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 Quering

with Neo4j and Cypher

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Open Data Science Conference

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Learning goals

- What are graphs?
  - Definition
  - Use cases
- Starting with Neo4j and Cypher
  - Configuration and start
  - CRUD operations with Cypher
- Indexes
- Quering 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)

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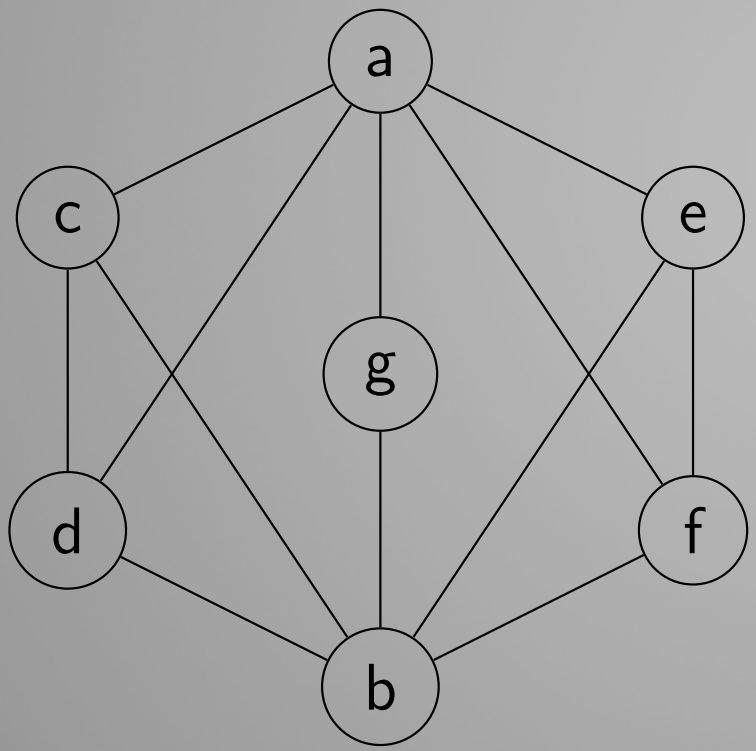

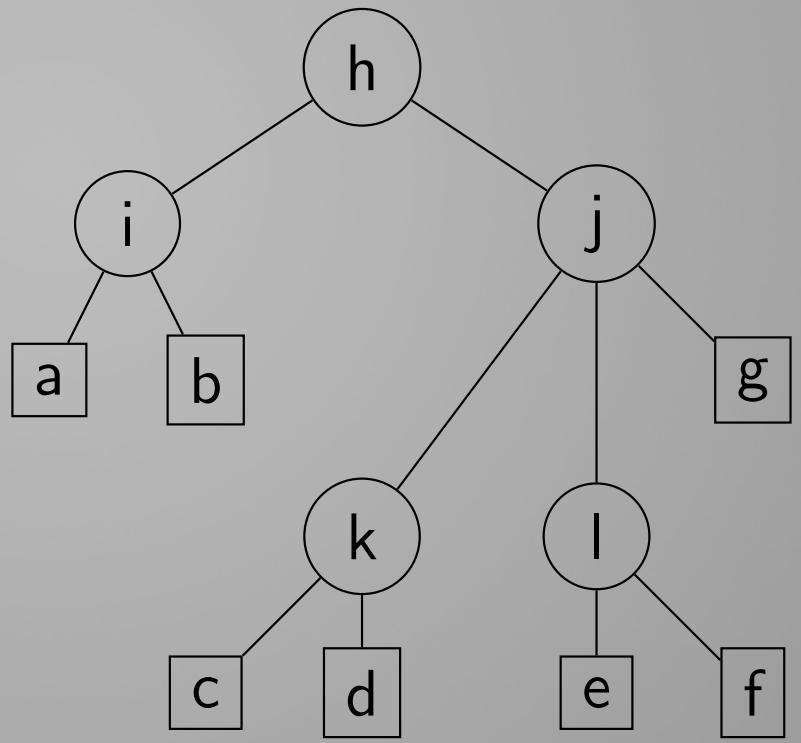

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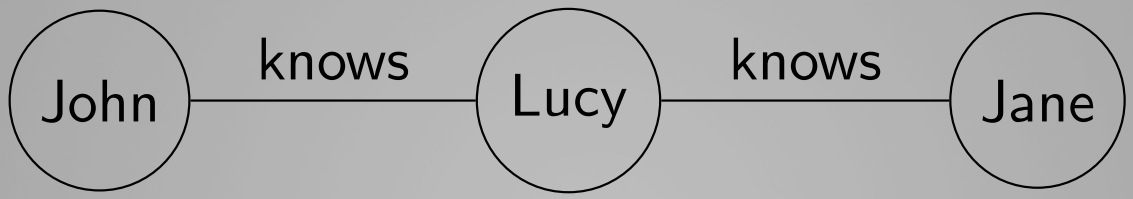
Use Cases

Use Cases

- Networks
  - Social networks



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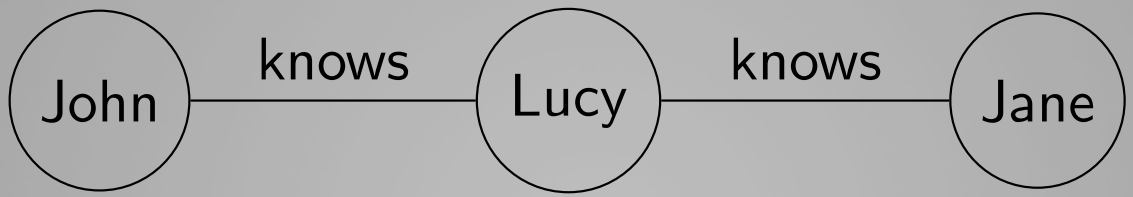
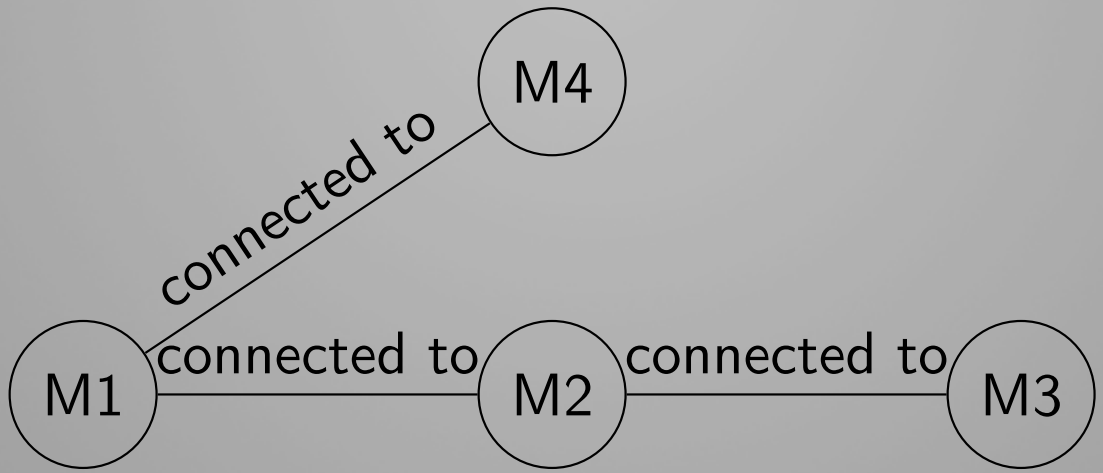
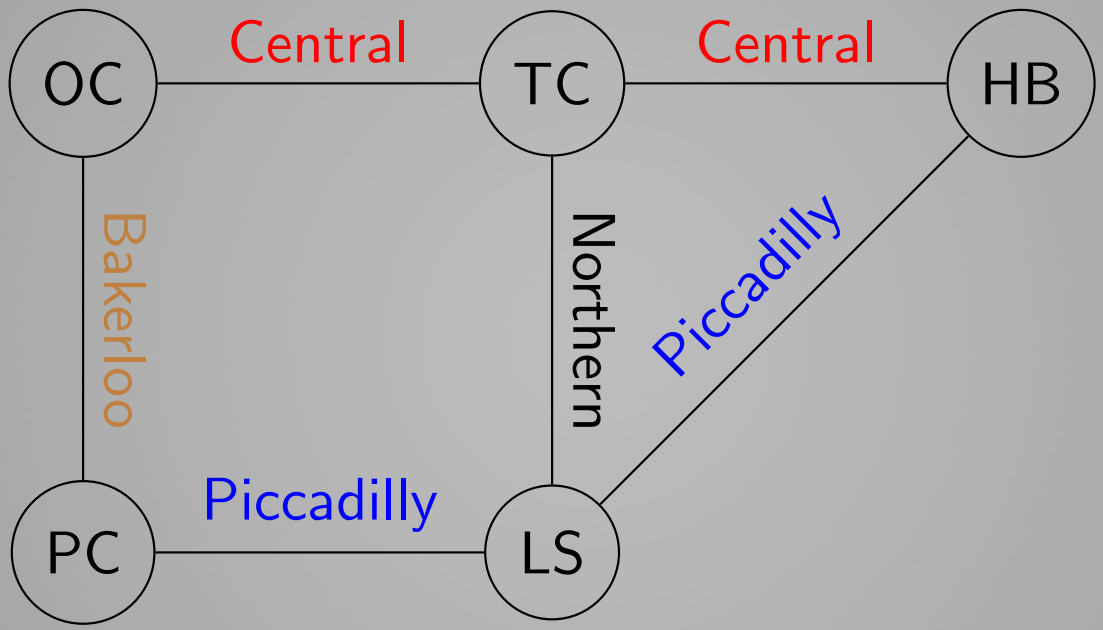


  - Computer networks



Use Cases

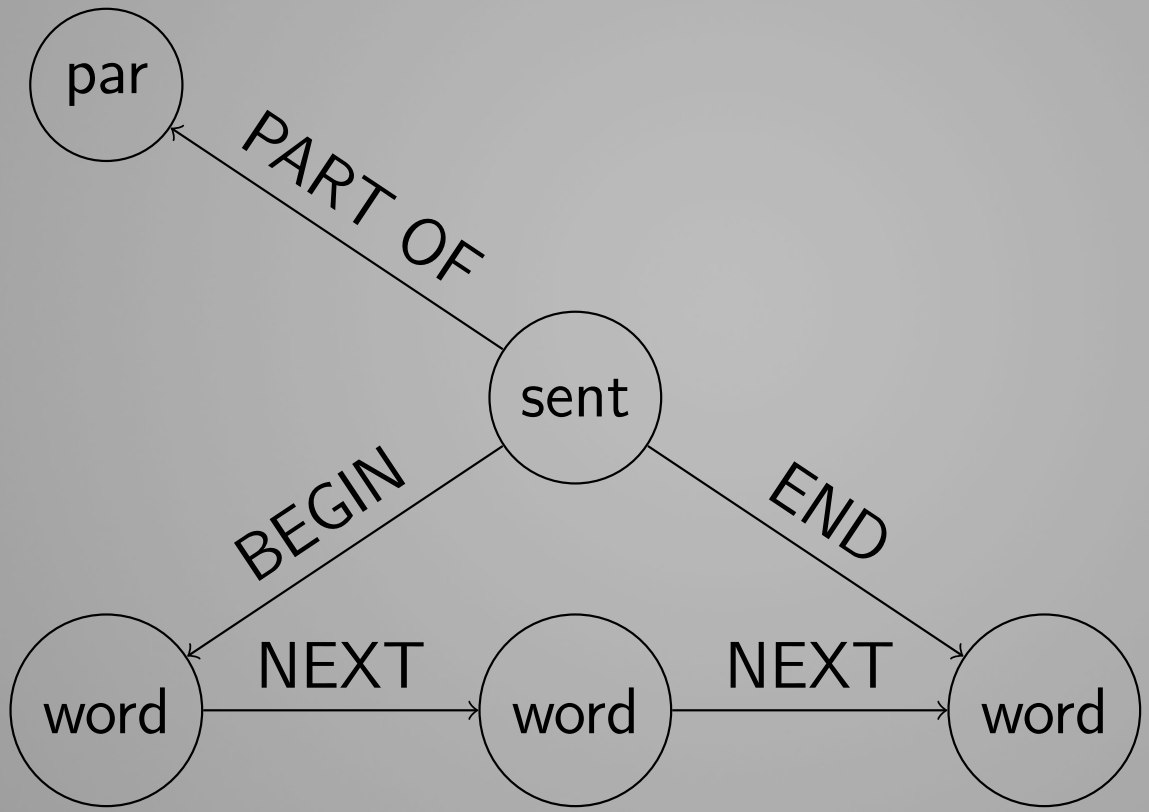
- Networks
  - Transport networks



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

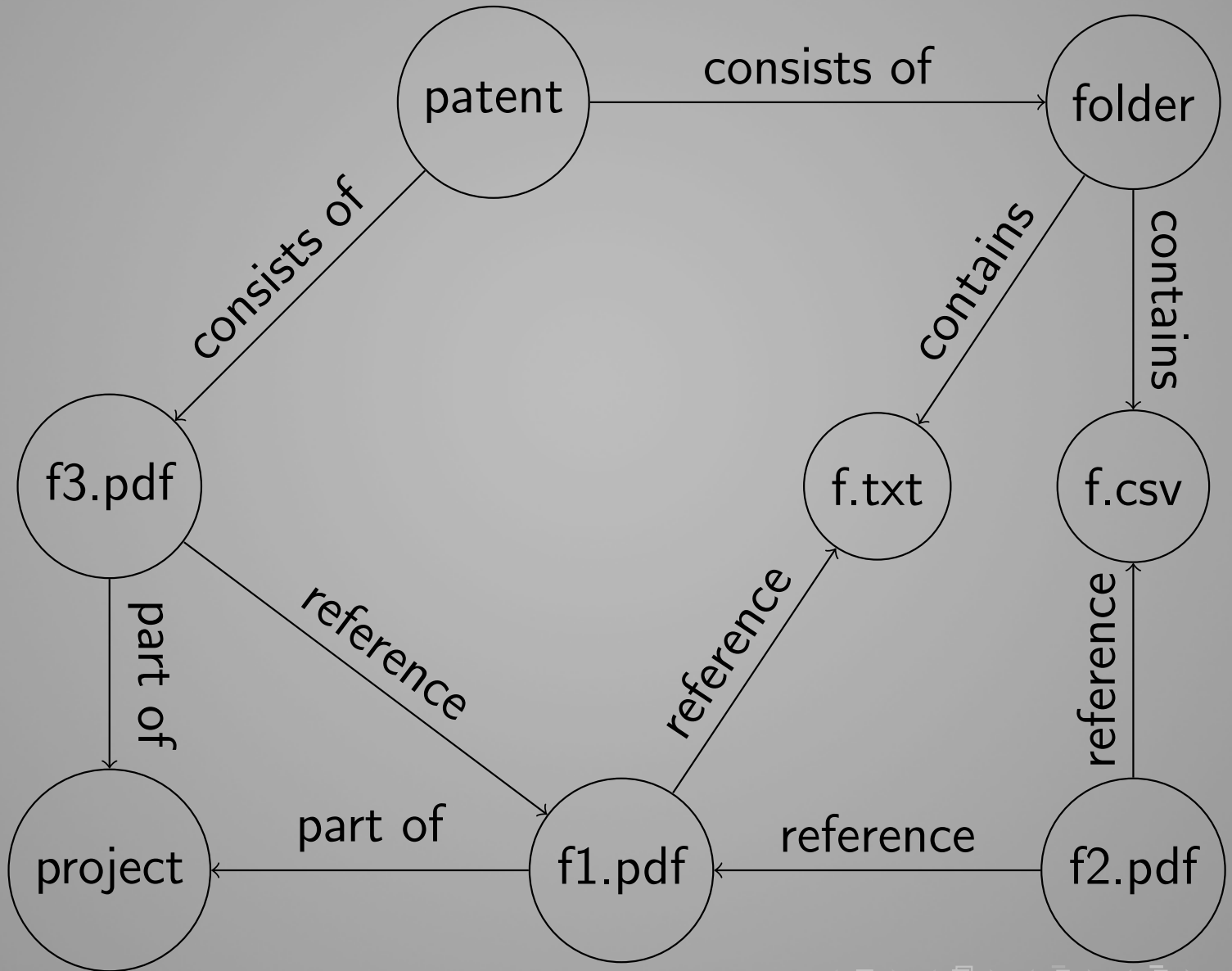
Use Cases

- Natural Language Processing



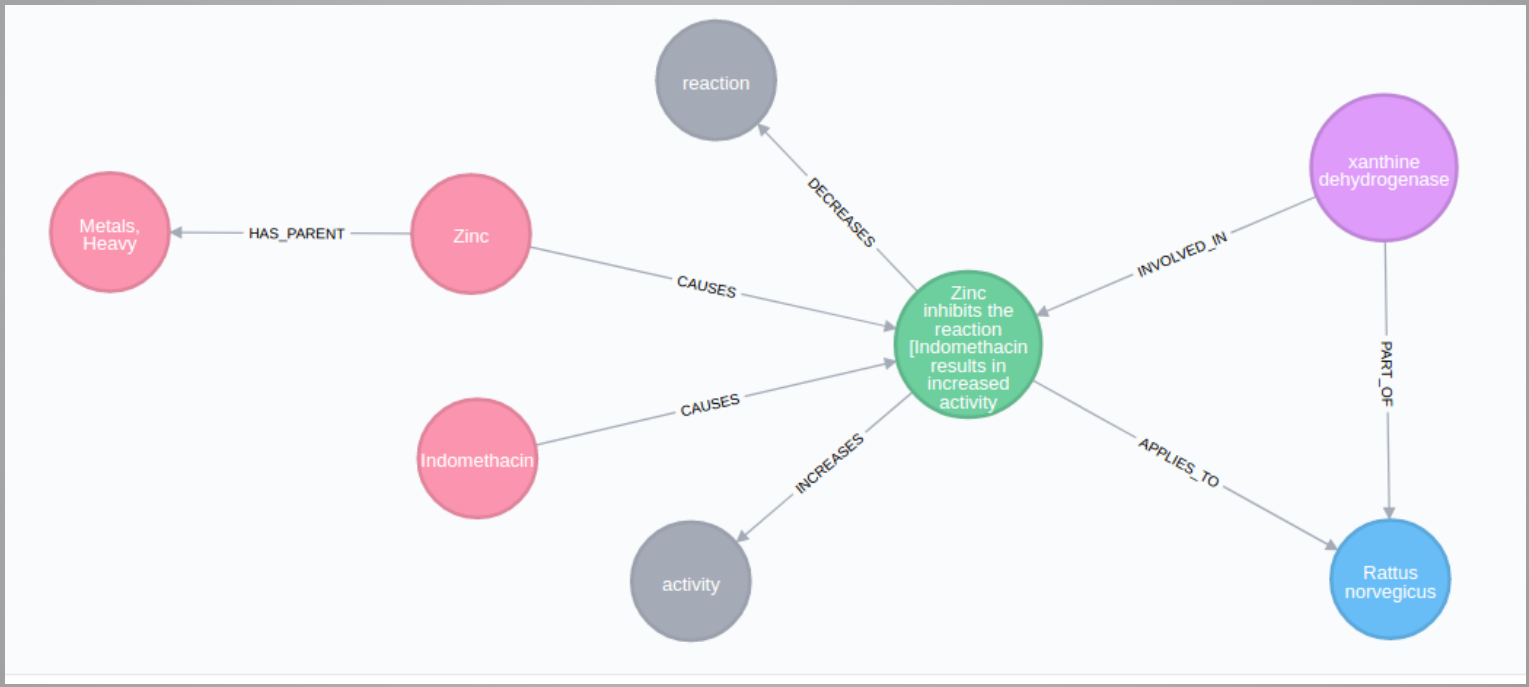
Use Cases

- Document management



Use Cases

- Biochemistry / Genomics



[1] http://ctdbase.org/

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

Starting Neo4j

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

Demonstration

Important configuration entries

dbms.active_database=odsc.db
dbms.security.auth_enabled=false
dbms.security.procedures.unrestricted=algo.*,apoc.*
apoc.import.file.enabled=true

Live coding session

- create node
  CREATE (c:Chemical {name: 'Helium'}) RETURN c
- update node
  MERGE (c:Chemical {name: 'Helium'}) SET c.symbol = 'He' RETURN c
- delete node
  - without relations
    MATCH (c:Chemical {name:'Helium'}) DELETE c
    MATCH (c:Chemical)
    WHERE c.name = 'Helium'
    DELETE c
  - with existing relations
    MATCH (c:Chemical {name:'Helium'})
    DETACH DELETE c

Live coding session

- create relation
  - between new nodes
    CREATE (c:Chemical chemicalName:'Helium')-[:BELONGS_TO]-¿(g:ChemicalGroup groupName:'Noble gases') RETURN c,g
  - between existing nodes
    MATCH (g:ChemicalGroup groupName:'Noble gases'), (p:ChemicalGroup groupName:'Gases') CREATE (g)-[:HAS_PARENT]-¿(p) RETURN g,p
- update relation
  MATCH ()-[r:BELONGS_TO]-() SET r.updateTime = timestamp() RETURN r
- delete relation
  MATCH ()-[r:BELONGS_TO]-() DELETE r

Indexes

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

Live coding session

Examples:

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

- MATCH p = (c:Chemical)-[*2]-(d:Disease) where d.diseaseName STARTS WITH 'Osteo' RETURN p LIMIT 20
- MATCH (c:Chemical)¡-[:HAS_PARENT*3..4]-(descendant:Chemical) WITH c, count(descendant) AS descendants , collect(descendant.chemicalName) as names ORDER BY descendants DESC LIMIT 10 RETURN c.chemicalName, names[1..10], descendants
- 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
- MATCH (type:InteractionType typeName:'degradation')¡-[:INCREASES—:DECREASES]-(i:Interaction)-[:APPLIES_TO]-¿(o:Organism organismName:'Cricetulus griseus') RETURN i.description

Live coding session

Shortest path

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

[2] en.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
```

[3] en.wikipedia.org/wiki/Centrality#Betweenness_centrality

Live coding session

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

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

Closeness

CALL algo.closeness('Chemical', 'HAS_PARENT', write:true, writeProperty:'centrality') YIELD nodes,loadMillis, computeMillis, writeMillis
match (c:Chemical) where c.centrality ¿ 200 return c.chemicalName, c.centrality order by c.centrality desc limit 10

LOAD CSV

```
USING PERIODIC COMMIT 500 LOAD CSV WITH
HEADERS FROM
"file:///neo4j-training-files/data/CTD/CTD_Disease-
GO_biological_process_associations.csv" AS line RETURN line
LIMIT 10
USING PERIODIC COMMIT 500 LOAD CSV WITH
HEADERS FROM
"file:///neo4j-training-files/data/CTD/CTD_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

```
CALL apoc.load.csv( 'file:///neo4j-training-files/data/CTD/CTD_chem_go_enriched.csv', ) YIELD lineNo, map AS line RETURN lineNo, line limit 5
CALL apoc.periodic.iterate( "CALL apoc.load.csv( 'file:///neo4j-training-files/data/CTD/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 )
```

Live coding session

```
MATCH (n:Movie) CALL apoc.create.addLabels( id(n), [
n.genre ] ) YIELD node REMOVE node.genre RETURN node
CALL apoc.periodic.iterate( "MATCH (p:Person) WHERE
(p)-[:ACTED_IN]-¿() RETURN p", "SET p:Actor",
batchSize:10000, parallel:true)
call apoc.refactor.setType(rel, 'NEW-TYPE')
```