

Introduction

Please find two other learning partners,

- ▶ form a standing group and
- ▶ tell them what you already know about
 - ▶ graphs,
 - ▶ graph databases and
 - ▶ Neo4j.

Graph Data - Modelling and Querying

with Neo4j and Cypher

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Graph Database - NRW Meetup

6 December 2017



Learning goals

What are graphs?

- Definition

- Use cases

Starting with Neo4j and Cypher

- Configuration and start

- CRUD operations with Cypher

Querying for paths and patterns

Using graph algorithms

- apoc library

- algo library

Importing data

Refactoring graph data model

Graph

Definition

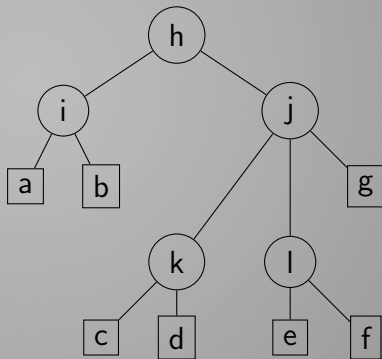
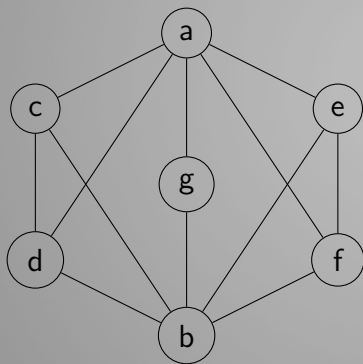
Graph is an ordered pair $G = (V, E)$ comprising a set V of *vertices*, *nodes* or *points* together with a set E of *edges*, *arcs* or *lines*, which are 2-element subsets of V .¹

¹[en.wikipedia.org/wiki/Graph_\(discrete_mathematics\)](https://en.wikipedia.org/wiki/Graph_(discrete_mathematics))

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Use Cases

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- ▶ Networks

Use Cases

- ▶ Networks
 - ▶ Social networks



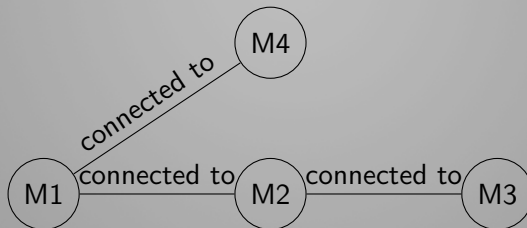
Use Cases

- ▶ Networks

- ▶ Social networks

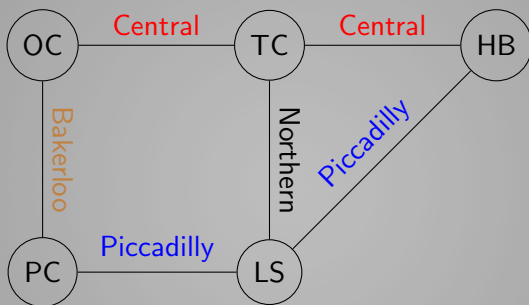


- ▶ Computer networks



Use Cases

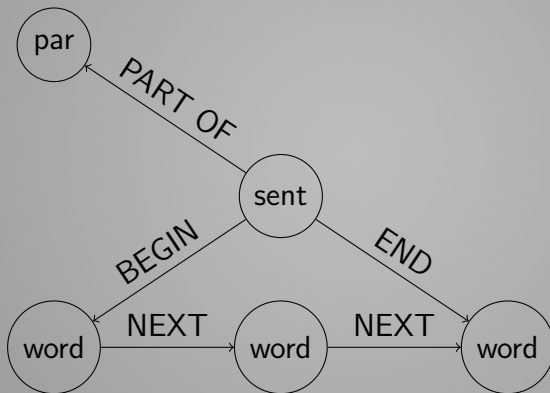
- ▶ Networks
 - ▶ Transport networks



OC = Oxford Circus, *LS* = Leicester Square
HB = Holborn, *PC* = Piccadilly Circus
TC = Tottenham Court Road

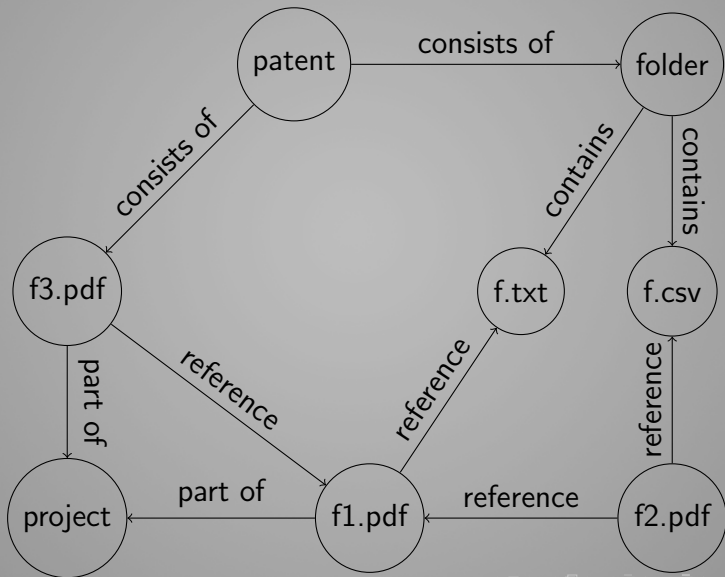
Use Cases

- Natural Language Processing



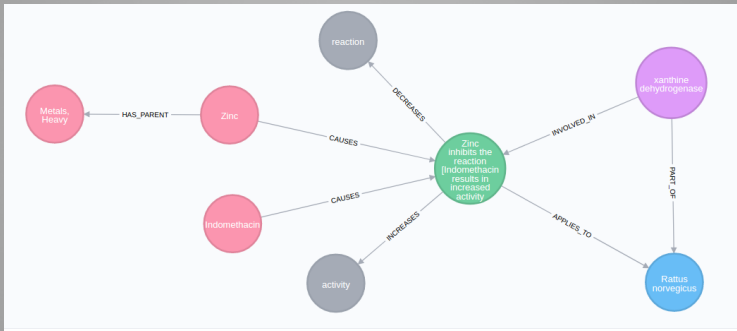
Use Cases

- ▶ Document management



Use Cases

► Biochemistry / Genomics



Practice activity - Graph modeling

- ▶ Come up with any use case idea of your choice.
- ▶ Model it as a graph on a sheet of paper.
- ▶ Introduce it to at least one of the attendees.

Installation

- ▶ Find the right installation file for your OS at `neo4j-training-files/neo4j` on the flash drive and install the software.

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- ▶ Mac-Users: Copy the plugins directory into your `/Application/Neo...` and into `graph.db/plugins`

Installation

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- ▶ Mac-Users: Copy the plugins directory into your `/Application/Neo...` and into `graph.db/plugins`
- ▶ Windows-Users: Follow the installation and start client.

Installation

- ▶ Replace the `NEO4J_HOME/conf/neo4j.conf` configuration file with the one found on the flash drive at `neo4j-training-files/conf/neo4j.conf`.

Installation

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- ▶ Copy the `neo4j-training-files/data/ctdbase.db` folder into your `NEO4J_HOME/data/databases/` directory

Starting Neo4j

- ▶ Start the database with
`NEO4J_HOME/bin/neo4j console`

Starting Neo4j

- ▶ Start the database with
`NEO4J_HOME/bin/neo4j console`
- ▶ Go to `http://localhost:7474` within you browser

Practice activity

- ▶ Please separate in 4 groups:
 - ▶ Chemical
 - ▶ Disease
 - ▶ Organism
 - ▶ Gene

Practice activity

- ▶ Please separate in 4 groups:
 - ▶ Chemical
 - ▶ Disease
 - ▶ Organism
 - ▶ Gene
- ▶ Explore the dashboard in groups
- ▶ What can you find out about your node type?
- ▶ What questions arise?

Demonstration

Important configuration entries

```
dbms.active_database=ctdbase.db
```

```
dbms.security.auth_enabled=false
```

```
dbms.security.procedures.unrestricted=algo.*,apoc.*
```

```
apoc.import.file.enabled=true
```

Live coding session - CRUD operations

create node

```
CREATE (c:Chemical {name: 'Helium'})  
      RETURN c
```

update node

```
MERGE (c:Chemical {name: 'Helium'})  
      SET c.symbol = 'He'      RETURN c
```

Live coding session - CRUD operations

delete node without relations

```
MATCH (c:Chemical {name:'Helium'})  
DELETE c
```

delete node without relations

```
MATCH (c:Chemical)  
WHERE c.name = 'Helium'  
DELETE c
```

delete node with existing relations

```
MATCH (c:Chemical {name:'Helium'})  
DETACH DELETE c
```

Live coding session - CRUD operations

create relation between new nodes

```
CREATE (c:Chemical {chemicalName:'Helium'})  
      -[:BELONGS_TO]->  
      (g:ChemicalGroup {groupName:'Noble gases'})  
RETURN c,g
```

create relation between existing nodes

```
MATCH (g:ChemicalGroup {groupName:'Noble gases'}),  
      (p:ChemicalGroup {groupName:'Gases'})  
CREATE (g)-[:HAS_PARENT]->(p)  
RETURN g,p
```

Live coding session - CRUD operations

update relation

```
MATCH ()-[r:BELONGS_TO]-()  
      SET r.updateTime = timestamp()  
      RETURN r
```

delete relation

```
MATCH ()-[r:BELONGS_TO]-()  
      DELETE r
```

Practice activity

- ▶ Go back to your graph model from the beginning of the training.
- ▶ Create about
 - ▶ 10 nodes and
 - ▶ 15 relations
 - ▶ with properties.

FINISH: PART ONE

Live coding session

Check your indexes

```
CALL db.indexes
```

```
CREATE INDEX ON :Disease(diseaseId)
```

```
CREATE INDEX ON :Gene(geneName, geneSymbol)
```


Live coding session

Example

```
MATCH (g:Gene)
      WHERE g.geneSymbol = 'CTSD'
      RETURN g
```

Example

```
MATCH (g:Gene)<-[:ASSOCIATED_WITH]-(d:Disease)
      WHERE g.geneSymbol = 'CTSD'
      RETURN g, d
```

Example

```
MATCH (g:Gene)<-[:ASSOCIATED_WITH]-(d:Disease)
      WHERE g.geneSymbol = 'CTSD'
      RETURN g, count(d)
```

Live coding session

Example

```
MATCH (g:Gene)<-[:ASSOCIATED_WITH]-(d:Disease)
      WITH g, count(d) as diseases
      WHERE diseases >50
      RETURN g.geneName, g.geneSymbol, diseases
      ORDER BY diseases DESC
```

Example

```
MATCH (g:Gene)<-[:ASSOCIATED_WITH]-(d:Disease)
      -[:ASSOCIATED_WITH]->(otherGene:Gene)
      WHERE g.geneSymbol = 'CTSD'
      AND d.diseaseName = 'Osteoarthritis'
      RETURN otherGene.geneName, otherGene.geneSymbol
```

Live coding session

Example

```
MATCH p = (c:Chemical)-[*2]-(d:Disease)
      WHERE d.diseaseName STARTS WITH 'Osteo'
      RETURN p LIMIT 20
```

Example

```
MATCH (c:Chemical)<-[:HAS_PARENT*3..4]-(d:Chemical)
      WITH c, count(d) AS descendants,
      collect(d.chemicalName) AS names
      ORDER BY descendants DESC LIMIT 10
      RETURN c.chemicalName, names[1..10], descendants
```

Live coding session

Example

```
MATCH (c:Chemical)
      WHERE c.chemicalName = 'Zinc Acetate'
MATCH (d:Disease)
      WHERE d.diseaseName = 'Alzheimer Disease'
MATCH p = (c)-[*1..3]-(d)
RETURN p LIMIT 20
```

Example

```
MATCH (:InteractionType {typeName:'degradation'})
      <-[:INCREASES|:DECREASES]-
      (i:Interaction)-[:APPLIES_TO]->
      (:Organism {organismName:'Cricetulus griseus'})
RETURN i.description
```

Practice activity

For each group (Chemical, Disease, Organism, Gene):

- ▶ Please check your questions from the first practice activity.
 - ▶ Can you answer any of them now?
- ▶ Think about new questions as you explore the graph with the querying techniques just learned.
- ▶ Present one question, appropriate query and an answer to your classmates.

Live coding session

Shortest path example

```
MATCH (zinc:Chemical {chemicalName:'Zinc Acetate'}),  
      (metals:Chemical {chemicalName:'Metals, Heavy'}),  
      p = shortestPath((zinc)-[*..15]-(metals))  
RETURN p
```

Shortest path example

```
MATCH (zinc:Chemical {chemicalName:'Zinc Acetate'}),  
      (metals:Chemical {chemicalName:'Metals, Heavy'}),  
      p = shortestPath((zinc)-[*..15]-(metals))  
WHERE NONE(r IN relationships(p)  
           WHERE type(r)='CAUSES')  
RETURN p
```

Live coding session

Shortest path example

```
MATCH (c:Chemical {chemicalName:'Zinc Acetate'}),  
      (d:Disease {diseaseName:'Alzheimer Disease'})  
MATCH path = allShortestPaths( (c)-[*..3]-(d) )  
RETURN path
```

Calling procedures

- ▶ `CALL db.schema`
- ▶ `CALL dbms.procedures`
- ▶ `CALL dbms.functions`
- ▶ `CALL apoc.help('dijkstra')`

Live coding session

Definition

In a connected graph, the normalized *closeness centrality* of a node is the average length of the shortest path between the node and all other nodes in the graph. Thus the more central a node is, the closer it is to all other nodes.²

Closeness Centrality Example

```
MATCH (node:Chemical)
```

```
    WHERE node.chemicalName CONTAINS 'Vitamin'
```

```
    WITH collect(node) AS nodes
```

```
CALL apoc.algo.closeness(['HAS_PARENT'],nodes,'BOTH')
```

```
    YIELD node, score
```

```
RETURN node, score
```

```
    ORDER BY score DESC
```

²en.wikipedia.org/wiki/Centrality#Closeness_centrality

Live coding session

Definition

Betweenness centrality quantifies the number of times a node acts as a bridge along the shortest path between two other nodes.³

Betweenness Centrality Example

```
MATCH (node:Disease)
      WHERE node.diseaseName CONTAINS 'deficiency'
      WITH collect(node) AS nodes
CALL apoc.algo.betweenness(['HAS_PARENT'],
                           nodes,'BOTH')
      YIELD node, score
RETURN node.diseaseName, score
      ORDER BY score DESC LIMIT 10
```

³en.wikipedia.org/wiki/Centrality#Betweenness_centrality 🔍🔍🔍

Live coding session

Definition

In graph theory, a *clique* is a subset of vertices of an undirected graph such that every two distinct vertices in the clique are adjacent.

Clique example query

```
MATCH (startNode:Category
      {name:'Endocrine system disease'})
  CALL apoc.algo.cliquesWithNode(startNode, 4)
  YIELD clique
RETURN clique
```

Practice activity

Explore the APOC library:

- ▶ read the documentation,
- ▶ try out different queries,
- ▶ make notes to about your questions and results.

Live coding session

PageRank example

```
CALL algo.pageRank.stream('InteractionType',  
    'HAS_PARENT', {iterations:20})  
    YIELD node, score  
WITH * ORDER BY score DESC LIMIT 5  
RETURN node.typeName, node.code, score;
```

Partitioning into connected components

```
CALL algo.unionFind('InteractionType',  
    'HAS_PARENT', write:true,  
    partitionProperty:"partition")  
YIELD nodes, setCount, loadMillis,  
    computeMillis, writeMillis
```

Live coding session

Closeness

```
CALL algo.closeness('Chemical', 'HAS_PARENT',  
    {write:true, writeProperty:'centrality'})  
YIELD nodes, loadMillis, computeMillis, writeMillis
```

Closeness

```
MATCH (c:Chemical)  
    WHERE c.centrality >200  
RETURN c.chemicalName, c.centrality  
    ORDER BY c.centrality DESC LIMIT 10
```

LOAD CSV

View the data

USING PERIODIC COMMIT 500

LOAD CSV WITH HEADERS FROM

"file:///.../_Disease-GO_biological_process_associations.csv"

AS line

RETURN line LIMIT 10

³<http://ctdbase.org/>

LOAD CSV

Import the data

```
USING PERIODIC COMMIT 500
```

```
LOAD CSV WITH HEADERS FROM
```

```
"file:///.../Disease-GO_biological_process_associations.csv"
```

```
AS line LIMIT 20
```

```
MATCH (d:Disease)
```

```
WHERE last(split(d.diseaseID,':')) = line.DiseaseID
```

```
MERGE (b:BiologicalProcess goid:line.GOID)
```

```
SET b.goName = line.GOName
```

```
MERGE (b)<-[:AFFECTED_BY
```

```
{inferenceGeneQty:line.InferenceGeneQty,
```

```
inferenceGeneSymbols:line.InferenceGeneSymbols}]- (d)
```


apoc.load.csv

View the data

```
CALL apoc.load.csv(  
    'file:///.../CTD_chem_go_enriched.csv',  
)  
YIELD lineNo, map AS line RETURN lineNo, line limit 5
```

³<http://ctdbase.org/>

Loading big files

```
CALL apoc.periodic.iterate(  
    "CALL apoc.load.csv(  
        'file:///.../CTD_chem_go_enriched.csv',  
    )  
    YIELD lineNo, map AS line RETURN lineNo, line",  
    "MATCH (c:Chemical {chemicalID : line.ChemicalID})  
    MERGE (o:Ontology {name : line.Ontology})  
    MERGE (t:Term {termID : line.GOTermID})  
        SET t.termName = line.GOTermName  
        SET t.level = line.HighestGOLevel  
    MERGE (c)-[r:AFFECTED_BY]-(t)-[:TERM_OF]->(o)  
        SET r.pValue = line.PValue  
        SET r.correctedPValue = line.CorrectedPValue",  
    {batchSize:10000, iterateList:true}  
)
```

³<http://ctdbase.org/>

Practice activity

- ▶ Choose a CSV file from `neo4j-training-files/data/CTD`.
- ▶ Load and show first 15 lines.
- ▶ Import some of the columns of the first 15-20 lines and connect it to existing graph nodes.

Refactor your graph

Add labels

```
MATCH (p:Pathway)
      WHERE toLower(p.pathwayName)
            CONTAINS 'reaction'
CALL apoc.create.addLabels(id(p), ['Reaction'])
YIELD node
RETURN count(node)
```

Rename relation

```
MATCH ()-[r:PART_OF]-()
CALL apoc.refactor.setType(r, 'BELONGS_TO')
YIELD input, output
RETURN count(input), count(output)
```

Practice activity

- ▶ Rename the relation :INVOLVED_IN in :INVOLVES
- ▶ and invert the direction.
- ▶ Can you find out how to invert the direction of the relation?
- ▶ First rename, then invert? Or first invert and then rename?

References

- ▶ Curated chemical–gene, chemical–disease and gene–disease interactions data were retrieved from the Comparative Toxicogenomics Database (CTD), MDI Biological Laboratory, Salisbury Cove, Maine, and NC State University, Raleigh, North Carolina. URL: <http://ctdbase.org/>. [October, 2017].
- ▶ Cypher Reference Card <https://neo4j.com/docs/cypher-refcard/current/>
- ▶ APOC User Guide <https://neo4j-contrib.github.io/neo4j-apoc-procedures/>
- ▶ Efficient Graph Algorithms in Neo4j <https://neo4j.com/blog/efficient-graph-algorithms-neo4j/>

Getting Help

Slack




`neo4j.com/blog/public-neo4j-users-slack-group/`

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Contact details

- ▶  @ira_res
- ▶ **in** `www.linkedin.com/in/ifeuerstein/`
- ▶  `github.com/IraRe`
- ▶  `iryna.feuerstein@prodyna.com`

Home work

- ▶ Pick an organism from the data base (for example the Chinese Hamster aka *Cricetulus griseus*).



- ▶ Find some interesting information about it in the database.
- ▶ Tweet to me a piece of information with the hashtag #cricetulus.
- ▶ Get a coffe mug for an interesting tweet!