Neo4J-commands:

Data bulk insertion

i1: Loading the CSV files (genes, enhancers, TFPairs)

LOAD CSV FROM "file:///genenames.csv" AS line CREATE (:Gene { genename: toString(line[0])});

c1: Assigning a uniqueness constraints to nodes

CREATE CONSTRAINT ON (g:Gene) ASSERT g.genename IS UNIQUE;

i2: Loading the CSV files (genes, enhancers, TFPairs)

LOAD CSV FROM "file:///enhids.csv" AS line CREATE (:Enhancer { enhancerID: toString(line[0])});

c2: Assigning a uniqueness constraints to nodes

CREATE CONSTRAINT ON (e:Enhancer) ASSERT e.enhancerID IS UNIQUE;

i3: Loading the CSV files (genes, enhancers, TFPairs)

LOAD CSV FROM "file:///tfpairs.csv" AS line CREATE (p:TFPair {name:toString(line[4]), pwm1:toString(line[0]), pwm2:toString(line[1]), knownCompelPair:toBoolean(line[2]), knownBioGridPair:toBoolean(line[3])}) RETURN p.name;

c3: Assigning a uniqueness constraints to nodes

CREATE CONSTRAINT ON (t:TFPair) ASSERT t.name IS UNIQUE;

i4: Loading relationship data from CSV files (EPI and binds)

LOAD CSV FROM "file:///enh2promo.csv" AS line MATCH (e:Enhancer {enhancerID:toString(line[0])}) MATCH (g:Gene {genename:toString(line[1])}) MERGE (e)-[r:EPI]->(g) RETURN e.enhancerID, g.genename;

i5: Loading relationship data from CSV files (EPI and binds)

LOAD CSV FROM "file:///tf2gene.csv" AS line MATCH (p:TFPair {name:toString(line[5])}) MATCH (g:Gene {genename:toString(line[4])}) CREATE (p)-[r:binds {zscore:toFloat(line[2])}]->(g) RETURN p.name,g.genename,r.zscore;

i6: Loading relationship data from CSV files (EPI and binds)

LOAD CSV FROM "file:///tf2enh.csv" AS line MATCH (p:TFPair {name:toString(line[4])}) MATCH (e:Enhancer {enhancerID:toString(line[3])}) CREATE (p)-[r:binds {zscore:toFloat(line[2])}]->(e) RETURN p.name,e.enhancerID,r.zscore;

Path queries

Q1a: For a given genename, find all enhancers interacting with that gene.

MATCH (g:Gene)-[:EPI]-(e:Enhancer)

WHERE g.genename="SLC25A45" RETURN g,e

Q1b: For a genename set, find all enhancers interacting with the genes.

MATCH (g:Gene)-[:EPI]-(e:Enhancer)

WHERE g.genename IN ["IER5L", "SLC25A45"] RETURN g,e

Q2a: For a given genename, find all TFPairs bound to that gene.

MATCH (g:Gene)-[:binds]-(t:TFPair)

WHERE g.genename="SLC25A45" RETURN g,t

Q2b: Restrict to the known TFPairs with AND operator.

MATCH (g:Gene)-[:binds]-(t:TFPair)

WHERE g.genename="SLC25A45"

AND t.knownCompelPair=TRUE RETURN g,t

Q2c: Restrict to the known TFPairs with AND and OR operator

MATCH (g:Gene)-[:binds]-(t:TFPair)

WHERE g.genename="SLC25A45"

AND (t.knownCompelPair=TRUE OR t.knownBioGridPair=TRUE)

RETURN g,t

Q2d: Find the TFPairs of an enhancer that interact with a certain gene.

MATCH p=(g:Gene)-[:EPI]-(e:Enhancer)-[:binds]-(t:TFPair)

WHERE g.genename="BATF2" RETURN p

Q2e: Restrict to z-score larger than 4.

MATCH p=(g:Gene)-[:EPI]-(e:Enhancer)-[:binds]-(t:TFPair)

WHERE g.genename="BATF2" AND r.zscore>4 RETURN p

Q3a: For all genenames find all other genenames that are bound by at least one common TFPair.

MATCH p=(g:Gene)-[:binds]-(t:TFPair)-[:binds]-(g2:Gene)

RETURN p

Q3b: For a specific gene find all other genenames that are bound by at least one common TFPair.

MATCH p=(g:Gene)-[:binds]-(t:TFPair)-[:binds]-(g2:Gene)

WHERE g.genename="MYL12B" RETURN p

Q3c: For a specific enhancerID find all other enhancerIDs that are bound by at least one common TFPair.

MATCH p=(e:Enhancer)-[:binds]-(t:TFPair)-[:binds]-(e2:Enhancer)

WHERE e.enhancerID="chr11:65239550-65239870-enhancer"

RETURN p

Q3d: For a specific enhancerID find genenames that are bound by at least one common TFPair.

MATCH p=(e:Enhancer)-[:binds]-(t:TFPair)-[:binds]-(g:Gene)

WHERE e.enhancerID="chr11:65239550-65239870-enhancer"

Q4a: For a given enhancer ID (or a prefix of the ID), find all the TFPairs bound to the enhancer.

MATCH (e:Enhancer)-[:binds]-(t:TFPair)
WHERE e.enhancerID STARTS WITH "chr1:" RETURN e,t

Q5a: For a given enhancerID, find all genes interacting with the enhancer.

MATCH (e:Enhancer)-[:EPI]-(g:Gene)
WHERE e.enhancerID STARTS WITH "chr11:" RETURN e,g

Q6a: For a given genename, find all TFPairs bound to the gene.

MATCH p=(g:Gene)-[r:binds]-(t:TFPair)
WHERE g.genename="SLC25A45" RETURN p

Q6b: For a given genename, find all TFPairs bound to the gene restricting to those bindings with a high zscore.

MATCH p=(g:Gene)-[r:binds]-(t:TFPair)
WHERE g.genename="SLC25A45" AND r.zscore>4 RETURN p

Q7a: For a given TF find all TFPairs that contain the TF.

MATCH (t:TFPair)
WHERE t.pwm1="V\$ELK1_02" OR t.pwm2="V\$ELK1_02"
RETURN t

Q7b: For a given TF find the names of the two transcription factors in the TFPairs that contain the transcription factor.

MATCH (t:TFPair)
WHERE t.pwm1="V\$ELK1_02" OR t.pwm2="V\$ELK1_02"
RETURN t.pwm1,t.pwm2

Statistical queries

G1a: Count the total number of TFPairs that one enhancer has in common with any other.

MATCH p=(e:Enhancer)-[:binds]-(t:TFPair)-[:binds]-(e2:Enhancer) RETURN e.enhancerID, COUNT(t)

G1b: Count the TFPairs that two specific enhancers have in common

MATCH p=(e:Enhancer)-[:binds]-(t:TFPair)-[:binds]-(e2:Enhancer) RETURN e.enhancerID, COUNT(t), e2.enhancerID