

Graph Databases

Lecture 8 of NoSQL Databases (PA195)

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Agenda



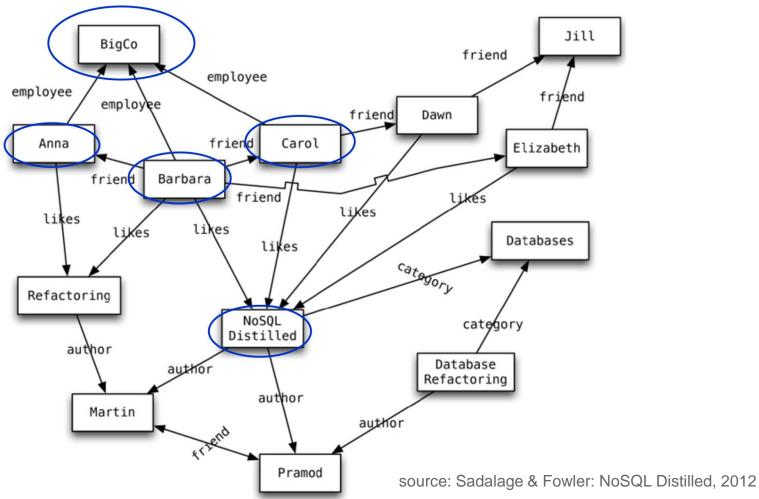
- Graph Databases: Mission, Data, Example
- A Bit of Graph Theory
 - o Graph Representations
 - Algorithms: Improving Data Locality (efficient storage)
 - o Graph Partitioning and Traversal Algorithms

• Graph Databases

- Transactional databases
- Non-transactional databases
- Neo4j
 - Basics, Native Java API, Cypher, Behind the Scene

Graph Databases: Example





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Graph Databases: Mission



- To store entities and relationships between them
 - Nodes are instances of objects
 - Nodes have properties, e.g., name
 - Edges connect nodes and have directional significance
 - Edges have types, e.g., likes, friend, ...
- Nodes are organized by relationships
 - Allows finding interesting patterns
 - **Example:** Get all nodes that are "employee" of "Big Company" and that "likes" "NoSQL Distilled"







Ranked list: <u>http://db-engines.com/en/ranking/graph+dbms</u>



A Bit of a Theory

Basics and graph representations

Basic Terminology



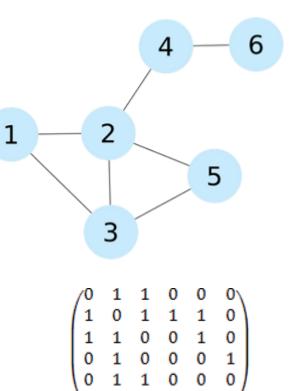
- Data: a set of entities and their relationships
 > we need to efficiently represent graphs
- Graph G = (V, E) is usually modelled as
 - set of nodes (vertices) V, |V| = n
 - o set of (directed) edges $E = (v_1, v_2), v_1, v_2 \in V, |E| = m$
- Basic operations:
 - finding the neighbors of a node,
 - checking if two nodes are connected by an edge,
 - updating the graph structure, ...
 - o => we need efficient graph operations
- What data structure to use?

Data Structure: Adjacency Matrix

- Two-dimensional array A of n × n Boolean values
 - Indexes of the array = node
 identifiers of the graph
 - Boolean value A_{ij} indicates
 whether nodes *i*, *j* are connected

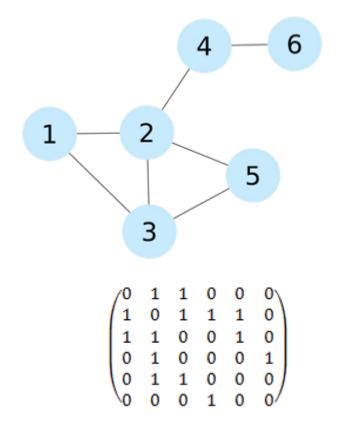
• Variants:

- o Directed graphs,
- o Weighted graphs, ...



Adjacency Matrix: Properties





• Pros:

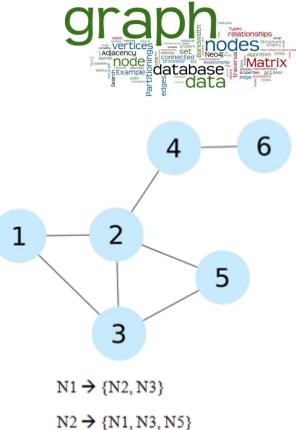
- Checking if 2 nodes are connected
- Adding/removing edges

• Cons:

- Quadratic space: O(n²)
- We usually have sparse graphs
- Retrieval of all the neighboring nodes takes linear time: O(n)
- Adding/Deleting nodes is expensive

Data Structure: Adjacency List

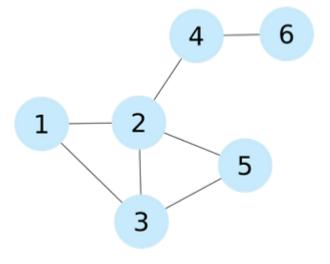
- A set of lists, each enumerating neighbors of one node
 - Vector of *n* pointers to adjacency lists
- Undirected graph:
 - An edge connects nodes *i* and *j*
 - => the adjacency list of *i* contains node *j* and vice versa
- Often compressed
 - Exploiting regularities in graphs



- $N3 \rightarrow \{N1, N2, N5\}$
- N4 → {N2, N6}
- N5 → {N2, N3}
- N6 → {N4}

Adjacency List: Properties





- $\text{N1} \not \rightarrow \{\text{N2},\text{N3}\}$
- N2 → {N1, N3, N5}
- N3 → {N1, N2, N5}

N4 → {N2, N6}

 $\rm N5 \not \rightarrow \{N2,N3\}$

N6 → {N4}

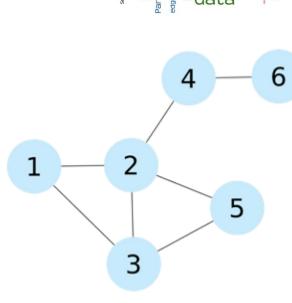
• Pros:

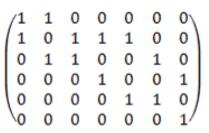
- More compact representation of sparse graphs
- Getting the neighbors of a node
- Cheap addition of nodes
- Cons:
 - Checking if there is an edge between two nodes
 - Optimization: sorted lists => logarithmic scan, but also logarithmic insertion

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Data Structure: Incidence Matrix

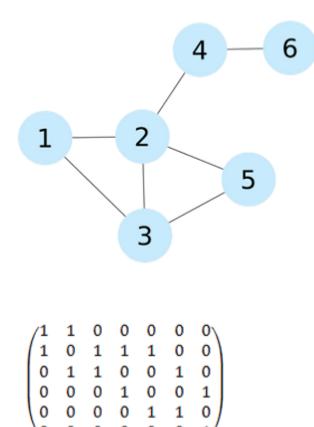
- Two-dimensional array of bools
 - n rows and m columns
 - Each row represents a node
 - All edges that are connected to the node
 - Each column represents an edge
 - Nodes that are connected by a certain edge
 - Directed graphs:
 - $-1 \text{edge } e_i \text{ leaves the node } n_i$
 - +1 edge e_i enters the node n_i
 - Weighted graphs





Incidence Matrix: Properties



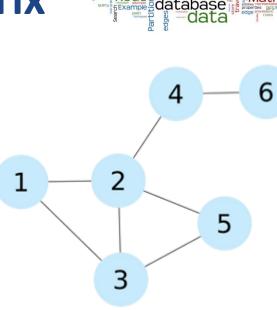


• Pros:

- Representation of hypergraphs
 - where one edge connects an arbitrary number of nodes
- Cons:
 - Requires n × m bits (for most graphs, m ≫ n)
 - Listing neighborhood is slow

Data Structure: Laplacian Matrix

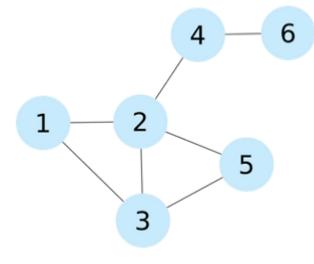
- Two-dimensional array of *n* × *n* integers
 - Similar structure as adjacency matrix
 - Diagonal of the Laplacian matrix indicates the degree of the node
 - The rest of positions are set to
 - O -1 if the two vertices are connected,
 - O *0* otherwise



 $\begin{pmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 4 & -1 & -1 & -1 & 0 \\ -1 & -1 & 3 & 0 & -1 & 0 \\ 0 & -1 & 0 & 2 & 0 & -1 \\ 0 & -1 & -1 & 0 & 2 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}$

Laplacian Matrix: Properties





$$\begin{pmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 4 & -1 & -1 & -1 & 0 \\ -1 & -1 & 3 & 0 & -1 & 0 \\ 0 & -1 & 0 & 2 & 0 & -1 \\ 0 & -1 & -1 & 0 & 2 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}$$

All features of adjacency matrix

- Pros:
 - Analyzing the graph structure by means of spectral analysis
 - Calculating the number of spanning trees
 - Approximation of the sparsest cut of the graph
 - Calculate eigenvalues of the matrix
 - A good summary: <u>Wikipedia</u>



A Bit of a Theory

Selected graph algorithms

Basic Graph Algorithms



- Access all nodes reachable from a given source:
 - Breadth-first Search (BFS)
 - Depth-first Search (DFS)
- Shortest path between two nodes
- Single-source shortest path problem
 - o BFS (unweighted),
 - Dijkstra (nonnegative weights),
 - Bellman-Ford algorithm
- All-pairs shortest path problem
 - o Floyd-Warshall algorithm

Improving Data Locality



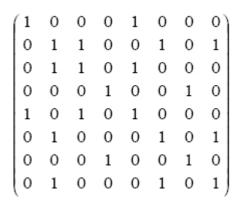
- Performance of the read/write operations
 - Depends also on physical organization of the data
 - Objective: Achieve the best "data locality"
- **Spatial** locality:
 - if a data item has been accessed, the nearby data items are likely to be accessed in the following computations
 - e.g., during graph traversal

• Strategy:

- in graph adjacency matrix representation, exchange rows and columns to improve the disk cache hit ratio
- Specific methods: BFSL, Bandwidth of a Matrix, ...







	(1	1	0	0	0	0	0	0)
	1	1	0	0	0	0	0	0
	0	0	1	1	1	0	0	0
	0	0	1	1	1	0	0	0
	0	0	1	1	1	1	0	0
	0	0	0	0	1	1	1	0
	0	0	0	0	0	1	1	1
	0	0	0	0	0	0	1	1)
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This matrix has better data locality, more efficient traversal

Breadth First Search Layout (BFSL)

- Input: vertices of a graph
- Output: a permutation of the vertices
 - with better cache performance for graph traversals
- BFSL algorithm:
 - 1. Select a node (at random, the origin of the traversal)
 - 2. Traverse the graph using the BFS alg.
 - generating a list of vertex identifiers in the order they are visited
 - 3. Take the generated list as the new vertices permutation

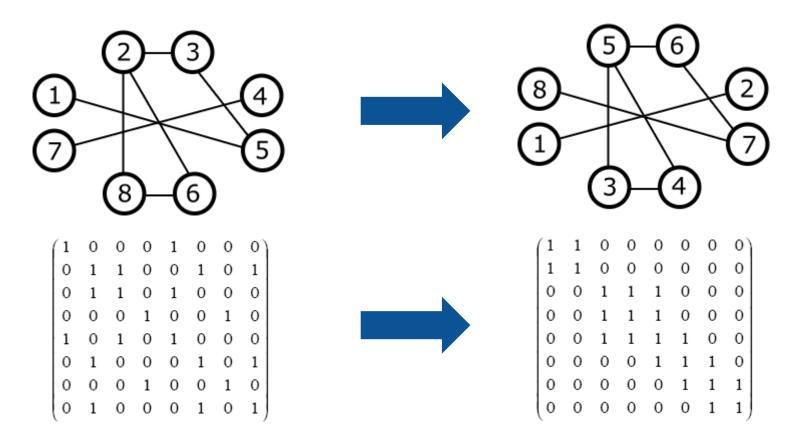
Breadth First Search Layout (2) Let us recall: Breadth First Search (BFS) FIFO queue of frontier vertices 5 8 9

- Pros: optimal locality for traversal from the root
- Cons: starting traversal from other nodes
 The further, the worse

Matrix Bandwidth: Motivation



• Graph represented by adjacency matrix



Matrix Bandwidth: Formalization



- The minimum bandwidth problem
 - Bandwidth of a row in a matrix = the maximum distance between nonzero elements, where one is left of the diagonal and the other is right of the diagonal
 - Bandwidth of a matrix = maximum bandwidth of its rows
- Low bandwidth matrices are more cache friendly
 Non zero elements (edges) clustered around the diagonal
- Bandwidth minimization problem: NP hard
 o For large matrices the solutions are only approximated



A Bit of a Theory

Graph partitioning

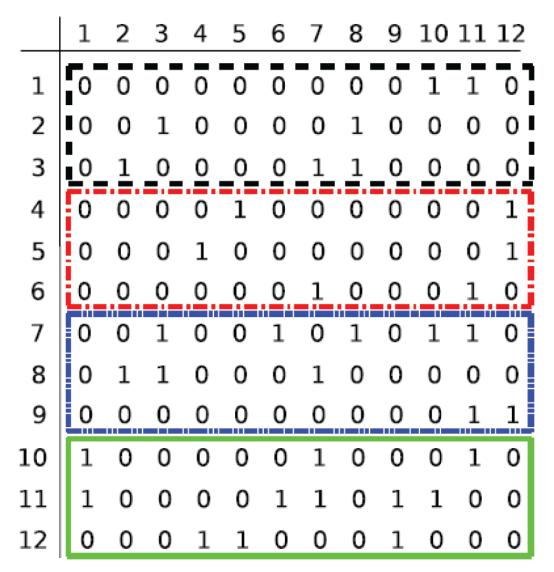
Graph Partitioning



- Some graphs are too large to be fully loaded into the main memory of a single computer
 - Usage of secondary storage degrades the performance
 - Scalable solution: distribute the graph on multiple nodes
- We need to partition the graph reasonably
 - Usually for a particular (set of) operation(s)
 - The shortest path, finding frequent patterns, BFS, spanning tree search

Example: 1-Dimensional Partitionin

- Aim: Partition the graph to solve BFS efficiently
 - Distributed into shared-nothing parallel system
 - Partitioning of the adjacency matrix
- 1D partitioning of Adjacency Matrix:
 - Matrix rows are randomly assigned to the P nodes (processors) in the system
 - Each vertex (and its edges) are owned by one processor





Starting BFS traversal at node 1:

- 1. (at black) 1 -> 10, 11 visit green server
- 2. (at green) 10, 11 ->
 - a. 1, back to black
 - b. 6, visit red
 - c. 7,9, visit blue
 - d. 10, 11, myself (green)
- 3. (at red) 6 -> 7 visit blue
- 3. (at blue) 7,9 ->
 - a. 3, back to black ...
 - b. 6, back to red
 - c. 8 -> 2,3, back to black
 - d. 10,11,12, back to green

Traversing Graph



- Traversing with 1D partitioning (e.g., BFS)
 - 1. Each **processor** keeps information about frontier vertices
 - 2. ...and also list of neighboring vertices in other processors
 - 3. Messages are sent to other processors...
- 1D partitioning leads to high messaging
 - o => 2D-partitioning of adjacency matrix
 - ... lower messaging but still very demanding

Efficient sharding of a graph is very difficult

• and thus graph DBs are often centralized



Graph Databases

Types of Graphs



• Single-relational graphs

- Edges are homogeneous in meaning
 - e.g., all edges represent friendship
- Multi-relational (property) graphs
 - Edges are typed or labeled
 - e.g., friendship, business, communication
 - Vertices and edges maintain a set of key/value pairs
 - Representation of non-graphical data (properties)
 - e.g., name of a vertex, the weight of an edge

Graph Databases



• A graph database = a set of graphs

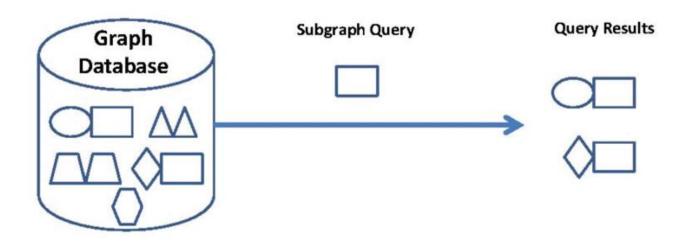
- Types of graph databases:
 - Transactional = a large set of small graphs
 - e.g., chemical compounds, biological pathways, ...
 - Searching for graphs that match the query
 - Non-transactional = few numbers of very large graphs
 - or one huge (not necessarily connected) graph
 - e.g., Web graph, social networks, ...

Transactional DBs: Queries



• Types of Queries

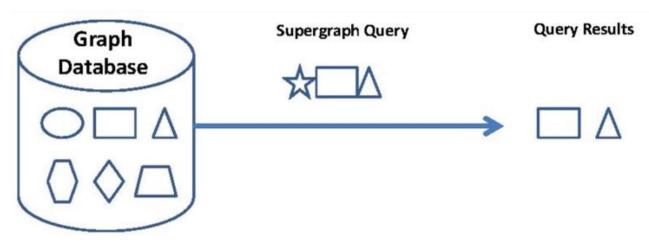
- o Subgraph queries
 - Searches for a specific pattern in the graph database
 - Query = a small graph
 - or a graph, where some parts are uncertain, e.g., vertices with wildcard labels
 - More general type: allow sub-graph isomorphism



Transactional DBs: Queries (2)



- o Super-graph queries
 - Search for graphs whose whole structure is contained in the query graph



- Similarity (approximate matching) queries
 - Finds graphs which are similar to a given query graph
 - but not necessarily isomorphic
 - Key question: how to measure the similarity

Indexing & Query Evaluation



- Extract certain characteristics from each graph
 And index these characteristics for each G₁,..., G_n
- Query evaluation in transactional graph DB
 - 1. Extraction of the characteristics from query graph q
 - 2. Filter the database (index) and identify a candidate set
 - Subset of the $G_1, ..., G_n$ graphs that should contain the answer
 - 3. Refinement check all candidate graphs

Subgraph Query Processing



- 1. Mining-based Graph Indexing Techniques
 - Idea: if some features of query graph q do not exist in data graph G, then G cannot contain q as its subgraph
 - Apply graph-mining methods to extract some features (sub-structures) from the graph database members
 - e.g., frequent sub-trees, frequent sub-graphs
 - An inverted index is created for each feature

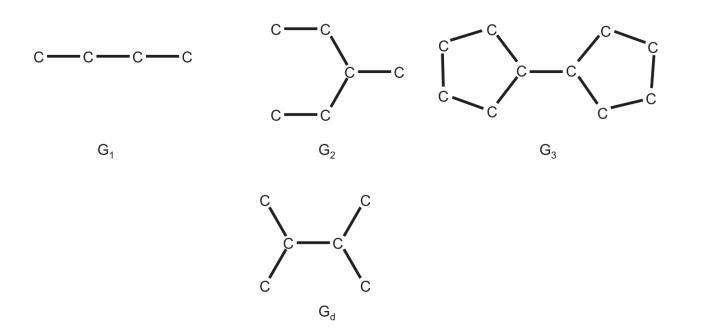
2. Non Mining-Based Graph Indexing Techniques

- Indexing of the whole constructs of the graph database
 - Instead of indexing only some selected features

Mining-based Technique



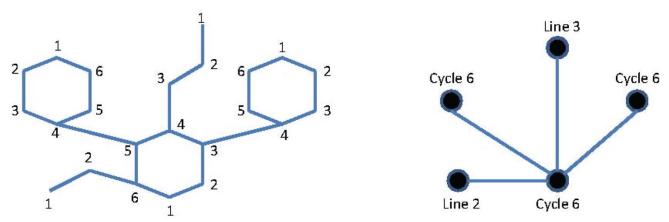
- Example method: GIndex [2004]
 - Indexing "frequent discriminative graphs"
 - Build inverted index for selected discriminative subgraphs



Non Mining-based Techniques



- **Example:** GString (2007)
 - Model the graphs in the context of organic chemistry using basic structures
 - Line = series of vertices connected end to end
 - Cycle = series of vertices that form a close loop
 - Star = core vertex directly connects to several vertices

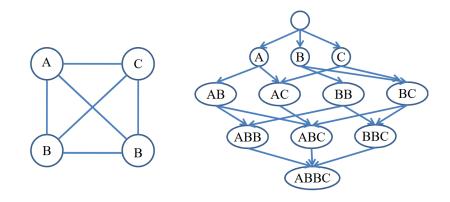


Non Mining-based Techniques



• GDIndex (2007)

- all connected and induced subgraphs of a given graph are enumerated (at most 2ⁿ)
- o due to isomorphisms, there are much fewer subgraphs.
 - if all labels are identical, a complete graph of size n is decomposed into just n+1 subgraphs.





Graph Databases

Non-transactional Databases

Non-transactional Databases



- A few very large graphs
 - o e.g., Web graph, social networks, ...

• Queries:

- Nodes/edges with properties
- Neighboring nodes/edges
- Paths (all, shortest, etc.)
- Our example: Neo4j

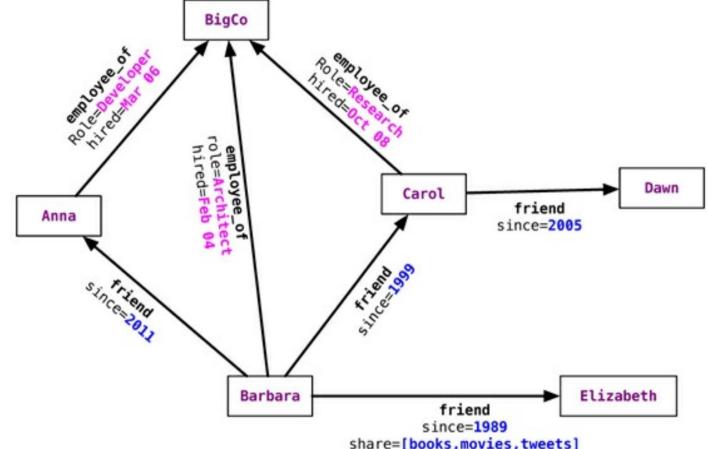
Basic Characteristics



- Different types of relationships between nodes
 - To represent relationships between domain entities
 - Or to model any kind of secondary relationships
 - Category, path, time-trees, spatial relationships, ...
- No limit to the number and kind of relationships
- Relationships have properties
 - E.g., since when did they become friends?

Barbara friend since=1989 share=[books,movies,tweets] Source: Sadalage & Fowler: NoSQL Distilled, 2012

Relationship Properties: Example



les

Adjacency During Node

Example database

da

Graph DB vs. RDBMS



- RDBMS designed for a single type of relationship
 "Who is my manager"
- Adding another relationship usually means a lot of schema changes
- In RDBMS, we model the graph beforehand based on the traversal we want
 - If the traversal changes, the data will have to change
 - Graph DBs: the relationship is not calculated but persisted

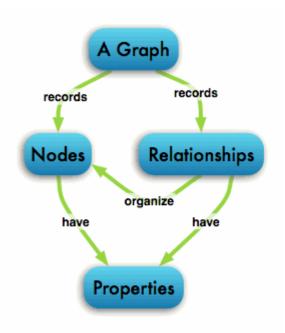


Neo4J: Basics & Concepts

Neo4j: Basic Info



- Open source graph database
 - o The most popular
- Initial release: 2007
- Written in: Java
- OS: cross-platform
- Stores data as nodes connected by directed, typed relationships
 - With properties on both nodes and relationships



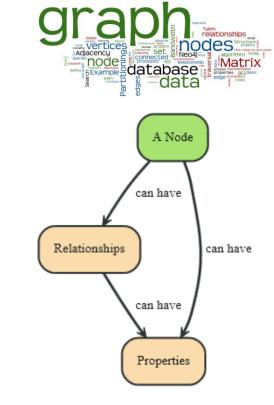
Neo4j: Basic Features

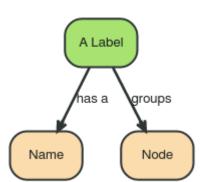


- reliable with full ACID transactions
- durable and fast disk-based, native storage engine
- scalable up to several billion nodes/relationships/properties
- highly-available when distributed (replicated)
- expressive powerful, human readable graph query language
- fast powerful traversal framework
- embeddable in Java program
- accessible simple REST interface & Java API

Data Model: Nodes

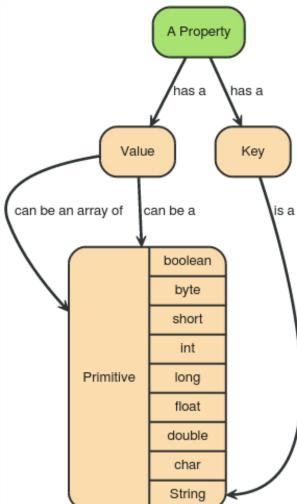
- Fundamental unit: node
- Nodes have properties
 - Key-value pairs
 - o null is not a valid property value
 - nulls can be modelled by the absence of a key
- Nodes have labels
 - labels typically express "type of node"





Data Model: Properties





Туре	Description	
boolean	true/false	
byte	8-bit integer	
short	16-bit integer	
int	32-bit integer	
long	64-bit integer	
float	32-bit IEEE 754 floating-point number	
double	64-bit IEEE 754 floating-point number	
char	16-bit unsigned integer representing a Unicode character	
String	sequence of Unicode characters	
DateTime	temporal types	

Data Model: Relationships

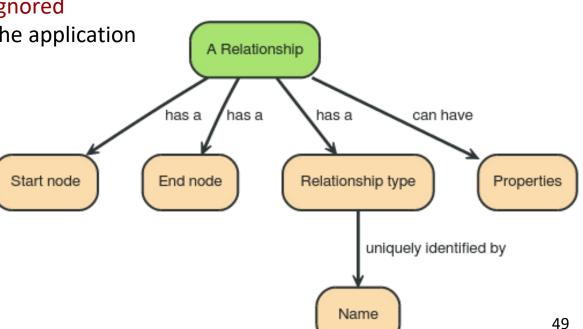


- Directed relationships (edges)
 - Incoming and outgoing edge
 - Equally efficient traversal in both directions
 - Direction can be ignored if not needed by the application
 - o Always a start

and an end node

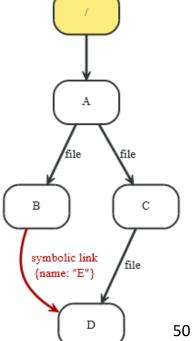
■ Can be recursive





Maja Alice	What		How	
follows follows	get wh	o a person follows	outgoing follows relati	ionships, depth one
Oscar	get the followers of a person		incoming follows relationships, depth one	
Usta	get wh	o a person blocks	outgoing blocks relationships, depth one	
William				
What		How		
get the full path of a file ii		incoming file relationships		
get all paths for a file		incoming <i>file</i> and <i>symbolic link</i> relationships		file file

get all files in a directory outgoing file and symbolic link relationships, depth one get all files in a directory, excluding outgoing file relationships, depth one symbolic links get all files in a directory, recursively outgoing file and symbolic link relationships



Access to Neo4j



- Embedded database in Java system
- Language-specific connectors
 - o Libraries to connect to a running Neo4j server
- Cypher query language
 - Standard language to query graph data
- HTTP REST API
- Gremlin graph traversal language (plugin)
- etc.



Neo4J: Native Java API & Graph Traversal

Native Java Interface: Example



```
Node irena = graphDb.createNode();
irena.setProperty("name", "Irena");
Node jirka = graphDb.createNode();
jirka.setProperty("name", "Jirka");
```

```
Relationship i2j = irena.createRelationshipTo(jirka, FRIEND);
Relationship j2i = jirka.createRelationshipTo(irena, FRIEND);
```

i2j.setProperty("quality", "a good one");

j2i.setProperty("since", 2003);

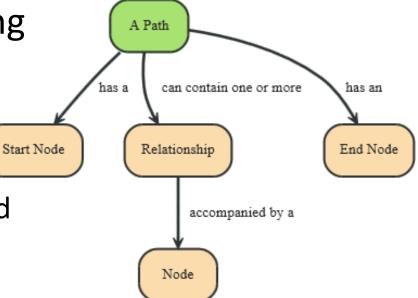
• Undirected edge:

- Relationship between the nodes in **both directions**
- INCOMING and OUTGOING relationships from a node

Data Model: Path & Traversal



- Path = specific nodes + connecting relationships
 Path can be a result of a query or a traversal
- Traversing a graph = visiting its nodes, following relationships according to some rules
 - Typically, a subgraph is visited
 - Neo4j: Traversal framework
 in Java API, Cypher, Gremlin



Traversal Framework



• A traversal is influenced by

- Starting node(s) where the traversal begins
- Expanders define what to traverse
 - i.e., relationship direction and type
- Order depth-first / breadth-first
- Uniqueness visit nodes (relationships, paths) only once
- Evaluator what to return and whether to stop or continue beyond current position

Traversal = TraversalDescription + starting node(s)

Traversal Framework – Java API



- org.neo4j...TraversalDescription
 - The main interface for defining traversals
 - Can specify branch ordering breadthFirst() / depthFirst()
- .relationships()
 - Specify the relationship types to traverse
 - e.g., traverse only edge types: FRIEND, RELATIVE
 - Empty (default) = traverse all relationships
 - Can also specify direction
 - Direction.BOTH
 - Direction.INCOMING
 - Direction.OUTGOING

Traversal Framework – Java API (2)

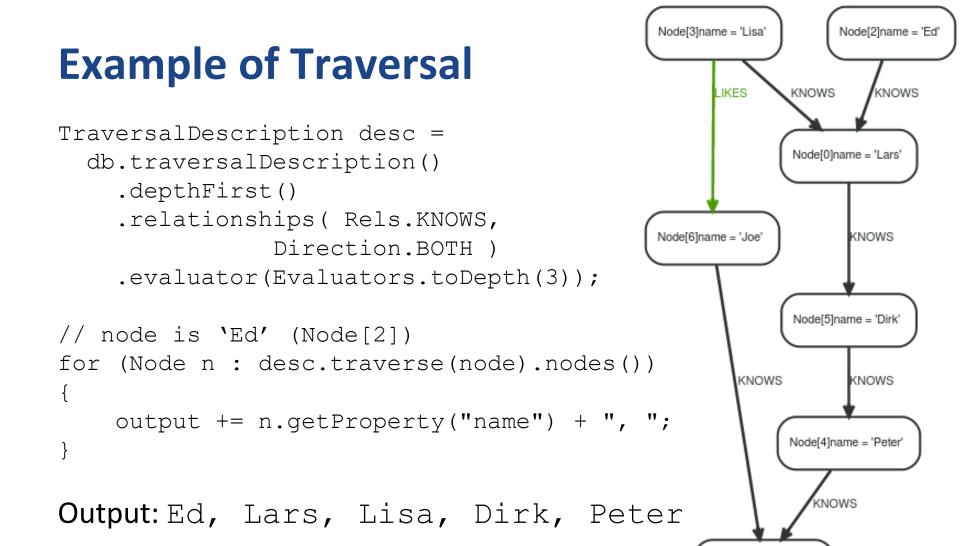
• org.neo4j...Evaluator

- Used for deciding at each node: should the traversal continue, and should the node be included in the result
 - INCLUDE_AND_CONTINUE: Include this node in the result and continue the traversal
 - INCLUDE_AND_PRUNE: Include this node, do not continue traversal
 - EXCLUDE_AND_CONTINUE: Exclude this node, but continue traversal
 - EXCLUDE_AND_PRUNE: Exclude this node and do not continue
- Pre-defined evaluators:
 - Evaluators.toDepth(int depth) / Evaluators.fromDepth(int depth),
 - Evaluators.excludeStartPosition()

Traversal Framework – Java API (3)

- org.neo4j...Uniqueness
 - Indicates under what circumstances a traversal may revisit the same position in the graph

- Traverser
 - Starts actual traversal given a TraversalDescription and starting node(s)
 - Returns an iterator over "steps" in the traversal
 - Steps can be: Path (default), Node, Relationship
 - The graph is actually traversed "lazily" (on request)



http://neo4j.com/docs/stable/tutorial-traversal-java-api.html

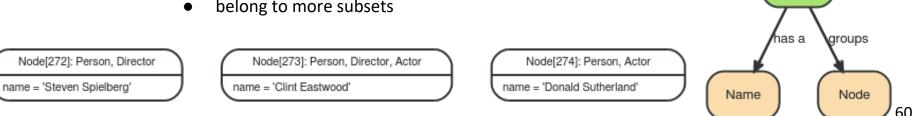
Node[1]name = 'Sara'

Access to Nodes



A Label

- How to get to the starting node(s) before traversal
 - 1. Using internal identifiers (generated IDs)
 - not recommended Neo4j generates IDs for memory objs and reuses IDs
 - 2. Using properties of nodes
 - one of the properties is typically "ID" (user-specified ID)
 - recommended, properties can be indexed
 - automatic indexes
 - 3. Using "labels"
 - group nodes into "subsets" (named graph)
 - a node can have more than one label
 - belong to more subsets





Neo4J: Cypher Language

Cypher Language



- Neo4j graph query language
 - For querying and updating
- Declarative we say what we want
 - Not how to get it
 - Not necessary to express traversals
- Human-readable
- Inspired by SQL and SPARQL
- Still growing = syntax changes are often

Cypher: Clauses



- **MATCH**: The graph **pattern** to match
- WHERE: Filtering criteria
- **RETURN**: What to return
- WITH: Divides a query into multiple parts
 o can define starting points in the graph
- **CREATE**: Creates nodes and relationships.
- **DELETE**: Remove nodes, relationships, properties
- SET: Set property values



CREATE (n);

(create a node, assign to var **n**)

Created 1 node, returned 0 rows

Cypher: Creating Relationships



MATCH (a {name:'John'}), (b {name:'Jack'}) CREATE a-[r:Friend]->b RETURN r ;

(create a relation Friend between John and Jack)

Created 1 relationship, returned 1 row

```
MATCH (a {name:'John'}), (b {name:'Jack'})
CREATE p = a-[:Friend {name: a.name + '->' + b.name }]->b
RETURN p
(set property 'name' of the relationship)
```

Created 0 nodes, set 1 property, returned 1 row





MATCH (p: Person) WHERE p.age >= 18 AND p.age < 30 RETURN p.name

(return names of all adult people under 30)

MATCH (user: Person {name: 'Andres'})-[:Friend]->(buddy) **RETURN** user.name, buddy.name

(find all 'Friends' of 'Andres')





MATCH (andres: Person {name: 'Andres'})-[*1..3]-(node) **RETURN** andres, node ;

(find all 'nodes' within three hops from 'Andres')

MATCH p=shortestPath(

(andres:Person {name: 'Andres'})-[*]-(david {name:'David'})

RETURN p ;

(find the shortest connection between 'Andres' and 'David')



Neo4J: Behind the Scene

Neo4j Internals: Indexes



CREATE INDEX ON :Person(name);

(Create index on property name of nodes with label Person) Indexes added: 1

Since Neo4j v.2, indexes are used automatically

 Can be specified explicitly (which index to use)

 MATCH (n:Person)

 USING INDEX n:Person(surname)
 WHERE n.surname = 'Taylor'
 RETURN n

Neo4j Internals: Transactions



- Transactions in Neo4j
 - Support for ACID properties
 - All write operations must be performed in a transaction
 - Default transaction isolation level: Read committed
 - Operation can see the last committed value
 - Reads do not block or take any locks
 - If the same row is retrieved twice within a transaction, the values in the row can differ
 - Higher level of isolation can be achieved
 - By explicit acquiring the read locks

Neo4j Internals: High Availability



- Master-slave replication
 - Several Neo4j slave databases can be configured to be exact replicas of a single Neo4j master database
- Speed-up of read operations
 - Enables to handle more read load than a single node
- Fault-tolerance
 - In case a node becomes unavailable
- Transactions are still atomic, consistent and durable, but eventually propagated to the slaves



Graph Databases: When (not) to Use

Graph DBs: Suitable Use Cases



- Connected Data
 - o Social networks
 - Any link-rich domain is well suited for graph databases
- Routing, Dispatch, and Location-Based Services
 - Node = location or address that has a delivery
 - Graph = nodes where a delivery has to be made
 - Relationships = distance
- Recommendation Engines
 - o "your friends also bought this product"
 - o "when buying this item, these others are usually bought"

Graph DBs: Modeling Issues



- Node modeling:
 - tradeoff between placing all attributes and properties in a single node,
 - and separating each attribute into an individual node.
- Relationship modeling:
 - o "unlabeled" all,
 - e.g., person **connected_to** person/address/product
 - versus semantic meaning encoded labels
 - e.g., person peters_work_colleague person, person peters_home_address address

Graph DBs: When Not to Use



- If we want to update all or a subset of entities
 - Changing a property on many nodes is not straightforward
 - e.g., analytics solution where all entities may need to be updated with a changed property
- No BLOBs (large binary objects) in byte arrays.
- Some graph databases may be unable to handle lots of data
 - Distribution of a graph is difficult





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