

# **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**





3

## **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
- 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
- Graph G = (V, E) is usually modelled as
  - set of nodes (vertices) V, |V| = n
  - o set of (directed) edges  $E = (V_1, V_2), |E| = m$
- Which 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<sub>ij</sub> indicates
    whether nodes *i*, *j* are connected

### • Variants:

- o (Un)directed graphs
- o Weighted graphs...



## **Adjacency Matrix: Properties**





• Pros:

- Adding/removing edges
- Checking if 2 nodes are connected
- Cons:
  - Quadratic space: O(n<sup>2</sup>)
  - We usually have sparse graphs
  - Adding nodes is expensive
  - Retrieval of all the neighboring nodes takes linear time: O(n)

# **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



- N1 → {N2, N3}
- $N2 \rightarrow \{N1, N3, N5\}$
- $\text{N3} \not \rightarrow \{\text{N1}, \text{N2}, \text{N5}\}$
- N4 → {N2, N6}
- N5 → {N2, N3}
- N6 → {N4}

### **Adjacency List: Properties**





- N1 → {N2, N3}
- N2 → {N1, N3, N5}
- N3 → {N1, N2, N5}

N4 → {N2, N6}

N5 → {N2, N3}

[2, N3}

• Pros:

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

### **Data Structure: Incidence Matrix**

- Two-dimensional Boolean matrix of 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







### **Incidence Matrix: Properties**





• Pros:

- Representation of hypergraphs
  - where one edge connects an arbitrary number of nodes
- Cons:
  - O 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 -1 if the two vertices are connected, 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),
  - o 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) |
| $\left(\begin{array}{cccccccccccccccccccccccccccccccccccc$ |    |   |   |   |   |   |   |    |

# 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



- 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 about 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
- 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 G<sub>1</sub>,..., G<sub>n</sub>
- 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 2<sup>n</sup>)
- o due to isomorfisms, there much less 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?

# Relationship Properties: Example



source: Sadalage & Fowler: NoSQL Distilled, 20122

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des

Matrix

### 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
  - 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 |                               | incoming file relationships                                 |   | A                   |
| get all paths for a file    |                               | incoming <i>file</i> and <i>symbolic link</i> relationships |   | file file           |
|                             |                               |   |   |                     |

get all files in a directoryoutgoing file and symbolic link relationships,<br/>depth oneget all files in a directory, excluding<br/>symbolic linksoutgoing file relationships, depth oneget all files in a directory, recursivelyoutgoing 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
  - o 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]->(follower) **RETURN** user.name, follower.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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