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#### UNIVERSITY OF CALIFORNIA SAN DIEGO

#### Semantic Optimizations in Modern Hybrid Stores

A dissertation submitted in partial satisfaction of the requirements for the degree Doctor of Philosophy

in

**Computer Science** 

by

#### Rana Bijad M Alotaibi

Committee in charge:

Professor Alin Deutsch, Chair Professor Michael J. Carey Professor Ranjit Jhala Professor Arun Kumar Professor Ramesh Rao

2022

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University of California San Diego

2022

## DEDICATION

This dissertation is gratefully dedicated to My beloved parents, Bijad Alotaibi and Hussah Alzyadi My siblings, Norah, Mohammed, Fares, and Rose.

### EPIGRAPH

It is good to have an end to journey towards; but it is the journey that matters, in the end. —Ursula K.Leguin, The Left Hand of Darkness, 1969.

### TABLE OF CONTENTS

Dissertation A	Approval Page
Dedication .	iv
Epigraph	
Table of Cont	ents
List of Figure	six
List of Tables	xii
Acknowledge	ements
Vita	xvii
Abstract of th	e Dissertation
Chapter 1	Introduction11.1Summary of Research Contributions31.1.1ESTOCADA: Bringing Semantic Optimization to Hybrid Stores31.1.2HADAD: Extending Benefits of Semantic Optimization to
	Hybrid Relational and Linear Algebra Computation41.2Dissertation Organization51.3Acknowledgement6
Chapter 2	Heterogeneous Data Management72.1Mediator: Data Integration and Federated Systems72.2Hybrid Warehouses92.3Modern Hybrid Stores102.4Relationship to This Work11
Chapter 3	Background       13         3.1       Conjunctive Query       13         3.1.1       Semantics       14         3.1.2       Query Containment and Equivalence       15         3.2       Integrity Constraints (Dependencies)       16
	<ul> <li>3.2.1 Expressing Constraints in First-Order Logic</li></ul>
	3.3.2 The Provenance-Directed C&B: PACB

Chapter 4	ESTOCADA: Bringing Semantic Optimization to Hybrid Stores 26				
	4.1	Introduction			
		4.1.1 Motivating example			
	4.2	Problem statement			
	4.3	ESTOCADA Overview			
	4.4	The $QBT^{XM}$ Language			
		4.4.1 Query Block Trees (QBT)			
		4.4.2 Integration Language: $QBT^{XM}$			
	4.5	Reduction from Cross-Model to Single-Model Setting			
		4.5.1 JSON Model			
		4.5.2 Key-Value Model			
		4.5.3 Graph Model			
		4.5.4 XML Model			
		4.5.5 Relational Model			
		4.5.6 Binding Patterns			
		4.5.7 Equality and Multiple Treatment of Nulls			
		4.5.8 Comparison and Arithmetic Operators			
		4.5.9 Denial Constraints			
	4.6	Encoding $QBT^{XM}$ Queries into the Pivot Language			
	4.7	Encoding $QBT^{XM}$ Views as Constraints			
	4.8	From Rewritings to Integration Plans			
	4.9	PACB Optimization and Extension			
		4.9.1 $PACB^{OPT}$ : Optimized PACB			
	4.10	Extending PACB <sup><math>OPT</math></sup> to Bag Semantics			
	4.11	PACB $_{OBT}^{OPT}$ : Extending PACB $^{OPT}$ to QBTs			
	4.12	Guarantees on the Reduction			
	4.13	Experimental Evaluation			
		4.13.1 Experiment Setup			
		4.13.2 Cross-Store Rewritings Evaluation			
		4.13.3 PACB vs. PACB $OPT$			
		4.13.4 Summary of Experimental Findings			
	4.14	Conclusion			
	4.15	Acknowledgement			
Chapter 5	Had	AD: Extending Benefits of Semantic Optimization to Hybrid Relational			
-	and I	Linear Algebra Computation			
	5.1	Introduction			
	5.2	HADAD Optimizations			
		5.2.1 LA Pipeline Optimization			
		5.2.2 Hybrid RA-LA Optimization			
	5.3	Problem Statement			
	5.4	HADAD Overview			
	5.5	LA Reduction to the Relational Model			

		5.5.1 Supported Matrix Algebra
		5.5.2 VREM Schema and Relational Encoding
		5.5.3 LA Relational Rewriting Using Constraints
	5.6	Choice of an Efficient Rewriting
	5.7	Cost Model
		5.7.1 LA-based Sparsity Estimators
		5.7.2 Pruning Rewritings: $PACB^{++}$
	5.8	Guarantees on the Reduction
	5.9	Experimental Evaluation
		5.9.1 Experiment Setup
		5.9.2 LA-based Experiments
		5.9.3 Hybrid (RA and LA) Experiments
		5.9.4 Experiments Takeaway
	5.10	Limitations
	5.11	Conclusion
	5.12	Acknowledgement
Chapter 6	Relat	ted Wrok
	6.1	Related Work for ESTOCADA
	6.2	Related Work for HADAD
	6.3	Acknowledgement
Chapter 7	Conc	clusion and Future Directions
$\Delta$ ppendix $\Delta$	Δnne	endix: Estocada 138
Appendix A		Ouery Templates Example 138
	$\Delta 2$	Snippet of $OBT^{XM}$ Overy Language Grammar 140
	A 3	Encoding of $OBT^{XM}$ Views: $V_1$ and $V_2$ 142
	A 4	Encoding of $QBT^{XM}$ Overy $Q_1$ and Decoding $RWQ_1$ 143
	1 1. 1	Encoding of $\mathcal{G}$ is a constant of $\mathcal{G}$ in a possibility $\mathcal{G}_1$ is a constant of $\mathcal{G}_2$
Appendix B	Appe	endix: HADAD
	<b>B</b> .1	LA Operators Encoding Relations
	B.2	Key Constraints of LA Encoding Relations 146
	B.3	Properties of LA Operations Encoded as Constraints
	<b>B.</b> 4	SystemML Rewrite Rules Encoded as Constraints
	B.5	Additional Results: $\mathcal{P}^{\neg Opt}$ and $\mathcal{P}^{Views}$ Pipelines Rewrites
	<b>B.6</b>	Additional Results: $\mathcal{P}^{\neg Opt}$ Pipelines: Naïve Cost Model
	<b>B</b> .7	Additional Results: $\mathcal{P}^{\neg Opt}$ Pipelines: MNC Cost Model
	B.8	Additional Results: $\mathcal{P}^{Views}$ Pipelines
Bibliography		

### LIST OF FIGURES

Figure 4.1:	ESTOCADA reduction outline.	. 31
Figure 4.2:	QBT query example.	36
Figure 4.3:	View definitions expressed in $QBT^{XM}$	38
Figure 4.4:	JSON view V and query $Q$	42
Figure 4.5:	Graph view V and query $Q$	47
Figure 4.6:	Snippet of supported denail constraints.	58
Figure 4.7:	Motivating scenario $QBT^{XM}$ query $Q_1$ .	59
Figure 4.8:	Relational encoding of $QBT^{XM}$ view $V_2$ defined in Figure 4.3.	59
Figure 4.9:	Rewriting $RWQ_1$ of $QBT^{XM}$ query $Q_1$ .	60
Figure 4.10:	Integration plan of the motivating scenario using Tatooine hybrid engine.	. 61
Figure 4.11:	Rewriting time (28 relevant views).	72
Figure 4.12:	Rewriting time (128 relevant views)	73
Figure 4.13:	ESTOCADA (Relational and JSON views in PostgreSQL, text view in Solr)	
C	vs. single-store evaluation.	74
Figure 4.14:	ESTOCADA (Relational and JSON views in PostgreSQL) vs. single-store	
C	evaluation.	75
Figure 4.16:	PACB vs PACB $OPT$ rewriting performance.	78
Figure 4.15:	Queries and rewritings evaluation in polystore engines	79
Figure 5.1:	HADAD reduction outline.	88
Figure 5.2:	Snippet of $\mathcal{MMC}_{IA_{new}}$ constraints	94
Figure 5.3:	Relational encoding of view V	94
Figure 5.4:	Equivalent rewritings of $Q_n$	99
Figure 5.5:	Relational equivalent rewritings of $Q_n$ .	99
Figure 5.6:	Naïve sparsity estimation scheme. $\ldots$	. 101
Figure 5.7:	P1.1, P1.4, P1.15, and P2.12 evaluation before and after rewriting.	112
Figure 5.8:	P1.13, and P1.25 evaluation before and after rewriting.	113
Figure 5.9:	R speedup on $\mathcal{P}^{\neg Opt}$	115
Figure 5.10:	P2.14, P2.21, P2.25 and P2.27 evaluation before and after rewriting using $V_{exc}$	
Figure 5.11:	Speedups of MorpheusR (with HADAD rewrites) over MorpheusR (without	
U	HADAD Rewrites) for pipelines P1.12, P2.10, P2.11 and P2.15 on synthetic	
	data for a PK-FK join.	118
Figure 5.12:	HADAD $RW_{find}$ overhead as a percentage (%) of the total time ( $Q_{exec}$ +	-
8	$RW_{find}$ ) for pipelines P1.10, P1.16, and P1.18 running on Morpheus R	119
Figure 5.13:	Results of micro-hybrid benchmark using Twitter dataset.	. 121
Figure 5.14:	Results of micro-hybrid benchmark using MIMIC dataset	126
Figure A.1:	Ouery templates $OT_0$ , $OT_1$ and $OT_2$ ,, $OT_1$ and $OT_2$ .	138
Figure A.2:	Ouery O produced from combining templates $OT_0$ . $OT_1$ and $OT_2$ .	139
Figure A.3:	Ouery $O$ (in AsterixDB SOL++ syntax) produced from combining $OT_0$ $OT_1$	
0	and $QT_2$ .	139

Figure A.4:	View $V_1$ forward and backward constraints
Figure A.5:	View $V_2$ backward constraint
Figure A.6:	Relational encoding of $QBT^{XM}$ query $Q_1$
Figure A.7:	Decoding of rewriting $RWQ_1$
Figure B.1:	P1.2 evaluation before and after rewriting
Figure B.2:	P1.2 evaluation before and after rewriting
Figure B.3:	P1.6 evaluation before and after rewriting
Figure B.4:	P1.8 evaluation before and after rewriting
Figure B.5:	P1.8 evaluation before and after rewriting
Figure B.6:	P1.9 evaluation before and after rewriting
Figure B.7:	P1.10 evaluation before and after rewriting
Figure B.8:	P1.10 evaluation before and after rewriting
Figure B.9:	P1.11 evaluation before and after rewriting
Figure B.10:	P1.11 evaluation before and after rewriting
Figure B.11:	P1.12 evaluation before and after rewriting
Figure B.12:	P1.14 evaluation before and after rewriting
Figure B.13:	P1.15 evaluation before and after rewriting
Figure B.14:	P1.16 evaluation before and after rewriting
Figure B.15:	P1.16 evaluation before and after rewriting
Figure B.16:	P1.17 evaluation before and after rewriting
Figure B.17:	P1.18 evaluation before and after rewriting
Figure B.18:	P1.18 evaluation before and after rewriting
Figure B.19:	P1.25 evaluation before and after rewriting
Figure B.20:	P2.1 evaluation before and after rewriting
Figure B.21:	P2.2 evaluation before and after rewriting
Figure B.22:	P2.3 evaluation before and after rewriting
Figure B.23:	P2.4 evaluation before and after rewriting
Figure B.24:	P2.4 evaluation before and after rewriting
Figure B.25:	P2.5, P2.6 and P2.8 evaluation before and after rewriting
Figure B.26:	P2.9 evaluation before and after rewriting
Figure B.27:	P2.10 evaluation before and after rewriting
Figure B.28:	P2.11 evaluation before and after rewriting
Figure B.29:	P2.11 evaluation before and after rewriting
Figure B.30:	P2.13 evaluation before and after rewriting
Figure B.31:	P2.14 evaluation before and after rewriting
Figure B.32:	P2.15 evaluation before and after rewriting
Figure B.33:	P2.15 evaluation before and after rewriting
Figure B.34:	P2.16 evaluation before and after rewriting
Figure B.35:	P2.18 evaluation before and after rewriting
Figure B.36:	P2.18 evaluation before and after rewriting
Figure B.37:	P1.2 evaluation before and after rewriting
Figure B.38:	P1.6 evaluation before and after rewriting

Figure B.39:	P1.8 evaluation before and after rewriting	185
Figure B.40:	P1.9 evaluation before and after rewriting	185
Figure B.41:	P1.10 evaluation before and after rewriting	186
Figure B.42:	P1.11 evaluation before and after rewriting	187
Figure B.43:	P1.12 evaluation before and after rewriting	188
Figure B.44:	P1.14 evaluation before and after rewriting	188
Figure B.45:	P1.15 evaluation before and after rewriting	189
Figure B.46:	P1.16 evaluation before and after rewriting.	189
Figure B.47:	P1.17 evaluation before and after rewriting	190
Figure B.48:	P1.18 evaluation before and after rewriting.	190
Figure B.49:	P1.25 evaluation before and after rewriting	191
Figure B.50:	P2.1 evaluation before and after rewriting	191
Figure B.51:	P2.4 evaluation before and after rewriting	192
Figure B.52:	P2.5, P2.6, P2.8 and P2.9 evaluation before and after rewriting.	193
Figure B.53:	P2.10 evaluation before and after rewriting.	194
Figure B.54:	P2.11 evaluation before and after rewriting.	195
Figure B.55:	P2.13 evaluation before and after rewriting.	196
Figure B.56:	P2.14 evaluation before and after rewriting.	196
Figure B.57:	P2.15 evaluation before and after rewriting.	197
Figure B.58:	P2.16 evaluation before and after rewriting.	197
Figure B.59:	P2.18 evaluation before and after rewriting.	198
Figure B.60:	P1.2 and P1.3 evaluation before and after rewriting	199
Figure B.61:	P1.4 and P1.11 evaluation before and after rewriting	200
Figure B.62:	P1.17, P1.19, P1.20 and P1.21 evaluation before and after rewriting	201
Figure B.63:	P1.22, P1.23, P1.24 and P1.29 evaluation before and after rewriting	202
Figure B.64:	P2.2, P2.4 and P2.5 evaluation before and after rewriting	203
Figure B.65:	P2.9, P2.11 and P2.16 evaluation before and after rewriting	204

### LIST OF TABLES

Table 4.1: Table 4.2:	Models and languages supported by ESTOCADA
Table 4.3:	Snippet of $\mathcal{VREG}$ schema 46
Table 4.4:	Snippet of $V\mathcal{R}\mathcal{E}\mathcal{X}$ schema
Table 5.1:	Snippet of the $\mathcal{VREM}$ schema
Table 5.2:	LA benchmark pipelines (part 1)
Table 5.3:	LA benchmark pipelines (part 2)
Table 5.4:	Overview of used real datasets
Table 5.5:	Syntactically generated dense datasets
Table 5.6:	Matrices used for each matrix name in a pipeline
Table 5.7:	LA pipelines used in micro-hybrid benchmark
Table B.1:	The $\mathcal{VREM}$ schema (part 1)
Table B.2:	The $\mathcal{VREM}$ schema (part 2)
Table B.3:	Key constraints of LA operators relations (part 1)
Table B.4:	Key constraints of LA encoding relations (part 2)
Table B.5:	Properties of addition of matrices encoded as integrity constraints 148
Table B.6:	Properties of addition and transposition of matrices encoded as integrity
	constraints
Table B.7:	Properties of inverse, determinant and trace of matrices encoded as integrity
	constraints
Table B.8:	Properties of direct sum and exponential of matrices encoded as integrity
Table D O.	Constraints
Table B.9:	Matrix decompositions properties captured as integrity constraints (part1) 151
Table D.10.	Matrix decompositions properties captured as integrity constraints (part2). 152
Table D.11:	Dush down Unorga Age Transpose On rewrite miles encoded as integrity constraints 155
Table D.12: Table D 12: Table	FushdownOnaryAggTransposeOp rewrite rules encoded as integrity constraints. 154
Table D.13. Table D 14.	Simplify TraceWath Xinth Tewnite rules encoded as integrity constraint 154
Table D.14.	Simplify ColWise A gg requirite rules encoded as integrity constraints 155
Table D.13.	SimplifyColwiseAgg lewine fulles encoded as integrity constraints
Table D.10.	SimplifyRow wiseAgg fewrite rules encoded as integrity constraints 150 DushdownSumOn Add rowrite rules encoded as integrity constraints 156
Table D.17.	FushdownSumonAdd Tewhite Tules encoded as integrity constraints 150
Table B.10.	Colsums/lowsums/live visual rewrite rules encoded as integrity constraints 150 $\mathcal{O}^{-Qpt}$ pipelines rewrites (part 1)
Table $\mathbf{B}$ 20.	$\mathcal{D}^{\neg Opt} \text{ pipelines rewrites (part 2)} $ 157
Table R $21$ .	$T = piperines rewrites (part 2), \dots 157$ The set of views V 157
Table B 221.	$\mathcal{P}^{Views}$ ninelines rewrites 158
10010 D.22.	$\perp$ pipennes termines

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xiii

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xiv

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XV

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#### PUBLICATIONS

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**Rana Alotaibi**, Damian Bursztyn, Alin Deutsch, Ioana Manolescu, and Stamatis Zampetakis, "Towards Scalable Hybrid Stores: Constraint-Based Rewriting to the Rescue.", *BDA Conference on Data Management*, 2019.

#### ABSTRACT OF THE DISSERTATION

#### Semantic Optimizations in Modern Hybrid Stores

by

Rana Bijad M Alotaibi

Doctor of Philosophy in Computer Science

University of California San Diego, 2022

Professor Alin Deutsch, Chair

In recent years, big data applications often involve dealing with diverse datasets in terms of structure: relations flat or nested, complex-structure graphs, documents (JSON or XML), poorly structured logs, or even text data. To handle the heterogeneity of the data, application designers usually rely on several data stores used side-by-side, each supporting a different data model, associated query language (or data access API), and very efficient for some, but not all, kinds of processing on the data. Systems capable of querying disparate data in this fashion are advocated by the database community under terms such as hybrid- or poly-stores.

These systems provide no support for semantic query optimizations, which include (i) exploiting possible data redundancy when the same data may be accessible (with different

performance) from distinct data stores; (*ii*) taking advantage of partial query results (in the style of materialized views), which may be available in the stores; and (*iii*) reasoning semantically about various data models and query operations' properties, which can enhance the hybrid workload performance. Motivated by these optimization opportunities, this dissertation makes the following two main contributions:

We design and demonstrate ESTOCADA, an extensible lightweight framework for providing semantic query optimization on top of hybrid stores without modifying their internals. ESTOCADA transparently enables each query to benefit from the best combination of stored data and available processing capabilities. It leverages recent advances in the area of view-based query rewriting under constraints, which we use to describe various data models and stored data. We demonstrate the effectiveness of our approach with an experimental evaluation using the MIMIC real-world dataset and show significant performance gains achieved by ESTOCADA.

Going beyond query workloads covering a variety of data models (relational, JSON, Graph, XML) in hybrid stores, modern applications increasingly need to blend querying and learning on the data, which is primarily expressed using a mix of relational algebra (RA)- and linear algebra (LA)-based languages. Existing specialized solutions for evaluating such hybrid analytical tasks either optimize RA and LA tasks separately, exploiting only RA properties while leaving LA-specific optimizations unexploited, or focus heavily on physical optimizations, leaving semantic query optimization opportunities unexplored. In our second contribution, we take a major step towards filling this gap by proposing HADAD. The novelty of HADAD is to extend the benefits of semantic query rewriting and view-based optimization introduced in ESTOCADA to LA computations, crucial for ML hybrid analytical tasks. Our solution can be naturally and portably applied on top of pure LA and hybrid RA-LA platforms. An extensive empirical evaluation shows that HADAD yields significant performance gains on diverse workloads, ranging from LA-centered to hybrid RA-LA workloads.

## Chapter 1

## Introduction

Nowadays, big data applications often involve dealing with diverse datasets in terms of structure: relations flat or nested, complex-structure graphs, documents (JSON or XML), poorly structured logs, or even text data. Such datasets are routinely hosted in heterogeneous stores. One reason is that the fast pace of application development prevents consolidating all the sources into a single data format and loading them into a single store. In addition, a system efficient on some tasks may perform poorly or not support other tasks, making it impossible to use a single data management system for a given application. Instead, the data model often dictates the choice of the store, e.g., relational data gets loaded into a relational or "Big Table"-style system, JSON documents in a JSON store [4, 11], graphs in a Graph store [14]. Heterogeneous stores also "accumulate" in an application along the time, e.g., at some point, one decision is made to host dataset  $D_1$  in PostgreSQL and  $D_2$  in MongoDB. Later on, another application needs to use  $D_1$  and  $D_2$  together. The database community advocates systems capable of exploiting diverse big data systems in this fashion under the term *hybrid stores*<sup>1</sup> (*a.k.a. polystores*) [68, 136, 27, 95, 35, 55].

Current hybrid stores support multiple query languages to seamlessly query datasets that reside in multiple backends. This feature distinguishes them from previous federations [49, 134],

<sup>&</sup>lt;sup>1</sup>We use the terms hybrid stores, hybrid systems and polystores interchangeably in this monograph.

which were based mainly on SQL. Users are often wedded to SQL for querying structured data, semi-structured language for querying JSON data, path-oriented language for querying Graph data, etc. Such mixed query notations workload is often referred to as a *hybrid* workload [68].

Query evaluation in hybrid systems recalls, to some extent, mediator systems [49, 134, 41, 103, 64, 110, 139]; in both cases, sub-queries, each expressed in its own query language, are delegated to their corresponding underlying stores, while the remaining operations are applied in the upper integration layer. Hybrid systems process a query assuming that each of its input datasets is available in exactly one store (often chosen for its support of a given data model).

Further, going beyond query workloads covering a variety of data models (relational, JSON, Graph, XML) in hybrid stores, modern applications increasingly need to blend querying and learning on the data, which is primarily expressed using a mix of relational algebra (RA)- and linear algebra (LA)-based languages. To run such hybrid RA-LA analytical tasks, various works propose *specialized* hybrid RA-LA integration solutions, where both algebraic styles can be used together [105, 52, 18, 94, 97, 137, 44]. Some solutions [105, 94, 18] suggest extending RDBMS to treat LA objects as first-class citizens by using built-in functions to express LA operations. Others offer to call LA packages through user-defined functions (UDFs), where libraries like NumPy are embedded in the host language. Moreover, some systems [137, 44] only optimize LA expressions by converting them into RA expressions, optimizing the latter, and then converting the result back to an (optimized) LA expression. They only focus on optimizing LA pipelines containing operations that can be expressed in RA. More advanced hybrid RA-LA soultion [52] speeds up LA pipelines over large joins by pushing computation into each joined table, thereby avoiding expensive materialization. Recently, several soultions [97] focus on low-level physical optimization by exploiting data layouts (e.g., column-wise) to choose LA operators' physical implementations.

This dissertation identifies optimization opportunities in the scope of hybrid solutions/systems, of which special hybrid RA-LA integration systems are a subset. These solutions provide no support for *cross-models semantic query optimization*. Semantic optimization uses semantic knowledge about the data and query operations to *rewrite* a query into another equivalent form that can be executed more efficiently than the original query [26]. In a hybrid setting, this includes (*i*) exploiting possible data redundancy: the same data could be stored in several stores, some of which may support a query operation much more efficiently than others; (*ii*) taking advantage of the presence of partially computed query results (in the style of materialized views), which may be available in one or several stores, when the data model of the queried dataset differs from the data model of the store hosting the view; and (*iii*) reasoning semantically about various data models and query operations supported by them, which can enhance hybrid queries performance.

Enabling semantic query optimizations in a hybrid setting is challenging since user queries, views, and query rewritings are expressed across different data models and query languages. Existing semantic query optimization solutions were designed to work within a *single* data model and query language (i.e., mostly relational or XML) [103, 34, 64, 26].

## **1.1 Summary of Research Contributions**

We critically need a new and innovative solution to enable the aforementioned optimization opportunities and tackle challenges in a hybrid setting. With this in mind, this dissertation presents new innovations in enabling *cross-models semantic query optimization* on top of hybrid systems, with no need to modify their internals. In the following subsections, we describe the contributions of this dissertation in further detail.

### 1.1.1 ESTOCADA: Bringing Semantic Optimization to Hybrid Stores

We propose ESTOCADA (Chapter 4), a novel approach for allowing an application to transparently exploit data stored in a set of heterogeneous stores (in a hybrid setting) as a set of potentially overlapping data fragments (views). Further, if fragments store results of partial computations applied on the data, we show how to speed up queries using them as materialized views. This reduces query processing time and seeks to take the maximum advantage of each store's efficient query processing features. Importantly, our approach does not require any change to the application code. ESTOCADA enables such semantic optimization based on a common abstraction that facilitates unified reasoning: a relational model endowed with integrity constraints, which we use to capture the key aspects of the data models in circulation today, properties of query operation, and stored views. The system fully appeared in SIGMOD'19 [31] and later was demonstrated in PVLDB'20 [32]. The technical contributions we make in ESTOCADA can be summarized as follows:

- We propose an extensible lightweight approach for bringing semantic query optimization to hybrid systems.
- We formalize the cross-models rewriting problem in the context of hybrid systems.
- We design a reduction from cross-models view-based rewriting to relational rewriting under integrity constraints.
- We prototype our cross-models views-based rewriting approach on top of some existing hybrid systems.
- We optimize the state-of-the-art rewriting algorithm to scale to a hybrid setting.
- We show that our approach improves the performance in natural scenarios for both crossmodels and single model user queries.

## **1.1.2 HADAD: Extending Benefits of Semantic Optimization to Hybrid Re**lational and Linear Algebra Computation

As described previously, existing specialized hybrid RA-LA solutions do not support semantic query optimization, which includes views-based, integrity constraint-based, and LA property-based rewriting and can bring significant performance saving in hybrid RA-LA and even plain LA settings.

To enable such fruitful optimizations, we introduce HADAD (Chapter 5), which extends the benefits of semantic query rewriting and view-based optimization introduced in ESTOCADA to LA computations, which are crucial for ML-hybrid workloads. Our solution can be naturally and portably applied on top of hybrid RA-LA and pure LA platforms. The system was partially demonstrated at PVLDB'20 [32] and later fully appeared in SIGMOD'21 [33]. The technical contributions we make in this work can be summarized as follows:

- We propose an extension to ESTOCADA [31] (Chapter 4). In particular, we extend ESTO-CADA's intermediate relational abstraction to support reasoning about LA operations. The RA part is already captured in the target formalism.
- To the best of our knowledge, our approach is the first work that brings views-based rewriting under integrity constraints in the context of LA-based pipelines and hybrid analytical tasks.
- We extend the query rewriting engine, integrating two different cost models, to help prune out inefficient rewritings at the early stages of the rewriting candidates' search phase.
- We prototype our approach on top of popular LA-oriented and hybrid RA-LA platforms.
- We conduct an extensive set of empirical experiments on typical LA- and hybrid-based expressions, which show the benefits of HADAD.

## **1.2 Dissertation Organization**

The remainder of this dissertation is organized as follows. Chapter 2 briefly gives an overview of heterogeneous data management systems and their relationship to this work. In

Chapter 3, we describe the necessary background to understand the details in this monograph. Chapter 4 introduces ESTOCADA, a novel lightweight framework that enables semantic query optimization on top of hybrid systems. Chapter 4 describes HADAD, which capitalizes on ESTOCADA and extends its benefits of semantic query rewriting and view-based optimization to LA computations. We discuss ESTOCADA and HADAD related work in Chapter 6. Finally, Chapter 7 concludes this dissertation and discusses potential future research directions.

## 1.3 Acknowledgement

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## Chapter 2

## **Heterogeneous Data Management**

Since the 1970's, the data management field has faced several challenges raised by dealing with heterogeneous data sources, yielding a proliferation of approaches and systems which range from mediator systems [49, 134, 41, 103, 64, 110, 139, 47], of which federated database systems (FDSs) are a subset, and some of which use XML or Ontology as the integration model [64, 110, 116, 139] to hybrid warehouses [132, 133, 66, 99], which are special FDSs providing an integration between Hadoop-like big data platforms and parallel data warehouses and finally modern hybrid stores (a.k.a. polystores) [68, 136, 27, 95, 35, 55] (also called hybrid systems).

This chapter briefly gives an overview of the evolution of heterogeneous data management systems over the years. This overview is not intended to be comprehensive, and we refer a reader to a more robust treatment of these topics [126, 96, 119, 140, 46] for details beyond the scope of this thesis.

## 2.1 Mediator: Data Integration and Federated Systems

Traditional heterogeneous data management systems aim at providing transparent access to a collection of autonomous (i.e., managed independently) heterogeneous data sources. Two main centralized system architectures were devised for that purpose: data warehouse [86] and mediator [67]. They both rely on the design of a global integration schema (*global schema* in short), which provides an *homogeneous* view of the source data, and w.r.t. which queries are formulated in a single language (e.g., SQL, XQuery). This way, the existence of multiple heterogeneous data sources is hidden from applications and users. However, the two architectures significantly differ in how they answer queries based on the source data. In a warehouse, data is first extracted from the sources and then transformed so as to be loaded as a global schema instance within a database. Thus, the warehouse approach eliminates heterogeneity by bringing all the data into a single store. In contrast, in a mediator, data remains in the heterogeneous sources, and every incoming query is decomposed into subqueries to be evaluated by the sources. Possible post-processing steps are usually applied in the mediator to integrate their results and provide the final query answer to the user.

Mediator systems follow *mediator-wrapper* architecture. In this architecture, each data source has a *wrapper* that passes on information about the source query processing capabilities and the local schema to the mediator (middleware). Wrappers translate queries received from the mediator, expressed in a common query language, to the query language of the source. Moreover, they reformat answers of each subquery from the source to conform to the internal data model of the middleware.

In mediator systems, the data is stored in the data sources and organized under local schemas. Hence, in order to for the mediator system to answer queries, there must be some descriptions (or explicit mapping rules) of how the relations in the sources are related to the ones in the global schema. These mapping rules virtually specify the global schema instance that applications and users can access through the mediator. There are two main types of mapping [101]:

**Global-As-View** (GAV). The global schema is defined as a set of views over the data source schemas. These view definitions indicate how the tuples (i.e., elements) of the global

schema relations can be derived from the tuples of the data source schemas. That is, for each relation R in the global schema, we write a query over the source relations specifying how to obtain R's tuples from the data sources schema. In a GAV mediator [101, 49, 134, 41, 79, 47], a query reformulation is simply unfolding, i.e., replacing each global schema relation in the query with its view definition. The reason is that relations in the global schema are defined in terms of the source relations; we only need to unfold the definitions of the global schema relations.

Local-As-View (LAV). The LAV approach is the opposite of the GAV approach. In a LAV mediator [103, 64, 110, 102], the global schema definition exists, and each data source schema is defined as a view over it. In other words, the contents of a data source are described as a query over the global schema. The query reformulation in LAV is not relatively straightforward as in GAV because it is not possible to simply unfold the definitions of the relations in the global schema. It amounts to finding combinations of views, hence of local schema tuples, that satisfy the query.

In [75], the authors describe the GLAV language that combines the expressive power of LAV and GLAV. They show that the query reformulation complexity is the same as for LAV.

**Data Integration vs. Federated Systems**. Data integration systems offer a level of data integration beyond what FDSs provide in that their global schema relation's tuples can be combined from multiple data sources' relations. In contrast, FDSs do not offer the ability to create such a composite "virtual" relation. Instead, the global schema in FDSs is just a collection of data sources' relations conforming to the schema model (primarily relational).

## 2.2 Hybrid Warehouses

With the emergence of Hadoop and its advantages in high-volume data processing, there has been a substantial move towards "Big Data" systems for massive data storage (i.e., HDFS) and analysis. Many applications (e.g., healthcare and enterprise businesses) require co-analyzing

data stored in HDFS and parallel relational database management systems (RDBMS), which have long been a superior storage and query processing engine for data warehousing applications. This has created a need for a special integration between Hadoop-like big data processing platforms (e.g., SQL-on- Hadoop) and parallel RDBMS.

Several solutions have emerged and most of these solutions statically *pre-load* HDFS data into the relational databases [22, 7, 23] through connectors [8, 22], bulk loading [7, 23] or external tables [1, 7], whereas some other solutions move the relational database data to the HDFS side [23, 22]. As stated in [133, 132], it is not always feasible to move the HDFS data into the relational database side since the HDFS data is typically very large, and bulk reading of the HDFS data into the database might incur an unnecessary load for the RDBMS resources [66]. Moreover, the parallel RDBMS data gets updated frequently. Thus, it is not beneficial to move the data to the HDFS side since it does not support updates properly.

*Hybrid warehouses* [132, 133, 66, 99, 38] propose to leave data in the storage engine where the data was originally located and allow splitting the query processing between the parallel RDBMS and HDFS side (i.e., Hadoop-like big data processing platform). They share some similarities with federated database systems. Both provide a global schema that conforms to a single data model (relational) and describes the data stored in RDBMS and HDFS. Further, they feature a single standard query language to the application layer. However, the key feature that distinguishes hybrid warehouses from other federation systems is that they follow the *lightweight-middleware* principle [46]. They mainly utilize the parallel RDBMS query engine as a *middleware* to orchestrate the query processing between two massively parallel systems.

## 2.3 Modern Hybrid Stores

Recently, we have witnessed a proliferation of data sources of different data models and query languages, which has rendered a mediator approach [10, 130, 80, 46], where using a *single* 

*global schema* to interact with all data sources is unfeasible. Developed specifically for this setting, hybrid systems (a.k.a. polystores) [68, 136, 27, 95, 35, 55] do not hide the heterogeneity of the data sources and are proposed to combine domain-specific databases that specialize in specific data models and execution. They provide integrated access to a number of heterogeneous data stores through one or more query languages [10, 46]. For example, BigDAWG [68], at its core, is the abstraction of an *island*, a collection of data stores of a common data model, which can be accessed with a single query language. For instance, SQL is used to pose queries in the scope of the relational island. CloudMDSQL [95] and SparkSQL [35] support SQL-like queries with the extended capabilities for subqueries expressed in terms of each data store's native query interface/language. Myria [136] provides an imperative-declarative hybrid language called MyriaL. The language resembles relational queries but with an imperative form. The language can be seen as an extension of PigLatin for cross-platform settings, where users can specify which platform to execute their queries (or sub-queries).

Moreover, these systems utilize (or extend) various query processing techniques from classical distributed database systems (e.g., data/function shipping, query decomposition). Query optimization is also supported by either a cost- or heuristics-based approach [46].

## 2.4 Relationship to This Work

Our work mainly focuses on enabling semantic query optimization (including crossmodels views- and integrity constraints-based rewriting) on top of hybrid systems. Mediator systems [103, 64, 110, 139] that follow the LAV approach address semantic optimization mostly in a single-model (typically relational or XML) setting, where cross-models query rewriting does not occur. Moreover, several information integration systems [102, 81] focus on finding not-necessarily equivalent (but maximally-contained) rewritings. In contrast, this thesis targets equivalent query rewriting, which leads to a very different algorithm. Further, setting our work apart is the scale and usage of integrity constraints.

## Chapter 3

## Background

In this chapter, we provide a brief introduction to conjunctive queries [50, 26], query containment and equivalence [50, 26], integrity constraints [26] and query reformulation under constraints [84]. These concepts are at the core of the approaches proposed in this monograph.

## **3.1** Conjunctive Query

A conjunctive query (or simply CQ) is an expression of the form:

$$Q(\vec{x})$$
:-  $R_1(\vec{y}_1), \ldots, R_n(\vec{y}_n)$ 

where each  $R_i$  for every i = 1, ..., n is a predicate (relation) of some finite arity, and Q is a *fresh* relation name, and it is called intensional relation since its content is given by definition through the query.  $\vec{x}, \vec{y}_1, ..., \vec{y}_n$  are free tuples of variables or constants. Each  $R_i(\vec{y}_i)$  is called a relational atom or subgoal. It is also called extensional relation since it is provided as input to the query.

The expression  $Q(\vec{x})$  is the *head* of the query, while the conjunction of relational *atoms*  $R_1(\vec{y}_1), \ldots, R_n(\vec{y}_n)$  is its *body*. The body can contain a conjunction (possibly empty) of relational

equality *atoms* of the form y = y'. All variables in the head are called *distinguished* variables. Also, every variable in  $\vec{x}$  ( $\vec{x}$  can be empty) must appear at least once in  $\vec{y}_1, \dots, \vec{y}_n$  tuples. Below some examples of conjunctive queries.

Example 3.1.1 (Examples of Conjunctive Query).

$$Q_1(x,z):= R(x,y), S(y,z)$$
  
 $Q_2(x,z):= R(x,y), S(y,z), R(x,e)$   
 $Q_3():= R(x,y), S(y,z), T(y)$   
 $Q_4(x,y):= R(x,y), y = c, where c is a constant$ 

 $Q_3$  is a *boolean* conjunctive query since its head is empty. In other words, its head is in the form of Q(). Equivalently, a conjunctive query is a query expressible by a SQL expression of the form: SELECT-FROM-WHERE.

#### 3.1.1 Semantics

Given a database instance D, a valuation v from Q to D is a total function (defined for all possible input values) that maps the variables of Q to constants in D and is the identity on the constants in Q. Moreover, the image of every relational atom R of Q under v is an R-tuple in D, and for every equality atom u = v of Q, u, v have the same image under v.

**Example 3.1.2** (Valuation From the Query to a Database Instance). For query  $Q_1$  (shown in *Example 3.1.1*), the function v, where v(x) = x', v(y) = y', v(z) = z', and  $v(\langle x, y \rangle) = \langle v(x), v(y) \rangle = \langle x', y' \rangle$ , is a valuation.

The answer of a conjunctive query Q on an instance D, denoted Q(D), is the set of all tuples t for which there is a valuation v from Q into D, such that the image of the head tuple under v is t.

#### **3.1.2** Query Containment and Equivalence

We now formally define query containment and equivalence [50, 26] for conjunctive queries:

**Definition 1** (Query Containment). We say that query  $Q_1$  is contained in query  $Q_2$ , denoted  $Q_1 \subseteq Q_2$ , if for every database instance D, we have  $Q_1(D) \subseteq Q_2(D)$  (the set  $Q_1(D)$  is included in the set  $Q_2(D)$ ).

**Definition 2** (Query Equivalence). We say that query  $Q_1$  is equivalent to query  $Q_2$ , denoted  $Q_1 \equiv Q_2$ , if for every database instance D, we have  $Q_1(D) \equiv Q_2(D)$ 

Two queries  $Q_1$  and  $Q_2$  are equivalent if and only if they are contained in each other  $(Q_1 \subseteq Q_2 \text{ and } Q_2 \subseteq Q_1).$ 

To check whether  $Q_1 \subseteq Q_2$ , we need to introduce the following core concepts:

**Definition 3** (Canonical Instance). *Given a conjunctive query Q, the canonical database D^Q is the database instance where each atom in Q becomes a fact in the instance.* 

**Example 3.1.3** (Canonical Instance). *The canonical database for the query*  $Q_2$  *in Example 3.1.1 is the instance*  $D^{Q_2} = \{R(x,y), S(y,z), R(x,e)\}.$ 

**Definition 4** (Homomorphism). A homomorphism h (a.k.a. containment mapping) from  $Q_2$  to  $Q_1$  is a function h:  $var(Q_2) \rightarrow var(Q_1) \cup const(Q_1)$  such that:

(i) for every atom  $R(x_1, x_2, ...)$  in  $Q_2$ , there is an atom  $R(h(x_1), h(x_2), ...)$  in  $Q_1$ 

(*ii*) 
$$h(head(Q_2)) = head(Q_1)$$

where **var** denotes the set of variables in a query Q and **head** denotes the denotes the head variables of Q.

**Example 3.1.4** (Homomorphism Example). Consider the following two queries  $Q_1$  and  $Q'_1$ :

$$Q_1(x,y):= R(x,y), S(y,y), R(x,e)$$
  
 $Q'_1(u,d):= R(u,d), S(d,f), R(u,w)$ 

There is a homomorphism  $h_1 = \{u \to x, d \to y, f \to y, w \to e\}$  from  $Q'_1$  to  $Q_1$ .

We now state the core theorem for query containment.

**Theorem 3.1.1** (Query Containment [50]). *Given two conjunctive queries*  $Q_1$ ,  $Q_2$ , the following statements are equivalent: (i)  $Q_1 \subseteq Q_2$ (ii) There is a homomorphism h from  $Q_2$  to  $Q_1$ .

(*iii*) *head*( $Q_1$ )  $\in Q_2(D^{Q_1})$ 

## **3.2** Integrity Constraints (Dependencies)

Different forms of *integrity constraints* (a.k.a. database dependencies in the relational model) have been introduced and studied in the literature [53, 69, 72]. They are used to express properties that must be satisfied by all instances of a database schema. These properties arise in a specific application domain. We refer a reader to several survey papers [72, 90, 135] for more details on constraints and their history.

### 3.2.1 Expressing Constraints in First-Order Logic

Constraints can be expressed using a fragment of the language of first-order logic, known as the class of *embedded dependencies* [26].

$$\forall x_1,\ldots,x_n\phi(x_1,\ldots,x_n) \rightarrow \exists z_1,\ldots,z_k\psi(y_1,\ldots,y_m)$$
where  $\{z_1, \ldots, z_k\} = \{y_1, \ldots, y_m\} \setminus \{x_1, \ldots, x_n\}$ . The constraint's *premise*  $\phi$  is a conjunction (possibly empty) of relational atoms over variables  $x_1, \ldots, x_n$  or constants. The constraint's *conclusion*  $\psi$  is a non-empty conjunction of relational atoms and/or equality atoms – of the form w = w' – over variables  $y_1, \ldots, y_m$  or constants. The case when all atoms in  $\psi$  are relational atoms is called Tuple Generating Dependencies (**TGD**s), while the case when all atoms in  $\psi$  are equalities defines Equality Generating Dependencies (**EGD**s).

**Example 3.2.1** (Example of Dependencies From [58]). *Consider a relation Review(paper, re-viewer, 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. The fact that a paper can only be submitted to a single track is captured by the following EGD:* 

$$\forall p \forall r \forall t \forall r' \forall t' Review(p, r, t) \land Review(p, r', t') \rightarrow t = t'$$

We can also express that papers be reviewed only by PC members by the following TGD:

$$\forall p \forall r \forall t \ Review(p,r,t) \rightarrow \exists a \ PC(r,a)$$

### 3.2.2 Reasoning With Integrity Constraints: The Chase

The chase procedure is a fundamental algorithm for tackling the implication problem of data dependencies [108, 40, 26] and optimizing conjunctive queries under data dependencies [89]. The algorithm has played a central role in semantic query optimizations [122, 63, 124, 101, 71] for a variety of database applications such as query answering using views [122, 63], data integration and exchange [101, 71] and probabilistic databases [117].

The core concept of the chase is that it fixes constraint violations for a given *fixed* database instance D and a set of data dependencies  $\Sigma$ .

**Chase Application**. Given a conjunction of atoms *A* and an embedded dependency  $\sigma \in \Sigma$  of the from:  $\forall \vec{x} \vec{y} \phi(\vec{x}, \vec{y}) \rightarrow \exists \vec{z} \psi(\vec{x}, \vec{z})$ , then  $\sigma$  is applicable to *A* with a premise homomorphism *h* 

iff *h* is a homomorphism from  $\phi$  to *A* (i.e., the premise holds in *A*), such that *h* cannot be extended to cover  $\phi$  (i.e., the conclusion is not already satisfied). We then apply the dependency  $\sigma$  by adding its conclusion to *A*.

A chase step adds  $\psi(h(\vec{x}), f(\vec{z}))$  to *A*, where *h* is the premise homomorphism, and *f* creates "fresh" variables, known as fresh null value or skolems for all of existential variables  $\vec{z}$ .

**Example 3.2.2** (Example of the Chase Application From [111]). Consider two atoms S(X) and E(X,Y), where E stores directed edges from node x to node y, and S contains nodes with some distinguished properties, which are enforced by constraints. Now, suppose we have only the following constraint  $\Sigma$  and database instance D:

 $\Sigma : \forall x \ S(x) \to \exists y \ E(x, y)$  $D = \{S(x_1), S(x_2), E(x_1, x_2)\}$ 

The constraint  $\Sigma$  states that each node in S has at least one outgoing edge. The example shows that the instance D does not satisfy the constraint  $\Sigma$  since it does not contain an outgoing edge from node  $x_2$ . The chase would fix the constraint violation in D by creating the tuple  $t = E(x_2, y')$ , where y' is a "fresh" variable. After applying the chase, the resulting database instance  $D' = D \cup \{t\}$  satisfies the constraint  $\Sigma$ . At this point, the chase terminates and returns the database instance D'.

The standard chase is a series of chase steps. These steps may be finite or infinite depending on the constraints. One well-known termination condition is *weak acyclicity* [70].

**Weak Acyclicity.** The key idea of weak acyclicity [70] is to assert that no "fresh" values are created over and over again during the execution of the chase.

**Definition 5** (Weakly Acyclic Set of TGDs [70]). Let  $\Sigma$  be a set of TGDs over a fixed schema. Construct a directed graph, called the dependency graph, as follows: (i) there is a node for every pair (R,a), where R is a relation symbol of the schema and a is an attribute of R; we call such pair (R,a) a position;(ii) for every TGD:  $\forall \vec{x} \ \phi(\vec{x}) \rightarrow \exists \vec{y} \ \psi(\vec{x}, \vec{y}) \in \Sigma$  and for every and for every x in  $\vec{x}$  that occurs in  $\psi$  add the following edges:

- For every occurrence of x in  $\phi$  in position  $(R, a_i)$ ;
  - 1. for every occurrence of x in  $\psi$  in position  $(S, b_j)$ , add an edge  $(R, a_i) \rightarrow (S, b_j \text{ (if it does not already exist)})$
  - 2. for every existentially quantified variable  $y \in \vec{y}$  and for every occurrence of y in  $\psi$  in position  $(E, c_k)$ , add a special edge  $(R, a_i) \xrightarrow{*} (E, c_k)$

A set  $\Sigma$  of embedded dependencies is called weakly acyclic iff the dependency graph of  $\Sigma$  has no cycles going through a special edge.

**Example 3.2.3** (Example of Weakly and Not Weakly Acyclic Constraints Adopted From [70]). Consider a schema S that has a relation  $DEPT(D_ID, E_ID, MGR_N)$ , listing departments with their manager IDs and names, and a separate relation for  $EMP(E_ID, D_ID)$ . The following set of constraints using DEPT and EMP relations is not weakly acyclic since finite chase may not exist. The first constraint states that each manager of a department is an employee of some department (not necessarily the one they manage).

 $\forall D \forall E \forall N \ DEPT(D, E, N) \rightarrow \exists d \ EMP(E, d)$  $\forall E \forall D \ EMP(E, D) \rightarrow \exists e \exists n \ DEPT(D, e, n)$ 

However, if we assume that we know that each manager of a department is employed by the same department, then we have the following weakly acyclic constraints where it is guaranteed that every chase setp is finite.

 $\forall D \forall E \forall N \ DEPT(D, E, N) \rightarrow EMP(E, D)$  $\forall E \forall D \ EMP(E, D) \rightarrow \exists e \exists n \ DEPT(D, e, n)$ 

We refer a reader to [111, 70] for more details on the chase termination under other permissive and sufficient conditions.

### **3.3 Query Reformulation Under Integrity Constraints**

One of the main problems in query processing is reformulating a query Q expressed against a source schema S to an equivalent query R against a target schema T, by exploiting the relationship between S and T. Examples of query reformulation problems include semantic query optimization (e.g., eliminating redundant joins and reformulating queries under integrity constraints), rewriting queries using views and physical access path selection in query optimization.

In [62], the authors introduce a *uniform* solution for these problems in the form of the Chase & Backchase (C&B) algorithm for query reformulation under constraints. They show how the above query reformulation problems can be expressed as particular query reformulation instances where the relationship between the schemas S and T is expressed by constraints.

In the following sections, we first give an overview of the C&B algorithm (Section 3.3.1), and then we briefly introduce the *Provenance-Directed C&B* [84] (Section 3.3.2), which is an improved version of the C&B algorithm.

### 3.3.1 The Chase&Backchase (C&B) Algorithm

The Chase&Backchase (C&B) is an algorithm for rewriting queries under integrity constraints [62]. We illustrate the algorithm on a very restricted case of a query reformulation problem, which is *finding total rewriting (i.e., base tables are disallowed) of queries using materialized views*.

**Reformulation Under Constraints.** We write  $D \models \Sigma$  if a database instance D satisfies all the constraints in a set  $\Sigma$ . Query  $Q_1$  is contained in query  $Q_2$  under the set  $\Sigma$  of constraints (denoted  $Q_1 \sqsubseteq_{\Sigma} Q_2$ ) if and only if  $Q_1(D) \subseteq Q_2(D)$  for every database  $D \models \Sigma$ , where Q(D) denotes the result of Q on D.  $Q_1$  is equivalent to  $Q_2$  under C (denoted  $Q_1 \equiv_{\Sigma} Q_2$ ) if and only if  $Q_1 \sqsubseteq_{\Sigma} Q_2$ and  $Q_2 \sqsubseteq_{\Sigma} Q_1$ .

Let *S* and *T* be relational schemas related by set  $\Sigma$  of constraints, and *Q* a query formulated against *S*. A reformulation of *Q* under  $\Sigma$  is a query *R* formulated against *T*, such that  $Q \equiv_{\Sigma} R$ 

The C&B algorithm is based on expressing queries as conjunctive queries and the view definitions as a set  $C_{\mathcal{V}}$  of *embedded dependencies*. Then, chasing with  $C_{\mathcal{V}}$  as well as with other integrity constraints *I*. We denote the result of chasing a query *Q* with  $\Sigma = C_{\mathcal{V}} \cup I$  as  $Q^{\Sigma}$ .

Phases of The C&B algorithm: The algorithm proceeds in two phases:

**Chase:** The input query Q is chased with  $\Sigma$ , to obtain a chase result  $Q^{\Sigma}$ . Then, the subquery U of  $Q^{\Sigma}$  is obtained by restricting  $Q^{\Sigma}$  to the schema of the views (a.k.a. target schema). U is called the *universal plan*.

**Backchase:** In this phase, the subqueries of the universal plan U are checked for equivalence (under  $\Sigma$ ) to Q. The output of this phase is all *minimal*-equivalent subqueries (i.e., contain no subqueries that are already equivalent to Q). This equivalence check is performed by chasing "back" each subquery sq in U, and checking whether Q has a containment mapping into  $sq^{\Sigma}$ .

We illustrate the algorithm on the following running example (the example adopted from [84, 59]). For simplicity, we discuss the example in the absence of integrity constraints *I* and only use  $C_{\psi}$  constraints.

Example 3.3.1 (Example of The C&B Algorithm from [84, 59]). Consider the query

$$Q(x): -R(x, w, y), S(y, z), T(z, e)$$

and assume that we have the following views defined:

$$V_R(x, y) : -R(x, w, y)$$
$$V_S(y, z) : -S(y, z)$$

$$V_{RS}(x,z) : -R(x,w,y), S(y,z)$$
$$V_T(z,e) : -T(z,e)$$

The reader realizes easily that

$$R_1(x) : -V_{RS}(x,z), V_T(z,e)$$
  
 $R_2(x) : -V_R(x,y), V_S(y,z), V_T(z,e)$ 

are equivalent views-based rewritings of Q. In addition,  $R_1$  and  $R_2$  are minimal rewritings since non of them contain subqueries that are already equivalent to Q.

In order to find these two rewritings, the algorithm requires capturing the view definitions by a set  $C_{V}$  of embedded dependencies.  $C_{V}$  is obtained by stating the inclusion (in both directions) between the result of the query defining each view and the view's extent [34]. For example,  $C_{V}$  is the following set of embedded dependencies:

$$\begin{split} V_R^{IO} &: \forall x \forall w \forall y \ R(x, w, y) \to V_R(x, y) \\ V_R^{OI} &: \forall x \forall y \ V_R(x, y) \to \exists w \ R(x, w, y) \\ V_S^{IO} &: \forall y \forall z \ S(y, z) \to V_S(y, z) \\ V_S^{OI} &: \forall y \forall z \ V_S(y, z) \to S(y, z)) \\ V_{RS}^{IO} &: \forall x \forall w \forall y \forall z \ R(x, w, y), S(y, z) \to V_{RS}(x, z) \\ V_{RS}^{OI} &: \forall x \forall z \ V_{RS}(x, z) \to \exists w \exists y \ R(x, w, y), S(y, z) \\ V_T^{IO} &: \forall z \forall e \ T(z, e) \to V_T(z, e) \\ V_T^{OI} &: \forall z \forall e \ V_T(z, e) \to T(z, e) \end{split}$$

**The Chase Phase**: When chasing Q with  $C_{V}$ , the only applicable chase steps involve  $V_{R}^{IO}$ ,  $V_{S}^{IO}$ ,  $V_{T}^{IO}$  and  $V_{RS}^{IO}$ , yielding the following chase result:

$$Q^{\mathcal{C}_{\mathcal{V}}}(x) : -R(x, w, y), S(y, z), T(z, e), V_R(x, y), V_S(y, z), V_T(z, e), V_{RS}(x, z)$$

Restricting  $Q^{C_{V}}$  to the schema of the views results into the following universal plan U:

$$U(x) : -V_R(x, y), V_S(y, z), V_T(z, e), V_{RS}(x, z)$$

**The Backchase Phase**: Now, the input to the backchase is U, where the subqueries of U are inspected for equivalence with Q. The rewritings  $R_1$  and  $R_2$  above are among these subqueries. To determine that a subquery sq in U is equivalent to Q, we chase sq back with  $C_{V}$ , and we search for a containment mapping from Q into sq $C_{V}$ . In this example, we illustrate only for the subquery of U corresponding to  $R_1$ . The only applicable chase steps involve  $V_{RS}^{OI}$  and  $V_T^{OI}$ , which yields:

$$R_1^{\mathcal{C}_{\mathcal{V}}}(x) : -V_{RS}(x,z), V_T(z,e), R(x,w,y), S(y,z), T(z,e)$$

Since there is a containment mapping h(Q) from Q into  $R_1^{C_V}$ ,  $R_1$  is an equivalent and minimal rewriting of Q.

One major problem with the backchase is that it inspects exponentially many subqueries of U, even when there were only very few minimal rewritings. In the next section, we briefly introduce the PACB algorithm [84], which employs much more goal-directed search techniques and inspects up to exponentially fewer reformulation candidates than the C&B algorithm. PACB is provably sound and complete for conjunctive queries and large classes of constraints and has been shown to outperform by orders of magnitude the commercial optimizer of a major relational vendor even when limited to the key and foreign key constraints that commercial optimizers understand.

#### **3.3.2** The Provenance-Directed C&B: PACB

The C&B algorithm enumerates the subqueries of the universal plan U in a bottomup fashion and chases each of them in isolation to determine equivalence to the query Q. This approach leads to redundant chasing of the atoms, and it also leads to useless chasing of subqueries that are not equivalent to Q.

The goal of the PACB algorithm [84] is to replace the many isolated subqueries chases with a single chase of the universal plan U. To do so, PACB keeps track of the provenance of each atom, where the provenance of an atom a gives the set of subqueries of U, whose chasing led to the creation of a. We illustrate the algorithm by revisiting Example 3.3.1 from Section 3.3.1.

**Example 3.3.2** (The Example of PACB Approch From [84]). *Revisiting Example 3.3.1, applicable chase steps of U with*  $C_{V}$  *involve*  $V_{R}^{OI}$ ,  $V_{S}^{OI}$ ,  $V_{T}^{OI}$  and  $V_{RS}^{OI}$ , yielding

$$U^{C_{\mathcal{V}}}(x) := -V_{R}(x, y), V_{S}(y, z), V_{T}(z, u), V_{RS}(x, z),$$
  
$$R(x, w_{1}, y), S(y, z), T(z, e), R(x, w_{2}, y_{1}), S(y_{1}, z)$$

Notice that they query Q has two containment mappings into  $U^{C_{V}}$ :

$$h_1 = \{x \to x, y \to y_1, w \to w_2, z \to z, e \to e\}$$
$$h_2 = \{x \to x, y \to y, w \to w_1, z \to z, e \to e\}$$

Now, we show  $U^{C_{\eta}}$ , this time annotating its atoms with a unique ID called a provenance term. The provenance annotations appear as superscripts:

$$U^{\mathcal{C}_{\mathcal{V}}}(x) := -V_{R}(x, y)^{V_{R}}, V_{S}(y, z)^{V_{S}}, V_{T}(z, u)^{V_{T}}, V_{RS}(x, z)^{V_{RS}},$$
  
$$R(x, w_{1}, y)^{V_{R}}, S(y, z)^{V_{S}}, T(z, e)^{V_{T}}, R(x, w_{2}, y_{1})^{V_{RS}}, S(y_{1}, z)^{V_{RS}}$$

The view atoms in  $U^{C_{V}}$  are annotated by themselves since they are not introduced by chasing. The R, S and T atoms are introduced by chasing  $V_{R}^{OI}$ ,  $V_{S}^{OI}$ ,  $V_{T}^{OI}$  and  $V_{RS}^{OI}$ . For instance, the first R atom:  $R(x,w_{1},y)$  is introduced by chasing  $V_{R}(x,y)$  with the dependency  $V_{R}^{OI}$ , while the second R atom:  $R(x,w_{2},y_{1})$  is introduced by chasing  $V_{RS}(x,z)$  with  $V_{RS}^{OI}$ . The provenance formula  ${}^{I} \pi(h_{1})$  of the first image  $h_{1}$  of Q is  $V_{RS} \wedge V_{T}$ , which corresponds to the rewriting  $R_{1}$  in

<sup>&</sup>lt;sup>1</sup>Provenance formulas are constructed from provenance terms using logical conjunction and disjunction with their expected properties such as commutativity, distributivity, idempotency and absorption.

Example 3.3.1, while the provenance formula  $\pi(h_2)$  of the second image  $h_2$  of Q is  $V_R \wedge V_S \wedge V_T$ , which corresponds to the rewriting  $R_2$  in the same running example.

Notice that we immediately identify the two rewritings of Q by reading them off directly from the provenance formulas:  $\pi(h_1)$  and  $\pi(h_2)$  of Q images in  $U^{C_V}$ . With this approach, the PACB algorithm avoids fruitless individual chases of the subqueries in U.

## **Chapter 4**

# **ESTOCADA: Bringing Semantic Optimization to Hybrid Stores**

### 4.1 Introduction

This chapter presents ESTOCADA, an extensible lightweight framework for bringing semantic query optimization on top of hybrid stores. The novelty of ESTOCADA is to find a semantically equivalent views-based rewriting of a given hybrid query via a reduction from multi-models views-based query rewriting to relational rewriting under integrity constraints. We formalize our guarantees in terms of soundness and completeness and show that ESTOCADA improves the performance in natural scenarios for both cross-models and single model user queries.

### 4.1.1 Motivating example

Consider the Medical Information Mart for Intensive Care III (MIMIC-III) [88] dataset, comprising health data for more than 40.000 Intensive Care Unit (ICU) patients from 2001 to 2012. The total size of **46.6 GB**, and it consists of : (*i*) all charted data for all patients and

their hospital admission information, ICU stays, laboratory measurements, caregivers' notes, and prescriptions; (*ii*) the role of caregivers (e.g., MD stands for "medical doctor"), (*iii*) lab measurements (e.g., ABG stands for "arterial blood gas") and (*iv*) diagnosis-related groups (DRG) codes descriptions.

**Our motivation query**  $Q_1$  is: "for the patients transferred into the ICU due to "coronary artery" issues, with abnormal blood test results, find the date/time of admission, their previous location (e.g., emergency room, clinic referral), and the drugs of type "additive" prescribed to them". Evaluating this query through the AsterixDB JSON store (v9.4) [4] took more than 25 minutes; this is because the system does not support full-text search by an index if the text occurs within a JSON array. In SparkSQL (v2.3.2), the query took more than an hour due to its lack of indexes for selective data access. In the MongoDB JSON store (v4.0.2) [11], it took more than 17 minutes due to its limited join capability. Finally, in PostgreSQL with JSON support (v9.6), denoted Postgres in the sequel,  $Q_1$  took  $\approx 12.6$  minutes.

Now, consider we had at our disposal three *materialized views* which pre-compute partial results for  $Q_1$ . SOLR is a well-known highly efficient full-text server. It is also capable of handling JSON documents. Consider a SOLR server that stores a view  $V_1$  storing the IDs of patients, their hospital admission IDs, and the caregivers' reports, including notes on the patients' stay (e.g., detailed diagnosis). Full-text search on  $V_1$  for "coronary artery" allows retrieving the IDs of the respective patients efficiently. Further, consider that a Postgres server stores a view  $V_2$  with the patient's meta-data information and their hospital admission information, such as admission time and patients' location prior to admission. Finally, assume available a view  $V_3$ , which stores all drugs that are prescribed for each patient that has "abnormal blood" test results as a JSON document stored in Postgres.

Now, we are able to evaluate  $Q_1$  by a full-text search on  $V_1$  followed by a BindJoin [123] with the result of filtering  $V_3$ , and projecting prescribed drugs as well as patients' admission time and prior location from  $V_2$ . Using Tatooine [45], a Java-based hybrid execution engine

(implementing select, project, join, etc.), to access the views and join them, this takes about  $\approx 5.7$  mins, or a **speedup of 5**× w.r.t. plain JSON query evaluation in SparkSQL and AsterixDB. This is also a **speedup of 2**× and **speedup of 3**× w.r.t. plain JSON query evaluation in Postgres and MongoDB, respectively.

**Lessons learned.** We can draw the following conclusions from the above example. (1.) Unsurprisingly, materialized views drastically improve query performance since they precompute partial query results. (2.) More interestingly: materialized views can strongly improve performance even when stored across several data stores, although such a hybrid scenario incurs a certain performance penalty due to the marshaling of data from one data model/store to another. In fact, exploiting the different strengths of each system (e.g., SOLR's text search, Postgres' efficient join algorithms, etc.) is the second reason (together with materialized view usage) for our performance gains. (3.) Different system combinations work best for different queries; thus it *must be easy to add/remove a view in one system*, without disrupting other queries that may be currently well-served. As known from classical data integration research [81], such flexibility is attained through the "local-as-view" (LAV) approach (see Chapter 2), where the content of each data source is described as a view. Thus, adding or removing a data source from the system is easily implemented by adding or removing the respective view definition. (4.) Application data sets may come in a variety of formats, e.g., Apache log data is often represented in CSV. However, while the storage model may change as data migrates, applications should not be disrupted. A simple way of achieving this is to guarantee them access to the data in its native format, regardless of where it is stored.

Observe that the combination of **2.**, **3.** and **4.** above goes well beyond the-state-of-the-art. Most LAV systems assume both the application data and the views are organized according to the same data model (mostly relational or XML). Thus, their view-based query rewriting algorithms are designed specifically within the bounds of that model, e.g., relational [102], or XML [51, 120, 118]. Different from these, some LAV systems [109, 64] allow different data

Data model	Query language/API	Systems
Relational	SQL	Major vendors
JSON	SparkSQL	Spark [35]
JSON	AQL/SQL++	AsterixDB [4]
JSON	SQLw/JSON	Postgres
Key-value	Redis API	Redis
Full-text and JSON	Solr API	Solr
XML	XQuery, XPath	Saxon [19]
Property Graph	Cypher	Neo4j [14]

**Table 4.1**: Models and languages supported by ESTOCADA.

models for the stored views but consider only the case when the application data model is XML. Consequently, the query answering approach adopted in these systems is tailored toward the XML data model and query language. In contrast, we aim at a unified approach, supporting *any data model both at the application and at the view level*. The core technical question to be answered in order to attain such performance benefits without disrupting applications is *view-based query rewriting across an arbitrary set of data models*. We introduce a novel approach for cross-models view-based rewriting. Our approach is currently capable of handling the systems listed in Table 4.1, together with their data models and query languages.

**Chapter Outline.** The chapter is organized as follows. Section 4.2 formalizes the rewriting problem we solve. Section 4.3 outlines our approach; at its core is a view-based query rewriting algorithm based on an internal relational model, invisible to users and applications, but which crucially supports rewriting under integrity constraints. Section 4.4 describes the language we use for (potentially cross-models) views and queries. Section 4.5 shows how we reduce the multi-data model rewriting problem to one within this internal pivot model, then transform rewritings obtained there into a hybrid integration query. Section 4.9 describes a set of extensions we contributed to the rewriting engine at the core of our approach to make it scale in a hybrid setting. Section 4.12 formalizes the guarantees of our approach. We present our experimental evaluation in Section 4.13, and conclude in Section 4.14.

### 4.2 **Problem statement**

We assume a set of data model-query language pairs  $\mathcal{P} = \{(M_1, L_1), (M_2, L_2), \dots, (M_n, L_n)\}$ such that for each  $i \ge 1$ , an  $L_i$  query evaluated against an  $M_i$  instance returns an answer which is also an  $M_i$  instance. The same model may be associated to several query languages; for instance, AsterixDB, MongoDB and Postgres have different query languages for JSON. As we shall see, we consider *expressive languages for realistic settings, supporting conjunctive querying, nesting, aggregation, and object creation.* Without loss of generality, we consider that a language is paired with one data model only.

We consider a hybrid setting comprising a set of stores  $S = \{S_1, S_2, ..., S_n\}$  such that each store  $S \in S$  is characterized by a pair  $(M_S, L_S) \in \mathcal{P}$ , indicating that *S* can store instances of the model  $M_S$  and evaluate queries expressed in  $L_S$ .

We consider a set of datasets  $\mathcal{D} = \{D_1, D_2, \dots, D_n\}$ , such that each data set  $D \in \mathcal{D}$  is an instance of a data model  $M_D$ . A dataset D is stored as a set of (potentially overlapping) **materialized views**  $\mathcal{V}=\{V_D^1, V_D^2 \dots\}$ , such that for every  $j \ge 1$ ,  $V_D^j$  is stored within the storage system  $S_D^j \in \mathcal{S}$ . Thus,  $V_D^j$  is an instance of a data model supported by  $S_D^{j-1}$ .

We consider a *hybrid integration language IL*, capable of expressing computations to be made within each store and across all of them, as follows:

- For every store S and query  $q_S \in L_S$ , IL allows that  $q_S$  should be evaluated over S directly;
- Further, *IL* allows expressing powerful processing over the results of one or several such source queries (e.g., join results).

Such integration language has been proposed in several hybrid systems [95, 68]; we use it to express queries and computations over the views. An *IL* expression bears obvious similarities with an execution plan in a wrapper-mediator system (see Chapter 2); its evaluation is split

<sup>&</sup>lt;sup>1</sup>For uniformity, we describe any collection of stored data as a view, e.g., a table stored in an RDBMS is an (identity) view over itself.



Figure 4.1: ESTOCADA reduction outline.

between computations pushed to the stores and subsequent operations applied by the mediator on top of their results. The main distinction is that *LL* remains declarative, abstracting the details of each in-store computation, which is simply specified by a query in the store's language.

We assume *available a cost model* which, given an *LL* expression *e*, returns an estimation of the cost of evaluating *e* (including the cost of its source sub-queries). The cost may reflect e.g., disk I/O, memory needs, CPU time, transfer time between distributed sites. *Devising a cost-based model for a hybrid setting is beyond the scope of this work*.

We term a *rewriting* of a query q as an integration query expressed in IL, which is equivalent to q. We consider the following rewriting problem:

**Definition 6** (Cross-Model Rewriting Problem). *Given a query*  $q \in IL$  *over several datasets*  $D_i$ ,  $1 \le i \le n$ , and a set of views V materialized over these datasets, find the minimum-cost equivalent rewriting RW of q using the views.

Most modern query languages include primitives such as arithmetic operations, aggregation, and calls to arbitrary UDFs; these suffice to preclude the decidability of checking whether two queries are equivalent. Therefore, we aim at finding rewritings *under black-box (uninterpreted) function semantics (UFS)*: we seek rewritings that make the same function calls, with the same arguments as the original query.

### 4.3 ESTOCADA Overview

We outline here our approach for solving the problem introduced in Section 4.2:

**Our integration language:**  $QBT^{XM}$ . We devised  $QBT^{XM}$ , a concrete integration language which supports queries over several data stores, each with its own data model and query language.  $QBT^{XM}$  follows a *block*-based design, with blocks organized into a tree in the spirit of the classical Query Block Trees (QBT) introduced in System R [125], slightly adapted to accommodate subsequent SQL developments, in particular, the ability to nest sub-queries within the select clause [85]. The main difference in our setting is that each block may be expressed in a different query language and carried over data of a different data model (e.g., SQL for relational data, key-based search API for key-value data, different JSON query languages). We call the resulting language  $QBT^{XM}$ , for *cross-models QBT* (detailed in Section 4.4.2). We note that exiting hybrid query languages [95, 68] resembles  $QBT^{XM}$ , and they can be translated directly to  $QBT^{XM}$ , as demonstrated in [32]. Excerpts of  $QBT^{XM}$  grammar are delegated to Appendix A.2.

 $QBT^{XM}$  Views. Each materialized view V is defined by an  $QBT^{XM}$  query (or other hybrid integration languages); it may draw data from one or several data sources of the same or different data models. Each view returns (holds) data following <u>one</u> data model, and is stored in a data store supporting that model.

**Encoding into a Single Pivot Model.** We reduce the cross-models rewriting problem to a single-model setting, namely *relational constraint-based query reformulation*, as follows (see also Figure 5.1; yellow background identifies the areas where we bring contributions in this work.). First, we *encode relationally*: the structure of original datasets, the view specifications, and the application query.

Note that the relations used in the encoding are *virtual*, i.e., no data is migrated into them; they are also *hidden*, i.e., invisible to both the application designers and to users. They only serve to support query rewriting via relational techniques. The virtual relations are accompanied by *integrity constraints* that reflect the features of the underlying data models (for each model M, a set enc(M) of constraints). For instance, we describe the organization of a JSON document data model using a small set of relations such as *Child(parentID, childID, key, type)* together with the constraint specifying that every child has just one parent. Such modeling had first been introduced in local-as-view XML integration works [109, 64]. The constraints are TGDs and EGDs (see Chapter 3), extended with such well-researched constraints as denial constraints [77] and disjunctive constraints [76]. We detail the pivot model in Section 4.5.

**Reduction From Cross-Model to Single-Model Rewriting.** Our reduction translates the declaration of each view V to additional constraints enc(V) that reflect the correspondence between V's input data and its output. Constraints have been used to encode single-model views [65] and correspondences between source and target schemas in data exchange [71]. The novelty here is the rich collection of supported models, and the cross-models character of the views.

An incoming query Q over the original datasets  $DS_1, \ldots, DS_l$ , whose data models respectively are  $M_1, \ldots, M_l$ , is encoded as a relational query enc(Q) over the dataset's relational encoding. enc(Q) is centered around conjunctive queries, with extensions such as aggregates, UDFs, and nested sub-queries.

The reformulation problem is thus reduced to a purely relational setting: given a relational query enc(Q), a set of relational integrity constraints encoding the views,  $enc(V_1) \cup ... \cup enc(V_n)$ , and the set of relational constraints obtained by encoding the data models  $M_1, ..., M_l$ , find the queries  $RW_r^i$  expressed over the relational views, for some integer k and  $1 \le i \le k$ , such that each  $RW_r^i$  is equivalent to enc(Q) under these constraints.

The challenge in coming up with the reduction consists in designing a *faithful* encoding, i.e., one in which rewritings found by (*i*) encoding relationally, (*ii*) solving the resulting relational reformulation problem, and (*iii*) decoding each reformulation  $RW_r^i$  into a  $QBT^{XM}$  query R =  $dec(RW_r^i)$  over the views in the polystore, correspond to rewritings found by solving the original problem. That is, *R* is a rewriting of *Q* given the views  $\{V_1, \ldots, V_n\}$  if  $R = dec(RW_r^i)$ , where  $RW_r^i$  is a relational reformulation of enc(Q) under the constraints obtained from encoding  $V_1, \ldots, V_n$ ,  $M_1, \ldots, M_l$ . The reduction is detailed in Sections 4.5, 4.6 and 4.7.

**Relational Rewriting Under Constraints.** To solve the single-model rewriting problem, we need to reformulate relational queries under constraints. The algorithm of choice is known as Chase & Backchase (C&B, in short, see Chapter 3), introduced in [63] and improved in [84] to yield the *Provenance-Aware C&B algorithm* (PACB, in short, see Chapter 3). PACB was designed to work with relatively few views and constraints. In contrast, in the hybrid setting, each of the many data sources is described by a view, and each view is encoded by many constraints. For instance, the JSON views in our experiments (Section 4.13) are encoded via  $\approx 45$  TGDs involving 10-way joins in the premise. To cope with this complexity, we incorporated into PACB novel scale-up techniques (discussed in Section 4.9.1) to make it scalable in a hybrid setting. PACB was designed for conjunctive queries under set semantics. Towards supporting a richer class of queries, we extended it to bag semantics (Section 4.10) and QBTs (Section 4.11).

**Decoding the Relational Rewritings.** On any relational reformulation  $RW_r^i$  issued by our modified PACB rewriting, a *decoding step dec*( $RW_r^i$ ) is performed to:

(*i*) Group the reformulation atoms by the view they pertain to by following the connections among atoms and knowledge of the encoded data model.

*(ii)* Reformulate each such atom group into a query that can be completely evaluated over a single view.

(*iii*) If several views reside in the same store, identify the largest subquery that can be delegated to that store, along the lines of query evaluation in wrapper-mediator systems [79].

**Evaluation of Non-Delegated Operations.** A decoded rewriting may be unable to push (delegate) some query operations to the store hosting a view if the store does not support them; for instance, most key-value stores do not support joins. In this case, operations have to be executed

outside of that store. For instance, to evaluate such "last-step" operations, our *lightweight execution (hybrid) engine* [45] supports many logical and physical operators, including bind joins [123] (with sideways information passing) to evaluate nested subqueries, and many other operators.

**Choice of the Most Efficient Rewriting.** Decoding may lead to several rewritings  $R_1, \ldots, R_k$ ; for each  $R_i$ , several evaluation plans may lead to different performance. The problem of choosing the best rewriting and best evaluation plan in this setting recalls query optimization in distributed mediator systems [119]. For each rewriting  $R_i$ , we denote by  $c(R_i)$  the lowest cost of an evaluation plan that we can find for  $R_i$ ; we choose the rewriting  $R_{best}$  that minimizes this cost. While devising cost models for hybrid settings is beyond the scope of this paper, we architected ESTOCADA to take the cost model as a configuration parameter (using the hybrid engine's own cost estimator, typically accessible via an API).

### 4.4 The *QBT*<sup>XM</sup> Language

We present here the language we use for views and queries. First, we recall the classical Query Block Trees (QBTs), then we extend them to cross-model views and queries.

### 4.4.1 Query Block Trees (QBT)

Since many of the languages that ESTOCADA supports allow for nested queries and functions (user-defined or built-in such as aggregates), our pivot language *Query Block Trees* (QBTs) also supports these features. These are essentially the classical System R QBTs [125], slightly adapted to accommodate subsequent SQL extensions, such as nesting in the select clause (introduced in SQL-1999 [85]). We first illustrate QBTs on a SQL example.

**Example 4.4.1** (QBT Query). *Consider the SQL query in Figure 4.2, which computes for each student who is not enrolled in any course for the Spring'16 quarter, the number of Spring'16* 

SELECT	s.ssn, COUN	F (SELECT FROM WHERE	w.cno Waitlist w w.ssn = s.ssn AND w.qtr = 'Spring 2016' ) AS cnt
FROM	Student s		
WHERE	NOT EXISTS	(SELECT FROM WHERE	c.no Course c, Enrollment e c.no = e.cno AND s.ssn = e.ssn AND e.gtr = 'Spring 2016')

Figure 4.2: QBT query example.

courses she is waitlisted for (a count of 0 is expected if the student is not waitlisted). While this query could be written using joins, outer joins, and group by operations, we show a natural alternative featuring nesting (which illustrates how we systematically normalize away such operations):

This query consists of three blocks. The outermost SELECT-FROM-WHERE expression corresponds to the root block; call it  $B_0$ . The two nested SELECT-FROM-WHERE expressions are modeled as children blocks of the root block, call them  $B_{00}$  and  $B_{01}$  for the block nested in the SELECT clause and the block nested in the WHERE clause, respectively

The variables occurring in a block B can be either defined by B (in which case we call them **bound** in B), or by one of its ancestors (in which case they are called **free** in B). We assume W.l.o.g. that the bound variables of B have fresh names, i.e., they share no names with variables bound in B's ancestors. For example, variable s is bound in  $B_0$ , but it occurs free in both  $B_{00}$  and  $B_{01}$ .

QBTs model SELECT-FROM-WHERE expressions as blocks, organized into a tree whose parent-child relationship reflects block nesting. Nested blocks always appear as arguments to functions, be they built-in (e.g., COUNT for  $B_{00}$  and NOT EXISTS for  $B_{01}$  in Example 4.4.1) or user-defined. While not shown in Example 4.4.1, the case of blocks nested within the FROM clause corresponds to the identity function.

### 4.4.2 Integration Language: *QBT*<sup>XM</sup>

To specify cross-model queries and views, we adopted a *block-based design*, similar to QBTs, but in which each block is expressed in its own language, signaled by an annotation on the block. We call the resulting language  $QBT^{XM}$ , which stands for *cross-model QBT*.  $QBT^{XM}$  queries comprise FOR and RETURN clauses. The FOR clause introduces several variables and specifies their legal bindings. The RETURN clause specifies what data should be constructed for each binding of the variables. Variables can range over different data models, which is expressed by possibly several successive blocks, each pertaining to its own model. In SQL style, this defines a Cartesian product of the variable bindings computed by each block from the FOR clause; this Cartesian product can be filtered through WHERE clause. We impose the restriction that *variables shared by blocks spanning different data models must be of text or numeric type*, so as to avoid dealing with conversions automatically, the topic is beyond the scope of this work. We describe *QBT<sup>XM</sup>* informally, by examples; the grammar of *QBT<sup>XM</sup>* is delegated to Appendix A.2.

**Example 4.4.2** (View Definition Expressed in  $QBT^{XM}$ ). We illustrate the  $QBT^{XM}$  definition of views  $V_1$  and  $V_2$  from Section 4.1 in Figure 4.3, using AsterixDB's SQL++ syntax (easier to read than the JSON syntax of PostgreSQL). FOR clauses bind variables, while RETURN clauses specify how to construct new data based on the variable bindings. Blocks are delimited by braces annotated by the language whose syntax they conform to. The annotations AJ, PR, and SJ stand for the SQL++ language of AsterixDB, the languages of Postgres and Solr, respectively. Also, below, PJ and RK stand respectively for PostgreSQL' JSON query language and for a simple declarative key-value query language that we designed for Redis.

```
Figure 4.3: View definitions expressed in QBT^{XM}.
```

### 4.5 Reduction from Cross-Model to Single-Model Setting

A key requirement in our setting is the ability to reason about queries and views involving multiple data models and query languages. This is challenging for several reasons. First, not every data model/query language setting supported in ESTOCADA comes with a known *view-based query rewriting (VBQR, in short) algorithm:* consider key-value pairs as the data model and declarative languages over them, or JSON data and its query languages in circulation, etc. Second, even if we had these algorithms for each model/language pair, neither would readily extend to a solution of the *cross-model* VBQR setting in which views may be defined over data from various models, materializing their result in yet again distinct models, and in which query rewritings access data from potentially different models than the original query. Third, for the feasibility of development and maintenance as the set of supported model/language pairs evolves, any cross-model VBQR solution needs to be modularly extensible to additional models/languages, in the sense that no modification to the existing code is required and it suffices to just add code dealing with the new model/language pair. Moreover, the developer of this additional code should not need to understand any of the other model/language pairs already supported in ESTOCADA.

To address these challenges, we reduce the cross-model VBQR problem to a single-

$CollectionName_J(ID)$		
$Child_J(parentID, childID, key, type)$		
$Eq_J(x,y)$		
Value(x, y)		

**Table 4.2**: Snippet of  $\mathcal{VREI}$  schema.

*model VBQR problem*. That is, we propose a unique *pivot data model*, on which QBT (Section 4.4.1) serves as a *pivot query language*. Together, they allow us to capture data models, queries, and views so that cross-model rewritings can be found by searching for rewritings in the single-model pivot setting instead.

Our pivot model is relational, and it makes prominent use of expressive integrity constraints. This is sufficiently expressive to capture the key aspects of the data models in circulation today, including: freely nested collections and objects, object identity (e.g., for XML element nodes and JSON objects), limited binding patterns (as required by key-value stores), relationships (in the E/R and ODL sense), functional dependencies, and much more. The integrity constraints we use are TGDs or EGDs (see Chapter 3), extended to denial constraints [77] and disjunctive constraints [76].

#### 4.5.1 JSON Model

We represent JSON documents as relational instances conforming to the schema  $\mathcal{VREI}$ (Virtual Relational Encoding of JSON) in Table 4.2. We emphasize that these relational instances are *virtual*, i.e., the JSON data is not stored as such. Regardless of the physical storage of the JSON data, we only use  $\mathcal{VREI}$  to encode JSON queries and views relationally, in order to reason about them.

 $\mathcal{VREI}$  constraints express the fact that JSON databases are organized into named collections of JSON values, which in turn can be objects (consisting of a set of key-value pairs), arrays of values, and scalar values (numeric or text).

We model objects, arrays, and values in an object-oriented fashion, i.e. they have identities. This is because some JSON stores, e.g., MongoDB and AsterixDB, support query languages that refer to identity and/or distinguish between equality by value versus equality by identity. Our modeling supports both the identity-aware and the identity-agnostic view of JSON via appropriate translation of queries and views into pivot language expressions over the  $\mathcal{VREI}$  schema.

Relation *CollectionName*<sup>J</sup> (see Table 4.2) attaches to each persistent collection name an ID. *Value*<sup>J</sup> attaches a scalar value y to a given variable x. *Child*<sup>J</sup> states that the value identified by *childID* is immediately nested within the value identified by *parentID*. The *type* attribute records the type of the parent (array "a" or object "o") and determines the kind of nesting and the interpretation of the *key* attribute: if the parent is an array, *key* holds the position at which the child occurs; if the parent is an object, then *key* holds the name of the key whose associated value is the child.

Our modeling of the parent-child (immediate nesting) relationship between JSON values provides the type of value *only in conjunction with a navigation step where this value is a parent*, and the step leads to a child value of undetermined type. This modeling reflects the information one can glean statically (at query rewriting time, as opposed to query runtime) from JSON query languages in circulation today.

Recall that JSON data is semi-structured, i.e., it may lack a schema. Queries can, therefore, express navigation leading to values whose type cannot be determined statically if these values are not further navigated into. The type of a value can be inferred only from the type of navigation step into it.

**Example 4.5.1** (JSON Navigation). *If query navigation starts from a named JSON collection* "coll" and proceeds to the fifth element e therein, we can infer that "coll" is of array type, but we do not know the type of e. Only if the query specifies an ensuing lookup of the value v associated to key "k" in e can we infer e's type (object). However, absent further navigation steps, we cannot tell the type of the child value v.

Importantly, we assume that fields' values are homogenous in this work. The reason is that different systems have different semantics and behavior on handling queries that access fields with heterogeneous types (e.g., failing, warning, returning null, or missing (see Section 4.5.9)). We leave capturing such different semantics to future work.

Finally, relation  $Eq_J$  is intended to model value-based equality for JSON (id-based equality is captured directly as equality of the id attributes).

We capture the intended meaning of the  $\mathcal{VREI}$  relations via constraints that are inherent in the data model (i.e. they would hold if we actually stored JSON data as a  $\mathcal{VREI}$  instance). We illustrate a few of these below:

The fact that a persistent name uniquely refers to a value is expressed by the EGD (4.1) below. EGD (4.2) states that an object cannot have two distinct key-value pairs sharing the same key, or that an array cannot have two distinct elements at the same position. TGDs (4.3) and (4.4) state that value-based equality is symmetric, respectively transitive, and TGD (4.5) states that value-equal parents must have value-equal children for each parent-child navigation step. EGD (4.6) states that no two distinct scalar values may correspond to a given id.

$$\forall x \forall y \ CollectionName_J(x) \land CollectionName_J(y) \rightarrow x = y$$

$$(4.1)$$

$$\forall p \forall c_1 \forall c_2 \forall k \forall t \ Child_J(p, c_1, k, t) \land Child_J(p, c_2, k, t) \rightarrow c_1 = c_2$$

$$(4.2)$$

$$\forall x \forall y \ Eq_J(x, y) \quad \rightarrow \quad Eq_J(y, x) \tag{4.3}$$

$$\forall x \forall y \forall z \ Eq_J(x, y) \land Eq_J(y, z) \quad \rightarrow \quad Eq_J(x, z) \tag{4.4}$$

$$\forall p \forall p' \forall c \forall k \forall t \; Eq_J(p,p') \land Child_J(p,c,k,t) \quad \rightarrow$$

$$\exists c' \, Eq_J(c,c') \wedge Child_J(p',c',k,t) \tag{4.5}$$

$$\forall x \forall v_1 \forall v_2 \ Value(x, v_1) \land Value(x, v_2) \rightarrow v_1 = v_2 \tag{4.6}$$

**Encoding JSON Views and Queries.** We present in this subsection how we encode JSON queries and views using the  $\mathcal{VREI}$  schema. JSON queries (or views) can be nested:

```
V:
SELECT VALUE {"CAaddresses": (SELECT VALUE D
FROM P.Addresses AS D
WHERE D.state="CA")}
FROM persons AS P
Q:
SELECT D.zip, D.street
FROM persons AS P, P.Addresses AS D
WHERE D.state="CA"
```

Figure 4.4: JSON view V and query Q.

the SELECT clause (a.k.a. RETURN clause in some languages [4]) may (*i*) constructs fresh elements (i.e., JSON objects), (*ii*) refers to variables bound in the FROM clause, (*iii*) contains SELECT-FROM-WHERE<sup>2</sup> expressions (a.k.a. FWR expressions in some languages.)

We call a block *b*, a fragment of a nested JSON query delimited as follows: it has the "FROM" clause, "WHERE" clause (if present), and "SELECT" clause. If a JSON object is created in the SELECT clause, we refer to it hereafter as a return template for a block *b*, denoted as rt(b). The local variables of a block *b*, denoted as localDefVars(b), represent a collection of variables introduced in *b*. Moreover, free variables of *b*, denoted as freeVars(b), represent variables mentioned in *b* but introduced in its ancestors. We call a collection of variables in a block *b* visible, denoted as visibleVars(b) if other blocks use them.

In the example below, we show how we encode a JSON query relationally using the  $\mathcal{VREI}$  schema, and translate a JSON view into additional relational integrity constraints, capturing the correspondence between the view input and output, with the knowledge of each block information described above.

**Example 4.5.2.** (Encoding JSON View and Query). Consider the JSON query Q and view V (using AsterixDB's SQL++ syntax) in Figure 4.4; the query Q asks to find the zip code and street name of "CA" addresses for each person. The nested view V constructs a JSON object that has a list of "CA" addresses for each person. The view V consists of two blocks. The outermost

<sup>&</sup>lt;sup>2</sup>The fragment of the supported JSON language in this work includes select-project-join queries with nested blocks, JSON object navigation, array unnest and object construction.

SELECT-FROM expression corresponds to the root block; call it  $V_0$ . The nested SELECT-FROM-WHERE block in the SELECT clause is modeled as a child block of  $V_0$ ; call it  $V_{00}$ . Notice that finding the rewriting of Q using V requires reasoning about the nested blocks and the construction of a new JSON object in the SELECT clause of V. The view V cannot be directly matched against Q.

**Encoding of View** V as a Set of Constraints. The view V will be partitioned into two blocks:  $V_0$  and  $V_{00}$ . For each block b, we capture rt(b), localDefVars(b), freeVars(b), and visibleVars(b). For example, for the block  $V_0$ , we have:

 $rt(V_0) = \{\{\text{``CAaddresses'':}\}\}$  $localDefVars(V_0) = \{P\}$  $freeVars(V_0) = \emptyset$  $visibleVars(V_0) = \{P\}$ 

Notice that  $freeVars(V_0)$  is empty since  $V_0$  is the root block. However,  $visibleVars(V_0) = \{P\}$  since P is visiable to the block  $V_{00}$ . In the same fashion, we capture the following information for the block  $V_{00}$ :

$$rt(V_{00}) = \emptyset$$
$$localDefVars(V_{00}) = \{D\}$$
$$freeVars(V_{00}) = \{P\}$$
$$visibleVars(V_{00}) = \emptyset$$

 $rt(V_{00})$  is empty since there is no object creation in the SELECT clause in  $V_{00}$ .

Now, given the information above for each block b, b will be encoded as a set of constraints. First, we encode the root block  $V_0$ , the following constraints are introduced for  $V_0$ :

$$\forall P \ persons(P) \to V_0 ExtrJ(P) \tag{4.7}$$

$$\forall P V_0 ExtrJ(P) \rightarrow \exists d_0 \exists d_1 V_0 CreateJ(d_0, d_1) \land V_0 SkJ0(d_0, P) \land V_0 SkJ1(d_1, P)$$
(4.8)

$$\forall d_0 \forall d_1 V_0 \ CreateJ(d_0, d_1) \rightarrow V(d_0) \land Child_J(d_0, d_1, ``CAaddresses", ``o")$$

$$(4.9)$$

The TGD (4.7) extracts the visible variable P to be accessed later by the constraint of the child block  $V_{00}$ . To enable rewriting, we would like the view V head exposes the ID of the constructed JSON object in the SELECT clause  $(rt(V_0))$ . This can be achieved by introducing the TGDs (4.8) and (4.9). The TGD (4.8) creates two IDs:  $d_0$  and  $d_1$ , the former represents the ID of the constructed JSON object, and the latter represents the ID of the array "CAaddresses", which is immediately nested within the parent ID  $d_0$ . These IDs are created using the Skolem functions, which are modeled relationally using the relations  $V_0SkJ0$  and  $V_0SkJ1$ . The variable P in both relations corresponds to arguments of the Skolem call. Furthermore, we need to express the fact that these relations model function and injective functions. We do this by means of key constraints, basically stating that:

$$\forall d_0^1 \forall d_0^2 \forall P \ V_0 SkJ0(d_0^1, P) \land V_0 SkJ0(d_0^2, P) \rightarrow d_0^1 = d_0^2 \ (function)$$
  
$$\forall d_0 \forall P_1 \forall P_2 \ V_0 SkJ0(d_0, P_1) \land V_0 SkJ0(d_0, P_2) \rightarrow P_1 = P_2 \ (injective)$$

*Now, we encode the nested block*  $V_{00}$  *by introducing the following constraint:* 

$$V_0ExtrJ(P) \land V_0SkJ1(d_1, P) \land Child_J(P, A, ``addresses", ``o") \land Child_J(A, D, ``*", ``a") \land$$
$$Child_J(D, S, ``state", ``o") \land Value(S, ``CA") \rightarrow$$
$$Child_J(d_1, D, ``*", ``a")$$

The nested block  $V_{00}$  is created within the return template  $rt(V_0)$  of the root block  $V_0$ . The result of the nested block  $V_{00}$  is an array of "CA" addresses for each person P. The ID of the array is  $d_1$ , created by the Skolem function  $V_0SkJ1(d_1,P)$ . The constraint encodes the fact that each element in  $d_1$  is represented by the variable D obtained from unnesting the "addresses" array and applying the condition (state="CA"), as shown in the premise of the constraint. To encode the unnest operator, we use the Child<sub>J</sub> relation, where we specify the key attribute as \*. For example, the relation Child<sub>J</sub>( $d_1$ ,D,"\*","a") indicates that  $d_1$  is an array and D binds to each element in  $d_1$ .

**Encoding of Query** Q. The following is the relational encoding of the query Q using the VREJ schema:

$$\begin{aligned} Q(Z,ST) &: -persons(P), Child_J(P,A, ``addresses", "o"), \\ Child_J(A,D, ``*", ``a"), Child_J(D,S, ``state", ``o"), \\ Value(S, ``CA"), Child_J(D,ST, ``street", ``o"), Child_J(D,Z, ``zip", ``o"); \end{aligned}$$

Taking as input the query Q, set of the view V constraints, and constraints of  $\mathcal{VREI}$  relations, the constraints-based rewriting algorithm (see Chapter 3) finds the following equivalent relational V-based rewriting of Q:

$$\begin{split} R(Z,ST) &: -V(d_0), Child_J(d_0, d_1, ``CAaddresses", ``o"), \\ Child_J(d_1, D, ``*", ``a"), Child_J(D, ST, ``street", ``o"), Child_J(D, Z, ``zip", ``o"); \end{split}$$

For brevity, we omit introducing the encoding of the unnest operator hereafter.

### 4.5.2 Key-Value Model

Our interpretation of the key-value pairs model is compatible with many current systems, in particular *Redis*, supported by ESTOCADA. Calling a *map* a set of key-value pairs, the store accommodates a set of persistently named maps (called *outer* maps). Within each outer map, the value associated to a key may be either a map (called an *inner* map), or a scalar value. In the case of an *inner* map, the value associated to a key is a scalar value.

Given the analogy between key-value and JSON maps, we model the former similarly to the latter, as instances of the relational schema  $\mathcal{VREK}$ , consisting of the relations:  $Map_{KV}(name,mapId)$ ,  $Child_{KV}(parentID,childID,key,type)$  and  $Eq_{KV}(x,y)$ . Here,  $Map_{KV}$ 

$\begin{tabular}{ll} \hline Connection_G(sID, dID, lID) \end{tabular}$		
$Label_G(lID, name)$		
$Property_G(lID, key, vID)$		
$Kind_G(lID, type)$		
Value(x, y)		

**Table 4.3**: Snippet of  $\mathcal{VREG}$  schema.

models the association between a persistent name and (the id of) an outer map.  $Child_{KV}$  reflects the immediate nesting relationship between a map (the parent) and a value associated to one of its keys (the child). The *type* attribute tells us whether the parent map is an outer or an inner map (these are treated asymmetrically in some systems). The  $Eq_{KV}$  relation models value-based equality, analogously to  $Eq_J$  for JSON.

The intended semantics of these relations is enforced by similar constraints to the JSON model, e.g., in a map, there is only one value for a key

$$\forall p \forall c_1 \forall c_2 \forall k \forall t \ Child_{KV}(p, c_1, k, t), \ Child_{KV}(p, c_2, k, t) \rightarrow c_1 = c_2$$

persistent map names are unique

$$\forall n \forall x \forall y \ Map_{KV}(n,x), \ Map_{KV}(n,y) \rightarrow x = y$$

#### 4.5.3 Graph Model

We discuss in this subsection our relational encoding of property graph queries and views using the schema  $\mathcal{VREG}$  (Virtual Relational Encoding of Graph) in Table 4.3. The relation *Connection*<sub>G</sub> states that there is a relationship between a source node *sID* and a destination node *dID* with the label ID *lID*. Every label in a graph has a name, and we capture that using the *Label*<sub>G</sub> relation. In addition, a label in a graph can be an "edge" (relationship) or a "node", and the type of a label is modeled using the *Kind*<sub>G</sub> relation, where *lID* is the label ID, and *type* indicates whether *lID* is an edge or a node. Nodes and relationships can have properties (key-value pairs).

```
V:
MATCH (po:Post) <-[:REPLY-OF]-(m:Message)-[:HAS-CREATOR]->
(p:Person {firstName: "Amelie"})
CREATE (po) <-[:REPLY-OF-V]-(:Message_V
{creationDate:m.creationDate})
-[:HAS-CREATOR-V]->(p)
Q:
MATCH (:Person {firstName: "Amelie"}) <-[:HAS_CREATOR]-
(m:Message)-[:REPLY_OF]->(p:Post)
MATCH (p)-[:HAS_CREATOR]->(c)
RETURN
m.creationDate AS mCreationDate,
p.postId AS pPostId,
c.personId AS originalPostAuthorId,
c.lastName AS originalPostAuthorLastName
```

Figure 4.5: Graph view V and query Q.

Property attached to a label *IID* is encoded using the  $Property_G$  relation, where vID is the value associated with the key *key*.

We currently support a fragment of Cypher graph-based language. This fragment includes (*i*) pattern-matching (MATCH), (*ii*) WHERE clause, containing simple predicates, and (*ii*) construction of a new node and a relationship between nodes. We note that we currently do not support the encoding of "Variable-length pattern matching" in the form:  $(n_1)$ -[\*] $\rightarrow$ ( $n_2$ ). This kind of matching can not be expressed directly in a conjunctive query form. In addition, we do not support filtering on patterns in the WHERE clause. We leave the investigation of addressing these limitations to future work.

**Example 4.5.3** (Encoding Graph View and Query). Consider the Gypher query Q and view V in Figure 4.5; the query Q asks to find the IDs of all posts that "Amelie" replies to, the information of the creators of these posts, and the creation dates of "Amelie"'s replies. The view V creates a new node "Message – V" that stores the creation date of "Amelie"'s reply "m" to a post "po". In addition, the view creates the "REPLY-OF-V" relationship that connects the new node "Message – V" with the original post "po" and the "HAS-CREATOR-V" relationship, which indicates that "Amelie" is the creator of the "Message – V" message. <sup>3</sup>

<sup>&</sup>lt;sup>3</sup>We note that the query Q is a simplified version of the query "interactive-short-2.cypher" in idbc benchmark.

**Encoding of View** V as a Constraint. The view V is translated into the following TGD using the set of relations in VREG schema:

$$\begin{split} Label_G(po, ``Post"), Label_G(m, ``Message"), Label_G(id0, ``REPLY - OF"), \\ Connection_G(m, po, id0), Label_G(p, ``Person"), Property_G(p, ``firstName", vID0), \\ Label_G(id1, ``HAS - CREATOR"), Connection_G(m, p, id1), Value(vId0, ``Amelie"), \\ Property_G(m, ``creationDate", vID1) \rightarrow \\ Label_G(id2, ``Message - V"), Property_G(id2, ``creationDate", vID1), \\ Label_G(id3, ``REPLY - OF - V"), Connection_G(id2, po, id3), \\ Label_G(id4, ``HAS - CREATOR - V"), Connection_G(id2, p, id4) \end{split}$$

**Encoding of Query** Q. The following conjunctive query is the relational encoding of the query Q:

 $\begin{aligned} Q(vID1, vID2, vID2, vID4) &: -Label_G(id0, ``Person"), Property_G(id0, ``firstName", vId0), \\ Value(vId0, ``Amelie"), Label_G(m, ``Message"), Label_G(id1, ``HAS - CREATOR"), \\ Connection_G(m, id0, id1), Label_G(p, ``Post"), Label_G(id2, ``REPLY - OF"), \end{aligned}$ 

 $\begin{aligned} &Connection_G(m, p, id2), Label_G(id3, ``HAS - CREATOR"), Connection_G(p, c, id3), \\ &Property_G(m, ``creationDate", vID1), Property_G(p, ``postId", vID2), \\ &Property_G(c, ``personId", vID3), Property_G(c, ``lastName", vID4); \end{aligned}$ 

*The query Q is equivalent to the V-based relational rewriting R:* 

 $R < vID1, vID2, vID3, vID4 >: -Property_G(p, "postId", vID2),$   $Property_G(c, "personId", vID3), Property_G(c, "firstName", vID0),$   $Property_G(c, "lastName", vID4), Property_G(id4, "creationDate", vID1),$   $Connection_G(p, c, id3), Connection_G(id4, p, id5), Connection_G(id4, id0, id6),$   $Label_G(id3, "HAS - CREATOR"), Label_G(id4, "Message - V"),$   $Label_G(id5, "REPLY - OF - V"), Label_G(id6, "HAS - CREATOR - V");$ 

Root(x)	Elem(x)
$Child_X(x,y)$	DescOrSelf(x,y)
Attrib(x,n,v)	Tag(x,n,v)

**Table 4.4**: Snippet of  $\mathcal{VREX}$  schema.

#### 4.5.4 XML Model

Query reformulation for XML has already been reduced in prior work to a purely relational setting using constraints. We refer the reader to [65, 64] for more details. At high-level, an XML document was represented as a *virtual* instance of the relational schema  $\mathcal{VREX}$  consisting of the relations: {*Root*, *Elem*, *Child*<sub>X</sub>, *DescOrSelf*, *Tag*, *Attrib*, *Id*, *Text*} (their schemas are shown in Table 4.4).

The intended meaning of the relations in  $\mathcal{VREX}$  reflects the fact that XML data is a tagged tree. The unary predicate *Root* denotes the root element of the XML document, and the unary relation *Elem* is the set of all elements. *Child<sub>X</sub>* and *DescOrSelf* are subsets of *Elem* × *Elem* and they say that their second component is a child, respectively a descendant of the first component.  $Tag \subseteq Elem \times string$  associates the tag in the second component to the element in the first. *Attrib*  $\subseteq Elem \times string \times string$  gives the element, attribute name and attribute value in its first, second, respectively third component.  $Id \subseteq string \times Elem$  associates the element in the second component to a string attribute in the first that uniquely identifies it (if DTD-specified ID-type attributes exist, their values can be used for this).  $Text \subseteq Elem \times string$  associates to the element in its first component the string in its second component.

[65] shows that some of the intended meaning of schema  $\mathcal{VREX}$  is captured by a set *TIX* (True In XML) of constraints expressible as TGDs and EGDs, in some cases extended with disjunction. We list below the most interesting ones:

(base)  $\forall x \forall y Child_X(x,y) \rightarrow DescOrSelf(x,y)$ (trans)  $\forall x \forall y \forall z \ DescOrSelf(x,y) \wedge DescOrSelf(y,z) \rightarrow DescOrSelf(x,z)$ 

(refl) 
$$\forall x \ Elem(x) \rightarrow Desc Or Self(x, x)$$
  
(someTag)  $\forall x \ Elem(x) \rightarrow \exists t Tag(x, t)$   
(oneTag)  $\forall x \forall t_1 \forall t_2 \ Tag(x, t_1) \land Tag(x, t_2) \rightarrow t_1 = t_2$   
(keyID)  $\forall x \forall t_1 \forall t_2 \ Id(s, e_1) \land Id(s, e_2) \rightarrow t_1 = t_2$   
(oneAttrib)  $\forall x \forall n \forall v_1 \forall v_2 \ Attrib(x, n, v_1) \land Attrib(x, n, v_2) \rightarrow v_1 = v_2$   
(oneLoop)  $Desc Or Self(x, y) \land Desc Or Self(y, x) \rightarrow y = x$   
(oneParent)  $\forall x \forall y \forall z \ Child_X(x, z) \land Child_X(y, z) \rightarrow x = y$   
(oneRoot)  $\forall x \forall y \ Root(x) \land Root(y) \rightarrow x = y$   
(topRoot)  $\forall x \forall y \ Desc Or Self(x, y) \land Root(y) \rightarrow Root(x)$ 

Intuitively, (oneRoot) states that the root of the XML tree is unique, and by (topRoot) has no ancestors beside itself. (someTag) and (oneTag) say that every element has precisely one tag.

The treeness of the data model is (partially) enforced by such constraints as (oneParent) (every element has at most one parent), (noLoop) (only trivial cycles are allowed). Observe that (base), (trans), (refl) above only guarantee that *DescOrSelf* contains its intended interpretation, namely the reflexive, transitive closure of the *Child* relation.

There are many models satisfying these constraints, in which *DescOrSelf* is interpreted as a proper superset of its intended interpretation, and it is well-known that we have no way of ruling them out using first-order constraints because transitive closure is not first-order definable. Similarly, the "treeness" property of the *Child*<sub>X</sub> relation cannot be fully captured in first-order logic.

**Example 4.5.4** (Relational Encoding of XML Tree Navigation). Consider an XPath expression Q defined as //a, which returns the set of nodes reachable by navigating to a descendant of the root and from there to a child tagged "a". Assume also that we materialize the view v defined as //.//a, i.e. which contains all "a"-children of descendants of descendants of the root. We can encode q, v as conjunctive queries Q = enc(q), V = enc(v) over schema VREX.

$$\begin{aligned} Q(y) &: -Root(r), DescOrSelf(r, x), Child(x, y), Tag(y, "a") \\ V(y) &: -Root(r), DescOrSelf(r, u), DescOrSelf(u, x), Child(x, y), Tag(y, "a") \end{aligned}$$

It is easy to see that the decoding operation, which takes a relational query over VREX back to XQuery/XPath syntax, is straightforward.

Clearly, under arbitrary interpretations of the DescOrSel f relation, the two encodings are not equivalent, and Q cannot be reformulated to use V. But on intended interpretations, the DescOrSel f relation is transitive and reflexive, therefore v itself is equivalent to q and

$$R(y):-V(y)$$

is a relatioanl reformulation of Q using V.

#### 4.5.5 Relational Model

It is well known that the relational data model endowed with key, uniqueness and foreign key constraints is captured by our pivot model (see Chapter 3): key/uniqueness constraints are expressible by EGDs, and foreign key constraints by TGDs.

### 4.5.6 Binding Patterns

We have seen above a natural way to model sets of key-value pairs using a relation. To simplify the discussion, we abstract from the *parentId* and *type* attributes of relation  $Child_{KV}$  above, focusing on the binary relationship between keys and values:

Note that typical key-values store APIs require that values can be looked up only given their key, but not conversely. If we do not capture this limitation, the rewriting algorithm may produce rewritings that correspond to no executable plan. For instance, consider a rewriting of the form:

$$R(v):-KV(k,v).$$

*R* corresponds to no legal plan given the access limitation of KV, because *R* requires the direct extraction of all values stored in the store, without looking them up by key.

This setting involving relations with limited lookup access is well-known in the literature and is modeled via the concept of relations adorned with *binding patterns* [123]. Binding patterns are strings over the alphabet  $\{i, o\}$ . If position  $p^{th}$  in the pattern holds character *i*, this signals that the  $p^{th}$  attribute must be provided as input in a lookup. An *o* at position *p* signals that the  $p^{th}$  attribute can be extracted by the lookup.

In the key-value store modeling example, one would use  $KS^{io}$  to specify the lookup limitation, and the candidate rewriting would turn to a conjunctive query over binding-pattern-annotated atoms:

$$R'(v):-KV^{io}(k,v).$$

The binding pattern now carries sufficient information to determine that R' requires k as input in order to look up v.

In a relational setting, query rewriting when access to the views is limited by binding patterns has been studied for conjunctive queries and views [74, 115], yet complete rewriting under both integrity constraints and binding patterns was not considered until [60]. [60] shows how to encode binding patterns using TGD constraints, which fit nicely into our pivot model. The idea is to introduce a unary relation, say D(x) to state that x is accessible, and for each binding pattern a TGD stating that when all required input attributes of a relation are accessible, then the output attributes are accessible as well. This allows the chase with such TGDs to determine which attributes of a rewriting are accessible.

**Example 4.5.5** (Binding Pattern Constraints). *This example shows a query* Q(y,z) : -R(x,y,z) *that can be rendered executable only after exploiting an integrity constraint and a binding pattern.*
Let us consider a store S that imposes a binding access constraint on a relation R(x, y, z), which requires that y and z can be extracted (projected) only when x is given. Given this constraint, Q is not executable as such. Moreover, consider that we have a constraint that states an inclusion, which guarantees that all values of R's first column (x) are among those in the relation S's first column.

$$\forall x \forall y \forall z \ R(x, y, z) \to S(x)$$

In order to make the query executable, we first introduce a view for each access pattern on a given relation:

$$orall x orall y orall z R(x, y, z) o R^{ioo}(x, y, z)$$
  
 $orall x S(x) o S^o(x)$ 

The above constraints state that x is required as input to project y and z from the relation R, and x is always accessible (can be extracted) from the relation S, respectively. Then, we need to introduce extractability constraints for access pattern modeling:

$$\forall x \ S^o(x) \to D(x) \tag{4.10}$$

$$\forall x \forall y \forall z \ R^{ioo}(x, y, z) \land D(x) \to D(y) \land D(z)$$
(4.11)

*The extractability constraint 4.11 states that when x is accessible, then the attributes y and z are accessible as well.* 

The access pattern modeling above reduces the problem from rewriting under binding patterns to rewriting only under constraints. This means that if we have an algorithm for rewriting under constraints, we can "trick" it into rewriting under binding patterns even though it is unaware of them and does not treat them as first-class citizens. As a result, the found rewriting (the executable version of Q) is:

$$R'(y,z) - : R^{ioo}(x,y,z), S^{o}(x)$$

which extracts all x values from the relation S, and uses these values as a look-up key to extract y and z from the relation R.

#### 4.5.7 Equality and Multiple Treatment of Nulls

An important issue raised by the polystore context is the fact that the notion of null values is treated differently across the spectrum of data models/stores, which in turn has implications on such fundamental primitives as equality and hence equi-joins, etc. Even in the single-model relational scenario, the classical theory of conjunctive queries, constraints, and view-based rewritings defines this real-life problem away by focusing on idealized relations without null values.

Direct application of classical theory would result in potentially unsound reformulation algorithms, because they would ignore the fact that for instance a MongoDB query joining <sup>4</sup> JSON data has a different semantics of equality from a SQL query joining two relations. For example, in MongoDB, join variables can match null values, but this is not the case in SQL. Such null-agnostic algorithms would generate a spurious reformulation of the query using the view.

To mitigate this issue, our current idea is to model each equality flavor by its own relational predicate, capturing *as much as possible of their intended semantics using constraints*. We use constraints to capture relationships between various equality flavors. For instance, the fact that whenever two values are equal according to flavor  $Eq_{S1}$  (e.g., Store  $S_1$ ) they are also equal according to flavor  $Eq_{S2}$  (e.g., Store  $S_2$ ), but only if they are both non-null could be captured as follows:

$$\forall x \forall y \ Eq_{S1}(x, y) \land \text{notnull}(x) \land \text{notnull}(y) \to Eq_{S2}(x, y) \tag{4.12}$$

$$\forall x \forall y \ Eq_{S2}(x, y) \to Eq_{S1}(x, y) \land \text{notnull}(x) \land \text{notnull}(y)$$
(4.13)

<sup>&</sup>lt;sup>4</sup>Whenever we mention join, we refer to equi-join.

We introduce an isnull predicate, as well as a notnull predicate, relating them to equality. To correctly model the fact that null and notnull are mutually exclusive, we add denial constraints (see Section 4.5.9) such as :

$$orall x ext{ isnull}(x) \wedge ext{notnull}(x) o ext{false}$$

Example 4.5.6 (Null Treatment Accross Different Equality Flavors). Consider the query

$$Q(y,z): -R(x_1,y), S(x_2,z), Eq_{S2}(x_1,x_2)$$

which joins R and S relations (in the store  $S_2$ ) on  $x_1$  and  $x_2$  using the equality flavor  $Eq_{S2}$ , where join variables cannot match null values (the standard SQL semantics).

Now, suppose we have the following two views, which are materialized in the store  $S_1$ , where join variables can match null values (i.e., null = null is evaluated to true):

$$V_1^{S_1}(x_1, y) : -R(x_1, y)$$
$$V_2^{S_1}(x_2, z) : -S(x_2, z)$$

Taking as inputs Q,  $V_1^{S_1}$ ,  $V_2^{S_1}$ , and the set of constraints 4.12 and 4.13, the relational rewriting algorithm under integrity constraints will find the following rewriting:

$$R(y,z):-V_1^{S_1}(x_1,y),V_2^{S_1}(x_2,z),Eq_{S_1}(x_1,x_2),\text{notnull}(x_1),\text{notnull}(x_2)$$

which joins  $V_1^{S_1}$  and  $V_1^{S_1}$  (in the store  $S_1$ ) using the equality flavor  $Eq_{S_1}$  and filtering out the null values of  $x_1$  and  $x_2$ .

The rewriting R is equivalent to Q under null-aware semantics. Now, suppose that we do not appropriately capture different null-semantics across stores, in other words, we treat equality similarly across stores. For example, the constraint  $Eq_{S2}(x,y) \rightarrow Eq_{S1}(x,y)$  indicates that the semantic of equality in S<sub>1</sub> is the same as the one in S<sub>2</sub>. This will result in the following rewriting:

$$R'(y,z):-V_1^{S_1}(x_1,y),V_2^{S_1}(x_2,z),Eq_{S_1}(x_1,x_2)$$

which is not equivalent to Q under null-aware semantic. The reason is that join variables can match null values when using the equality flavor  $Eq_{S1}$ , which is different from the equality flavor used in the original query.

We use isnull and notnull predicates not only to model equality constraints but also to translate "is null" and "is not null" conditions in a query. For example, consider the SQL WHERE clause: "r.b is null AND s.b is null", it will be translated to :

$$R(b_1, y), S(b_2, x), \text{isnull}(b_1), \text{isnull}(b_2)$$

Given a rewriting with isnull and notnull predicates, they will be decoded to "is null" and "is not null" conditions, respectively.

In addition to supporting null value, JSON stores have a notion of missing data value [4, 11], which is produced by attempts to access non-existent fields or out-of-bound array elements. We leave the investigation of how far this constraint-based approach can be used to capture missing semantics across these stores to future work.

#### 4.5.8 Comparison and Arithmetic Operators

To maintain extensibility, we adopt a uniform way to incorporate any additional language primitives by treating them as *user-defined functions with worst-case black-box semantics*, attempting to "make the box more transparent" by adding constraints that capture some of their intended semantics.

**Comparison Operators.** We use the relations Lt(x,y), Gt(x,y), Lte(x,y), and Gte(x,y) to encode "*x* is less than *y*", "*x* is greator than *y*", "*x* is less than or equal *y*", "*x* is greator than or equal *y*" comparison operators, respectively. We capture capture some of their properties via

constraints as follows:

$$\forall x \forall y \forall z \ Lt(x,y) \land Lt(y,z) \to Lt(x,z) \tag{4.14}$$

$$\forall x \forall y \forall z \ Gt(x, y) \land Gt(y, z) \to Gt(x, z)$$
(4.15)

$$\forall x \forall y \forall z \ Lte(x, y) \land Lte(y, z) \to Lte(x, z)$$
(4.16)

$$\forall x \forall y \forall z \ Gte(x, y) \land Gte(y, z) \to Gte(x, z)$$
(4.17)

$$\forall x \forall y \ Lt(x, y) \to Gt(y, x) \tag{4.18}$$

$$\forall x \forall y \ Gt(x, y) \to Lt(y, x) \tag{4.19}$$

The constraints from (4.14) to (4.17) capture the transitive property, and the constraints from (4.18) to 4.18) capture the reversal property.

Arithmetic Operators. The arithmetic operators such as addition operator would be modeled as a relation  $add(arg_1, arg_2, res)$  with intended meaning  $res = arg_1 + arg_2$ , which one could partially capture with constraints stating that add is a functional relation:

$$\forall x \forall y \forall res_1 \forall res_2 \ add(x, y, res_1) \land add(x, y, res_2) \rightarrow res_1 = res_2$$

that is commutative, associative, and has zero:

$$(\text{comm}) \quad \forall x \forall y \forall res_1 \ add(x, y, res_1) \rightarrow add(y, x, res_1)$$

$$(\text{asso}) \quad \forall x \forall y \forall res_1 \forall z \forall res_3 \ add(x, y, res_1) \land add(res_1, z, res_3) \rightarrow$$

$$\exists res_4 \ add(y, z, res_4) \land add(x, res_4, res_3)$$

$$(\text{identity}) \quad \forall x \forall res \ add(x, 0, res) \rightarrow res = x$$

#### 4.5.9 Denial Constraints

A natural way of handling mutual exclusion of domains in the various models considered is by extending our pivot model to support *denial constraints*. They are constraints whose premise  $\forall x \forall y \ Eq(x,y) \land Lt(x,y) \rightarrow \text{false} \\ \forall x \forall y \ Eq(x,y) \land Gt(x,y) \rightarrow \text{false} \\ \forall x \forall y \ Lt(x,y) \land Gt(x,y) \rightarrow \text{false} \\ \forall x \forall y \ Lte(x,y) \land Gt(x,y) \rightarrow \text{false} \\ \forall x \forall y \ Lte(x,y) \land Lt(x,y) \rightarrow \text{false} \\ \forall x \forall y \ Gt(x,y) \land Lt(y,x) \rightarrow \text{false} \\ \forall x \forall y \ Gt(x,y) \land Gt(y,x) \rightarrow \text{false} \\ \forall x \forall y \ Gt(x,y) \land Gt(y,x) \rightarrow \text{false} \\ \forall x \text{notnull}(x) \land null(x) \rightarrow \text{false} \\ \end{cases}$ 

Figure 4.6: Snippet of supported denail constraints.

has the same form as that of TGDs and EGDs, but whose conclusion contains simply the boolean value false.

**Example 4.5.7** (Denail Constraints). Let us consider the relations Gt(x,y) and Lt(x,y), which we use to encode that x is greator than y, and x is less than y, respectively. Then to state that x cannot be both greator than y and less than y, we would use the denial constraint  $\forall x, y \ Gt(x,y) \land$  $Lt(x,y) \rightarrow false$ . Chasing with this denial constraint, a query Q that attempts to specify a condition, where x is greator than y and x is less than y, would add the atom false to its body, thus signaling Q's unsatisfiability (the query returns an empty answer).

Figure 4.6 illustrates a snippet of denial constraints that ESTOCADA currently supports.

# **4.6** Encoding *QBT<sup>XM</sup>* Queries into the Pivot Language

The purpose of the pivot language is to reduce the VBQR problem to a single-model setting. The pivot model enables us to represent relationally queries expressed in the various languages supported in our system (recall Table 4.1), and which can be combined into a single  $QBT^{XM}$  query. As shown in Figure 4.1, an incoming query Q is *encoded* as a relational conjunctive enc(Q) over the relational encoding of the datasets it refers to (with extensions such as aggregates,

FOR AJ	: { SELECT	M.PATIENTID AS patientID,
		A.ADMISSIONLOC AS admissionLoc,
		A.ADMISSIONTIME <b>AS</b> admissionTime,
		P.DRUG <b>AS</b> drug
	FROM	LABITEM L, MIMIC M, M.ADMISSIONS A,
		A.LABEVENTS LE, A.NOTEEVENTS NE, A.PRESCRIPTIONS P
	WHERE	L.ITEMID=LE.LABITEMID <b>AND</b>
		L.CATEGORY='blood' AND
		L.FLAG = 'abnormal' AND
		P.DRUGTYPE=`additive' AND
		<pre>contains(NE.REPORT, `coronary artery')}</pre>
RETURN	patientID	, admissionLoc, admissionTime, drug

**Figure 4.7**: Motivating scenario  $QBT^{XM}$  query  $Q_1$ .

```
MIMIC(M),
Child<sub>J</sub>(M,PID,"PATIENTID","o"),
Child<sub>J</sub>(M,A,"ADMISSIONS","o"),
Child<sub>J</sub>(A,AID,"ADMISSIONID","o"),
Child<sub>J</sub>(A,ALOC,"ADMISSIONLOC","o"),
Child<sub>J</sub>(A,ATIME,"ADMISSIONTIME","o")->
V<sub>2</sub>(PID,AID,ALOC,ATIME);
```

**Figure 4.8**: Relational encoding of  $QBT^{XM}$  view  $V_2$  defined in Figure 4.3.

user-defined functions, and nested queries). Figure 4.7 shows the  $QBT^{XM}$  query  $Q_1$  of the motivating scenario, and its relational encoding  $enc(Q_1)$  appears in Appendix A.4.

# **4.7** Encoding *QBT<sup>XM</sup>* Views as Constraints

We translate each view definition V expressed in  $QBT^{XM}$  into additional relational integrity constraints enc(V) showing how the view inputs are related to its output. Figure 4.8 illustrates the relational encoding of  $QBT^{XM}$  view  $V_2$  from Section 4.4, and constraints resulting from  $V_1$ appears in Appendix A.3. We note that  $QBT^{XM}$  view definitions do not have aggregation. We leave the investigation of extending the rewriting algorithm to reason about views involving aggregations to future work.

# **4.8** From Rewritings to Integration Plans

We translate each query rewriting into a *logical plan* specifying (*i*) the (native) query to be evaluated within each store, and (*ii*) the remaining logical operations to be executed within the integration engine. The translation first decodes  $RW_r$  into  $QBT^{XM}$  syntax. Based on the heuristic that the store where a view resides is more efficient than the middleware, and thus it should be preferred for all the operations it can apply, decoding tries to delegated to the stores as much as possible.

To that end, the decoding phase first partitions each rewriting  $RW_r$  into view-level subqueries, which are sets of atoms referring to the virtual relations of a *same view*. If a group of view-level subqueries pertains to the same store (we record the store reference where each view is stored in a catalog) and if the store supports joins, we translate the group to a single query to be pushed to the store.

```
\begin{split} RWQ_1 <& \text{PID}, \text{ALOC}, \text{ATIME}, \text{DRUG} >: -\\ V_1(d_1), \\ Child_J(d_1, \text{PID}, "PATIENTID", "o"), \\ Child_J(d_1, \text{AID}, "ADMISSIONID", "o"), \\ Child_J(d_1, \text{REPORT}, "REPORT", "o"), \\ Value(report, "contains-coronary artery"), \\ V_2(\text{PID}, \text{AID}, \text{ALOC}, \text{ATIME}), \\ V_3(d_2), \\ Child_J(d_2, \text{PID}, "PATIENTID", "o"), \\ Child_J(d_2, \text{AID}, "ADMISSIONID", "o"), \\ Child_J(A, P, "PRESCRIPTIONS", "o"), \\ Child_J(P, DRUG, "DRUG", "o"), \\ Child_J(P, DRUGTYPE, "DRUGTYPE", "o"), \\ Value(DRUGTYPE, "additive"); \end{split}
```

**Figure 4.9**: Rewriting  $RWQ_1$  of  $QBT^{XM}$  query  $Q_1$ .

**Example 4.8.1** (Delegation-Aware Decoding). Consider the rewriting  $RWQ_1$  of  $QBT^{XM}$  query  $Q_1$  shown in Figure 4.9. First, we delimit the view-wide subqueries (delimited by empty lines in the figure), calling them  $RWQ_1^1$ ,  $RWQ_1^2$  and  $RWQ_1^3$  in order from the top. The subquery heads contain variables from the head of  $RWQ_1$  and join variables shared with other subqueries. For



Figure 4.10: Integration plan of the motivating scenario using Tatooine hybrid engine.

example, the head of  $RWQ_1^2$  contains the variables ALOC and ATIME (in the head of  $RWQ_1$ ), and also PID, AID, needed to join with  $RWQ_1^1$ , and  $RWQ_1^3$ . These relational subqueries are then decoded to the native syntax of their respective stores, each constituting a block of the resulting  $QBT^{XM}$  rewriting dec( $RWQ_1$ ) (shown in Appendix A.4).

ESTOCADA's plan generator next translates the decoded  $QBT^{XM}$  rewriting to a logical plan that pushes leaf blocks to their native store, applying last-step operators on the results. The integration plan for  $RWQ_1$  is shown in Figure 4.10. We note that when using ESTOCADA's polystore engine Tatooine [45], the results of sources' subqueries are translated into Tatooine's internal nested-valued tuple-based model (nested relation [57]).

#### Algorithm 1: Delegation-aware decoding *QBT<sup>XM</sup>*.

```
Input :CQ rw(\bar{x}) : -a_1 \wedge \cdots \wedge a_n, Catalog c
   Output : Delegation-Aware Decoded Rewriting into QBT<sup>XM</sup>
 1 cqs \leftarrow split rw atoms by store reference
2 foreach cq_1 \in cqs, cq_2 \in cqs do
       if cq_1 \neq cq_2 and cq_1, cq_2 share variables and cq_1, cq_2 are in the same store s and
 3
         s supports join then
            remove cq_1 from cqs;
 4
            remove cq_2 from cq_s;
 5
           add cq_1 \cup cq_2 to cqs;
 6
       end
 7
8 end
9 returnClause \leftarrow 0;
10 foreach x \in \bar{x} do
       add x to returnClause;
11
12 end
13 where Clause \leftarrow \emptyset:
14 foreach (cq_1, s_1) \in cqs, (cq_2, s_2) \in cqs, do
       if head(cq_1) share same variable z in head(cq_2) then
15
            (cq'_2, s_2) \leftarrow rename z in head(cq_2) and body(cq_2) to z_i;
16
            remove (cq_2, s_2) from cqs;
17
            add (cq'_2, s_2) to cqs;
18
            add z = z_i to where Clause;
19
       end
20
21 end
22 forBlocks \leftarrow \emptyset;
23 foreach (cq, s) \in cqs do
       add decode(cq, s) to blocks;
24
25 end
26 decodedRW \leftarrow concat(forBlocks, whereClause, returnClause)
27 return plan;
```

## **4.9 PACB Optimization and Extension**

We detail below just enough of the PACB algorithm's inner working to explain our optimization. Then, Section 4.9.1 introduces our optimization in the original PACB setting (conjunctive relational queries and set semantics). Section 4.10 extends this to bag semantics, Section 4.11 extends it to  $QBT^{XM}$ .

A key ingredient of the PACB algorithm is to *capture views as constraints*, in particular TGDs, thus reducing the view-based rewriting problem to constraints-only rewriting. For a given view V, the constraint  $V_{IO}$  states that for every match of the view body against the input data there is a corresponding tuple in the view output; the constraint  $V_{OI}$  states the converse inclusion, i.e., each view tuple is due to a view body match. Then, given a set  $\mathcal{V}$  of view definitions, PACB defines a set of view constraints  $C_{\mathcal{V}} = \{V_{IO}, V_{OI} \mid V \in \mathcal{V}\}$ .

The constraints-only rewriting problem thus becomes: given the source schema  $\sigma$  with a set of integrity constraints *I*, a set  $\mathcal{V}$  of view definitions over  $\sigma$  and the target schema  $\tau$  which includes  $\mathcal{V}$ , given a conjunctive query *Q* expressed over  $\sigma$ , find reformulations  $\rho$  expressed over  $\tau$  that are equivalent to *Q* under the constraints  $I \cup C_{\mathcal{V}}$ .

For instance, if  $\sigma = \{R, S\}$ ,  $I = \emptyset$ ,  $\tau = \{V\}$  and view *V* materializes the join of tables *R* and *S*, V(x, y) : -R(x, z), S(z, y), the constraints capturing *V* are:

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

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

(*i*) chasing Q with the set of constraints  $I \cup C_{\mathcal{V}}^{IO}$  where  $C_{\mathcal{V}}^{IO} = \{V_{IO} \mid V \in \mathcal{V}\};$ 

(*ii*) restricting the chase result to only the  $\tau$ -atoms (the result is the *universal plan*) U;

(*iii*) chasing U with the constraints in  $I \cup C_{\mathcal{V}}^{OI}$ , where  $C_{\mathcal{V}}^{OI} = \{V_{OI} \mid V \in \mathcal{V}\}$ ; the result is

denoted *B* and called the *backchase*; finally:

(*iv*) matching Q against B and outputting as rewritings those subsets of U that are responsible for the introduction (during the backchase) of the atoms in the image of Q.<sup>5</sup>

In our example, *I* is empty,  $C_{q_{\ell}}^{IO} = \{V_{IO}\}$ , and the result of the chase in phase (*i*) is  $Q_1(x, y)$ : -R(x,z), S(z,y), V(x,y). The universal plan obtained in phase (*ii*) by restricting  $Q_1$  to  $\tau$  is U(x,y): -V(x,y). The result of backchasing *U* with  $C_{q_{\ell}}^{OI}$  in phase (*iii*) is B(x,y) : -V(x,y), R(x,z), S(z,y)and in phase (*iv*) we find a match from *Q*'s body into the *R* and *S* atoms of *B*, introduced during the backchase due to *U*'s atom V(x,y). This allows us to conclude that  $\rho(x,y) : -V(x,y)$  is an equivalent rewriting of *Q*.

# **4.9.1 PACB** $^{OPT}$ : **Optimized PACB**

The idea for our optimization was sparked by the following observation. The backchase phase (step (*iii*)) involves the  $V_{OI}$  constraints for all  $V \in \mathcal{V}$ . The backchase attempts to match the left-hand side of each  $V_{OI}$  for each V repeatedly, leading to wasted computation for those views that have no match. In a polystore setting, the large number of data sources and stores lead to a high number of views, most of which are often irrelevant for a given query Q.

This observation leads to the following modified algorithm. Define the set of views mentioned in the universal plan U as relevant to Q under I, denoted  $relev_I(Q)$ . Define the optimized PACB algorithm PACB<sup>OPT</sup> identical with PACB except phase (*iii*) where PACB<sup>OPT</sup> replaces  $C_{V}^{OI}$  with  $C_{relev_I(Q)}^{OI}$ . That is, PACB<sup>OPT</sup> performs the backchase only with the OIconstraints of the views determined in phase (*i*) to be relevant to Q, ignoring all others. This modification is likely to save significant computation when the polystore includes many views. In our example assume that, besides V, V contained 1000 other views  $\{V^i\}_{1 \le i \le 1000}$ , each irrelevant to Q. Then the universal plan obtained by PACB would be the same as U above, and yet

<sup>&</sup>lt;sup>5</sup>Recall that a chase step *s* with constraint *c* matches *c*'s premise against existing atoms *e* and adds new atoms *n* corresponding to *c*'s conclusion. To support fast detection of responsible atoms in Phase (*iv*), *s* records that the *e* atoms are responsible for the introduction of the *n* atoms [84]. Our optimization does not affect Phase (*iv*).

 $\{V_{OI}^i\}_{1 \le i \le 1000}$  would still be considered by the backchase phase, which would attempt at every step to apply each of these 1000 constraints. In contrast, PACB<sup>OPT</sup> would save this work in particular, in our setting, where the premises of  $V_{OI}$  views can have up to 10-way joins.

In general, ignoring even a single constraint c during backchase may lead to missed rewritings [121]. This may happen *even when* c *mentions elements of schema*  $\sigma$  *that are disjoint from those mentioned in* U, if the backchase with I exposes semantic connections between these elements. In our setting, we prove that this is not the case:

# **Theorem 4.9.1.** Algorithm $PACB^{OPT}$ finds the exact same rewritings as the original PACB.

This is because we only ignore some *view-capturing constraints*, which can be shown (by analyzing the backchase evolution) *never* to apply, regardless of the constraints in *I*.

*Proof.* Assume for the sake of contradiction that the set  $\mathcal{RW}^{O\mathcal{PT}}$  of rewritings found by PACB  $\mathcal{OPT}$  is not the same as the set  $\mathcal{RW}$  of rewritings found by the original PACB ( $\mathcal{RW}^{O\mathcal{PT}} \neq \mathcal{RW}$ ). Let  $\mathcal{V}$  be the set of views and  $V_{irr} \in \mathcal{V}$  be the set of irrelevant views to the query Q.

By applying the PACB<sup>OPT</sup> algorithm, the chase introduces the relevant views  $V_{rel} \in \mathcal{V}$  (i.e.,  $V_{rel} = \mathcal{V} - V_{irr}$ ) into the universal plan U. Now, in the backchase phase, only the premise of each backward constraint  $v \in V_{rel}$  can be fully matched against U. This makes the chase step applicable, where the conclusion of each v will be added to the evolving backchase instance B. When no further chase steps are applied, the query Q will be matched against B, and the output will be the rewritings  $\mathcal{RW}^{OPT}$ , which are those subsets of U that are responsible for the introduction (during the backchase) of the atoms in the image of Q in B. When applying the original PACB, similarly, the chase phase introduces only  $V_{rel}$  into U. During the backchase phase,  $V_{irr}$  will never be applied since their premises cannot be fully matched into U, resulting into the same instance B as in the PACB<sup>OPT</sup> algorithm. Thus, when Q is matched against B, this outputs the rewritings  $\mathcal{RW}$ , which are exactly the same as  $\mathcal{RW}^{OPT}$ . However, this contradicts that  $\mathcal{RW}^{OPT} \neq \mathcal{RW}$ . Hence, our original statement is true that the algorithm PACB<sup>OPT</sup> finds the exact same rewritings as the original PACB.

Combined with the main result from [84], Theorem 4.9.1 yields the completeness of PACB<sup>OPT</sup> in the following sense:

**Corollary 4.9.1.** Whenever the chase of input conjunctive query Q with the constraints in I terminates<sup>6</sup>, we have:

(a) algorithm  $PACB^{OPT}$  without a cost model enumerates all join-minimal<sup>7</sup> V-based rewritings of Q under I, and

(b) algorithm PACB<sup>OPT</sup> equipped with a cost model c finds the c-optimal join-minimal rewritings of Q.

In Section 4.13.3, we evaluate the performance gains of PACB<sup>OPT</sup> over the original PACB, measuring up to 40x speedup when operating in the polystore regime.

# **4.10** Extending PACB OPT to Bag Semantics

We extended PACB<sup>OPT</sup> to find equivalent rewritings of an input conjunctive query under bag semantics (the original PACB only addresses set semantics). The extension involves a modification to phase (*iv*). In its original form, the matches from *Q* into the backchase result *B* are not necessarily injective, being based on *homomorphisms* [26]. These allow multiple atoms from *Q* to map into the same atom of *B*. To find bag-equivalent rewritings, we disallow such matches, requiring match homomorphisms to be injective.

66

<sup>&</sup>lt;sup>6</sup>Termination of the chase with TGDs is undecidable [61], but many sufficient conditions for termination are known, starting with weak acyclicity [70]. Our constraints are chosen so as to ensure termination.

<sup>&</sup>lt;sup>7</sup>A rewriting of Q is join-minimal if none of its joins can be removed while preserving equivalence to Q.

# **4.11 PACB**<sup>*OPT*</sup><sub>*OBT*</sub>: Extending PACB<sup>*OPT*</sup> to QBTs

The original PACB algorithm (and our extensions thereof) have so far been defined for conjunctive queries only. However, recall that QBTs (Section 4.4.1) are nested.

We extend the PACB  $^{OPT}$  algorithm to nested QBTs as follows. Each block *B* is rewritten in the context of its ancestor blocks  $A_1, \ldots, A_n$ , to take into account the fact that the free variables of *B* are instantiated with the results of the query corresponding to the conjunction of its ancestor blocks. We therefore replace *B* with the rewriting of the query  $A_1 \wedge A_2 \wedge \ldots \wedge A_n \wedge B$ . We call the resulting algorithm PACB  $^{OPT}_{QBT}$ , using the notation PACB  $^{OPT}_{QBT} \langle C, c \rangle$  to emphasise the fact that it is parameterized by the constraints *C* and the cost model *c*.

Recalling the uninterpreted (black-box) function semantics from Section 4.2, Corollary 4.9.1 implies:

**Corollary 4.11.1.** Under uninterpreted-function semantics, Corollary 4.9.1 still holds when we replace conjunctive queries with QBT queries and PACB<sup>OPT</sup> with PACB<sup>OPT</sup><sub>QBT</sub>.

# 4.12 Guarantees on the Reduction

We provide the following formal guarantees for our solution to the cross-model rewriting problem based on the reduction to single-model rewriting. Recall from Section 5.4 that enc(M)are the relational constraints used to encode  $M \in M^i$  in virtual relations, enc(Q) encodes a  $QBT^{XM}$ query Q as a QBT query over the virtual relations, and dec(R) decodes a QBT query over the virtual relations into a  $QBT^{XM}$  query. Also recall from Section 4.9 that given a set  $\mathcal{V}$  of  $QBT^{XM}$ views,  $C_{\mathcal{V}}$  are the relational constraints used to capture  $\mathcal{V}$ . We have:

**Theorem 4.12.1** (Soundness of the reduction). Let Q be a  $QBT^{XM}$  query over a polystore over the set of data models  $M^i$ . Let I be a set of integrity constraints satisfied by the data in the polystore

and enc(I) be their relational encoding. For every rewriting R obtained via our reduction, i.e.

$$R = dec(PACB_{QBT}^{OPT} \langle enc(I) \cup \bigcup_{M \in M^{i}} enc(M) \cup C_{V}, c \rangle (enc(Q))),$$

*R* is a *c*-optimal V-based rewriting equivalent to Q under I, assuming black-box function semantics (Section 4.2).

In the above,  $enc(I) \cup \bigcup_{M \in M^i} enc(M) \cup C_{\mathcal{V}}$  is the set of constraints used by the PACB $_{QBT}^{OPT}$  algorithm; Theorem 4.12.1 states the correction of our approach, outlined in Figure 5.1.

*Proof sketch.* Let  $F_r$  be a family of virtual relations detailed in Section 4.5. The core strategy of our approach is to compile the operations in a query Q and a set of views V to virtual relations in  $F_r$ . The relations in  $F_r$  may not fully specify the exact properties of the operations they capture. They are interpreted as a proper superset of their intended interpretations. However, they can satisfy some constraints I. In other words, this large class of relations can contain the intended relations interpretations, which we capture via constraints enc(I). While the encoded constraints enc(I) do not contradict the intended operations interpretations and properties (this holds for our encoded constraints enc(I)), the theoretical result in [65] combined with the soundness of PACB [84] and Thereom 4.9.1 guarantee that soundness is preserved for any query Q that is compilable relationally. If a relational reformulation is found, then it is the encoding of  $QBT^{XM}$  rewriting, which can be retrieved by the decoding phase that follows the connections among atoms and knowledge of the encoded data models.

**Completeness Discussion.** The natural question to be asked is whether we capture all constraints that follow from the original data model. If we miss some constraints, then our rewriting approach, which includes encoding, rewriting with constraints, and finally decoding the rewriting, remains sound, returning only equivalent rewritings. It may not be complete, meaning that it may miss existing rewritings.

The question has to be answered in a nuanced way because of the following reason: classical results from logic [129] tell us that for any tree-like models (including XML and JSON) the the answer is no, and it is impossible to capture all constraints that follow from these models even when using full-fledged first-order logic to express constraints (TGDs and EGDs are merely particular cases of first-order constraints).

But it is possible to capture all constraints that matter to a certain language L, in the sense that L does not have sufficient expressivity to distinguish among models that satisfy all constraints and models that satisfy only the ones we capture. For practicality, we support the entire language via black-box encodings of the primitives with undecidable/ computationally expensive reasoning, giving up on the completeness guarantee while adopting a solution that allows progressive enhancements of a best-effort approach to completeness. In other words, the more relevant constraints we add, the fewer rewritings we miss, allowing progressive refinement of the rewriting algorithm without changing code, simply by adding constraints.

Not guaranteeing completeness has no discernible practical impact, since already for SQL absolute completeness of the rewriting procedure is precluded by the undecidability of reasoning about primitives that render SQL (and related languages) Turing-complete (e.g., user-defined functions and arithmetic). In practice, completeness is not attained by commercial SQL optimizers, even when the user queries fall in a restricted class with theoretically feasible rewriting completeness, due to the combinatorial explosion of searching for all possible plans and the imperfection of the cost model.

# 4.13 Experimental Evaluation

In this section, we describe our experimental evaluation to show the effectiveness of our cross-models rewriting technique. Section 4.13.1 describes our experiment setup. In Sections 4.13.2 and 4.13.3, we discuss the results of our noval cross-models rewriting approach. We

summarize our experimental finding and takeaways in Section 4.13.4.

#### 4.13.1 Experiment Setup

We use a single machine with an Intel(R) Xeon(R) CPU E5-2640 v4@2.40GHz, 20 physical cores (40 logical cores), and 123GB RAM of main memory. The machine is equipped with a 1TB SSD storage device, where the read speed is 616 MB/s, and the write speed is 455 MB/s (interesting since some systems write intermediate results to disk).

**Polystore Configuration.** For our main polystore setting (called "ESTOCADA polystore engine" hereafter), we use Tatooine [45], a lightweight execution engine and a set of data stores, selected for their capabilities and popularity: an RDBMS (PotsgreSQL v9.6), JSON document stores/engines (PostgreSQL v9.6, MongoDB v4.0.2, AsterixDB v0.9.4, and SparkSQL v2.3.2) and a text search engine (Solr v6.1). We set a memory budget of 60GB for all systems. We configure the number of utilizable cores to 40 (for systems with such a configurable parameter). We set the compiler frame size of AsterixDB (for its batch-at-a-time query processor) to 6MB.

Dataset. We use the real-life 46.6 GB MIMIC-III dataset [88] described in Section 4.1.1.

Generating Query and View Families. We create a micro-benchmark based on MIMIC dataset. We define a set QT of 25 query templates, each checking meaningful conditions against patients' data. These are parameterized by selection constants, and they involve navigation into the JSON document structure. Each query/view is obtained by joining a subset of QT and picking values for the selection constants, leading to an exponential space of meaningful queries and views. Among them, we identify those with non-empty results: first, non-empty instantiations of QT queries then join of two such queries, then three etc., in an adaptation of the Apriori algorithm [29].

**Example 4.13.1** (Generating Queries/Views based on Query Templates). Consider the query templates  $QT_0$ ,  $QT_1$  and  $QT_2$  in Appendix A, shown directly in relationally encoded form.  $QT_0$  asks for patients' information including patient's PATIENTID, DOB, and GENDER.  $QT_1$  asks

for all "abnormal" lab measurement results for patients.  $QT_2$  asks for bloodwork-related lab measurements. The natural join of  $QT_0$ ,  $QT_1$  and  $QT_2$  yields a query Q which seeks information on patients with abnormal blood test results. The query Q and its translation in AsterixDB SQL++ syntax appear in Appendix A.

**The Queries.** We choose 50 queries  $Q_{EXP}$  among those described above. 58% of the queries  $(Q_{01}, \ldots, Q_{29})$  contain full-text operations; all involve joins, selections, and at least two-level-deep navigation into the JSON document structure.

**The Views.** We materialized a set of views  $V_{EXP}$  as follows: We store in PostgreSQL six relational views  $V_{PostgreSQL} \subset V_{EXP}$  of the MIMIC-III dataset, comprising the uniformly structured part of the dataset (including all patient metadata and admission under specific services such as Cardiac Surgery, Neurologic Medical, etc).

We also stored in PostgreSQL a set  $V_{PostgresJSON} \subset V_{EXP}$  of 21 views which are most naturally represented as nested JSON documents. These views store for instance: (*i*) lab tests conducted for each patient with "abnormal" test results (e.g., blood gas, Cerebrospinal Fluid (CSF)); (*ii*) data about drugs prescribed to patients sensitive to certain types of antibiotics (e.g., CEFEPIME); (*iii*) data about drugs and lab tests prescribed to each patient who underwent specific types of procedures (e.g., carotid endarterectomy); (*iv*) microbiology tests were conducted for each patient; (*v*) lab tests for each patient who was prescribed certain drug types (e.g. additive, base); etc. We placed in Solr a view  $V_{Solr} \in V_{EXP}$ , storing for each admitted patient the caregivers' reports (unstructured text). The usage of AsterixDB, SparkSQL, and MongoDB is detailed below.

#### 4.13.2 Cross-Store Rewritings Evaluation

In this section, we study the effectiveness of ESTOCADA cross-store query rewriting: (*i*) compared to single-store query evaluation and (*ii*) improving performance in the pre-existing polystore engines: BigDAWG [68] and ESTOCADA polystore engine (Tatooine) [45].



Figure 4.11: Rewriting time (28 relevant views).

**Single-Store Evaluation Comparison.** Figure 4.11 shows the rewriting time for the query set using the views described above. Notice that most queries are rewritten within 100ms, and the few outliers require at most 190ms, which is negligible compared to the query execution time (in the order of minutes, as seen in Figures 4.13 and 4.14). Figure 4.12 shows the distribution of rewriting time over the same query set when we scale up the number of relevant views (we did not materialize them) to 128 views (this is for stress-test purposes, as 128 views relevant to the data touched by a single query is implausible).

Queries with Text Search Predicates. Figure 4.13 reports the total execution time plus rewriting time of ESTOCADA using the views  $V_{EXP}$  for  $Q_{01}$  to  $Q_{29}$ , all of which feature a text search predicate against the text notes in the caregiver's report. For each query, cross-model rewriting and evaluation significantly improve the performance of a direct query evaluation in a single store.

For SparkSQL and AsterixDB, queries  $(Q_{01}, \ldots, Q_{29})$  took over 25 minutes (the timeout value we used). The bottleneck is the text search operation, and a JSON array unnest operator: full-text indexing is lacking in SparkSQL, and limited to exclude text occurring within JSON arrays in AsterixDB<sup>8</sup>. This confirms our thesis that cross-models redundant storage of data into

<sup>&</sup>lt;sup>8</sup>AsterixDB v9.8 supports array indexing.



Figure 4.12: Rewriting time (128 relevant views).

the stores most suited for an expected operation is worthwhile.

For MongoDB and PostgreSQL, the execution time is correlated with the number of JSON array unnest operators. For instance, query  $Q_{25}$  has five unnest operators, whereas query  $Q_{17}$  has 2. PostgreSQL outperforms MongoDB because the latter lacks join-reordering optimization, and it does not natively support inner joins. These must be simulated by left outer joins – using the \$lookup operator – followed by a scan and selection for non-null values –using the \$match operator.

Queries without Text Search Predicates. Figure 4.14 repeats this experiment for queries  $Q_{30,...,Q_{50}}$ , which do not perform a text search. These queries each feature join, selection and navigation into the JSON document structure (at least two levels deep). The relevant views for these queries are  $V_{PostgreSQL} \cup V_{PostgresJSON}$ ; again, exploiting them improves single-store evaluation. SparkSQL has the highest query execution time; this is because it supports navigation into JSON arrays through the EXPLODE function, which is highly inefficient. We observe that in a single-store evaluation, PostgreSQL is more efficient; this is why we choose it to store  $V_{PostgresJSON}$ .



Timeout







Execution time in minutes (includes rewriting time for

**Polystore Evaluation Comparison.** We study the benefits that ESTOCADA can bring to an existing polystore system by transparently rewriting queries using materialized views stored across different stores. We used two polystore engines: (*i*) ESTOCADA polystore engine instantiated with two PostgreSQL servers (instances), one stores relational data while the other stores JSON, and Solr v6.1 for storing text; (*ii*) the latest release of the BigDAWG polystore. A key BigDAWG concept is an *island*, or collection of data stores accessed with a single query language. BigDAWG supports islands for relational, array, and text data, based on the PostgreSQL, SciDB [20] and Apache Accumulo [3] stores, respectively. BigDAWG queries use explicit CAST operators to *migrate* an intermediary result from one island to another.

To work with BigDAWG, we extended it with two new CAST operators: (*i*) to migrate Solr query results to PostgreSQL; (*ii*) to migrate PostgreSQL JSON query results to a PostgreSQL relational instance and vice-versa. The main difference between our ESTOCADA polystore engine and BigDAWG is that we join subquery results *in the mediator* using a BindJoin[123], whereas BigDAWG *migrates* such results to a store in an island capable of performing the join.

**Data Storage.** We store the MIMIC-III dataset (in both systems) as follows: patient metadata in PostgreSQL relational instance; caregivers' reports in Solr; patients' lab events, prescriptions, microbiology events, and procedures information in the PostgreSQL JSON instance.

**Polystore Queries.** We rewrite  $Q_{01}, \ldots, Q_{29}$  in BigDAWG syntax, referring to each part of the data from its respective island (as BigDAWG requires); we refer to the resulting query set as  $Q_{BigDAWG}$ . We have the same set of queries in  $QBT^{XM}$  syntax; we call these queries  $Q_{ESTOCADA Polystore}$ .

**The Views.** To the view set  $V_{EXP}$  introduced above, we have added a new set of views  $V_{NEW}$  which can benefit  $Q_{BigDAWG}$  and  $Q_{ESTOCADA Polystore}$  queries as we detail below.

The queries vary in terms of full-text search predicates selectivity.  $\approx 60\%$  of  $Q_{BigDAWG}$ and  $Q_{ESTOCADA}$  queries consist of full-text search predicates, which are *not highly selective* (e.g., "low blood pressure"). We refer to these queries as  $Q_{BigDAWG}^{60\%}$  and  $Q_{ESTOCADA}^{60\%}$ . We observed that the cost of such queries in BigDAWG is dominated by moving and ingesting the results of Solr queries in PostgreSQL (JSON instance) to join them with the results of other sub-queries. To alleviate this overhead, we materialized *in the PostgreSQL instance storing JSON* a set of 6 views  $V_{NEW}$ , which join the data from Solr (using those full-text predicates in the views definitions) with JSON data from the PostgreSQL JSON instance.

Given the  $Q_{BigDAWG}^{60\%}$  queries,  $V_{PostgresJSON}$ ,  $V_{PostgreSQL}$  and  $V_{NEW}$ , our cross-model viewsbased rewriting approach finds rewritings using views from PostgreSQL (relational instance) and PostgreSQL (JSON instance). The performance saving is due to the fact that we no longer have to move data from Solr to a PostgreSQL instance (see Figure 4.15 for queries labeled \*). Although ESTOCADA polystore engine does not require any data movement, it still benefits from utilizing  $V_{PostgresJSON}$ ,  $V_{PostgreSQL}$  and  $V_{NEW}$  to answer  $Q_{ESTOCADA}^{60\%}$  queries as shown in Figure 4.15 (queries labeled with \*). In contrast, the remaining 40% of  $Q_{BigDAWG}$  and  $Q_{ESTOCADA}^{40\%}$ and  $Q_{ESTOCADA}^{40\%}$  polystore).

The high selectivity of these queries reduces the overhead of moving the data from Solr to PostgreSQL in BigDAWG, and in general the data movement is not a bottleneck for these queries. However, both systems can benefit from the materialized views  $V_{EXP}$  to evaluate these queries, as shown in Figure 4.15 (queries labeled with +).

As mentioned earlier, ESTOCADA polystore engine and BigDAWG differ in terms of multi-store join evaluation strategies, leading to different performance variations when the queries and/or views change. On the queries  $Q_{BigDAWG}^{60\%}$  and  $Q_{ESTOCADA Polystore}^{60\%}$ , where the full-text search predicates are not very selective, BigDAWG execution time is dominated by moving partial results to the join server. In contrast, ESTOCADA polystore engine performs better since it computes the join in memory in the mediator; thus, it does not need to pay the intermediary result storage cost.

For the other 40% of queries (with very selective full-text search predicates), BigDAWG data movement cost is negligible; thus its evaluation time is dominated by evaluating the join



**Figure 4.16**: PACB vs PACB  $^{OPT}$  rewriting performance.

between sub-queries results in the PostgreSQL island, where join algorithms and orders may be better chosen than in the ESTOCADA polystore engine (the two platform support different sets of join algorithms). However, the differences are negligible. The main conclusion of this experiment, however, is that our cross models views-based rewriting approach *improves performance in both polystore engines*.

## 4.13.3 PACB vs. PACB OPT

This experiment demonstrates the performance gains of PACB<sup>OPT</sup> over PACB in a polystore setting. We consider the queries  $Q_{EXP}$  and the 28 views  $V_{EXP}$  that can be utilized to answer  $Q_{EXP}$ , introduced above. We add to  $V_{EXP}$  some *irrelevant* views  $V_{irrel} \subseteq (\mathcal{V} - V_{EXP})$ . The backward constraints of  $V_{irrel}$  can partially match against the universal plan of chasing each query in the benchmark. However, they cannot be used to answer a query; therefore, we call them "irrelevant". The premises of the backward constraints of  $V_{irrel}$  can have up to 10-way joins. PACB<sup>OPT</sup> would save attempts performed by PACB at every step to apply each of these constraints. We scale the size of  $V_{irrel}$  from 1000 to 4000 (from 2000 to 4000, the premises (backward) of the newly added constraints have up to 3-ways joins). Figure 4.16 presents the *average rewriting time* of  $Q_{EXP}$  in the presence of  $V_{EXP} \cup V_{irrel}$ ; the y axis is in log scale.



Figure 4.15: Queries and rewritings evaluation in polystore engines.

#### 4.13.4 Summary of Experimental Findings

We have shown that our cross-models views-based rewriting approach is *portable* across polystore engines. Moreover, it is *worthwhile*, as it improves their performance in natural scenarios for both cross-models and even single-model user queries; the latter are improved by rewritings using a cross-store (and cross-models) set of materialized views (even when accounting for the time it takes to find the rewriting). We have also shown that the time spent searching for rewritings is a small fraction of the query execution time and hence a worthwhile investment. As we confirm experimentally, the performance of the rewriting search is due to our optimized PACB<sup>OPT</sup> algorithm, shown to outperform standard PACB by up to  $40 \times$ .

# 4.14 Conclusion

We have shown that multi-store architectures have the potential to significantly speed up query evaluation by materializing views in the systems most suited to expected workload operations, even when these views are distributed across stores and data models. ESTOCADA supports this functionality by a local-as-view approach whose immediate benefit is flexibility since it requires no work when the underlying data storage changes. In our experiments, we achieve performance gains by simply placing the materialized views according to a few common-sense guidelines (e.g., place large unstructured text collections in a store with good full-text indexing support, and place inherently nested data in JSON document stores).

# 4.15 Acknowledgement

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# Chapter 5

# HADAD: Extending Benefits of Semantic Optimization to Hybrid Relational and Linear Algebra Computation

# 5.1 Introduction

This chapter presents HADAD, which capitalizes on ESTOCADA framework previously introduced in [31] (Chapter 4) for rewriting queries across many data models, using materialized views in a hybrid setting that does not include the LA model. The novelty of HADAD is to extend the benefits of semantic rewriting and views optimizations under integrity constraints to pure LA and hybrid RA-LA computations, which are crucial for ML-hybrid workloads.

This approach makes it very easy to extend HADAD's semantic knowledge of LA operations, RA-LA, or LA rewrite rules by simply declaring appropriate constraints, with no need to change HADAD code. Moreover, as we will show, constraints are sufficiently expressive to declare (and thus allow HADAD to exploit) more properties of LA operations than previous work could consider. **Chapter Outline.** The rest of this chapter is organized as follows: Section 5.2 highlights HADAD's optimizations that go beyond the state-of-the-art based on *real-world* scenarios. In Section 5.3, we formalize the query optimization problem in the context of pure LA and hybrid RA-LA settings. Section 5.4 provides an end-to-end overview of our approach. We present our novel reduction of the rewriting problem, focusing on LA computation, into one that can be solved by existing techniques from the relational setting (Chapter 4) in Section 5.5. Section 5.6 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 guarantees in Section 5.8 and present the experiments in Section 5.9. We conclude in Section 5.11.

# 5.2 HADAD Optimizations

We highlight below examples of performance-enhancing opportunities that are exploited by HADAD and not being addressed by LA-oriented and cross RA-LA existing solutions.

#### 5.2.1 LA Pipeline Optimization

**Example 5.2.1.** Consider the Ordinary Least Squares Regression (OLS) pipeline:  $(X^TX)^{-1}(X^Ty)$ , where X is a square matrix of size  $10K \times 10K$  and y is a vector of size  $10K \times 1$ . Suppose available a materialized view  $V = X^{-1}$ .

HADAD rewrites the pipeline to  $(V(V^T(X^Ty)))$ , by exploiting the LA properties  $(CD)^{-1} = D^{-1}C^{-1}$ , (CD)E = C(DE) and  $(D^T)^{-1} = (D^{-1})^T$  as well as the view V. The rewriting is more efficient than the original pipeline since it avoids computing the expensive inverse operation. Moreover, it optimizes the matrix chain multiplication order to minimize the intermediate result size. This leads to a 70× speedup on R. Current popular LA-oriented systems [17, 16, 42, 25, 112] are not capable of exploiting such rewrites due to the lack of systematic exploration of standard LA properties and views.

#### 5.2.2 Hybrid RA-LA Optimization

Cross RA-LA platforms such as MorpheusR [52], SparkSQL [35] and others [97, 91] can greatly benefit from HADAD's cross-model optimizations, which can find rewrites that they miss.

**Example 5.2.2** (Factorization of LA Operations over Joins). *Morpheus R* [52] *implements a powerful optimization that factorizes an LA operation on a matrix* **M** *obtained by joining tables* **R** *and* **S** *and casting the join result as a matrix. Factorization pushes the LA operation on* **M** *to operate on* **R** *and* **S**, *cast as matrices.* 

Consider a specific instantiation of factorization: colSums(MN), where matrix M has size  $20M \times 120$  and N has size  $120 \times 100$ ; both matrices are dense. The colSums operation sums up the elements in each column, returning the vector of these sums (the operation is common in ML algorithms such as K-means clustering [107]). On this pipeline, MorpheusR applies a left matrix multiplication factorization rule to push the multiplication by N down to R and S. The size of MN intermediate result is  $20M \times 100$ . Finally, colSums is applied to the intermediate result, reducing to a  $1 \times 100$  vector.

HADAD can help Morpheus R do better by pushing the colSums operator to R and S (instead of the multiplication with N), then concatenating the resulting vectors. This leads to much smaller intermediate results, since the combined size of vectors colSums(R) and colSums(S) is only  $1 \times 120$ .

To this end, HADAD rewrites the pipeline to colSums(M)N by exploiting the property colSums(AB) = colSums(A)B and applying its cost estimator, which favors rewritings with a small intermediate result size. Evaluating this HADAD-produced rewriting, MorpheusR's multiplication pushdown rule no longer applies, while the colSums pushdown rule is now enabled, leading to  $125 \times$  speedup.

**Example 5.2.3** (Cross-Model Optimizations). *Consider another hybrid example on a Twitter dataset* [24]. *The JSON dataset contains tweet ids, extended tweets, entities including hashtags,* 

filter-level, media, URL, tweet text, etc. We implemented it on SparkSQL (with SystemML [42]). In the preprocessing stage, our SparkSQL query constructs a tweet-hashtag filter-level matrix N of size  $2M \times 1000$ , for all tweets posted from "USA" mentioning "covid", where rows are tweets, columns are hashtags, and values are filter-levels<sup>1</sup>.

*N* is then loaded into SystemML, where rows with filter-level less than four are selected. The result undergoes an Alternating Least Square (ALS) [114] computation. A core building block of the ALS computation is the LA pipeline  $(uv^T - N)v$ . In our example, *u* is a tweet feature vector (of size  $2M \times 1$ ) and *v* is a hashtag feature vector (of size  $1000 \times 1$ ).

We have two materialized views available:  $V_1$  stores the tweet id and text as a text data source in Solr, and  $V_2$  stores tweet id, hashtag id, and filter-level for all tweets posted from "USA", and is materialized on disk as CSV file. The rewriting modifies the preprocessing of N by introducing  $V_1$  and  $V_2$ ; it also pushes the filter-level selection from the LA pipeline into the preprocessing stage. To this end, it rewrites  $(uv^T - N)v$  to  $uv^Tv - Nv$ , which is more efficient for two reasons. First, N is ultra sparse (0.00018% non-zero), which renders the computation of Nv extremely efficient. Second, SystemML evaluates the chain  $uv^Tv$  efficiently, computing  $v^Tv$  first, which results in a scalar, instead of computing  $uv^T$ , which results in a dense matrix of size  $2M \times 1000$  (HADAD's cost model realizes this). Without the rewriting help from HADAD, SystemML is unable to exploit its own efficient operations for lack of awareness of the distributivity property of vector multiplication over matrix addition, Av + Bv = (A+B)v. The rewriting achieves  $14 \times$  speedup.

HADAD detects and applies all the above-mentioned optimizations combined. It captures RA-, LA-, and cross-model optimizations precisely because it reduces all rewrites to a single setting in which they can interact and synergize: *relational rewrites under integrity constraints*.

<sup>&</sup>lt;sup>1</sup>Matrix N is represented in MatrixMarket Format (MTX) since it is sparse.

# 5.3 **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, and two basic data types: *relations (sets of tuples)* 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 each tuple would become a matrix line, in some order that is unknown, unless the relation was explicitly sorted before the conversion. In other words, resulting relations are cast as matrices.

We consider a hybrid RA-LA language  $\mathcal{L}$ , comprising a set  $R_{ops}$  of (unary or binary) *RA* operators; concretely,  $R_{ops}$  comprises the standard relational selection, projection, and join. We also consider a set  $L_{ops}$  of *LA* operators, comprising: unary (e.g., inversion and transposition) and binary (e.g., matrix product) operators. The full set  $L_{ops}$  of LA operations we support is detailed in Section 5.5.1. A hybrid expression in  $\mathcal{L}$  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 an expression, where  $ro_1 \in R_{ops}$  is a unary relational operator, and E's type matches  $ro_1$ '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);
- (LA operators): given some expressions *E*, *E'* that are either numeric matrices or numbers (which can be seen as 1 × 1 matrices), and some real number *r*, the following are also expressions: *lo*<sub>1</sub>(*E*) where *lo*<sub>1</sub> ∈ *L*<sub>ops</sub> is a unary operator, and *lo*<sub>2</sub>(*E*, *E'*) where *lo*<sub>2</sub> ∈ *L*<sub>ops</sub> is a binary operator (again, provided that *E*, *E'* match the expected input types of the operators).

Clearly, an important set of *equivalence rules* that we focus on in this work are LA equivalence rules (i.e., properties of LA operations). These equivalences lead to *alternative evaluation strategies* for each expression. Further, we assume given a (possibly empty) set of *materialized views*  $\mathcal{V} \in \mathcal{L}$ , 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 rewrite** derived from E by: (*i*) exploiting integrity constraints, (*ii*) exploiting equivalence rules, and/or (*iii*) 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 setting. Importantly, our solution (based on a *relational encoding with integrity constraints*) capitalizes on ESTOCADA framework previously introduced in (Chapter 4) [31], where it was used to *rewrite queries using materialized views in a polystore setting*, where the data, views and queries cover a variety of data models (relational, JSON, XML, etc. ). Those queries can be expressed in a combination of query languages, including SQL, JSON query languages, 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 used. The novelty of HADAD is to **extend the benefits of rewriting and view-based optimization to LA computations, crucial for ML workloads**. In Section 5.5, we focus on capturing matrix data and LA computations in the relational framework, along with relational data naturally; this enables our novel, holistic optimization.

## 5.4 HADAD Overview

We outline here our approach as an extension to ESTOCADA [31] (see Chapter4) for solving the rewriting problem introduced in Section 5.3.

RA-LA Hybrid Expressions and Views. A hybrid RA-LA expression (whether asked



Figure 5.1: HADAD reduction outline.

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 [50]. Other expressions are purely LA ones; we assume that they are defined in a dedicated LA language such as R [17], DML [42], etc., using LA operators from our set  $L_{ops}$  (see Section 5.5.1), commonly used in real-world ML 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.

Our approach is based on a reduction to a relational model. Below, we focus on showing how to bring LA components under a relational form (the RA part of each expression is already in the target formalism, see Chapter4).

Encoding of LA Operations into the Relational Model. Let *E* be an LA expression (query), and  $\mathcal{V}$  be a set of materialized views. We reduce the LA views-based rewriting problem to the relational rewriting problem under integrity constraints, as follows (see Figure 5.1). First, we *encode relationally E*,  $\mathcal{V}$ , and the set  $L_{ops}$  of LA operators. Note that the relations used in the encoding are *virtual* and *hidden*. They only serve to support query rewriting via relational techniques, as we show in Chpater 4. 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  $L_{ops}$  operations. For instance, we model the *matrix addition* operation using a relation  $add_M(M,N,R)$ , denoting that *R* is the result of M + N, together with a set of constraints (see Section 5.5.2) stating that  $add_M$  is a *functional* relation that is *commutative*, *associative*, etc. We detail our relational encoding in Section 5.5.

Reduction From LA-based to Relational Rewriting. Our reduction translates the dec-
laration of each view  $V \in \mathcal{V}$  to constraint  $enc_{LA}(V)$  that reflects 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 matrices.

The reformulation problem is reduced to a purely relational setting (as shown before in Chapter 4) as follows. We are given a (purely LA or RA-LA hybrid) query expression  $E \in \mathcal{L}$  and a set  $\mathcal{V} \subseteq \mathcal{L}$  views. We encode E as the relational query  $enc_{LA}(E)$ , the views as the relational integrity constraints  $C_{\mathcal{V}} = enc_{LA}(V_1) \cup \ldots \cup enc_{LA}(V_n)$ . We add as further input the set of relational constraints  $enc_{LA}(LA_{prop})$  mentioned above, which specify properties of the LA operators. We call them Matrix-Model encoding Constraints, or  $\mathcal{MMC}$  in short. We must find a rewriting  $RW_e$  expressed over the relational views  $C_{\mathcal{V}}$ , such that  $RW_e$  is equivalent to  $enc_{LA}(E)$ under the constraints  $(C_{\mathcal{V}} \cup \mathcal{MMC})$  and is optimal according to our cost model. Note that  $RW_e$ is a *relationally encoded rewriting* of E; a final *decoding* step is needed to obtain  $E' \in \mathcal{L}$ , the (LA or hybrid) rewriting of E.

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' (see Section 5.5).

**Relational Rewriting Using Constraints.** To solve the relational rewriting problem under constraints, the engine of choice is PACB [84] (previously used in ESTOCADA, see Chapter 4). We extend PACB engine ( $PACB^{++}$  hereafter) to utilize the  $Pruned_{prov}$  algorithm discussed in [83], which prunes inefficient rewritings during the equivalent rewritings search phase, based on simple cost models (see Section 5.6).

**Decoding of the Relational Rewriting.** In a similar fashion as what we have seen in Chapter 4, the selected relational reformulation  $RW_e$  found by  $PACB^{++}$ , a *decoding step dec*( $RW_e$ ) is performed to translate  $RW_e$  into the native syntax of its respective underlying system language (e.g., R, DML, etc.).

Operation	Encoding	Operation	Encoding	
Matrix scan	name(M,n)	Inversion	$ ext{inv}_M(M,R)$	
Multiplication	reliantion multi (M N R) Scalar		[mu] + i (a M D)	
winnpheation	$\operatorname{Multl}(M(M,N,\mathbf{K}))$	Multiplication	$\left  \begin{array}{c} \operatorname{mull} MU(s,M,K) \\ \end{array} \right $	
Addition	$\operatorname{add}_M(M,N,R)$	Cells Sum	$\operatorname{sum}(M,s)$	
Division	$\operatorname{div}_M(M,N,R)$	Trace	trace(M,s)	
Hadamard	$m_{11} + i - (M N P)$	Pow sum	rowSums $(M,R)$	
product	$\begin{bmatrix} 111111111111111111111111111111111111$			
Transposition	tr(M,R)	Colsums	colSums(M,R)	

**Table 5.1**: Snippet of the  $\mathcal{VREM}$  schema.

## **5.5 LA Reduction to the Relational Model**

Our internal model is relational, and it makes prominent use of expressive integrity constraints. This framework suffices to describe the features and properties of most data models used today, notably including relational, XML, JSON, graph, etc [31, 32] (see Chapter 4).

Going beyond, in this section, we present a novel way to *reason relationally about LA* operations by treating them as un-interpreted 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 (Section 5.5.1). Then, in Section 5.5.2, we show how matrices and their operations can be 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 MMC that capture the properties of these operations. Section 5.5.3 exemplifies relational rewritings obtained via our reduction.

#### 5.5.1 Supported Matrix Algebra

We consider a wide range of matrix operations [98, 37], which are common in realworld ML algorithms [9]: element-wise multiplication (multi<sub>E</sub>), matrix-scalar 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), diagonal (diag), exponential (exp), adjoints (adj), direct sum (sum<sub>D</sub>), direct product (product<sub>D</sub>), summation (sum), rows/columns summation (rowSums, colSums, respectively), QR (QR), Cholesky (CHO), LU (LU), and pivoted LU (LUP) decompositions. The full list of supported operations appear in Appendix B.1.

### 5.5.2 VREM Schema and Relational Encoding

To model LA operations on the  $\mathcal{VREM}$  relational schema (part of which appears in Table 5.1), we also rely on a set of integrity constraints  $\mathcal{MMC}$ , which are encoded using relations in  $\mathcal{VREM}$ . We detail the encoding below.

**Base Matrices and Dimensionality Modeling.** We denote by  $M_{k\times z}(\mathcal{D})$  a matrix of k rows and z columns, whose values come from a domain  $\mathcal{D}$ , e.g., the domain of real numbers  $\mathbb{R}$ . For brevity we just use  $M_{k\times z}$ . We define a virtual relation  $name(M,n) \in \mathcal{VREM}$  attaching a unique ID M to any matrix identified by a name denoted n (which may be e.g., of the form "/M.csv"). This relation (shown at the top left in Table 5.1) is accompanied by an EGD key constraint  $I_{name} \in \mathcal{MMC}_m$ , where  $\mathcal{MMC}_m \subset \mathcal{MMC}$ , stating that *two matrices with the same name n have the same ID*:

$$I_{name}: \forall M \forall N \; name(M, n) \land name(N, n) \rightarrow M = N$$

Note that the matrix ID in *name* relation (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. In Table 5.1, we use M and N to denote input matrices' IDs, R for the resulting matrix ID, and s for scalar input and output.

Accessing a particular cell in matirx M can be modeled using a cell(M, i, j, v) relation, where i is the row, j is the column and v is the cell value. To state that there is no cell that has two distinct values, we need to introduce the following EGD:

$$I_{cell}: \forall M \forall i \forall j \forall v_1 \forall v_2 \ cell(M, i, j, v_1) \land cell(M, i, j, v_2) \rightarrow v_1 = v_2$$

Currently, we do not support encoding *matrix slicing operator*, which involves selecting certain rows and columns of a matrix, and forming a new matrix, possibly in a different dimension from the original. We leave this to future work.

The dimensions of a matrix are captured by a size(M,k,z) relation, where k and z are the number of rows, resp. columns and M is an ID. An EGD constraint  $I_{size} \in \mathcal{MMC}_m$  holds on the *size* relation, stating that the ID determines the dimensions:

$$I_{size}: \forall M \forall k_1 \forall z_1 \forall k_2 \forall z_2 \ size(M, k_1, z_1) \land size(M, k_2, z_2) \rightarrow k_1 = k_2 \land z_1 = z_2$$

The identity and zero matrices are captured by Zero(O) and Identity(I) relations, where O and I denote their IDs, respectively. They are accompanied by EGD constraints  $I_{iden}$ ,  $I_{zero} \in \mathcal{MMC}_m$ , stating that zero matrices with the same sizes have the same IDs, and this also applies for identity matrices with the same size:

$$\begin{split} I_{zero}: \forall O_1 \forall O_2 \forall k \forall z \ Zero(O_1) \land size(O_1,k,z) \land Zero(O_2) \land size(O_2,k,z) \rightarrow O_1 = O_2 \\ I_{iden}: \forall I_1 \forall I_2 \ Identity(I_1) \land size(I_1,k,k) \land Identity(I_2) \land size(I_2,k,k) \rightarrow I_1 = I_2 \end{split}$$

**Encoding Matrix Algebra Expressions.** LA operations are encoded into dedicated relations, as shown in Table 5.1. We now illustrate the encoding of an LA expression on the  $\mathcal{VREM}$  schema. The full list of encoding relations appears in Appendix B.1.

**Example 5.5.1** (Encoding LA Expression Using  $\mathcal{VREM}$  Schema). Consider the LA expression E:  $((MN)^T)$ , where the two matrices  $M_{100\times 1}$  and  $N_{1\times 10}$  are stored as "M.csv" and "N.csv", respectively. The encoding function  $enc_{LA}(E)$  takes as argument the LA expression E and returns a conjunctive query whose: (i) body is the relational encoding of E using  $\mathcal{VREM}$  (see below), and (ii) head has one distinguished variable, denoting the equivalence class of the result. For instance:

$$enc(((MN)^{T}) = Let enc(MN) = Let enc(M) = Q_{0}(M):- name(M, "M.csv"); enc(N) = Q_{1}(N):- name(N, "N.csv"); R_{1} = freshId() in Q_{2}(R_{1}):- multi_{M}(M, N, R_{1}), Q_{0}(M), Q_{1}(N); R_{2} = freshId() in Q(R_{2}):- tr(R_{1}, R_{2}), Q_{2}(R_{1});$$

In the above, nesting is dictated by the syntax of E. From the inner (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  $R_1$ ), using the multi<sub>M</sub> relation and encoding the relationship between this product and its inputs in the definition of  $Q_2(R_1)$ . Next, we create a fresh ID  $R_2$  used to encode the full E (the transposed of  $Q_2$ ) via relation tr, in  $Q(R_2)$ . For brevity, we omit the matrices' size relations in this example and hereafter. Unfolding  $Q_2(R_1)$  in the body of Q yields:

$$Q(R_2) := tr(R_1, R_2), multi_M(M, N, R_1), Q(R_2) Q_0(M), Q_1(N);$$

Now, by unfolding  $Q_0$  and  $Q_1$  in Q, we obtain the final encoding of  $((MN)^T)$  as a conjunctive query Q:

$$Q(R_2) := tr(R_1, R_2), multi_M(M, N, R_1), Q(R_2), name(M, "M.csv"), name(N, "N.csv");$$

**Encoding LA Properties as Integrity Constraints.** Figure 5.2 shows some of the constraints  $\mathcal{MMC}_{LA_{prop}} \subset \mathcal{MMC}$ , which capture textbook LA properties [98, 37] of our LA operations (Section 5.5.1). The TGDs (5.1), (5.2) and (5.3) state that matrix addition is commutative, matrix transposition is distributive with respect to addition, and the transposition of the

$$\forall M \forall N \forall R \text{ add}_M(M, N, R) \to \text{add}_M(N, M, R)$$

$$\forall M \forall N \forall R \text{ add}_M(M, N, R) \to \text{add}_M(N, M, R)$$
(5.1)

$$\exists R_2 \exists R_4 \pm r(M, R_2) \land \pm r(N, R_4) \land \operatorname{add}_M(R_2, R_4, R_2) \qquad (5.2)$$

$$\forall M \forall R_1 \forall R_2 \operatorname{inv}_M(M, R_1) \wedge \operatorname{tr}(R_1, R_2) \rightarrow \tag{3.2}$$

$$\exists R_3 \operatorname{tr}(M, R_3) \wedge \operatorname{inv}_M(R_3, R_2) \tag{5.3}$$

**Figure 5.2**: Snippet of  $\mathcal{MMC}_{LA_{prop}}$  constraints

$$\begin{array}{c} \forall M \forall N \forall R_1 \forall R_2 \forall R_3 \forall R_4 \\ name(M, ``M.csv") \land name(N, ``N.csv") \land \\ \texttt{tr}(N, R_1) \land \texttt{tr}(M, R_2) \land \\ \texttt{inv}_M(R_2, R_3) \land \texttt{add}_M(R_1, R_3, R_4) \rightarrow name(R_4, ``V.csv") \end{array}$$

Figure 5.3: Relational encoding of view V

inverse of matrix M is equivalent to the inverse of the transposition of M, respectively. We also express that the *virtual relations are functional* by using EGD key constraints. For example, the following  $I_{multi_M} \in \mathcal{MMC}_{LA_{prop}}$  constraint states that  $multi_M$  is functional, that is the products of pairwise equal matrices are equal.

$$\begin{split} &I_{multi_M}:\forall M\forall N\forall R_1\forall R_2\\ &\text{multi}_M(M,N,R_1)\wedge \text{multi}_M(M,N,R_2)\rightarrow R_1=R_2 \end{split}$$

Other properties [37, 98] of the LA operations we consider are similarly encoded (See Appendix B.3).

**Encoding LA Views as Constraints.** We translate each view definition V (defined in LA language) into relational constraints  $enc_{LA}(V) \in C_{\mathcal{V}}$ , where  $C_{\mathcal{V}}$  is the set of relational constraints used to capture the views  $\mathcal{V}$ . These constraints show how the view's inputs are related to its output over the  $\mathcal{VREM}$  schema. Figure 5.3 illustrates the encoding as a TGD constraint of the view  $V : (N)^T + (M^T)^{-1}$  stored in a file "V.csv" and computed using matrices N and M(e.g., stored as "N.csv" and "M.csv", respectively). **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 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 decompositions (LU, QR, and Pivoted LU or PLU) as a set of virtual relations  $\mathcal{VREM}_{dec}$ , which we add to  $\mathcal{VREM}$ . For instance, for CD, we associate a relation CHO(M,L), which denotes that L is the output of the CD decomposition for a given matrix M whose ID is M. CHO is a functional relation, meaning every symmetric positive definite matrix has a unique CD decomposition. This functional aspect is captured by an EGD, conceptually similar to the constraint  $I_{multiM}$  (Section 5.5.2). The property  $M = LL^T$  is captured as a TGD constraint  $I_{cho} \in \mathcal{MMC}_{LA_{num}}$ :

$$I_{cho}: \forall M \ type(M, "S") \to \exists \ L_1 \exists L_2 \ cho(M, L_1) \land$$
$$type(L_1, "L") \land tr(L_1, L_2) \land multi_M(L_1, L_2, M)$$
(5.4)

The atom type(M, "S") indicates the type of matrix M, where the constant "S" denotes a matrix that is *symmetric positive definite*; similarly,  $type(L_1, "L")$  denotes that the matrix  $L_1$  is a lower triangular 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:

$$\forall M name(M, ``M.csv") \rightarrow type(M, ``S")$$
(5.5)

**Example 5.5.2** (Cholesky Decomposition Rewriting). Consider a view  $V=N+LL^T$ , where L = cho(M) and M is a symmetric positive definite matrix encoded as in (5.5). 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 (5.4), and since M+N = N+M, which is encoded

*in* (5.1). *However, at the syntactic level, V and E are very dissimilar. Knowledge of* (5.1) *and* (5.4) *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 necessarily a symmetric positive definite matrix, 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 real square matrix, *Q* is an orthogonal matrix [98] 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  $\mathcal{MMC}_{LAprop}$ :

$$\forall M \forall n \forall k \; name(M,n) \land size(M,k,k) \rightarrow \exists Q \exists R$$
$$QR(M,Q,R) \land type(Q,"O") \land type(R,"U") \land multi_M(Q,R,M)$$
(5.6)

$$\forall Q \ type(Q, "O") \to \exists I \ QR(Q, Q, I) \land identity(I) \land multi_M(Q, I, Q)$$
(5.7)

$$\forall R \ type(R, "U") \to \exists I \ QR(R, I, R) \land identity(I) \land multi_M(I, R, R)$$
(5.8)

$$\forall I \ identity(I) \to QR(I,I,I) \tag{5.9}$$

Known LA properties of the other matrix decompositions (LU and PLU) are similarly encoded in Appendix B.3.

Encoding LA-Oriented System Specific Rewrite Rules. Most LA-oriented systems [17, 16] execute an incoming LA expression *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 [42] 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 the

following rule to rewrite sum(MN) (summing all cells in the matrix product), where  $\odot$  is a matrix element-wise multiplication, to avoid actually computing MN and materializing it.

$$sum(MN) = sum(colSums(M)^T \odot rowSums(N))$$
 (i)

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 5.5.3.** Consider an LA expression  $E = ((M^T)^k (M + N)^T)$ , where M and N are square matrixes, and expression E' = sum(E), which computes the sum of all cells in E. E' can be rewritten to

$$RW_1: sum(colSums(M+N)^T \odot rowSums(M^k))$$

Failure to exploit the LA properties  $M^T N^T = (NM)^T$ ,  $(M^n)^T = (M^T)^n$  and  $sum((MN)^T) = sum(MN)$  together prevents from finding the rewriting  $RW_1$ .

E' admits the alternative rewriting:

$$RW_2$$
:  $sum((colSums((M^T)^k))^T \odot (colSums(M+N)^T))$ 

which can be obtained by directly applying the rewrite rule (i) given previously and the LA property  $rowSums(M^T)=colSums(M)^T$ . However,  $RW_2$  creates more intermediate results than  $RW_1$ .

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

$$\begin{split} &I_{sum}: \forall M \forall N \forall R \; \text{multi}_M(M,N,R) \wedge \text{sum}(R,s) \rightarrow \\ &\exists R_1 \exists R_2 \exists R_3 \exists R_4 \text{colSums}(M,R_1) \wedge \text{tr}(R_1,R_2) \\ &\wedge \text{rowSums}(N,R_3) \wedge \text{multi}_E(R_2,R_3,R_4) \wedge \text{sum}(R_4,s) \end{split}$$

We refer the reader to Appendix B.4 for a list of supported SystemML's rewrite rules and their encoding into integrity constraints.

#### 5.5.3 LA Relational Rewriting Using Constraints

With the set of views constraints  $C_{V}$  and  $\mathcal{MMC} = \mathcal{MMC}_m \cup \mathcal{MMC}_{LA_{prop}} \cup \mathcal{MMC}_{StatAgg}$ , we rely on  $PACB^{++}$  to rewrite a given expression under integrity constraints. We exemplify this below, and detail  $PACB^{++}$ 's inner workings in Section 5.6.

**Example 5.5.4** (LA View-based Rewriting). The view V shown in Figure 5.3 can be used to fully rewrite (return the answer for) the pipeline  $Q_p = (M^{-1} + N)^T$  by exploiting the TGDs (5.1), (5.2) and (5.3) listed in Figure 5.2, which describe the following three LA properties, denoted  $LA_{prop_1}$ : M + N = M + N;  $((M + N))^T = (M)^T + (N)^T$  and  $((M)^{-1})^T = ((M)^T)^{-1}$ . The relational rewriting RW<sub>0</sub> of  $Q_p$  using the view V is RW<sub>0</sub>(R<sub>4</sub>):- name(R<sub>4</sub>, "V.csv"). In this example, RW<sub>0</sub> is the only views-based rewriting of  $Q_P$ . However, five other rewritings exist (shown in Figure 5.4 and their relational form in Figure 5.5), which reorder its operations just by exploiting the set LA<sub>prop1</sub> of LA properties.

Rewritings have different evaluation costs. We discuss next how we estimate which among these alternatives (including evaluating  $Q_p$  directly) is likely the most efficient.

$$RW_{1}: (M^{-1})^{T} + N^{T} \qquad RW_{2}: (M^{T})^{-1} + N^{T}$$
  

$$RW_{3}: N^{T} + (M^{-1})^{T} \qquad RW_{4}: N^{T} + (M^{T})^{-1}$$
  

$$RW_{5}: (N + M^{-1})^{T}$$

**Figure 5.4**: Equivalent rewritings of  $Q_p$ .

$$\begin{split} RW_1(R_4) &: -name(M, ``M.csv"), name(N, ``N.csv"), \\ \text{tr}(N,R_1), \text{inv}_M(M,R_2), tr(R_2,R_3), \text{add}_M(R_3,R_1,R_4) \\ RW_2(R_4) &: -name(M, ``M.csv"), name(N, ``N.csv"), \\ \text{tr}(N,R_1), \text{tr}(M,R_2), \text{inv}_M(R_2,R_3), \text{add}_M(R_3,R_1,R_4) \\ RW_3(R_4) &: -name(M, ``M.csv"), name(N, ``N.csv"), \\ \text{tr}(N,R_1), \text{inv}_M(M,R_2), tr(R_2,R_3), \text{add}_M(R_1,R_3,R_4) \\ RW_4(R_4) &: -name(M, ``M.csv"), name(N, ``N.csv"), \\ \text{tr}(N,R_1), \text{tr}(M,R_2), \text{inv}_M(R_2,R_3), \text{add}_M(R_1,R_3,R_4) \\ RW_5(R_4) &: -name(M, ``M.csv"), name(N, ``N.csv"), \\ \text{inv}_M(M,R_1), \text{add}_M(N,R_1,R_2), \text{tr}(R_2,R_4) \end{split}$$

**Figure 5.5**: Relational equivalent rewritings of  $Q_p$ .

# 5.6 Choice of an Efficient Rewriting

We introduce our cost model in Section 5.7, which can take two different sparsity estimators (Section 5.7.1). Then, we detail our extension to the PACB rewriting engine based on the  $Prune_{prov}$  algorithm (Section 5.7.2) to prune out inefficient rewritings.

# 5.7 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 admits 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 5.7.1) into our framework.

**Example 5.7.1.** 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  $\gamma(E_2) = 100 \times 100$ .

### 5.7.1 LA-based Sparsity Estimators

We outline below two existing *sparsity estimators* [137, 42] that we have incorporated into our framework to estimate  $nnz^2$ .

**Naïve Metadata Estimator.** The naïve metadata estimator [43, 137] 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 [43, 137, 44], which aims to provide an upper bound for worst-case memory estimates. Figure 5.6 illustrates the naïve worst-case sparsity estimation scheme that we use<sup>3</sup>. *S<sub>E</sub>* denotes the estimated sparsity of an input LA expression. We define *sparsity* = *nnz/size*. We note that we assign "zero" as the sparsity of the scalar output (e.g., *S<sub>E</sub>*[trace(*D*)] = 0, *S<sub>E</sub>*[sum(*M*)] = 0, *S<sub>E</sub>*[det(*D*)] = 0, etc. ). The operator  $\odot$  denotes a matrix-element wise multiplication. For complex operations such as inverse, we assume the sparsity of the output matrix is the same as the sparsity of the input matrix<sup>4</sup>.

**Matrix Non-zero Count (MNC) Estimator.** The MNC estimator [128] exploits matrix structural properties such as single non-zero per row or columns with varying sparsity for efficient,

<sup>&</sup>lt;sup>2</sup>Solving the problem of sparsity estimation is beyond the scope of this work.

<sup>&</sup>lt;sup>3</sup>The figure illustrates the sparsity estimation for LA operators used in our experiments (Section 5.9)

<sup>&</sup>lt;sup>4</sup>Most of the existing sparsity estimators focus on basic matrix operations such as matrix products, transportation, element-wise multiply, etc. To the best of our knowledge, we are not aware of existing work on estimating the sparsity of matrices resulting from complex operators (e.g., inverse)

 $S_E[cM] = S_E[M]$ where *c* is a non -zero scalar  $S_E[M^T] = S_E[M]$   $S_E[M \odot N] = min(S_E[M], S_E[N])$   $S_E[M + N] = min(\mathbf{1}, (S_E[M] + S_E[N]))$   $S_E[M - N] = min(\mathbf{1}, (S_E[M] + S_E[N]))$   $S_E[M/N] = min(\mathbf{1}, (S_E[M] + (1 - S_E[N])))$   $S_E[MN] = min(\mathbf{1}, (S_E[M] * \mathbf{n}) * min(\mathbf{1}, (S_E[N] * \mathbf{n}))$ where *n* is the common dimension of *M* and *N*  $S_E[rowSums(M)] = min(\mathbf{1}, \mathbf{m} * S_E[M])$ where *m* is the number of rows of *M*  $S_E[colSums(M)] = min(\mathbf{1}, \mathbf{n} * S_E[M])$ where *n* is the number of columns of *M* 

Figure 5.6: Naïve sparsity estimation scheme.

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 our experiments (Section 5.9). MNC also lacks the support of estimating the sparsity of complex matrix operations. For this reason, we made the same assumptions discussed in the naïve metadata estimator.

### **5.7.2 Pruning Rewritings:** *PACB*<sup>++</sup>

We extended the PACB rewriting engine with the  $Prune_{prov}$  algorithm discussed in [83, 84], 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 suffices on the scenarios considered in [84, 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. In this Section, we recall below just enough of the *PACB*'s inner working to explain *Prune*<sub>prov</sub> (see Section 3.3.2 for details).

**Provenance-Directed Rewritings Search.** Given a source schema  $\sigma$  with a set of integrity constraints *I*, a set  $\mathcal{V}$  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 *Q* under the constraints  $I \cup C_{\mathcal{V}}$ .

**Example 5.7.2.** For instance, if  $\sigma = \{R, S\}$ ,  $I = \emptyset$ ,  $\tau = \{V\}$  and we have a view V materializing the join of relations R and S, V(x,y):-  $R(x,z) \land S(z,y)$ , the pair of constraints capturing V is the following:

$$V_{IO} : \forall x \forall z \forall y \ R(x,z) \land S(z,y) \to V(x,y)$$
$$V_{OI} : \forall x \forall y V(x,y) \to \exists z \ R(x,z) \land S(z,y)$$

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

(i) chasing Q with the constraints  $I \cup C_{\mathcal{V}}^{IO}$ , where  $C_{\mathcal{V}}^{IO} = \{V_{IO} \mid V \in \mathcal{V}\}$ ; intuitively, this enriches (extends) Q with all the consequences that follow from its atoms and the constraints  $I \cup C_{\mathcal{V}}^{IO}$ .

(ii) restricting the chase result to only  $\mathcal{V}$ -atoms; the result is called a universal plan U.

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

(iv) chasing U with the constraints in  $I \cup C_{V}^{OI}$ , where  $C_{V}^{OI} = \{V_{OI} \mid V \in V\}$ , and annotating each relational atom **a** introduced by these chase steps with a provenance formula  $\pi(a)$ , 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,  $C_{qv}^{IO} = \{V_{IO}\}$ , and the result of the chase in phase (i) is  $Q_1(x,y):-R(x,z) \wedge S(z,y) \wedge V(x,y)$ . The universal plan obtained in (ii) by restricting  $Q_1$  to the schema of view names is  $U(x,y):-V(x,y)^{p_0}$ , where  $p_0$  denotes the provenance term of atom V(x,y). The result of backchasing U with  $C_{qv}^{OI}$  in phase (iv) is  $B(x,y):-V(x,y)^{p_0} \wedge R(x,z)^{p_0} \wedge S(z,y)^{p_0}$ . Note that the  $\pi(R)$  and  $\pi(S)$  of the R and S atoms (a simple term  $p_0$ , 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  $\pi(h(Q))$  of the image h of Q is  $p_0$ , which corresponds to an equivalent rewriting: RW(x,y):-V(x,y).

*Prune*<sub>prov</sub> Minimum-Cost Rewriting. The minimal rewritings of a query Q are obtained by first finding the set  $\mathcal{H}$  of all matches (i.e., containment mappings) from Q to the result Bof backchasing the universal plan U. Denoting with  $\pi(A)$  the provenance formula of a set of atoms A, 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 guaranteed to be a rewriting of Q.

The idea behind cost-based pruning is that, whenever the naïve 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 minimum-cost 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 5.7.3** (Applying  $Prune_{prov}$ ). 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:

$$\begin{split} U(R_2) &: -name(M, ``M.csv")^{p_0}, size(M, ``50000", ``100")^{p_1}, name(N, ``N.csv")^{p_2}, \\ size(N, ``100", ``50000")^{p_3}, multi_M(M, N, R_1)^{p_4}, multi_M(R_1, M, R_2)^{p_5}, \\ multi_M(N, M, R_3)^{p_6}, multi_M(M, R_3, R_2)^{p_7} \end{split}$$

*Now, consider in the backchase the associativity constraint C:* 

$$\forall M \forall N \forall R_1 \forall R_2$$

$$multi_M(M,N,R_1) \land multi_M(R_1,M,R_2) \rightarrow$$

$$\exists R_4 multi_M(N,M,R_4) \land multi_M(M,R_4,R_2)$$

There exists a match 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 U' which has additional  $\pi(h(P))$ -annotated atoms:  $\operatorname{multi}_M(N,M,R_4)^{p_4 \wedge p_5} \wedge \operatorname{multi}_M(M,R_4,R_2)^{p_4 \wedge p_5}$ . 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  $sq(c_1)$  corresponding to the rewriting (MN)M, of cost  $(50K)^2$ .

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

The naïve PACB would find both rewritings, cost them, and drop the former ,which introduces a large intermediate result ( $\gamma(sq(\pi(h(P))) = (50K)^2)$ ), above the threshold, in favor of the latter.

With pruning, the threshold T is the cost of the original expression  $100^2$ . The chase step with C is never applied, as it would introduce the provenance conjunct  $\pi(h(P))$  which determines U-subquery  $sq(\pi(h(P)) = multi_M(M,N,R_1)^{p_4} \wedge multi_M(R_1,M,R_2)^{p_5}$  of cost  $(50K)^2$  exceeding T. The atoms needed as an image of E under  $h_1$  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 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  $rw \in \mathcal{R}W$  whenever the pruned chase step is applied again for another constraint.

To address this issue, in our modified version of  $Prune_{prov}$ , we keep track of the rewritings that their costs are already estimated to prevent such redundant work. Additionally, the search for *minimal-rewritings* "so far" (matches of the query Q into the evolving universal plan instance U'), whenever the pruned chase step is applied, is modeled as a query evaluation of Q against U'(viewed as a symbolic/canonical database [26]). 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 that step, while most of the instance is unchanged. Therefore, instead of evaluating the query plan from scratch, we employ incremental evaluation as in [84]. 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.

## 5.8 Guarantees on the Reduction

We detail the conditions under which we guarantee that our approach is *sound* (i.e., generates only equivalent, cost-optimal rewritings), and *complete* (i.e., finds all equivalent cost-optimal rewritings).

Let  $\mathcal{V} \subseteq \mathcal{L}$  be a set of materialized view definitions, where  $\mathcal{L}$  is the language of hybrid expressions described in Section 5.3.

Let  $LA_{prop}$  be a set of properties of the LA operations in  $L_{ops}$  that admits relational encoding over  $\mathcal{VREM}$ . 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  $LA_{prop}$ ).

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  $E \in \mathcal{L}$  ( $\gamma, LA_{prop}, \mathcal{V}$ )-optimal if for every  $E' \in \mathcal{L}$  that is  $(LA_{prop}, \mathcal{V})$ -equivalent to E we have  $\gamma(E') \geq \gamma(E)$ .

Let  $\text{Eq}^{\gamma}\langle LA_{prop}, \mathcal{V} \rangle(E)$  denote the set of all  $(\gamma, LA_{prop}, \mathcal{V})$ -optimal expressions that are  $(LA_{prop}, \mathcal{V})$ -equivalent to *E*.

We denote with  $HADAD\langle LA_{prop}, \mathcal{V}, \gamma \rangle$  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 5.1). Given  $E \in \mathcal{L}$ ,  $HADAD\langle LA_{prop}, \mathcal{V}, \gamma \rangle(E)$ denotes all expressions returned by  $HADAD\langle LA_{prop}, \mathcal{V}, \gamma \rangle$  on input *E*.

**Theorem 5.8.1** (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  $rw \in Eq^{\gamma} \langle LA_{prop}, \mathcal{V} \rangle(E)$ .

The proof sketch parallels that of Theorem 4.12.1 (shown in Section 4.12). The only difference is that we extended HADAD to use  $Prune_{prov}$ , where the soundness still holds.

**Completeness Discussion.** We state that our approach is complete within theoretically imposed limitations, meaning if  $\gamma$  is monotonic and  $LA_{prop}$  is terminating, then for every  $E \in \mathcal{L}$ and every  $rw \in Eq^{\gamma} \langle LA_{prop}, \mathcal{V} \rangle (E)$ , we have  $rw \in HADAD \langle LA_{prop}, \mathcal{V}, \gamma \rangle (E)$ . The completeness of PACB  $Prune_{prov}$  [83] (which was proven under terminating chase and monotonic cost function) guarantees that it *returns* all and precisely the *minimum-cost reformulations* of enc(E) under  $C_{\mathcal{V}} \cup enc_{LA}(LA_{prop})$ ). However, LA operations can satisfy more properties that we cannot fully capture with our class of constraints. The rewriting algorithm will not exploit those properties. Thus, with respect to those properties, our approach is incomplete necessarily so because these tasks are undecidable.

## 5.9 Experimental Evaluation

We evaluate HADAD to answer the research questions below about our approach:

- Section 5.9.2 and Section 5.9.3: Can HADAD find rewrites with/without views that lead to a greater performance improvement than original pipelines without modifying the internals of the existing systems?. Are the identified rewrites found by state-of-the-art platforms?.
- Section 5.9.2 and Section 5.9.3: Is HADAD's optimization overhead compensated by the performance gains in execution?.

We evaluate our approach, first on **LA-based pipelines** (Section 5.9.2), then on **hybrid expressions** (Section 5.9.3).

### 5.9.1 Experiment Setup

We use a single machine with an Intel(R) Xeon(R) CPU E5-2640 v4@2.40GHz, 20 physical cores (40 logical cores) and 123GB RAM, running CentOS Linux release 7.9.2009. The machine is equipped with a 1TB SSD storage device, where the disk read and write speeds are 616 MB/s and 455 MB/s, respectively. We run our PACB++ engine on OpenJDK Java 8 VM. As for LA systems/libraries, we use R 3.6.0, Numpy 1.16.6 (python 2.7), TensorFlow r1.4.2, Spark 2.4.5 (MLlib), SystemML 1.2.0. For hybrid experiments, we use MorpheusR [12] and SparkSQL [35]. We use Scala version 2.11.12 for SparkMLlib and SystemML.

We use a JVM-based linear algebra library for SystemML as recommended in [131], at the optimization level 4. Additionally, we enable multi-threaded matrix operations in a single node. We run Spark in a single node setting and configure Spark to import OpenBLAS (we

No.	Expression	No.	No. Expression		Expression
P1.1	$(MN)^T$	P1.2	$A^T + B^T$	P1.3	$C^{-1}D^{-1}$
P1.4	$(A+B)v_1$	P1.5	$((D)^{-1})^{-1}$	P1.6	$trace(s_1D)$
P1.7	$((A)^T)^T$	P1.8	$s_1A + s_2A$	P1.9	$\det(D^T)$
P1.10	$\operatorname{rowSums}(A^T)$	P1.11	$rowSums(A^T + B^T)$	P1.12	colSums((MN))
P1.13	$\operatorname{sum}(MN)$	P1.14	$ ext{sum(colSums((} N^T M^T)))$	P1.15	(MN)M
P1.16	$\operatorname{sum}(A^T)$	P1.17	$\det(CDC)$	P1.18	sum(colSums((A)))
P1.19	$(C^T)^{-1}$	P1.20	$ trace(C^{-1})$	P1.21	$(C+D^{-1})^T$
P1.22	$\mathrm{trace}((C+D)^{-1})$	P1.23	$\det((CD)^{-1}) + D)$	P1.24	$ extsf{trace}((CD)^{-1})) +  extsf{trace}(D)$
P1.25	$egin{array}{c} M \odot (N^T / \ (MNN^T)) \end{array}$	P1.26	$N \odot (M^T / (M^T M N))$	P1.27	$trace(D(CD)^T)$
P1.28	$A \odot (A \odot B + A)$	P1.29	DCCC	P1.30	$NM \odot NMR^T$

 Table 5.2: LA benchmark pipelines (part 1).

compiled from the source as detailed in [13]) as a linear algebra backend library to take advantage of its accelerations [131]. SparkMLlib's datatypes do not support many basic LA operations, such as scalar-matrix multiplication, Hadamard-product. To support them, we use the Breeze Scala library [5], convert MLlib's datatypes to Breeze types and express the basic LA operations. The driver memory allocated for Spark and SystemML is 115GB.

To maximize TensorFlow performance, we compile it from the source to enable architecturespecific optimizations (e.g., SMID instructions). For all systems/libraries, we set the number of **cores** to **24** (i.e., we use the command **taskset** -c **0–23** when running R, NumPy and TensorFlow scripts, as used in [131]). All system use double precision numbers (**double**) by default, while TensorFlow uses single precision floating point numbers (**float**). To enable fair companion with other systems, we use a double precision (**tf.float64**) for Tensorflow.

### 5.9.2 LA-based Experiments

In this experiment, we study the performance benefits of our approach on LA-based pipelines as well as our optimization overhead.

No.	Expression	No.	Expression	No.	Expression
P2.1	trace(C+D)	P2.2	$\det(D^{-1})$	P2.3	$ t trace(D^T)$
P2.4	$s_1A + s_1B$	P2.5	$\det((C+D)^{-1})$	P2.6	$C^T (D^T)^{-1}$
P2.7	$DD^{-1}C$	P2.8	$\det(C^TD)$	P2.9	$trace(C^TD^T+D)$
P2.10	rowSums(MN)	P2.11	sum(A+B)	P2.12	$sum(rowSums(N^TM^T))$
P2.13	$((MN)M)^T$	P2.14	((MN)M)N	P2.15	sum(rowSums(A))
P2.16	$\begin{array}{c} \texttt{trace}(C^{-1}D^{-1}) \\ +\texttt{trace}(D) \end{array}$	P2.17	$\begin{array}{c} ((((C+D)^{-1})^{T}) \\ ((D^{-1})^{-1})C^{-1}C \end{array}$	P2.18	$\operatorname{colSums}((A^T+B^T)$
P2.19	$(C^T D)^{-1}$	P2.20	$(M(NM))^T$	P2.21	$(D^T D)^{-1} (D^T v_1)$
P2.22	$\exp((C+D)^T)$	P2.23	$\frac{\det(C)*\det(D)}{*\det(C)}$	P2.24	$(D^{-1}C)^T$
P2.25	$(u_1v_2^T - X)v_2$	P2.26	$\exp((C+D)^{-1})$	P2.27	$((((C+D)^T)^{-1})D)C$

**Table 5.3**: LA benchmark pipelines (part 2).

Table 5.4: Overview of used real datasets.

Name	<b>Rows</b> <i>n</i>	<b>Cols</b> <sub>m</sub>	<b>Nnz</b> $  X  _0$	$\mathbf{S}_X$
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%
Netflix/(NS)	50K	100	69559	1.3911%
Netflix/( <i>NM</i> )	100K	100	139344	1.3934%
Netflix/ $(NL_1)$	1M	100	665445	0.6654%
Netflix/ $(NL_2)$	10M	100	665445	0.0665%
Netflix/ $(NL_3)$	100K	50K	15357418	0.307%

 Table 5.5:
 Syntactically generated dense datasets.

Name	<b>Rows</b> <i>n</i>	<b>Cols</b> <sub>m</sub>	][	Name	<b>Rows</b> <i>n</i>	<b>Cols</b> <sub>m</sub>
Syn <sub>1</sub>	50K	100	][	Syn <sub>6</sub>	20K	20K
Syn <sub>2</sub>	100	50K	1[	Syn7	100	1
Syn <sub>3</sub>	1M	100	1	Syn <sub>8</sub>	50K	1
Syn <sub>4</sub>	5M	100	1[	Syn <sub>9</sub>	100K	1
Syn <sub>5</sub>	10K	10K	1[	<i>Syn</i> <sub>10</sub>	100	100

**Datasets.** We used several **real-world**, **sparse matrices**, for which Table 5.4 lists the dimensions and the sparsity ( $S_X$ ): (*i*) we used several subsets of an Amazon books review dataset [2] (in JSON), and similarly (*ii*) subsets of a Netflix movie rating dataset [15]. They

Matrix Name	Used Data
A and B	$AM, AL_1, AL_2, NM, NL_1, NL_2,$ Syn <sub>3</sub> or Syn <sub>4</sub>
C  and  D	Syn <sub>5</sub> or Syn <sub>6</sub>
M	$AS, NS, $ or $Syn_1$
N	$Syn_2$
R	Syn <sub>10</sub>
X	$AL_3$ or $NL_3$
$v_1, v_2$ and $u_1$	Syn <sub>7</sub> , Syn <sub>8</sub> and Syn <sub>9</sub> , respectively.

**Table 5.6**: Matrices used for each matrix name in a pipeline.

were easily converted into matrices where columns are items and rows are customers [137]; 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 of **synthetic, dense matrices**, described in Table 5.5.

LA benchmark. We use a set  $\mathcal{P}$  of 57 LA pipelines used in prior studies and/or frequently occurring in real-world LA computations, as follows:

- Real-world Pipelines (10): include: a chain of matrix self products used for reachability queries and other graph analytics [128] (P1.29 in Table 5.2); expressions used in Alternating Least Square Factorization (ALS) [137] (P2.25 in Table 5.3); Poisson Nonnegative Matrix Factorization (PNMF)(P1.13 in Table 5.2) [137]; Nonnegative Matrix Factorization (NMF)(P1.25 and P1.26 in Table 5.2) [131]; recommendation computation [128] (P1.30 in Table 5.2); finally, Ordinary Least Squares Regression (OLS) [131] (P2.21 in Table 5.3).
- Synthetic Pipelines (47): were also generated, based on a set of basic matrix operations (inverse, multiplication, addition, etc.), and a set of combination templates, written as a Rule-Iterated Context-Free Grammar (RI-CFG) [113]. Examples of synthetic pipelines include P2.16, P2.16, P2.23, P2.24 in Table 5.2. Expressions thus generated include P2.16, P2.23, P2.24 in Table 5.3.

Methodology. We first show the performance benefits of our approach to LA-oriented

systems/tools mentioned above using a set  $\mathcal{P}^{\neg Opt} \subset \mathcal{P}$  of **38** pipelines in Table 5.2 and Table 5.3, and the matrices in Table 5.6. The performance of these pipelines can be improved *just by exploiting LA properties* (in the absence of views). For TensorFlow and NumPy, we present the results only for dense matrices due to limited support for sparse matrices. Then, we show how our approach improves the performance of **30** pipelines from  $\mathcal{P}$ , denoted  $\mathcal{P}^{Views}$ , using pre-materialized views. Finally, we study our rewriting performance and *optimization overhead* for the set  $\mathcal{P}^{Opt} = \mathcal{P} \setminus \mathcal{P}^{\neg Opt}$  of **19** pipelines that are already optimized. For the purpose of the discussion, we discuss a selection of these experiments below. The detailed set of results appears in Appendix B.5, Appendix B.6, Appendix B.7, and Appendix B.8.

Effectiveness of LA Rewriting (No Views). For each system, we run the original pipeline and our rewriting five times; we report the average of the last four running times. We exclude the data loading time [131]. For fairness, we ensure SparkMLib and SystemML compute the entire pipeline (despite their lazy evaluation mode). So, we print a random matrix cell value to force the systems to compute the entire pipeline. Additionally, for SystemML, we insert a "break block" (e.g., WHILE (FALSE)) after each pipeline and before the cell print statement to prevent computing only the value of a single cell and force it to compute all the outputs.

**Discussion.** Figure 5.7 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 the figure. For brevity in the figures, we use **SM** for SystemML, **NP** for NumPy, **TF** for Tensorflow, and **SP** for SparkMLlib.

For **P1.1** (see Figure 5.7(a)), both matrices are dense. The speedup  $(1.3 \times \text{to } 4 \times)$  comes from rewriting  $(MN)^T$  (intermediate result size to  $(50K)^2$ ) into  $N^T M^T$ , much cheaper since both  $N^T$  and  $M^T$  are of size  $50K \times 100$ . We exclude MLlib from this experiment since it failed to allocate memory for the intermediate matrix (Spark/MLLib limits the maximum size of a dense



Figure 5.7: P1.1, P1.4, P1.15, and P2.12 evaluation before and after rewriting.

matrix). As a variation (not plotted in the Figure), we run 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 leads to a runtime exception, and to avoid it, we cast M during load time to a dense matrix type. Thus, the speedup achieved is the same as if M and N were both dense. If, instead, NS (1.3911% non-zeros) plays the role of M, our rewrite achieves  $\approx 1.8 \times$  speedup for SystemML.

For **P1.4** (Figure 5.7(b)), we rewrite  $(A + B)v_1$  to  $Av_1 + Bv_1$ . Adding Amazon sparse matrix  $AL_1$  (0.0065% nnz) used as A to a dense matrix B results into a dense intermediate of size  $1M \times 100$ . Instead,  $Av_1 + Bv_1$  has intermediate results of sizes  $1M \times 1$  and  $1M \times 1$ , respectively.



Figure 5.8: P1.13, and P1.25 evaluation before and after rewriting.

In addition,  $Av_1$  can be computed efficiently thanks to the sparsity in A. The MNC sparsity estimator has a noticeable overhead. We run the same pipeline, where the dense  $5M \times 100$  matrix plays both A and B (not shown in the Figure). This leads to speedup of up to  $2.7 \times$  for SystemML,  $1.4 \times$  for R, and  $9 \times$  for MLlib, which does not natively support matrix addition; thus, we convert its matrices to Breeze types in order to perform it [131].

**P1.15** (Figure 5.7(c)) 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 50*K*. Instead, the rewriting M(NM) only needs an  $O(m^2)$  intermediate matrix, where *m* is 100, and is much faster. To avoid MLLib memory failure on **P1.15**, we use the distributed matrix of type BlockMatrix, which we can run locally 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 always produce dense matrices) [21]. SystemML does optimize the multiplication order if the user does not enforce it (based on our experiments). Further (not shown in the Figure), we run **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 (discussed earlier).

Figure 5.7(d) shows speedups of up to  $42 \times$  when rewriting P2.12 into  $sum((colSums(M))^T$ 

 $\bigcirc$ rowSums(N)). This exploits several properties:

- (i)  $(MN)^T = N^T M^T$ , (ii) sum $(M^T) =$ sum(M), (iii) sum(rowSums(M)) =sum(M), and
- $(iv) \operatorname{sum}(MN) = \operatorname{sum}((\operatorname{colSums}(M))^T \odot \operatorname{rowSums}(N)).$

SystemML captures (*ii*), (*iii*), and (*iv*) as rewrite rules, however, it is unable to find this rewrite since it is unaware of (*i*). Other systems do not exploit these properties. *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.

Figures 5.8(a) and 5.8(b) study **P1.13** and **P1.25**, two real-world pipelines involved in ML algorithms, using the MNC cost model; note the log-scale y axis. Rewriting **P1.13** to sum(t(colSums((M)) \* rowSums(N)) yields a speedup of 50×; while SystemML *has* this rewrite as a dynamic rewrite rule, it did not apply it during optimization. In addition, our rewrite allows other systems to benefit from it. Not shown in the Figure, we re-run this pipeline with *M* ultra sparse (using *AS*) and SystemML: the rewrite did not bring benefits, since *MN* is already efficient. For **P1.25**, the important optimization is selecting the multiplication order in *MNN<sup>T</sup>* (Figure 5.8(b)). SystemML is efficient here, due to its dedicated operator tsmm for transpose-self matrix multiplication and mmchain for matrix multiply chains. MLlib is excluded as it does not support divisions on BlockMatrixes.

Figure 5.9 shows the distribution of the significant rewriting speedup on  $\mathcal{P}^{\neg Opt}$  running on R, and using the MNC-based cost model. For clarity, we split the distribution into two figures: on the left, 25  $\mathcal{P}^{\neg Opt}$  pipelines with speedup lower than 10×; on the right, the remaining 13 with greater speedup. Among the former, 87% achieved at least 1.5× speedup. The latter are sped up by 12× to 58×. **P1.5** is an extreme case here (not plotted): it is sped up by about 1000×, simply by rewriting  $((D)^{-1})^{-1}$  into *D*.

Effectiveness of Views-based LA Rewriting. We define a set  $V_{exp}$  of 12 views that



**Figure 5.9**: R speedup on  $\mathcal{P}^{\neg Opt}$ .

pre-compute the result of some expensive operations (multiplication, inverse, determinant, etc. ), which can be used to answer our  $\mathcal{P}^{Views}$  pipelines and materialize them on disk as CSV files. The experiments outlined below used the naïve cost model; all graphs have a log-scale y axis. The list of all view definitions appears in Appendix B.5.

**Discussion**. For **P2.14** (Figure 5.10(a)), using the view  $V_3 = NM$  by and the multiplication associativity leads to up to  $2.8 \times$  speedup.

Figure 5.10(b) shows the performance gain due to using the view  $V_1 = D^{-1}$ , for the 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  $V(V^T(D^Tv_1))$ , since it introduces small intermediate results due to the optimal matrix chain multiplication order. This rewrite leads to  $70 \times$ ,  $55 \times$ ,  $115 \times$ , and  $150 \times$  speedups on R, NumPy, TensorFlow, and MLlib, respectively; On SystemML, the original pipeline timed out (> 1000 seconds).

Pipeline **P2.25** (Figure 5.10(c)) benefits from the view  $V_4 = u_1 v_2^T$ , which pre-computes a dense intermediate vector multiplication result. The rewrite of  $(u_1 v_2^T - X)v_2$  to  $V_4 v_2 - X v_2$  is



Figure 5.10: P2.14, P2.21, P2.25 and P2.27 evaluation before and after rewriting using V<sub>exp</sub>.

based on exploiting the property (A + B)v = Av + Bv, which leads to  $65 \times$  speedup in SystemML. For MLlib, as discussed before, to avoid memory failure, we used BlockMatrix types. for all matrices and vectors, thus they were treated as dense. In R, the original pipeline triggers a memory allocation failure for the intermediate result, which the rewriting avoids.

Figure 5.10(d) shows that for **P2.27** exploiting the views  $V_9 = (D+C)^{-1}$  and  $V_5 = DC$ leads to speedups of  $4 \times$  to  $41 \times$  on different systems. Properties enabling rewriting here are C+D = D+C,  $(D^T)^{-1} = (D^{-1})^T$  and (CD)E = C(DE). The matrix multiplication order does not have an effect for this pipeline since all matrices are squares.

**Rewriting Performance and Overhead.** We now study the running time *RW*<sub>find</sub> 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 run 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  $\mathcal{P}^{\neg Opt}$  pipelines, on the dense and sparse matrices listed in Table 5.6, 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 38  $\mathcal{P}^{\neg Opt}$  pipelines, SystemML finds efficient rewritings for a set of 9, denoted  $\mathcal{P}_{SM}^{\neg Opt}$ , while TensorFlow optimizes a different set of 11, denoted  $\mathcal{P}_{TF}^{\neg Opt}$ . On these subsets, where HADAD's optimization is redundant, using *dense* matrices, the rewriting overhead is very low: with the *MNC* model, 0.48% to 1.12% on  $\mathcal{P}_{SM}^{\neg Opt}$  (0.64% on average), and 0.0051% to 3.51% on  $\mathcal{P}_{TF}^{\neg Opt}$  (1.38% on average). Using the *naïve* estimator 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, and 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 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* 



**Figure 5.11**: Speedups of MorpheusR (with HADAD rewrites) over MorpheusR (without HADAD Rewrites) for pipelines P1.12, P2.10, P2.11 and P2.15 on synthetic data for a PK-FK join.

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.

### 5.9.3 Hybrid (RA and LA) Experiments

We now study the benefits of rewriting on hybrid scenarios combining RA and LA operations. We first show the performance benefits of HADAD to a cross RA-LA platform, MorpheusR [12]. We then evaluate our hybrid micro-benchmark on SparkSQL+SystemML.



**Figure 5.12**: HADAD  $RW_{find}$  overhead as a percentage (%) of the total time ( $Q_{exec} + RW_{find}$ ) for pipelines P1.10, P1.16, and P1.18 running on MorpheusR.

**MorpheusR Experiments.** We use the same experimental setup introduced in [52] for generating synthetic datasets for the PK-FK join of tables **R** and **S**. The quantities varied are the *tuple ratio*  $(n_S/n_R)$  and feature ratio  $(d_R/d_S)$ , where  $n_S$  and  $n_R$  are the number of rows and  $d_R$  and  $d_S$  are the number of columns (features) in **R** and **S**, respectively. We fix  $n_R = 1M$  and  $d_S = 20$ . The join of **R** and **S** outputs  $n_S \times (d_R + d_S)$  matrix **M**, which is always dense. We evaluate on MorpheusR a set of 8 pipelines and their rewritings found by HADAD using the naïve cost model.

**Discussion**. P1.12: colSums(MN) is the example from Section 5.2, with M the output

(viewed as dense matrix) of joining tables **R** and **S** generated as described above. *N* is a  $ncol(\mathbf{M}) \times 100$  dense matrix. HADAD's rewriting yields up to  $125 \times$  speedup (see Figure 5.11(a)).

Figure 5.11(b) shows up to  $15 \times$  speedup for **P2.10**: rowSums(N**M**), where the size of N is  $100 \times nrow(\mathbf{M})$ . This is due to HADAD's rewriting:  $NrowSums(\mathbf{M})$ , which enables MorpheusR to push the rowSums operator to **R** and **S** instead of computing the matrix multiplication.

**P2.11**: sum(N+M) is run *as-is* by MorpheusR since it does not factorize element-wise operations, e.g., addition. However, HADAD rewrites **P2.11** into sum(N)+sum(M), which avoids the (large and dense) intermediate result of the element-wise matrix addition. The HADAD rewrite enables MorpheusR to execute sum(M) by pushing sum to **R** and **S**, for up to  $20 \times$  speedup (see Figure 5.11(c)).

MorpheusR evaluates P2.15:  $sum(rowSums(\mathbf{M}))$  by pushing the rowSums operator to **R** and **S**. HADAD finds the rewriting  $sum(\mathbf{M})$ , which enables MorpheusR to push the sum operation instead, achieving up to  $4.5 \times$  speedup (see Figure 5.11(d)).

Since MorpheusR does not exploit the associative property of matrix multiplication, it cannot reorder multiplication chains to avoid large intermediate results, which leads to runtime exception in R (MorpheusR's backend). For example, for the chain  $N^T N \mathbf{M}$  (variation of **P1.26**), when the size of **M** is  $1\mathbf{M}\times40$  and the size of N is  $40\times1\mathbf{M}$ , the size of the  $N^TN$  intermediate result is  $1\mathbf{M}\times1\mathbf{M}$ , which causes out of memory in R. HADAD exploits associativity and selects the rewriting  $N^T(N\mathbf{M})$  of intermediate result size ( $40\times40$ ).

For pipelines **P1.14** and **P2.12**, that involve transpose operator, MorpheusR applies its special rewrite rules that replace an operation on  $\mathbf{M}^T$  with an operation on  $\mathbf{M}$  before pushing the operation to the base tables. HADAD rewrites both pipelines to  $sum(N\mathbf{M})$ , enabling MorpheusR to apply its factorized rewrite rule on  $N\mathbf{M}$ . This rewrite achieves speedup from  $1.3 \times$  up to  $1.5 \times$ .

**Rewriting Overhead.** For pipelines that are already optimized or MorpheusR finds the same rewriting found by HADAD, the rewriting overhead is very negligible compared to  $Q_{exec}$ . For example, for pipelines that contain matrix multiplication expressions, the rewriting time is



Figure 5.13: Results of micro-hybrid benchmark using Twitter dataset.

generally less than 0.1% of the total time. However, for the other pipelines, such as **P1.10**, **P1.16**, and **P1.18**, which contain only aggregate operations, the rewriting time is up to 9% of the total time (when the data size is very small (0.32GB), and the computation is extremely efficient) and less than 1% (when the data size is large (19.2GB), and the computation is expensive) as shown in Figure 5.12.

**Micro-hybrid Benchmark Experiments.** In this experiment, we create a *micro-hybrid benchmark* on Twitter[24] and MIMIC [88] datasets to empirically study HADAD's rewriting benefits in a hybrid setting (SparkSQL+SystemML). The benchmark comprises ten different queries combining relational and linear algebra expressions.

Twitter Dataset Preparation. We obtain from Twitter API [24] 16GB of tweets (in

No.	Expression
P3.1	$rowSums(X\mathbf{M}) + (uv^T + \mathbf{N}^T)v$
P3.2	${f u}$ col ${f S}$ ums $((X{f M})^T)$ + ${f N}$
P3.3	$((\mathbf{N}{+}X)v)$ colSums $(\mathbf{M})$
P3.4	$ ext{sum}(C + \mathbf{N}  ext{rowSums}(X\mathbf{M})  u)$
P3.5	$u$ colSums $(\mathbf{M}X)$ + $\mathbf{N}$
P3.6	$rowSums((\mathbf{M}X)^T) + (uv^T + \mathbf{N})v$
P3.7	$X\mathbf{N}u+ ext{rowSums}((\mathbf{M})^T)$
P3.8	$N \odot$ trace $(C + v$ colSums $(MX)C)$
P3.9	$X \odot$ sum $( ext{colSums}(\mathbf{C})^T \odot$ rowSums $(\mathbf{M}))$ + $\mathbf{N}$
P3.10	$\mathbf{N}\odot$ sum $((X+C)\mathbf{M})$

**Table 5.7**: LA pipelines used in micro-hybrid benchmark.

JSON). We extract the structural parts of the dataset, which include user and tweet information, and store them in tables **User (U)** and **Tweet (T)**, linked via PK-FK relationships. The dataset is detailed in Section 5.2. The tables **User** and **Tweet** as well as **TweetJSON (TJ)** are stored in Parquet format.

Twitter Queries and Views. Queries consist of two parts: (*i*) RA preprocessing ( $Q_{RA}$ ) and (*ii*) LA analysis ( $Q_{LA}$ ). In the  $Q_{RA}$  part, queries construct two matrices: **M** and **N**. The matrix **M** (2M×12; *dense*) is the output of joining **T** and **U**. The construction of matrix **N** is described in Section 5.2. We fix the  $Q_{RA}$  part across all queries and vary the  $Q_{LA}$  part using a set of LA pipelines detailed below. In addition to the views defined in Section 5.2, we define three hybrid RA-LA materialized views:  $V_1^H$ ,  $V_2^H$  and  $V_3^H$ , which store the result of applying rowSums, colSums and matrix multiplication operations over base tables **T** and **U** (viewed as matrices), respectively. Importantly, rewritings based on these views can only be found by *exploiting together LA properties* and *Morpheus's rewrites rules* (we incorporated them in our framework as a set of integrity constraints).

**Discussion**. After construction of **M** and **N** by the  $Q_{RA}$  part in SparkSQL, both matrices are loaded to SystemML to be used in the  $Q_{LA}$  part. Before evaluating an LA pipeline on **M** and **N**, all queries select **N**'s rows ( $Q_{F_{LA}}$ ) with *filter-level* less than 4 (medium). For all of them,

HADAD rewrites the  $Q_{RA}$  part of N as described in Section 5.2.

Q1: For the  $Q_{LA}$  part, the query runs P3.1 (see Table 5.7). HADAD applies several optimizations: (*i*) it rewrites  $(uv^T + \mathbf{N}^T)v$  to  $uv^Tv + \mathbf{N}^Tv$ , where *u* and *v* are synthetic vectors of size  $1000 \times 1$  and  $2\mathbf{M} \times 1$ . First, **N** is ultra sparse, which makes the computation of  $\mathbf{N}^Tv$  extremely efficient. Second, SystemML evaluates  $uv^Tv$  efficiently in one go without intermediates, taking advantage of **t** smm operator (discussed earlier) and mmchain for matrix multiply chains, where the best way to evaluate it computes  $v^Tv$  first, which results in a scalar, instead of computing  $uv^T$ , which results in a dense matrix of size  $2\mathbf{M} \times 1000$ . Alone, SystemML is unable to exploit its own efficient operations for lack of awareness of the LA property Av + Bv = (A + B)v; (*ii*) HADAD also rewrites  $rowSums(X\mathbf{M})$  into  $XV_1^H$ , where  $V_1^H = rowSums(\mathbf{T}) + KrowSums(\mathbf{U})$ , by exploiting the property  $rowSums(X\mathbf{M}) = XrowSums(\mathbf{M})$  together with Morpheus's rewrite rule:  $rowSums(\mathbf{M}) \rightarrow rowSums(\mathbf{T}) + KrowSums(\mathbf{U})^5$ . The rewriting achieves up to  $16.5 \times$  speedup.

Q2: The speedup of 2.5× comes from rewriting the pre-processing part and turning P3.2: ucolSums $((X\mathbf{M})^T)$ +N to  $u(XV_1^H)^T$ +N, where u and X are synthetic matrices of size 2M×1 and 1000×2M, respectively. HADAD exploits colSums $((X\mathbf{M})^T) = (rowSums(X\mathbf{M}))^T$ and  $rowSums(X\mathbf{M}) = XrowSums(\mathbf{M})$  together with Morpheus's rewrite rule:  $rowSums(\mathbf{M}) \rightarrow$  $rowSums(\mathbf{T}) + KrowSums(\mathbf{U})$ . Both the rewriting and the original LA pipeline introduce an unavoidable large dense intermediate of size 2M×1000.

Q3: The query runs ((N+X)v)colSums(M) in the  $Q_{LA}$  part, where dense matrices X and v are of size  $2M \times 1000$  and  $1000 \times 1$ , respectively. HADAD avoids the dense intermediate (N+X) by distributing the multiplication by v and realizing that the sparsity of N yields efficient multiplication. It also directly rewrites colSums(M) to  $V_2^H$ , where  $V_2^H = [colSums(T), colSums(K)U]$  by utilizing one of Morpheus's rewrite rules: colSums $(M) \rightarrow [colSums(T), colSums(K)U]$ . The rewriting  $(Nv + Xv) V_2^H$  and including the rewriting of the  $Q_{RA}$  part of N, achieves  $9.2 \times$  speedup (Figure 5.13(a)-Q3).

 $<sup>{}^{5}</sup>K$  is the unique sparse indicator matrix that captures the primary/foreign key dependencies between **T** and **U**, introduced by Morpheus's rewrite rules [52].

Q4: In the  $Q_{LA}$  part, the query runs P3.4: sum(C+NrowSums(XM)v) (inspired by the COX proportional hazard regression model used in SystemML's test suite [6]), where synthetic dense matrices C, X and v have size  $2M \times 1000, 1000 \times 2M$  and  $1 \times 1000$ , respectively. HADAD (*i*) distributes the sum operation to avoid introducing the dense result of the addition (SystemML includes this rewrite rule but fails to apply it); (*ii*) rewrites rowSums(XM) to  $XV_1^H$ , where  $V_1^H = rowSums(T) + KrowSums(U)$ , by exploiting rowSums(XM) = XrowSums(M) together with Morpheus's rewrite rule  $rowSums(M) \rightarrow rowSums(T) + KrowSums(U)$ . The multiplication chain in the rewriting and the query is efficient since N is sparse. The rewriting of this query (including the rewriting of the  $Q_{RA}$  part of N ) achieves  $3.63 \times$  speedup (Figure 5.13(a)-Q4).

Q5: HADAD's rewriting speeds up this query by 2.3×. It rewrites ucolSums(MX) in P3.5 to  $uV_2^HX$  (see Q3 for  $V_2^H$ 's definition). The view is exploited by HADAD due to utilizing colSums(MX) = colSums(M)X together with the Morpheus's rewrite rule (shown in Q3) for pushing the colSums to the base tables (viewed as matrices) U and T. With the found rewriting, SystemML optimizes the matrix-chain multiplication by computing  $V_2^HX$  first, resulting in the intermediate 1×1000 matrix (X is 12×1000 dense matrix) instead of computing  $uV_2^H$  (u is a dense vector of size 2M×1), which results in the intermediate of size 2M×12. The rewriting and the original pipeline still introduce an unprevented dense intermediate of size 2M×1000.

Q6: The LA pipeline (P3.6) in this query is a variation of P3.1. In addition to distributing the multiplication of v, HADAD rewrites  $rowSums((\mathbf{M} X)^T)$  to  $(V_2^H X)^T$  (see Q3 for  $V_2^H$ 's definition) by exploiting  $rowSums((\mathbf{M} X)^T) = colSums(\mathbf{M} X)^T$  and  $colSums(\mathbf{M} X) = colSums(\mathbf{M})X$ , all together with Morpheus's rewrite rule as illustrated in Q3. The obtained rewriting, including the rewriting of  $Q_{RA}$  part, achieves a speedup of  $13.4 \times$ .

Q7: In the  $Q_{LA}$  part, the query runs the pipeline P3.7:  $XNu + rowSums((M)^T)$ , where sizes of synthetic dense matrices X and u are  $12 \times 2M$  and  $1000 \times 1$ , respectively. HADAD rewrites the pipeline to  $XNu + (V_2^H)^T$ . It discovers the view  $V_2^H$  by exploiting the property  $rowSums((M)^T) =$  $(colSums(M))^T$  and Morpheus rewrite rule  $colSums(M) \rightarrow [colSums(T), colSums(K)U]$ . Notice
that SystemML computes XNu (in the rewriting and the original query) efficiently since N is ultra sparse.

**Q8:** The  $Q_{LA}$  part executes  $\mathbf{N} \odot \text{trace}(C + v \text{colSums}(\mathbf{M}X)C)$ , where the size of v, X and C are  $20K \times 1$ ,  $12 \times 20K$  and  $20K \times 20K$ , respectively. First, HADAD distributes the trace operation (which SystemML does not apply) to avoid the dense intermediate addition. Second, HADAD enables the exploitation of view  $V_2^H$  (see **Q2**) by utilizing  $\text{colSums}(\mathbf{M}X) = \text{colSums}(\mathbf{M})X$ . The resulting multiplication chain is optimized by the order  $v((V_2^H X)C)$ . The final element-wise multiplication with **N** is efficient since **N** is ultra-sparse. The combined  $Q_{RA}$  and  $Q_{LA}$  rewriting speeds up **Q8** by 5.94× (Figure 5.13(a)-Q8).

**Q9:** In addition to the rewriting of the  $Q_{RA}$  part, the speedup of  $3 \times$  also attributes to turning sum(colSums(C)<sup>T</sup> $\odot$ rowSums( $\mathbf{M}$ )) in **P3.9** to sum( $V_3^H$ ), where  $V_3^H = [C\mathbf{T}, (CK)\mathbf{U}]$ . The view  $V_3^H$  is utilized by exploiting the property sum( $C\mathbf{M}$ ) = sum(colSums(C)<sup>T</sup> $\odot$  rowSums( $\mathbf{M}$ )) together with Morpheus's rewrite rule:  $C\mathbf{M} \rightarrow [C\mathbf{T}, (CK)\mathbf{U}]$ . The result of an element-wise multiplication with the dense matrix X in the rewriting and the original pipelines is a dene intermediate (see Figure 5.13(a)-Q9).

Q10: HADAD's rewrite the  $Q_{LA}$ :  $\mathbf{N} \odot \operatorname{sum}((X + C)\mathbf{M})$ , where X and C are dense matrices of size  $1000 \times 1$ M, to  $\mathbf{N} \odot (\operatorname{sum}(X\mathbf{M}) + \operatorname{sum}(V_3^H))$ . The  $V_3^H = [C\mathbf{T}, (CK)\mathbf{U}]$  is utilized by exploiting  $(X + C)\mathbf{M} = X\mathbf{M} + C\mathbf{M}$  together with Morpheus's rewrite rule:  $C\mathbf{M} \rightarrow [C\mathbf{T}, (CK)\mathbf{U}]$ . This optimization goes beyond SystemML's optimization since it does not consider distributing the multiplication of  $\mathbf{M}$ , which then enables exploiting the view and distributing the sum operation to avoid a dense intermediate. The obtained rewriting (with the rewriting of the  $Q_{RA}$  part of  $\mathbf{N}$ ) achieves  $3.91 \times$  (Figure 5.13(a)-Q8).

Twitter Varying Filter Selectivity. We repeat the benchmark for two different textsearch selection conditions: "Trump" and "US election", obtaining 1M and 0.5M rows for N, respectively (we adjust the size of the synthetic matrices for dimensional compatibility). As shown in Figures 5.13(b) and 5.13(c), the benefit of the combined  $Q_{RA}$  and  $Q_{LA}$  stage rewriting



Figure 5.14: Results of micro-hybrid benchmark using MIMIC dataset.

increases with data size, remaining significant across the spectrum.

**MIMIC Dataset Preparation**. MIMIC dataset [88] comprises health data for patients. The total size of the dataset is 46.6 GB, and it consists of : (i) all charted data for all patients and their hospital admission information, ICU stays, laboratory measurements, caregivers' notes, and prescriptions; (ii) the role of caregivers (e.g., MD stands for "medical doctor"), (iii) lab measurements (e.g., ABG stands for "arterial blood gas") and (iv) diagnosis-related groups (DRG) codes descriptions. We use a subset of the dataset, which includes **Patients (P)**, **Admission (A)**, **Service (S)**, and **Callout (C)** tables. Using one-hot encoding, we convert tables' categorical features (columns) to numeric. **MIMIC Queries and Views**. Similar to the Twitter's dataset benchmark, queries consist of two parts: (*i*) pre-processing ( $Q_{RA}$ ) and (*ii*) analysis ( $Q_{LA}$ ). In the  $Q_{RA}$  part, the queries construct two main matrices: **M** and **N**. The matrix **M** (40K×82; *dense*) is the output of joining tables **P** and **A**. The matrix **N** (40K×30K; *ultra-sparse*) is *patient-service* outcome (e.g., cancelled (1), serving (2), etc) matrix, constructed from joining **C** and **S** for all patients who are in "CCU" care unit. We fix the  $Q_{RA}$  part across all queries and vary the  $Q_{LA}$  part using a set of LA pipelines in Table 5.7. For views, we define three cross RA-LA materialized views:  $V_4^H$ ,  $V_5^H$  and  $V_6^H$ , which store the result of applying rowSums, colSums and matrix multiplication operations over **P** and **A** base tables (matrices), respectively. These views can only be found by *exploiting together LA properties* and *Morpheus rewrites' rules* in the same fashion as we detailed in the Twitter's dataset experiment.

**Discussion.** The results exhibit similar trends to Twitter's benchmark. The first run of the benchmark is shown in Figure 5.14(a); both matrices **M** and **N** are loaded in SystemML to be used for the analysis part (varied using the set of pipelines in Table 5.7). Before evaluating an LA pipeline, all queries filter **N**'s rows, where the *outcome* is equal to 2. HADAD applies the same set of optimizations as described in Twitter's benchmark. For the second and third runs of the queries (see Figures 5.14(b) and 5.14(c)), we construct the **N** matrix for patients who are in "TSICU" and "MICU" care units, where **N**'s rows are 20K and 10K, respectively.

#### 5.9.4 Experiments Takeaway

Our experiments with both real-life and synthetic datasets show performance gains across the board, for small rewriting overhead, in both pure LA and hybrid RA-LA settings. This is due to the fact that HADAD's rewriting power strictly subsumes that of optimizers of reference platforms like R, Numpy, TensorFlow, Spark (MLlib), SystemML and MorpheusR. Moreover, HADAD enables optimization where it was not previously feasible, such as across a cascade of unintegrated tools, e.g., SparkSQL for pre-processing followed by SystemML for analytics.

#### 5.10 Limitations

In our LA relational-based reduction, we primarily focus on treating matrices and LA operations expressed over them as a block-box, where we capture important properties of LA operators via integrity constraints. However, it turns out that we can discover more interesting rewrites by opening this block-box, as we show in the example below:

**Example 5.10.1** (LA Rewriting Follows From Standard Properties of Operations Over Numeric Values). Consider an LA expression  $E = sum((X - UV)^2)$ , which defines a typical loss function for approximating a matrix X with a low-rank matrix  $UV^T$  [137], and a view B = XV. After applying standard LA properties, which include expanding the square and distributing the sum, we obtain the following expression:

$$sum(X^2)$$
-2 $sum(X \odot UV^T) + sum((UV^T)^2)$ 

Interestingly, the expression  $sum(X \odot UV^T)$  can be rewritten as  $sum(U \odot XV)$ , where we can match the view B. However, this rewrite does not seem to follow from just using standard LA properties, where we treat matrices as a black box. The equivalence of expressions  $sum(X \odot UV^T)$  and  $sum(U \odot XV)$  follows from standard properties of operations over numeric values.

$$sum(X \odot UV^{T}) = \sum_{i} \sum_{k} x_{ik} \circ (\sum_{j} u_{ij} \circ v_{kj})$$

$$= \sum_{i} \sum_{k} \sum_{j} x_{ik} \circ (u_{ij} \circ v_{kj}) \quad by \ distributivity \ of \ product \ over \ addition$$

$$= \sum_{i} \sum_{j} \sum_{k} u_{ij} \circ (v_{kj} \circ x_{ik}) \quad by \ associativity \ and \ commutativity \ of \ product$$

$$= \sum_{i} \sum_{j} u_{ij} \circ (\sum_{k} x_{ik} \circ v_{kj}) \quad by \ distributivity \ of \ product \ over \ addition$$

$$= sum(U \odot XV)$$

$$= sum(U \odot B)$$

To obtain the rewriting in the example above, this requires extending HADAD rewriting capabilities to rewrite nested conjunctive queries with aggregation under integrity constraints where the body of views can have nested aggregation. Existing studies [54] consider rewriting conjunctive queries with aggregation in the absence of constraints.

Moreover, LA expressions can contain matrix slicing operations. Rewriting such operations requires complex index bounds analysis. Further, some complex analytics tasks can be naturally expressed by iterative LA programs, or LA expressions can be recursively rewritten given special constraints imposed over base matrices. We leave these extensions and investigations to future work. We plan to start from existing work on the safety and equivalence of index-based queries [106] and recent work on recursive query rewriting and optimization [138] and study their applicability in the presence of integrity constraints.

#### 5.11 Conclusion

In this chapter, we presented HADAD, an extensible lightweight framework for optimizing hybrid analytics queries, based on the powerful intermediate abstraction of *a relational model with integrity constraints*. HADAD extends the capability of [31] (Chapter 4) with a reduction from LA (or 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 significant performance gains on various LA and hybrid workloads across popular LA and cross RA-LA platforms.

#### 5.12 Acknowledgement

This chapter contains material from "HADAD: A Lightweight Approach for Optimizing Hybrid Complex Analytics Queries" by Rana Alotaibi, Bogdan Cautis, Alin Deutsch, and Ioana Manolescu, which appeared in Proceedings of the 2019 International Conference on Management of Data (SIGMOD 2021). The dissertation author was the primary investigator of this paper.

This chapter contains material from "HADAD: A Lightweight Approach for Optimizing Hybrid Complex Analytics Queries (Extended Version)" by Rana Alotaibi, Bogdan Cautis, Alin Deutsch, and Ioana Manolescu. This paper is on ArXiv. The dissertation author was the primary investigator of this paper.

# **Chapter 6**

# **Related Wrok**

#### 6.1 Related Work for ESTOCADA

Heterogeneous data integration is an old topic [102, 81, 79, 109] addressed mostly in a single-model (typically relational) setting (see Chapter 2), where cross-models query rewriting was therefore not an issue in these settings. The reference federated Garlic system [79] considered true multi-model settings, but the non-relational stores did not support their own declarative query language (they included, for instance, text documents, spreadsheets, etc.), being instead wrapped to provide an SQL API. Consequently, works on federated databases did not need cross-models rewriting.

The remark "one-size does not fit all" [130] has been recently revisited [104, 87] for heterogeneous stores. [99] uses a relational database as a "cache" for partial results of a MapReduce computation, while [100] considers view-based rewriting in a MapReduce setting. Unlike our work, these algorithms need the data, views, and queries to be in the same data model.

Polystores [68, 27] allow querying heterogeneous stores by grouping similar-model platform into "islands" and explicitly sending queries to one store or another; datasets can also be migrated by the users. Our Local-as-View (LAV) (see Chapter 3 for an overview of LAV systems)

approach is novel and, as we have shown, enables improving the performance of such stores also. The integration of "NoSQL" stores has been considered e.g., in [36] again in a Global-as-View (GAV) (see Chapter 3 for an overview of GAV systems) approach, without the benefits of LAV view-based rewriting.

Adaptive stores for a single data model have been studied e.g., in [82, 30, 56, 93, 92]; views have been also used in [127, 28] to improve the performance of a large-scale distributed relational store. The novelty of ESTOCADA here is to support multiple data models by relying on powerful query reformulation techniques under constraints.

Data exchange tools such as Clio [70, 78] allow migrating data between two different schemas of the same (typically relational and sometimes XML) model (and thus not focused on cross-models rewriting). View-based rewriting and view selection are grounded in the seminal works [102, 81]; the latter focuses on maximally contained rewritings, while we target exact query rewriting, which leads to very different algorithms. Further setting our work apart is the scale and usage of integrity constraints. Our pivot model recalls the ones described in [64, 109] but ESTOCADA generalizes these works by allowing multiple data models both at the application and storage level.

CloudMdsQL [95] is an integration language resembling *QBT<sup>XM</sup>*, and our cross-models view-based rewriting approach could be easily adapted to use CloudMdsQL as its integration language, just like we adapted it to use BigDAWG's. The polystore engine supporting CloudMdsQL does not feature our cross-models view-based query rewriting functionality.

Works on publishing relational data as XML [73] followed the GAV paradigm thus did not raise the (cross-models) view-based rewriting problem we address here.

#### 6.2 Related Work for HADAD

LA Systems/Libraries. SystemML [42] offers high-level R-like LA language, called Declarative Machine Learning (DML). The language offers physical data independence, where the users do not need to specify any data layout or formats. It applies some logical LA pattern-based rewrites and physical execution optimizations based on cost estimates for the latter. The system also supports sparse and dense matrices. SparkMLlib [112] provides LA operations and built-in function implementations of popular ML algorithms on Spark RDDs. The library supports sparse and dense matrices, but the user has to select this type explicitly.

R [17] and NumPy [16] 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 providing a rich set of built-in LA operations. However, LA properties in most of these systems remain unexploited, which makes them *miss opportunities to use their own highly efficient operators* (recall the scenario in Section 5.2). Our experiments (Section 5.9.2) show that evaluation of LA pipelines in these systems can be sped up by more than  $10 \times$  using our rewriting that utilizes: (*i*) LA properties and (*ii*) materialized views.

**Bridging the Gap: RA and LA.** There has been a recent increase in research for unifying the execution of RA and LA expressions [105, 18, 94, 52]. A key limitation of these approaches is that *the semantics of LA operations remains hidden* behind built-in functions or UDFs, preventing performance-enhancing rewrites, as shown in Section 5.9.3.

SPORES [137], SPOOF [44], LARA [97] and RAVEN [91] are closer to our work. SPORES and SPOOF optimize LA expressions by converting them into RA, optimizing the latter, and then converting the result back to an (optimized) LA expression. They are restricted to a small set of selected LA operations (the ones that can only be expressed in RA), while we support significantly more (Section 5.5.1) and model properties, allowing to optimize with them. LARA relies on a declarative domain-specific language for collections and matrices, which can enable optimization (i.e., *selection pushdown*) across the two algebraic abstractions. It heavily focuses on low-level optimization, such as exploiting the choice of data layouts for physical LA operators' optimization. RAVEN takes a step forward by providing intermediate representation to enable cross-optimization between ML and database operators and enhance in-database model inferencing performance. It transforms many classical ML models (e.g., decision tree) into equivalent neural networks (NN) to leverage highly optimized ML engines on CPU/GPU. [39, 48] study the expressive power of cross RA–LA [39] / LA [48] query languages, but do not address semantic optimizations / rewriting under integrity constraints and/or views.

In contrast to HADAD, as all aforementioned solutions do not reason with constraints, they provide no capabilities for *holistic* semantic query optimizations, including RA/LA views-based and LA pure rewritings; such optimizations can bring large performance savings, as shown in Section 5.9. We see HADAD as complementary to all of these platforms, on top of which it can be naturally and portably applied, providing an algorithm for RA/LA views- and constraint-based rewriting.

#### 6.3 Acknowledgement

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This chapter contains material from "HADAD: A Lightweight Approach for Optimizing Hybrid Complex Analytics Queries" by Rana Alotaibi, Bogdan Cautis, Alin Deutsch, and Ioana Manolescu, which appears in Proceedings of the 2019 International Conference on Management of Data (SIGMOD 2021). The dissertation author was the primary investigator of this paper.

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# Chapter 7

## **Conclusion and Future Directions**

In this dissertation, we first presented ESTOCADA (see Chapter 4), which is an extensiblelightweight framework designed to enable semantics query optimizations (including cross-models views-based and integrity constraint-based rewriting) in a polystores context. At the core of ES-TOCADA lies a powerful intermediate abstraction of a *relational model with integrity constraints*, which we used to describe various data models' properties and cross model views. The novelty of ESTOCADA is to reduce the multi-data model rewriting problem to one within the internal relational pivot model, then transform rewritings obtained there into hybrid integration plans. For scalability, we presented a set of optimizations and extensions we contributed to the rewriting engine at the core of ESTOCADA, making it scalable in a polystore setting. Our experiments showed that ESTOCADA improves the performance in natural scenarios for both cross-models and single model user queries.

Then, in Chapter 5, we introduced HADAD, a framework that extends the benefits of semantic query optimizations introduced in ESTOCADA to LA computations, which are crucial for hybrid complex workloads. HADAD is the first framework that brings views-based rewriting under integrity constraints in the context of LA pipelines. It extends the intermediate abstraction used in ESTOCADA to enable reasoning about LA and cross RA-LA computations. This approach makes

it very easy to extend HADAD's semantic knowledge of LA operations or RA-LA rewrite rules by simply declaring appropriate constraints, with no need to change HADAD code, and ensures portability across pure LA and cross RA-LA platforms. Our extensive empirical evaluation showed significant performance gains on diverse LA and RA-LA workloads.

As a natural future work step in the space of hybrid systems, we are targeting the costbased recommendation of optimal cross-models views placement, which suggests views to materialize within each underlying data store to obtain the best performance for a given *hybrid* workload. This task is related to the field of automatic view selection, with the significant difference that prior work was conducted in a single-model setting. View selection starts from an expected query workload and proposes a collection of views to materialize to best support the workload, subject to cost constraints (e.g., the available space). A majority of view selection results were developed for the relational model but mostly abstract away from integrity constraints and thus do not apply directly to our context, in which expressive constraints are prominent and views are expressed as a particular case of constraints. Extending these results to the presence of constraints is a fertile research proposition. Moreover, an interesting follow-up work would be designing efficient incremental maintenance of fragments as the native dataset is updated in a cross-models setting.

# Appendix A

# **Appendix: ESTOCADA**

### A.1 Query Templates Example

 $QT_0 < PID, DOD, GENDER > :-$ MIMIC (M), Child<sub>J</sub> (M, PID, "PATIENTID", "o"), Child<sub>J</sub> (M, DOB, "DOB", "o"), Child<sub>J</sub> (M, DOD, "DOD", "o"), Child<sub>J</sub> (M, GENDER, "GENDER", "o");

QT2<ITID>:-LABITEMS(L), Child<sub>J</sub>(L, ITID, "ITEMID","o"), Child<sub>J</sub>(L,FLUID, "FLUID","o"), Value<sub>J</sub>(FLUID,"Blood");  $\begin{array}{l} QT_1 < \texttt{PID}, \texttt{ITID}, \texttt{VAL}, \texttt{CHT} > :-\\ \texttt{MIMIC}(\texttt{M}),\\ Child_J(\texttt{M}, \texttt{PID}, \texttt{"PATIENTID"}, \texttt{"o"}),\\ Child_J(\texttt{M}, \texttt{A}, \texttt{"ADMISSIONS"}, \texttt{"o"}),\\ Child_J(\texttt{A}, \texttt{LE}, \texttt{"LABEVENTS"}, \texttt{"o"}),\\ Child_J(\texttt{LE}, \texttt{ITID}, \texttt{"ITEMID"}, \texttt{"o"}),\\ Child_J(\texttt{LE}, \texttt{VAL}, \texttt{"VALUE"}, \texttt{"o"}),\\ Child_J(\texttt{LE}, \texttt{CHT}, \texttt{"CHART"}, \texttt{"o"}),\\ Child_J(\texttt{LE}, \texttt{FLAG}, \texttt{"FLAG"}, \texttt{"o"}),\\ Child_J(\texttt{LE}, \texttt{FLAG}, \texttt{"abnormal"}); \end{array}$ 

**Figure A.1**: Query templates  $QT_0$ ,  $QT_1$  and  $QT_2$ .

```
Q<PID, DOB, GENDER, ITID, VAL, CHT> :-
MIMIC(M),
Child<sub>J</sub>(M, PID, "PATIENTID", "o"),
Child<sub>J</sub>(M, DOB, "DOB", "o"),
Child<sub>J</sub>(M, DOD, "DOD", "o"),
Child<sub>J</sub>(M, GENDER, "GENDER", "o"),
Child<sub>J</sub>(M, A, "ADMISSIONS", "o"),
Child<sub>J</sub>(A, LE, "LABEVENTS", "o"),
Child<sub>J</sub>(LE, ITID, "ITEMID", "o"),
Child<sub>J</sub>(LE, CHT, "CHARTTIME", "o"),
Child<sub>J</sub>(LE, CHT, "CHARTTIME", "o"),
Child<sub>J</sub>(LE, FLAG, "FLAG", "o"),
Value<sub>J</sub>(FLAG, "abnormal");
LABITEMS(L),
Child<sub>J</sub>(L, FLUID, "ITEMID", "o"),
Child<sub>J</sub>(L, FLUID, "FLUID", "o"),
Value<sub>J</sub>(FLUID, "Blood");
```

Figure A.2: Query Q produced from combining templates  $QT_0$ ,  $QT_1$  and  $QT_2$ .

SELECT	M.PATIENTID AS PID, M.DOB AS DOB, M.GENDER AS GENDER, L.ITEMID AS ITID, LE.VALUE AS VAL, LE.CHARTTIME AS CHT
FROM	MIMIC AS M, LABITEMS AS L, M.ADMISSIONS AS A,
WHERE	LE.ITEMID=L.ITEMID AND LE.FLAG="abnormal" AND L.FLUID ="Blood"

**Figure A.3**: Query Q (in AsterixDB SQL++ syntax) produced from combining  $QT_0$ ,  $QT_1$  and  $QT_2$ .

# A.2 Snippet of *QBT<sup>XM</sup>* Query Language Grammar

$\langle Query \rangle$	::=	(ForClause) (WhereClause)? (ReturnClause)
$\langle ForClause \rangle$	::=	'FOR' $\langle Block \rangle$ (', ' $\langle Block \rangle$ )*
$\langle WhereClause \rangle$	::=	'WHERE' $\langle Condition \rangle$
<i>(ReturnClause)</i>	::=	'RETURN' $\langle ReturnStatement \rangle$
$\langle Block \rangle$	::=	$\langle Annotation \rangle$ ':' '{' $\langle ModelBlock \rangle$ '}'
$\langle Annotation \rangle$	::=	'PR'   'RK'   'PJ'   'AJ'
$\langle ModelBlock \rangle$	::=	$\langle PRModelBlock \rangle$
		$\langle RKModelBlock \rangle$
		$\langle PJModelBlock \rangle$
		$\langle AJModelBlock \rangle$
$\langle Condition \rangle$	::=	$\langle Atom \rangle$
		('(Condition)')'
		$\langle Condition \rangle$ 'AND' $\langle Condition \rangle$
$\langle Atom \rangle$	::=	$\langle Term \rangle$ '=' $\langle Term \rangle$
$\langle Term \rangle$	::=	$\langle Constant \rangle$
		$\langle Variable \rangle$
$\langle Constant \rangle$	::=	<i>(StringConstant)</i>
		$\langle NumericConstant \rangle$
$\langle ReturnStatement \rangle$	::=	$\langle ModelConstructor \rangle$
		$\langle Variable \rangle$ (',' $\langle Variable \rangle$ )*
$\langle PRModelBlock \rangle$	::=	$\langle PR-Syntax-Specific \rangle$
$\langle RKModelBlock \rangle$	::=	$\langle RK$ -Syntax-Specific $\rangle$

**Notes.** Whenever mentioned "syntax-specific," the understanding is that the parser of the supported fragment of the language corresponding to the annotation will be called. Importantly, the comparison between variables of the same data model conforms to that data model. However, the comparisons between variables of distinct data models are only legal when both variables have string or numeric types.

### **A.3** Encoding of $QBT^{XM}$ Views: $V_1$ and $V_2$

 $V_1$  Forward (IO) Constraints MIMIC(M), Child<sub>J</sub> (M, PID, "PATIENTID", "o"), Child<sub>J</sub> (M, A, "ADMISSIONS", "o"), Child<sub>J</sub> (A, AID, "ADMISSIONID", "o"), Child<sub>J</sub> (A, NE, "NOTEEVENTS", "o"), Child<sub>J</sub> (A, REPORT, "REPORT", "o") ->  $V_1(d_1)$  , Child<sub>J</sub>(d<sub>1</sub>, PID, "PATIENTID", "o"), Child<sub>J</sub>(d<sub>1</sub>, AID, "ADMISSIONID", "o"),  $Child_J(d_1, \text{REPORT}, "\text{REPORT"}, "\circ");$  $V_1$  BACKWARD (OI) CONSTRAINTS:  $V_1(d_1)$ ,  $Child_J(d_1, PID, "PATIENTID", "o"),$ Child<sub>J</sub>(d<sub>1</sub>, AID, "ADMISSIONID", "o"), Child<sub>J</sub>(d<sub>1</sub>, REPORT, "REPORT", "o") -> MIMIC(M), Child<sub>J</sub>(M, PID, "PATIENTID", "o"), Child<sub>J</sub>(M, A, "ADMISSIONS", "o"), Child<sub>J</sub>(A, AID, "ADMISSIONID", "o"), Child<sub>J</sub>(A, NE, "NOTEEVENTS", "o"), Child<sub>J</sub> (NE, REPORT, "REPORT", "o")

Figure A.4: View V<sub>1</sub> forward and backward constraints.

```
V2 (PID, AID, ALOC, ATIME) ->
MIMIC(M),
Child<sub>J</sub>(M, PID, "PATIENTID", "o"),
Child<sub>J</sub>(M, A, "ADMISSIONS", "o"),
Child<sub>J</sub>(A, AID, "ADMISSIONID", "o"),
Child<sub>J</sub>(A, ALOC, "ADMISSIONLOC", "o"),
Child<sub>J</sub>(A, ATIME, "ADMISSIONTIME", "o");
```

Figure A.5: View V<sub>2</sub> backward constraint.

### A.4 Encoding of $QBT^{XM}$ Query $Q_1$ and Decoding $RWQ_1$

 $Q_1 < \text{PID}$ , ALOC, ATIME, DRUG >: -MIMIC(M), Child<sub>J</sub>(M, PID, "PATIENTID", "o"), Child<sub>J</sub>(M, A, "ADMISSIONS", "o"),  $Child_J$  (A, AID, "ADMISSIONID", "o"),  $Child_J$  (A, NE, "NOTEEVENTS", "o"), Child, (NE, REPORT, "REPORT", "o"), Value (REPORT, "contains - coronary artery"), Child<sub>J</sub> (A, ALOC, "ADMISSIONLOC", "o"), Child<sub>J</sub> (A, ATIME, "ADMISSIONTIME", "o"), Child<sub>J</sub>(A, LE, "LABEVENTS", "o"),  $Child_J$ (LE,FLAG,"FLAG","o"), Value(FLAG, "abnormal"), Child<sub>J</sub>(LE, ITEMID, "LABITEMID", "o"), Child<sub>J</sub> (A, P, "PRESCRIPTIONS", "o"), Child<sub>J</sub>(P,DRUG,"DRUG","o") Child<sub>J</sub>(P, DRUGTYPE, "DRUGTYPE", "o"), Value(DRUGTYPE, "additive"), LABITEMS(L), Child<sub>J</sub>(L, ITEMID, "ITEMID", "o"), Child<sub>J</sub>(L, CATEGORY, "CATEGORY", "o"), Value(CATEGORY, "blood");

**Figure A.6**: Relational encoding of  $QBT^{XM}$  query  $Q_1$ .

```
FOR SJ: {V_1/query?q=REPORT: `coronary artery'&
           fl=PID1:PATIENTID, AID1:ADMISSIONID},
                                   AS PID2,
     PR:{SELECT patientID
                       admissionID AS AID<sub>2</sub>,
                       admissionLoc AS ALOC,
                       admissionTime AS ATIME
           FROM
                    V_2},
     PJ:{SELECT v3->'PATIENTID'
                                           AS PID3,
                    v<sub>3</sub>-> 'ADMISSIONID' AS AID<sub>3</sub>,
                    D \rightarrow  DRUG '
                                             AS DRUG
          FROM V_3 v_3,
          jsonb_array_elements(v<sub>3</sub>-> 'PRESCRIPTIONS') D
WHERE D->> 'DRUGTYPE' = 'additive' }
WHERE PID_1 = PID_2 AND
          AID_1 = AID_2 AND
          PID<sub>2</sub>=PID<sub>3</sub> AND
          AID_2 = AID_2
RETURN PID1, AID1, ALOC, ALOC, DRUG
```

**Figure A.7**: Decoding of rewriting *RWQ*<sub>1</sub>.

# **Appendix B**

# Appendix: HADAD

## **B.1 LA Operators Encoding Relations**

Operator	Input(s)	Output	<b>Relational Encoding</b>
Multiplication	Matrices <i>M</i> and <i>N</i>	Matrix <i>R</i>	$\operatorname{multi}_M(M,N,R)$
Hadamard Product	Matrices <i>M</i> and <i>N</i>	Matrix <i>R</i>	$\operatorname{multi}_E(M,N,R)$
Matrix-Scalar Multiplication	Scalar <i>s</i> and Matrix <i>M</i>	Matrix <i>R</i>	$multi_{MS}(s,M,R)$
Addition	Matrices M and N	Matrix <i>R</i>	$\operatorname{add}_M(M,N,R)$
Scalar Addition	Scalars $s_1$ and $s_2$	Scalar <i>r</i>	$\operatorname{add}_S(s_1,s_2,r)$
Division	Matrices M and N	Matrix <i>R</i>	$\operatorname{div}_M(M,N,R)$
Transposition	Matrix M	Matrices R	tr(M,R)
Inversion	Matrix <i>M</i>	Matrices R	$ ext{inv}_M(M,R)$
Scalar Inversion	Scalar s	Scalar <i>r</i>	$ ext{inv}_S(s,r)$
Trace	Matrix <i>M</i>	Scalar s	t trace(M,s)
Matrix Sum	Matrix M	Scalar s	$\operatorname{sum}(M,s)$
Matrix mean	Matrix M	Scalar s	$ extsf{mean}(M,s)$
Matrix max	Matrix M	Scalar s	$\max(M,s)$
Matrix min	Matrix M	Scalar s	$\min(M,s)$
Row sum	Matrix M	Vector R	${\tt rowSums}(M,R)$
Column sum	Matrix M	Vector R	colSums(M,R)
Row Min	Matrix M	Vector R	rowMin $(M,R)$

**Table B.1**: The  $\mathcal{VREM}$  schema (part 1).

Operator	Input(s)	Output	<b>Relational Encoding</b>
Column Min	Matrix M	Vector R	$\operatorname{colMin}(M,R)$
Row Max	Matrix M	Vector R	rowMax $(M,R)$
Column Max	Matrix M	Vector R	colMax(M,R)
Row Mean	Matrix M	Vector R	rowMean $(M,R)$
Column Mean	Matrix M	Vector R	colMean(M,R)
Row Variance	Matrix M	Vector R	rowVar $(M,R)$
Column Variance	Matrix M	Vector R	$ ext{colVar}(M,R)$
Determinant	Matrix M	Scalar s	$\det(M,s)$
Exponential	Matrix M	Matrix <i>R</i>	$\exp(M,R)$
Direct Product	Matrices <i>M</i> and <i>N</i>	Matrix <i>R</i>	$product_D(M,N,R)$
Direct Sum	Matrices <i>M</i> and <i>N</i>	Matrix <i>R</i>	$\operatorname{sum}_D(M,N,R)$
Adjoints	Matrix M	Matrix <i>R</i>	adj $(M,R)$
Diagonal	Matrix M	Matrix <i>R</i>	diag $(M,R)$
Cholesky Decomposition	Matrix M	Matrix L	$ ext{CHO}(M,L)$
QR Decomposition	Matrix <i>M</i>	Matrices $Q$ and $R$	QR(M,Q,R)
LU Decomposition	Matrix <i>M</i>	Matrices L and U	$\mathtt{LU}(M,L,U)$
Pvioted LU Decomposition	Matrix M	Matrices $L, U$ and $P$	$\mathtt{LUP}(M,L,U,P)$

**Table B.2**: The  $\mathcal{VREM}$  schema (part 2).

## **B.2** Key Constraints of LA Encoding Relations

LA Encoding Relation	Key Constraint
name(M,n)	$\forall n, M_1, M_2 \ name(M_1, n) \land name(M_2, n) \rightarrow M_1 = M_2$
size(M, r, c)	$\forall M, r_1, r_2, c_1, r_1 \ size(M, r_1, c_1) \land size(M, r_2, c_2) \rightarrow r_1 = r_2 \land c_1 = c_2$
$\operatorname{multi}_M(M,N,R)$	$orall M, N, R_1, R_2$ multi $_M(M, N, R_1) \wedge$ multi $_M(M, N, R_2) \rightarrow R_1 = R_2$
$ ext{multi}_E(M,N,R)$	$orall M, N, R_1, R_2$ multi $_E(M, N, R_1) \wedge$ multi $_E(M, N, R_2) \rightarrow R_1 = R_2$
$multi_{MS}(s,M,R)$	$\forall s, M, R_1, R_2 \; \texttt{multi}_{MS}(s, M, R_1) \land \texttt{multi}_{MS}(s, M, R_2) \rightarrow R_1 = R_2$
$\operatorname{add}_M(M,N,R)$	$orall M, N, R_1, R_2$ add $_M(M, N, R_1) \wedge  ext{add}_M(M, N, R_2)  o R_1 = R_2$
$\operatorname{add}_S(s_1,s_2,r)$	$\forall s_1, s_2, r_1, r_2 \text{ add}_S(s_1, s_2, r_1) \land \text{add}_S(s_1, s_2, r_2)  ightarrow r_1 = r_2$
$\operatorname{div}_M(M,N,R)$	$orall M, N, R_1, R_2 \operatorname{div}_M(M, N, R_1) \wedge \operatorname{div}_M(M, N, R_2)  ightarrow R_1 = R_2$
tr(M,R)	$orall M, R_1, R_2 \operatorname{tr}(M, R_1) \wedge \operatorname{tr}(M, R_2)  o R_1 = R_2$
$ ext{inv}_M(M,R)$	$orall M, R_1, R_2  ext{ inv}_M(M, R_1) \wedge  ext{inv}_M(M, R_2)  o R_1 = R_2$
$ ext{inv}_S(s,r)$	$orall s, r_1, r_2  ext{ inv}_S(s, r_1) \wedge  ext{ inv}_S(s, r_2)  ightarrow r_1 = r_2$
t trace(M,s)	$orall M, s_1, s_2 \operatorname{trace}(M, s_1) \wedge \operatorname{trace}(M, s_2)  o s_1 = s_2$
$\operatorname{sum}(M,s)$	$orall M, s_1, s_2 \operatorname{sum}(M, s_1) \wedge \operatorname{sum}(M, s_2)  o s_1 = s_2$
${\tt mean}(M,s)$	$orall M, s_1, s_2  ext{ mean}(M, s_1) \wedge  ext{mean}(M, s_2)  o s_1 = s_2$
$\max(M,s)$	$\forall M, s_1, s_2 \max(M, s_1) \land \max(M, s_2) \rightarrow s_1 = s_2$
$\min(M,s)$	$orall M, s_1, s_2 \min(M, s_1) \wedge \min(M, s_2)  ightarrow s_1 = s_2$
<code>rowSums(<math>M,R)</math></code>	$orall M, R_1, R_2$ rowSums $(M, R_1) \wedge$ rowSums $(M, R_2)  o R_1 = R_2$
colSums(M,R)	$orall M, R_1, R_2  ext{ colSums}(M, R_1) \wedge  ext{colSums}(M, R_2)  o R_1 = R_2$
<code>rowMin(<math>M,R)</math></code>	$orall M, R_1, R_2$ rowMin $(M, R_1) \wedge$ rowMin $(M, R_2)  o R_1 = R_2$
$\operatorname{colMin}(M,R)$	$orall M, R_1, R_2  ext{ colMin}(M, R_1) \wedge  ext{ colMin}(M, R_2)  o R_1 = R_2$
$\operatorname{rowMax}(M,R)$	$orall M, R_1, R_2$ rowMax $(M, R_1) \wedge$ rowMax $(M, R_2)  ightarrow R_1 = R_2$

**Table B.3**: Key constraints of LA operators relations (part 1).

LA Encoding Relation	Key Constraint
$ ext{colMax}(M,R)$	$orall M, R_1, R_2  ext{ colMax}(M, R_1) \wedge  ext{ colMax}(M, R_2)  ightarrow$
	$R_1 = R_2$
<code>rowMean(<math>M,R)</math></code>	$orall M, R_1, R_2$ rowMean $(M, R_1) \wedge$ rowMean $(M, R_2)  o$
	$R_1 = R_2$
<code>colMean(<math>M,R)</math></code>	$orall M, R_1, R_2$ colMean $(M, R_1) \wedge$ colMean $(M, R_2)  o$
	$R_1 = R_2$
rowVar $(M,R)$	$orall M, R_1, R_2$ rowVar $(M, R_1) \wedge$ rowVar $(M, R_2)  ightarrow$
	$R_1 = R_2$
$ ext{colVar}(M,R)$	$orall M, R_1, R_2  ext{ colVar}(M, R_1) \wedge  ext{colVar}(M, R_2)  ightarrow$
	$R_1 = R_2$
$\det(M,s)$	$orall M, s_1, s_2$ diag $(M, s_1) \wedge$ diag $(M, s_2)  ightarrow$
	$s_1 = s_2$
$\exp(M,R)$	$\forall M, R_1, R_2 \exp(M, R_1) \wedge \exp(M, R_2) \rightarrow$
	$R_1 = R_2$
$product_D(M,N,R)$	$orall M, N, R_1, R_2  ext{ product}_D(M, N, R_1) \wedge  ext{ product}_D(M, N, R_2)  ightarrow$
	$R_1 = R_2$
$\operatorname{sum}_D(M,N,R)$	$\forall M,N,R_1,R_2 \; \text{sum}_D(M,N,R_1) \land \text{sum}_D(M,N,R_2) \rightarrow$
	$R_1 = R_2$
adj $(M,R)$	$orall M, R_1, R_2$ adj $(M, R_1) \wedge$ adj $(M, R_2)  ightarrow$
	$R_1 = R_2$
diag $(M,R)$	$orall M, R_1, R_2$ diag $(M, R_1) \wedge$ diag $(M, R_2)  ightarrow$
	$R_1 = R_2$
$ ext{CHO}(M,L)$	$orall M, L_1, L_2$ cho $(M, L_1) \wedge$ cho $(M, L_2) \rightarrow$
	$L_1 = L_2$
CHO $(M,L)$	$orall M, L_1, L_2$ cho $(M, L_1) \wedge$ cho $(M, L_2)  ightarrow$
	$L_1 = L_2$
${ t QR}(M,Q,R)$	$orall M, Q_1, Q_2, R_1, R_2 \ { m QR}(M, Q_1, R_1) \wedge { m QR}(M, Q_2, R_2)  ightarrow$
	$Q_1 = Q_2 \wedge R_1 = R_2$
LU $(M,L,U)$	$orall M, L_1, L_2, U_1, U_2 \ { m LU}(M, L_1, U_1) \wedge { m LU}(M, L_2, U_2)  ightarrow$
	$L_1 = L_2 \wedge U_1 = U_2$
t LUP(M,L,U,P)	$\forall M, L_1, L_2, U_1, U_2, P_1, P_2 \sqcup U(M, L_1, U_1, P_1) \land \sqcup U(M, L_2, U_2, P_2) \rightarrow $
	$L_1 = L_2 \wedge U_1 = U_2 \wedge P_1 = P_2$

 Table B.4: Key constraints of LA encoding relations (part 2).

## **B.3** Properties of LA Operations Encoded as Constraints

LA Property	Integrity Constraint		
Addition of Matrices			
M + N = N + M	$orall M, N, R$ add $_M(M, N, R)  ightarrow$ add $_M(N, M, R)$		
(M+N)+D=M+(N+D)	$orall M, N, D, R_1, R_2$ add $_M(M, N, R_1) \wedge \operatorname{add}_M(R_1, D, R_2)$		
	$ ightarrow \exists R_3 \;  ext{add}_M(N,D,R_3) \wedge \;  ext{add}_M(M,R_3,R_2)$		
c(M+N) = cM + cN	$\forall c, M, N, R_1, R_2 \; \; \text{add}_M(M, N, R_1) \land \; \text{multi}_{MS}(c, R_1, R_2)$		
	$ ightarrow \exists R_3, R_4$ multi $_{MS}(c, M, R_3) \land$ multi $_{MS}(c, N, R_4) \land$		
	$\operatorname{add}_M(R_3,R_4,R_2)$		
(c+d)M = cM + dM	$\forall c, d, s, M, R_1 a d d_S(c, d, s) \land \texttt{multi}_{MS}(s, M, R_1)$		
	$ ightarrow \exists R_2, R_3$ multi $_{MS}(c, M, R_2) \land$ multi $_{MS}(d, M, R_3) \land$		
	$\operatorname{add}_M(R_2,R_3,R_1)$		
M + 0 = M	$\rightarrow \exists Zero(O)$		
	$\forall M, n, O  name(M, n) \land Zero(O) \rightarrow \operatorname{add}_M(M, O, M)$		
	$orall O \;\; Zero(O)  ightarrow  ext{add}_M(O,O,O)$		

**Table B.5**: Properties of addition of matrices encoded as integrity constraints.

LA Property	Integrity Constraint		
Multiplication of Matrices			
(MN)D = M(ND)	$orall M, N, D, R_1, R_2$ multi $_M(M, N, R_1) \wedge$		
	$multi_M(R_1,D,R_2)$		
	$ ightarrow \exists R_3$ multi $_M(N,D,R_3) \land$ multi $_M(M,R_3,R_2)$		
M(N+D) = MN + MD	$orall M, N, D, R_1, R_2$ add $_M(N, D, R_1) \wedge$		
	$multi_M(M,R_1,R_2)$		
	$ ightarrow \exists R_3, R_4 \; { m multi}_M(M,N,R_3) \wedge { m multi}_M(M,D,R_4) \wedge$		
	$\operatorname{add}_M(R_3,R_4,R_2)$		
(M+N)D = MD + MD	$orall M, N, D, R_1, R_2$ add $_M(M, N, R_1) \wedge$		
	$\texttt{multi}_{M}(R_1,D,R_2) \rightarrow$		
	$\exists R_3, R_4$ multi $_M(M, D, R_3) \land$ multi $_M(N, D, R_4) \land$		
	$add_M(R_3,R_4,R_2)$		
d(MN) = (dM)N	$orall d, M, N, R_1, R_2$ multi $_M(M, N, R_1) \wedge$		
	$\texttt{multi}_{MS}(d,R_1,R_2) \rightarrow$		
	$\exists R_{3} \text{multi}_{MS}(d, M, R_{3}) \land \text{multi}_{M}(R_{3}, N, R_{2})$		
c(dM) = (cd)M	$\forall c, dM, R_1, R_2$		
	$\operatorname{multi}_{MS}(d,M,R_1) \wedge \operatorname{multi}_{MS}(c,R_1,R_2) \rightarrow$		
	$\exists s \ multi_{S}(c,d,s) \land multi_{MS}(s,M,R_{2})$		
$I_k M = M = M I_z$	$\forall M, n, k, z \text{ name}(M, n) \land size(M, k, z) \rightarrow$		
	$\exists I \ Identity(I) \land size(I,k,k)$		
	$\forall M, n, k, z \text{ name}(M, n) \land size(M, k, z) \rightarrow$		
	$\exists I_1 \ Iaemity(I_1) \land size(I, z, z)$		
	$\forall M, I_1, n, k, z \text{ name}(M, n) \land Size(M, k, z) \land$		
	$1 \operatorname{denuuy}(1) \land \operatorname{Size}(1, \kappa, \kappa) \rightarrow \dots$		
	$\forall M \ L \ n \ k \ z \ name(M \ n) \ \land size(M \ k \ z) \land$		
	$Identity(I) \land size(I, z, z) \rightarrow$		
	multin(M I M)		
Transposition of Matrices			
$(MN)^T = N^T M^T$	$\forall M \ N \ R_1 \ R_2 \text{multi} M (M \ N \ R_1) \land \forall r (R_1 \ R_2) \rightarrow$		
	$\exists R_3, R_4 \operatorname{tr}(M, R_3) \wedge \operatorname{tr}(N, R_4) \wedge \operatorname{multi}_M(R_4, R_3, R_2)$		
$(M+N)^T = M^T + N^T$	$\forall M, N, R_1, R_2 \text{ add}_M(M, N, R_1) \land \text{tr}(R_1, R_2)$		
	$\rightarrow \exists R_3, R_4 \operatorname{tr}(M, R_3) \wedge \operatorname{tr}(N, R_4) \wedge \operatorname{add}_M(R_3, R_4, R_2)$		
$(cM)^T = c(M)^T$	$\forall c, M, R_1, R_2 \text{ multi}_{MS}(c, M, R_1) \land \text{tr}(R_1, R_2)$		
	$\rightarrow \exists R_3 \texttt{tr}(M, R_3) \land \texttt{multi}_{MS}(c, R_3, R_2)$		
$((M)^T)^T = M$	$\forall n, M \ name(M, n) \rightarrow \exists R_1 \operatorname{tr}(M, R_1) \wedge \operatorname{tr}(R_1, M)$		

**Table B.6**: Properties of addition and transposition of matrices encoded as integrity constraints.

LA Property	Integrity Constraint	
Inverses of Matrices		
$((M)^{-1})^{-1} = M$	$\forall n, M \ name(M, n)$	
	$ ightarrow \exists R_1$ inv $_M(M,R_1)$ $\land$ inv $_M(R_1,M)$	
$(MN)^{-1} = N^{-1}M^{-1}$	$\forall M, N, R_1, R_2 $ multi $_M(M, N, R_1) \land inv_M(R_1, R_2)$	
	$ ightarrow \exists R_3, R_4$ inv $_M(M,R_3) \wedge$ inv $_M(N,R_4) \wedge$	
	$multi_M(R_4,R_3,R_2)$	
$((M)^T)^{-1} = ((M)^{-1})^T$	$orall M, R_1, R_2  ext{tr}(M, R_1) \wedge  ext{inv}_M(R_1, R_2)$	
	$ ightarrow \exists R_3  ext{inv}_M(M,R_3) \wedge  ext{tr}(R_3,R_2)$	
$((kM))^{-1} = k^{-1}M^{-1}$	$\forall k, M, R_1, R_2$ multi $_{MS}(k, M, R_1) \land \text{inv}_M(R_1, R_2)$	
	$ ightarrow \exists R_3, s \ inv_S(k,s) \wedge  ext{inv}_M(M,R_3) \wedge$	
	$multi_{MS}(s,R_3,R_2)$	
$M^{-1}M = I = MM^{-1}$	$orall M, R_1, R_2 \operatorname{inv}_M(M, R_1) \wedge \operatorname{multi}_M(R_1, M, R_2)$	
	$\rightarrow$ Identity( $R_2$ )	
	$\forall M, R_1, R_2 \text{ inv}_M(M, R_1) \land \text{multi}_M(M, R_1, R_2)$	
	$\rightarrow$ Identity(R <sub>2</sub> )	
	eterminant of Matrices	
$\det(MN) = \det(M) * \det(N)$	$\forall M, N, R_1, d $ multi $_M(M, N, R_1) \land \det(R_1, d)$	
	$ ightarrow \exists d_1, d_2 \det(M, d_1) \wedge \det(N, d_2) \wedge$	
((z, z), T) $(z, z)$	$multi_{S}(d_{1}, d_{2}, d)$	
$\det((M)^{I}) = \det(M)$	$\forall M, R_1, d \operatorname{tr}(M, R_1) \land \det(R_1, d) \to \det(M, d)$	
$\det((M)^{-1}) = (\det(M))^{-1}$	$orall M, R_1, d$ inv $_M(M, R_1) \wedge \det(R_1, d)  ightarrow$	
	$\exists d_1 \det(M, d_1) \land inv_S(d_1, d)$	
$\det((cM)) = c^{\kappa}\det(M)$	$\forall M, c, k, d \ size(M, k, k) \land multi_{MS}(c, M, d) \rightarrow$	
	$\exists s_1, s_2 pow(c, k, s_1) \land \det(M, s_2) \land \operatorname{multi}_{S}(s_1, s_2, d)$	
$\det((I)) = 1$	$\forall I_1, d \ Identity(I_1) \land \det(I_1, d) \to d = 1$	
	Trace of Matrices	
trace(M+N) = trace(M)	$\forall M \ N \ R_1 \ s_1 \ add_M (M \ N \ R_1) \land$	
+trace $(N)$		
	$\texttt{trace}(R_1,s_1) \rightarrow \exists s_2, s_3 \texttt{trace}(M,s_2) \land$	
	$\texttt{trace}(N,s_3) \land \texttt{add}_S(s_2,s_3,s_1)$	
trace(MN) = trace(NM)	$\forall M, N, R_1, s_1 \text{ multi}_M(M, N, R_1) \land$	
	$trace(R_1,s_1) \to \exists R_2 \; multi_M(N,M,R_2) \land$	
	$trace(R_2, s_1)$	
trace(M') = trace(M)	$\forall M, K_1, s_1  \text{tr}(M, K_1) \land \text{trace}(K_1, s_1) \rightarrow$	
	$trace(M, s_1)$	

**Table B.7**: Properties of inverse, determinant and trace of matrices encoded as integrity constraints.

LA Property	Integrity Constraint	
Direct Sum		
$(M \oplus N) + (C \oplus D) = (M+C) \oplus (N+D)$	$\forall M, N, R_1, C, D, R_2, R_3 $ sum $_D(M, N, R_1)$	
	$\wedge  ext{sum}_D(C,D,R_2) \wedge  ext{add}_M(R_1,R_2,R_3)  o$	
	$\exists R_4, R_5$ add $_M(M, C, R_4) \wedge  ext{add}_M(N, D, R_5)$	
	$\wedge  ext{sum}_D(R_5,R_{3)}$	
$(M \oplus N)(C \oplus D) = (MC) \oplus (ND)$	$\forall M, N, R_1, C, D, R_2, R_3 \text{ sum}_D(M, N, R_1)$	
	$\wedge  ext{sum}_D(C,D,R_2) \wedge  ext{multi}_M(R_1,R_2,R_3)  o$	
	$\exists R_4, R_5$ multi $_M(M, C, R_4) \land$ multi $_M(N, D, R_5)$	
	$\wedge  ext{sum}_D(R_5,R_{3})$	
Exponential of Matrices		
$\exp(0) = I$	$\forall O, R_1 \ Zero(O) \land \exp(O, R_1) \rightarrow Identity(R_1)$	
$\exp(M^T) = \exp(M)^T$	$\forall M, R_1, R_2 \texttt{tr}(M, R_1) \land \exp(R_1, R_2) \rightarrow$	
	$\exists R_3 \exp(M, R_3) \wedge \exp(R_3, R_2)$	

**Table B.8**: Properties of direct sum and exponential of matrices encoded as integrity constraints.

**Table B.9**: Matrix decompositions properties captured as integrity constraints (part1).

Decomposition Property	Integrity Constraint	
Cholesky Decomposition (CD)		
CHO(M) = L		
such that $M = LL^{I}$ ,	$\forall M \ type(M, ``S") \rightarrow \exists \ L_1 \exists L_2 \ CHO(M, L_1) \land$	
where M is SPD		
	$type(L_1, L') \wedge tr(L_1, L_2) \wedge multi_M(L_1, L_2, M)$	
QR Decomposition		
QR(M) = [Q, R] such that $M = QR$	$\forall M \forall n \forall k \; name(M,n) \land size(M,k,k) \rightarrow \exists Q, R$	
	$QR(M,Q,R) \land type(Q,"O") \land type(R,"U") \land$	
	$multi_M(Q,R,M)$	
	$\forall Q type(Q, "O") \rightarrow \exists I QR(Q, Q, I) \land identity(I)$	
	$\wedge$ multi $_M(Q,I,Q)$	
	$\forall R type(R, "U") \rightarrow \exists I QR(R, I, R) \land identity(I)$	
	$\wedge$ multi $_M(I,R,R)$	
	$\forall I \ identity(I) \rightarrow QR(I,I,I)$	

<b>Decomposition Property</b>	Integrity Constraint	
LU Decomposition		
LU(M) = [L, U] such that $M = LU$	$\forall M \forall n \forall k \; name(M,n) \land size(M,k,k) \rightarrow \exists L, U$	
	$\mathtt{LU}(M,L,U) \wedge type(L,``L") \wedge type(U,``U") \wedge \mathtt{multi}_M(L,U,M)$	
	$\forall L type(L, ``L") \rightarrow \exists I LU(L,L,I) \land identity(I) \land multi_M(L,I,L)$	
	$\forall U \ type(U, "U") \rightarrow \exists I \ LU(U, I, U) \land identity(I)$	
	$\wedge$ multi $_M(I,U,U)$	
	$\forall I \ identity(I)  ightarrow  extsf{LU}(I,I,I)$	
Pi	voted LU Decomposition	
LUP(M) = [L, U, P] such that $PM = LU$ , where <i>M</i> is a square matrix	$\forall M \forall n \forall k \; name(M,n) \land size(M,k,z) \rightarrow \exists L,U,P,R$	
	$\begin{split} & \texttt{LUP}(M,L,U,P) \land type(L,``L'') \land type(U,``U'') \land \\ & type(P,``P'') \land \texttt{multi}_M(L,U,R) \land \texttt{multi}_M(P,M,R) \end{split}$	
	$ \forall L type(L, ``L") \land size(L, k, z) \rightarrow \exists I \ \texttt{LUP}(L, L, I, I) \land identity(I) \ \land \texttt{multi}_M(L, I, L) \land \texttt{multi}_M(I, L, L) $	
	$ \begin{array}{l} \forall U \ type(U, ``U") \rightarrow \exists I \ \texttt{LUP}(U, I, U, I) \land \\ identity(I) \land \texttt{multi}_M(I, U, U) \end{array} $	
	$\forall I \ identity(I)  ightarrow  ext{LU}(I, I, I)$	

**Table B.10**: Matrix decompositions properties captured as integrity constraints (part2).

## **B.4** SystemML Rewrite Rules Encoded as Constraints

Rule	Integrity Constraint
$\texttt{sum}(\texttt{tr}(M)) {\rightarrow} \texttt{sum}(M)$	$orall M, R_1, s \operatorname{tr}(M, R_1), \operatorname{sum}(R_1, s)  ightarrow$
	$\operatorname{sum}(M,s)$
$\texttt{sum}(\texttt{rowSums}(M)) {\rightarrow} \texttt{sum}(M)$	$orall M, R_1, s$ rowSums $(M, R_1),$ sum $(R_1, s)  ightarrow$
	$\operatorname{sum}(M,s)$
$\texttt{sum(colSums}(M)) \rightarrow \texttt{sum}(M)$	$orall M, R_1, s$ colSums $(M, R_1),$ sum $(R_1, s)  ightarrow$
	$\operatorname{sum}(M,s)$
$\min(\text{tr}(M)) \! \to \min(M)$	$\forall M, R_1, s \operatorname{tr}(M, R_1), \min(R_1, s) \rightarrow$
	$\min(M,s)$
$\texttt{min}(\texttt{rowMin}(M)) {\rightarrow} \texttt{min}(M)$	$orall M, R_1, s$ rowMin $(M, R_1),$ min $(R_1, s)  ightarrow$
	$\min(M,s)$
$\texttt{min}(\texttt{colMin}(M)) {\rightarrow} \texttt{min}(M)$	$orall M, R_1, s$ colMin $(M, R_1),$ min $(R_1, s)  ightarrow$
	$\min(M,s)$
$\max(\texttt{tr}(M)) \! \to \! \max(M)$	$\forall M, R_1, s \operatorname{tr}(M, R_1), \max(R_1, s) \rightarrow$
	$\max(M,s)$
$\texttt{max(colMax}(M)) {\rightarrow} \texttt{max}(M)$	$orall M, R_1, s$ colMax $(M, R_1),$ max $(R_1, s)  ightarrow$
	$\max(M,s)$
$\texttt{max(rowMax}(M)) {\rightarrow} \texttt{max}(M)$	$orall M, R_1, s$ rowMax $(M, R_1),$ max $(R_1, s)  ightarrow$
	$\max(M,s)$

**Table B.11**: UnnecessaryAggregates rewrite rules encoded as integrity constraints.

Rule	Integrity Constraint
$rowSums(tr(M)) \rightarrow tr(colSums(M))$	$\forall M, R_1, R_2 \operatorname{tr}(M, R_1) \land \operatorname{rowSums}(R_1, R_2)$
	$ ightarrow \exists R_3  ext{ colSums}(M,R_3) \wedge  ext{tr}(R_3,R_2)$
$colSums(tr(M)) \rightarrow tr(rowSums(M))$	$\forall M, R_1, R_2 \operatorname{tr}(M, R_1) \land \operatorname{colSums}(R_1, R_2)$
	$ ightarrow \exists R_3 \;  ext{rowSums}(M,R_3) \wedge  ext{tr}(R_3,R_2)$
$rowMean(tr(M)) \rightarrow tr(colMean(M))$	$\forall M, R_1, R_2 \operatorname{tr}(M, R_1) \wedge \operatorname{colMean}(R_1, R_2)$
	$ ightarrow \exists R_3 \;  ext{rowMean}(M,R_3) \wedge  ext{tr}(R_3,R_2)$
$colMean(tr(M)) \rightarrow tr(rowMean(M))$	$\forall M, R_1, R_2 \operatorname{tr}(M, R_1) \land \operatorname{rowMean}(R_1, R_2)$
	$ ightarrow \exists R_3  ext{ colMean}(M,R_3) \wedge  ext{tr}(R_3,R_2)$
$rowVar(tr(M)) \rightarrow tr(colVar(M))$	$orall M, R_1, R_2 \operatorname{tr}(M, R_1) \wedge \operatorname{rowVar}(R_1, R_2)$
	$ ightarrow \exists R_3 \ { m colVar}(M,R_3) \wedge { m tr}(R_3,R_2)$
$colVar(tr(X)) \rightarrow tr(rowVar(X))$	$orall M, R_1, R_2 \operatorname{tr}(M, R_1) \wedge \operatorname{colVar}(R_1, R_2)$
	$ ightarrow \exists R_3 \;  ext{rowVar}(M,R_3) \wedge  ext{tr}(R_3,R_2)$
$rowMax(tr(M)) \rightarrow tr(colMax(M))$	$orall M, R_1, R_2 \operatorname{tr}(M, R_1) \wedge \operatorname{rowMax}(R_1, R_2)$
	$ ightarrow \exists R_3 \operatorname{colMax}(M,R_3) \wedge \operatorname{tr}(R_3,R_2)$
$\texttt{colMax}(\texttt{tr}(M)) { ightarrow} \texttt{tr}(\texttt{rowMax}(M))$	$orall M, R_1, R_2 \operatorname{tr}(M, R_1) \wedge \operatorname{colMax}(R_1, R_2)$
	$ ightarrow \exists R_3 \;  ext{rowMax}(M,R_3) \wedge  ext{tr}(R_3,R_2)$
$\texttt{rowMin}(\texttt{tr}(M)) {\rightarrow} \texttt{tr}(\texttt{colMin}(M))$	$orall M, R_1, R_2 \operatorname{tr}(M, R_1) \wedge \operatorname{rowMin}(R_1, R_2)$
	$ ightarrow \exists R_3  ext{ colMin}(M,R_3) \wedge  ext{tr}(R_3,R_2)$
$\operatorname{colMin}(\operatorname{tr}(M)) \rightarrow \operatorname{tr}(\operatorname{rowMin}(M))$	$\forall M, R_1, R_2 \operatorname{tr}(M, R_1) \land \operatorname{colMin}(R_1, R_2)$
	$ ightarrow \exists R_3 \;  ext{rowMin}(M,R_3) \wedge  ext{tr}(R_3,R_2)$

**Table B.12**: PushdownUnaryAggTransposeOp rewrite rules encoded asintegrity constraints.

**Table B.13**: SimplifyTraceMatrixMult rewrite rules encoded as integrity constraint.

Rule	Integrity Constraint
$\texttt{trace}(MN) {\rightarrow} \texttt{sum}(M {\odot} \texttt{tr}(N))$	$\forall M, N, R_1, r \text{ multi}_M(M, N, R_1) \land \texttt{trace}(R_1, r)$
	$ ightarrow \exists R_3, R_4  ext{tr}(N, R_3) \land  ext{multi}_E(M, R_3, R_4)$
	$\wedge \texttt{sum}(R_4,r)$

Rule	Integrity Constraint
$\begin{array}{c} \texttt{sum}(MN) \rightarrow \\ \texttt{sum}(\texttt{tr}(\texttt{colSums}(M)) \odot \texttt{rowSums}(N)) \end{array}$	$orall M, N, R_1, r \;  ext{multi}_M(M, N, R_1) \wedge  ext{sum}(R_1, r)  o$
	$\exists R_2, R_3, R_4, R_5 \text{ colSums}(M, R_2) \land \text{tr}(R_2, R_3) \land$
	<code>rowSums</code> $(N,R_4)$ $\wedge$ <code>multi<math>_E(R_3,R_4,R_5)</math></code>
	$\wedge \texttt{sum}(R_5,r)$
$\texttt{colSums}(MN) \rightarrow \texttt{colSums}(M)N$	$orall M, N, R_1, R_2$ multi $_M(M, N, R_1) \wedge$
	<code>colSums</code> ( $R_1,R_2) ightarrow$
	$\exists R_3 \ { t colSums}(M,R_3) \land { t multi}_M(R_3,N,R_2)$
$\texttt{rowSums}(MN) \to M\texttt{rowSums}(N)$	$orall M, N, R_1, R_2$ multi $_M(M, N, R_1) \wedge$
	<code>rowSums</code> $(R_1,R_2) ightarrow$
	$\exists R_3 \; \texttt{rowSums}(N,R_3) \land \texttt{multi}_M(M,R_3,R_2)$

**Table B.14**: SimplifySumMatrixMult rewrite rules encoded as integrityconstraints.

**Table B.15**: SimplifyColWiseAgg rewrite rules encoded as integrity constraints.

Rule	Integrity Constraint
$colSums(M) \rightarrow M$ if x is row vector	$\forall M, n, j \ name(M, n) \land size(M, "1", j)$
	$ ightarrow  ext{colSums}(M,M)$
$colMean(M) \rightarrow M$ if x is row vector	$\forall M, n, j \ name(M, n) \land size(M, "1", j)$
	$ ightarrow  ext{colSums}(M,M)$
$colVar(M) \rightarrow M$ if x is row vector	$\forall M, n, j \ name(M, n) \land size(M, "1", j)$
	ightarrowcolVar $(M,M)$
$colMax(M) \rightarrow M$ if x is row vector	$\forall M, n, j \ name(M, n) \land size(M, "1", j)$
	$ ightarrow  ext{colMax}(M,M)$
$colMin(M) \rightarrow M$ if x is row vector	$\forall M, n, j \ name(M, n) \land size(M, "1", j)$
	$ ightarrow  ext{colMin}(M,M)$
$colSums(M) \rightarrow sum(M)$ if x is col vector	$\forall M, i, R_1 \text{ colSums}(M, R_1) \land size(M, i, "1")$
	$ ightarrow  extsf{sum}(M,R_1)$
$colMean(M) \rightarrow mean(M)$ if x is col vector	$\forall M, i, R_1 \text{ colMean}(M, R_1) \land size(M, i, "1")$
	$ ightarrow$ mean $(M,R_1)$
$colMax(X) \rightarrow max(M)$ if x is col vector	$\forall M, i, R_1 \text{ colMax}(M, R_1) \land size(M, i, ``1")$
	$ ightarrow  extsf{max}(M,R_1)$
$\operatorname{colMin}(M) \rightarrow \min(X)$ if x is col vector	$\forall M, i, R_1 \text{ colMin}(M, R_1) \land size(M, i, ``1")$
	$ ightarrow  extsf{min}(M,R_1)$
$colVar(M) \rightarrow var(M)$ if x is colvector	$orall M, i, R_1$ colVar $(M, R_1) \wedge size(\overline{M, i, ``1`')}$
	$ ightarrow$ var $(M,R_1)$

Rule	Integrity Constraint
rowSums(M) $\rightarrow$ M, if x is col vector	$\forall M, n, i \ name(M, n) \land size(M, i, "1")$
	ightarrowrowSums $(M,M)$
rowMean(M) $\rightarrow$ M, if x is col vector	$\forall M, n, i \ name(M, n) \land size(M, i, "1")$
	ightarrowSums $(M,M)$
rowVar(M) $\rightarrow$ M, if x is col vector	$\forall M, n, i \ name(M, n) \land size(M, i, "1")$
	ightarrow Var $(M,M)$
$rowMax(M) \rightarrow M$ , if x is col vector	$\forall M, n, i \ name(M, n) \land size(M, i, "1")$
	ightarrowMax $(M,M)$
$rowMin(M) \rightarrow M$ , if x is col vector	$\forall M, n, i \ name(M, n) \land size(M, i, "1")$
	ightarrow rowMin $(M,M)$
$rowSums(M) \rightarrow sum(M)$ , if x is row vector	$orall M, j, R_1$ rowSums $(M, R_1) \wedge$
	$size(M, ``1", j) \rightarrow sum(M, R_1)$
$rowMean(M) \rightarrow mean(M)$ , if x is row vector	$orall M, j, R_1$ rowMean $(M, R_1) \wedge$
	$\mathit{size}(M, ``1", j) { ightarrow} \mathtt{mean}(M, R_1)$
$rowMax(X) \rightarrow max(M)$ , if x is row vector	$orall M, j, R_1$ rowMax $(M, R_1) \wedge$
	$size(M, "1", j) \rightarrow \max(M, R_1)$
$rowMin(M) \rightarrow min(X)$ , if x is row vector	$orall M, j, R_1$ rowMin $(M, R_1) \wedge$
	$size(M, "1", j) \rightarrow \min(M, R_1)$
$rowVar(M) \rightarrow var(M)$ , if x is row vector	$orall M, j, R_1$ rowVar $(M, R_1) \wedge$
	$size(M, "1", j) \rightarrow var(M, R_1)$

 Table B.16:
 SimplifyRowWiseAgg rewrite rules encoded as integrity constraints.

 Table B.17:
 PushdownSumOnAdd rewrite rules encoded as integrity constraints.

Rule	Integrity Constraint
$sum(M+N) \rightarrow sum(A) + sum(B)$	$\forall M, N, s \text{ add}_M M, N, s_1) \land \text{sum}(M, s_1) \rightarrow$
	$\exists s_2, s_3 \;  ext{sum}(M, s_2) \wedge  ext{sum}(N, s_3) \wedge$
	$add_s(s_2, s_3, s_1)$

**Table B.18**: ColSums/rowSumsMVMult rewrite rules encoded as integrity constraints.

Rule	Integrity Constraint
$colSums(M*N) \rightarrow tr(N)M,$	
if N is col vector	$\forall M, N, R_1, R_2, i \ size(N, i, "1") \land$
	$\texttt{multi}_E(M,N,R_1) \land \texttt{colSums}(R_1,R_2) \rightarrow$
	$\exists R_3 \texttt{tr}(N,R_3) \land \texttt{multi}_M(R_3,M,R_2)$
$rowSums(M*N) \rightarrow Mtr(N),$	
if N is row vector	$\forall M, N, R_1, R_2, j \ size(N, "1", j) \land$
	$multi_E(M,N,R_1)\land rowSums(R_1,R_2) \rightarrow$
	$\exists R_3 \texttt{tr}(N, R_3) \land \texttt{multi}_M(M, R_3, R_2)$

# **B.5** Additional Results: $\mathcal{P}^{\neg Opt}$ and $\mathcal{P}^{Views}$ Pipelines Rewrites

No.	Rewrite	No.	Rewrite	No.	Rewrite
P1.1	$N^T M^T$	P1.2	$(A+B)^T$	P1.3	$(DC)^{-1}$
P1.4	$Av_1 + Bv_1$	P1.5	D	P1.6	$s_1$ trace $(D)$
P1.7	A	P1.8	$(s_1+s_2)A$	P1.9	$\det(D)$
P1.10	$\operatorname{colSums}(A)^T$	P1.11	$\operatorname{colSums}(A+B)^T$	P1.12	$\operatorname{colSums}(M)N$
D1 13	$\operatorname{sum}(\operatorname{colSums}(M)^T*$	D1 1/	$\operatorname{sum}(\operatorname{colSums}(M)^T*)$	D1 15	M(NM)
11.15	$\operatorname{rowSums}(N))$	1 1.14	$\operatorname{rowSums}(N))$	11.15	
P1 16	$\operatorname{cum}(A)$	D1 17	$\det(C) * \det(D) *$	D1 18	$\operatorname{Sum}(A)$
1 1.10		$\det(C)$	11.10	Sum(A)	
P1.25		M	$T \odot (N^T / (M(NN^T)))$		

**Table B.19**:  $\mathcal{P}^{\neg Opt}$  pipelines rewrites (part 1).

**Table B.20**:  $\mathcal{P}^{\neg Opt}$  pipelines rewrites (part 2).

No.	Rewrite	No.	Rewrite	No.	Rewrite
P2.1	trace(C)+ trace(D)	P2.2	$1/\det(D)$	P2.3	trace(D)
P2.4	$s_1(A+B)$	P2.5	$1/\det((C+D))$	P2.6	$(D^{-1}C)^T$
P2.7	С	P2.8	$\det(C)*\det(D)$	P2.9	trace(DC)+
P2.10	MrowSums(N)	P2.11	$\operatorname{sum}(A) + \operatorname{sum}(B)$	P2.12	$\operatorname{sum}(\operatorname{colSums}(M)^T*$ rowSums $(N))$
P2.13	$(M(NM))^T$	P2.14	(M(NM))N	P2.15	$\operatorname{sum}(A)$
P2.16	$ ext{trace}((DC)^{-1}) +  ext{trace}(D)$	P2.17	$((((C+D)^{-1})^T)D)$	P2.18	$\operatorname{rowSums}(A+B)^T$
P2.25			$u_1v_2^Tv_2 - Xv_2$		

**Table B.21**: The set of views  $V_{exp}$ .

No.	Expression	No.	Expression	No.	Expression
$V_1$	$(D)^{-1}$	<i>V</i> <sub>2</sub>	$(C^T)^{-1}$	<i>V</i> <sub>3</sub>	NM
$V_4$	$u_1v_2^T$	V5	DC	<i>V</i> <sub>6</sub>	A+B
<i>V</i> <sub>7</sub>	$C^{-1}$	$V_8$	$C^T D$	$V_9$	$(D+C)^{-1}$
V <sub>10</sub>	det(CD)	<i>V</i> <sub>11</sub>	det(DC)	V <sub>12</sub>	$(DC)^T$

No.	Rewrite	No.	Rewrite	No.	Rewrite
P1.2	$(V_6)^T$	P1.3	$V_7V_1$	P1.4	$(V_6)v_1$
P1.11	$\operatorname{colSums}(V_6)^T$	P1.15	$M(V_3)$	P1.17	$V_{10}*\det(C)$
P1.19	$V_2$	P1.20	$trace(V_7)$	P1.21	$(C+V_1)^T$
P1.22	$trace(V_9)$	P1.24	$\frac{\texttt{trace}(V_1V_7) +}{\texttt{trace}(D)}$	P1.29	V <sub>5</sub> CCC
P1.30	$V_3 \odot V_3 R^T$	P2.2	$\det(V_1)$	P2.4	$s_1(V6)$
P2.5	$\det(V_9)$	P2.6	$(V_1C)^T$	P2.9	$\frac{\texttt{trace}(V_{12})+}{\texttt{trace}(D)}$
P2.11	$\operatorname{sum}(V_6)$	P2.13	$(MV_3)^T$	P2.14	$MV_3N$
P2.16	$trace(V_7V_1) + traceD)$	P2.17	$(V_9^T)D$	P2.18	$rowSums(V_6)^T$
P2.20	$(MV_3)^T$	P2.21	$V_1(V_1^T(D^Tv_1))$	P2.25	$V_4v_1 - Xv_1$
P1.23	$\det((V_7V_1)+D)$	P2.26	$exp(V_9)$	P2.27	$V_9^T V_5$

**Table B.22**:  $\mathcal{P}^{Views}$  pipelines rewrites.

## **B.6** Additional Results: $\mathcal{P}^{\neg Opt}$ Pipelines: Naïve Cost Model



Figure B.1: P1.2 evaluation before and after rewriting.



Figure B.2: P1.2 evaluation before and after rewriting.



Figure B.3: P1.6 evaluation before and after rewriting.


Figure B.4: P1.8 evaluation before and after rewriting.



Figure B.5: P1.8 evaluation before and after rewriting.



Figure B.6: P1.9 evaluation before and after rewriting.



Figure B.7: P1.10 evaluation before and after rewriting.



Figure B.8: P1.10 evaluation before and after rewriting.



Figure B.9: P1.11 evaluation before and after rewriting.



Figure B.10: P1.11 evaluation before and after rewriting.



Figure B.11: P1.12 evaluation before and after rewriting.



Figure B.12: P1.14 evaluation before and after rewriting.



Figure B.13: P1.15 evaluation before and after rewriting.



Figure B.14: P1.16 evaluation before and after rewriting.



Figure B.15: P1.16 evaluation before and after rewriting.



Figure B.16: P1.17 evaluation before and after rewriting.



Figure B.17: P1.18 evaluation before and after rewriting.



Figure B.18: P1.18 evaluation before and after rewriting.



Figure B.19: P1.25 evaluation before and after rewriting.



Figure B.20: P2.1 evaluation before and after rewriting.



Figure B.21: P2.2 evaluation before and after rewriting.



Figure B.22: P2.3 evaluation before and after rewriting.



Figure B.23: P2.4 evaluation before and after rewriting.



Figure B.24: P2.4 evaluation before and after rewriting.



Figure B.25: P2.5, P2.6 and P2.8 evaluation before and after rewriting.



Figure B.26: P2.9 evaluation before and after rewriting.



Figure B.27: P2.10 evaluation before and after rewriting.



Figure B.28: P2.11 evaluation before and after rewriting.



Figure B.29: P2.11 evaluation before and after rewriting.



Figure B.30: P2.13 evaluation before and after rewriting.



Figure B.31: P2.14 evaluation before and after rewriting.



Figure B.32: P2.15 evaluation before and after rewriting.



Figure B.33: P2.15 evaluation before and after rewriting.



Figure B.34: P2.16 evaluation before and after rewriting.



Figure B.35: P2.18 evaluation before and after rewriting.



Figure B.36: P2.18 evaluation before and after rewriting.

## **B.7** Additional Results: $\mathcal{P}^{\neg Opt}$ Pipelines: MNC Cost Model



Figure B.37: P1.2 evaluation before and after rewriting.



Figure B.38: P1.6 evaluation before and after rewriting.



Figure B.39: P1.8 evaluation before and after rewriting.



Figure B.40: P1.9 evaluation before and after rewriting.



Figure B.41: P1.10 evaluation before and after rewriting.



Figure B.42: P1.11 evaluation before and after rewriting.



Figure B.43: P1.12 evaluation before and after rewriting.



Figure B.44: P1.14 evaluation before and after rewriting.



Figure B.45: P1.15 evaluation before and after rewriting.



Figure B.46: P1.16 evaluation before and after rewriting.



Figure B.47: P1.17 evaluation before and after rewriting.



Figure B.48: P1.18 evaluation before and after rewriting.



Figure B.49: P1.25 evaluation before and after rewriting.



Figure B.50: P2.1 evaluation before and after rewriting.



Figure B.51: P2.4 evaluation before and after rewriting.



Figure B.52: P2.5, P2.6, P2.8 and P2.9 evaluation before and after rewriting.



Figure B.53: P2.10 evaluation before and after rewriting.



Figure B.54: P2.11 evaluation before and after rewriting.



Figure B.55: P2.13 evaluation before and after rewriting.



Figure B.56: P2.14 evaluation before and after rewriting.


Figure B.57: P2.15 evaluation before and after rewriting.



Figure B.58: P2.16 evaluation before and after rewriting.



Figure B.59: P2.18 evaluation before and after rewriting.



## **B.8** Additional Results: $\mathcal{P}^{Views}$ Pipelines

Figure B.60: P1.2 and P1.3 evaluation before and after rewriting.



Figure B.61: P1.4 and P1.11 evaluation before and after rewriting.



Figure B.62: P1.17, P1.19, P1.20 and P1.21 evaluation before and after rewriting.



Figure B.63: P1.22, P1.23, P1.24 and P1.29 evaluation before and after rewriting.



Figure B.64: P2.2, P2.4 and P2.5 evaluation before and after rewriting.



Figure B.65: P2.9, P2.11 and P2.16 evaluation before and after rewriting.

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