What we talk about when we talk about graphs

George Fletcher

Eindhoven University of Technology
The Netherlands

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Open research directions

In general, I am interested in guiding MSc research projects on any topic in data engineering (both theory and systems), broadly conceived.

- relational data, XML data, RDF data, graph data, JSON data, key-value data, ...
- query language design
- query language engineering
- physical and distributed storage strategies (e.g., index design)
- data privacy and security
- data integration
- (big) data analytics
- ...

In this presentation, I will talk about some of my recent research in graph data management. I will conclude with a discussion of several concrete research project proposals.

Open research directions

Before we jump into this presentation, I would like to introduce three concrete research proposals with company partners

- Philips Research (Eindhoven)
- Semaku (Eindhoven)
- Semmtech (Amsterdam)

Open research directions: Philips Research

Context

- Located on the High Tech campus here in Eindhoven.
- Headquarters of the R & D arm of a large, multinational company, so lots of potential to learn, grow, and make many interesting connections
- 1,500 staff, 50 nationalities
- Strong connections with TU/e and the Computer Science faculty

Focus

- is on helping Health Care researchers and professionals to discover and understand connections between patient data and research trial data

Open research directions: Philips Research

Project proposals

(a) Investigate and develop a general methodology for integrating data sources in the so-called TranSMART platform with the Common Information Model (CIM) used at Philips. The CIM is built upon well-known ontologies such as the HL7 RIM, SNOMED CT and LOINC. Trial (or study) data in tranSMART does not enforce or use(s) a standard ontology.

(b) Investigate and develop flexible approaches to modeling clinical trial information and elaborate corresponding formalisms to support machine-processability and reasoning with this information, to be leveraged by a range of relevant applications in the medical domain.

Full details are posted on the seminar homepage

Open research directions: Semaku

Context

- Startup company located in the Strijp-S, here in Eindhoven
- Spin-off of NXP (located on the HTC, in Eindhoven) this year
- Early phase of R & D, so lots of potential for major impact and professional growth

Focus

- is on development of a corporate Semantic Framework/Platform, building on Linked Data standards, and data management as a service. All projects are in cooperation with NXP.

Open research directions: Semaku

Project proposals

(a) Develop an efficient standard data transformation process. The aim is to use as much as possible a "standardized" transformation and update propagation mechanism. The process will be added as a basic service to the Semantic platform, i.e., as core Base Module functionality.

(b) Data modeling: develop an optimal mix for data quality validation when transporting data from source environments to the meta data "cloud" triple store. These validations are a core functionality to the Base Module and will be presented in a Dashboard.

(c) Define a generic strategy for modeling and conversion of data into RDF. What are the pro's and con's for positioning the modeling process at source or destination location or even in between in the enterprise services environment.

Full details are posted on the seminar homepage

Open research directions: Semmtech

Context

- Startup company located in Hoofddorp (next to Amsterdam)
- Established client base, in both public and private sectors
- Early phase of R & D, so lots of potential for major impact and professional growth
- One successful MSc thesis project already with the WE group (Cai 2013)

Focus

- is on development of a generic platform for maintaining and sharing semantically structured information, leveraging Web standards and open-source solutions

Open research directions: Semmtech

Project proposals

(a) Investigate and develop a SPARQL query builder for clients without knowledge of SPARQL. The solution is a module in the generic framework, and should help users understand and reformulate executable queries on semantic data.

(b) Study and develop solutions to rate the (relative) value of a 'resource' in a semantic model by means of a so called 'density-coefficient'. This coefficient should provide modelers and/or administrators more insight into the intensity of use of individual resources, e.g., in ranking search results.

(c) Develop approaches for modeling basic mathematical operations and formulas within a semantic model, e.g., cost calculations of activities, or geometrical calculations for physical objects. After conceptualizing these formulas, the modeled calculations can be automatically performed, using the concepts described by the model.

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What we talk about when we talk about graphs

What we talk about when we talk ...

Sapir-Whorf: "the structure of a language affects the ways in which its speakers conceptualize their world" (Wikipedia)

- Wilhelm von Humboldt (1767-1835): linguistics and philology
  - *The heterogeneity of language and its influence on the intellectual development of mankind* (1836)

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- Franz Boas (1858-1942): anthropology
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  - *Language, mind, and reality* (1942)

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- and in sociology, psychology, philosophy, history (e.g., Kuhn's "Structure of scientific revolutions", Wittgenstein's language games), ...
  - deep and lasting impact across the sciences

What we talk about when we talk ... about graphs

Over the past few years, my colleagues and I have been investigating the ways in which graph query languages affect the way in which clients structure their world.

- i.e., how the choice of query language restricts and shapes concrete graph instances.

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- i.e., how the choice of query language restricts and shapes concrete graph instances.

I will briefly survey this work, which is the result of collaborations with my wonderful colleagues at Delft University of Technology, Eindhoven University of Technology, Hasselt University, Indiana University - Bloomington, and Université Libre de Bruxelles.

Full bibliographic details can be found on the last slide and on my homepage.

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part 1. a brief history of query language expressivity

- “query” expressivity
- “instance” expressivity

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part 2. case studies in instance expressivity

- simple graph languages
- structural indexing for efficient SPARQL query processing

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Notions of language expressivity

Codd (1972)

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- *Codd's solution:* introduce notion of "relational completeness"
  - is your language as expressive as mine (i.e., the relational calculus)?

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  - is your language as expressive as mine (i.e., the relational calculus)?
- ... rather ad hoc

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Towards language-independent notions of expressivity ....

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- for example,
  - *expressible:* nonmonotonic queries
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... primary focus of research community

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- fact: T is expressible from S in Codd's algebra if and only if

$$atoms(T) \subseteq atoms(S)$$

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  and

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i.e., characterization in terms of the structure of S.

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On an (arbitrary) fixed instance S, characterize output space of a given language $\mathcal{L}$

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Given a source instance S and target instance T, can S be mapped to T in $\mathcal{L}$?

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For two objects $o_1, o_2 \in S$, can they be distinguished by an expression $e \in \mathcal{L}$?

$$o_1 \in e(S) \qquad\qquad o_2 \notin e(S)$$

Instance expressivity

The BP result is for the relational calculus on relational databases. Similar structural characterizations later discovered for query languages on nested relations and object-oriented DBs.

However, no significant application was made of these results towards engineering of data management systems.

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Recent results (including applications!)

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- **tree structured data**
  - structural characterizations of XPath fragments (Gyssens et al. PODS 2006)
  - structural indexing for XPath evaluation (Fletcher et al. *Information Systems* 2009, ...)

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  - structural indexing for XPath evaluation (Fletcher et al. *Information Systems* 2009, ...)
- **(arbitrary) graph structured data**
  - structural characterizations of Tarski's relation algebra on directed edge-labeled graphs (Fletcher et al. ICDT 2011; arXiv 2012; FoIKS 2012)
  - structural characterizations of SPARQL fragments (Fletcher et al. DBPL 2011, Picalausa et al. ICDT 2014)
  - structural indexing for accelerated SPARQL evaluation (Picalausa et al. ESWC 2012)

Instance expressivity

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- **tree structured data**
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  - structural indexing for XPath evaluation (Fletcher et al. *Information Systems* 2009, ...)
- **(arbitrary) graph structured data** My focus today
  - structural characterizations of Tarski's relation algebra on directed edge-labeled graphs (Fletcher et al. ICDT 2011; arXiv 2012; FoIKS 2012)
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web, linked data, dataspaces, social networks,
biological networks, ...

graph structured data

Paths in graphs

Relation Algebra already proposed by Alfred Tarski in the 1940s as a basic query language for reasoning about paths in graphs

Paths in graphs

- clear understanding of expressive power of path navigation is essential
- we study Tarski's relation algebra, on arbitrary graphs (as binary relations)
  - query expressiveness
  - instance expressiveness

Graphs

We are interested in navigating over graphs whose edges are labeled by symbols from a finite, nonempty set of labels Λ.

A graph is a relational structure G, consisting of

- a set of nodes V and,
- for every $R \in \Lambda$, a relation $G(R) \subseteq V \times V$, the set of edges with label R.

Graphs

For example, suppose we have

$$V = \mathit{people} \cup \mathit{hospitals} \cup \mathit{diseases}$$

and edge labels

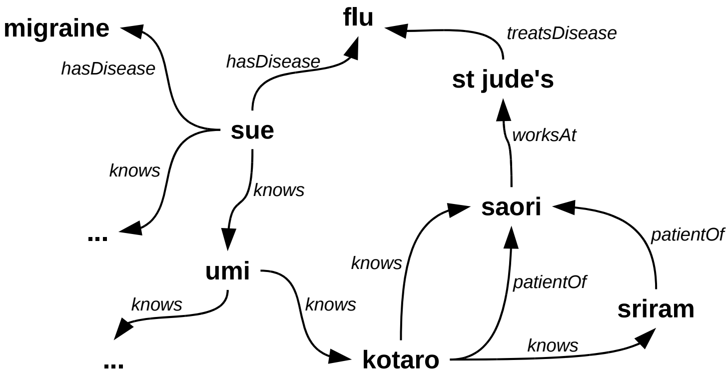
$$\Lambda = \{\text{knows}, \text{worksAt}, \text{patientOf}, \text{hasDisease}, \text{treatsDisease}\}$$

with semantics restricted as:

$$\begin{aligned}
\text{knows} &\subseteq \mathit{people} \times \mathit{people} \\
\text{worksAt} &\subseteq \mathit{people} \times \mathit{hospitals} \\
\text{patientOf} &\subseteq \mathit{people} \times \mathit{people} \\
\text{hasDisease} &\subseteq \mathit{people} \times \mathit{diseases} \\
\text{treatsDisease} &\subseteq \mathit{hospitals} \times \mathit{diseases}.
\end{aligned}$$

Graphs

A small fragment of such a graph



Basic language features

Basic navigational language: algebra $\mathcal{N}$ whose expressions are built recursively from

- the edge labels Λ,
- the primitive $\emptyset$, and
- the primitive id,

using

- composition $(e_1 \circ e_2)$, and
- union $(e_1 \cup e_2)$.

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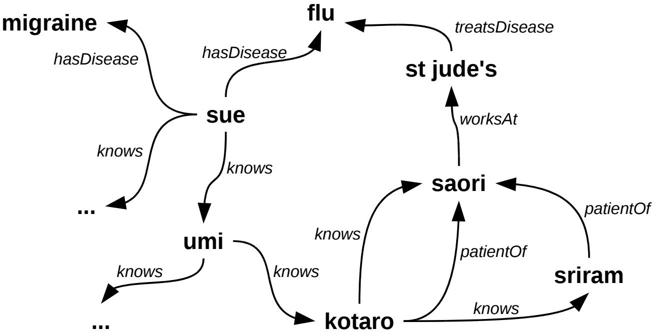
On input graph G, each expression $e \in \mathcal{N}$ defines a path query $e(G) \subseteq \text{adom}(G) \times \text{adom}(G)$, i.e., a binary relation on the *active domain* of G.

Basic language features

In particular, the semantics of $\mathcal{N}$ is inductively defined as follows:

$$
\begin{aligned}
R(G) &= G(R)\,; \\
\emptyset(G) &= \emptyset\,; \\
id(G) &= \{(m,m) \mid m \in \mathrm{adom}(G)\}\,; \\
e_1 \circ e_2(G) &= \{(m,n) \mid \exists p\,((m,p) \in e_1(G) \;\&\; (p,n) \in e_2(G))\}\,; \\
e_1 \cup e_2(G) &= e_1(G) \cup e_2(G)\,.
\end{aligned}
$$

Basic language features



Example: by person, the doctors of their friends

$$\text{knows} \circ \text{patientOf}(G) = \{(\mathit{umi}, \mathit{saori}), (\mathit{kotaro}, \mathit{saori}), \ldots\}$$

Nonbasic language features

The basic algebra $\mathcal{N}$ is extended with the following features:

- diversity (di),
- converse (e^{-1}),
- intersection ($e_1 \cap e_2$),
- difference ($e_1 \setminus e_2$),
- projections ($\pi_1(e)$ and $\pi_2(e)$), and,
- coprojections ($\overline{\pi}_1(e)$ and $\overline{\pi}_2(e)$).

Tarski's algebra consists of the language having all basic and nonbasic features.

Nonbasic language features

The semantics of these language extensions is as follows:

$$
\begin{aligned}
di(G) &= \{(m,n) \mid m,n \in \mathrm{adom}(G) \ \&\ m \neq n\}\,;\\
e^{-1}(G) &= \{(m,n) \mid (n,m) \in e(G)\}\,;\\
e_1 \cap e_2(G) &= e_1(G) \cap e_2(G)\,;\\
e_1 \setminus e_2(G) &= e_1(G) \setminus e_2(G)\,;\\
\pi_1(e)(G) &= \{(m,m) \mid m \in \mathrm{adom}(G) \ \&\ \exists n\,(m,n) \in e(G)\}\,;\\
\pi_2(e)(G) &= \{(m,m) \mid m \in \mathrm{adom}(G) \ \&\ \exists n\,(n,m) \in e(G)\}\,;\\
\overline{\pi}_1(e)(G) &= \{(m,m) \mid m \in \mathrm{adom}(G) \ \&\ \neg\exists n\,(m,n) \in e(G)\}\,;\\
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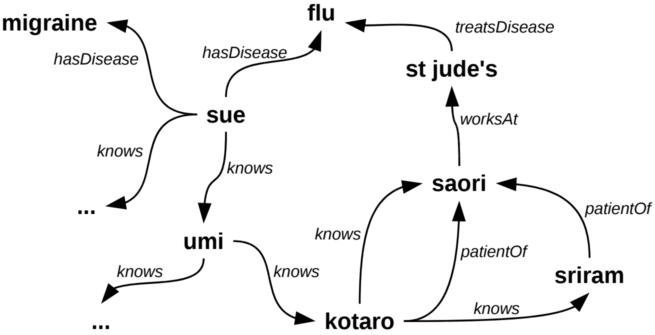
Nonbasic language features



Example: people with untreatable diseases

$$\text{hasDisease} \setminus (\text{hasDisease} \circ \pi_2(\text{treatsDisease}))(G) = \{(\textit{sue}, \textit{migraine}), \ldots\}$$

Language equivalence

A marked structure $\mathbf{G}$ is a triple (G, a, b) where G is a graph, and (a, b) is an ordered pair of nodes from G.

For two marked structures $\mathbf{G}_1 = (G_1, a_1, b_1)$ and $\mathbf{G}_2 = (G_2, a_2, b_2)$, we write $\mathbf{G}_1 \equiv \mathbf{G}_2$ if $\mathbf{G}_1$ and $\mathbf{G}_2$ are indistinguishable in the RA, i.e., for every expression e in the algebra, whenever $(a_1, b_1) \in e(G_1)$, it also holds that $(a_2, b_2) \in e(G_2)$, and vice versa.

Structural equivalence

Let G_1 and G_2 be two graphs with node sets V_1 and V_2, respectively. A non-empty relation $Z \subseteq V_1^2 \times V_2^2$ is a bisimulation between G_1 and G_2 if it satisfies the following conditions

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Atoms if (a_1, b_1, a_2, b_2) is in Z, then $(a_1, b_1) \in R(G_1)$ if and only if $(a_2, b_2) \in R(G_2)$, for all $R \in \Lambda$;

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Forth if $(a_1, b_1, a_2, b_2) \in Z$, then

- for each $c_1 \in V_1$ there exist $c_2 \in V_2$ such that both (a_1, c_1, a_2, c_2) and (c_1, b_1, c_2, b_2) are in Z;
- if $a_1 = b_1$ then $a_2 = b_2$; and,
- $(b_1, a_1, b_2, a_2) \in Z$.

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- if $a_1 = b_1$ then $a_2 = b_2$; and,
- $(b_1, a_1, b_2, a_2) \in Z$.

Back is the same as *Forth*, only with the roles of G_1 and G_2 reversed.

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Coupling Theorem

Let $\mathbf{G}_1 = (G_1, a_1, b_1)$ and $\mathbf{G}_2 = (G_2, a_2, b_2)$ be finite marked structures. Then

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For positive algebra fragments, we similarly obtained new simulation characterizations, where the *Back* condition is dropped.

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part 2. case studies in instance expressivity

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- **structural indexing for efficient SPARQL query processing**

part 3. research directions

Structural indexing

Up to this point, our investigations of Tarski's algebra have focused on the relative expressive power of the various fragments of the algebra.

We have also obtained structural characterizations for a core fragment of SPARQL, the W3C's recommendation language for the RDF graph data model, with an eye towards "structural" index design (Fletcher et al. DBPL 2011, Picalausa et al. ICDT 2014)

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The basic idea here is to group together structurally equivalent RDF triples, since the language cannot distinguish them, and build access mechanisms on top of these "blocks."

We then use this index to accelerate query processing on a reduced search space (Picalausa et al. ESWC 2012).

Partitioning massive graphs under bisimulation

Note that this approach only works if computing bisimulation partitioning of a graph is practical.

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Efficient *main memory* approaches to bisimulation partitioning have been studied since the 80's, as bisimilarity is a fundamental notion arising in a wide range of contexts (e.g., set theory, distributed computing, process modeling, ...).

However, there has been no approach to compute bisimulation on massive disk-resident graphs.

Partitioning massive graphs under bisimulation

To address this, we have developed the first I/O-efficient approaches to bisimulation partitioning of massive graphs (Hellings et al. SIGMOD 2012; Luo et al. CIKM 2013).

We have also developed the first effective MapReduce solution for this problem (Luo et al. BNCOD 2013).

Structural indexing for SPARQL

SaintDB: quad-store based structural indexing and query processing (Picalausa et al. ESWC 2012).

- We introduced the first triple-based structural index for RDF.
- This index is formally coupled to practical core fragment of SPARQL.
- Our initial empirical study shows that the approach is profitable
  - Empirical analysis on community benchmark data/queries demonstrates competitiveness with RDF-3X on broad range of query scenarios, with up to multiple orders of magnitude reduction in query processing costs.

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- query language engineering
- physical and distributed storage strategies (e.g., index design)
- data privacy and security
- data integration
- (big) data analytics
- ...

Open research directions

(a) Building on the work on path indexing for tree-structured data, study structural path indexing and query optimization for fragments of Tarski's algebra on graph-structured data. (see Fletcher et al. *Information Systems*, 2009; and Sofía Brenes Barahona, *Structural summaries for efficient XML query processing*, PhD thesis, Indiana University, Bloomington, 2011)

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(b) Luo et al. (CIKM 2013) just use flat files and other simple data structures, to establish I/O efficient bisimulation. Study more sophisticated data structures and (join) algorithms, towards applications of the partition (e.g., in path query processing).

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(c) Picalausa et al. (ESWC 2012) studied three basic approaches to physical plan optimization/generation over the quad-store representation of a bisimulation-partitioned triple store. Develop and study a general framework for query optimization over RDF structural indexes.

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(d) Study other basic applications of structural characterizations of query languages, e.g.,

- query language design in social network analysis (cf. Marx and Masuch, *Social Networks* 25(1), 2003; Fan ICDT 2012)
- structure-sensitive privacy and security mechanisms
- dynamic structure (e.g., ontology) extraction, via language-distinguishability (cf. Cai, MSc Thesis, TU/e, 2013)
- visualizing language-induced structures (e.g., interplay of ontological knowledge)

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(e) Structure preserving network sampling: how to preserve graph structure while sampling massive graphs (e.g., the sample should have the same degree-distribution structure and the same bisimulation reduction graph as the original graph, or some good approximation(s) thereof).

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(f) JSON vs. XML: what is different? what is the same? Study JSON native storage and indexing (external memory and distributed), for JSONiq queries.

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