Non-Standard-Datenbanken und Data Mining

Graphdatenbanken

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Acknowledgements for slides 2-36

Graph databases and graph querying

Advances in Data Management, 2019

Dr. Petra Selmer
Query languages standards & research group, Neo4j

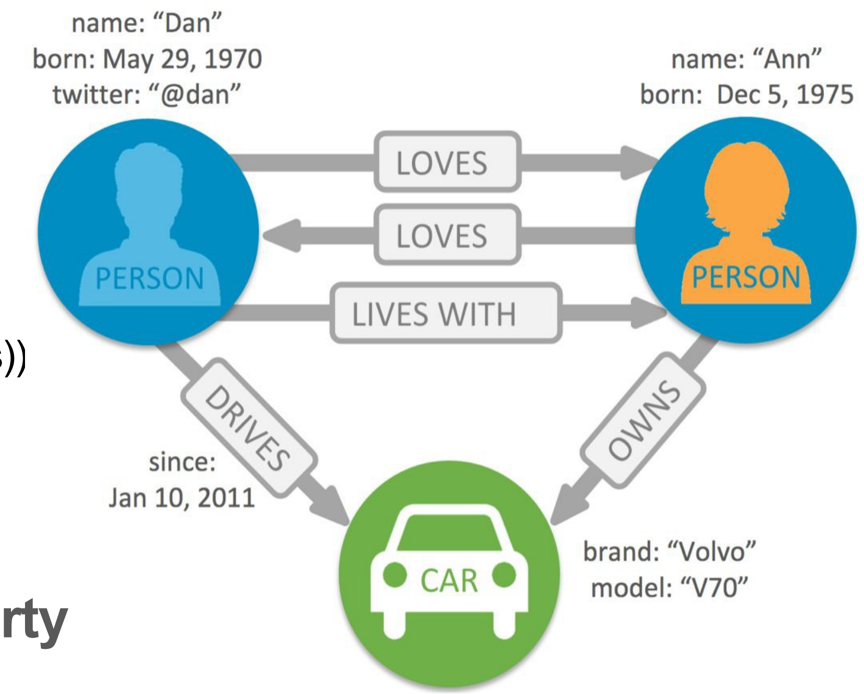
Property graph

Node

- Represents an entity within the graph
- Has zero or more *labels*
- Has zero or more *properties*
  (which may differ across nodes with the same label(s))

Edge

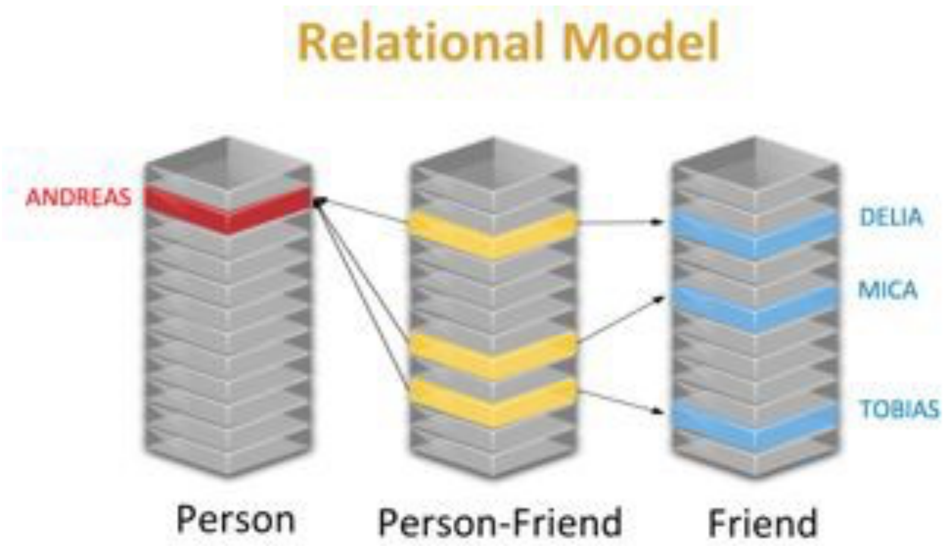
- Adds structure to the graph
  (provides semantic context for nodes)
- Has one *type*
- Has zero or more *properties*
- Relates nodes by *type* and *direction*
- Must have a start and an end node

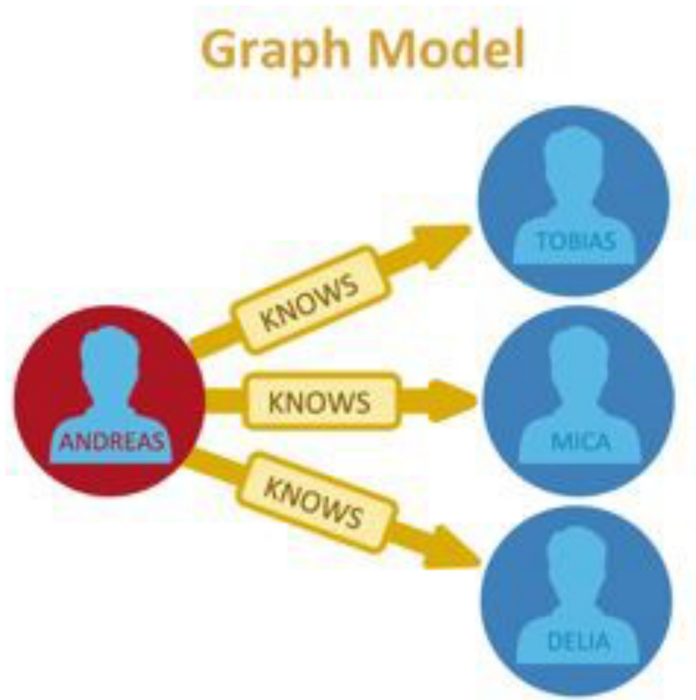


Property

- Name-value pair (map) that can go on nodes and edges
- Represents the data: e.g. name, age, weight etc
- *String* key; typed value *(string, number, bool, list)*

Relational vs. graph models





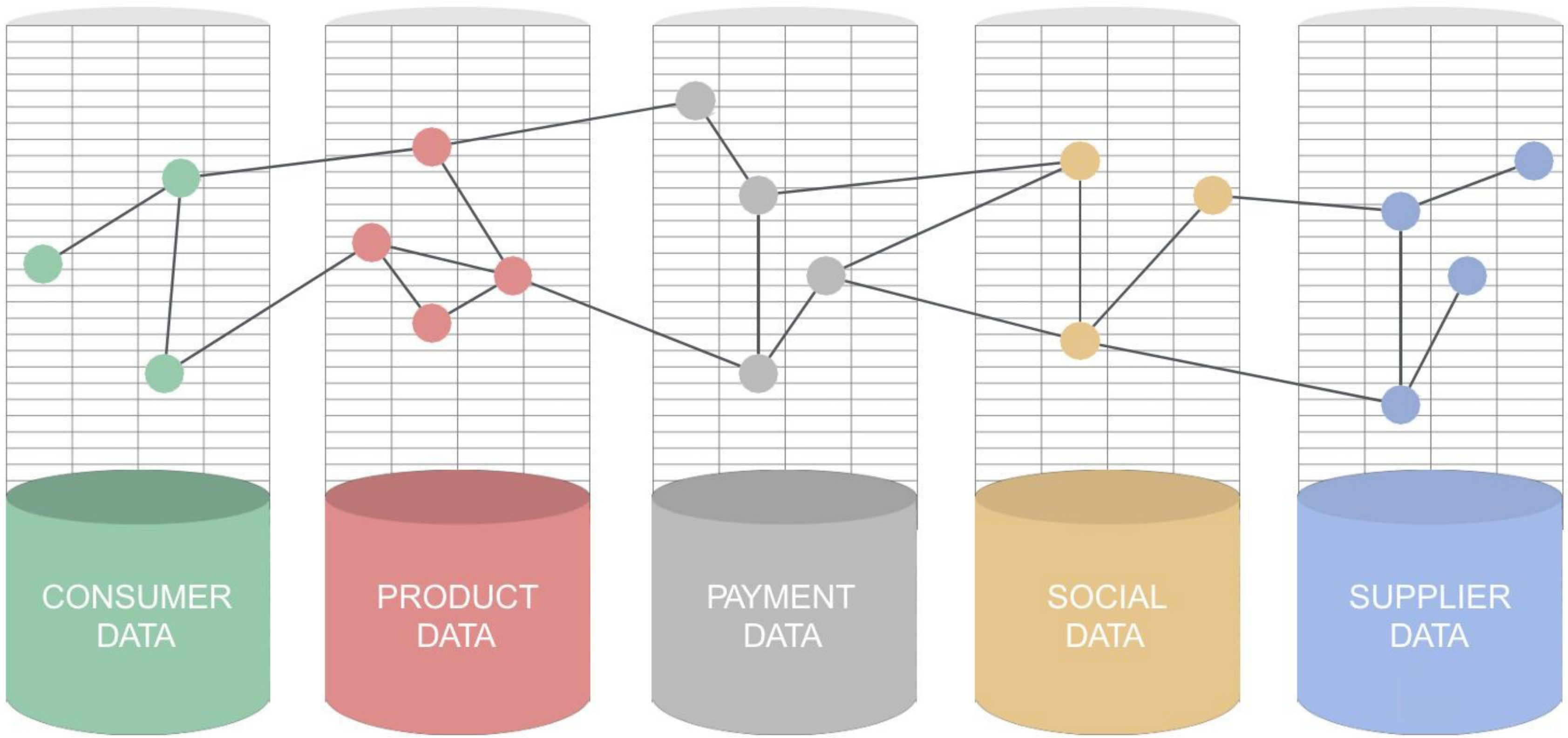
Relationship-centric querying

Query complexity grows with need for JOINs

Graph patterns not *easily* expressible in SQL

- Recursive queries
- Variable-length relationship chains
- Paths cannot be returned natively

Data Integration



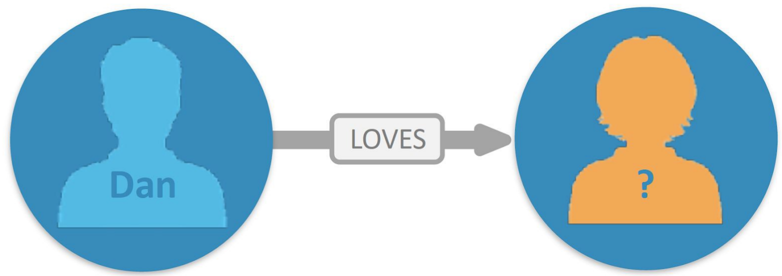
Introducting Cypher

Declarative **graph pattern matching** language

SQL-like syntax

- DQL for reading data
- DML for creating, updating and deleting data
- DDL for creating constraints and indexes

Searching for (matching) graph patterns



NODE   Relationship   NODE

MATCH (:Person { name:"Dan"}) -[:LOVES]-> (whom) **RETURN** whom

LABEL   PROPERTY   VARIABLE

Nodes:

- () or (n)
  - Surround with parentheses
  - Use an alias n to refer to our node later in the query
- (n:Label)
  - Specify a Label starting with a colon :
  - Used to group nodes by roles or types (similar to tags)
- (n:Label {prop: 'value'})
  - Nodes can have properties

Edges/Relationships:

- --> or -[r:TYPE]->
  - Wrapped in hyphens and square brackets
  - A relationship type starts with a colon :
- <>
  - Specify the direction of the relationships
- -[:KNOWS {since: 2010}]->
  - Relationships can have properties

Cypher: patterns

Used to query data

```
(n:Label {prop: 'value'})-[:TYPE]->(m:Label)
```

Find Alice who knows Bob In other words:

find Person with the name 'Alice'

who KNOWS

a Person with the name 'Bob'

```
(p1:Person {name: 'Alice'})-[:KNOWS]->(p2:Person {name: 'Bob'})
```

DML: Creating and updating data

```
// Data creation and manipulation
CREATE (you:Person)
SET you.name = ‘Jill Brown’
CREATE (you)-[:FRIEND]->(me)


// Either match existing entities or create new entities.
// Bind in either case
MERGE (p:Person {name: ‘Bob Smith’})
    ON CREATE SET p.created = timestamp(), p.updated = 0
    ON MATCH SET p.updated = p.updated + 1
RETURN p.created, p.updated
```

DQL: Reading data

```
// Pattern description (ASCII art)
MATCH (me:Person)-[:FRIEND]->(friend)
// Filtering with predicates
WHERE me.name = 'Frank Black'
AND   friend.age > me.age
// Projection of expressions
RETURN toUpper(friend.name) AS name, friend.title AS title
// Order results
ORDER BY name, title DESC
```

Multiple pattern parts can be defined in a single match clause (i.e. *conjunctive* patterns); e.g:
MATCH (a)-(b)-(c), (b)-(f)

Input: a property graph
Output: a table

Queries are graphs

Cypher patterns

Node patterns

```
MATCH ( ),  (node), (node:Node), (:Node), (node {type:"NODE"})
```

Relationship patterns

```
MATCH()-->(),  ()<--(),  ()--()                  // Single relationship
MATCH()-[edge]->(),  (a)-[edge]->(b)             // With binding
MATCH()-[:RELATES]->()                           // With specific relationship type
MATCH()-[edge {score:5}]->()                     // With property predicate
MATCH()-[r:LIKES|:EATS]->()                      // Union of relationship types
MATCH()-[r:LIKES|:EATS {age: 1}]->()             // Union with property predicate
                                                 (applies to all relationship types specified)
```

Cypher patterns

Variable-length relationship patterns

```
MATCH (me)-[:FRIEND*]-(foaf)             // Traverse 1 or more FRIEND relationships
MATCH (me)-[:FRIEND*2..4]-(foaf)         // Traverse 2 to 4 FRIEND relationships
MATCH (me)-[:FRIEND*0..]-(foaf)          // Traverse 0 or more FRIEND relationships
MATCH (me)-[:FRIEND*2]-(foaf)            // Traverse 2 FRIEND relationships
MATCH (me)-[:LIKES|HATES*]-(foaf)        // Traverse union of LIKES and HATES 1 or more times

// Path binding returns all paths (p)
MATCH p = (a)-[:ONE]-()-[:TWO]-()-[:THREE]-()
// Each path is a list containing the constituent nodes and relationships, in order
RETURN p

// Variation: return all constituent nodes of the path
RETURN nodes(p)
// Variation: return all constituent relationships of the path
RETURN relationships(p)
```

Cypher: linear composition and aggregation

Parameters: $param

```
1: MATCH (me:Person {name: $name})-[:FRIEND]-(friend)
2: WITH me, count(friend) AS friends
3: MATCH (me)-[:ENEMY]-(enemy)
4: RETURN friends, count(enemy) AS enemies
```

Aggregation
(grouped by 'me')

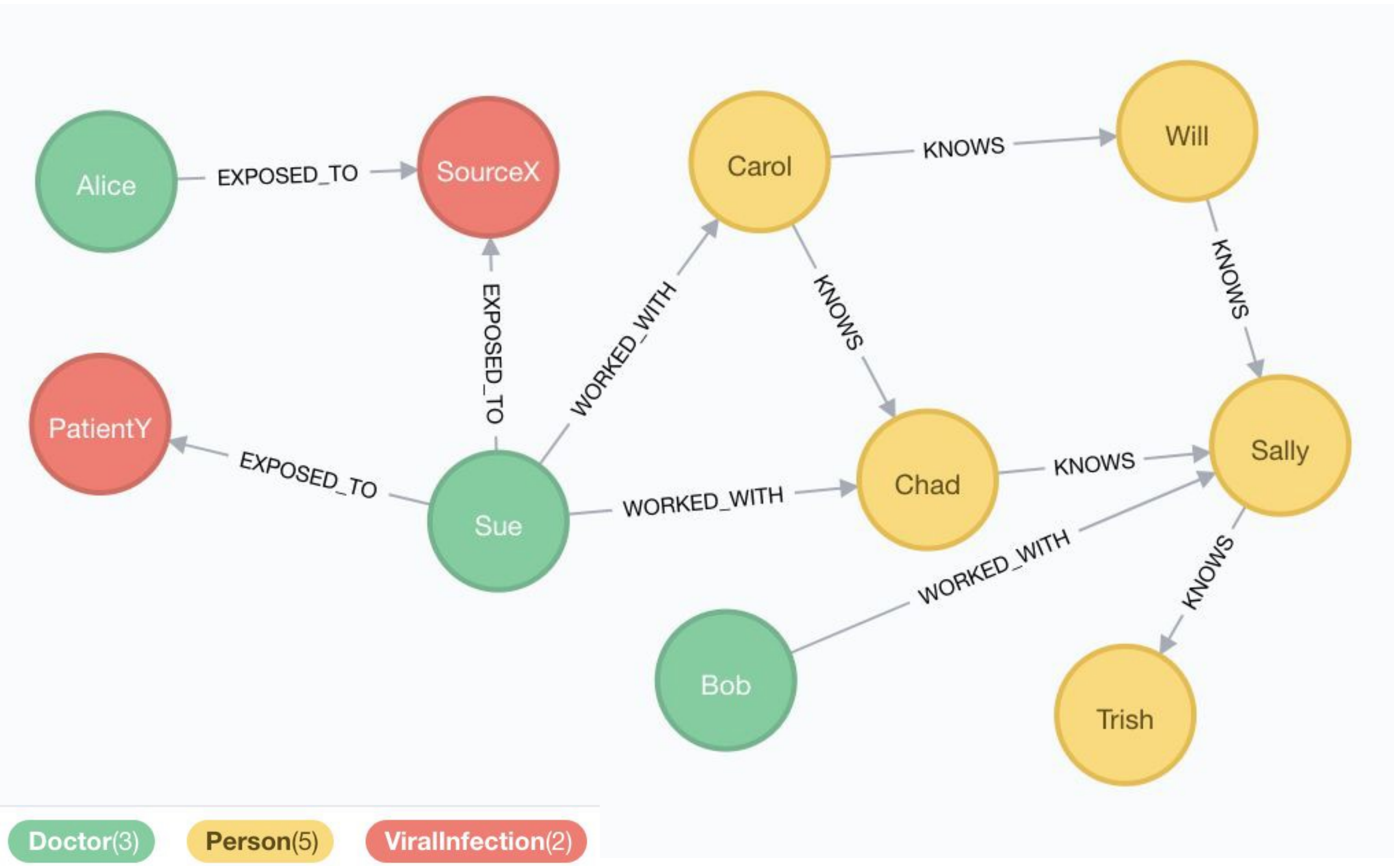
WITH provides a *horizon*, allowing a query to be subdivided:

- Further matching can be done after a set of updates
- Expressions can be evaluated, along with aggregations
- Essentially acts like the pipe operator in Unix

Linear composition

- Query processing begins at the top and progresses linearly to the end
- Each clause is a function taking in a table **T** (*line 1*) and returning a table **T'**
- **T'** then acts as a driving table to the next clause (*line 3*)

Example query: epidemic!



Assume a graph G containing doctors who have potentially been infected with a virus….

Example query

The following Cypher query returns the name of each doctor in G who has perhaps been exposed to some source of a viral infection, the number of exposures, and the number of people known (both directly and indirectly) to their colleagues

```
MATCH (d:Doctor)
 OPTIONAL MATCH (d)-[:EXPOSED_TO]->(v:ViralInfection)
  WITH d, count(v) AS exposures
MATCH (d)-[:WORKED_WITH]->(colleague:Person)
 OPTIONAL MATCH (colleague)<-[:KNOWS*]-(p:Person)
RETURN d.name, exposures, count(DISTINCT p) AS thirdPartyCount
```

Example query

```
1: MATCH (d:Doctor)
2: OPTIONAL MATCH (d)-[:EXPOSED_TO]->(v:ViralInfection)
```

Matches all :Doctors, along with whether or not they have been :EXPOSED_TO a :ViralInfection

OPTIONAL MATCH analogous to outer join in SQL

- Produces rows provided entire pattern is found
- If no matches, a single row is produced in which the binding for *v* is `null`

d	v
Sue	SourceX
Sue	PatientY
Alice	SourceX
Bob	*null*

Although we show the *name* property (for ease of exposition), it is actually the *node* that gets bound

Example query

`3: WITH d, count(v) AS exposures`

WITH projects a subset of the variables in scope - *d* - and their bindings onwards (to 4).
WITH also computes an aggregation:

- *d* is used as the grouping key implicitly (as it is not aggregated) for count()
- All non-null values of v are counted for each unique binding of d
- Aliased as *exposures*

The variable *v* is no longer in scope after 3

This binding table is now the driving table for the **MATCH** in 4

d	exposures
Sue	2
Alice	1
Bob	0

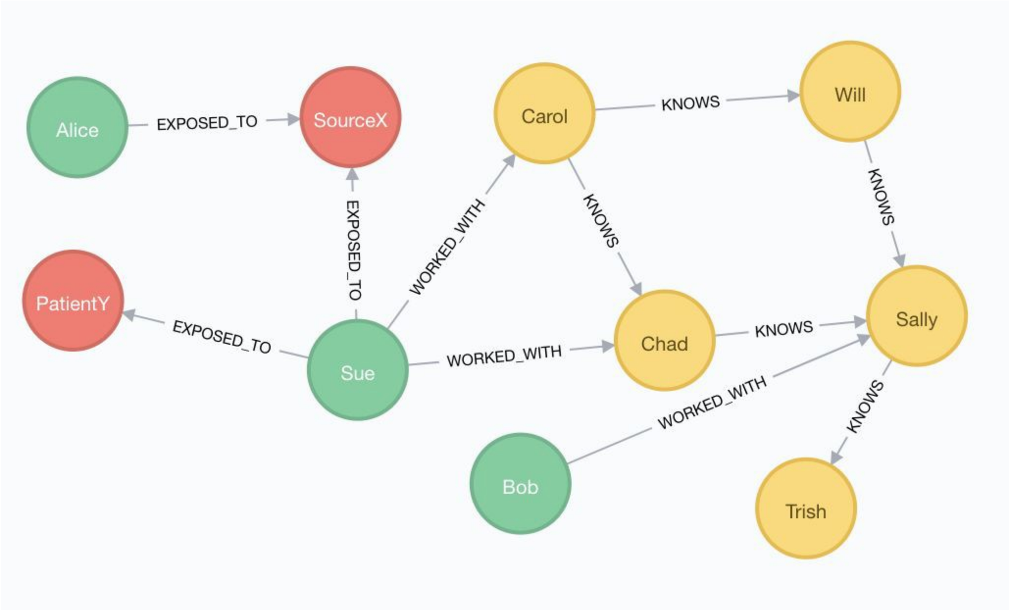
Example query

4 : **MATCH**(d)-[:WORKED_WITH]->(colleague:Person)

Uses as driving table the binding table from 3

Finds all the colleagues (:Person) who have :WORKED_WITH our doctors

d	exposures	colleague
Sue	2	Chad
Sue	2	Carol
Bob	0	Sally



Example query

5: **OPTIONAL MATCH** (colleague)<-[:KNOWS*]-(p:Person)

Finds all the people (:Person) who :KNOW our doctors' colleagues (only in the one direction), both directly and indirectly (using :KNOWS* so that one or more relationships are traversed)

d	exposures	colleague	p
Sue	2	Chad	Carol
Sue	2	Carol	*null*
Bob	0	Sally	Will
Bob	0	Sally	Chad
Bob	0	Sally	Carol*
Bob	0	Sally	Carol*

No (Carol)<-[:KNOWS]-() pattern in G

* This is due to the :KNOWS* pattern: *Carol* is reachable from *Sally* via *Chad* and *Will*
(*Carol* :KNOWS *Will* and *Chad*)

Example query results

```
MATCH (d:Doctor)
OPTIONAL MATCH (d)-[:EXPOSED_TO]->(v:ViralInfection)
WITH d, count(v) AS exposures
MATCH (d)-[:WORKED_WITH]->(colleague:Person)
OPTIONAL MATCH (colleague)<-[:KNOWS*]-(p:Person)
RETURN d.name, exposures, count(DISTINCT p) AS thirdPartyCount
```

d.name	exposures	thirdPartyCount
Bob	0	3 (Will, Chad, Carol)
Sue	2	1 (Carol)

Other functionality

Aggregating functions

`count(), max(), min(), avg(), ...`

Operators

Mathematical, comparison, string-specific, boolean, list

Map projections

Construct a map projection from nodes, relationships and properties

CASE expressions

Functions (scalar, list, mathematical, string, UDF, procedures)

Property graphs are everywhere

Many implementations

Amazon Neptune, Oracle PGX, Neo4j Server, SAP HANA Graph, AgensGraph (over PostgreSQL), Azure CosmosDB, Redis Graph, SQL Server 2017 Graph, Cypher for Apache Spark, Cypher for Gremlin, SQL Property Graph Querying, TigerGraph, Memgraph, JanusGraph, DSE Graph, ...

Multiple languages

ISO SC32.WG3 → SQL PGQ (Property Graph Querying)
Neo4j → openCypher
LDBC → G-CORE (augmented with paths)
Oracle → PGQL
W3C → SPARQL (RDF data model)
Tigergraph → GSQL

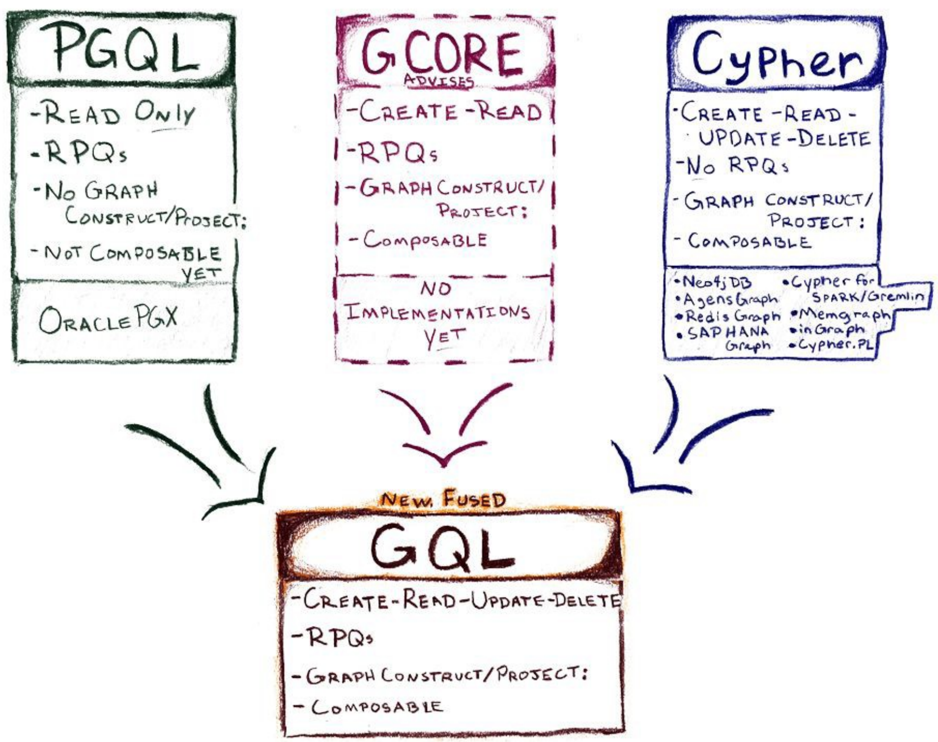
SQL 2020
Participation from major DBMS vendors.
Neo4j's contributions freely available*.

...also imperative and analytics-based languages

* http://www.opencypher.org/references#sql-pg

Graph Query Language(GQL)

Graphs **first**, not graphs “extra”



A new stand-alone / native query language for graphs

Targets the labelled PG model

Composable graph query language with support for updating data

Based on

- “Ascii art” pattern matching
- Published formal semantics (Cypher, G-CORE)
- SQL PG extensions and SQL-compatible foundations (some data types, some functions, ...)

https://www.gqlstandards.org

GQL Documents also available at http://www.opencypher.org/references#sql-pg

Example GQL Query

```
//from graph or view 'friends' in the catalog
FROM friends

//match persons 'a' and 'b' who travelled together
MATCH (a:Person)-[:TRAVELLED_TOGETHER]-(b:Person)
WHERE a.age = b.age
    AND a.country = $country
    AND b.country = $country

//from view parameterized by country
FROM census($country)

//find out if 'a' and 'b' at some point moved to or were born in a place 'p'
MATCH SHORTEST (a)-[:BORN_IN|MOVED_TO*]->(p)<-[:BORN_IN|MOVED_TO*]->(b)

//that is located in a city 'c'
MATCH (p)-[:LOCATED_IN]->(c:City)

//aggregate the number of such pairs per city and age group
RETURN a.age AS age, c.name AS city, count(*) AS num_pairs
    GROUP BY age
```

Illustrative syntax only!

Regular path queries

Complex path patterns

Regular path queries (RPQs)

X, (likes.hates)*(eats|drinks)+, Y

Find a path whose edge labels conform to the regular expression, starting at node X and ending at node Y

(X and Y are node bindings)

Plenty of research in this area since 1987!

SPARQL 1.1 has support for RPQs: "property paths"

I. F. Cruz, A. O. Mendelzon, and P. T. Wood
A graphical query language supporting recursion
In Proc. ACM SIGMOD, pages 323–330, **1987**

Complex paths in the property graph data model

Property graph data model:

Properties need to be considered

Node labels need to be considered

Specifying a cost for paths (ordering and comparing)

Path patterns (e.g., GXPATH)

Concatenation
a.b - a is followed by b
Alternation
a|b - either a or b
Transitive closure
***** - 0 or more
+ - 1 or more
{m, n} - at least m, at most n
Optionality:
?- 0 or 1
Grouping/nesting
() - allows nesting/defines scope

L. Libkin, W. Martens, and D. Vrgoč
Querying Graphs with Data
ACM Journal, pages 1-53, **2016**

Composition of Path Patterns

Provisional syntax

Sequence / Concatenation:	( ) - / αβ / - ( )
Alternation / Disjunction:	( ) - / α | β / - ( )
Transitive closure:	
1 or more	( ) - / α* / - ( )
2or more	( ) - / α+ / - ( )
n ormore	( ) - / α*n.. / - ( )
At least n, at most m	( ) - / α*n..m / - ( )
Overriding direction forsub-pattern:	
Left to right direction	( ) - / α > / - ( )
Right to left direction	( ) - / < α / - ( )
Any direction	( ) - / <α> / - ( )

Path Pattern:example

```
PATH PATTERN
  older_friends = (a)-[:FRIEND]-(b) WHERE b.age > a.age

MATCH p=(me)-/~older_friends+/-(you)
WHERE me.name = $myName AND you.name = $yourName
RETURN p AS friendship
```

Nested Path Patterns: Example

```
PATH PATTERN
  older_friends = (a)-[:FRIEND]-(b) WHERE b.age > a.age

PATH PATTERN
  same_city = (a)-[:LIVES_IN]->(:City)<-[:LIVES_IN]-(b)

PATH PATTERN
  older_friends_in_same_city = (a)-/~older_friends/-(b)

    WHERE EXISTS { (a)-/~same_city/-(b) }
```

Cost function for cheapest path search

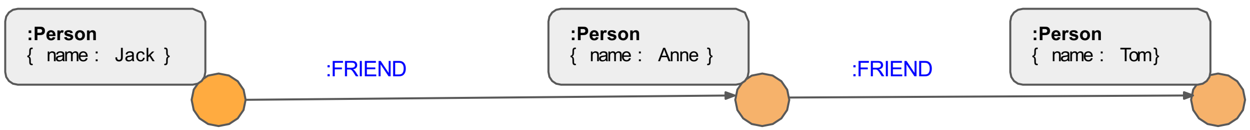
```
PATH PATTERN road = (a)-[r:ROAD_SEGMENT]-(b) COST r.length

MATCH route = (start)-/~road*/-(end)
WHERE start.location = $currentLocation
    AND end.name = $destination
RETURN route
ORDER BY cost(route) ASC LIMIT 3
```

“Cyphermorphism”

Usefulness proven **in practice** over multiple industrial verticals: we have not seen any worst-case examples

Pattern matching today uses **edge isomorphism** (no repeated relationships)



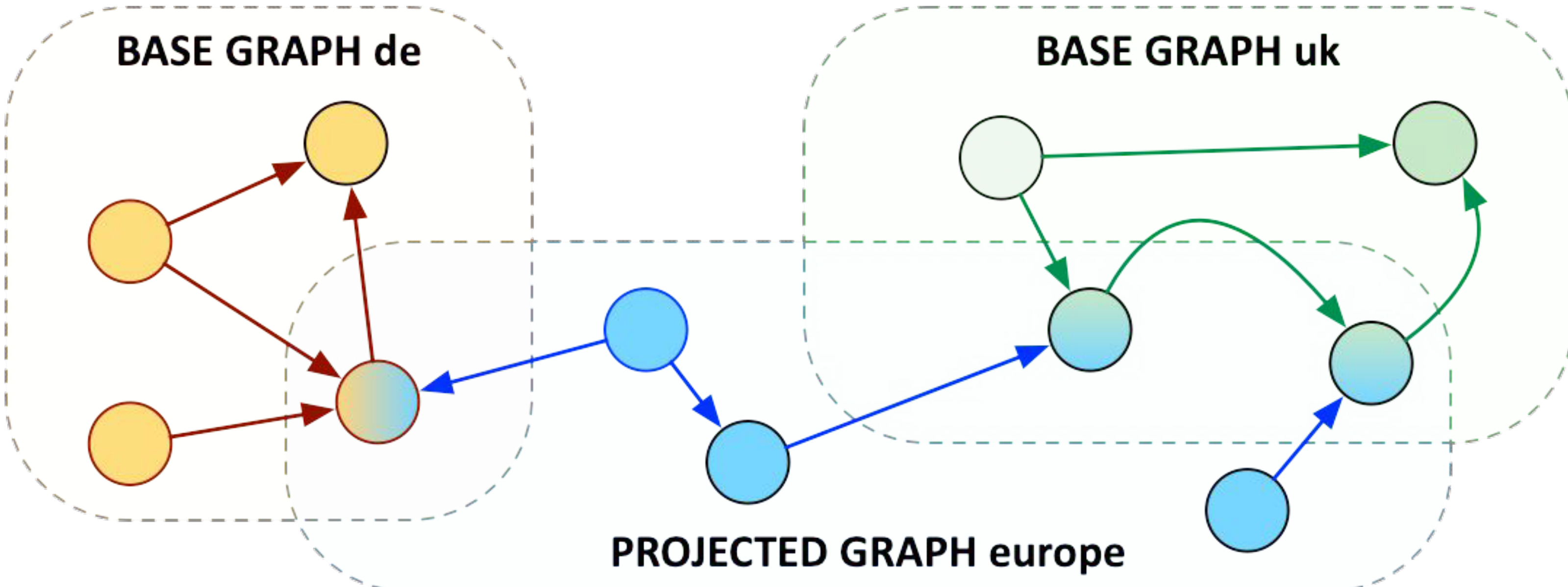

```
MATCH (p:Person {name: Jack})-[r1:FRIEND]-()-[r2:FRIEND]-(friend_of_a_friend)
RETURN friend_of_a_friend.name AS fofName
```

```
+---------+
| fofName |
+---------+
| “Tom”   |
+---------+
```

r1 and **r2** may not be bound to the same relationship *within the same pattern*

Rationale was to avoid **potentially** returning infinite results for varlength patterns when matching graphs containing cycles (this would have been different if we were just checking for the *existence* of a path)

Graph projection

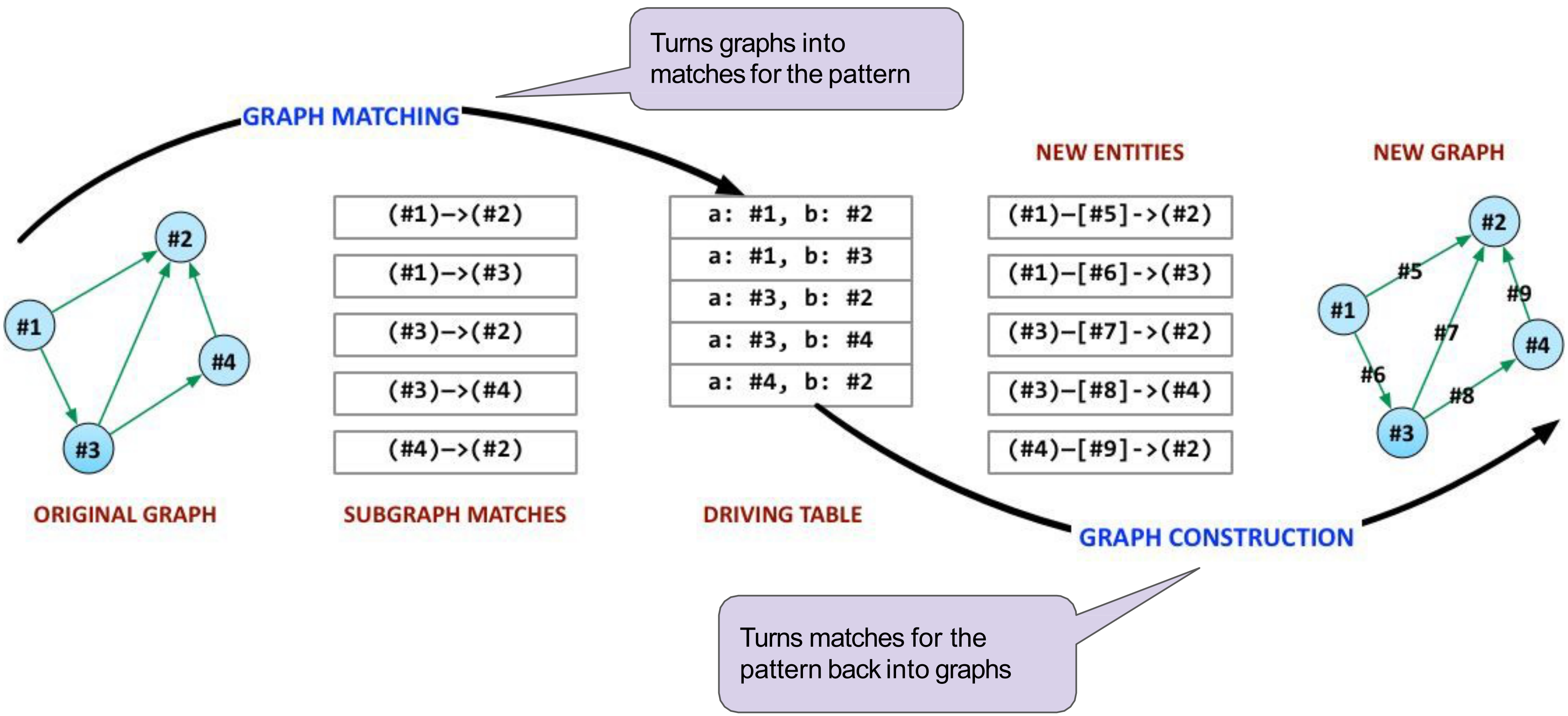


Sharing elements in the projected graph

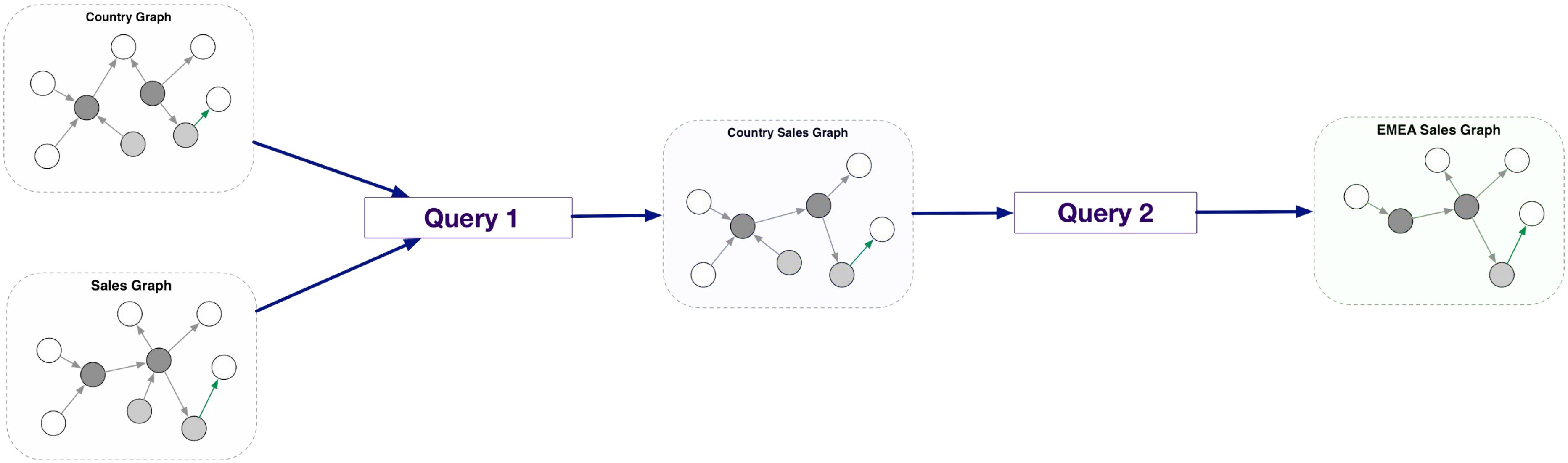
Deriving new elements in the projected graph

Shared edges always point to the same (shared) endpoints in the projected graph

Projection is the inverse of pattern matching



Queries are composable procedures



- Use the output of one query as input to another to enable abstraction and views
- Applies to queries with tabular output and graph output
- Support for nested subqueries
- Extract parts of a query to a view for re-use
- Replace parts of a query without affecting other parts
- Build complex workflows programmatically

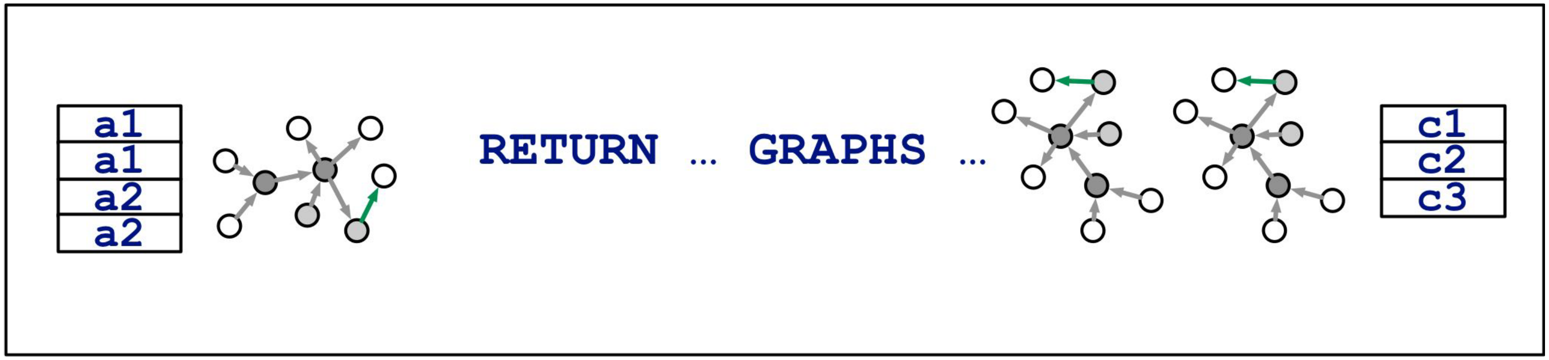
Implications

Pass both multiple graphs and tabular data into a query

Return both multiple graphs and tabular data from a query

Select which graph to query

Construct new graphs from existing graphs



based on slide by S. Plantikow

Acknowledgements for slides 38-48

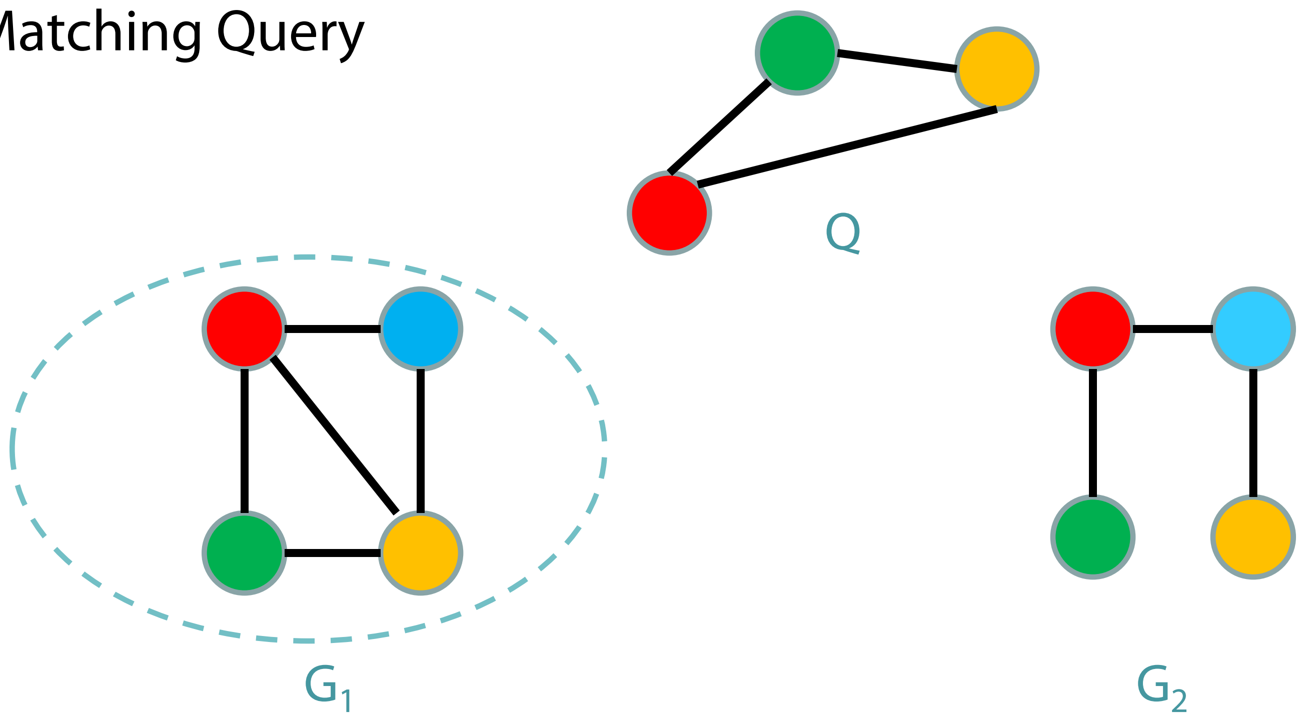
- Slides are taken from the following Presentation
- Emerging Graph Queries in Linked Data
  - Arijit Khan, Yinghui Wu, Xifeng Yan
  - Department of Computer Science
  - University of California, Santa Barbara

- All errors are mine

Graph Search Queries

- **Containment Query**
- Similarity Query
- Matching Query

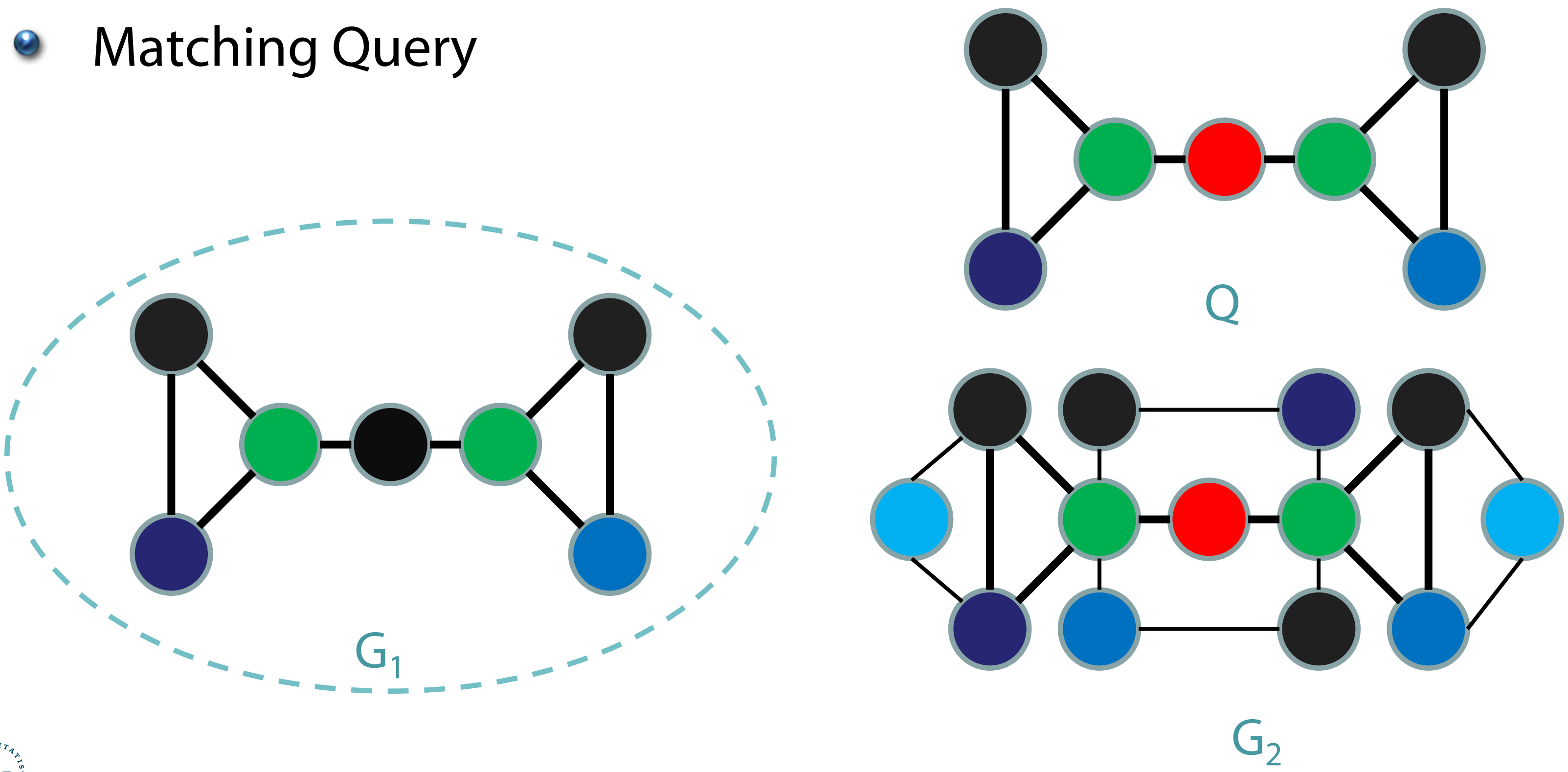
Retrieves all graphs from a graph database, such that they **contain** a given query graph (exact and approximate).



Graph Search Queries

- Containment Query
- **Similarity Query**
- Matching Query

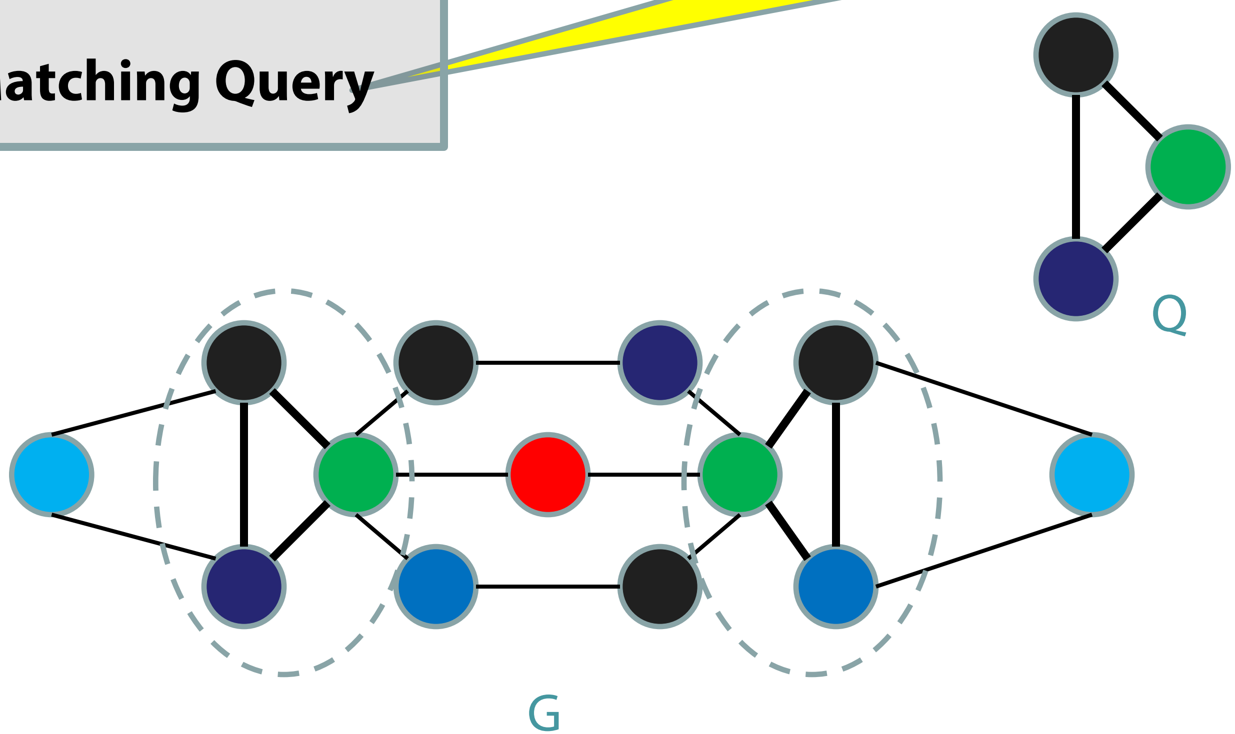
Retrieves all graphs from a graph database, that are **similar** to the query graph (exact and approximate).



Graph Search Queries

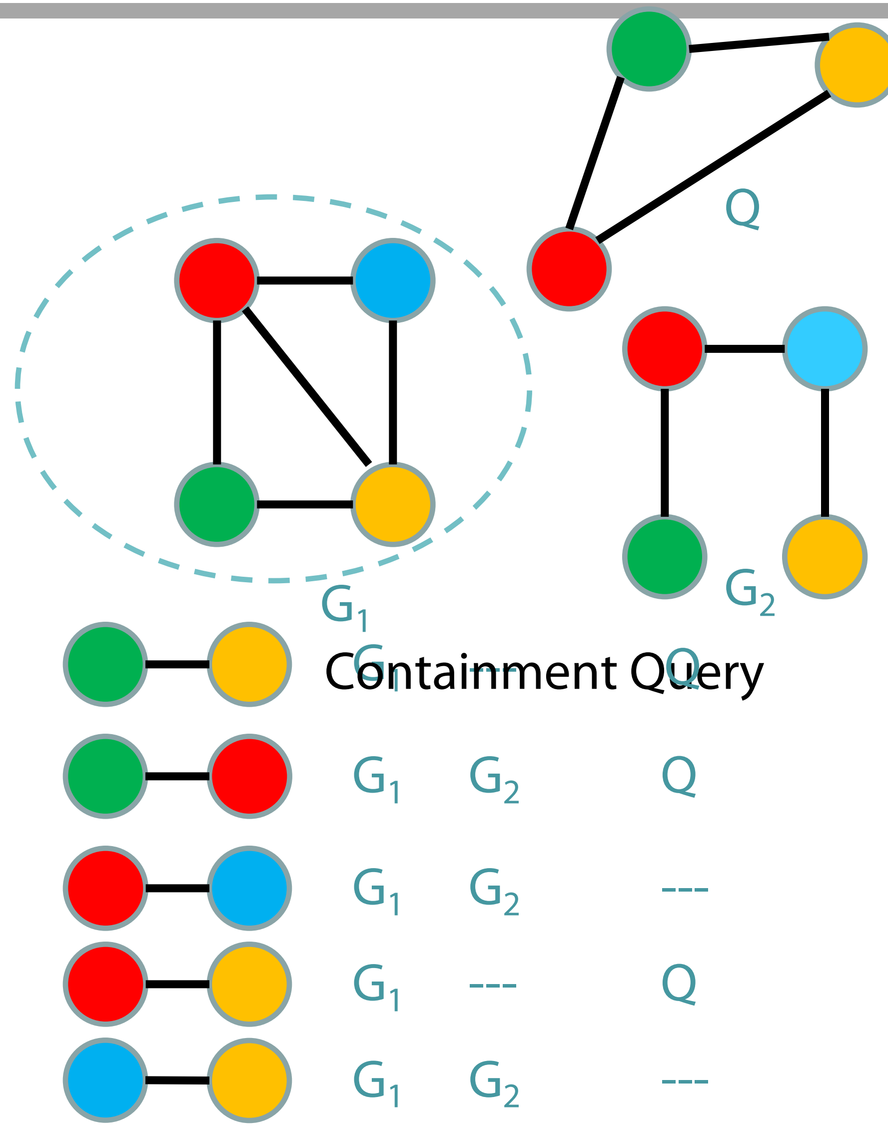
- Containment Query
- Similarity Query
- **Matching Query**

Find all occurrences of a query graph in a large target network (exact and approximate).



Containment Query

- Subgraph Isomorphism Problem is **NP-hard**.
- Filtering and Verification
- **Filtering Phase:**
  Feature-based index is used to filter out the negative results and generate candidate sets.
- **Verification Phase:**
  Precise Subgraph Isomorphism Testing to generate final results from the candidate set.



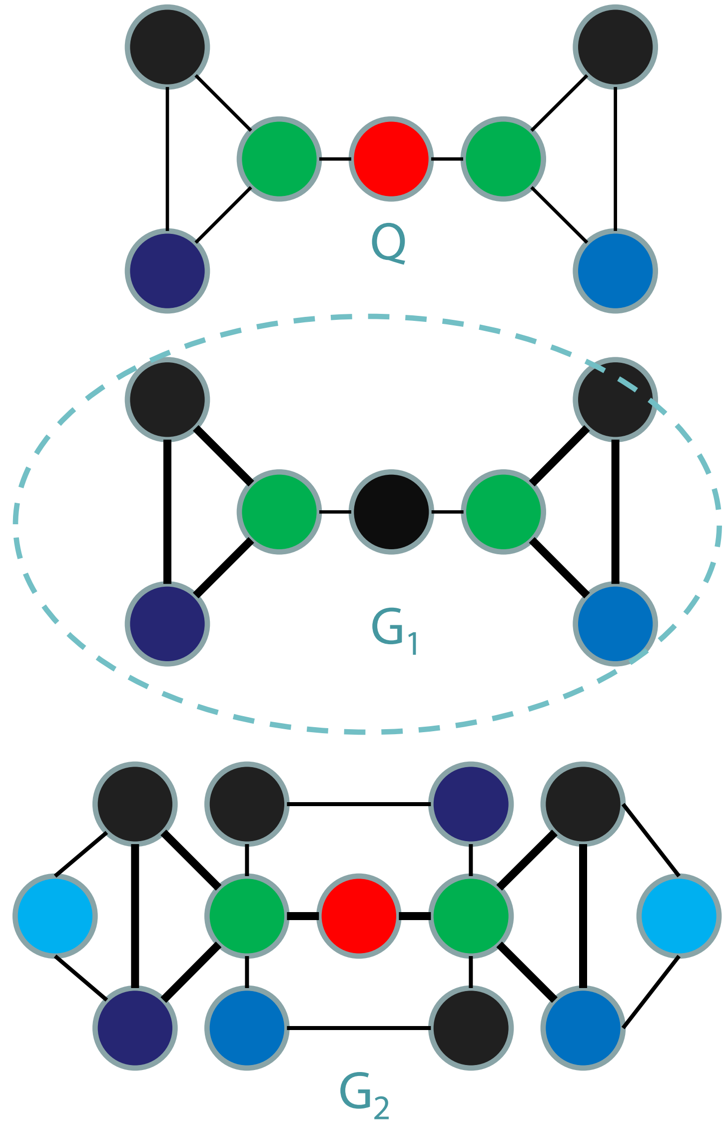
Edge Based Index

Filtering

Similarity Query

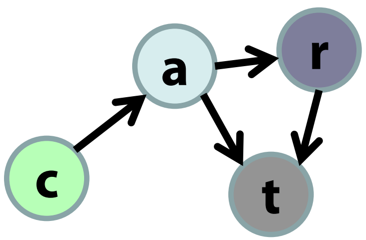
- Graph Isomorphism is **neither known to be Polynomial or NP-Complete**
- **Graph Edit Distance** NP-hard
- **Maximum Common Subgraph (MCS)** based approach.
  - $\Delta = |d(Q, MCS(Q,G))| + |d(G, MCS(Q,G))|$
  - MCS is NP-hard.
  - Efficiently Finding MCS of two large networks (Approximate) – *Zhu et al., CIKM '11*
  - Indexing based on MCS in Filtering Phase – *Zhu et. al., EDBT '12*

- **Maximum Common Subgraph (MCS)** based approach.
  - $|d(Q, MCS(Q,G_1))| = 2$
  - $|d(G_1, MCS(Q,G_1))| = 2$
  - $\Delta = |d(Q, MCS(Q,G_1))| + |d(G_1, MCS(Q,G_1))| = 4$
  - $|d(Q, MCS(Q,G_2))| = 0$
  - $|d(G_2, MCS(Q,G_2))| = 10$
  - $\Delta = |d(Q, MCS(Q,G_1))| + |d(G_1, MCS(Q,G_1))| = 10$



Similarity Query

- **Kernel Based Approach.**
  - Measure similarity of two graphs by comparing their substructures.
  - Map two graphs G_1 and G_2 via mapping φ into feature space H.



$\varphi \equiv$ length of all walks between every ordered pair of labels.

e.g., $\varphi_{(c\,,\,a)} = \varphi_{(a\,,\,r)} = \varphi_{(r\,,\,t)} = 1$

$\varphi_{(a\,,\,t)} = 1+2 = 3$

$\varphi_{(c\,,\,t)} = 2+3 = 5$

$\varphi_{(c\,,\,c)} = 0$ etc.

  - Measure their similarity in H as scalar product $<\varphi(G_1), \varphi(G_2)>$.
  - **Kernel Trick:** Compute inner product in H as kernel in input space $k(G_1, G_2) = <\varphi(G_1), \varphi(G_2)>$; e.g., compute walks in the product graph $G_1 \times G_2$.

- Positive Definite.

Similarity Query

- **Complete Graph Kernel:** Let $k(G_1, G_2) = \langle \varphi(G_1), \varphi(G_2) \rangle$ be a graph kernel. If φ is injective, k is called a complete graph kernel.

- **Example:** The graph kernel that has one feature Φ_H for each possible graph H, each feature $\Phi_H(G)$ measuring how many subgraphs of G have the same structure as graph H.

- The above example of Complete Graph Kernel is NP-hard.

Theorem: Computing any complete graph kernel is at least as hard as deciding whether two graphs are isomorphic *[Gärtner et. al., COLT '03]*

Graph Kernels

- **Polynomial Time Computable Graph Kernels:**

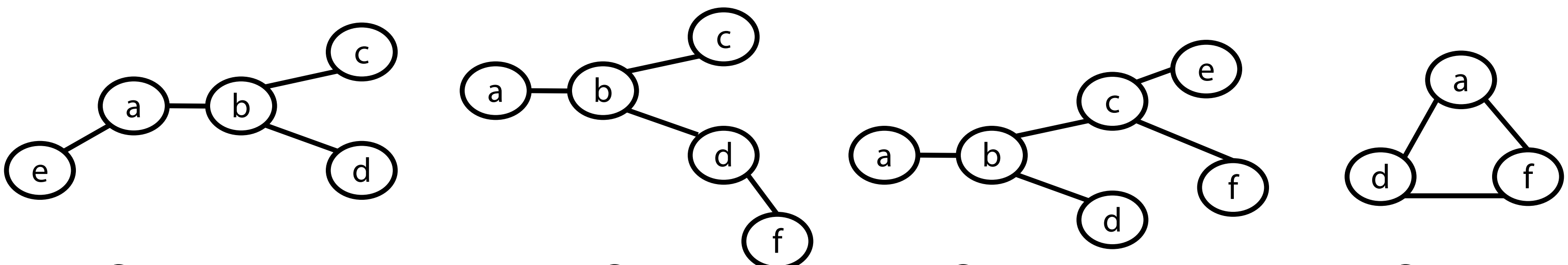
  - **Random Walk** - Kashima et al., *ICML '03*
    - Gaertner et al., *COLT '03*
    - Mahe et al., *ICML '04*
    - Vishwanathan et al., *NIPS '06*
  - **Shortest Path** - Borgwardt et. al., *ICDM '05*
  - **Optimal assignment kernel** - Froehlich et al, *ICML '05*
    [NOT Positive definite, Vert, *'08*]
  - **Weighted Decomposition Kernel** - Menchetti et al., *ICML '05*
  - **Edit-Distance Kernel** - Neuhaus et. al., *SSPR/SPR '06*
  - **Subtree Kernel** - Ramon et. al., *Mining Graphs, Trees and Sequences '04*
    - Shervashidze et. al., *NIPS '09*
  - **Cyclic Pattern Kernel** - Horvath et al., *KDD '04*
  - **Neighborhood Kernel** - Wang et. al., *EDBT '09*

Graph Pattern Mining

Given a graph dataset D, find all subgraphs g, s.t.

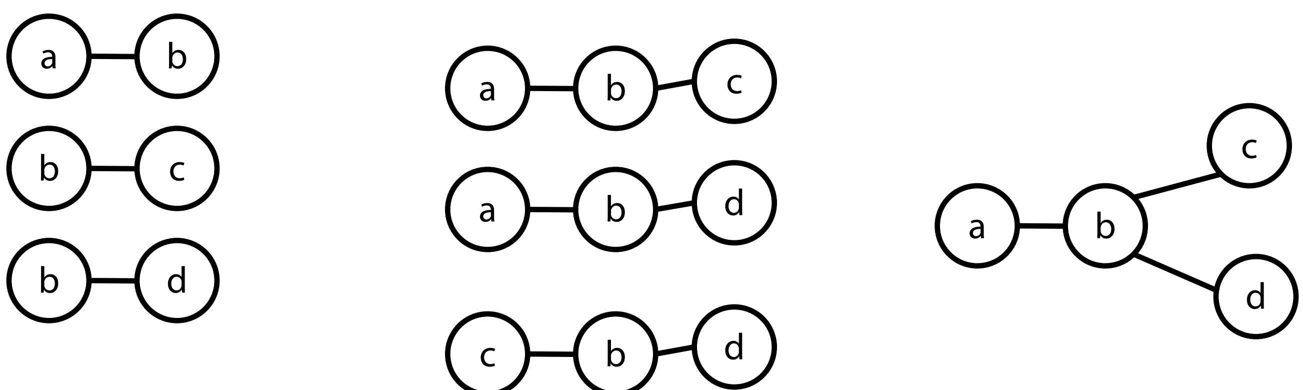
$$freq(g) \geq \theta$$

Where $freq(g)$ is the (relative) number of graphs that contain g.



G_1 G_2 G_3 G_4

Θ=3



UNIVERSITÄT ZU LÜBECK
INSTITUT FÜR INFORMATIONSSYSTEME

Why Mine Graph Patterns?

- Direct Use:
  - Mining over-represented sub-structures in chemical databases.
  - Mining conserved sub-networks.
  - Program control flow analysis.
- Indirect Uses:
  - Index the data graph and query graph using local features.
  - Building block of further analysis, i.e., Classification, Clustering, Similarity Searches, Indexing

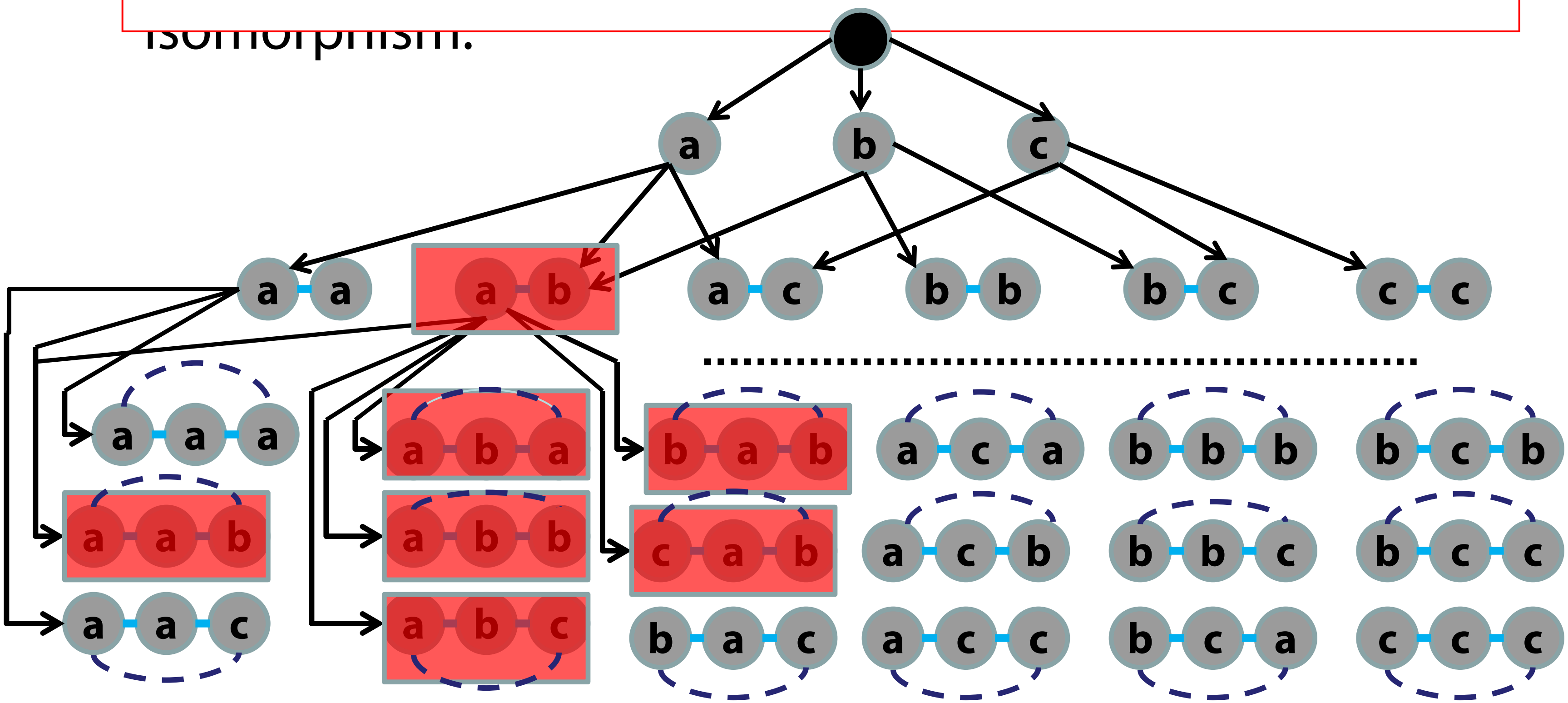
Why is Graph Mining Hard?

Apriori Property

If a graph is frequent, all of its subgraphs are frequent.

graph

isomorphism.



Pattern Search Tree

Summary

- Graph database language
  - Cypher and others → GQL
- Hardness results
- Implementation issues
  - Containment and matching
    - Indexing / filtering (still false positive, no false negatives)
    - Verification (eliminate false positives)
  - Similarity
    - Mapping into feature space
      with polynomial graph kernels
- Graph mining