduced into S a class of objects called dataframes, which can be used if convenient to organize all of the variables relevant to a particular analysis...” Chambers and Hastie then extended this paper into a 1992 book [26], which states “Data frames are more general than matrices in the sense that matrices in S assume all elements to be of the same mode—all numeric, all logical, all character string, etc.” and “… data frames support matrix-like computation, with variables as columns and observations as rows.
and, in addition, they allow computations in which the variables act as separate objects, referred to by name.”

The R programming language, an open-source implementation of S with some additional innovations, was first released in 1995, with a stable version released in 2000, and gained instant adoption among the statistics community. Finally, in 2008, Wes McKinney developed pandas in an effort to bring dataframe capabilities with R-like semantics to Python, which as we described in the introduction, is now incredibly popular. In fact, pandas is often cited as the reason Python’s popularity [19], now surpassing Java and C++ [8]. We discuss other dataframe implementations in Section 7.

3.2 Dataframe Data Model

As Chambers and Hastie themselves state, dataframes are not familiar mathematical objects. Dataframes are not quite relations, nor are they matrices or tensors. In our definitions we borrow textbook relational terminology from Abiteboul, et al. [18] Chapter 3 but adapt it to our use.

The elements in the dataframe have to come from a known set of domains \( \text{Dom} = \{ \text{dom}_1, \text{dom}_2, \ldots \} \). For simplicity, we assume in our discussion that domains are taken from the set \( \text{Dom} = \{ \Sigma^*, \text{int}, \text{float}, \text{bool}, \text{category} \} \), though a few other useful domains like datetimes are common in practice. The domain \( \Sigma^* \) is the set of finite strings over an alphabet \( \Sigma \), and serves as a default, uninterpreted domain; in some dataframe libraries it is called \text{Object}. Each domain \( \text{dom} \) contains a distinguished \text{null} value, sometimes written as \text{NA}. Each domain \( \text{dom} \), also includes a \text{parsing function} \( \text{parse} \) : \( \Sigma^* \rightarrow \text{dom} \), allowing us to interpret the values in dataframe cells as domain values (including possibly \text{null}).

A key aspect of a dataframe is that the domains of its columns may be induced from data \text{post hoc}, rather than being declared \text{a priori} as in the relational model. We define a schema induction function \( S : \Sigma^* \rightarrow \text{Dom} \) that assigns an array of \( m \) strings to a domain in \( \text{Dom} \). This schema induction function is applied to a given column and returns a domain that describes this array of strings; we will return to this function later.

Armed with these definitions, we can now define a dataframe:

\textbf{Definition 3.1. A dataframe is} a tuple \((A_m, R_m, C_n, D_n)\), where \(A_m\) is an array of entries from the domain \( \Sigma^* \), \(R_m\) is a vector of row labels from \( \Sigma^* \), \(C_n\) is a vector of column labels from \( \Sigma^* \), and \(D_n\) is a vector of \( n \) domains from \( \text{Dom} \), one per column, each of which can also be left unspecified. We call \( D_n \) the schema of the dataframe. If any of the \( n \) entries within \( D_n \) is left unspecified, then that domain can be induced by applying \( S(\cdot) \) to the corresponding column of \( A_m \).

We depict our conceptualization of dataframes in Figure 2. From our example in Figure 1, the dataframe \texttt{products} in \texttt{Out[1]} has \( R_m \) corresponding to an array of labels \{Display, Camera, \ldots\}; \( C_n \) corresponding to an array of labels \{iPhone 11 Pro, iPhone Pro Max, \ldots\}. \( A_m \) corresponding to the matrix of values beginning with 5.8-inch, with \( m = 6, n = 4 \). Here, \( D_n \) is left unspecified, and may be inferred using \( S(\cdot) \) per column to possibly correspond to \{\( \Sigma^* \), \( \Sigma^* \), \( \Sigma^* \), \( \Sigma^* \)\}, since each of the columns contains strings.

Rows and columns are symmetric in many ways in dataframes. Both can be referenced explicitly, using either numeric indexing (positional notation) or label-based indexing (named notation). In our example in Figure 1, the \texttt{products} dataframe is referenced using positional notation in step C1 with \texttt{products.iloc[2, 0]} to modify the value in the third row and first column, and by named notation in step C3 using \texttt{products["Wireless Charging"]} to modify the column corresponding to "Wireless Charging". The relational model traditionally provides this kind of referencing only for columns. Note that row ordering is exogenous to the data—it \textit{need not} be correlated in any way to the data values, unlike sort orderings found in relational extensions like SQL’s \texttt{ORDER BY} clause. The positional notation allows for (row, col) references to index individual values, as is familiar from matrices.

A subtler distinction is that row and column labels are from the same set of domains as the underlying data (\text{Dom}), whereas in the traditional relational model, column names are from a separate domain (sometimes called \texttt{att} [18]). This is important because there are dataframe operators that copy data values into labels, or copy labels into data values, discussed further in Section 3.3.

Despite the notational symmetry between rows and columns, \( D_n \) introduces a \textit{schematic asymmetry} that we will need to reason about. Consider a schema like \( D_n = \{ \text{category}, \text{int}, \text{float} \} \). Note that the column types differ, but the type of each row is the same (namely \{\text{category}, \text{int}, \text{float}\}). Moreover, each column has a single domain (an atomic type), but each row has a vector of domains (a tuple type). Once seen through the lens of a schema and its parsing functions, rows and columns are quite different.

When the schema \( D_n \) has the same domain \text{dom} for all \( n \) columns, we call this a \textit{homogeneous} dataframe, and its rows and columns can be considered symmetrically to have the domain \text{dom} differing only in dimension. As a special case, consider a homogeneous dataframe with a domain like \text{float} or \text{int} and operators +, × that satisfy the algebraic definition of a field. We call this a \textit{matrix} dataframe, since it has the algebraic properties required of a matrix, and can participate in linear algebra operations simply by parsing its values and ignoring its labels. The dataframe \texttt{iphone_df} in \texttt{Out[6]} in Figure 1 is one such example; thus it was possible to perform the covariance operation via \texttt{.cov()} in step C3.

When the domain for any column is left unspecified, it can be induced via the schema induction function \( S \). In doing so, \( S \) must examine every value in that column to determine the most specific domain from \text{Dom} that can be used to classify the data in that column. Since \( S \) is applied by the system on-demand, it can be done lazily or eagerly, presenting optimization opportunities that we will describe later on. For example, the \texttt{map} operation in step C3 in Figure 1 involves a function that explicitly transforms elements in a given column into boolean values, allowing us to infer the output type for that column. As another example, prior to the \texttt{.cov()} operation in step A3, we need to verify that the dataframe is a matrix dataframe; this could be done lazily when the \texttt{.cov()} is called.

In summary, a dataframe can be viewed in two equivalent ways. From a relational viewpoint, dataframes are ordered relations with named rows and a lazily-induced schema. From a linear algebra viewpoint, dataframes are heterogeneous matrices with added labels for rows and columns. We will exploit these two viewpoints in our dataframe algebra to allow us to define both relational and linear algebra operations.

\textit{Data model Comparisons}

Before we go on, we address some key distinctions between dataframes and other familiar data models.

\textbf{Comparison with matrices.} All matrices can be represented as dataframes (with null labels). Not all dataframes can be matrices, however, even if we strip off their labels! Matrices are homogeneous in schema, but dataframes allow for schemas with multiple domains. Even if we ignore the schema, a dataframe is still not a matrix—opaque strings from \( \Sigma^* \) do not satisfy the properties of a field as required by a matrix.

\textbf{Comparison with relational tables.} A relation is defined by a declared schema, and there are many possible \textit{instances} of a relation—sets of tuples that satisfy the schema. An instance can be thought of as a fixed relational table. Dataframes are something like rel-
tion instances: they represent a fixed set of data. However their schema can be unspecified and hence induced based on their content by a schema induction function \( S \). This flexibility is critical to dataframes.

Moreover, dataframes impose an ordering and naming on their rows. Object-oriented relational extensions such as the Postgres data model also introduced implicit row identifiers \([59]\), but typically relational models do not impose a row ordering. Of course, we can capture this semantics in a relational model via design discipline: we can ensure that all our relations have a unique key (for naming), and an ordering key (for ordering), which are exogenous to the actual data columns in the table. In this sense, all dataframes can be represented as relation instances conforming to some (potentially induced) schema with appropriate keys.

Even so, a key difference between dataframes and relations is the symmetry between rows and columns. This aspect, along with the freedom to induce a schema on a per-instance basis, make it possible to define a transpose operator on dataframes. Since the underlying representation is uninterpreted, we are free to induce a different relational schema after transposition of a dataframe.

**Comparison with spreadsheets.** At a high level, a spreadsheet is an array of heterogeneously-typed cells that may contain strings or formulae. A spreadsheet thus stores code as well as data. The strings are dynamically interpreted into a variety of domains. It is tempting to think of formula-free spreadsheets as being similar to dataframes, given the common row/column indexing scheme and the dynamic typing. But in general they are quite different. The data representations possible in spreadsheets are quite free, and in practice often quite irregular. Dense regions of data are often interspersed with empty regions, or with cells containing comments and other forms of human-centric annotation or metadata. Spreadsheets have a notion of a “range”—a subarray or even a set of subarrays—which may be sparsely located in the data grid and represent diverse or unrelated data sets stored in the same spreadsheet. As a result of this freedom of structure, bulk algebraic operations are difficult to define generally within spreadsheets. Some modern spreadsheets allow a range to be labeled as a “table” that is interpreted with a schema and maintains an ordering; further extensions to “pivot tables” allow for row and column labels. Using these constructs it is possible for a spreadsheet to represent one or more dataframes. But the relative simplicity of dataframes enables a much simpler algebra and easier implementation and optimization of the algebra’s operators.

### 3.3 Dataframe Algebra

We now propose an algebra that encompasses the functionality provided by dataframe implementations like pandas and R. The purpose of this section is to help frame the dataframe definition and explicitly contrast dataframe algebra with relational algebra. We do not argue that this set of operators is minimal, but we do feel it is both expressive and elegant; we demonstrate via examples in Section 4 how these operators can express various functions in pandas. Based on the contrast with relational algebra, we are in a position to articulate research challenges in optimizing dataframe algebra expressions in subsequent sections.

To the best of our knowledge, an algebra for dataframes has never been defined previously. Recent work by Hutchinson et al. \([55,57]\) proposes an algebra called Lara that combines linear and relational algebra, exposing only three operators: JOIN, UNION, and Ext (also known as “flatmap”); however, the operators below that manipulate metadata would not be possible in Lara without placing the metadata as part of the data. Other differences stem from the flexible data model and lazily induced schema. That said, as we continue to refine our algebra, we will draw on Lara as a reference.

We list the algebra operators we have defined in Table 1; the rows correspond to the operators, and the columns correspond to their properties. The operators encompass ordered analogs of extended relational algebra operators (from \textit{SELECT} to \textit{RENAME}), one operator that is not part of extended relational algebra but is found in many database systems (\textit{WINDOW}), as well as four new operators (\textit{TRANSPOSE}, \textit{MAP}, \textit{TOLABELS}, and \textit{FROMLABELS}). We briefly describe the first two categories first, followed by the three new operators.

The ordered analogs of the extended relational algebra operators preserve the ordering of the input dataframe(s). If there are multiple arguments, the result is ordered by the first argument first, followed by the second. For example, \textit{UNION} simply concatenates the two input dataframes in order, while \textit{CROSS-PRODUCT} preserves a nested order, where each tuple on the left is associated, in order, with each tuple on the right, with the order preserved. The operator \textit{WINDOW} is straightforward: \textit{WINDOW} applies a sliding window function, in order, to values present in a subset of columns. This application is similar to window functions in SQL \([43]\), supporting the computation of windowed aggregates such as cumulative sum.

It is important to point out that the presence of a schema induction function means that the output schema of certain operators like \textit{TRANSPOSE} can be defined to be unspecified (see the Schema (\textit{D}) column in Table 1), meaning they are unknown in the absence of a specific array of data. This can lead to runtime type errors in algebraic expressions based on the values of data in the inputs, which is impossible in either relational or linear algebra. Due to this feature, it is no surprise that dataframes are most natural in languages like Python and R, which support dynamic typing and runtime type errors.

Note that languages choose different approaches to inferring the schema after a \textit{TRANSPOSE} with important implications for usability. For example, in R, a \textit{TRANSPOSE} with heterogeneous \( D_n \) ends up coercing everything to \textit{string}, which may make it impossible to apply another \textit{TRANSPOSE} and yield a dataframe equivalent to the original \( D_n \). In Python, everything is coerced to \textit{Object}, which has typing information embedded at runtime, so the schema induction function can always recover the original \( D_n \) after two transposes.

The output schema for most other operators one would find in a relational database can be carried over from the inputs (indicated as preserved in Table 1).

**Transpose.** \textit{TRANSPOSE} interchanges rows and columns, so that the columns of the dataframe become the rows, and vice-versa. Formally, given a dataframe \( DF = (A_{mn}, R_m, C_n, D_n) \), we define \textit{TRANSPOSE}(\textit{DF}) to be a dataframe \( (A_{mn}^T, C_m, R_n, null) \), where \( A_{mn}^T \) is the array transpose of \( A_{mn} \). Note that the schema of the result may be induced by \( S \), and may not be similar to the schema of the input. \textit{TRANSPOSE} is useful both for matrix operations on homogenous dataframes, and for data cleaning or for presentation of “crosstabs” data. In step C2 in our example in Figure 1, the table was not oriented properly from ingest, and a transpose was required to give us the desired table orientation.

In pandas and other dataframe implementations, it is possible to perform many operations along either the rows or columns via the \textit{axis} argument. Instead, to minimize redundancy, we define operators on collections of rows, as in relational algebra, and enable operations across columns by first performing a \textit{TRANSPOSE}, applying the operation, and then a \textit{TRANSPOSE} again to return to the original orientation. That said, performing \textit{TRANSPOSE} can be expensive (as we will see in Section 4), so one of our goals will be to postpone performing it or avoid it entirely. Moreover, given the presence of \textit{TRANSPOSE} in the algebra, we need to be prepared to...
handle dataframes that are not only extremely high in cardinality ("tall") but also extremely high in arity ("wide").

The asymmetry of row and column types in the relational model makes TRANSPOSE impossible to define for relations with non-homogeneous column domains (for which the sets in \( D_n \) differ): there is no data-independent way to derive a relational output schema for TRANSPOSE from the input schema. In the dataframe data model, the data-dependent schema induction function provides an output schema.

**Map.** The map operator takes some function \( f \) and applies it to each row individually, returning a single output row of fixed arity. The purpose of the map operator is to alter each dataframe row uniformly. MAP is useful for data cleaning and feature engineering (e.g., step 3 in Figure 1). Given a dataframe \( DF = (A_{mn}, R_m, C_n, D_n) \), the result of \( MAP(DF, f) \) is a dataframe \( (A'_{mn'}, R_m, C'_n, D'_n) \) with \( f : D_n \rightarrow D'_n \), where \( A'_{mn'} \) is the result of applying function \( f \) to each row, \( C'_n \) is the resulting column labels, and \( D'_n \) is the resulting vector of domains. Notice that in this definition, the number of columns (\( n' \)) and the column labels (\( C'_n \)) can change based on this definition, but they must be changed uniformly for every row. The vector of domains \( D'_n \) may, in many cases, be inferred from the type of the function \( f \).

Extended relational algebra supports map via the use of functions in the subscripts of projection operators (i.e., in the `SELECT` clause of SQL). However, this projection syntax is linear in the arity of the relation, which is cumbersome for very wide schemas (e.g., after a TRANSPOSE). In this definition, MAP is passed an entire row as an argument so it can reason across columns in a generic fashion without enumerating them, whereas SQL expressions (including UDFs) typically require specific fields from the row as scalar arguments. For example, consider a transformation that needs to ensure every row. The vector of domains \( D'_n \) may, in many cases, be inferred from the type of the function \( f \).

**ToLabels.** The TOLABELS operator projects one column out of the matrix of data, \( A_{mn} \), to be set as new row labels for the resulting dataframe, replacing the old labels. Given \( DF = (A_{mn}, R_m, C_n, D_n) \) and some column label \( L \), \( TOLABELS(DF, L) \) returns a dataframe \( (A_{mn(n-1)}, L, C_n, D'_n) \), where \( C_n \) (respectively \( D'_n \)) is the result of removing the label \( L \) from \( C_n \) (respectively \( D_n \)). With this capability, data from \( A_{mn} \) can be promoted into the metadata of the dataframe and referenced by name during future interactions.

From a relational perspective, this operator is rather unusual in that it converts data into metadata. Dataframe users are interested in wrangling and cleaning data, so operations that let them move entries between metadata and data are popular and convenient to use. In fact, TOLABELS followed by TRANSPOSE is, in effect, promoting data values into column labels, which is impossible using relational operators.

**FromLabels.** FROMLABELS creates a new dataframe with the row labels inserted into the array \( A_{mn} \) as a new column of data at position 0 with a provided column label. The data type of the new column starts as `null` until it can be induced by the schema induction function \( S \). The row labels of the resulting dataframe are set to the default label: the order rank of each row (positional notation). Formally, given a dataframe \( DF = (A_{mn}, R_m, C_n, D_n) \) and a new column label \( L \) we define \( FROMLABELS(DF, L) \) to be a dataframe \((R_m + A_{mn}, P_n, [L] + C_n, [null] + D_n)\), where \( R_m + A_{mn} \) is the concatenation of the row labels \( R_m \) with the array of data \( A_{mn}, P_n \) is the positional notation values for all of the rows: \( P_n = (0, \ldots, m - 1) \), and \([L] + C_n \) is the result of prepending the new column label \( L \) to the column labels \( C_n \).

FROMLABELS is the opposite of the TOLABELS operator, and the two of these give the user complete control over moving data to and from the dataframe’s labels. This allows users to apply operators on the dataframe’s metadata (specifically the row labels), which is particularly useful for operators like JOIN and GROUPBY. Conceptually, this operator also allows the positional notation of the dataframe to be treated as data if multiple FROMLABELS are chained together. However, because the order is immutable, it is impossible to update the order of the dataframe directly in this way. Despite providing the ability to promote data to row labels (named notation), it is impossible in this algebra to promote data to positional notation. If the users wished to reorder the data, they may JOIN with another dataset with a specific order or SORT based on some column(s).

From a relational point of view, FROMLABELS enables the capability to push metadata into the data to be queried and operated on. Thanks to this operator and TOLABELS specifically, column and row labels must be of type \( \Sigma^* \) so that these operators make sense. FROMLABELS also has some interesting interaction with the schema induction function \( S \), where labels can be interpreted as any type in \( Dom \) when they are added to the data via FROMLABELS and then operated on. It is important to point out here in the definition, but we leave the enumeration of the nuances of this interaction to future work.

3.4 Rewriting Examples

To demonstrate the expressiveness of the algebra above, we show how it can be used to capture a range of pandas functions.

To start off, many pandas functions provide essentially identical functionality to dataframe operators, e.g., `sort_values` for `SORT`, `merge` for `JOIN`, `groupby` for `GROUPBY`, `append` for `UNION`, `reset_index` for `FROMLABELS`, and `set_index` for `TOLABELS`. | Operator | Metadata | Data | Schema (\( D \)) | Origin | Order | Description |
|---|---|---|---|---|---|---|
| **SELECTION** | × | static | REL | Parent | Eliminate rows |
| **PROJECTION** | × | static | REL | Parent | Eliminate columns |
| **UNION** | × | static | REL | Parent | Set union of two dataframes |
| **DIFFERENCE** | × | static | REL | Parent | Set difference of two dataframes |
| **CROSS-PRODUCT / JOIN** | × | static | REL | Parent | Combine two dataframes by element |
| **DROP DUPLICATES** | × | static | REL | Parent | Remove duplicate rows |
| **GROUPBY** | × | static | REL | New | Group identical attributes |
| **SORT** | × | static | REL | New | Lexicographically order rows |
| **RENAME** | × | static | REL | Parent | Change the name of a column |
| **WINDOW** | × | static | SQL | Parent | Apply a function via a sliding-window (either direction) |
| **TRANSPOSE** | × | dynamic | DF | Parent | Swap data and metadata between rows and columns |
| **MAP** | × | inferred/dynamic | DF | Parent | Apply a function uniformly to every row |
| **TOLABELS** | × | dynamic | DF | Parent | Set a data column as the row labels column |
| **FROMLABELS** | × | dynamic | DF | Parent | Convert the row labels column into a data column |

Table 1: Dataframe Algebra. †: Ordered by left argument first, then right to break ties. ©: Order of columns is inherited from order of rows and vice-versa.
The function `transform` is a special case of `MAP` that applies a fixed function to each value within a row, thereby preserving the input arity, while apply is another special case where a fixed function is applied on a per-row-basis to combine values across multiple columns to generate a new column.

A number of pandas functions correspond to dataframe operators, with specific UDFs. As examples for `WINDOW`, `cummax` computes the cumulative max of values for one or more columns, `diff` takes the difference between elements in a column and preceding values, and `shift` shifts rows down to align with a new row label, maintaining the order of the data. Likewise, for `MAP`, `fillna` converts all null values to another value, `iina` replaces each value with a boolean based on whether or not they are null, and `str.upper` converts all the string values to upper case. In fact, pandas has many functions that implement string and date-time transformations.

Finally, there are several pandas functions that are compositions of dataframe operators. We list a few examples below, with informal descriptions on how they may be rewritten using the algebra.

The pandas function `transform` function in pandas computes aggregate functions `f1`, `f2`, ..., for each of the columns individually, with the result containing dataframe corresponding to one per aggregate, i.e., the first row corresponds to the f1 aggregate, the second to the f2 aggregate, and so on. This function can be rewritten using one `GROUPBY` operator per aggregate function to produce a single row corresponding to the aggregates, followed by a `UNION` to append these rows to each other in the order the aggregates are listed. Another approach is to perform a `TRANSPOSE`, then a `MAP` to compute all the necessary aggregates, one per column, followed by another `TRANSPOSE` to bring the result to the right orientation.

The pandas function `target` function supports changing a given dataframe (the target) by reordering its rows and columns to match those of another dataframe (the reference). This operator is useful for aligning two dataframes for comparison purposes. One way to express this function using dataframe operators would be to first `FROMLABELS` on both dataframes to allow the row labels to become part of the data, followed by a `JOIN` between the two dataframes on the row labels, with the reference as the left operand; followed by a `MAP` to project out the reference dataframe attributes (leaving behind reference's ordering). Finally, `TOLABELS` can be used to move the row labels back from the data.

In pandas, the pivot operator elevates data into the column labels and creates a new dataframe reshaped around the new column labels (see Figure [3]). A pivot operator has been implemented in relational systems before [23], but it is simpler to express in the algebra from Section [3.3] primarily because there is no need to know the names of the new columns a priori. Recall that it is possible to elevate data to the column labels by using `TOLABELS` followed by `TRANSPOSE`. In this case, the `TOLABELS` operator would be applied on the label of the column being pivoted over. After this step, we perform a `GROUPBY` on the other attributes followed by the `MAP` operator with a function that transforms the grouped data into the correct orientation. This will result in a table pivoted around the attribute selected for the `TOLABELS` operator.

### 3.5 Extensions to the Formalism

Our data model so far is quite simple. We now describe a few additional extensions for our data model that do not provide any additional expressive power, but make certain operations more convenient.

#### Multiple label columns

The data model can, optionally, have multiple row label columns or multiple column label rows. Often, these are presented in a hierarchical or nested manner in pandas. As an example, in a dataframe tabulating sales, we could have two row label rows that are nested, with the first (external) row label row corresponding to the years, and the second (internal) row label row corresponding to the quarters within each year. In our representation, we can simply capture this by repeating the external row label values, and combining the row label columns to give a single composite value, as shown below:

\[
\begin{array}{ccc}
2017 & Q1 & (2017, Q1) \\
2018 & Q1 & (2018, Q1) \\
\end{array}
\]

#### Label flexibility and types

Row labels can have a predefined type or domain from `Dom`—this type can be recorded separately and used to augment the schema `Dn` when performing an AS `LABELS` operation, thereby avoiding having to induce it using `S`. Due to the symmetry between columns and rows, column labels also have this constraint. Additionally, labels can have duplicate values or be null; so labels are not like primary keys.

We finally define another notion that will come in handy in future sections: a dataframe-like system is one that supports some, but not all dataframe properties as defined in the data model and algebra above. For example, a dataframe-like system might support unordered weakly-typed relations, with queries being composed incrementally over the course of many statements.

We return to this notion and provide some example systems in Section [7].

### Workflow Definitions

We now briefly introduce some terms that will allow us to describe how dataframes are manipulated during a data analysis workflow.

**Operator.** A dataframe operator, or simply an operator, is an atomic dataframe processing step that takes multiple dataframe arguments and returns a dataframe as a result. We will describe the operators in the context of the dataframe algebra in Section [3.3].

**Statement.** A dataframe statement is an expression composed entirely of dataframe operators and is the unit of interaction between the user and the system. In a notebook environment, a statement corresponds to a single cell; each of which is executed one at a time, as we saw in Figure [1]. In an interpreted environment (e.g., IPython), a statement is a single block of code.

**Query.** A sequence of statements chained together form a dataframe query. Following variable references, a query can be represented as a DAG of operators and dataframes, with the input dataframes at the leaves, and the queries as the root(s). A dataframe query is analogous to a SQL query, but it is composed incrementally across many statements.

**Session.** A session is a complete, end-to-end analysis workflow, comprising one or more queries issued across many statements. A session begins when the user starts a notebook or interpreter environment and ends when the user shuts down that environment.
3.6 Dataframe Usage Statistics

To study how dataframe users interact with the pandas API, we analyzed a comprehensive dataset of 1 million Jupyter notebooks hosted on GitHub from Rule et al. [6]. Out of the 1 million Jupyter notebooks, about 40% used pandas. We used the jupyter nbconvert module to convert each notebook into a python script, the 2to3 module to transform python 2 to python 3, and the python ast module to parse and extract method invocation calls. We note that there may be some issues in our extraction; for example, `append` is both a python built-in list method as well as a pandas method. However, we expect our trends to largely hold.

We will focus on three questions to investigate how people work with pandas.

What are some high-density functions used in interactive analysis? We studied the total occurrence of each pandas dataframe function in our data. The most notable ones are those used to inspect the data (plot, shape, head), perform numeric aggregation (mean, sum, product), and perform relational operations (groupby, join). It is worth noting that the notebooks contained a lot of data modification operations (both point queries as well as column and row queries) using `loc`, `iloc`, `drop`, `append`. Columns and index metadata inspection and manipulation are common as well with `index`, `columns`.

What kinds of functions are common in day-to-day usage? We counted the number of files that each pandas function has occurred in. The occurrence measures the frequency of usage per analytic job. The most commonly used functions are those that create dataframes (`read_csv, DataFrame`), inspect partial results (head, shape), visualizing result (plot), perform aggregation (mean, sum, max), perform point queries (loc, iloc, ix), add or remove data (append, drop), apply arbitrary user defined transformations (apply), and perform relational operations (groupby, join). It is worth noting that type-casting (astype) and direct access or manipulation of columns and index metadata, and underlying data storage (columns, index, values) are also high in the list.

Which functions are common used together? We also investigated the number of co-occurrence of functions in the same line of code. This typically involves the user chaining pandas functions together or calling them inside a single invocation. For example, `df.dropna().describe()` is fairly common across our sample. It is also common for pandas users to perform multiple operations in single execution cell. For example, `print(result = df["col1"].mean(), df["col1"].max())` prints a tuple of summary statistics. The popularity of chained or parallel invocation suggests opportunities for acceleration, going beyond one operation at a time to more complex queries.

4. THE MODIN DATAFRAME SYSTEM

MODIN is our open-source dataframe system that implements the data model and algebra described in Section 3. The MODIN source-code is available at [https://github.com/modin-project/modin](https://github.com/modin-project/modin). MODIN supports the pandas API by rewriting the API calls into a sequence of algebraic operators. MODIN is implemented in Python using over 30,000 lines of code and emulates all the functionality of pandas.DataFrame, pandas.Series, and pandas utilities (e.g., pd.concat), while also yielding substantial (30x) speedups over pandas for certain operations. To use MODIN instead of pandas, users can simply invoke “import modin.pandas”, instead of “import pandas”, and proceed as they would with pandas. In this section, we outline MODIN’s architecture and describe an initial set of optimizations we have implemented in MODIN.

4.1 The MODIN Architecture

MODIN’s architecture is modular for easy integration of new storage and execution engines, APIs, and optimizations. It consists of four layers: the API layer, the query processing and optimization layer, the execution layer, and the storage layer, shown in Figure 5.

API layer. Users can leverage MODIN via a pandas-based API, or directly via a leaner and simpler MODIN API based on the algebra in Section 3.3. In either case, the API layer translates each call into a dataframe algebraic expression, and passes that to the next layer for execution. The layer isolates users from changes to the layers below, while allowing users to leverage the API modality they are most comfortable with. Future implementations may support other user APIs for working with dataframes, such as SQL or relational algebra. Our pandas-based API currently supports about 150 of over 200 pandas dataframe APIs, and rewrites each of them into dataframe algebraic expressions.

Query processing and optimization layer. As shown in Figure 5, the query processing layer follows a “narrow waist” design, exposing a small API based on the dataframe algebra, and implements the data model from Section 3.2. This layer parses, optimizes, and executes dataframe queries with the help of layers below. As we will describe in Section 4.2, MODIN leverages parallel execution

1MODIN’s name comes from the Korean word for every, as in every pandas operator or every dataframe API.
of dataframe queries on multiple dataframe partitions, scheduled on execution engines in the next layer. This layer also keeps track of dataframe metadata including row labels, column labels, and column data types. Recall that data types may not be specified on dataframe creation, so MODIN induces types on-the-fly (using the $S$ function) when needed for a specific operation.

**Execution layer.** MODIN supports distributed processing of dataframe partitions using two execution frameworks: Ray [48] and Dask [29]. Both Ray and Dask are task-parallel asynchronous execution engines exposing an API that requires defining a task or function and providing data for the task to run on. Integration of a new execution framework is simple, often requiring fewer than 400 lines of code.

**Storage layer.** MODIN’s modular storage layer supports both main memory and persistent storage out-of-core (also called memory spillover), allowing intermediate dataframes to exceed main-memory limitations while not throwing memory errors, unlike pandas. To maintain pandas semantics, the dataframe partitions are freed from persistent storage once a session ends.

### 4.2 Existing Optimizations

We have started exploring two classes of optimizations within MODIN: parallel execution and support for billions of columns.

**Parallel execution.** Parallelization is commonly used to improve performance in a relational context due to the embarrassingly parallel nature of relational operators. Dataframes have some unique properties and requirements that enable different degrees of parallelism depending on the data dimensions and operations being performed. Some operations, e.g., MAP, are embarrassingly parallel and can be performed on each row independently. In contrast, WINDOW operations do not admit row-wise parallelism because computation for each subsequent row must wait for the result of the prior row. Our current simple approach to partitioning is to do it on a per-operation basis, and to pick between row-based (i.e., each partition has a collection of rows), column-based (i.e., each partition has a collection of columns), or block-based partitioning (i.e., each partition has a subset of rows and columns), depending on the operation. Each partition is then processed independently by the execution engine, with the results communicated across partitions if need be. For example, MAP, in general, requires row-based partitioning, but in certain cases, depending on the function, could also use column-based or block-based partitioning, e.g., when we are replacing all null values with another predetermined value. On the other hand, when applying WINDOW functions on multiple columns, or GROUP BY aggregates on multiple columns, column-based partitioning could be a good option. Finally, TRANSPOSE, especially on dataframes that have many rows and columns, can be done more efficiently with block-based partitioning, as we will discuss next.

**Supporting billions of columns.** Most modern database systems cannot support tables with billions of columns; however, with the dataframe algebra, it is possible to TRANSPOSE a dataframe with billions of rows into one with billions of columns. In many settings, e.g., when dealing with large graph adjacency matrices in neuroscience or genomics, the number of rows and number of columns can both be very large. For these reasons, MODIN treats rows and columns essentially equivalently, modulo $S(\cdot)$, as discussed in Section 4.2. In particular, for transposing a large dataframe, MODIN uses block-based partitioning on the large dataframe, where each block consists of a subset of rows and columns. Each of the blocks are individually transposed, followed by a simple change of the overall metadata tracking the new locations of each of the blocks.

We evaluated MODIN’s performance against that of pandas using microbenchmarks on an EC2 x1.32xlarge (128 cores and 1.952 GB RAM) node using a New York City taxicab dataset [50] that was replicated 1 to 11 times to yield a dataset size between 20 to 250 GB with up to 1.6 billion rows. We consider four queries:

- **map:** check if each value in the dataframe is null, and replace it with a TRUE if so, and FALSE if not.
- **groupby (n):** group by the non-null “passenger_count” column and count the number of rows in each group.
- **transpose:** swap the columns and rows of the dataframe and apply a simple (map) function across the new rows.

We wanted to highlight the difference between one group and $n$ groups, because in a group by with $n$ groups, it is important to be careful about data shuffling, while a single group is a simple aggregation that can use any partitioning scheme. We include transpose followed by a map (in this case, an identity function, to verify that the transpose completed correctly) to demonstrate that MODIN can handle data with billions of columns. This query also shows where pandas crashed or did not complete in more than 2 hours.

Figure 4.2 shows that for the group by (n) and group by (1) operations, MODIN yields a speedup of up to $19 \times$ and $30 \times$ relative to pandas, respectively. For example, a group by (n) on a 250GB dataframe, pandas takes about 359 seconds and MODIN takes $18.5 \times$ seconds, a speedup of more than $19 \times$. For map operations, MODIN is about $12 \times$ faster than pandas. These performance gains come from simple parallelization of operations within MODIN, while pandas only uses a single core. During the evaluation of transpose, pandas was unable to transpose even the smallest dataframe of 20 GB ($\approx150$ million rows) after 2 hours. Through separate testing, we observed that pandas can only transpose dataframes of up to 6 GB ($\approx6$ million rows) on the hardware we used for testing.

These performance numbers are preliminary results that demonstrate the promise of our approach. We plan to perform further analyses in support of future optimizations.

5. **Optimizing Dataframe Queries**

In this section, we discuss research challenges in efficiently supporting the dataframe data model and executing dataframe algebraic expressions. In the next section, we discuss additional optimization opportunities that stem from how dataframes are actually operated on over the course of a session, i.e., incremental construction of queries, with inspection of intermediate results for debugging.

As we discussed previously, the dataframe data model neither corresponds to relations nor to matrices—supporting this model efficiently leads to new challenges in data representation, memory management, indexing, and metadata management. Subsequently, we discuss challenges in efficiently executing dataframe algebraic expressions, which encompasses ordered relational operations, as well as other types of operations; we discuss pipelining, rewriting, cost modeling, and optimization.

**Physical data representation.** Since dataframes are a hybrid of relations and matrices, there are opportunities to leverage, combine, and extend physical data layout approaches from the database and scientific computing communities.

From a relational context, current approaches for representing dataframes, e.g., in pandas, do not observe physical data independence. In particular, the dataframe is physically stored in the same conceptual order defined by the user. This constraint is not necessary, and removing it may open up certain optimization opportunities.
For example, a sort operation can be “conceptual” in that a new order can be defined without actually performing the expensive sorting operation. Likewise, a transpose operation doesn’t require the data to be reoriented on physical storage unless beneficial for subsequent operations, with metadata being updated to reflect the new orientation of the dataframe.

Extending physical data independence even further, the database community has explored many ways for physically representing relations, optimized for the types of operations being performed. For example, columnar storage, or row-column hybrid storage may be beneficial [17]. Finally, drawing on the scientific computing [27], array database [62] or spreadsheet context [23], ordered tabular data can also be represented via key-value pairs, where the key corresponds to the (row number, column number) pair. This representation is especially effective when the dataframe is “sparse”, allowing us to omit pairs where the value is null. Automatically detecting the right representation, and updating it over the course of dataframe query execution, is a substantial challenge.

One possible starting point for an in-memory representation format is Apache Arrow [10], an efficient in-memory column store that aims to be a cross-language standard for flat and hierarchical tabular data, with high-performance compute kernels. Arrow is not designed to be a user-facing dataframe library, but instead aims to be the canonical in-memory tabular storage format across systems. In fact, MODIN uses Apache Arrow for serialization of dataframe partitions when they being shuffled. However, Arrow’s representation does not support vectors of row labels \( R_i \) (unlike our model), nor does it support TRANSPOSE; it is also not clear what the new column labels of a TRANSPOSE would be without any row labels.

**Buffer management and partitioning.** Once we have decided on a data representation, the next question is where to store it. Current dataframe systems, e.g., pandas, operate on modest-size datasets that fit in the RAM of a single machine. Supporting larger datasets can be achieved by exploiting a memory hierarchy, e.g., by spilling data to secondary storage via out-of-core algorithms, or using a paginated buffer cache as in traditional database systems, or by exploiting the aggregate RAM across many machines using data partitioning (“sharding”). None of these techniques are new, but the requirements of the data model and diversity of access patterns lead to additional challenges beyond prior work. The design space is further complicated by technology trends, such as the use of GPU acceleration for matrix operations, as well as multi-level storage hierarchies in new hardware and cloud storage services, and the ability to autoscale cloud resources (including RAM) for bursts of memory- and compute-intensive work. Vectorization of execution is important for certain dataframe operations and depends heavily on the physical data layout. Compression [17] can be important for minimizing memory footprint and improving I/O bandwidth as in columnar databases, but may be a bad fit to certain access patterns.

**Indexing and views.** Given a certain physical representation, operations on dataframes, from a relational perspective, often make use of ordered access, e.g., editing the \( i \)th row, as well as access based on the row labels, e.g., filtering based on row labels. Automatically maintaining indexes for this purpose can be beneficial. Recent work has developed positional indexing [24], allowing ordered access to be supported in \( O(\log n) \), in the presence of edits (e.g., adding or removing rows). Column stores take a different approach to avoid expensive edits across columns, instead recording edits separately as deltas, and periodically merging them back in [17]; it would be interesting to see which approach works better given a certain set of operations. Similarly, for matrices, accesses often happen in a row-major or column-major order, and identifying the right indexes to efficiently support them in conjunction with relational-style accesses, is an important challenge. In particular, when a dataframe has many rows and many columns, we may need both row- and column-oriented indexing.

Another approach to speed up dataframe queries would be to defer the creation of new dataframes as a result of queries and instead allow for the results of dataframe queries to be essentially non-materialized “views”. This could be useful, for example, when a dataframe query essentially adds a new derived column for feature engineering. In this case, we don’t actually add the derived column and create a new dataframe, simply recording the operations instead, and materializing the result on-demand. Deferring the operations also opens up opportunities for pipelining through subsequent operations, saving overall computation costs. In fact, the Vaex project [16], which is a dataframe-like system (as we described in Section 3.2) that supports querying on HDF5 files, implements virtual columns. With virtual columns, the column is not actually materialized until required for output, printing, or for a query. In cases where the computation that creates a column is expensive, virtual columns will need to be paired with intelligent caching mechanisms that prioritize caching columns that were expensive to generate.

**Metadata management.** An important new concern in dataframes, since they are lazily typed, is when and how to infer the types of columns and maintain them across operations. One approach is to defer type inference to when the operation is performed. However, this could lead to errors being detected too late, e.g., an arithmetic operation on a given column, which contains numbers except for a string in the \( n \)th row that throws an error. If, instead, we kept track of the types after operations, e.g., a given column contains mainly floats, except for strings in positions \( n_1, n_2, \ldots, n_k \), this could accelerate the detection of such errors. However, maintaining this typing information also introduces overhead, and therefore must be balanced against the potential benefit. Types are often cumbersome to detect after a transpose; to ameliorate this, types could also be maintained at both the row and column level across operations, allowing type inference to be faster. For example, in Figure 1 if we had detected that each row in Out[1] had a uniform type, we could have skipped columnar type inference after a transpose.

**Pipelining and rewriting.** The next challenge emerges when processing queries involving the new dataframe algebra. Existing data-
frame systems execute queries in an imperative way, one step at a
time, and do not perform any query rewriting. Pipelining
is performed only when explicitly requested using the pipe
command. Pipelining can prove to be effective in reducing
latencies; for example, instead of materializing the result in-between
two map operations, we could use pipelining to perform both at the
time.

With respect to rewriting rules, some of the same rewriting rules apply
to the ordered analogs of relational algebra, but many don’t.
For example, \( R \Join S \neq S \Join R \); however, this identity can be
repaired if the right hand side is subject to an additional sort of the
rows and a rearranging of the columns. Likewise, the set oriented
operations do not obey commutativity due to an incorrect output
order, but the incorrect order can be fixed with an appropriate sort-
ing of the result rows and columns. However, filters still commute
even under ordered semantics, when combined with the ordered rela-
tional operations. The \( \text{T} \text{RANSPOSE} \) operation
presents some particularly interesting opportunities and challenges,
in some cases the operation itself can be avoided entirely using
clever rewrite rules. For example, the query \( \text{T} \text{RANSPOSE}, \text{SORT}, \text{T} \text{RANSPOSE} \) to reorder columns can be rewritten as a
\text{MAP} and \text{REN}AME. And a query \( \text{T} \text{RANSPOSE}, \text{SELECTION}, \text{T} \text{RANSPOSE} \) to drop columns can be rewritten similarly.

\text{Cost modeling and optimization.} Once we have rewrite
rules, the next step is to support cost modeling and query optimization.
Current dataframe users perform manual query optimization by trying
out various possible rewritten query variants to find one with low
latency, often turning to external resources for guidance. Unlike
Selinger-style query optimization, where the notion of inter-
esting orders is simply for performance reasons, here, ordering is
a first-class citizen, and therefore, gains special prominence. Thus,
operations that generate the output in the “correct order”, e.g., a
nested loop join as opposed to a hash join, are more valuable. When
employing partitioned parallelism, query optimization becomes even
more challenging, since it may be beneficial to change the partition-
ing scheme between operations. For example, we may start with a
row-oriented partitioning well-suited for map operations, followed
by re-partitioning to a block-oriented partitioning to allow for an
efficient transpose. Determining how and when to repartition in the
query plan is an interesting challenge.

\text{Summary.} Overall, there is a rich panoply of research challenges
in supporting the dataframe data model and algebra by revisiting all
the typical layers of a “database stack”, from layout and indexing,
to query planning and optimization.

6. OPTIMIZING ACROSS SESSIONS

A unique characteristic of the way users work with dataframes is
that they construct queries incrementally, where multiple statements
together compose a larger overall query. Several queries are built
over the course of a session, in a trial-and-error fashion with query
sub-expressions often reused multiple times. In this section, we
describe research challenges that leverage this session-based mode
of operation to further optimize the user experience. We identify two
classes of optimization opportunities. First, recognizing the fact that
users often wish to quickly examine the results of each intermediate
statement along the way towards accomplishing a larger query, we
target immediate feedback for a given statement. Second, over the
course of a session, there are often many different statements and
queries that are assembled, by building on top of each other, so we
target sharing and reuse across the session.

6.1 Immediate Feedback

Providing immediate feedback to the user during data explo-
ration would greatly improve the usability of dataframe systems.
In fact, recent work has shown that delays of execution greater
than 500 ms often leads to fewer hypotheses explored and insights
generated. We describe three classes of optimizations: two of
which—opportunistic evaluation and prefix computation—preserve
dataframe semantics, and reduce latencies, while the third, approx-
nimate execution, changes the semantics slightly, for even larger
reductions in latency.

6.1.1 Opportunistic Evaluation

There are two standard modes of query evaluation in data pro-
cessing systems: lazy and eager. In the eager paradigm, adopted by
current dataframe systems like pandas, program control is not re-
turned to the user until the statement has been completely evaluated,
forcing the user to be idle during the computation. Query optimiza-
tion is not possible in an eager system because each operator within
the statement must be completely evaluated as it is called. Thus, a
significant amount of computation is wasted for statements that are
never used or inspected, and users are either rewarded or punished
based on the efficiency of a query as it is written.

On the other hand, in the lazy paradigm, which has recently
emerged as a popular alternative in some systems [21\textsuperscript{29}]. control is
returned to the user immediately, and the system defers the compu-
tation until the user requests the result. By scheduling computation
later, the system can wait for larger query sub-expressions to be
assembled, leading to greater opportunities for optimization, as is
done in systems such as Spark [27]. For example, if the user com-
poses a cross-product in one step, followed by a filter in the next
step, this filter can be rewritten to be performed first. The downside
of lazy evaluation is that computation only begins when the user
requests the result of a query. This introduces new burdens for users,
particularly for debugging, since bugs are not revealed until com-
putation is triggered. Moreover, during the time a user is thinking
or typing, the system could be working toward a result—however,
in the lazy paradigm, the system is idle during think time, leading
to lost computation. For smaller datasets or simple queries this can
potentially lead to a longer overall runtime if there are periods of
think time that exceed the runtime of the statements in the query.
In fact, most users of such systems end up requesting the results after
each operation, essentially defaulting to the eager mode.

Instead, we propose a middle ground that aims to preserve the ben-
efits of both lazy and eager evaluation; a mode we call opportunistic
evaluation, that we have started to implement in MODIN, which
makes the best use of system resources during user think time. Like
lazy evaluation, opportunistic evaluation does not require the user to
wait after each statement. Instead, the system opportunistically starts
execution, while passing control back to users with a pointer to the
eventually computed dataframe, which is asynchronously computed
in the background. In this manner, opportunistic evaluation makes
use of system resources to compute results in the background as
users are composing the next step of the query. Like eager evalu-
aton, opportunistic evaluation does not wait for users to complete
the entire query to begin evaluation. However, when a user requests
to view a certain output, opportunistic evaluation prioritizes producing
that output over all else. Opportunistic evaluation allows queries to
be rewritten as new statements are submitted to get to the requested
answer as fast as possible, taking into account the statements that
are partially computed. There are also new opportunities within
opportunistic evaluation to do speculative query execution, where
during idle time the system can start executing statements that com-
monly follow previous statements. Optimistic evaluation also leads
to new challenges in sharing and reuse across many query fragments.
whose computation has been scheduled in the background, which we will discuss in Section 6.2.

6.1.2 Prefix/Suffix Computation

As we saw in Section 4, building queries incrementally through trial-and-error typically involves printing the first or last few rows of the dataframe, via the head or tail commands, or other print commands. The head and tail commands, in pandas, print the first or last k rows (5 by default), respectively, while printing a dataframe displays both the first and last k rows. When building queries through trial-and-error, the user relies heavily on the order of the displayed data in judging the correctness of the intermediate query sub-expression, and deciding what to do next. When the user employs these printing commands, they expect the same k rows to be displayed, in order.

One way to give the users immediate feedback is to return the output to the user as soon as these k rows are assembled, computing the rest of the output in the background using opportunistic evaluation. This is reminiscent of techniques that try to optimize for early results for LIMIT queries, or for representative tuple identification, but special care must be taken to make sure that the displayed rows and their order are indeed correctly computed. Therefore, techniques that try to find samples anywhere in the data that match query predicates as in Kim et al., will not apply. We might be able to address this challenge by opting for physical operators that not just prioritize high output rate, but also preserve order, thereby ensuring that the first k rows will be produced as quickly as possible. An example, if only the first k rows of an ordered join were to be computed, a nested loop join, with the result displayed after k rows are computed, might work well. Returning the first k rows following a TRANSPOSE, especially when using columnar storage, can be fairly efficient as well. However, certain blocking operators will cause problems. For example, it is hard to produce the first k tuples of a GROUP BY or SORT without examining the entire data first. (Indeed, for small enough k, sorting may be faster than O(n log n), but still requires an O(n) sequential scan.) We may be able to exploit approximation (see next section) to produce the prefix/suffix early for these blocking operators. For example, a GROUP BY might correctly produce an approximate estimate of the first k groups without filling in the aggregates, and a SORT might be able to produce an approximation of the top-k after reading a large enough random sample—however guarantees on correctness may be minimal.

6.1.3 Approximate Execution

Since immediate feedback is essential, and since users often do not require exact results when simply inspecting results for debugging purposes, approximate query processing (AQP) techniques may be employed to quickly display inexact results at significantly reduced latencies. Traditional AQP has been applied to accelerate the generation of specific aggregates, e.g., SUM or AVG, and bound their estimates with confidence intervals. AQP is performed either offline, or online, where the former involves maintenance of materialized stratified samples, with some sample selection happening online, and the latter involves sampling on-the-fly with no pre-materialization decisions. Due to the highly ad-hoc nature of dataframe processing, we expect online sampling to be more effective. Specifically, online aggregation-type schemes can be used to produce progressively improving aggregates to the user—and these schemes will work well in the context of opportunistic evaluation, as discussed in Section 6.1.1, but we expect the dataframe model and algebra to introduce new challenges. Recent work has also introduced the notion of guarantees across collections of aggregates, often optimizing for user tasks or perceptual guarantees, e.g., ensuring that the ordering of the aggregates matches the correct ordering, even if the values of the aggregates are inexact, and these techniques may be a good fit to a dataframe setting.

While it is well known that some aggregates like MAX cannot be approximated, even blocking operators such as SORT can return early approximate results, using results from the 1990s. There may be additional opportunities for approximation if the user simply wants to inspect the approximate structure of the result for debugging purposes, especially in conjunction with prefix/suffix computation. For example, we can provide the overall structure of the output of a pivot table computation (displaying the row-wise groups and column headers), without actually filling in any of the aggregate values, and doing so progressively. Similar ideas of adding “placeholder” values for in-progress tuples have been proposed in streaming, web-database hybrid, and crowdsourcing contexts, but not, as far as we can tell, for a group-by aggregation setting. This idea could also be applied, for example, to TRANSPOSE, where the structure of the output dataframe is prepared first, with the values filled in progressively.

Other notions of approximation may also be valuable, e.g., the incomplete/phantom notions in Lang et al., wherein the result may contain additional rows not present in the dataframe query result, or rows that should be present, but are absent. This could be valuable, for example, for expensive filters. In fact, we could also exploit correlations between the filtering attribute and the other attributes in order to quickly approximate the rows that might pass the filter and quickly display them to the user, refining as additional filter evaluations are performed.

As we discussed in the previous subsection, this is a setting where ordering, in conjunction with prefix computation can actually help us achieve lower latencies—a reasonable estimate of the prefix of the output (which usually corresponds to some prefix of the input dataframe) would suffice. For example, we don’t need to produce an estimate of all of the groups, in a GROUP BY, just the first k that appear in the input.

Finally, when used in conjunction with optimistic evaluation, exact results may be scheduled in the background, and displayed explicitly to the user (e.g., as a pop-up) for later verification, as in Moritz et al., where they found that this approach of showing users an inexact result, while allowing them to proceed with their analysis, and letting them know when the exact results are ready, is an effective approach to optimization. However, this may result in many exact queries getting queued in the background as the user rapidly issues statements and achieves immediate approximate feedback. To increase throughput of these statements that build up in the execution queue, we can apply multiquery optimization techniques and take advantage of opportunities for shared computation, to be described in detail in Section 6.2.1.

6.2 Sharing and Reuse

Our final set of optimizations recognizes the fact that with many incremental query sub-expressions constructed and executed over the course of a session, there are opportunities for shared computation via multi-query optimization, by computing many query sub-expressions at the same time, and for reuse via materialization, by caching intermediate dataframe results and reusing to process subsequent query sub-expressions.

6.2.1 Multi-query Optimization

As a result of opportunistic evaluation, there are often many statements that are not completely executed when the user specifies it, and are instead executed in the background asynchronously. More-
over, by prioritizing the return of partial or approximate results, often, many statements are not computed entirely, with the computation either deferred (in lazy or eager evaluation), or being scheduled in the background (in opportunistic evaluation). Thus, there are many statements that may be scheduled for execution at the same time. These statements may operate over similar or identical subsets of data. To accelerate the computation of these many statements jointly, we have a perfect use-case for multi-query optimization (MQO), e.g., [32][34][60][64]. In fact, while some have argued that MQO has limited applicability in a general relational context: “One problem of MQO is its limited applicability (...)” In many workloads (...) there aren’t many opportunities to factor out common subexpressions” [32], with another problem with traditional MQO being “the synchronization of the execution of queries with common subexpressions when queries are submitted at different moments in time” [32]. In our setting, both these reasons for limited applicability do not hold: there are often many statements executed essentially in sync, and there are lots of opportunities to factor out common subexpressions since these statements essentially build on top of each other.

One simple approach to multi-query optimization is to allow operations that share inputs to share scans or seeks, thereby reducing the overhead required to access data. We can go even further if we recognize that many statements are essentially portions of a query composed incrementally (e.g., a cross-product followed by a filter, in two separate statements, to simulate a join). Therefore, we simply need to construct a query plan wherein sub-plans that correspond to intermediate dataframe results are materialized as a by-product. This poses an interesting conundrum, because ensuring that the sub-plan results are materialized “along the way” may result in suboptimal overall plan selection, which is problematic when the user cares more about the final dataframe than intermediates. For example, the optimal way to compute the overall join may not be to first compute the cross-product and then do the filter, while the latter does have the benefit of producing the appropriate intermediate results. By using partial results to help users avoid debugging mistakes, we may be able to reduce the importance of constructing many of the intermediate results in entirety, unless requested by the user explicitly. Moreover, by observing the user’s likelihood of inspecting the intermediates over the course of many sessions, we can do a weighted joint optimization of all query subexpressions, where the weights for each intermediate dataframe corresponds to its importance.

Going one step further, we can try to jointly optimize not just the evaluation of intermediate and final result dataframes, but also the partial or approximate results—a challenging endeavor. We can estimate probabilities for what the user might do next, e.g., inspect an intermediate, or compose the next statement, and the time they may take to do so. We can couple that with quantifying the benefit of the user seeing a certain portion of an intermediate result at a certain time, to construct a globally optimal query plan.

6.2.2 Materialization and Reuse

The incremental and exploratory nature of dataframe query construction over the course of a session leads to nonlinear code paths where the users revisit the same intermediate results repeatedly as a step towards constructing just the right queries they want. In such cases, the intermediate results gain special prominence. For example, if the user intends to try several filters along the way towards constructing their intended join, constructing a cross-product intermediate first may be sensible. The system can try to predict which intermediates may be likely to be used more in the future, and use that to guide automatic materialization decisions, thereby removing redundant computation and reducing execution time for subsequent statements. As is typical in this setting, there is a trade-off between the materialization overhead, including both the storage and the time to persist the results, and the expected reduced execution time due to reuse. There are two components to this optimization. First, we need to identify reusable intermediate results, which can be accomplished using standard program analysis. Then, we need to decide whether an intermediate result should be stored and reused, and the optimizer needs to utilize storage in a way that maximizes saved compute—small objects that are time-consuming to compute and reused frequently should be prioritized over large objects that are fast to compute. Recent work has shown that the optimal reuse policy given a dataflow graph can be identified in PTIME [69]. Storage can refer to either memory or disk, depending on whether reuse takes place within a single session or across multiple sessions. A special wrinkle in our setting is that we may be able to get away with partial view materialization, e.g., materializing a prefix of the cross-product, to be able to efficiently support prefix computation of the results of several filters applied to that cross-product.

7. OTHER IMPLEMENTATIONS

While our focus on pandas is driven by its popularity, in this section, we discuss other existing dataframe and dataframe-like implementations. Table 2 outlines the features of these dataframe and dataframe-like implementations. We will discuss how existing dataframe implementations fit into our framework, thus showing how our proposed research is applicable to these systems.

7.1 Dataframe Implementations: R

As we discussed in Section 3.1, the R language (and the S language before it), both support dataframes in a manner similar to pandas, and can be credited for initially popularizing the use of dataframes for data analysis [38]. R is still quite popular, especially among the statistics community. An R dataframe is a list of variables, each represented as a column, with the same number of rows. While both the rows and columns in an R dataframe have names, row names have to be unique; thus the pandas dataframe is more permissive than the R one. As shown in Table 2, R supports all of the operations in our algebra. The R dataframe fully captures our definition of a dataframe, and thus, implementational support of R dataframes requires only conforming the R API to our proposed algebra. External R packages such as readr, dplyr, and ggplot2 operate on R dataframes and provide functionalities such as data loading, transformation, and visualization, similar to ones from the pandas API [5][68].

7.2 Dataframe-like Implementations

There is a class of libraries that provide a functional or object-oriented programming layer on top of what is essentially relational algebra. These libraries include SparkSQL dataframes [2], SQL generator libraries like QueryDSL [2] and JOOQ [1], and object-relational-mapping systems (ORMs) such as Ruby on Rails [9] and SQLAlchemy [22]. All of these systems share some of the benefits with respect to incremental query construction mentioned in Section 6. However, they generally do not support the richness and expressiveness of the dataframe data model and algebra, including keys aspects like ordering of rows, and symmetry between rows and columns, and operations such as transpose.

SparkSQL and Dask are scalable dataframe-like systems that take advantage of distributed computing to handle large datasets. However, as shown in Table 2, Spark and Dask do so at the cost of limiting the supported dataframe functionalities. For example, a dataframe in SparkSQL does not treat columns and rows equivalently.
We introduced our ongoing effort to bring database optimizations as well as those that stem from how dataframes are leveraged—in an incrementally constructed manner, with inspection of intermediate results. We hope our work serves as a roadmap for others in the database community to start contributing to the important area of optimization techniques pioneered by the database community to make dataframes more efficient, targeting optimizations that revisit every step of a typical stack of a database-like system, as well as those that stem from how dataframes are leveraged—in an incrementally constructed manner, with inspection of intermediate results. We hope our work serves as a roadmap for others in the database community to start contributing to the important area of developing better dataframe systems for exploratory data analysis.

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