

# Scalable Linear Algebra on a Relational Database System

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**Abstract**—As data analytics has become an important application for modern data management systems, a new category of data management system has appeared recently: the scalable linear algebra system. In this paper, we argue that a parallel or distributed database system is actually an excellent platform upon which to build such functionality. Most relational systems already have support for cost-based optimization—which is vital to scaling linear algebra computations—and it is well-known how to make relational systems scale.

We show that by making just a few changes to a parallel/distributed relational database system, such a system can be a competitive platform for scalable linear algebra. Taken together, our results should at least raise the possibility that brand new systems designed from the ground up to support scalable linear algebra are not absolutely necessary, and that such systems could instead be built on top of existing relational technology. Our results also suggest that if scalable linear algebra is to be added to a modern dataflow platform such as Spark, they should be added on top of the system’s more structured (relational) data abstractions, rather than being constructed directly on top of the system’s raw dataflow operators.

## I. INTRODUCTION

Data analytics, including machine learning and large-scale statistical processing, is an important application domain and such computations often require linear algebra. Thus a new category of data processing system has appeared recently: the scalable linear algebra system.

Unlike established, long-lived efforts aimed at building scalable linear algebra APIs (such as ScaLAPACK [1]), these newer efforts are targeted more towards building complete data management systems. Not only do scalable linear algebra systems provide support for vectors and matrices and standard operations on them, but they also support storage/retrieval of data to/from disk, buffering/caching of data, and automatic logical/physical optimizations of computations (automatic rewriting of queries, pipelining, etc.). Such systems also typically offer some form of recovery, as well as offering a special-purpose domain-specific language.

There are three types of modern, scalable linear algebra systems that have been developed over the last few years:

- 1) The first type is built almost from the *ground up* to support scalable linear algebra, and provides support for all or most of the aforementioned features. A good example of this type of system is SystemML, developed at IBM [2].
- 2) The second type of system is what we term a *linear algebra dataflow API*, e.g., Spark’s `mllib.linalg` [3]. While such an API is closer in spirit to older efforts such as ScaLAPACK, such an API’s tight integration with a dataflow platform means that the API comes with the more general data management support that the underlying platform provides.

- 3) The third type of scalable linear algebra system is the *array database system* [4], [5]. such as SciDB [6].

**Is a New Type of System Actually Necessary?** While supporting scalable linear algebra in the context of a full-fledged data management system is clearly a desirable goal, the hypothesis underlying this paper is that with just a few changes, a classical, parallel relational database is actually an excellent platform for building a scalable linear algebra system.

In practice, many (or even most) distributed linear algebra computations have closely corresponding, distributed relational algebra computations. Given this, we believe that it is natural to build distributed linear algebra functionality on top of a distributed relational database system. Such systems are highly performant, reaping the benefits of decades of research and engineering effort targeted at building efficient systems. Further, relational systems already have software components such as a cost-based query optimizer to aid in performing efficient computations. In fact, much of the work that goes into developing a scalable linear algebra system from the ground up [7] requires implementing functionality that looks a lot like a database query optimizer [8].

Given that much of the world’s data currently sits in relational databases, and that dataflow systems increasingly provide at least some support for relational processing [9], [10], building linear algebra support into relational systems would mean that much of the world’s data would be sitting in systems capable of performing scalable linear algebra. This would have several obvious benefits:

- 1) It would eliminate the “extract-transform-reload nightmare”, particularly if the goal is performing analytics on data already stored in a relational system. It is difficult and expensive (in terms of computing/network costs and engineering dollars) to remove data from one system and put it in another, and if a database came off-the-shelf with the necessary functionality, there would be no reason to undertake such an often arduous task.
- 2) It would obviate the need for practitioners to adopt yet another type of data processing system in order to perform mathematical computations.
- 3) The design and implementation of high-performance distributed and parallel relational systems is well-understood. If it is possible to adapt such a system to the task of scalable linear algebra, most or all of the science performed over decades, aimed at determining how to build a distributed relational system, is directly applicable.

Along those lines, in this paper, we ask the question:

*Can we make a very small set of changes to the relational model and a RDBMS software to render them suitable for in-database linear algebra?*

**Our Contributions.** The approach we examine is simple: we consider adding new `LABELLED_SCALAR`, `VECTOR`, and `MATRIX` data types to relational database systems. Technically, this seems to be a rather minor change. After all, `array` has been available as a data types in most modern DBMSs—arrays can clearly be used to encode vectors and matrices—and some database systems (such as Oracle) offer a form of integration between arrays and linear algebra libraries such as BLAS [11] and LAPACK [12]. However, these previous, ad-hoc approaches do not offer complete integration with the database system. The query optimizer, for example, does not understand the semantics of the relational algebra, and this results in losing opportunities for optimization. Thus, we also consider a small set of changes to a relational query optimizer that can render it “linear algebra aware”, and able to make reasonable decisions in the face of linear algebra.

Specific contributions of this paper are as follows:

- We propose a very small set of changes to SQL that make it easy for a programmer to specify even complicated computations over vectors and matrices.
- We propose a set of simple language mechanisms for moving between purely relational data, vectors, and matrices, making it easily possible to combine relational and linear algebra as necessary, in one system.
- We implement these ideas in the context of the SimSQL parallel database system [13].
- We show experimentally that the resulting system has performance that is comparable to a special-purpose array system (SciDB), a special-purpose scalable linear algebra system (SystemML), and a linear algebra library built directly on top of a dataflow platform (Spark’s `mllib.linalg`).

Simplicity and ease of implementation should be considered a feature of our approach. Taken together, our results show the suitability of existing, relational systems for scalable linear algebra computations. As such, we believe that our results call into question the need to build yet another special-purpose data management system for linear-algebra-based analytics.

## II. LA ON TOP OF RA

In this section of the paper, we discuss why a relational database system might make an excellent platform for high-performance, distributed linear algebra. We then discuss the challenges in using a database system for linear algebra, as well as our basic approach.

### A. Linear and Relational Algebra

Development of distributed algorithms for linear algebra has been an active area of scientific investigation for decades, and many algorithms have become standard. Figure 1(a) shows the example of performing a distributed multiplication of two large, dense matrices,  $\mathbf{O} \leftarrow \mathbf{L} \times \mathbf{R}$ .

For efficiency and storage consideration, matrices to be multiplied in a distributed system are typically “blocked” or “chunked”; that is, they are divided into smaller matrices, which can then be moved around in bulk to specific processors where high-performance local computations are performed. Imagine that the six blocks making up each of the two input matrices  $\mathbf{L}$  and  $\mathbf{R}$  are distributed among three nodes as shown at the left of Figure 1(b). The blocks from  $\mathbf{L}$  are hash

partitioned randomly, while the blocks from  $\mathbf{R}$  are round-robin partitioned, based upon each block’s row identifier.

As a first step to perform the distributed multiplication, we would shuffle the blocks from  $\mathbf{L}$  so that all of the blocks from  $\mathbf{L}$ , column  $i$  are co-located with all of the blocks from  $\mathbf{R}$ , row  $i$ . Then, at each node, a local join (in this case, a cross product) is performed to iterate through all  $(L_{j.i}, R_{i.k})$  pairs that can be formed at the node. For each pair, a matrix multiply is performed, so that  $I_{i.j.k} \leftarrow L_{j.i} \times R_{i.k}$ . Finally, all of the  $I_{i.j.k}$  blocks are again shuffled so that all  $I_{i.j.k}$  are co-located based upon their  $(j, k)$  values—these blocks are then summed, so that the output block is computed as  $O_{j.k} \leftarrow \sum_i I_{i.j.k}$ .

The key observation underlying this paper is that *this is really just a relational algebra computation* over the blocks making up  $\mathbf{L}$  and  $\mathbf{R}$ . The first two steps of the computation are a distributed join that computes all  $(L_{j.i}, R_{i.k})$  pairs, followed by a projection that performs the matrix multiply. The next two steps—the shuffle and summation—are nothing more than a distributed grouping with aggregation.

The matrix multiplication example shows that distributed linear algebra computations are often nothing more than distributed relational algebra computations. This fact underlies our assertion that a relational database system makes an excellent platform for distributed linear algebra. Database researchers have spent decades studying efficient algorithms for distributed joins and aggregations, and many relational systems are mature and highly performant. Using a distributed database means that there is no need to reinvent the wheel.

A further benefit of using a distributed database system as a linear algebra engine is that decades of work in query optimization is directly applicable. In our example, we decided to shuffle  $\mathbf{L}$  because  $\mathbf{R}$  was already partitioned on the join key. Had  $\mathbf{L}$  been pre-partitioned and not  $\mathbf{R}$ , it would have been better to shuffle  $\mathbf{R}$ . This is *exactly* the sort of decision that a modern query optimizer makes with total transparency. Using a database as the basis for a linear algebra engine gives us the benefit of query optimization for free.

### B. The Challenges

However, there are two main concerns associated with implementing linear algebra directly on top of an existing relational system, without modification. First is the complexity of writing linear algebra computations on top of SQL. Consider a data set consisting of the vectors  $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$ , and imagine that our goal is to compute the distance

$$d_{\mathbf{A}}^2(\mathbf{x}_i, \mathbf{x}') = (\mathbf{x}_i - \mathbf{x}')^T \mathbf{A} (\mathbf{x}_i - \mathbf{x}')$$

for a Riemannian metric [14] encoded by the matrix  $\mathbf{A}$ . We might wish to compute this distance between a particular data point  $\mathbf{x}_i$  and every other point  $\mathbf{x}'$  in the database. This would be required, for example, in a  $k$ NN-based classification in the metric space defined by  $\mathbf{A}$ .

This can be implemented in SQL as follows. Assume the set of vectors is encoded as a table:

```
data (pointID, dimID, value)
```

with the matrix  $\mathbf{A}$  encoded as another table:

```
matrixA (rowID, colID, value)
```

Then, the desired computation is expressed in SQL as:

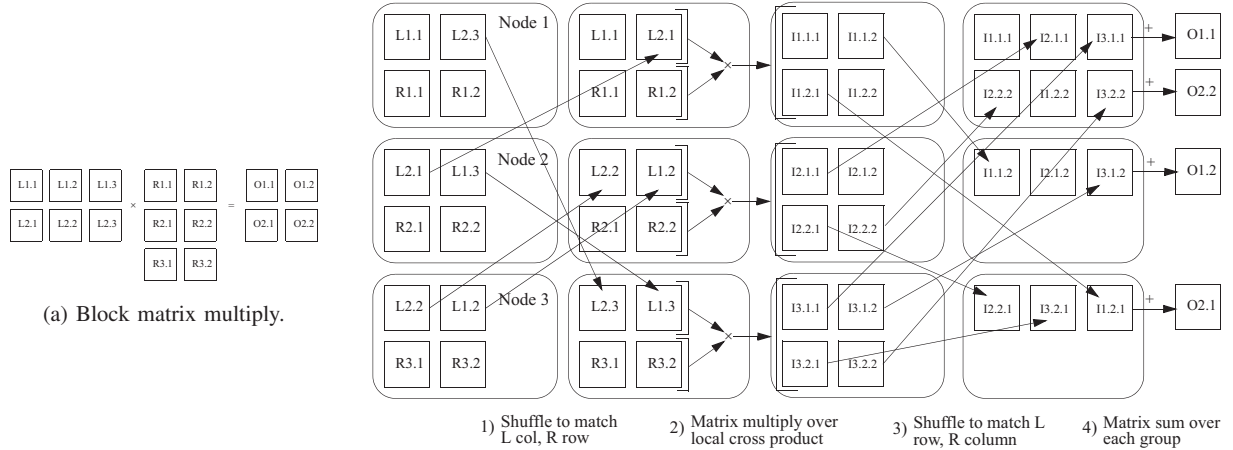


Fig. 1: Distributed processing of a block matrix multiply.

```

CREATE VIEW xDiff (pointID, dimID, value) AS
SELECT x2.pointID, x2.dimID, x1.value - x2.value
FROM data AS x1, data AS x2
WHERE x1.pointID = i and x1.dimID = x2.dimID

SELECT x.pointID, SUM (firstPart.value * x.value)
FROM (SELECT x.pointID AS pointID, a.colID AS
      colID, SUM (a.value * x.value) AS value
      FROM xDiff AS x, matrixA AS a
      WHERE x.dimID = a.rowID
      GROUP BY x.pointID, a.colID)
      AS firstPart, xDiff AS x
WHERE firstPart.colID = x.dimID
      AND firstPart.pointID = x.pointID
GROUP BY x.pointID

```

While it is clearly possible to write such a code, it is not necessarily a good idea.

The first obvious problem is that this is a very intricate specification, requiring a nested subquery and a view—without the view it is even more intricate—and it bears little resemblance to the original, simple mathematics.

The second problem is perhaps less obvious from looking at the code, but just as severe: performance. This code is likely to be inefficient to execute, requiring three or four joins and two groupings. Even more concerning in practice is the fact that if the data are dense and the number of data dimensions is large (that is, there are a lot of dimID values for each pointID), then the execution of this query will move a huge number of small tuples through the system, since a million, thousand-dimensional vectors are encoded as a billion tuples. In the classical, iterator-based execution model, there is a fixed cost incurred per tuple, which will translate to a very high execution cost. Vector-based processing can alleviate this somewhat, but the fact remains that satisfactory performance is unlikely. This fixed-cost-per-tuple problem was often cited as the impetus for designing new systems, specifically for vector- and matrix-based processing, or for processing of more general-purpose arrays.

### C. The Solution

As a solution, we propose a very small set of changes to a typical relational database system that include adding new LABELED\_SCALAR, VECTOR, and MATRIX data types

to the relational model. Because these non-normalized data types cause the contents of vectors and matrices to be manipulated as a single unit during query processing, the simple act of adding these new types brings significant performance improvements. It becomes easy to implement efficient, linear algebra computations on top of a database with these changes.

Further, we propose a very small number of SQL language extensions for manipulating these data types and moving between them. This alleviates the complicated-code problem. In our Riemannian metric example, the two input tables data and matrixA become data (pointID, val) and matrixA (val) respectively, where data.val is a vector, and matrixA.val is a matrix. The SQL code to compute the pairwise distances becomes dramatically simpler:

```

SELECT x2.pointID,
       inner_product (
         matrix_vector_multiply (
           a.val, x1.val - x2.val),
         x1.val - x2.val) AS value
FROM data AS x1, data AS x2, matrixA AS a
WHERE x1.pointID = i

```

In the next full section of the paper, we describe our proposed extensions in detail.

## III. OVERVIEW OF EXTENSIONS

### A. New Types

At the very highest level, we propose adding VECTOR, MATRIX, and LABELED\_SCALAR column types to SQL and the relational model, as well as a useful set of operations over those types (diag to extract the diagonal of a matrix, matrix\_vector\_multiply to multiply a matrix and a vector, matrix\_multiply to multiply two matrices, and so on). Overall, 22 different built-in functions over LABELED\_SCALAR, VECTOR and MATRIX types are present in our implementation. Each element of a VECTOR or a MATRIX is a Double.

In this particular subsection, we focus on introducing the VECTOR and MATRIX types; LABELED\_SCALAR will be considered in detail in a subsequent subsection.

For a simple example of the use of VECTOR and MATRIX types, consider the following table:

```
CREATE TABLE m (mat MATRIX[10][10],
                vec VECTOR[100]);
```

This code specifies a relational table, where each tuple in the table has two attributes, `mat` and `vec`, of types `MATRIX` and `VECTOR` respectively. In our language extensions, `VECTORS` and `MATRIXes` (as above) can have specified sizes, in which case operations such as `matrix_vector_multiply` are automatically type-checked for size mismatches. For example, the following query:

```
SELECT matrix_vector_multiply (m.mat, m.vec)
       AS res
FROM m
```

will not compile because the number of columns in `m.mat` does not match the number of entries in `m.vec`. However, if the original table declaration had been:

```
CREATE TABLE m (mat MATRIX[10][10],
                vec VECTOR[10]);
```

then the aforementioned SQL query would compile and execute, and the output would be a database table with a single attribute (called `res`) of type `VECTOR[10]`.

Note that in our extensions, there is no distinction between row and column vectors; whether or not a vector is a row or a column vector is up to the interpretation of each individual operation. `matrix_vector_multiply` interprets a vector as being a column vector, for example. To perform a matrix-vector multiplication treating the vector as a row vector, a programmer would first transform the vector into a one-row matrix (this transformation is described in the subsequent subsection) and then call `matrix_multiply`. Or, a programmer could transform the matrix first, then apply the `matrix_vector_multiply` function.

It is possible to create `MATRIX` and `VECTOR` types where the sizes are unspecified:

```
CREATE TABLE m (mat MATRIX[10][10],
                vec VECTOR[]);
```

In this case, the aforementioned `matrix_vector_multiply` SQL query would compile, but there could possibly be a runtime error if one or more of the tuples in `m` contained a `vec` attribute that did not have 10 entries.

It is also possible to have a `MATRIX` declaration where only one of the dimensionalities is given; for example, `MATRIX[10][ ]` is acceptable. However, it is generally a good idea for a programmer to specify the sizes in the table declaration, if possible. If a dimensionality *is* given, then the system ensures that there can be no runtime failures due to size mismatches. At load time, data is checked to ensure the correct dimensionality, and queries are fully type-checked to ensure that proper dimensionalities are used. Further, if dimensions are known, it can help the optimization process because the optimizer is aware of the sizes of intermediate results; a plan that uses a linear algebra operation that greatly reduces the amount of data early on (a multiplication of two “skinny” matrices, for example, which results in a small output matrix) may be chosen over other plans that would be preferred had the system not been aware of the output sizes of operations.

### B. Built-In Operations

In addition to a long list of standard relational algebra operations, the standard arithmetic operations `+`, `-`, `*` and `/`

(element-wise) are also defined over `MATRIX` and `VECTOR` types. For example, the SQL:

```
CREATE TABLE m (mat MATRIX[100][10]);
```

```
SELECT mat * mat
FROM m
```

returns a database table which stores the Hadamard product of each matrix in `m` with itself.

Since the standard arithmetic operations are all overloaded to work with `MATRIX` and `VECTOR` types, it means that the standard SQL aggregate operations all work as expected automatically. The `SUM` aggregate over `VECTOR` type attribute, for example, performs a `+` (entry-by-entry addition) over each `VECTOR` in a relation. This can be very convenient for implementing mathematical computations. For example, imagine that we have a matrix stored as a relational table of vectors, and we wish to perform a standard Gram matrix computation (if the matrix  $\mathbf{X}$  is stored as a set of columns  $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$ , then the gram matrix of  $\mathbf{X}$  is  $\sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^T$ ). This computation can be implemented using our extensions simply as:

```
CREATE TABLE v (vec VECTOR[]);
```

```
SELECT SUM (outer_product (vec, vec))
FROM v
```

Arithmetic between a scalar value and a `MATRIX` or `VECTOR` type performs the arithmetic operation between the scalar and *every* entry in the `MATRIX` or `VECTOR`. In this way, it becomes very easy to specify linear algebra computations of significant complexity using just a few lines of code. For example, consider the problem of learning a linear regression model. Given a matrix  $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$  and a set of outcomes  $\{y_1, y_2, \dots, y_n\}$ , the goal is to estimate a vector  $\hat{\beta}$  where for each  $i$ ,  $\mathbf{x}_i \hat{\beta} \approx y_i$ . In practice,  $\hat{\beta}$  is typically computed so as to minimize the squared loss  $\sum_i (\mathbf{x}_i \hat{\beta} - y_i)^2$ . In this case, the formula for  $\hat{\beta}$  is given as:

$$\hat{\beta} = \left( \sum_i \mathbf{x}_i \mathbf{x}_i^T \right)^{-1} \left( \sum_i \mathbf{x}_i y_i \right)$$

This can be coded as follows. If we have:

```
CREATE TABLE X (i INTEGER, x_i VECTOR []);
CREATE TABLE Y (i INTEGER, y_i DOUBLE);
```

then the SQL code to compute  $\hat{\beta}$  is:

```
SELECT matrix_vector_multiply (
       matrix_inverse (
           SUM (outer_product (X.x_i, X.x_i)),
           SUM (X.x_i * y_i))
FROM X, Y
WHERE X.i = Y.i
```

Note the multiplication `X.x_i * y_i` between the vector `X.x_i` and the scalar `y_i`, which multiplies `y_i` by each entry in `X.x_i`.

### C. Moving Between Types

By introducing `MATRIX` and `VECTOR` types, we then have new, de-normalized alternatives for storing data. For example, a matrix can be stored as a traditional relation:

```
mat (row INTEGER, col INTEGER, value DOUBLE)
```



or as a relation containing a set of row vectors, or as a set of column vectors using

```
row_mat (row INTEGER, vec_value VECTOR[])
or
col_mat (col INTEGER, vec_value VECTOR[])
```

Or, the matrix can be stored as a relation with a single tuple having the whole matrix:

```
mat (value MATRIX [[]])
```

It is of fundamental importance to be able to move around between these various representations, for several reasons. Most importantly, each has its own performance characteristics and ease-of-use for various tasks; depending upon a particular computation, one may be preferred over another.

Reconsider the linear regression example. Had we stored the data as:

```
CREATE TABLE X (mat MATRIX [[]]);
CREATE TABLE y (vec VECTOR []);
```

then the SQL code to compute  $\hat{\beta}$  would have been:

```
SELECT matrix_vector_multiply (
    matrix_inverse (
        matrix_multiply (trans_matrix (mat), mat)),
    matrix_vector_multiply (
        trans_matrix (mat), vec))
FROM X, y
```

Arguably, this is a more straightforward translation of the mathematics compared to the code that stores  $X$  as a set of vectors. However, it may not perform as well because it may be more difficult to parallelize on a shared-nothing cluster of machines. In comparison to the vector-based implementation, the matrix multiply  $X^T X$  is implicit in the relational algebra.

Since different representations are going to have their own merits, it may be necessary to construct (or deconstruct) `MATRIX` and `VECTOR` types using SQL. To facilitate this, we introduce the notion of a *label*. In our extension, each `VECTOR` attribute implicitly or explicitly has an integer label value attached to it (if the label is never explicitly set for a particular vector, then its value is  $-1$  by default). In addition, we introduce a new type called `LABELED_SCALAR`, which is essentially a `DOUBLE` with a label. Using those labels along with three special aggregate functions (`ROWMATRIX`, `COLMATRIX`, and `VECTORIZE`), it is possible to write SQL code that creates `MATRIX` types and `VECTOR` types, respectively, from normalized data.

For example, reconsider the table:

```
CREATE TABLE y (i INTEGER, y_i DOUBLE);
```

Imagine that we want to create a table with a single vector tuple from the table  $y$ . To do this, we simply write:

```
SELECT VECTORIZE (label_scalar (y_i, i))
FROM y
```

Here, the `label_scalar` function creates an attribute of type `LABELED_SCALAR`, attaching the label  $i$  to the `DOUBLE`  $y_i$ . Then the `VECTORIZE` operation aggregates the resulting values into a vector, adding each `LABELED_SCALAR` value to the vector at the position indicated by the label. Any “holes” (or entries in the vector for which no `LABELED_SCALAR` were found) in the resulting vector are set to zero. The overall

number of entries in the vector is set to be equal to the largest label of any entry in the vector.

As stated above, `VECTOR` attributes implicitly have labels, but they can be set explicitly, and those labels can be used to construct matrices. For example, imagine that we want to create a single tuple with a single matrix from the table:

```
mat (row INTEGER, col INTEGER, value DOUBLE)
```

We can do this with the following SQL code:

```
CREATE VIEW vecs AS
SELECT VECTORIZE (label_scalar (val, col))
    AS vec, row
FROM mat
GROUP BY row
```

followed by:

```
SELECT ROWMATRIX (label_vector (vec, row))
FROM vecs
```

The first bit of code creates one vector for each row, and the second bit of code aggregates those vectors into a matrix, using each vector as a row. It would have been possible to create a column matrix by first using a `GROUP BY col` and then `SELECT COLMATRIX`.

So far we have discussed how to de-normalize relations into vectors and matrices. It is equally easy to normalize `MATRIX` and `VECTOR` types. Assuming the existence of a table `label` (`id`) which simply lists the values 1, 2, 3, and so on, then one can move from the vectorized representation (found in the `vecs` view defined above) to a purely-relational representation using a `join` of the form:

```
SELECT label.id, get_scalar (vecs.vec, label.id)
FROM vecs, label
```

Code to normalize a matrix is written similarly.

## IV. IMPLEMENTATION

We have implemented all of these ideas on top of the SimSQL distributed database system [13]. SimSQL is a prototype database system designed to perform scalable numerical and statistical computations over large data sets, written mostly in Java, with a C/C++ foreign function interface.

In this section, we describe some details regarding our implementation. In building linear algebra capabilities into SimSQL, our mantra was “incremental, not revolutionary”. Our goal was to see whether, with a small set of changes, a relational database system could be a reasonable platform for distributed linear algebra.

### A. Distributed Matrices?

One of the very first questions that we had to ask ourselves when architecting the changes to SimSQL to support vectors and matrices was: should we allow individual matrices stored in an RDBMS to be large enough to exceed the size of RAM available on one machine? Should individual vectors and matrices be distributable objects?

After a lot of debate, we decided that, in keeping with a traditional RDBMS design, SimSQL would enforce a requirement that all vectors and matrices should be small enough to fit into the RAM of an individual machine, and that individual vectors and matrices would *not* be distributed across multiple machines. Since our mantra was “incremental, not

revolutionary,” we did not want to replace database tables with new linear algebra types—which would effectively give us an array database system. Thus, vectors/matrices are stored as attributes in tuples. And since distributing individual tuples or attributes across machines (or having individual tuples larger than the RAM available on a machine) is generally not supported by modern database systems, it seemed reasonable to not to support this in our system.

Of course, one might ask, *What if one has a matrix that is too large to fit into the RAM of an individual machine?* This might be a reasonably common use case, and it would be desirable to support very large matrices. Fortunately, it turns out that one can still handle efficient operations over very large matrices using an RDBMS. For example, a large, dense matrix with 100,000 rows and 100,000 columns and requiring nearly a terabyte to store in all can be stored as one hundred tuples in the table:

```
bigMatrix (tileRow INTEGER, tileCol INTEGER,
           mat MATRIX[10000][10000])
```

Efficient, distributed matrix operations are then easily possible via SQL. For example, to multiply `bigMatrix` with another `LargeMat`:

```
anotherLargeMat (tileRow INTEGER,
                 tileCol INTEGER, mat MATRIX[10000][10000])
```

We would use:

```
SELECT lhs.tileRow, rhs.tileCol,
       SUM (matrix_multiply (lhs.mat, rhs.mat))
FROM bigMatrix AS lhs, anotherLargeMat AS rhs
WHERE lhs.tileCol = rhs.tileRow
GROUP BY lhs.tileRow, rhs.tileCol
```

The resulting, very efficient computation is identical to what one would expect from a distributed matrix engine.

Of course, one might argue that there is some intricacy to this code, and that it is non-trivial to write. This may be a reasonable point, but it can be addressed with some syntactic sugar, allowing (for example) a programmer to write:

```
SELECT *
FROM matrix_multiply (bigMatrix, anotherLargeMat)
```

### B. Storage

Given such considerations, storage for vectors and matrices is quite simple. Vectors are stored in dense fashion, as lists of double-precision values, along with an integer label (since, as described in the previous section, all vectors are labeled with a row or a column number so that they can be used to construct matrices). This may sometimes represent a waste if vectors are indeed sparse, but if necessary vectors can easily be compressed before being written to secondary storage.

Matrices, on the other hand, are stored as sparse lists of vectors, using a run-length encoding scheme (missing vectors are treated as consisting entirely of zeros). As described previously, matrices can be stored as lists of column vectors or lists of row vectors; the exact storage format is specified during matrix construction (via either the `ROWMATRIX` or `COLMATRIX` aggregate function).

### C. Algebraic Operations

SimSQL is written mostly in Java, which presented something of a problem for us when implementing linear algebra

operations: some readers of this paper will no doubt disagree, but after much examination, we felt that Java linear algebra packages still lag behind their C/FORTRAN contemporaries in terms of raw performance. While a high-performance C implementation is (in theory) available to a Java system via JNI, passing through the Java/C barrier typically requires a relatively expensive data copy.

The solution that we implemented is, in the end, a compromise. We decided not to use any Java linear algebra package. The majority of SimSQL’s built-in linear algebra operations (indeed, the majority of *any* linear algebra system’s built-in operations), are simple and easy to implement efficiently: extracting/setting the diagonal of a matrix, computing the outer product of two vectors (which is of linear cost in the size of the output matrix), scalar/matrix multiplication, and so on. All such “simple” operations are implemented in Java, directly on top of our in-memory representation.

There is, however, another set of operations (matrix inverse, matrix-matrix multiply, etc.), that are much more challenging to implement in terms of achieving good performance and dealing with numerical instabilities. For those operations, we use SimSQL’s foreign function interface to transform vector- and matrix-valued inputs into C++ objects, where we then use BLAS implementations to fulfill the operations.

### D. Aggregation

The extensions proposed in this paper require two new types of aggregation. First, we must be able to perform standard aggregate computations (`SUM`, `AVERAGE`, `STD_DEV`, etc.) over vectors and matrices. Since, in SimSQL, these standard aggregate computations are all written in terms of basic arithmetic operations (+, −, \*, etc.), the standard aggregate computations over vectors and matrices all happen “for free” without any additional modifications to the system.

Second, our extensions require a few new aggregate functions with special semantics: `VECTORIZE`, `ROWMATRIX`, and `COLMATRIX`. The first constructs a vector out of a set of `LABELED_SCALAR` objects. The latter two construct a matrix out of a set of vectors. All are implemented within the system via hashing. For example, in the case of `VECTORIZE`, all of the `LABELED_SCALAR` objects used to build the vector are collected in a hash table (in the case of a `GROUP BY` clause, there would be many such hash tables). Since aggregation is performed in a distributed manner, hash tables from different machines that are being used to create the same vector will need to be merged into a single hash table on a single machine. Merging may also need to happen if there are enough groups during aggregation that memory is exhausted; in this case, a partially-complete hash table may need to be flushed to disk. Any merge (or insertion into the hash table) that causes two `LABELED_SCALAR` objects with the same label to be added to the vector results in a runtime error.

Once all of the `LABELED_SCALAR` objects for a vector have been collected into a single hash table, the objects are sorted based on the position labels, and are then converted into a vector. Any missing entries are treated as zero, and the length of the resulting vector is equal to the largest label used to construct the vector.

Matrices are constructed similarly, with one change being that the objects hashed to construct the matrix are `VECTOR` objects, rather than `LABELED_SCALAR` objects. Note that by

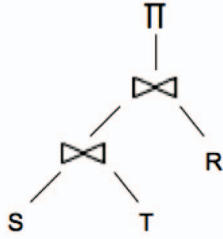


Fig. 2: A simple, suboptimal query plan. The projection at top computes `matrix_multiply (r_matrix, s_matrix)`.

definition, all `VECTOR` objects are labeled, and it is those labels that are used to perform the aggregation.

## V. TYPING AND OPTIMIZATION

### A. Vector and Matrix Sizes

In practical applications, the individual matrices stored in a database table can range from a few bytes in size to many gigabytes in size. Hence, knowing the size of individual linear algebra object stored in a database is going to be of fundamental importance during query optimization. Unfortunately, linear algebra objects are typically manipulated via a large set of user-defined and system-provided functions that change the sizes of the objects being manipulated in ways that are regular, but opaque to the system. This can easily result in the choice of a query plan that is far from optimal.

The problem can be illustrated by a simple example. Assume we have three tables defined as below:

```
R (r_rid INTEGER, r_matrix MATRIX[10][100000])
S (s_sid INTEGER, s_matrix MATRIX[100000][100])
T (t_rid INTEGER, t_sid INTEGER)
```

Imagine that the sizes of the tables R, S, and T are 100 tuples, 100 tuples, and 1,000 tuples, respectively. Now, suppose we want to calculate the product of a number of pairs of matrices from the relations R and S, where the pairs for which we need to obtain are indicated by T:

```
SELECT matrix_multiply (r_matrix, s_matrix)
FROM R, S, T
WHERE r_rid = t_rid AND s_sid = t_sid
```

A rule-based optimizer, or a cost-based optimizer without access to good information about the size of the linear algebra object being pushed through the system, is almost assuredly going to produce the query plan depicted in Figure 2.

The plan is straightforward. Since no predicate links tables R and S, the optimizer is going to first join either R and T or else S and T before joining the third table. After joining all three tables, the linear algebra computation `matrix_multiply (r_matrix, s_matrix)` is then computed as part of a relational projection operation.

In this example, the join between tables S and T produces about 1,000 tuples (estimated as  $\frac{1000 \times 100}{100}$ ), each containing an 8MB matrix (estimated as  $8 \times 100000 \times 10$  bytes). Thus, the total data produced in this join is about 8 GB.

However, this is clearly not the optimal query plan. It is possible to do a lot better, as illustrated in Figure 3.

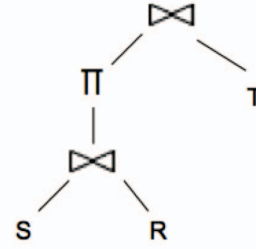


Fig. 3: A better query plan that computes the cross product of S and R first, which allows early evaluation of `matrix_multiply (r_matrix, s_matrix)`.

Here we first perform a join between the tables S and R, despite the lack of a join predicate. A projection on the join result calculates the product between `r_matrix` and `s_matrix`. While the join between the tables S and R produces 10,000 tuples, the early projection allows the optimizer to produce a plan that performs the `matrix_multiply (r_matrix, s_matrix)` early, to effectively remove all of the large matrices from the plan; the result of each matrix multiply is only 8KB (estimated as  $8 \times 10 \times 100$  bytes). Thus, the total data produced in this join and projection is about 80 MB, and it is likely far superior.

### B. Type Signatures

To make sure that the SimSQL optimizer has the information necessary to choose the correct plan, the type signature for any function that includes vectors and matrices is *templated*. The type signature takes (as an argument) the size and shape of the input, and returns the size and shape of the output. For example, the function signature of the built-in function `diag` (computing the diagonal of a matrix) is:

```
diag (MATRIX[a][a]) -> VECTOR[a]
```

This signature constrains the input matrix to be square, and it indicates that the output vector has a number of entries identical to the number of rows/columns of the input matrix. The signature for `matrix_multiply` is:

```
matrix_multiply (MATRIX[a][b], MATRIX[b][c]) ->
MATRIX[a][c]
```

In this signature, the arguments `a`, `b`, and `c` effectively parameterize the function signature. This information is then used by the optimizer to infer the exact dimensions of the output object. For example, consider the schema:

```
U (u_matrix MATRIX[1000][100])
V (v_matrix MATRIX[100][10000])
```

And the query:

```
SELECT matrix_multiply (u_matrix, v_matrix)
FROM U, V
```

The optimizer obtains the dimensions of the `u_matrix` and `v_matrix` objects by looking in the catalog. Note that the user-specified dimensionality for vector/matrix data is enforced by the system during data loading.

When the dimensions of `u_matrix` are retrieved from the catalog, the type parameter `a` is bound to 1000, and `b` is bound to 100. When the dimensions of `v_matrix` are retrieved,

`b` is bound a second time to 100 (a different value for `b` would cause a compile-time error) and `c` is bound to 10000. Hence, the output of the matrix multiply is a 1000-by-10000 matrix of approximately 80 MB in size; this information can subsequently be used by the optimizer.

By convention, the SimSQL optimizer always assumes that matrices are dense, and so a matrix of dimensions `a` and `b` has size (8 bytes)  $\times a \times b$ . While not always accurate, this is a pessimistic, and hence safe assumption, that will typically avoid choosing poor plans.

### C. unknown Dimensionalities

Note that size parameters can also take a special value `unknown`, so that it is possible to have:

```
U (u_matrix MATRIX[1000][])
```

Here, the number of columns in the matrix is unknown at compilation/optimization time—this is typically used when the table `U` has matrices with a different number of columns. In this case, when the optimizer encounters `matrix_multiply(u_matrix, v_matrix)`, the signature parameter `b` will get nothing from `u_matrix`, and it will be bound to 100 referring to the dimension of `v_matrix`.

Note that it is possible to have dimensions of `unknown` sizes that the optimizer is unable to resolve, so that planning must take place over vectors/matrices whose sizes are not known. This can be handled in a reasonable way by associating an estimated size with each `unknown` dimension value. In SimSQL, statistics are collected regarding the (approximate) number of distinct attribute values and the (approximate) average, physical size of those attribute values. This data is collected using a lightweight, randomized algorithm, as data are loaded, and also when materialized views are created. These statistics are then stored in the system catalog. Given this data, a `vector` attribute whose dimensionality is tagged as `unknown` can be given an estimated dimensionality of `estimated avg att size/8`, since the storage required for each entry in the vector is 8 bytes. A `matrix` attribute with one `unknown` dimensionality and another whose size is `m` can be given an estimated value of `estimated avg att size/(8×m)`. If both dimensions are unknown, then the matrix can be assumed to be square for estimation purposes.

Estimates produced in this way for the dimensionality of vectors will typically be highly accurate, since `vector` types are always stored densely. However, estimates for the dimensionality of matrices can be more problematic. As SimSQL matrices are stored as a (possibly) sparse list of column/row vectors, estimates for the size of `unknown` dimensions can be lower than the reality for sparse data. In terms of choosing a poor plan, this could pose a problem for the optimizer. As such, it is always good for a programmer to avoid the use of `unknown` dimensions if not absolutely necessary.

## VI. EXPERIMENTS

We have implemented all of the capabilities described in the paper on top of SimSQL, and in this section, we experimentally evaluate the utility of the new capabilities.

This section consists of two different sets of experiments. In the first set of experiments, we compare the efficiency of SimSQL with the new linear algebra types with several alternative platforms. In a second set of experiments, we

consider a couple of relatively complicated machine learning computations, and show how the addition of matrix and vector types to the relational model can greatly speed the underlying machine learning computations.

### A. Comparison Across Platforms

This subsection evaluates our proposed addition of `VECTOR` and `MATRIX` types by comparing SimSQL to a number of alternative platforms.

**Platforms Tested.** The platforms we evaluated are:

- (1) SimSQL. We tested several different SimSQL implementations: Without vector/matrix support (the original SimSQL implementation, without the improvements proposed in this paper), with data stored as vectors, and with data stored as vectors, then converted into blocks.
- (2) SystemML. This is SystemML V0.9, which provides the option to run on top of Hadoop. All computations are written in SystemML’s DML programming language.
- (3) SciDB. This is SciDB V14.8. All computations are written in SciDB’s AQL language which is similar to SQL.
- (4) Spark `mllib.linalg`. This is run on Spark V1.6 in standalone mode. All computations are written in Scala.

**Computations Performed.** In our experiments, we performed three different representative computations.

- (1) Gram matrix computation. A Gram matrix is the inner products of a set of vectors. It is a common computational pattern in machine learning, and is often used to compute the kernel functions and covariance matrices. If we use a matrix `X` to store the input vectors, then the Gram matrix `G` can be calculated as  $G = X^T X$ .
- (2) Least squares linear regression. Given a paired data set  $\{y_i, \mathbf{x}_i\}, i = 1, \dots, n$ , we wish to model each  $y_i$  as a linear combination of the values in  $\mathbf{x}_i$ . Let  $y_i \approx \mathbf{x}_i^T \beta + \epsilon_i$ , where  $\beta$  is the vector of regression coefficients. The most common estimator for  $\beta$  is the least squares estimator:  $\hat{\beta} = (X^T X)^{-1} X^T y$ .
- (3) Outlier detection in a vector space. As described in Section 2.2 of the paper, the distance between vectors  $\mathbf{x}_i$  and  $\mathbf{x}'$  is defined as  $d_A^2(\mathbf{x}_i, \mathbf{x}') = (\mathbf{x}_i - \mathbf{x}')^T A (\mathbf{x}_i - \mathbf{x}')$  for some metric space defined by the matrix `A`. For each data point  $\mathbf{x}_i$ , we first compute the minimum  $d_A^2(\mathbf{x}_i, \mathbf{x}')$  value over all  $\mathbf{x}' \neq \mathbf{x}_i$ ; this is the distance of the closest point to  $\mathbf{x}_i$  in the data set. An *outlier* is a point whose closest neighbor is far away, and hence we wish to compute the few data points for which this minimum distance is maximized among the data set.

**Implementation Details.** We now describe in some detail how we performed each of these three computations over the various platforms.

- (1) SimSQL. A SimSQL programmer uses queries and built-in functions to conduct computations. In SimSQL, we implemented each model using three different SQL codes. First, we wrote a pure-tuple based code (as on an existing, standard SQL-based platform). Second, we wrote an SQL code where each data point is stored as an individual vector, in the schema:

```
x_vm (id INTEGER, value VECTOR[])
```



Third, we wrote an SQL code where data points are grouped together in blocks of 1000 data points, and stored as a matrix with 1000 rows, so that they can be manipulated as a group.

The Gram matrix computation is written over tuples as:

```
SELECT x1.col_index, x2.col_index,
       SUM(x1.value * x2.value)
FROM x AS x1, x AS x2
WHERE x1.row_index = x2.row_index
GROUP BY x1.col_index, x2.col_index;
```

The Gram matrix is computed over vectors as:

```
SELECT SUM(outer_product(x.value, x.value))
FROM x_vm AS x;
```

For a block-based computation, the rows are first grouped into blocks (the table `block_index` (mi `INTEGER`) stores the indices for blocks):

```
CREATE VIEW MLX (m) AS
  SELECT ROWMATRIX(label_vector(
    x.value, x.id - ind.mi*1000))
  FROM x_vm AS x, block_index AS ind
  WHERE x.id/1000 = ind.mi
  GROUP BY ind.mi;
```

Note that this grouping step is not necessary if the data are already stored as blocks; in our experiments, we count the blocking time as part of the computation.

Then, the result is a sum of a series of matrix multiplies:

```
SELECT SUM(matrix_multiply(
  trans_matrix(mlx.m), mlx.m))
FROM mlx;
```

The calculation of linear regression is similar to Gram matrix computation. We omit the code for brevity. We also omit the code for tuple-based outlier detection.

The key codes of vector-based and block-based outlier detections are given below. There are three steps to compute the outlier. First, the distance between each pair of vectors is computed, then the distance to the closest neighbor is extracted from that all-distance list, and finally the points with the furthest nearest neighbors are determined. For the vector-based computation, we compute the distance to the nearest neighbor for each point as:

```
CREATE VIEW DISTANCESM (id, dist) AS
  SELECT a.dataID,
         MIN(inner_product (mxx.mx_data, a.data))
  FROM X_m AS a, MX AS mxx
  WHERE a.dataID <> mxx.id
  GROUP BY a.dataID;
```

And in the block-based computation we first calculate all distances using a set of matrix multiplies:

```
CREATE VIEW DISTANCES (id1, id2, dm) AS
  SELECT mxx.id, mx.id, matrix_multiply(
    mxx.m, matrix_multiply(mp.mapping,
    trans_matrix(mx.m)))
  FROM MLX AS mx, MLX AS mxx, MM AS mp;
```

Then, the minimum distance for each data point is computed via a series of operations on matrices.

(2) SystemML. Physically, the data in SystemML are stored and processed as *blocks*, which are square matrices.

Gram matrix computation in SystemML is:

```
result = t(X) %** X
```

Linear regression is omitted. The code of outlier detection is:

```
all_dist = X %** m %** X_t
all_dist = all_dist + diag(diag_inf)
min_dist = rowMins(all_dist)
result = rowIndexMax(t(min_dist))
```

(3) Spark `mllib.linalg`. A Spark `mllib.linalg` programmer must decide: should the input data be stored/processed as vectors, or as matrices? And, if a matrix is used, should it be a local matrix, or a distributed one? In our experiments, we tried different vector/local matrix/distributed matrix implementations, and selected the most efficient ones.

For Gram matrix computation, vector-based is the fastest:

```
val result = parsedData.map(
  x => x.transpose.multiply(
    x.asInstanceOf[DenseMatrix]
  ).toArray
).reduce((a, b) => (a, b).zipped.map(_+_))
```

For linear regression, vector-based is also the most efficient. We omit the code for brevity.

Outlier detection was challenging. After a lot of experimentation, we found that the distributed `BlockMatrix` was the best. The code is as follows:

```
val dist_matrix = block_matrix_x.
  multiply(block_matrix_m).
  multiply(block_matrix_x.transpose)

val result =
  dist_matrix.toIndexedRowMatrix.rows.map(
    x => (x.index, x.vector.toArray)).
  map{ case (i, a) =>
    {if (i==0) a(0)=a(1)
     else a(i.toInt)=a(0); (i, a.min);}
  }.max()(
    new Ordering[Tuple2[Long, Double]]() {
      override def compare(
        x: (Long, Double), y: (Long, Double)
      ): Int =
        Ordering[Double].compare(x._2, y._2)})
```

(4) SciDB. Data in SciDB are partitioned as *chunks*. We use 1000 as the chunk size for all arrays in our code.

The SciDB code of Gram matrix computation is:

```
SELECT * FROM gemm(transpose(x), x,
  build(<val:double>[t1=0:9,1000,0,
  t2=0:9,1000,0], 0));
```

Linear regression is similar. The implementation of outlier detection is:

```
SELECT * INTO mxt
FROM gemm(m, transpose(x),
  build(<val:double>[t1=0:999,1000,0,
  t2=0:99999,1000,0], 0));
```

```
SELECT * INTO all_distance
FROM filter(gemm(x, mxt,
  build(<val:double>[t1=0:99999,1000,0,
  t2=0:99999,1000,0], 0)), t1<>t2);
```

```
SELECT min(gemm) INTO distance
FROM all_distance
GROUP BY t1;
```

Gram Matrix Computation			
Platform	10 dims	100 dims	1000 dims
Tuple SimSQL	00:01:28	00:03:19	05:04:45
Vector SimSQL	00:00:37	00:00:43	00:05:43
Block SimSQL	00:01:18	00:01:23	00:02:53
SystemML	00:00:05*	00:00:51	00:02:34
Spark mllib	00:00:20	00:00:54	00:17:31
SciDB	00:00:03	00:00:17	00:03:20

Fig. 4: Gram matrix results. Format is HH:MM:SS. A star (\*) indicates running in local mode.

```

SELECT * INTO max_dist
FROM (SELECT max(min) FROM distance);

SELECT t1
FROM distance JOIN max_dist ON
      distance.min = max_dist.max;

```

**Experiment Setup.** We ran all experiments on 10 Amazon EC2 m2.4xlarge machines, each having eight CPU cores. For Gram matrix computation and linear regression, the number of data points per machine was  $10^5$ . For outlier detection, the number of data points per machine was  $10^4$ . All data sets were dense, and all data were synthetic—since we are only interested in running time; there is likely no practical difference between synthetic and real data. For each computational task, we considered three data dimensionalities: 10, 100, and 1000.

**Experiment Results and Discussion.** The results are shown in Figures 4, 5, and 6.

Vector- and block-based SimSQL clearly dominate the tuple-based implementation for each of the three computations. The results show that sometimes it is simply not possible to move enough tuples through a database system to implement linear algebra operations using only tuples.

To examine this further, we re-ran the tuple-based and vector-based Gram matrix computations over 1000-dimensional data on a five machine cluster, and this time we timed the individual operations that made up the computation. Note that in the 1000-dimensional computation, in the tuple-based computation, each tuple joins with the other 1000 values making up the same data point, and all of those tuples need to be aggregated. Since  $5 \times 10^5$  data points are stored as  $5 \times 10^8$  tuples, this results in  $5 \times 10^{11}$  tuples that need to be aggregated. Even though these operations are pipelined, they dominate the running time, as shown in Figure 7. Here we see—perhaps surprisingly—that the dominant cost is *not* the *join* in the tuple-based computation, but the *aggregation*. This illustrates the problem with tuple-based linear algebra: even a tiny fixed cost associated with each tuple is magnified when we must push  $5 \times 10^{11}$  tuples through the system.

Interestingly, we see that the vector-based computation was faster than block-based for 10- and 100-dimensional computations. This is because our experiments counted the time of grouping vectors into blocked matrices. This additional computation was not worthwhile for less computationally expensive problems. But for the 1000-dimensional computations, additional time savings could be realized via blocking.

For the higher-dimensional, computationally intensive computations, there was no clear winner among SystemML,

Linear Regression			
Platform	10 dims	100 dims	1000 dims
Tuple SimSQL	00:03:42	00:05:46	05:05:22
Vector SimSQL	00:00:45	00:00:49	00:06:35
Block SimSQL	00:02:23	00:02:22	00:04:22
SystemML	00:00:06*	00:00:53	00:02:38
Spark mllib	00:00:35	00:01:01	00:17:42
SciDB	00:00:15	00:00:33	00:06:04

Fig. 5: Linear regression results. Format is HH:MM:SS. A star (\*) indicates running in local mode.

Outlier Detection			
Platform	10 dims	100 dims	1000 dims
Tuple SimSQL	Fail	Fail	Fail
Vector SimSQL	00:10:14	00:11:49	00:13:53
Block SimSQL	00:03:14	00:04:43	00:10:36
SystemML	00:13:29	00:22:38	00:33:22
Spark mllib	01:22:59	01:15:06	01:13:06
SciDB	00:03:46	00:04:54	00:05:06

Fig. 6: Outlier detection results. Format is HH:MM:SS.

SciDB, and SimSQL. SimSQL was a bit slower for the lower-dimensional problems, because, as a prototype system, it is not engineered for high throughput. Spark mllib was not competitive on the higher-dimensional data. Over the three, 1000-dimensional computations, SimSQL, SystemML, and SciDB had geometric mean running times of 5 minutes 7 seconds, 6 minutes 5 seconds, and 4 minutes 41 seconds, respectively.

The results for SimSQL, SystemML, and SciDB are close enough to, in our opinion, be practically identical, at least on this suite of experiments. SciDB had the fastest mean because it lacked a particularly poor showing (unlike SimSQL, which was twice as slow as SciDB for outlier detection, and SystemML, which took more than six times as long), but the three means were still very close.

We spent a lot of time trying to tune both SimSQL and SystemML for the outlier computation. In the case of SimSQL, the problem appears to be that there are only  $10^5$  data points in all; when grouped into blocks of 1000 vectors, this results in only 100 matrices in all. This meant that each of our 80 compute cores had an average of 1.25 matrices mapped to it. Since SimSQL uses a randomized, hash-based partitioning, it is easily possible for one core to receive four or five of the 100 matrices. This resulted in a very unbalanced computation. We observed that most cores would finish in a short time, while just a few, overloaded cores would be left to finish the computation in a much longer period. Better load balancing would likely have solved this problem.

Finally, we ask the question: do these experiments support the hypothesis at the core of the paper, that a relational engine can be used with little modification to support efficient linear algebra processing? In terms of performance, they seem to, though there are some caveats in our findings. First, scalable linear algebra systems continue to improve. For example, the SystemML designers have recently shown that it is possible to greatly speed up SystemML via the use of the specialized compression methods [15]—had we evaluated a version of SystemML enhanced with those methods, our results may have been very different. Still, we feel that it should be possible

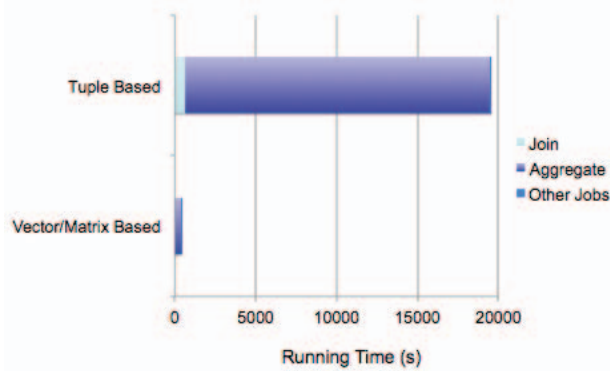


Fig. 7: Comparison of Gram matrix computation for tuple-based and vector-based SimSQL.

to build such methods into an enhanced relational database system, just as they can be built into SystemML. A second reasonable concern with our evaluation is that SimSQL is not a classical relational system, in that it is built upon Hadoop; hence, is SimSQL really any different from a special-purpose system such as SystemML? Though SimSQL is built upon Hadoop, in most ways, it is indistinguishable from a classical, relational system. SimSQL has an SQL compiler, a cost-based optimizer, and a very classical relational execution engine supporting various relational algorithms (joins, aggregations, etc.). In our implementation, we modified only SimSQL system components that are going to be found in any classical relational system: the type system and the compiler, SimSQL’s costing framework (so that operations over vectors/matrices could be costed), a set of new built-in functions, and a few new aggregation operations. We expect similar results were a more traditional relational system used, but this should be verified via future work.

### B. Machine Learning Computations

A reasonable critique of the experiments in the last section is that it focuses exclusively on computationally intensive, linear algebra computations. In more general machine learning computations, one might expect that the benefit of vector- and matrix-based computations vis-a-vis tuple-based computations would be less pronounced.

**Experiment Overview.** As an attempt to investigate this further, we ran two additional experiments, where the goal was to perform iterative machine learning computations aimed at learning a Gaussian Mixture Model (GMM) and the Bayesian Lasso (BL) [16].

The goal of learning a GMM is to estimate the mean and covariance for a set of Gaussian components in a clustering model. In our experiment, we generated a synthetic data set composed of  $5 \times 10^7$  data points, and distributed those data points across five Amazon EC2 m2.4xlarge machines.

The BL is a regularized Bayesian regression model. We produced a synthetic data set that had  $5 \times 10^5$  {response, regressor} pairs, also on five Amazon EC2 m2.4xlarge machines. Each regressor had 1000 dimensions.

We wrote both tuple-based implementation and vector/matrix based implementation for these two models. And we use Gibbs samplers for learning these models.

**Experiment Results.** Results are given in Figure 8. Since both

Model	Implementation	Iteration time	Init time
BL	Tuple SimSQL	00:07:28	02:38:46
BL	V/M SimSQL	00:04:04	00:04:44
GMM	Tuple SimSQL	00:21:16	00:11:22
GMM	V/M SimSQL	00:09:15	00:08:09

Fig. 8: Performance of GMM and BL learning. Format is HH:MM:SS per iteration.

learning tasks are iterative, requiring multiple scans over the data set until convergence, the time is measured as the average time for five iterations. We also report the initialization time, which includes the time required to set up the initial model parameters and to collect statistics required for initialization.

**Discussion.** While the disparity between the tuple-based and vector/matrix-based implementations is less when linear algebra objects are used as tools for building more complicated machine learning computations, the disparity is still significant. Note that this was the case even though our GMM computation only utilized 10-dimensional data—one would expect the disparity to become more acute with higher-dimensionality (because more tuples would be produced in tuple-based implementation). Also, note that since the BL requires a Gram matrix computation, the BL initialization time is brought down from more than two and a half hours to just a few minutes by using vectors and matrices for the computations.

## VII. RELATED WORK

ScaLAPACK [1] is the best-known and most widely-used framework for distributed linear algebra. However, ScaLAPACK is really an MPI-based API, and it is not a data management system.

As intimated in the introduction to this paper, there has been some recent interest in combining distributed/parallel data management systems and linear algebra to support analytics. One approach is the construction of a special purpose data management system for scalable linear algebra; SystemML [2] is the best example of this. Another good example of this is the Cumulon system [17], which has the notable capability of optimizing its own hardware settings in the cloud. MadLINQ [18], built on top of Microsoft’s LINQ framework, can also be seen as an example of this. Other work aims at scaling statistical/numerical programming languages such as R. Ricardo [19] aims to support R programming on top of Hadoop. Riot [20] attempts to plug an I/O efficient backend into R to bring scalability.

A second (and not completely distinct) approach is building scalable linear algebra libraries on top of a dataflow platform. In this paper, we have experimentally considered `mllib.linalg` [3]. Apache Hama [21] is another example of such a package. So is SciHadoop [22].

The idea of moving past relations onto arrays as a database data model, particularly for scientific and/or numerical applications, has been around for a long time. One of the most notable efforts is Baumann and his colleague’s work on Rasdaman [5]. In this paper, we have compared with SciDB [6], an array database for which linear algebra is a primary use case.

An array-based approach that is somewhat related to what we have proposed is SciQL [23], which is a system supporting an extended SQL that is implemented on top of the MonetDB system [24]. SciQL adds arrays (in addition to tables) as a sec-

ond data storage abstraction. Our proposed approach is much more modest; rather than allowing arrays as a fundamental data abstraction, we simply add vectors and matrices as new attribute types, with special support, into a relational database.

There is some support for linear algebra in modern, commercial relational database systems, but it is not well-integrated into the declarative (SELECT-FROM-WHERE) portion of SQL, and generally challenging to use. For example, Oracle provides the UTL\_NLA [25] package to support BLAS and LAPACK operations. To multiply two matrices using this package, and assuming two input matrices `m1` and `m2` declared as type `utl_nla_array_dbl` (and an output matrix `res` defined similarly), a programmer would write:

```
utl_nla.blas_gemm(
  transa => 'N', transb => 'N', m => 3, n => 3,
  k => 3, alpha => 1.0, a => m1, lda => 3,
  b => m2, ldb => 2, beta => 0.0, c => res,
  ldc => 3, pack => R);
```

This code specifies details about the input matrices, as well as details about the invocation of the BLAS library.

The MADlib project [26] is an effort to build analytics, including linear algebra functionality, on top of a database system. MADlib is closely related to what we have described here, in that this project showed the feasibility and potentially high performance of linear algebra on top of a database system. However, MADlib is not concerned with building linear algebra functionality *into* a database system.

## VIII. FUTURE WORK AND CONCLUSIONS

We have proposed a small set of changes to SQL that can render any distributed, relational database engine a high-performance platform for distributed relational algebra. We have shown that making these changes to a distributed relational database (SimSQL) results in a system for distributed linear algebra whose performance meets or exceeds special-purpose systems. Given that SimSQL is a prototype system written mostly in Java, it is not unreasonable to speculate that a commercial, high-performance database system with similar extensions could do even better. We believe that our results call into question the need to build yet another special-purpose data management system for linear-algebra-based analytics.

In terms of future work, the language and optimization extensions that we proposed do not automatically support chunking or blocking of very large matrices that cannot be stored in RAM, nor do they support transparent operations (multiplications, inversions, etc.) over blocked matrices. Ideally, the decision for when and how to block should be pushed to the query optimizer. A further extension would be getting rid of SQL as the typical front-end altogether, and instead translating a widely-used mathematical programming language such as MATLAB into SQL, or directly into a computation that can be optimized and then executed by the engine.

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## REFERENCES

- [1] L. S. Blackford, J. Choi, A. Cleary, E. D’Azevedo, J. Demmel, I. Dhillon, J. Dongarra, S. Hammarling, G. Henry, A. Petitet *et al.*, *ScaLAPACK users’ guide*. siam, 1997, vol. 4.
- [2] A. Ghoting, R. Krishnamurthy, E. Pednault, B. Reinwald, V. Sindhwani, S. Tatikonda, Y. Tian, and S. Vaithyanathan, “SystemML: Declarative machine learning on mapreduce,” in *ICDE*, 2011, pp. 231–242.
- [3] “Apache spark mllib: <http://spark.apache.org/docs/latest/mllib-data-types.html>.”
- [4] L. Libkin, R. Machlin, and L. Wong, “A query language for multidimensional arrays: Design, implementation, and optimization techniques,” in *SIGMOD*, 1996, pp. 228–239.
- [5] P. Baumann, A. Dehmel, P. Furtado, R. Ritsch, and N. Widmann, “The multidimensional database system rasdaman,” in *SIGMOD Record*, vol. 27, no. 2. ACM, 1998, pp. 575–577.
- [6] P. G. Brown, “Overview of SciDB: large scale array storage, processing and analysis,” in *SIGMOD*, 2010, pp. 963–968.
- [7] M. Boehm, D. R. Burdick, A. V. Evfimievski, B. Reinwald, F. R. Reiss, P. Sen, S. Tatikonda, and Y. Tian, “Systemml’s optimizer: Plan generation for large-scale machine learning programs.” *IEEE Data Eng. Bull.*, vol. 37, no. 3, pp. 52–62, 2014.
- [8] S. Chaudhuri, “An overview of query optimization in relational systems,” in *PODS*. ACM, 1998, pp. 34–43.
- [9] M. Armbrust, R. S. Xin, C. Lian, Y. Huai, D. Liu, J. K. Bradley, X. Meng, T. Kaftan, M. J. Franklin, A. Ghodsi *et al.*, “Spark sql: Relational data processing in spark,” in *SIGMOD*. ACM, 2015, pp. 1383–1394.
- [10] A. Thusoo, J. S. Sarma, N. Jain, Z. Shao, P. Chakka, S. Anthony, H. Liu, P. Wyckoff, and R. Murthy, “Hive: a warehousing solution over a map-reduce framework,” *VLDB*, vol. 2, no. 2, pp. 1626–1629, 2009.
- [11] L. S. Blackford, A. Petitet, R. Pozo, K. Remington, R. C. Whaley, J. Demmel, J. Dongarra, I. Duff, S. Hammarling, G. Henry *et al.*, “An updated set of basic linear algebra subprograms (blas),” *ACM TOMS*, vol. 28, no. 2, pp. 135–151, 2002.
- [12] E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, and D. Sorensen, *LAPACK Users’ guide*. Siam, 1999, vol. 9.
- [13] Z. Cai, Z. Vagena, L. L. Perez, S. Arumugam, P. J. Haas, and C. Jermaine, “Simulation of database-valued Markov chains using SimSQL,” in *SIGMOD*, 2013, pp. 637–648.
- [14] G. Lebanon, “Metric learning for text documents,” *IEEE PAMI*, vol. 28, no. 4, pp. 497–508, 2006.
- [15] A. Elgohary, M. Boehm, P. J. Haas, F. R. Reiss, and B. Reinwald, “Compressed linear algebra for large-scale machine learning,” *VLDB*, vol. 9, no. 12, pp. 960–971, 2016.
- [16] T. Park and G. Casella, “The Bayesian Lasso,” *JASA*, vol. 103, no. 482, pp. 681–686, 2008.
- [17] B. Huang, S. Babu, and J. Yang, “Cumulon: Optimizing statistical data analysis in the cloud,” in *SIGMOD*, 2013, pp. 1–12.
- [18] Z. Qian, X. Chen, N. Kang, M. Chen, Y. Yu, T. Moscibroda, and Z. Zhang, “Madlinq: large-scale distributed matrix computation for the cloud,” in *EuroSys*. ACM, 2012, pp. 197–210.
- [19] S. Das, Y. Sismanis, K. S. Beyer, R. Gemulla, P. J. Haas, and J. McPherson, “Ricardo: integrating R and Hadoop,” in *SIGMOD*, 2010, pp. 987–998.
- [20] Y. Zhang, W. Zhang, and J. Yang, “I/o-efficient statistical computing with riot,” in *ICDE*. IEEE, 2010, pp. 1157–1160.
- [21] S. Seo, E. J. Yoon, J. Kim, S. Jin, J.-S. Kim, and S. Maeng, “Hama: An efficient matrix computation with the mapreduce framework,” in *CloudCom*. IEEE, 2010, pp. 721–726.
- [22] J. B. Buck, N. Watkins, J. LeFevre, K. Ioannidou, C. Maltzahn, N. Polyzotis, and S. Brandt, “SciHadoop: Array-based query processing in Hadoop,” in *ACM SC*, 2011, p. 66.
- [23] Y. Zhang, M. Kersten, and S. Manegold, “Sciql: array data processing inside an rdbms,” in *SIGMOD*. ACM, 2013, pp. 1049–1052.
- [24] P. A. Boncz, M. Zukowski, and N. Nes, “Monetdb/x100: Hyper-pipelining query execution,” in *CIDR*, vol. 5, 2005, pp. 225–237.
- [25] “Oracle corporation: [https://docs.oracle.com/cd/B1930-6\\_01/index.htm](https://docs.oracle.com/cd/B1930-6_01/index.htm).”
- [26] J. M. Hellerstein, C. Ré, F. Schoppmann, D. Z. Wang, E. Fratkin, A. Gorajek, K. S. Ng, C. Welton, X. Feng, K. Li *et al.*, “The MADlib analytics library: or MAD skills, the SQL,” *VLDB*, vol. 5, no. 12, pp. 1700–1711, 2012.