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# HADAD: A Lightweight Approach for Optimizing Hybrid Complex Analytics Queries

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### ABSTRACT

Hybrid complex analytics workloads typically include  $(i)$  data management tasks (joins, filters, etc. ), easily expressed using relational algebra (RA)-based languages, and (ii) complex analytics tasks (regressions, matrix decompositions, etc.), mostly expressed in linear algebra (LA) expressions. Such workloads are common in a number of areas, including scientific computing, web analytics, business recommendation, natural language processing, speech recognition. Existing solutions for evaluating hybrid complex analytics queries – ranging from LA-oriented systems, to relational systems (extended to handle LA operations), to hybrid systems – fail to provide a unified optimization framework for such a hybrid setting. These systems either optimize data management and complex analytics tasks separately, or exploit RA properties only while leaving LA-specific optimization opportunities unexplored. Finally, they are not able to exploit precomputed (materialized) results to avoid computing again (part of) a given mixed (LA and RA) computation.

We describe HADAD, an extensible lightweight approach for optimizing hybrid complex analytics queries, based on a common abstraction that facilitates unified reasoning: a relational model endowed with integrity constraints, which can be used to express the properties of the two computation formalisms. Our approach enables full exploration of LA properties and rewrites, as well as semantic query optimization. Importantly, our approach does not require modifying the internals of the existing systems. Our experimental evaluation shows significant performance gains on diverse workloads, from LA-centered ones to hybrid ones.

#### 1 INTRODUCTION

Modern analytical tasks typically include  $(i)$  data management tasks (e.g., joins, filters) to perform pre-processing steps including feature selection, transformation, and engineering [18, 22, 34, 41, 43], tasks that are easily expressed using relational algebra (RA)-based languages, as well as (ii) complex analytics tasks (e.g., regressions, matrices decompositions), which are mostly expressed using linear algebra (LA) operations [33]. Such workloads are common in several application domains including scientific computing, web analytics, business recommendation, natural language processing [38], or speech recognition [29]. To perform such analytical tasks, data scientists can choose from a variety of systems, tools, and languages. Languages/libraries such as R [3] and NumPy [2], as well as LAoriented systems such as SystemML [19] and TensorFlow [11] treat matrices and linear algebra operations as first-class citizens: they offer a rich set of built-in LA operations and algorithms. However, it can be difficult to express data management tasks that include pre-processing and data transformation in these systems. Further,

expression rewrites, based on equivalences that hold due to wellknown LA properties, are not exploited in some of these systems, leading to missed optimization opportunities.

Many works haved sought to efficiently integrate RA and LA processing in a hybrid environment where both algebraic styles can be used together [1, 27, 32, 35, 37, 39, 45]. Some works propose calling LA packages through user defined functions (UDFs), where libraries such as R and NumPy are embedded in the host language [1]. Others suggest to treat LA objects as first-class citizens in a column-oriented store or RDBMS and using built-in functions to express LA operations [32, 37]. However, the semantics of LA operations remain hidden behind these built-in functions and UDFs, i.e., LA routines, which the optimizers treat as black-boxes. LARA [35] introduces a declarative domain-specific language for collections and matrices, which enables optimization across the two algebraic abstractions. SPORES [46] and SPOOF [21] optimize LA expressions, by converting them into RA, optimizing the latter, and then converting the result back to an (optimized) LA expression. Polystore or hybrid systems provide an environment, where mixed RA and LA programs can be written and executed across different systems [27, 45].

We identify *unexplored optimization opportunities* in existing solutions for evaluating hybrid complex analytics queries. First, they do not fully exploit LA properties and rewrites, whereas it has been shown that such rewrites can drastically enhance LA-based pipelines' performance [44]. Second, they do not support semantic query optimization [12], which includes taking advantage of partial materialized computation results, i.e., materialized views, known to improve the performance of a variety of queries.

We propose HADAD, an extensible, lightweight, holistic optimizer for analytical queries, based on reasoning on a common abstraction: relational model with integrity constraints. This brings within reach powerful cost-based optimizations across RA and LA, without the need to modify the internals of the existing systems; as we show, it is very easy to add within HADDAD knowledge about a wider range of LA operations than previous work could consider, while also enabling view-based rewriting and semantic query optimization using integrity constraints. The benefits of our optimized rewrites apply both to systems that provide a mixed-programming interface, such as polystores, and to LA-oriented systems designed and built for matrix operations. Last but not least, our holistic, cost-based approach enables to judiciously apply for each query the best available optimization. For instance, given the computation  $M(NP)$  for some matrices M, N and P, we may rewrite it into  $(MN)P$  if its estimated cost is smaller than that of the original expression, or we may turn it into MV if a materialized view V stores exactly the result of  $(NP)$ . HADAD capitalizes on a framework

previously introduced in [14] for rewriting queries across many data models, using materialized views, in a polystore setting. The novelty of HADAD is to extend the benefits of rewriting and views optimizations to LA computations, crucial for model analytics and ML workloads.

Contributions. This paper makes the following contributions:

- 1 We propose an extensible lightweight approach to optimize hybrid complex analytics queries. Our approach can be implemented on top of existing systems without the need to modify their internals; it is based on a powerful intermediate abstraction that supports reasoning about such a hybrid setting, namely, a relational model with integrity constraints.
- 2 We formalize the problem of rewriting computations using previously materialized views in this mixed setting. To the best of our knowledge, ours is the first work that brings viewsbased rewriting under integrity constraints in the context of LA-based pipelines and hybrid complex analytics queries.
- <sup>3</sup> We provide *formal guarantees* for our solution in terms of soundness and completeness.
- 4 We conduct an extensive set of experiments on typical LAbased and hybrid pipelines, which show the benefits of our approach.

Paper Organization. The rest of this paper is organized as follows. Section 2 formalizes the query optimization problem we solve in the context of a hybrid setting. After some preliminaries (Section 3), Section 4 provides an end-to-end overview of our approach. Section 5 presents our novel reduction of a rewriting problem with LA views into one that can be solved by existing techniques from the relational setting. Section 6 describes our extension to the query rewriting engine, integrating two different cost models, to help prune out inefficient rewritings as soon as they are enumerated. We formalize our solution's guarantees in Section 7 and present our experimental evaluation in Section 8. We then discuss related work and conclude in Section 9.

#### 2 PROBLEM STATEMENT

We consider a set of *value domains*  $\mathcal{D}_i$ , e.g.,  $\mathcal{D}_1$  denotes integers,  $\mathcal{D}_2$  denotes real numbers,  $\mathcal{D}_2$  strings, etc. We consider two basic  $\mathcal{D}_2$  denotes real numbers,  $\mathcal{D}_3$  strings, etc. We consider two basic data types: relations (sets of tuples) as in classical database modeling, and matrices (bi-dimensional arrays). Any attribute in a tuple or cell in a matrix is a value from some  $\mathcal{D}_i$ . We assume *a matrix can be implicitly converted into a relation* (the order among matrix rows is implicitly converted into a relation (the order among matrix rows is lost), and the opposite conversion (each tuple becomes a matrix line, in some order that is unknown, unless the relation was explicitly sorted before the conversion).

We consider a set  $R_{obs}$  of (unary or binary) relational algebra operators; concretely,  $R_{ops}$  comprises the standard relational selection, projection, and join. We also consider a set  $L_{ops}$  of linear algebra operators, comprising: unary operators which apply to a matrix and return a matrix (e.g., inversion and transposition), a number (e.g., the trace), or two matrices (e.g., the LU decomposition [36]); unary operations applied to a matrix and a number and returning a matrix, such as the scalar-matrix multiplication; binary operations applied to two matrices, or a matrix and a number, and returning a matrix or a number, such as matrix sum and product, scalar product, etc. The full set  $L_{ops}$  of LA operations we support is detailed in Section 5.1. A hybrid (RA and/or LA) expression is defined as follows:

- any value from a domain  $\mathcal{D}_i$ , any matrix, and any relation, is an expression;
- (RA operators): given some expressions E, E',  $ro_1(E)$  is also<br>an expression where  $ro_2 \in R$ , is a unary relational operaan expression, where  $ro_1 \in R_{ops}$  is a unary relational operator, and  $E$ 's type matches  $ro<sub>1</sub>$ 's expected input type. The same holds for  $ro_2(E, E')$ , where  $ro_2 \in R_{ops}$  is a binary relational operator (i.e., the join). operator (i.e., the join);
- (LA operators): given some expressions  $E, E'$  which are either numeric matrices or numbers (which can be seen as ther numeric matrices or numbers (which can be seen as degenerate matrices of  $1 \times 1$ ), and some real number r, the following are also expressions:  $lo_1(E)$  where  $lo_1 \in L_{ops}$  is a unary operator, and  $l_{O_2}(E, E')$  where  $l_{O_2} \in L_{ops}$  is a binary<br>operator (again, provided that  $E, E'$  match the expected input operator (again, provided that  $E, E'$  match the expected input<br>types of the operators) types of the operators).

Clearly, an important set of equivalence rules hold over our hybrid expressions, well-known respectively in the RA and the LA literature. These equivalences lead to alternative evaluation strategies for each expression.

Further, we assume given a (potentially empty) set of materialized views  $V$ , expressions which have been previously computed over some inputs (matrices and/or relations), and whose results are directly available (e.g., as a file on disk). Detecting when a materialized view can be used instead of evaluating (part of) an expression is another important source of alternative evaluation strategies.

Given an expression  $E$  and a cost model that assigns a cost (a real number) to an expression, we consider the problem of identifying the most efficient (lowest-cost) rewrite derived from  $E$  by:  $(i)$  exploiting RA and LA equivalence rules, and/or  $(ii)$  replacing part of an expression with a scan of a materialized view equivalent to that expression.

Below, we detail our approach, the equivalence rules we capture, and two alternative cost models we devised for this hybrid RA/LA setting. Importantly, our solution (based on a relational encoding with integrity constraints) capitalizes on the framework previously introduced in [14], where it was used to rewrite queries using materialized views in a polystore setting, where the data, views, and query cover a variety of data models (relational, JSON, XML, etc. ). Those queries can be expressed in a combination of standard database query languages, including SQL, JSON query languages, XQuery, etc. The ability to rewrite such queries using heterogeneous views directly and fully transfers to HADAD: thus, instead of a relation, we could have the (tuple-structured) results of an XML or JSON query; views materialized by joining an XML document with a JSON one and a relational database could also be reused. The novelty of our work is to extend the benefits of rewriting and viewbased optimization to LA computations, crucial for modern analytics and ML workloads. In what follows (Section 5), we focus on capturing matrix data and LA computations in the relational framework, along with relational data naturally; this enables our novel, holistic optimization of hybrid expressions.

#### 3 PRELIMINARIES

We recall conjunctive queries [23], integrity constraints [12], and query rewriting under constraints [31]; these concepts are at the core of our approach.

#### 3.1 Conjunctive Query and Constraints

A conjunctive query (or simply CQ)  $Q$  is an expression of the form  $Q(\overline{x})$ :-  $R_1(\overline{y}_1), \ldots, R_n(\overline{y}_n)$ , where each  $R_i$  is a predicate (relation)<br>of some finite arity and  $\overline{x}$ ,  $\overline{u}$  are tuples of variables or conof some finite arity, and  $\overline{x}, \overline{y}_1, \ldots, \overline{y}_n$  are tuples of variables or con-<br>stants. Each  $R(\overline{x})$  is called a relational atom. The expression  $Q(\overline{x})$ stants. Each  $R_i(\overline{y}_i)$  is called a relational atom. The expression  $Q(\overline{x})$ <br>is the *head* of the query while the conjunction of relational atoms is the head of the query, while the conjunction of relational atoms  $R_1(\overline{y}_1), \ldots, R_n(\overline{y}_n)$  is its *body*. All variables in the head are called distinguished. Also, every variable in  $\overline{x}$  must appear at least once in distinguished. Also, every variable in  $\overline{x}$  must appear at least once in  $\overline{y}_1, \ldots, \overline{y}_n$ . Different forms of constraints have been studied in the literature [12]. In this work, we use Tuple Generating Dependent  $y_1, \ldots, y_n$ <br>literature [12]. In this work, we use Tuple Generating Dependencies (TGDs) and Equality Generating Dependencies (EGDs), stated by formulas of the form  $\forall x_1, \ldots, x_n \phi(x_1, \ldots, x_n) \rightarrow \exists z_1, \ldots, z_k$  $\psi(y_1, \ldots, y_m)$ , where  $\{z_1, \ldots, z_k\} = \{y_1, \ldots, y_m\} \setminus \{x_1, \ldots, x_n\}$ .<br>The constraint's *premise*  $\phi$  is a possibly empty conjunction of rela-The constraint's *premise*  $\phi$  is a possibly empty conjunction of relational atoms over variables  $x_1, \ldots, x_n$  and possibly constants. The constraint's *conclusion*  $\psi$  is a non-empty conjunction of atoms over variables  $y_1, \ldots, y_m$  and possibly constants, atoms that are relational ones in the case of TGDs or equality atoms – of the form  $w = w'$  – in the case of **EGD**s. For instance, consider a relation Re-<br>view (paper reviewer track) listing reviewers of papers submitted to a view(paper, reviewer, track) listing reviewers of papers submitted to a conference's tracks, and a relation PC (member, affiliation) listing the affiliation of every program committee member [25].The fact that a paper can only be submitted to a single track is captured by the following EGD:  $\forall p \forall r \forall t \forall r' \forall t' \text{Review}(p, r, t) \land \text{Review}(p, r', t') \rightarrow t = t'$ .<br>'Y We can also express that papers can be reviewed only by PC mem. where  $\frac{1}{2}$ . We can also express that papers can be reviewed only by PC memthe calculation of the following TGD:  $\forall p \forall r \forall t$  Review $(p, r, t) \rightarrow \exists a \, PC(r, a)$ .

#### 3.2 Provenance-Aware Chase & Back-Chase

A key ingredient leveraged in our approach is relational query rewriting using views, in the presence of constraints. The stateof-the-art method for this task, called Chase & Backchase, was introduced in [26] and improved in [31], as the Provenance-Aware Chase & Back-Chase (PACB in short). At the core of these methods is the idea to model views as constraints, in this way reducing the view-based rewriting problem to constraints-only rewriting. Specifically, for a given view  $V$  defined by a query, the constraint  $V_{IO}$  states that for every match of the view body against the input data, there is a corresponding (head) tuple in the view output, while the constraint  $V_{OI}$  states the converse inclusion, i.e., each view output tuple is due to a view body match. From a set  $\mathcal V$  of view definitions, PACB therefore derives a set of view constraints  $C_V = \{V_{IO}, V_{OI} \mid V \in V\}.$ 

Given a source schema  $\sigma$  with a set of integrity constraints  $I$ , a set V of views defined over  $\sigma$ , and a conjunctive query Q over  $\sigma$ , the **rewriting problem** thus becomes: find every reformulation query  $\rho$  over the schema of view names  $\mathcal V$  that is equivalent to  $\mathcal Q$ under the constraints  $\mathcal{I} \cup \mathcal{C}_{V}$ .

For instance, if  $\sigma = \{R, S\}$ ,  $\mathcal{I} = \emptyset$ ,  $\tau = \{V\}$  and we have a view V materializing the join of relations R and S,  $V(x, y)$ :-  $R(x, z)$ ,  $S(z, y)$ , the pair of constraints capturing  $V$  is the following:

$$
V_{IO}: \quad \forall x \forall z \forall y \ R(x, z) \land S(z, y) \rightarrow V(x, y)
$$
  

$$
V_{OI}: \quad \forall x \forall y V(x, y) \rightarrow \exists z \ R(x, z) \land S(z, y).
$$

Given the query  $Q(x, y)$ :-  $R(x, z)$ ,  $S(z, y)$ , PACB finds the reformulation  $\rho(x, y)$ :-  $V(x, y)$ . Algorithmically, this is achieved by:



(i) chasing Q with the constraints  $I \cup C_{V}^{IO}$ , where  $C_{V}^{IO} = \{V_{IO} | V \in \emptyset\}$  is intuitively this enriches (extends) Q with all the consequences  $\mathcal{V}$ }; intuitively, this enriches (extends)  $\mathcal{Q}$  with all the consequences that follow from its atoms and the constraints  $I \cup C_V^{IO}$ .<br>(ii) restricting the chose result to only the V atoms: the

(*ii*) restricting the chase result to only the  $V$ -atoms; the result is called the *universal plan*) U.

 $(iii)$  annotating each atom of the universal plan  $U$  with a unique ID called a provenance term.

(iv) chasing U with the constraints in  $I \cup C_V^{OI}$ , where  $C_V^{OI} =$ <br> $\sim$   $\frac{1}{2}$   $V \in \Omega$ , and annotating seek relational stam a introduced  $\{V_{OI} \mid V \in \mathcal{V}\}$  , and annotating each relational atom  $a$  introduced by these chase steps with a *provenance formula*<sup>1</sup>  $\pi$ (*a*), which gives the set of  $U$ -subqueries whose chasing led to the creation of  $a$ ; the result of this phase, called the backchase, is denoted B.

(*v*) matching Q against B and outputting as rewritings the subsets of  $U$  that are responsible for the introduction (during the backchase) of the atoms in the image  $h(Q)$  of Q; these rewritings are read off directly from the provenance formula  $\pi(h(Q))$ .

In our example, *I* is empty,  $C_{V}^{IO} = \{V_{IO}\}$ , and the result of the results of the contract of the results of the results of the results of the results of the res chase in phase (i) is  $Q_1(x, y)$ :-  $R(x, z)$ ,  $S(z, y)$ ,  $V(x, y)$ . The universal plan obtained in (ii) by restricting  $Q_1$  to the schema of view names is  $U(x, y)$ :-  $V(x, y)$  $\dot{p}_0$ , where  $p_0$  denotes the provenance term of otom  $V(x, y)$ . The result of backgroups  $U$  with  $C^{OL}$  in phase (in) atom  $V(x, y)$ . The result of backchasing U with  $C_{Q}^{O I}$  in phase (iv)<br>in  $P(x, y)$ .  $V(x, y)P_0 P(x, z)P_0 S(x, y)P_0$ . Note that the provincing is  $B(x, y)$ :-  $V(x, y)^{p_0}$ ,  $R(x, z)^{p_0}$ ,  $S(z, y)^{p_0}$ . Note that the provenance formulas of the  $R$  and  $S$  atoms (a simple term, in this example) are introduced by chasing the view  $V$ . Finally, in phase  $(v)$  we find one match image given by h from  $Q$ 's body into the R and S atoms from B's body. The provenance formula  $\pi(h(Q))$  of the image h is  $p_0$ , which corresponds to an equivalent rewriting  $\rho(x, y)$ :-  $V(x, y)$ .

#### 4 HADAD OVERVIEW

We outline here our approach as an extension to [14] for solving the rewriting problem for LA-based computations.

Hybrid Expressions and Views. A hybrid expression (whether asked as a query, or describing a materialized view) can be purely relational (RA), in which case we assume it is specified as a conjunctive query. Other expressions are purely linear-algebra ones (LA); we assume that they are defined in a dedicated LA language such as R [3], DML [19], etc. , using linear algebra operators from our set  $L_{obs}$  (see Section 5.1), commonly used in real-world machine learning workloads. Finally, a hybrid expression can combine RA and LA, e.g., an RA expression (resulting in a relation) is treated as a matrix input by an LA operator, whose output may be converted again to a table and joined further, etc.

Our approach is based on a reduction to a relational model. Below, we show how to bring our hybrid expressions - and, most specifically, their LA components - under a relational form (the RA part of each expression is already in the target formalism).

 $^1$  Provenance formulas are constructed from provenance terms using logical conjunction and disjunction.

Encoding into a Relational Model. Let E be an LA expression (query) and  $V$  be a set of materialized views. We reduce the LAviews based rewriting problem to the relational rewriting problem under integrity constraints, as follows (see Figure 1). First, we encode *relationally E*,  $V$ , and the set  $L_{ops}$  of linear algebra operators. Note that the relations used in the encoding are virtual and hidden, i.e., invisible to both the application designers and users. They only serve to support query rewriting via relational techniques.

These virtual relations are accompanied by a set of relational integrity constraints enc<sub>LA</sub>( $LA_{prop}$ ) that reflect a set  $LA_{prop}$  of LA properties of the supported LA operations  $L_{ops}$ . For instance, we model the *matrix addition* operation using a relation  $add_M(M, N, R)$ to denote that O is the result of  $M + N$ , together with a set of constraints stating that  $add_M$  is a functional relation that is commutative, associative, etc. These constraints are EGDs or TGDs (recall Section 3). We detail our relational encoding in Section 5.

Reduction form LA-based to Relational Rewriting. Our reduction translates the declaration of each view  $V \in \mathcal{V}$  to additional constraints  $enc_{LA}(V)$  that reflect the correspondence between V's input data and its output. Separately, E is also encoded as a relational query  $enc_{LA}(E)$  over the relational encodings of  $L_{ops}$  and its basic ingredients (matrices).

Now, the reformulation problem is reduced to a purely relational setting, as follows. We are given a relational query  $enc<sub>LA</sub>(E)$  and a set  $C_V = enc_{LA}(V_1) \cup ... \cup enc_{LA}(V_n)$  of relational integrity constraints encoding the views  $\boldsymbol{\mathcal{V}}$ . We add as further input a set of relational constraints  $enc_{LA}(LA_{prop})$ , which encodes relationally the  $LA_{prop}$  operators; we called them Matrix-Model Encoding constraints, or MMC in short. We must find the rewritings  $RW_t^i$  expressed over the relational views  $C_{\alpha}$  and  $MAC$  for some integer pressed over the relational views  $\overline{C}_\mathcal{V}$  and  $\mathcal{MMC}$ , for some integer  $\vec{k}$  and  $1 \le i \le k$ , such that each  $RW_t^i$  is equivalent to enc<sub>LA</sub>(E) under these constraints (Ca+ | **MMC**). Solving this problem vields der these constraints ( $\overline{\mathcal{C}}_{\boldsymbol{\mathcal{V}}}\cup\overline{\mathcal{M}\mathcal{M}\mathcal{C}}$ ). Solving this problem yields a relationally encoded rewriting  $RW_e$  expressed over the (virtual) relations used in the encoding; a final decoding step is needed to obtain  $E'$ , the rewriting of the (LA or, more generally, hybrid)  $E$ <br>using the views  $\mathcal U$ using the views  $V$ .

The challenge in coming up with the reduction consists in designing an encoding, i.e., one in which rewritings found by (i) encoding relationally, (ii) solving the resulting relational rewriting problem, and (iii) decoding a resulting rewriting over the views, is guaranteed to produce an equivalent expression E ′ . The reduction is detailed in Section 5.

Relational Rewriting Using Constraints. To solve the relational rewriting problem under constraints, the algorithm of choice is PACB (recall Section 3). Our PACB rewriting engine (*PACB*<sup>++</sup> hereafter) has been extended to utilize the  $Pruned_{prov}$  algorithm sketched and discussed in [30, 31], which prunes inefficient rewritings during the rewritings search phase, based on a simple cost model using two different matrix sparsity estimators. Section 6 details the choice of an efficient rewriting utilizing the  $PACB^{++}$ engine.

Decoding of the Relational Rewriting. For the selected relational reformulation  $RW_e$  by  $PACB^{++}$ , a decoding step dec( $RW_e$ ) is performed to translate  $RW_e$  into the native syntax of its respective underlying store/engine (e.g., R, DML, etc.).

#### 5 REDUCTION TO THE RELATIONAL MODEL

Our internal model is relational, and it makes prominent use of expressive integrity constraints (TGDs and EGDs, recall Section 3). This framework suffices to describe the features and properties of most data models used today, notably including relational, XML, JSON, graph, etc [14, 15].

Going beyond, in this section, we present a novel way to reason relationally about LA primitives/operations by treating them as uninterpreted functions with black-box semantics, and adding constraints that capture their important properties. First, we give an overview of a wide range of LA operations that we consider in Section 5.1. Then, in Section 5.2, we show how matrices and their operations can be represented (encoded) using a set of virtual relations, part of a schema we call  $VREM$  (for Virtual Relational Encoding of Matrices), together with the integrity constraints  $\mathcal{MMC}$  that capture the LA properties of these operations. Regardless of matrix data's physical storage, we only use  $VREM$  to encode LA expressions and views relationally to reason about them. Section 5.3 exemplifies relational rewritings obtained via our reduction.

#### 5.1 Matrix Algebra

We consider a wide range of matrix operations [17, 36], which are common in real-world machine learning algorithms [5]: elementwise multiplication (i.e., Hadamard-product) ( $multi_E$ ), matrix-scalar multiplication ( $multiplication (multi<sub>MS</sub>)$ , matrix multiplication ( $multi<sub>M</sub>$ ), addition (add<sub>M</sub>), division (div<sub>M</sub>), transposition (tr), inversion (inv<sub>M</sub>), determinant (det), trace (trace), exponential (exp), adjoints (adj), direct sum (sum<sub>D</sub>), direct product (product<sub>D</sub>), summation (sum<sub>M</sub>), rows and columns summation (rowSum<sub>M</sub> and colSum<sub>M</sub>, respectively), QR decomposition (QR), Cholesky decomposition (cho), LU decomposition  $(LU)$ , and pivoted LU decomposition  $(LUP)$ .

#### 5.2 VREM Schema and Relational Encoding

To model LA operations on the VREM relational schema (part of which appears in Table 1), we also rely on a set of integrity constraints  $MMC$ , which are encoded using relations in  $VREM$ . We detail the encoding below.

5.2.1 Base Matrices and Dimensionality Modeling. We denote by  $M_{k\times z}(\mathcal{D})$  a matrix of k rows and z columns, whose entries (values) come from a domain  $D$ , e.g., the domain of real numbers R. For brevity we just use  $M_{k \times n}$ . We define a virtual relation bers K. For brevity we just use  $M_{k \times z}$ . We define a virtual relation<br>  $name(M_1^i, n) \in VREM$  attaching a unique ID  $M_1^i$  to any matrix<br>
identified by a name denoted n (which may be a g of the form identified by a name denoted  $n$  (which may be e.g. of the form "/data/M.csv"). This relation (shown at the top left in Table 1) is accompanied by an EGD key constraint  $I_{name} \in \mathcal{MMC}_m$ , where  $\mathcal{MMC}_m \subset \mathcal{MMC}$ , and  $I_{name}$  states that two matrices with the same name n have the same ID:

 $I_{name}: \forall M_1^i \forall M_2^i \ name(M_1^i, n) \land name(M_2^i, n) \rightarrow M_1^i = M_2^i$ 

Note that the matrix ID in name (and all the other virtual relations used in our encoding) are not IDs of individual matrix objects: rather, each identifies an equivalence class (induced by value equality) of expressions. That is, two expressions are assigned the same ID iff they yield value-based-equal matrices.

The dimensions of a matrix are captured by a size  $(M_1^i, k, z)$  rela-<br>n, where  $k$  and a sure the number of name, near, as lumnes and  $M_i^i$ . tion, where k and z are the number of rows, resp. columns and  $M_1^i$ <br>is an ID, An EGD constraint  $\overline{I}$ ,  $\epsilon$  **MMC** holds on the size is an ID. An EGD constraint  $I_{size} \in \mathcal{MMC}_m$  holds on the size relation, stating that the ID determines the dimensions:





$$
I_{size}(M_1^i \vee k_1 \vee z_1 \vee k_2 \vee z_2
$$
  

$$
size(M_1^i, k_1, z_1) \wedge size(M_1^i, k_2, z_2) \rightarrow k_1 = k_2 \wedge z_1 = z_2
$$

The identity I and zero O matrices are captured by the  $Zero(O)$ <br>d Identity(I) relations respectively which are accompanied by and  $Identity(I)$ , relations respectively, which are accompanied by EGD constraints  $I_{iden}$ ,  $I_{zero} \in MMC_m$ , stating that zero matri-<br>ces with the same sizes have the same IDs, and this also applies for ces with the same sizes have the same IDs, and this also applies for identity matrices with the same size:

$$
\begin{aligned} \label{eq:zero} I_{zero}\colon \forall O_1^i\forall O_2^i\forall k\forall z\\ Zero(O_1^i)\land size(O_1^i,k,z)\land Zero(O_2^i)\land size(O_2^i,k,z)\rightarrow O_1^i=O_2^i\\ I_{iden}\colon \forall I_1^i\forall I_2^i\forall i\\ Identity(I_1^i)\land size(I_1^i,k,k)\land Identity(I_2^i)\land size(I_2^i,k,k)\rightarrow I_1^i=I_2^i \end{aligned}
$$

5.2.2 Encoding Matrix Algebra Expressions. LA operations are encoded into dedicated relations, as shown in Table 1. We now illustrate the encoding of an LA expression on the  $VREM$  schema.

EXAMPLE 5.1. Consider the LA expression  $E: ((MN)^T)$ , where the two matrices  $M_{100\times1}$  and  $N_{1\times10}$  are stored as "M.csv" and "N.csv", respectively. The encoding function enc $(E)$  takes as argument the LA expression E and returns a conjunctive query whose: (i) body is the relational encoding of E using  $VREM$  (see below), and (ii) head has one distinguished variable, denoting the equivalence class of the result. For instance:

$$
enc(((MN)^{T}) =
$$
  
\nLet enc(MN) =  
\nLet enc(M) =  $Q_{0}(M_{1}^{i})$ : - name(M\_{1}^{i}, "M.csv");  
\nenc(N) =  $Q_{1}(N_{1}^{i})$ : - name(N\_{1}^{i}, "N.csv");  
\n $R_{1}^{o}$  = freshId()  
\nin  
\n $Q_{2}(R_{1}^{o})$ : - multi<sub>M</sub>(M\_{1}^{i}, N\_{1}^{i}, R\_{1}^{o}),  $Q_{0}(M_{1}^{i})$ ,  $Q_{1}(N_{1}^{i})$ ;  
\n $R_{2}^{o}$  = freshId()  
\n*O*( $R_{2}^{o}$ ): - tr( $R_{1}^{o}, R_{2}^{o}$ ),  $Q_{2}(R_{1}^{o})$ ;  
\n $Q_{2}^{o}$ :

In the above, nesting is dictated by the syntax of E. From the inner<br>(most indented) to the outer we first encode M and N as small queries (most indented) to the outer, we first encode M and N as small queries using the name relation, then their product (to whom we assign the newly created identifier  $R_1^0$ , ), using the multi<sub>M</sub> relation and encoding<br>the relationship between this product and its inputs in the definition the relationship between this product and its inputs in the definition of  $\mathbf{Q}_2(R_1^o)$ . Next, we create a fresh ID  $R_2^o$  used to encode the full E<br>(the transposed of  $\mathbf{Q}_2$ ) via relation tr, in the query  $\mathbf{Q}(R_2^o)$ . For brew the (the transposed of  $\mathbf{Q}_2$ ) via relation tr, in the query  $\mathbf{Q}(R_2^o)$ . For brevity, we omit the matrices' size relations in this example and hereafter we omit the matrices' size relations in this example and hereafter. Unfolding  $Q_2(R_1^0)$  in the body of  $Q$  yields:

$$
Q(R_2^o) - tr(R_1^o, R_2^o), multi_M(M_1^i, N_1^i, R_1^o),
$$
  
 
$$
Q_0(M_1^i), Q_1(N_1^i);
$$

$$
\forall M_1^i \forall M_2^i \forall R^o \ add_M(M_1^i, M_2^i, R^o) \rightarrow add_M(M_2^i, M_1^i, R^o)
$$
 (1)  

$$
\forall M_1^i \forall M_2^i \forall R_1^o \forall R_2^o \ add_M(M_1^i, M_2^i, R_1^o) \land tr(R_1^o, R_2^o) \rightarrow
$$

$$
\forall M_1^1 \forall M_2^1 \forall R_1^0 \forall R_2^0 \ add_M(M_1^1, M_2^1, R_1^0) \land tr(R_1^0, R_2^0) \rightarrow
$$
  
\n
$$
\exists R_3^0 \exists R_4^0 \ tr(M_1^i, R_3^0) \land tr(M_2^i, R_4^0) \land add_M(R_3^0, R_4^0, R_2^0)
$$
\n
$$
\forall M_1^1 \forall R_1^0 \forall R_2^0 \ inv_M(M_1^i, R_1^0) \land tr(R_1^0, R_2^0) \rightarrow
$$
  
\n
$$
\exists R_3^0 \ tr(M_1^i, R_3^0) \land inv_M(R_3^0, R_2^0)
$$
\n(3)

#### Figure 2: MMC Constraints Capturing Basic LA Properties

Now, by unfolding  $Q_0$  and  $Q_1$  in  $Q$ , we obtain the final encoding of  $((MN)^T)$  as a conjunctive query **Q**:<br> $Q(D^0)$ , tr(D<sup>0</sup>, D<sup>0</sup>), multi, (M

 $Q(R_2^o) = tr(R_1^o, R_2^o)$ , multi<sub>M</sub> $(M_1^i, N_1^i, R_1^o)$ ,<br>name(M<sup>i</sup><sup>a</sup>M cszy<sup>n</sup>) name(N<sup>i</sup><sup>a</sup>  $name(N_1^i, "M.csv"), name(N_1^i, "N.csv"),$ 

5.2.3 Encoding LA Properties as Integrity Constraints. Figure 2 shows some of the constraints  $\widetilde{MMC}_{LAprop} \subset \widetilde{MMC}$ ,<br>which conture to thook LA properties [17, 36] of our LA operations which capture textbook LA properties [17, 36] of our LA operations (Section 5.1). The TGDs (1), (2) and (3) state that matrix addition is commutative, matrix transposition is distributive with respect to addition, and the transposition of the inverse of matrix  $M_1^i$  is equiv-<br>along the inverse of the transposition of  $M_1^i$  acquestively. We also alent to the inverse of the transposition of  $M_1^i$ , respectively. We also<br>express that the *virtual relations are functional* by using ECD key express that the virtual relations are functional by using EGD key constraints. For example, the following  $I_{multi} \in \text{MMC}_{LAprop}$ mul t i<sup>M</sup> constraint states that multiM is functional, that is the products of pairwise equal matrices are equal.

$$
I_{multi_M}: \forall M_1^i \forall M_2^i \forall R_1^o \forall R_2^o
$$
  

$$
multi_M(M_1^i, M_2^i, R_1^o) \land multi_M(M_1^i, M_2^i, R_2^o) \rightarrow R_1^o = R_2^o
$$

Other properties [17, 36] of the LA operations we consider are similarly encoded; due to space constraints, we relegate them to the technical report [4].

5.2.4 Encoding LA Views as Constraints. We translate each view definition V (defined in LA language such as R, DML, etc) into relational constraints enc<sub>LA</sub>(V)  $\in C_V$ , where  $C_V$  is the set of relational constraints used to capture the views  $V$ . These constraints show how the view's inputs are related to its output over the  $VREM$  schema. Figure 3 illustrates the encoding as a TGD constraint of the view  $V : (N)^T + (M^T)^{-1}$  stored in a file "V .csv" and<br>computed based on the matrices N and M (e.g., stored as "N csv" computed based on the matrices  $N$  and  $M$  (e.g., stored as "N.csv" and "M.csv", respectively).

5.2.5 Encoding Matrix Decompositions. Matrix decompositions play a crucial role in many LA computations. For instance, for every symmetric positive definite matrix M there exists a unique

 $\forall M_1^i \forall N_1^i \forall R_1^o \forall R_2^o \forall R_3^o \forall R_4^o$  $name(M_1^i, "M.csv") \wedge name(N_1^i, "N.csv") \wedge tr(N_1^i, R_1^o) \wedge$ <br> $tr(M_1^i, R_2^o) \wedge int(M_1^i, R_2^o) \wedge$  $tr(M_1^i, R_2^o) \wedge inv_M(R_2^o, R_3^o) \wedge$ <br> $L(R^o, R^o, R^o) \rightarrow nume(R^o, W)$  $add_M(R_1^o, R_3^o, R_4^o) \rightarrow name(R_4^o, "V.csv")$ 

Figure 3: Relational Encoding of view V

Cholesky Decomposition (CD) of the form  $M = LL^T$ , where L is a lower triangular matrix. We model CD as well as other well-known lower triangular matrix. We model CD, as well as other well-known decompositions (LU, QR, and Pivoted LU or PLU) as a set of virtual relations  $VREM_{dec}$ , which we add to  $VREM$ . For instance, to CD we associate a relation cho( $M<sup>i</sup>$ ,  $I<sup>0</sup>$ ) which denotes that  $I<sup>0</sup>$  is the CD we associate a relation  $cho(M_1^i, L^o)$ , which denotes that  $L^o$  is the output of the CD decomposition for a given matrix M whose ID is output of the CD decomposition for a given matrix M whose ID is  $M_t^i$  cho is a functional relation meaning every symmetric positive  $m_{1}$ : *eno* is a functional relation, meaning every symmetric positive<br>definite matrix has a unique CD decomposition. This functional  $\frac{i}{1}$ , *cho* is a functional relation, meaning every symmetric positive  $\frac{1}{1}$ . aspect is captured by an EGD, conceptually similar to the constraint  $I_{multi_M}$  (Section 5.2.3). The property  $M = LL^T$  is captured as a  $TCD$  constraint  $I_{i,j} \in MMC$ ;  $T_{\text{Hill}}$  (section 5.2.5). The property<br>TGD constraint  $I_{cho} \in \text{MMC}_{LA_{prop}}$ :

$$
I_{cho}: \forall M_1^i \ type(M_1^i, \text{``S''}) \rightarrow \exists L_1^o \exists L_2^o \ cho(M_1^i, L_1^o) \land \ type(L_1^o, \text{``L''}) \land tr(L_1^o, L_2^o) \land \ multiple(L_1^o, L_2^o, M_1^i)
$$
\n
$$
\tag{4}
$$

The atom type( $M_1^i$ ,  $S^r$ ) indicates the type of matrix  $M_1^i$ , where the constant " $S^r$  denotes a matrix that is symmetric positive definite: constant "S" denotes a matrix that is symmetric positive definite; similarly, type( $L_1^o$ ",  $L$ ") denotes that the matrix  $L_1^o$  is a lower trian-<br>sular matrix. For each base matrix, its type (if available) (e.g., symgular matrix. For each base matrix, its type (if available) (e.g., symmetric, upper triangular, etc. ) is specified as TGD constraint. For example, we state that a certain matrix M (and any other matrix value-equal to  $M$ ) is symmetric positive definite as follows:

$$
\forall M_1 \ name(M_1^i, \text{``}M.csv\text{''}) \rightarrow type(M_1^i, \text{``}S\text{''})
$$
 (5)

EXAMPLE 5.2. Consider a view  $V = N + LL^T$ , where  $L = cho(M)$ <br>d M is a symmetric positive definite matrix encoded as in (5) Let and M is a symmetric positive definite matrix encoded as in (5). Let E be the LA expression  $M + N$ . The reader realizes easily that V can be used to answer E directly, thanks to the specific property of the CD decomposition (4), and since  $M + N = N + M$ , which is encoded in  $(1)$ . However, at the syntactic level, V and E are very dissimilar. Knowledge of  $(1)$  and  $(4)$  and the ability to reason about them is crucial in order to efficiently answer E based on V .

The output matrix of CD decomposition is a lower triangular matrix L, which is not symmetric positive definite, meaning that CD decomposition can not be applied again on L. For other decompositions, such as  $QR(M) = [Q, R]$  decomposition, where M is a square matrix,  $Q$  is an orthogonal matrix [36] and  $R$  is an upper triangular matrix, there exists a  $QR$  decomposition for the orthogonal matrix Q such that  $QR(Q) = [Q, I]$ , where I is an identity matrix and  $QR(R) = [I, R]$ . We say the *fixed point* of the QR decomposition is  $QR(I) = [I, I]$ . These properties of the Q decompositions are captured with the following constraints, which are part of  $\mathcal{MMC}_{LAprop}$ :

$$
\forall M_1^i \forall n \forall k \ name(M_1^i, n) \land size(M_1^i, k, k) \rightarrow \exists Q^o \exists R^o
$$
  
\n
$$
QR(M_1^i, Q^o, R^o) \land type(Q^o, "O") \land type(R^o, "U")
$$
  
\n
$$
\land \ multi_M(Q^o, R^o, M_1^i)
$$
  
\n
$$
\forall Q_1^i \ type(Q_1^i, "O") \rightarrow \exists I^o \ QR(Q_1^i, Q_1^i, I^o) \land identity(I^o)
$$
  
\n(6)

$$
\wedge \text{ multi } _{M}(Q_1^i, I^o, Q_1^i) \tag{7}
$$

$$
\forall R_1^i \text{ type}(R_1^i, \text{``}U\text{''}) \rightarrow \exists I^o \text{ QR}(R_1^i, I^o, R_1^i) \land identity(I^o)
$$

$$
\wedge \text{ multi }_{M}(I^{o}, R_{1}^{i}, R_{1}^{i})
$$
\n
$$
(8)
$$

$$
\forall I_1^i \text{ identity}(I_1^i) \rightarrow QR(I_1^i, I_1^i, I_1^i)
$$
\n
$$
\tag{9}
$$

Known LA properties of the other matrix decompositions (LU and PLU) are similarly encoded.

5.2.6 Encoding LA-Oriented System Rewrite Rules. Most LAoriented systems [2, 3] execute an incoming expression (LA pipeline) as-is, that is: run operations in a sequence, whose order is dictated by the expression syntax. Such systems do not exploit basic LA properties, e.g., reordering a chain of multiplied matrices in order to reduce the intermediate size. SystemML [19] is the only system that models some LA properties as static rewrite rules. It also comprises a set of rewrite rules which modify the given expressions to avoid large intermediates for aggregation and statistical operations such as  $rowsums(M), sum(M),$  etc. For example, SystemML uses rule:

$$
sum(MN) = sum(colSums(M)^{1} \odot rowSums(N))
$$
 (i)

to rewrite  $sum(MN)$  (summing all cells in the matrix product) where ⊙ is a matrix element-wise multiplication, to avoid actually computing MN and materializing it; similarly, it rewrites  $sum(M^T)$  into<br> $sum(M)$  to avoid materializing  $M^T$  ato However, the performance  $sum(M)$ , to avoid materializing  $M<sup>T</sup>$ , etc. However, the performance benefits of rewriting depend on the rewriting power (or, in other words, on how much the system understands the semantics of the incoming expression), as the following example shows.

EXAMPLE 5.3. Consider the LA expression  $E = ((M^T)^k (M + N)^T)$ ,<br>sere M and N are square matrixes, and expression  $E'$  sum(E), which where M and N are square matrixes, and expression  $E' = sum(E)$ , which<br>computes the sum of all cells in F. The expression  $F'$  can be rewritten computes the sum of all cells in E. The expression E' can be rewritten<br>to  $PW_0$ : sum( $F'$ ), where  $F''$  is: to  $\widetilde{RW}_0$  : sum(E''), where E'' is:

sum(colSums
$$
(M+N)^T
$$
  $\odot$  rowSums $(M^k)$ )

Failure to exploit the properties  $LA_{prop1} : (MN)^{T} = M^{T}N^{T}$  and/or  $LA_{prop2}:(M^n)^T=(M^T)^n$  prevents from finding rewriting RW<sub>0</sub>.<br>  $F'$  admits the alternative rewriting E' admits the alternative rewriting<br>PW sum(t(colSums((MT)k))

 $RW_1: sum(t(\text{colSums}((M^T)^k)) \odot t(\text{colSums}((M+N)))$ <br>wich can be obtained by directly applying the rewrite ry which can be obtained by directly applying the rewrite rule (i) above and rowSums( $M^T$ )=colSums( $M$ )<sup>T</sup>, without exploiting the properties<br>LA<sub>ster</sub> and LA<sub>ster</sub> However, BW, introduces more intermediate  $LA_{prop1}$  and  $LA_{prop2}$ . However, RW<sub>1</sub> introduces more intermediate results than RW<sub>0</sub>.

To fully exploit the potential of rewrite rules (for statistical or aggregation operations), they should be accompanied by sufficient knowledge of, and reasoning on, known properties of LA operations.

To bring such fruitful optimization to other LA-oriented systems lacking support of such rewrite rules, we have incorporated SystemML's rewrite rules into our framework, encoding them as a set of integrity constraints over the virtual relations in the schema  $\mathcal{V}\mathcal{R}\mathcal{E}\tilde{\mathcal{M}}$ , denoted  $\mathcal{M}\mathcal{M}\mathcal{C}_{StatAgg}$  (MM $\mathcal{C}$ ).

$$
RW_1: (M^{-1})^T + N^T \qquad RW_2: (M^T)^{-1} + N^T
$$
  
\n
$$
RW_3: N^T + (M^{-1})^T \qquad RW_4: (N^T)^{-1} + N^T
$$
  
\n
$$
RW_5: (N + M^{-1})^T
$$

Figure 4: Equivalent rewritings of the pipeline  $\mathcal{Q}_p$ .

Thus, these rewrite rules can be exploited together with other LA properties. For instance, the rewrite rule  $(i)$  is modeled by the following integrity constraint  $I_{sum} \in \mathcal{MMC}_{StatAgg}$ :

$$
\forall M_1^1 \forall N_1^1 \forall R^o \text{ multi}_M(M_1^1, N_1^1, R^o) \land \text{sum}(R^o, s) \rightarrow
$$
  

$$
\exists R_1^o \exists R_2^o \exists R_3^o \exists R_4^o \text{ colSums}(M_1^i, R_1^o) \land \text{tr}(R_1^o, R_2^o)
$$
  

$$
\land \text{rowSums}(N_1^i, R_3^o) \land \text{multi}_E(R_2^o, R_3^o, R_4^o) \land \text{sum}(R_4^o, s)
$$

We refer the reader to the extended version of the paper [4] for a full list of SystemML's encoded rewrite rules.

#### 5.3 Relational Rewriting Using Constraints

With the set of views constraints  $C_V$  and  $MMC = MMC_m \cup$  $MMC_{LA_{prop}} \cup MMC_{StatAgg}$ , we rely on  $PACB^{++}$  to rewrite a given expression under integrity constraints. We examplify this given expression under integrity constraints. We exemplify this below, and detail  $PACB^{++}$ 's inner workings in Section 6.

The view  $V$  shown in Figure 3 can be used to  $fully$  rewrite (return the answer for) the pipeline  $Q_p$ :  $(M^{-1} + N)^T$  by exploiting the TCDs (1) (2) and (3) listed in Figure 2, which describe the following TGDs (1), (2) and (3) listed in Figure 2, which describe the following three LA properties, denoted  $LA_{prop_1}: M+N = M+N; ((M+N))^T = (M^T + (M^T + M^T)(M^T - M^T + M^T))$  $(M)^T + (N)^T$  and  $((M)^{-1})^T = ((M)^T)^{-1}$ . The relational rewriting<br>*PW<sub>2</sub>* of *Q*, using the view *V* is *PW<sub>2</sub>*(*P*<sup>0</sup>) - name(*P*<sup>0</sup> <sup>e</sup>V cs;<sup>*r*</sup>)</sub>. In this  $RW_0$  of  $Q_p$  using the view V is  $RW_0(R_1^o)$ :- name  $(R_1^o, {}^vV \ncsc v)$ . In this example,  $RW_0$  is the only views-hased rewriting of  $Q$ . However example,  $RW_0$  is the only views-based rewriting of  $Q_p$ . However, five other rewritings exist (shown in Figure 4), which reorder its operations just by exploiting the set  $LA_{prop_1}$  of LA properties.<br>
Powritings  $P W_2$  to  $P W_4$  have different evaluation costs  $W_2$ 

Rewritings  $RW_0$  to  $RW_5$  have different evaluation costs. We discuss next how we estimate which among these alternatives (including evaluating  $Q_p$  directly) is likely the most efficient.<br>6 CHOICE OF AN EFFICIENT REWRIT

#### 6 CHOICE OF AN EFFICIENT REWRITING

We introduce our cost model (Section 6.1), which can take two different sparsity estimators (Section 6.2). Then, we detail our extension to the PACB rewriting engine based on the  $Prune_{prov}$  algorithm (Section 6.3) to prune out inefficient rewritings.

#### 6.1 Cost Model

We estimate the cost of an expression E, denoted  $\gamma(E)$ , as the sum of the intermediate result sizes if one evaluates  $E$  "as stated", in the syntactic order dictated by the expression. Real-world matrices may be dense (most or all elements are non-zero) or sparse (a majority of zero elements). The latter admit more economical representations that do not store zero elements, which our intermediate result size measure excludes. To estimate the number of non-zeros (nnz, in short), we incorporated two different sparsity estimators from the literature (discussed in Section 6.2) into our framework.

EXAMPLE 6.1. Consider  $E_1 = (MN)M$  and  $E_2 = M(NM)$ , where we assume the matrices  $M_{50K\times100}$  and  $N_{100\times50K}$  are dense. The total cost of  $E_1$  is  $\gamma(E_1) = 50K \times 50K$  and  $\gamma(E_2) = 100 \times 100$ .

#### 6.2 LA-based Sparsity Estimators

We outline below two existing sparsity estimators [19, 46] that we have incorporated into our framework to estimate nnz.

6.2.1 Naïve Metadata Estimator. The naïve metadata estimator [20, 46] derives the sparsity of the output of LA expression solely from the base matrices' sparsity. This incurs no runtime overhead since metadata about the base matrices, including the nnz, columns and rows are available before runtime in a specific metadata file. The most common estimator is the worst-case estimator [20], which we use in our framework.

6.2.2 Matrix Non-zero Count (MNC) Estimator. The MNC estimator [42] exploits matrix structural properties such as single non-zero per row, or columns with varying sparsity, for efficient, accurate, and general sparsity estimation; it relies on count-based histograms that exploit these properties. We have also adopted this framework into our approach, and compute histograms about the base matrices offline. However, the MNC framework still needs to derive and construct histograms for intermediate results online (during rewriting cost estimation). We study this overhead in Section 8.

#### 6.3 Rewriting Pruning: PACB++

We extended the PACB rewriting engine with the  $Prune_{prov}$  algorithm sketched and discussed in [30, 31], to eliminate inefficient rewritings during the rewriting search phase. The naïve PACB algorithm generates all minimal (by join count) rewritings before choosing a minimum-cost one. While this sufficies on the scenarios considered in [14, 31], the settings we obtain from our LA encoding stress-test the naïve algorithm, as commutativity, associativity, etc. blow up the space of alternate rewritings exponentially. Scalability considerations forced us to further optimize naïve PACB to find only minimum-cost rewritings, aggressively pruning the others during the generation phase. We illustrate Prune<sub>prov</sub> and our improvements next.

Pruneprov Minimum-Cost Rewriting. Recall from Section 3 that the minimal rewritings of a query  $Q$  are obtained by first finding the set  $H$  of all matches (i.e., containment mappings) from  $Q$  to the result B of backchasing the universal plan U. Denoting with  $\pi(S)$ the provenance formula of a set of atoms S, PACB computes the DNF form D of  $\bigvee_{h \in \mathcal{H}} \pi(h(Q))$ . Each conjunct c of D determines a subquery sq(c) of U which is quaranteed to be a rewriting of O subquery  $sq(c)$  of U which is guaranteed to be a rewriting of Q.

The idea behind cost-based pruning is that, whenever the naive PACB backchase would add a provenance conjunct c to an existing atom a's provenance formula  $\pi(a)$ , Prune<sub>prov</sub> does so more conservatively: if the cost  $\gamma(sq(c))$  is larger than the minimum cost threshold  $T$  found so far, then  $c$  will never participate in a minimumcost rewriting and need not be added to  $\pi(a)$ . Moreover, atom a itself need not be chased into  $B$  in the first place if all its provenance conjuncts have above-threshold cost.

EXAMPLE 6.2. Let  $E = M(NM)$ , where we assume for simplicity that  $M_{50K\times100}$  and  $N_{100\times50K}$  are dense. Exploiting the associativity of matrix-multiplication  $(MN)M = M(NM)$  during the chase leads to the following universal plan U annotated with provenance terms:

 $U(R_2^0)$ : name(M<sup>1</sup><sub>1</sub>, "M.csv")<sup>p<sub>0</sup></sub> ∧ size(M<sup>1</sup><sub>1</sub>, 50000, 100)<sup>p<sub>1</sub></sup> ∧<br>name(M<sup>1</sup><sup>4</sup>N sex")<sup>p</sup>2 ∧ size(N<sup>1</sup> 100, 50000)<sup>p</sup>3 ∧</sup>  $name(N_1^i, "N.csv")^{p_2} \wedge size(N_1^i, 100, 50000)^{p_3} \wedge$ <br>undti (M<sup>i</sup> N<sup>i</sup> P<sup>0</sup>)P<sub>4</sub> A quality (P<sup>0</sup> M<sup>i</sup> P<sup>0</sup>)P<sub>5</sub> A  $\frac{multi_1(M_1^i, N_1^i, R_1^o)^{p_4} \wedge multi_1(R_1^o, M_1^i, R_2^o)^{p_5} \wedge}{unit_1(M_1^i, R_2^o)M_1^i}$  $multiplying (N<sub>1</sub>, M<sub>1</sub>, R<sub>3</sub>)<sup>p<sub>6</sub></sup> \wedge multi<sub>M</sub>(M<sub>1</sub>, R<sub>3</sub>, R<sub>2</sub>)<sup>p<sub>7</sub></sup>$ 

Now, consider in the back-chase the associativity constraint C:

$$
\forall M_1^i \forall N_1^i \forall R_1^o \forall R_2^o
$$
  
\n
$$
multi_M(M_1^i, N_1^i, R_1^o) \land multi_M(R_1^o, M_1^i, R_2^o) \rightarrow
$$
  
\n
$$
\exists R_4^o multi_M(N_1^i, M_1^i, R_4^o) \land multi_M(M_1^i, R_4^o, R_2^o)
$$

There exists a containment mapping h embedding the two atoms in the premise  $P$  of  $C$  into the  $U$  atoms whose provenance annotations are  $p_4$  and  $p_5$ . The provenance conjunct collected from P's image is  $\pi(h(P))=p_4 \wedge p_5$ .

Without pruning, the backchase would chase  $U$  with the constraint C, yielding  $\bar{U}'$  which features additional  $\pi(h(P))$ -annotated atoms<br>multiv( $N^i$   $M^i$   $P^0$ ) $P^4$  $\wedge P^5$   $\wedge$  multiv( $M^i$   $P^0$   $P^0$ ) $P^4$  $\wedge P^5$ 

multi<sub>M</sub> $(N_1^i, N_1^i, R_4^o)^{p_4 \wedge p_5} \wedge multi_M(M_1^i, R_2^o, R_2^o)^{p_4 \wedge p_5}$ <br>F has precisely two matches h, he into  $N'$ , h, (F) i

mutt<sub>M</sub>( $N_1$ ,  $N_4$ ,  $K_4$ <sup>r</sup>,  $N_2$ )  $\land$  mutt<sub>M</sub>( $M_1$ ,  $K_4$ ,  $K_2$ )<sup> $\rightarrow$ </sup>,  $N_2$ <br>E has precisely two matches  $h_1$ ,  $h_2$  into U'.  $h_1(E)$  involves the newly added atoms as well as those annotated with  $p_0, p_1, p_2, p_3$ . Collecting all their provenance annotations yields the conjunct  $c_1 =$  $p_0 \wedge p_1 \wedge p_2 \wedge p_3 \wedge p_4 \wedge p_5$ .  $c_1$  determines the U-subquery sq( $c_1$ )  $\frac{1}{\pi}$  corresponding to the rewriting (MN)M, of cost  $(50K)^2$ .<br>  $\frac{1}{\pi}$  (F)'s image vialds the provenance conjunct co = 0.

 $h_2(E)$ 's image yields the provenance conjunct  $c_2 = p_0 \wedge p_1 \wedge p_2 \wedge p_2$  $p_3 \wedge p_6 \wedge p_7$ , which determines the rewriting  $M(NM)$  that happens to be the original expression  $E$  of cost  $100^2$ .<br>The naive PACB would find both rewrit

The naive PACB would find both rewritings, cost them, and drop the former in favor of the latter.

With pruning, the threshold  $T$  is the cost of the original expression 100<sup>2</sup>. The chase step with C is never applied, as it would intro-<br>duce the provenance conjunct  $\pi(b(P))$  which determines Leubouery duce the provenance conjunct  $\pi(h(P))$  which determines U-subquery  $sq(\pi(h(P)) = multi<sub>M</sub>(M<sub>1</sub><sup>i</sup>, N<sub>1</sub><sup>i</sup>, R<sub>1</sub><sup>o</sup>)<sup>p<sub>4</sub></sup> \wedge multi<sub>M</sub>(R<sub>1</sub><sup>o</sup>, M<sub>1</sub><sup>i</sup>, R<sub>2</sub><sup>o</sup>)<sup>p<sub>5</sub></sup>$ <br>of sort (50 K)<sup>2</sup> generating T. The stame needed as image of t

of cost  $(50K)^2$  exceeding T. The atoms needed as image of E under<br>are thus never produced while hackchasing II, so the expensive  $h_1$  are thus never produced while backchasing U, so the expensive rewriting is never discovered. This leaves only the match image  $h_2(E)$ , which corresponds to the efficient rewriting M(NM).

Our improvements on  $Prune_{prov}$ . Whenever the pruned chase step is applicable and applied for each TGD constraint, the original algorithm searches for all *minimal-rewritings*  $\mathcal{R}W$  that can be found "so far", then it costs each  $rw \in \mathcal{R}W$  to find the "so far" minimum-cost one  $rw_e$  and adjusts the threshold T to the cost of  $rw_e$ . However, this strategy can cause *redundant* costing of  $rw \in \mathbb{R}^2W$ whenever the pruned chase step is applied again for another constraint. Therefore, in our modified version of  $Prune_{prov}$ , we keep track of the rewriting costs already estimated, to prevent such redundant work. Additionally, the search for minimal-rewritings "so far" (matches of the query  $O$  into the evolving universal plan instance  $U'$ , see Section 3) whenever the pruned chase step is applied<br>is modeled as a guery evaluation of  $\Omega$  against  $U'$  (viewed as a symis modeled as a query evaluation of  $Q$  against  $U'$  (viewed as a symbolic/canonical database [12]). This involves repeatedly evaluating bolic/canonical database [12]). This involves repeatedly evaluating the same query plan. However, the query is evaluated over evolutions of the same instance. Each pruned chase step adds a few new tuples to the evolving instance, corresponding to atoms introduced by the step, while most of the instance is unchanged. Therefore, instead of evaluating the query plan from scratch, we employ incremental evaluation as in [31]. The plan is kept in memory along with the populated hash tables, and whenever new tuples are added to the evolving instance, we push them to the plan.

#### 7 GUARANTEES ON THE REDUCTION

We detail the conditions under which we guarantee that our approach is sound (i.e., it generates only equivalent, cost-optimal

rewritings), and complete (i.e., it finds all equivalent cost-optimal rewritings).

We denote with  $\mathcal L$  the language of hybrid expressions described in Section 2. Let  $V \subseteq \mathcal{L}$  be a set of materialized view definitions.

Let  $LA_{prop}$  be a set of properties of the LA operations in  $L_{ops}$ that admits relational encoding over  $VREM$ . We say that  $LA_{prop}$ is terminating if it corresponds to a set of TGDs and EGDs with terminating chase (this holds for our choice of  $LA_{\text{prop}}$ ).

Denote with  $\gamma$  a cost model for expressions from  $\mathcal{L}$ . We say that  $\gamma$  is *monotonic* if expressions are never assigned a lower cost than their subexpressions (this is true for both models we used).

We call  $E \in L(y, LA_{prop}, V)$ -optimal if for every  $E' \in L$  that <br>*LA*  $\leq$  *W*)-equivalent to *E* we have  $v(F') \geq v(F)$ is  $(LA_{prop}, V)$ -equivalent to E we have  $\gamma(E') \ge \gamma(E)$ .<br>Let Eq. (LA<sub>LLA</sub> V<sub>LE</sub>) denote the set of all (v, LA<sub>L</sub>

Let  $\text{Eq}^{\gamma}(LAprop, V)(E)$  denote the set of all  $(\gamma, LAprop, V)$ -optimal<br>pressions that are  $(I_{A} \cup V)$ -equivalent to  $F$ expressions that are  $(LA_{prop}, V)$ -equivalent to E.

We denote with  $HADAD\langle LA_{\text{prop}}, \mathcal{V}, \gamma \rangle$  our parameterized solution based on relational encoding followed by PACB++ rewriting and next by decoding all the relational rewritings generated by the cost-based pruning PACB++ (recall Figure 1). Given  $E \in$  $\mathcal{L}$ , HADAD $\langle LA_{\text{prop}}, \mathcal{V}, \gamma \rangle (E)$  denotes all expressions returned by  $HADAD\langle LA_{prop}, \hat{V}, \gamma \rangle$  on input E.

THEOREM 7.1 (SOUNDNESS). If the cost model  $\gamma$  is monotonic, then for every  $E \in \mathcal{L}$  and every  $rw \in HADAD\langle LA_{prop}, \mathcal{V}, \gamma \rangle (E)$ , we have  $rw \in Eq^{\gamma} \langle LA_{prop}, \mathcal{V} \rangle (E).$ 

THEOREM 7.2 (COMPLETENESS). If  $\gamma$  is monotonic and LA<sub>prop</sub> is terminating, then for every  $E \in \mathcal{L}$  and every  $rw \in Eq^{\gamma} \langle LA_{prop}, \mathcal{V} \rangle(E)$ ,<br>we have rw  $\in HADAD/I A$ ,  $\sim \mathcal{N}(\gamma(E))$ we have  $rw \in HADAD\langle LA_{prop}, V, \gamma \rangle (E)$ .<br> **8 EXPERIMENTAL EVALUATER** 

#### **EXPERIMENTAL EVALUATION**

We evaluate our approach, first on LA pipelines (Section 8.1), then on real-world hybrid scenarios (Section 8.2). Due to space constraints, we delegate other results to our extended version of the paper [4].

Experimental Environment. We used a single node with an Intel(R) Xeon(R) CPU E5-2640 v4 @ 2.40GHz, 40 Cores (hyperthreading), 123GB RAM, disk read speed 616 MB/s, and disk write speed 455 MB/s. We run on OpenJDK Java 8 VM. As for LA systems/libraries, we used R 3.6.0, Numpy 1.16.6 (python 2.7), TensorFlow 1.4.1, Spark 2.4.5 (MLlib), and SystemML 1.2.0; hybrid scenarios were evaluated in the **SparkSQL** [16] polystore.

Systems Configuration Tuning. We discuss here the most important installation and configuration details. We use a JVM-based linear algebra library for SystemML as recommended in [44], at the optimization level 4. Additionally, we enable multi-threaded matrix operations in a single node. We run Spark using the standalone cluster manager, and using OpenBLAS (built from the sources as detailed in [10]) to take advantage of its accelerations [44]. SparkM-Llib's datatypes do not support many basic LA operations, such as scalar-matrix multiplication, matrix element-wise multiplication, etc. To support them, we use the Breeze Scala library [7], convert MLlib's datatypes to Breeze types and express the basic LA operations in Spark. The driver memory allocated for Spark and SystemML is 115GB. To maximize TensorFlow performance, we compile it from sources. For all systems/libraries, we set the number of cores to 24; all systems use double precision numbers.

No.	Expression	No.	Expression	No.	Expression				
P1.1	$(MN)^T$	P1.2	$A^T + B^T$	P <sub>1.3</sub>	$C^{-1}D^{-1}$				
P1.4	$(A + B)v_1$	P <sub>1.5</sub>	$((D)^{-1})^{-1}$	P <sub>1.6</sub>	$trace(s_1D)$				
P <sub>1.7</sub>	$((A)^T)^T$	P <sub>1.8</sub>	$s_1A + s_2A$	P <sub>1.9</sub>	$det(D^T)$				
P <sub>1.10</sub>	$rowsums(A^T)$	P <sub>1.11</sub>	$rowsums(A^T + B^T)$	P <sub>1.12</sub>	colSums(MN)				
P1.13	sum(MN)	P1.14	$sum(colsums(NTMT))$	P1.15	(MN)M				
P1.16	$sum(A^T)$	P1.17	det(CDC)	P1.18	sum(colsums(A))				
P <sub>1.19</sub>	$(C^{T})^{-1}$	P <sub>1.20</sub>	$trace(C^{-1})$	P <sub>1.21</sub>	$(C+D^{-1})^T$				
P <sub>1.22</sub>	$trace((C+D)^{-1})$	P <sub>1.23</sub>	$det((CD)^{-1}) + D$	P1.24	$trace((CD)^{-1}))+trace(D)$				
P <sub>1.25</sub>	$M \odot (N^T/(MNN^T))$	P <sub>1.26</sub>	$N \odot (M^T/(M^T M N))$	P <sub>1.27</sub>	$trace(D(CD)^{T})$				
P <sub>1.28</sub>	$A \odot (A \odot B + A)$	P <sub>1.29</sub>	<b>DCCC</b>	P <sub>1.30</sub>	$NM \odot NMR^T$				
	Table 2: LA Benchmark Pipelines (Part 1)								

Name	Rows $n$	$\mathbf{Cols}_{m}$	$\textbf{Nnz} \,   X  _0$	$S_X$
DFV	1M	100	8050	0.0080%
2D 54019	50K	100	3700	0.0740%
Amazon/ $(AS)$	50K	100	378	0.0075%
Amazon/ $(AM)$	100K	100	673	0.0067%
Amazon/ $(AL_1)$	1M	100	6539	0.0065%
Amazon/ $(AL_2)$	10M	100	11897	0.0011%
Amazon/ $(AL_3)$	100K	50K	103557	0.0020%
Netfix/(NS)	50K	100	69559	1.3911%
Netfix/(NM)	100K	100	139344	1.3934%
Netflix/ $(NL_1)$	1M	100	665445	0.6654%
Netflix/ $(NL_2)$	10M	100	665445	0.0665%
$M_{\alpha}$ $\leftarrow$ $N$ $I$ $\rightarrow$	100V	$E \cap V$	1.5957410	0.20707

 $\frac{\text{Netflux}(NL_3)}{\text{Table 3: Overview of Used Real Datasets.}}$ 

Datasets. We used several real-world, sparse matrices, for which Table 3 lists the dimensions and the sparsity  $(\mathbf{S}_X)(i)$  dielFilterV3real (DFV in short) is an analysis of a microwave filter with different mesh qualities [24]; (ii) 2D\_54019\_highK (2D\_54019 in short) is a 2D semiconductor device simulation [24]; (iii) we used several subsets of an Amazon books review dataset [6] (in JSON), and similarly  $(iv)$  subsets of a Netflix movie rating dataset [8]. The latter two were easily converted into matrices where columns are items and rows are customers [46]; we extracted smaller subsets of all real datasets to ensure the various computations applied on them fit in memory (e.g., Amazon/(AS) denotes the small version of the Amazon dataset). We also used a set synthetic, dense matrices, described in Table 4.

LA benchmark. We select a set  $P$  of 57 LA expressions (pipelines) used in prior studies and/or frequently occurring in real-world LA computations, as follows:

Real-world matrix expressions include: a chain of matrix selfproducts used for reachability queries and other graph analytics [42] (P1.29 in Table 18); expressions used in Alternating Least Square Factorization (ALS) [46] (P2.25 in Table 17); Poisson Nonnegative Matrix Factorization (PNMF) [46] (P1.13 in Table 18); Nonnegative Matrix Factorization (NMF) [44](P1.25 and P1.26 in Table 18); complex predicate for image masking [42] (P1.30 in Table 18); recommendation computation [42] (P1.30 in Table 18); finally, Ordinary Least Squares Regression (OLS) [44] (P2.21 in Table 17).

Synthetic expressions were also generated, based on a set of basic matrix operations (inverse, multiplication, addition, etc.), and

Name	Rows $n$	$\mathbf{Cols}_{m}$		Name	Rows $n$	Cols <sub>m</sub>				
$Syn_1$	50K	100		$Syn_6$	20K	20K				
Syn <sub>2</sub>	100	50K		Syn <sub>7</sub>	100					
$Syn_3$	1M	100		$Syn_8$	50K					
$Syn_4$	5M	100		Syn <sub>9</sub>	100K					
Syn <sub>5</sub>	10K	10K		$Syn_{10}$	100	100				
<b>Table 4: Syntactically Generated Dense Datasets</b>										

<b>Matrix Name</b>	<b>Used Data</b>			
$A$ and $B$	AM, $AL_1$ , $AL_2$ , NM, $NL_1$ , $NL_2$ , dielFilter, $Syn_3$ or $Syn_4$			
$C$ and $D$	$Syn_5$ or $Syn_6$			
M	AS, NS, $Syn_1$ , or 2D 54019			
N	Syn <sub>2</sub>			
R	$Syn_{10}$			
X	$AL_3$ or $NL_3$			
$v_1$ , $v_2$ and $u_1$	$Syn_7$ , $Syn_8$ and $Syn_9$ , respectively.			

 $\begin{array}{|l|l|} \hline v_1,v_2 \text{ and } u_1 & Syn_7, Syn_8 \text{ and } Syn_9, \text{ respectively.} \ \hline \end{array}$  Table 5: Matrices used for each matrix name in a pipeline

. a set of combination templates, written as a Rule-Iterated Context-Free Grammar (RI-CFG) [40]. Expressions thus generated include P2.16, P2.16, P2.23, P2.24 in Table 18.

Methodology. We evaluate our approach using the LA pipelines in Table 18 and Table 17, systems/tools mentioned above, and the matrices in Table 5. For TensorFlow and NumPy, we present the results only for dense matrices, due to limited support for sparse matrices. In Section 8.1, we focus on LA pipeline rewriting, while Section 8.2 describes experiments on real-world, hybrid scenarios.

#### 8.1 Experiments on LA-based Pipelines

In Section 8.1.1, we show the performance benefits of our approach to existing LA systems using a set  $\mathcal{P}^{-Opt} \subset \mathcal{P}$  of 38 pipelines, whose performance can be improved just by exploiting LA properties (in the absence of views). In Section 8.1.2, we study our optimization overhead for the set  $P^{Opt} = P \setminus P^{-Opt}$  of 19 pipelines that are already optimized. Finally, in Section 8.1.3, we show how our approach improves the performance of 30 pipelines from  $P$ , denoted  $\mathcal{P}^{Views}$ , using pre-materialized views.

8.1.1 Effectiveness of LA Rewriting (No Views). For each system, we run the original pipeline and our rewriting 5 times; we report the average of the last 4 running times. We exclude the data loading time. For fairness, we ensured SparkMLib and SystemML compute the entire pipeline (despite their lazy evaluation mode).

Figure 5 illustrates the original pipeline execution time  $Q_{exec}$ and the selected rewriting execution time  $RW_{exec}$  for P1.1, P1.3, **P1.4**, and **P1.15**, including the rewriting time  $RW_{find}$ , using the MNC cost model. For each pipeline, the used datasets are on top of

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No.	Expression	No.	Expression	No.	Expression				
P <sub>2.1</sub>	$trace(C+D)$	P <sub>2.2</sub>	$det(D^{-1})$	P <sub>2.3</sub>	trace(D <sup>T</sup> )				
P <sub>2.4</sub>	$s_1A + s_1B$	P <sub>2.5</sub>	$det((C+D)^{-1})$	P <sub>2.6</sub>	$C^T(D^T)^{-1}$				
P <sub>2.7</sub>	$DD^{-1}C$	P <sub>2.8</sub>	$det(C^TD)$	P <sub>2.9</sub>	$trace(C^TD^T + D)$				
P <sub>2.10</sub>	rowSums(MN)	P <sub>2.11</sub>	$sum(A+B)$	P <sub>2.12</sub>	$sum(rowSums(NTMT))$				
P <sub>2.13</sub>	$((MN)M)^T$	P <sub>2.14</sub>	((MN)M)N	P <sub>2.15</sub>	sum(rowSums(A))				
P <sub>2.16</sub>	$trace(C^{-1}D^{-1}) + traceD)$	P <sub>2.17</sub>	$((((C+D)^{-1})^T)((D^{-1})^{-1})C^{-1}C$	P <sub>2.18</sub>	$colSums(A^T + B^T)$				
P <sub>2.19</sub>	$(C^{T}D)^{-1}$	P <sub>2.20</sub>	$(M(NM))^T$	P <sub>2.21</sub>	$(D^TD)^{-1}(D^T v_1)$				
P <sub>2.22</sub>	$exp((C+D)^T)$	P <sub>2.23</sub>	$det(C) * det(D) * det(C)$	P <sub>2.24</sub>	$(D^{-1}C)^T$				
P <sub>2.25</sub>	$(u_1v_2^T - X)v_2$	P <sub>2.26</sub>	$exp((C+D)^{-1})$	P <sub>2.27</sub>	$((((C+D)^{T})^{-1})D)C$				
	Table 6: LA Benchmark Pipelines (Part 2)								



the figure. For brevity in the figures, we use SM for SystemML, NP for NumPy, TF for Tensorflow, and SP for MLlib.

For P1.1 (see Figure 5(a)), both matrices are dense. The speed-up (1.5× to 4×) comes from rewriting  $(MN)^T$  (intermediate result size<br>to (50K)<sup>2</sup>) into  $N^T M^T$  much cheaper since both  $N^T$  and  $M^T$  are of to  $(50K)^2$ ) into  $N^T M^T$ , much cheaper since both  $N^T$  and  $M^T$  are of<br>size  $50K \times 100$ . We exclude MI lib from this experiment since it foiled  $T_{\text{SDE}}$  of  $T_{\text{M}}$  and  $N_{\text{M}}$  and  $N_{\text{M}}$  and  $N_{\text{M}}$  are ordered in the size 50K $\times$ 100. We exclude MLlib from this experiment since it failed to allocate memory for the intermediate matrix (Spark/MI I ib lim to allocate memory for the intermediate matrix (Spark/MLLib limits the maximum size of a dense matrix). As a variation (not plotted in the Figure), we ran the same pipeline with the ultra-sparse AS matrix (0.0075% non-zeros) used as M. The  $Q_{exec}$  and  $RW_{exec}$  time are very comparable using SystemML, because we avoid large dense intermediates. In R, this scenario lead to a runtime exception since the multiplication operator tries to densify the matrix M. To avoid it, we cast M during load time to a dense matrix type. Thus, the speed-up achieved is the same as if  $M$  and  $N$  were both dense. If, instead, NS (1.3860% non-zeros) plays the role of M, our rewrite achieves  $\approx 1.8 \times$  speed-up for SystemML.

For **P1.3** (Figure 5(b)), the speed-up comes from rewriting  $C^{-1}D^{-1}$ <br> $(DC)^{-1}$  Interestingly. TensorFlow is the only system that applies  $(DC)^{-1}$ . Interestingly, TensorFlow is the only system that applies<br>this optimization by itself. SystemMI timed out (>1000 secs) for this optimization by itself. SystemML timed-out (>1000 secs) for both original pipeline and its rewriting.



Figure 6: P1.13 and P1.25 evaluation before and after rewrite

For pipeline **P1.4** (Figure 5(c)), we rewrite  $(A + B)v_1$  to  $Av_1$  +  $Bv_1$ . Adding a sparse matrix A to a dense matrix B results into materializing a dense intermediate of size  $1M \times 100$ . Instead,  $Av_1$  +  $Bv_1$  has fewer non-zeros in the intermediate results, and  $Av_1$  can be computed efficiently since A is sparse. The MNC sparsity estimator has a noticeable overhead here. We run the same pipeline, where the dense  $Syn_4$  matrix plays both A and B (not shown in the Figure). This leads to speed-up of up to 9× for MLlib, which does not natively support matrix addition, thus we convert its matrices to Breeze types in order to perform it (as in [44]).

P1.15 (Figure 5(d)) is a matrix chain multiplication. The naïve left-to-right evaluation plan (MN)M computes an intermediate matrix of size  $O(n^2)$ , where n is 50K. Instead, the rewriting  $M(NM)$ <br>only needs an  $O(n^2)$  intermediate matrix, where m is 100, and is only needs an  $O(m^2)$  intermediate matrix, where *m* is 100, and is much faster. To avoid MI in memory failure on **P1.15**, we use the much faster. To avoid MLLib memory failure on P1.15, we use the distributed matrix of type **BlockMatrix** for both matrices. While M thus converted has the same sparsity, Spark views it as being of a dense type ( multiplication on BlockMatrix is considered to produce dense matrices) [9]. SystemML does optimize the multiplication order if the user does not enforce it. Further (not shown in the Figure), we ran **P.15** with AS in the role of M. This is  $4\times$  faster in SystemML since with an ultra sparse M, multiplication is more efficient. This is not the case for MLlib which views it as dense. For R, we again had to densify M during loading to prevent crashes.

Figure 6 studies P1.13 and P1.25, two real-world pipelines involved in ML algorithms, using the MNC cost model; note the logscale y axis. Rewriting P1.13:  $sum(MN)$  into  $sum(t(colSums(M))$  \*  $rowsums(N))$  yields a speed-up of 50 $\times$ ; while SystemML has this rewrite as a static rule, it did not apply it. Our rewrite allowed SystemML and the others to benefit from it. Not shown in the Figure, we re-ran this with M ultra sparse (using AS) and SystemML: the rewrite did not bring benefits, since MN is already efficient. In this







experiment and subsequently, whenever MLlib is absent, this is due to its lack of support for LA operations (here, sum of all cells in a matrix) on BlockMatrix. For P1.25, the important optimization is selecting the multiplication order in  $MNN^T$  (Figure 6(b)). SystemML is ef-<br>ficient here, due to its dedicated operator  $t$ smm for transpose-self ficient here, due to its dedicated operator tsmm for transpose-self matrix multiplication and mmchain for matrix multiply chains.

Figure 7 shows up to 42× rewriting speed-up achieved by turning P1.14 and P2.12 into  $sum(t(colsums(M)) * rowSums(N))$ . This exploits several properties: (i)  $(MN)^T = N^T M^T$ , (ii)  $sum(M)^T$ ) = sum(M) (iii) sum(MN) exploits several properties: (1)  $(MN)^{-} = N^{-}M^{-}$ , (11)  $sum(M)^{-} = sum(M)$ , (iii)  $sum(mN) = sum(t(c)Sum(M)) * rowSum(S)$ . SystemMI, contures (ii) (iii)  $sum(t(colsums(M)) * rowSums(N))$ . SystemML captures (ii), (iii), and  $(iv)$  as static rewrite rules, however, it is unable to exploit these performance-saving opportunities since it is unaware of (i). Other systems lack support for more or all of these properties.

Figure 8 shows the distribution of the significant rewriting speedup on  $\mathcal{P}^{-Opt}$  running on R, and using the MNC-based cost model. For clarity, we split the distribution into two figures: on the left, 25  $P^{-Opt}$  pipelines with speed-up lower than 10×; on the right, the remaining 13 with greater speed-up. Among the former, 87% achieved at least <sup>1</sup>.5<sup>×</sup> speed-up. The latter are sped up by <sup>10</sup><sup>×</sup> to 60×. P1.5 is an extreme case here (not plotted): it is sped up by about 1000×, simply by rewriting  $((D)^{-1})^{-1}$  into D.

8.1.2 Rewriting Performance and Overhead. We now study the running time  $RW_{find}$  of our rewriting algorithm, and the rewrite overhead defined as  $RW_{find}/(Q_{exec} + RW_{find})$ , where  $Q_{exec}$  is the time to run the pipeline "as stated". We ran each experiment 100 times and report the average of the last 99 times. The global trends are as follows. (i) For a fixed pipeline and set of data matrices, the overhead is slightly higher using the MNC cost model, since histograms are built during optimization. (ii) For a fixed pipeline and cost model, sparse matrices lead to a higher overhead simply because  $Q_{exec}$  tends to be smaller. (iii) Some (system, pipeline) pairs

lead to a low  $Q_{exec}$  when the system applies internally the same optimization that HADAD finds "outside" of the system.

Concretely, for the  $P^{-Opt}$  pipelines, on the dense and sparse matrices listed in Table 5, using the naïve cost model, 64% of the  $RW_{find}$  times are under 25ms (50% are under 20ms), and the longest is about 200m. Using the MNC estimator, 55% took less than 20ms, and the longest (outlier) took about 300ms. Among the 39  $\mathcal{P}^{-Opt}$ pipelines, SystemML finds efficient rewritings for a set of 6, denoted  $\mathcal{P}_{SM}^{-Opt}$ , while TensorFlow optimizes a different set of 11, denoted  $\mathcal{P}_{SM}^{-Opt}$ . On these subsets where  $HADAD^2$  extinting is reduced  $\varphi_{TF}^{\neg Opt}$  . On these subsets, where HADAD's optimization is redundant. using *dense* matrices, the overhead is very low: with the *MNC* dant, using dense matrices, the overhead is very low: with the MNC model, 0.48% to 1.12% on  $\mathcal{P}_{SM}^{-Opt}$  (0.64% on average), and 0.0051%<br>to 2.54% and  $\mathcal{P}_{SM}^{-Opt}$  (1.29% or array and History the polynomial transformation to 3.51% on  $\mathcal{P}_{TF}^{-Opt}$  (1.38% on average). Using the *naïve* estimator<br>slightly reduces this overhead, but across  $\mathcal{P}^{-Opt}$ , this model misses slightly reduces this overhead, but across  $\mathcal{P}^{\neg Opt}$  , this model misses 4 efficient rewritings. On sparse matrices, the overhead is at most 4.86% with the naïve estimator and up to 5.11% with the MNC one.

Among the already-optimal pipelines  $\mathcal{P}^{Opt}$  , 70% involve expensive operations such as inverse, determinant, matrix exponential, leading to rather long  $Q_{exec}$  times. Thus, the rewriting overhead is less than 1% of the total time, on all systems, using sparse or dense matrices, and the naïve or the MNC-based cost models. For the other  $\mathcal{P}^{Opt}$  pipelines with short  $Q_{exec}$ , mostly matrix multiplications chains already in the optimal order on dense matrices, the overhead chains already in the optimal order, on dense matrices, the overhead reaches 0.143% (SparkMlLib) to 9.8% (TensorFlow) using the naïve cost model, while the MNC cost model leads to an overhead of 0.45% (SparkMlib) up to 10.26% (TensorFlow). On sparse matrices, using the naïve and MNC cost models, the overhead reaches up to 0.18% (SparkMLlib) to 1.94% (SystemML), and 0.5% (SparkMLlib) to 2.61% (SystemML), respectively.

8.1.3 Effectiveness of view-based LA rewriting. We have defined a set  $V_{exp}$  of 12 views that pre-compute the result of some expensive operations (multiplication, inverse, determinant, etc.) which can be used to answer our  $\mathcal{P}^{Views}$  pipelines, and materialized them on disk as CSV files. The experiments outlined below used the naïve cost model; all graphs have a log-scale  $y$  axis.

**Discussion**. For **P2.14** (Figure 9(a)), using the view  $V_4 = NM$  by and the multiplication associativity leads to up to <sup>2</sup>.8<sup>×</sup> speed-up.

Figure 9(b) shows the gain due to the view  $V_1 = D^{-1}$ , for the linear least regression (OI S) nineline **P2.21** It has 8 requirings ordinary-least regression (OLS) pipeline P2.21. It has 8 rewritings, 4 of which use  $V_1$ ; they are found thanks to the properties  $(CD)^{-1} = D^{-1}C^{-1}$  (CD)  $E = C(DE)$  and  $(D^T)^{-1} = (D^{-1})^T$  among others The cheapest rewriting is  $V(V^T(D^{T}v_1))$ , since it introduces small<br>intermediates due to the optimal matrix chain multiplication order <sup>-1</sup>C<sup>-1</sup>,  $(CD)E = C(DE)$  and  $(D<sup>T</sup>)$ <sup>-1</sup> =  $(D<sup>-1</sup>)<sup>T</sup>$  among others. intermediates due to the optimal matrix chain multiplication order. This rewrite leads to 70×, 55× and 150× speed-ups on R, NumPy and MLlib, respectively; TensorFlow is omitted as matmul operator does not support matrix-vector multiplication. It could run this pipeline by converting the matrices to NumPy, whose performance we already report separately. On SystemML, the original pipeline timed out (> 1000 seconds).

Pipeline **P2.25** (Figure 9(c)) benefits from a view  $V_5$ , which precomputes a dense intermediate vector multiplication result; then, rewriting based on the property  $(A + B)v = Av + Bv$  leads to a 65 $\times$ speed-up in SystemML. For MLlib, as discussed before, to avoid memory failure, we used BlockMatrix types. for all matrices and

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Figure 10:  $Hyb<sub>1</sub>$  and  $Hyb<sub>2</sub>$  evaluation before and after rewrite

vectors, thus they were treated as dense. In R, the original pipeline triggers a memory allocation failure, which the rewriting avoids.

Figure 9(d) shows that for **P2.27** exploiting the views  $V_2 = (D +$ C)<sup>-1</sup> and  $V_3 = DC$  leads to speed-ups of 4× to 41× on different systems. Properties enabling rewriting here are  $C + D = D + C$ systems. Properties enabling rewriting here are  $C + D = D + C$ ,  $(D^T)^{-1} = (D^{-1})^T$  and  $(CD)E = C(DE)$ .<br>
9. 2. Hybrid (I.A. and P.A.) Soc

#### 8.2 Hybrid (LA and RA) Scenarios

We now study the benefits of rewriting on hybrid expressions combining relational and linear algebra.

Scenario 1 ( $Hyb_1$ ): Amazon reviews. This JSON dataset contains product information, product reviews (text) and reviewer information. We defined two materialized views:  $V_1$  stores review id, product id, and the overall rate for "Kindle-Edition" books as a relational table;  $V_2$  stores the reviewer id, product id, and the review text as a text datasource in Solr. A query constructs a product-review matrix  $X$  for "Kindle-Edition" books, where the review text mentions "mystery". This matrix is loaded in SystemML, where we filter rows with rating less than 2. Next, an analysis is run, through the computation:  $(u_1v_2^T - X)v_2$ , which appears in the ALS algorithm [46].<br>Note that  $u_1$  and  $v_2$  are synthetic dance vectors of size 100K  $\times$  1 and Note that  $u_1$  and  $v_2$  are synthetic dense vectors of size 100K  $\times$  1 and  $50K \times 1$ , respectively, and X is ultra sparse (0.00028% non-zeros). Rewriting modifies the pre-processing by introducing  $V_1$  and  $V_2$ ; it also pushes the rating filter into the pre-processing part. The analysis is rewritten into  $u_1v_2^T v_2 - Xv_2$ ; this is the main reason for the  $60 \times$  speed-up we bring to SystemMI. (Figure 10) First X is ultra  $60\times$  speed-up we bring to SystemML (Figure 10). First, X is ultra sparse which makes the computation of  $Xv_2$  extremely efficient. Second, SystemML evaluates  $u_1v_2^T v_2$  efficiently in one go without<br>intermediates, taking advantage of **temm** operator (discussed earintermediates, taking advantage of **tsmm** operator (discussed earlier) and **mmchain** for matrix multiply chains, where the best way to evaluate it computes  $v_2^T v_2$  first, which results in a scalar, instead of

computing  $u_1v_2^T$ , which results in a dense matrix of size 100K  $\times$  50K.<br>Alone, SystemMI is unable to exploit its own efficient operations Alone, SystemML is unable to exploit its own efficient operations for lack of awareness the LA property  $Av + Bv = (A + B)v$ .

Scenario 2 ( $H y b<sub>2</sub>$ ): Netflix reviews. The dataset is in CSV form, and it contains movie id, customer id, overall rate and rating time. A query (in the pre-processing part) constructs a review matrix  $X$ , where columns are movies, and rows are customers. In the same fashion as in the previous scenario,  $X$  is loaded for analysis in SystemML, where we filter rows with overall rate greater than 3. Next, we run the same analysis computation described in Scenario 1, where the obtained rewriting is also the same. The main difference here is that matrix  $X$  is much denser (0.261% non-zeros), and the rewriting does not involve using materialized views. The rewrite achieves ∼20× speed-up as shown in Figure 10.

#### 8.3 Experiments Summary

We have shown that HADAD brings significant performance-saving across LA-oriented and potentially polystore engines/systems without the need to modify their internals. It improves their performance by order of magnitudes on typical LA-based and hybrid pipelines. Moreover, as we confirm experimentally, the time spent searching for rewritings is a small fraction of the query execution time for  $\mathcal{P}^{-Opt}$  pipelines hence a worthwhile investment. In addition, the rewriting overhead of  $\mathcal{P}^{Opt}$  pipelines is very negligible compared to the original pipeline execution time in the presence of sparse/ dense matrices and using naïve and MNC-based cost models.

#### 9 RELATED WORK AND CONCLUSION

LA-oriented Systems, Libraries & Languages. SystemML [19] offers high-level R-like linear algebra abstractions, using a declarative language called Declarative Machine Learning (DML). The system applies some logical LA pattern-based rewrites and physical execution optimizations, based on cost estimates for the latter. SparkMLlib [39] provides LA operations and built-in function implementations of popular ML algorithms, such as linear regression, etc. on Spark RDDs. The library supports sparse and dense matrices, but the user has to select this type explicitly. R [3] and NumPy [2] are two of the most popular computing environments for statistical data analysis, widely used in academia and industry. They provide a high-level abstraction that can simplify the programming of numerical and statistical computations, by treating matrices as first-class citizens and by providing a rich set of built-in LA operations and ML algorithms. However, LA properties in most of these systems remain unexploited, which makes them miss opportunities to use their own highly efficient operators (recall  $Hyb_1$  in Section 8.2). Our

experiments (Section 8) show that LA pipeline evaluation in these systems can be sped up, often by more 10×, by our rewriting using  $(i)$  LA properties and  $(ii)$  materialized views.

Bridging the Gap: Linear and Relational Algebra. There has been a recent increase in research for unifying the execution of relational and linear algebra queries /pipelines [1, 27, 32, 35, 37, 39, 45]. A key limitation of these works is that the semantics of linear algebra operations remains hidden behind built-in functions and/or UDFs, preventing performance-enhancing rewrites. Some of these works call LA packages through UDFs, where libraries such as R and NumPy are embedded in the host language [1]. Other works treat LA objects as first-class citizens and use built-in functions to express LA operations [28, 32, 37]. Closer to our work, LARA [35] relies on a declarative domain-specific language for collections and matrices, which can enable optimization across the two algebraic abstractions. SPORES [46] and SPOOF [21] optimize LA expressions, by converting them into RA, optimizing the latter, and then converting the result back to an (optimized) LA expression. SPORES and SPOOF are restricted to a small set of selected LA operations (the ones that can be expressed in relational algebra), while we support significantly more (Section 5.1), and model properties allowing to optimize with them. Further, as they do not reason with constraints, they cannot exploit materialized views in an LA (or hybrid LA/RA) context; as shown in our experiments, such rewritings can bring large performance advantages. Our work can also complementing the optimizations of LARA, SPORES or SPOOF, to extend to these platforms the benefits of views-based rewriting.

Conclusion. HADAD is an extensible lightweight approach for optimizing hybrid complex analytics queries, based on the powerful intermediate abstraction of a a relational model with integrity constraints. HADAD extends [14] with a reduction from LA view-based rewriting to relational rewriting under constraints. It enables a full exploration of rewrites using a large set of LA operations, with no modification to the execution platform. Our experiments show performance gains of up to several orders of magnitude on LA and hybrid workloads. Future work includes reasoning about cell-wise operations, building upon the FAQ [13] framework.

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# A  $L_{ops}$  OPERATIONS PROPERTIES ( $LA_{prop}$ ) CAPTURED AS INTEGRITY CONSTRAINTS



### Table 7:  $L_{ops}$  Operations Properties ( $LA_{prop}$ ) Captured as Integrity Constraints

### Table 8:  $\mathcal{L}_{ops}$  Operations Properties  $(LA_{prop})$  Captured as Integrity Constraints





### Table 9: Matrix Decompositions Properties Captured as Integrity Constraints

### B SYSTEMML REWRITE RULES ENCODED AS INTEGRITY CONSTRAINTS



### Table 10: SystemML Algebraic Aggregate Rewrite Rules Captured as Integrity Constraints



## $C \quad \mathcal{P}^{-Opt}$  AND  $\mathcal{P}^{Views}$  PIPELINES REWRITES







Table 13: The set of views  $V_{exp}$ 

No.	Rewrite	No.	Rewrite	No.	Rewrite			
P <sub>1.2</sub>	$(V_6)^T$	P <sub>1.3</sub>	$V_7V_1$	P <sub>1.4</sub>	$(V_6)v_1$			
P <sub>1.11</sub>	$colSums(V_6)^T$	P <sub>1.15</sub>	$M(V_3)$	P <sub>1.17</sub>	$V_{10} * det(C)$			
P <sub>1.19</sub>	$V_2$	P <sub>1.20</sub>	$trace(V_7)$	P <sub>1.21</sub>	$(C + V_1)^T$			
P <sub>1.22</sub>	$trace(V_9)$	P <sub>1.24</sub>	$trace(V_1V_7) + trace(D)$	P <sub>1.29</sub>	$V_5CCC$			
P <sub>1.30</sub>	$V_3 \odot V_3 R^T$	P <sub>2.2</sub>	$det(V_1)$	P <sub>2.4</sub>	$s_1(V6)$			
P <sub>2.5</sub>	$det(V_9)$	P <sub>2.6</sub>	$(V_1C)^T$	P <sub>2.9</sub>	$trace(V_{12}) + trace(D)$			
P <sub>2.11</sub>	$sum(V_6)$	P <sub>2.13</sub>	$(MV_3)^T$	P <sub>2.14</sub>	$MV_3N$			
P <sub>2.16</sub>	$trace(V_7V_1) + traceD)$	P <sub>2.17</sub>	$(V_0^T)D$	P <sub>2.18</sub>	rowSums $(V_6)^T$			
P <sub>2.20</sub>	$(MV_3)^T$	P <sub>2.21</sub>	$V_1(V_1^T(D^Tv_1))$	P <sub>2.25</sub>	$V_4v_1-Xv_1$			
P <sub>1.23</sub>	$det((V_7V_1)+D)$	P <sub>2.26</sub>	$exp(V_9)$	P <sub>2.27</sub>	$V_0^T V_5$			
	Table 14: $\mathcal{P}^{Views}$ Pipelines Rewrites							



## D ADDITIONAL RESULTS:  $\mathcal{P}^{-Opt}$  PIPELINES - NAÏVE-BASED COST MODEL

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Figure 22: P1.14 evaluation time with and without rewriting

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Figure 26: P1.17 evaluation time with and without rewriting











## E ADDITIONAL RESULTS:  $\mathcal{P}^{-Opt}$  PIPELINES - MNC-BASED COST MODEL



Figure 50: P1.9 evaluation time with and without rewriting



Figure 54: P1.14 evaluation time with and without rewriting

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Figure 66: P2.14 evaluation time with and without rewriting



### **F** ADDITIONAL RESULTS:  $\mathcal{P}^{Views}$  pipelines





## G  $P^{-Opt}$  AND  $P^{View}$  pipelines rewrites







Table 17: The set of views  $V_{exp}$ 

No.	Rewrite	No.	Rewrite	No.	Rewrite			
P <sub>1.2</sub>	$(V_6)^T$	P <sub>1.3</sub>	$V_7V_1$	P <sub>1.4</sub>	$(V_6)v_1$			
P <sub>1.11</sub>	$colSums(V_6)^T$	P <sub>1.15</sub>	$M(V_3)$	P <sub>1.17</sub>	$V_{10} * det(C)$			
P <sub>1.19</sub>	$V_2$	P <sub>1.20</sub>	$trace(V_7)$	P <sub>1.21</sub>	$(C + V_1)^T$			
P <sub>1.22</sub>	$trace(V_9)$	P <sub>1.24</sub>	$trace(V_1V_7) + trace(D)$	P <sub>1.29</sub>	$V_5CCC$			
P <sub>1.30</sub>	$V_3 \odot V_3 R^T$	P <sub>2.2</sub>	$det(V_1)$	P <sub>2.4</sub>	$s_1(V6)$			
P <sub>2.5</sub>	$det(V_9)$	P <sub>2.6</sub>	$(V_1C)^T$	P <sub>2.9</sub>	$trace(V_{12}) + trace(D)$			
P <sub>2.11</sub>	$sum(V_6)$	P <sub>2.13</sub>	$(MV_3)^T$	P <sub>2.14</sub>	$MV_3N$			
P <sub>2.16</sub>	$trace(V_7V_1) + traceD)$	P <sub>2.17</sub>	$(V_0^T)D$	P <sub>2.18</sub>	rowSums $(V_6)^T$			
P <sub>2.20</sub>	$(MV_3)^T$	P <sub>2.21</sub>	$V_1(V_1^T(D^Tv_1))$	P <sub>2.25</sub>	$V_4v_1-Xv_1$			
P <sub>1.23</sub>	$det((V_7V_1)+D)$	P <sub>2.26</sub>	$exp(V_9)$	P <sub>2.27</sub>	$V_0^T V_5$			
	Table 18: $\mathcal{P}^{Views}$ Pipelines Rewrites							



#### H ADDITIONAL RESULTS: FACTORIZED LA EXPERIMENTS

Figure 76: Speed-ups of MorpheusR (with HADAD rewrites) over MorpheusR (without HADAD rewrites) for pipelines 1.12, 1.14 and 2.11 on synthetic data for a PK-FK join.



Figure 77: Speed-ups of MorpheusR (with HADAD rewrites) over MorpheusR (without HADAD rewrites) for pipelines 2.12 and 2.15 on synthetic data for a PK-FK join.





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Figure 79:  $RW_{find}$  overhead as a percentage (%) of the total time ( $Q_{exec}$  +  $RW_{f\,ond}$ ) for pipelines 1.16 and 1.18