GraphDB's & Applications

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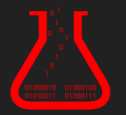
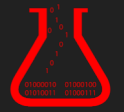
UC Berkeley School of information
Berkeley Data Science Group, LLC



Presentation Road Map

- Intro
- Background
- Examples
- Our Work
- Graph Databases



Intro

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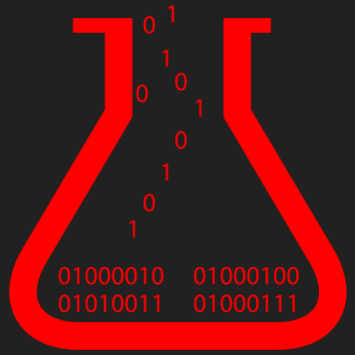
About Us: BDSG

Berkeley Data Science Group

Founded by UC Berkeley Data Science instructors and alumni with the goal of bringing Berkeley data science projects to market and commercializing Berkeley Data Science research.



About Us: the Speakers

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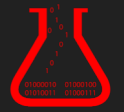

Why Graphs?

Why Graph Databases?

GraphDB's Optimized for Relationships

- Graph Databases store data in tables/rows/columns, just like a traditional RDBMS
- First Class Citizen is a relationship, not an entity
- GraphDB's are optimized for graph traversals
- This also makes them slow at data retrieval
- But, they're a LOT faster at traversing the nodes of a graph!

Intro

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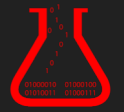
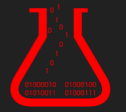


What is Graph Theory?

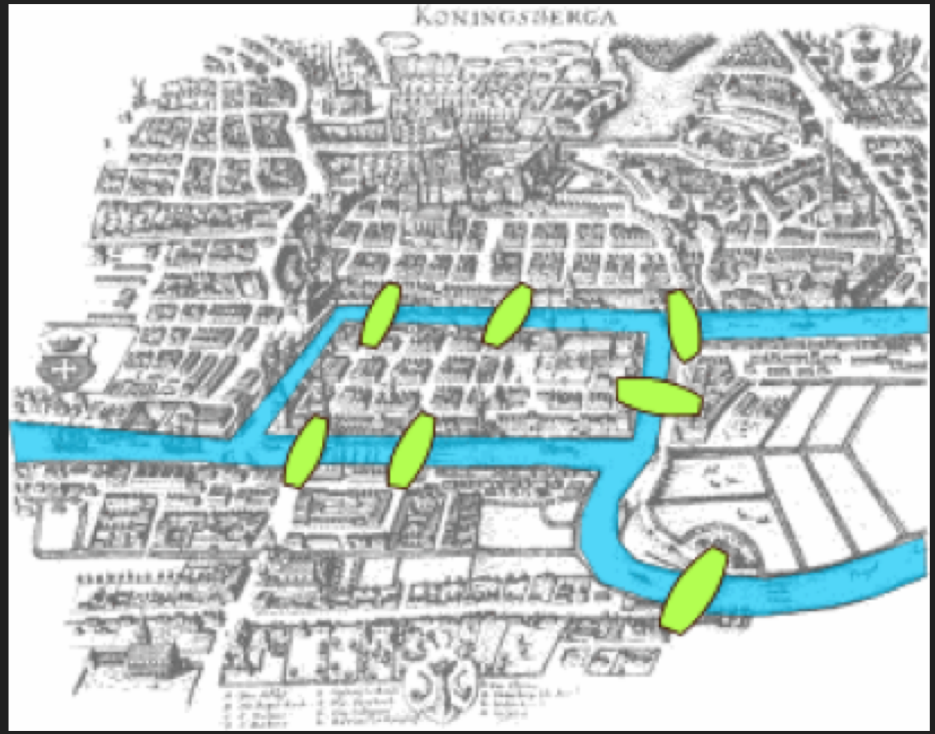
Dates back to 1736: Seven Bridges of Königsberg, by Leonhard Euler

Laid down the original groundwork for what became Graph Theory

Also evolved into modern day Network Analysis (or Network Graph Analysis) and Social Network Analysis (SNA)



The Seven Bridges of Konigsberg

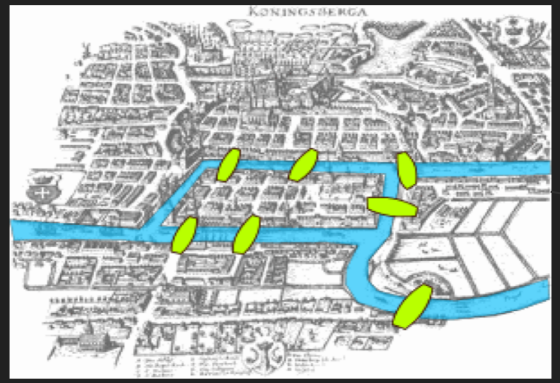


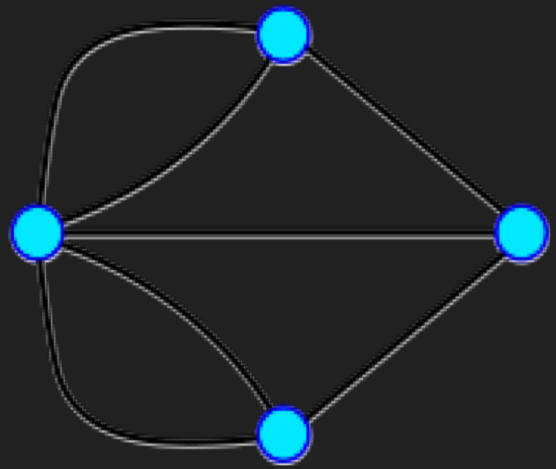
The two large islands in the city of Konigsberg were connected by 7 bridges.

Problem Statement: Can you visit each part of the town, using each bridge only once?

The Seven Bridges of Konigsberg

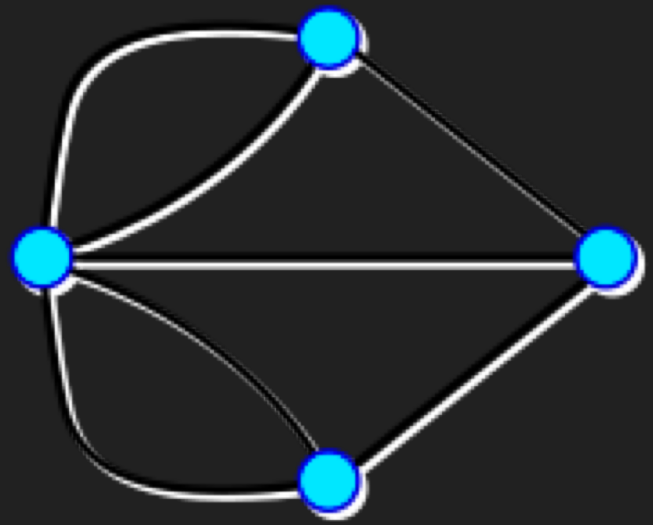
Leonhardt Euler came up with a new way of thinking about the problem, and in turn became the father of modern Graph Theory





The Seven Bridges of Konigsberg

Euler’s Final Answer: it is impossible. His analysis technique laid the foundations of graph theory.

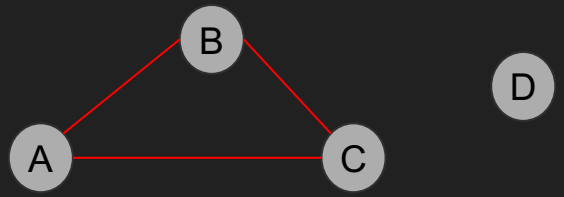


A Very Abridged Intro to Graph Theory

Terminology and Notation

A **graph** G is a set of vertices **V** that are connected by a set of edges **E**.

G = (V, E)

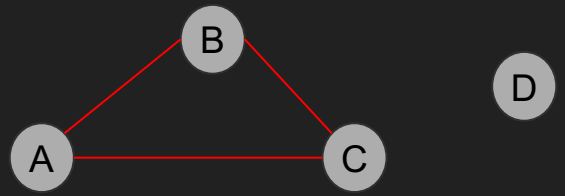


V = {A, B, C, D}

E = {AB, AC, BC}

A vertex A's "children" is the set of verteces that can be reached from vertex A by traversing an edge connected to A.

Terminology and Notation



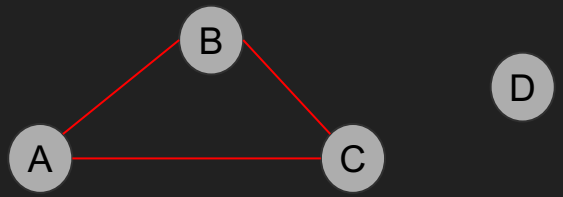
A **cycle** is a group of at least 3 vertices connected in a closed chain (ie, you can start and end a traversal of the vertices at the same vertex).

Vertices A, B, and C form a cycle above.

Terminology and Notation

- Edges of a graph may have **weights** that can be used to model various phenomena

- Edges may also be **directed**, pointing in a particular direction to indicate how the edge may be traversed
  - A graph that does not have any directed edges is **undirected**



Graph Searching Algorithms

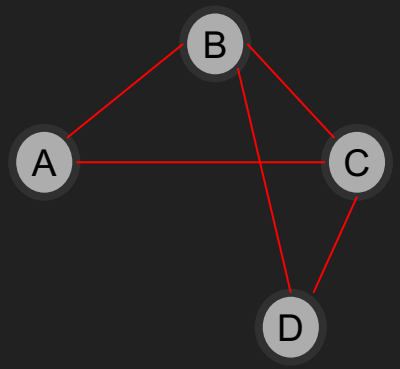
Breadth First Search: starting at a vertex N, add all nodes connected to N to a queue, and then continuously breadth first search the items in the queue, in order (adding new vertices to the queue in recursive calls).

Depth First Search: starting at a vertex N, recursively depth first search all vertices connected to N that have not been searched yet. *Alternatively, depth first search can be performed with the same exact code as breadth first search, replacing the queue with a stack.*

Representations in Code

There are two primary methods of representing graphs in code:

1) Adjacency matrix: each row / column represents a vertex, and the value in row i and column j represents the weight of the edge between vertices i and j.

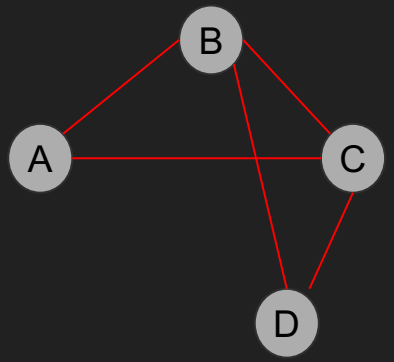


	A	B	C	D
A	0	1	1	0
B	1	0	1	1
C	1	1	0	1
D	0	1	1	0

Representations in Code

There are two primary methods of representing graphs in code:

2) Adjacency list: A list (usually a linked list) is stored for each vertex, representing its connections.



A: [B, C]

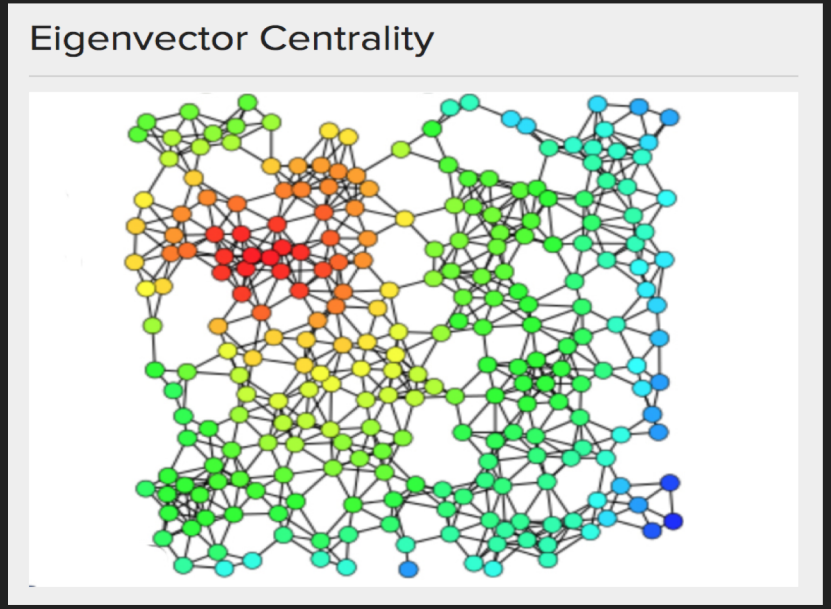
B: [C, D]

C: [A, B, D]

D: [B, C]

Node Level Indices

- Centrality Measures:
  - Degree
  - Betweenness
  - Closeness
  - Eigenvector

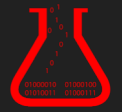


Google's PageRank is the quintessential example of Eigenvector Centrality

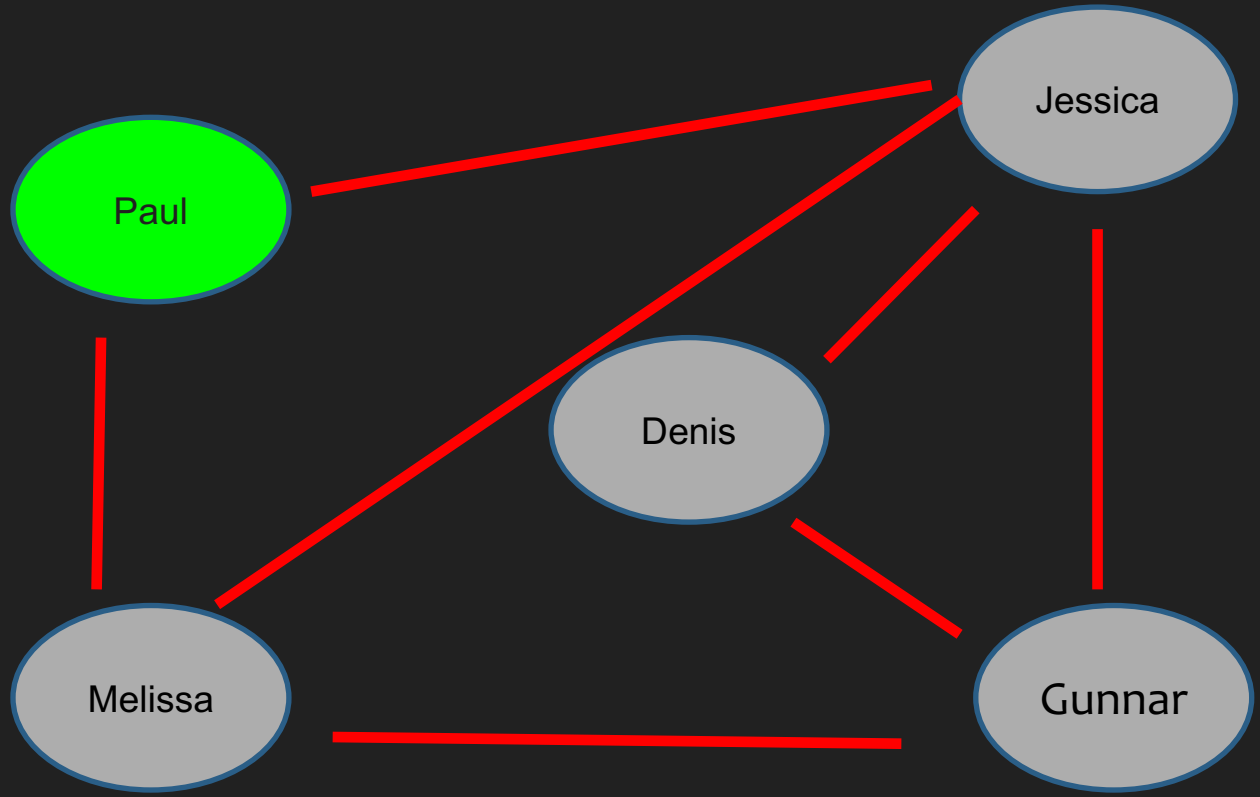
Picture: Wikipedia

Graph Level Metrics

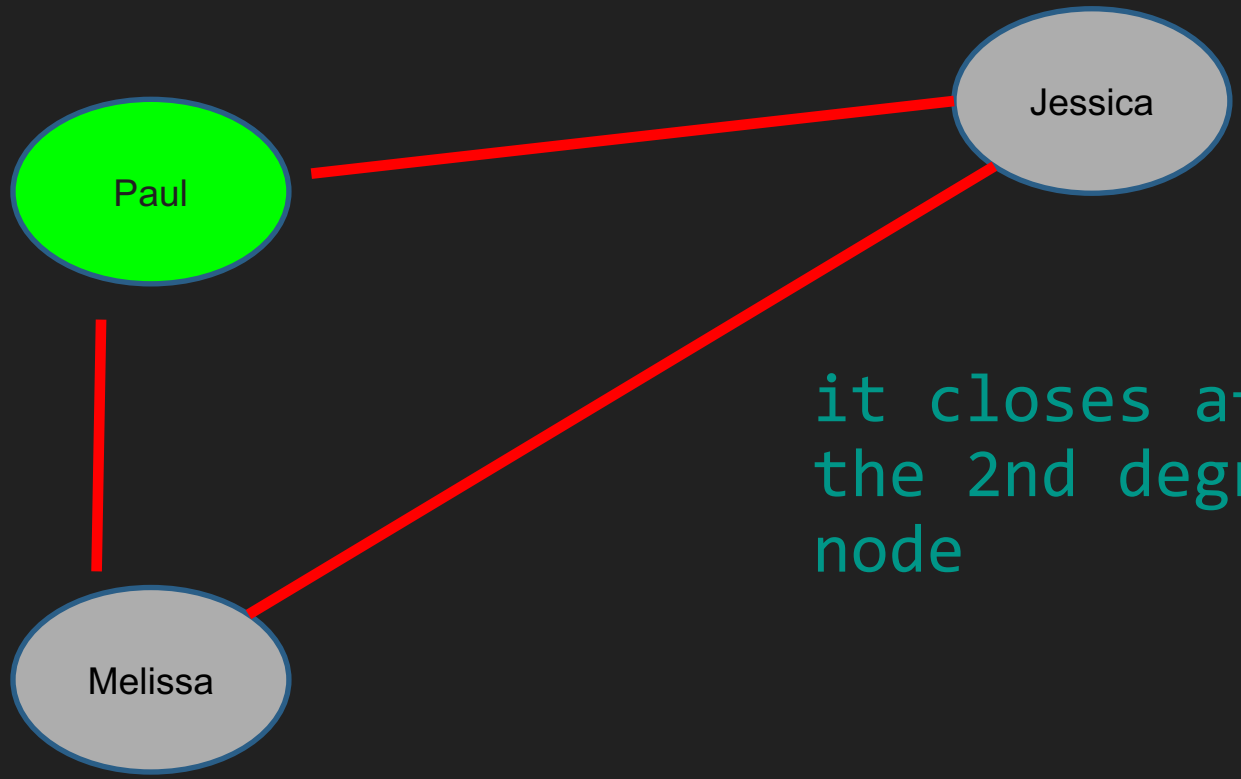
- Averages of Node Level Indices
- Distance
- Community-/Cluster-Based



Consider Paul in a simple social network

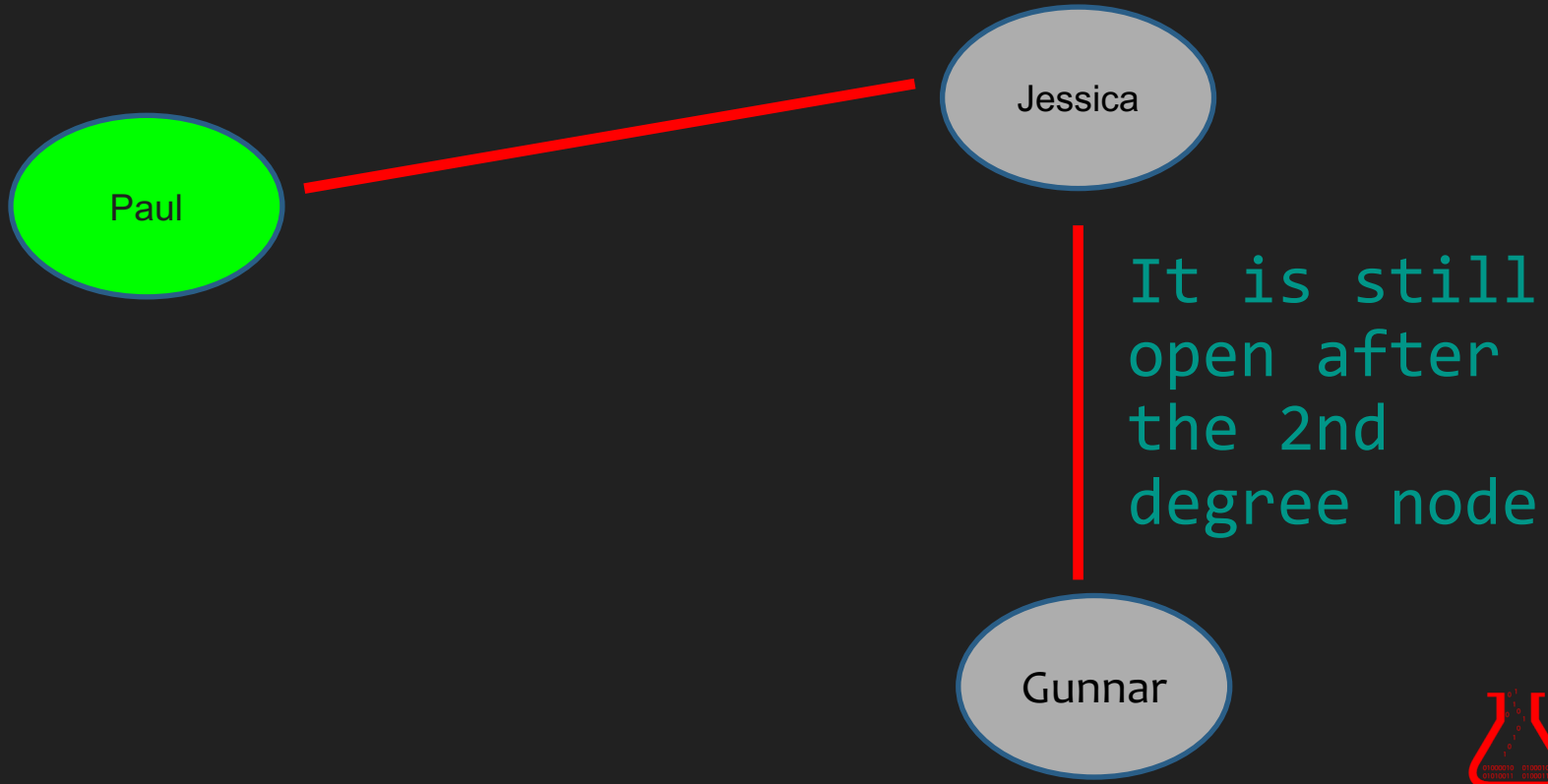


This relationship forms a triangle



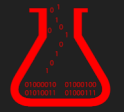
it closes after the 2nd degree node

This relationship forms a wedge

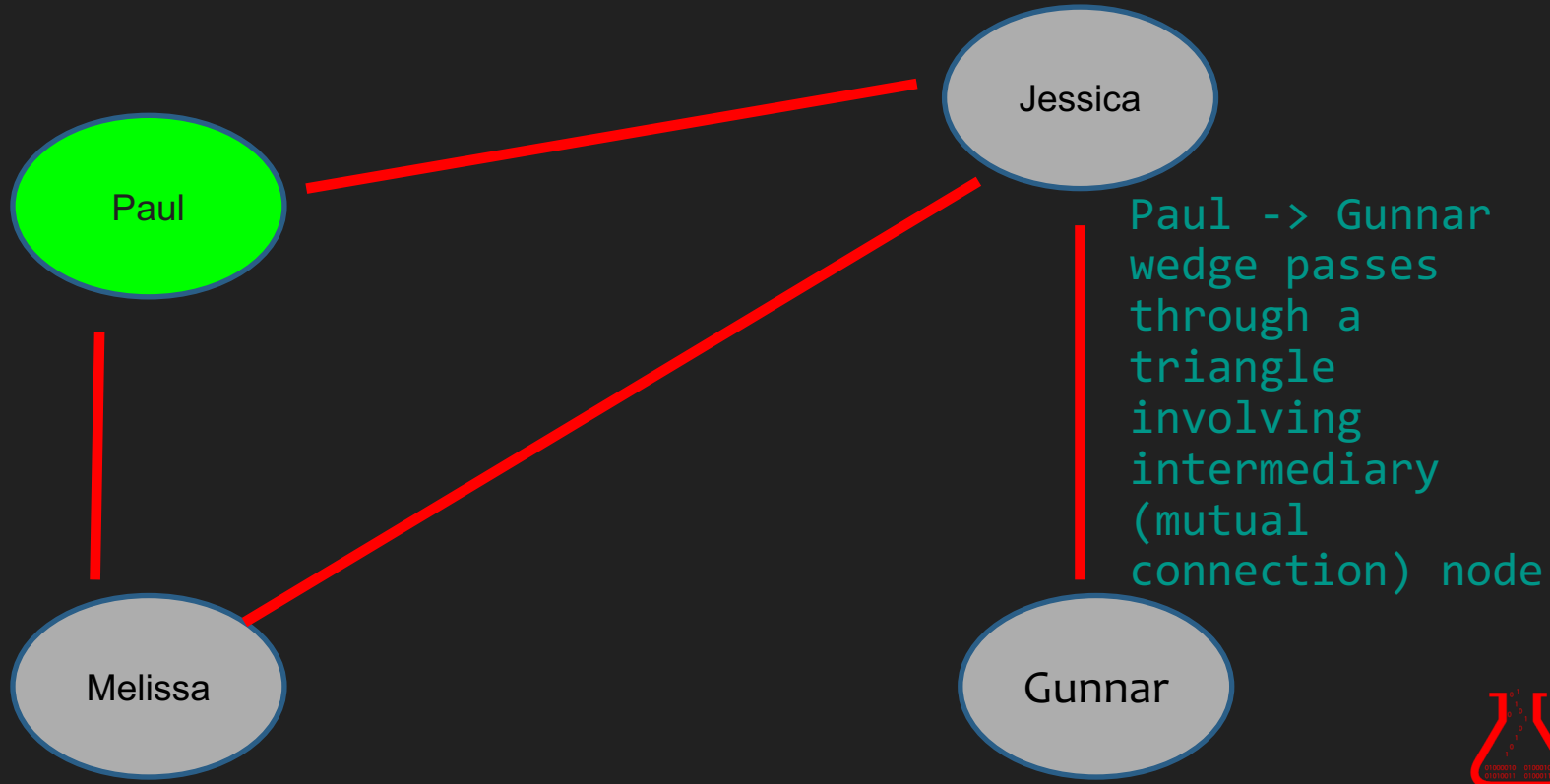


Strength of Wedge

- Number of Triangles that a Wedge pass through, where the intermediate nodes (mutual connection) is part of the triangle.
- This gives a measure of the strength of the 2nd degree connection.
- In other words: how well do you know the mutual friend that can connect you to the 2nd degree node?



Wedge through Triangle



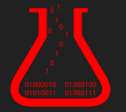
Recommender Systems: Traditional vs. Graph

Traditional:

- At Scale
- Production Deployments

Graph-Based:

- Exploratory
- Highly Contextual
- Known Rules



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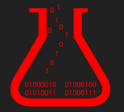
Applications of Graph Theory

- Social network analysis
- Map / GPS algorithms - shortest distance between two points, etc.
- AI algorithms
- Search engine algorithms

Examples of Graph Applications

- 9/11 Terrorist Network
- London Phone Network
- Enron Emails
- Panama Papers



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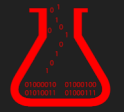

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Keyword Rec:

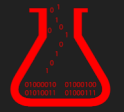
an HR Keyword Assistant

Consider a typical job requisition

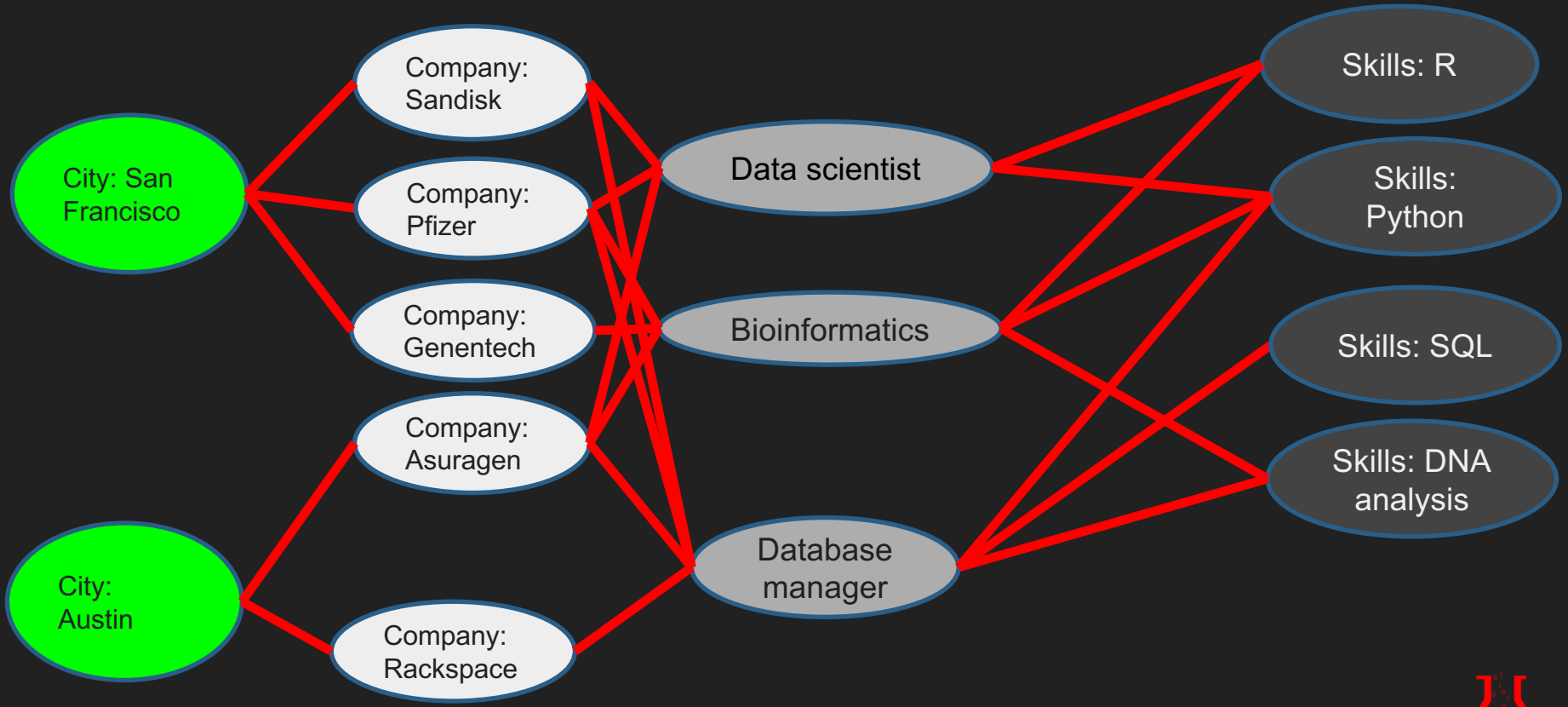
Job Title
- topic information

Company and institute
- workplace
- geographic location

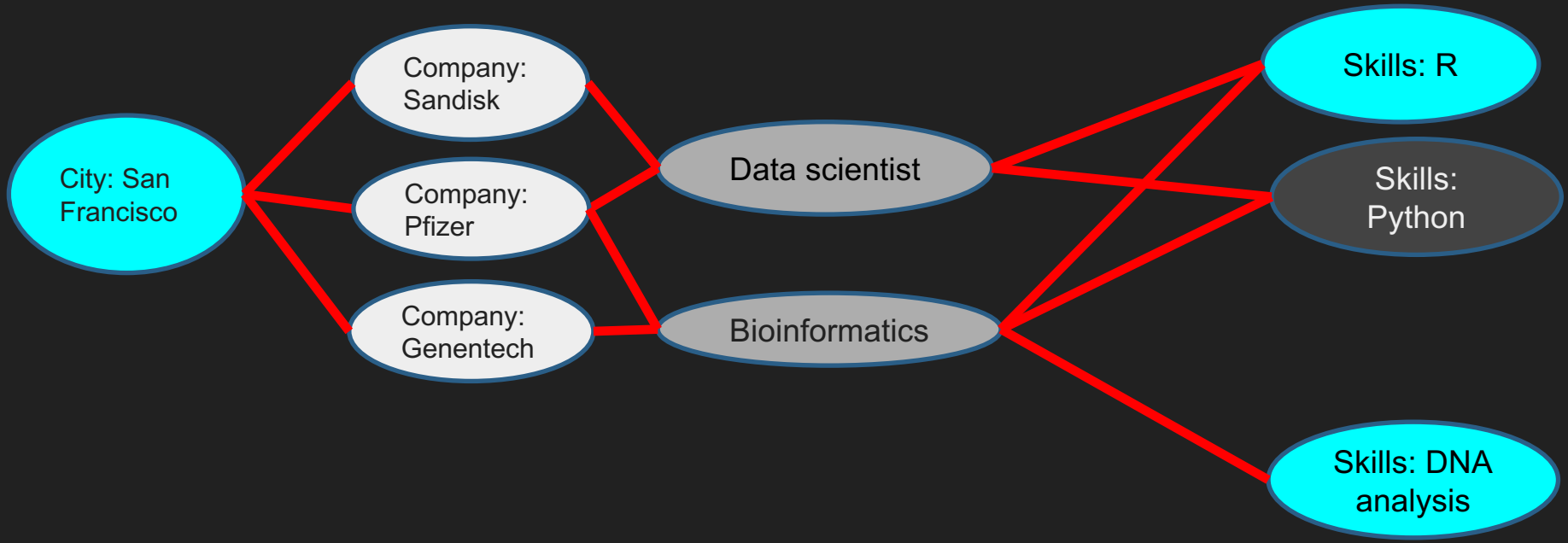
Keywords
- skills
- experience/focus



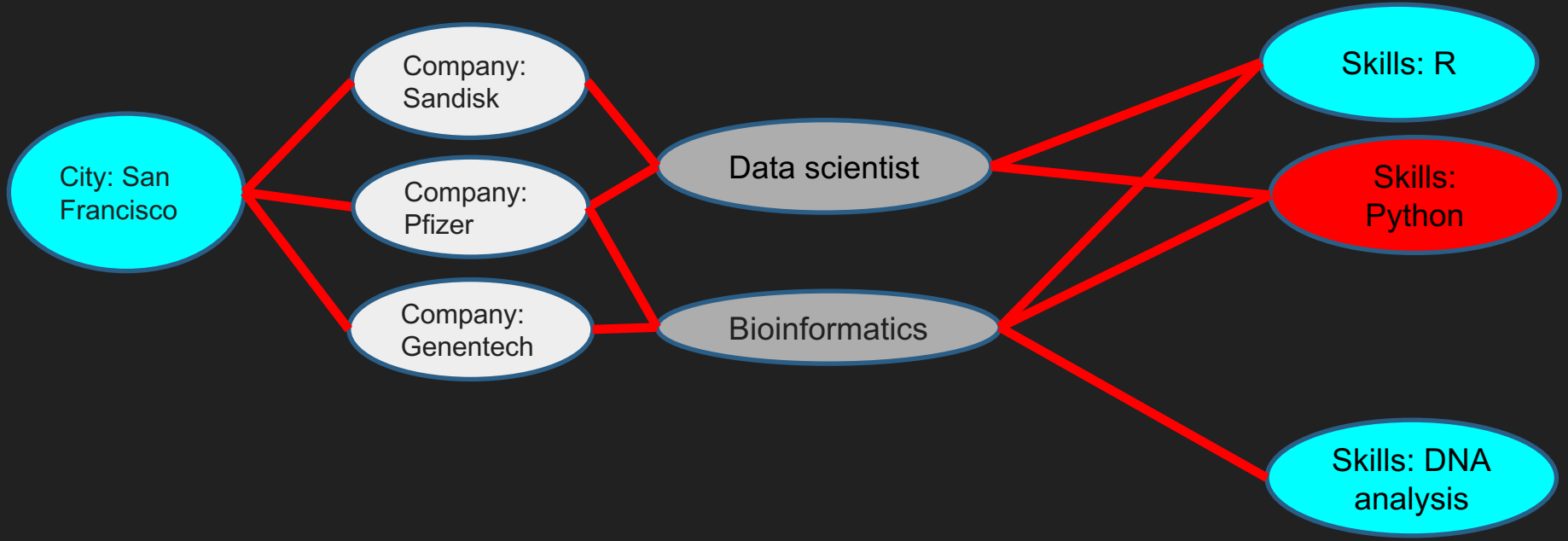
Job requisition analysis by skills



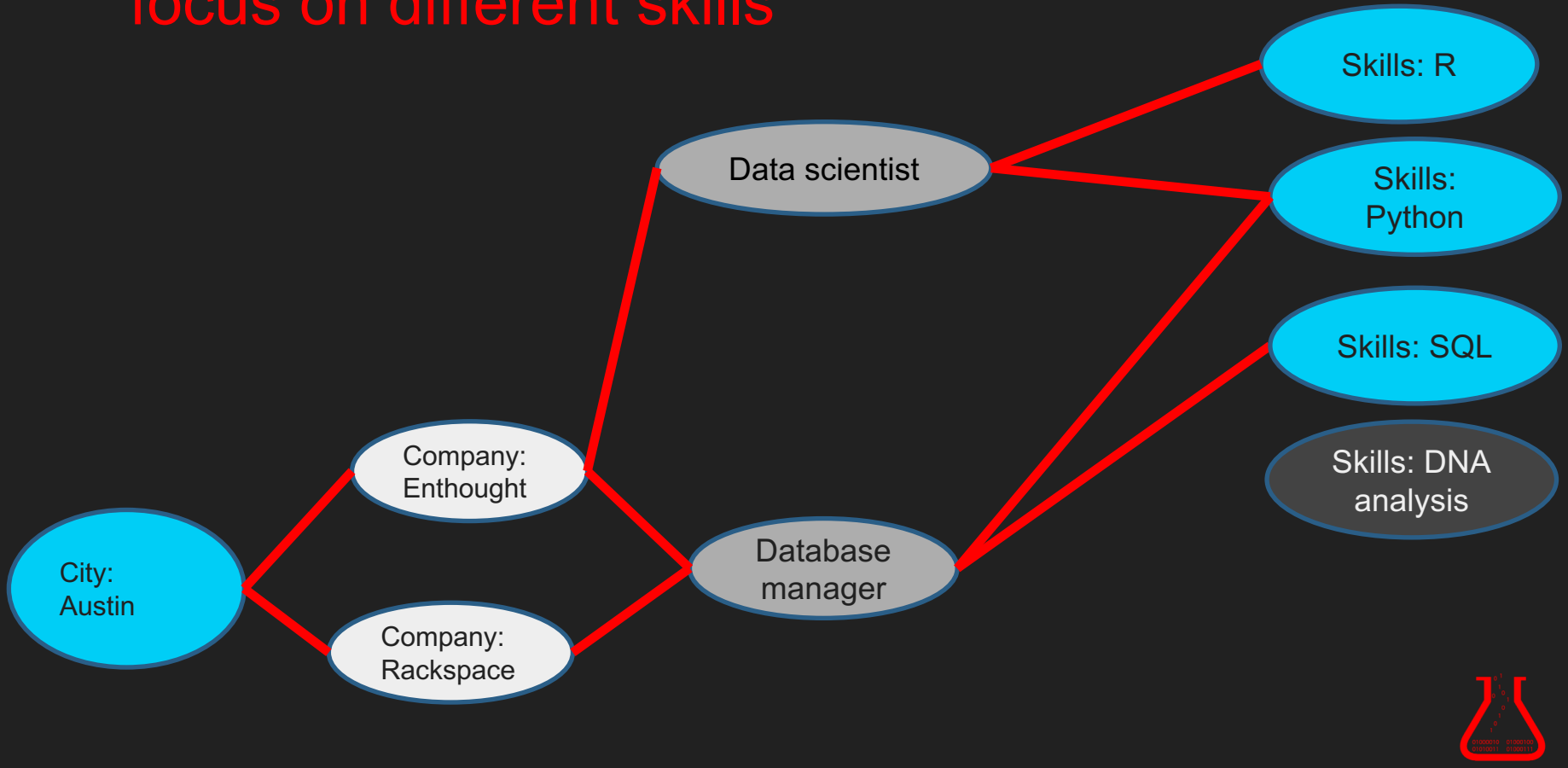
Or looking at a skill might suggest a geographic hub



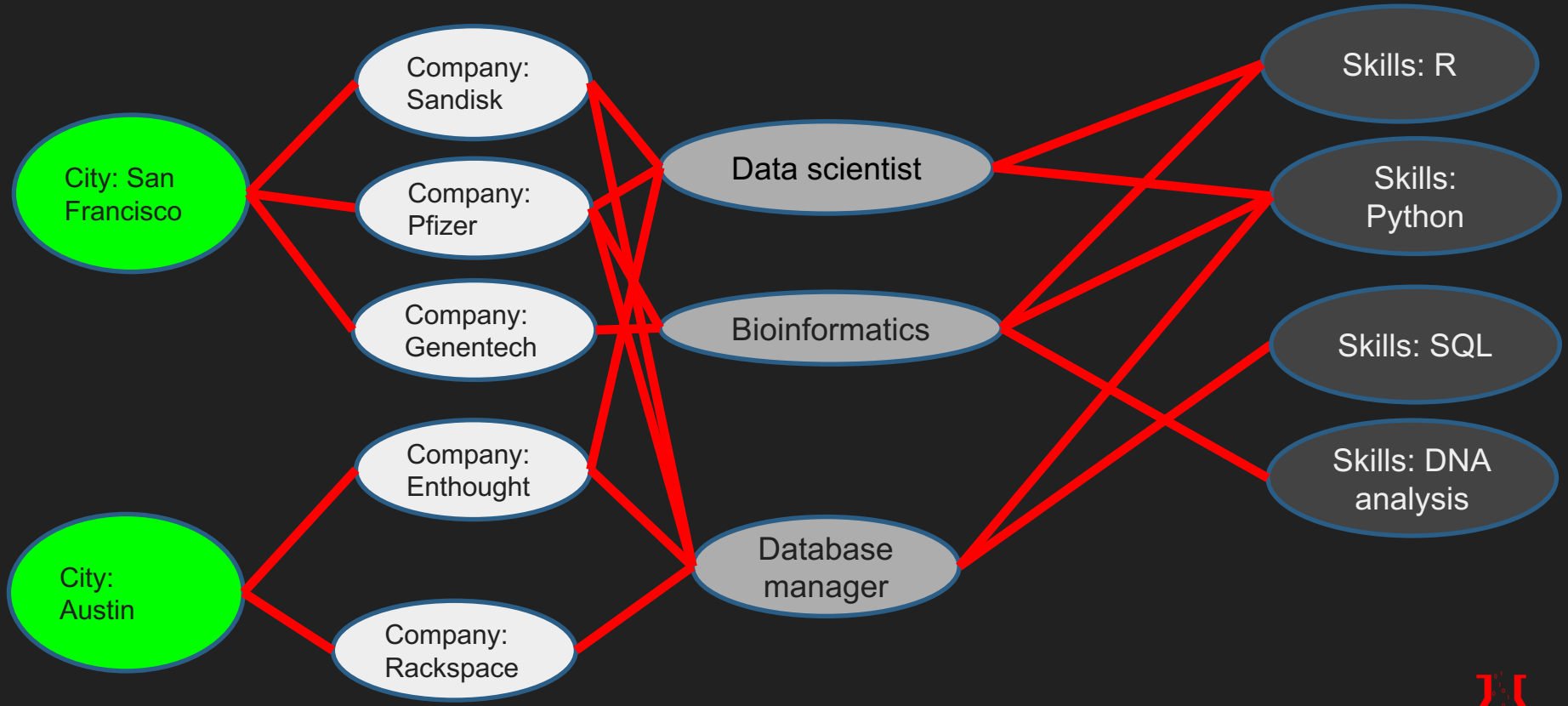
We can also recommend missing skills



If we focus on a specific region we might focus on different skills



Job requisition analysis by skills



The final API

File Edit View Insert Cell Kernel Help Trusted Python 2

Code

```
('gender identity', 3),
('world class', 3)]
```

In [16]:
```
relatedskills('data science','NY',5)
```

Out[16]:
```
[('data science', 3885),
('big data', 616),
('data engineering', 312),
('science communication', 310),
('information system', 297)]
```

In [20]:
```
relatedskills('Python','SV',5)
```

Out[20]:
```
[('python', 328),
('similar', 137),
('unix', 136),
('programming experience', 21),
('language', 15)]
```

In [21]:
```
relatedskills('Python','NY',5)
```

Out[21]:
```
[('plus', 636),
('programming experience', 615),
('python', 383),
('sql', 324),
('r', 320)]
```

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SF vs NY:

Who has better data scientists

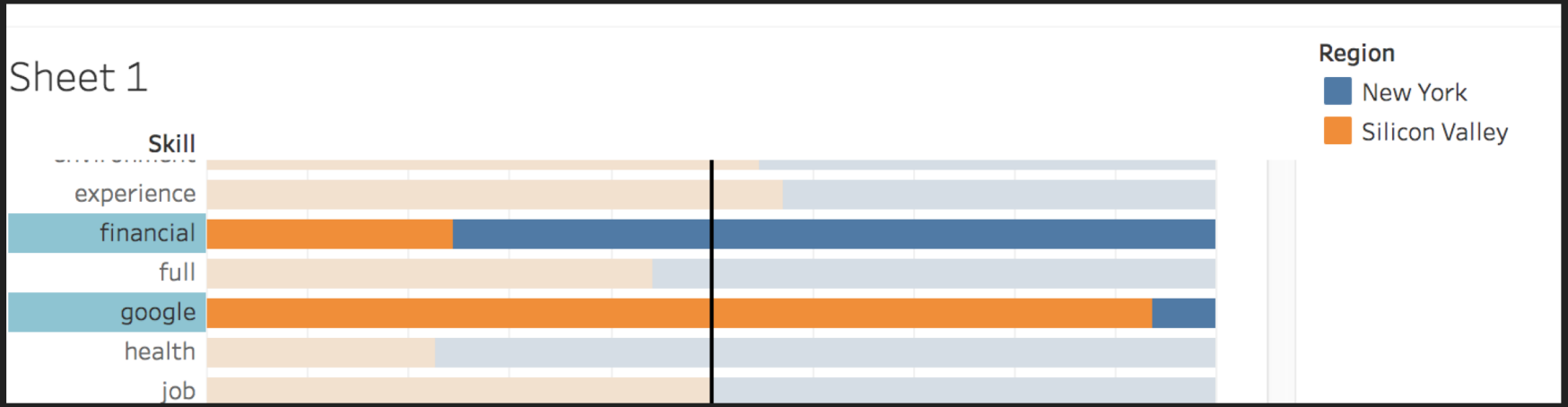
Who has Better Data Scientists?

- San Francisco/Silicon Valley
- or New York

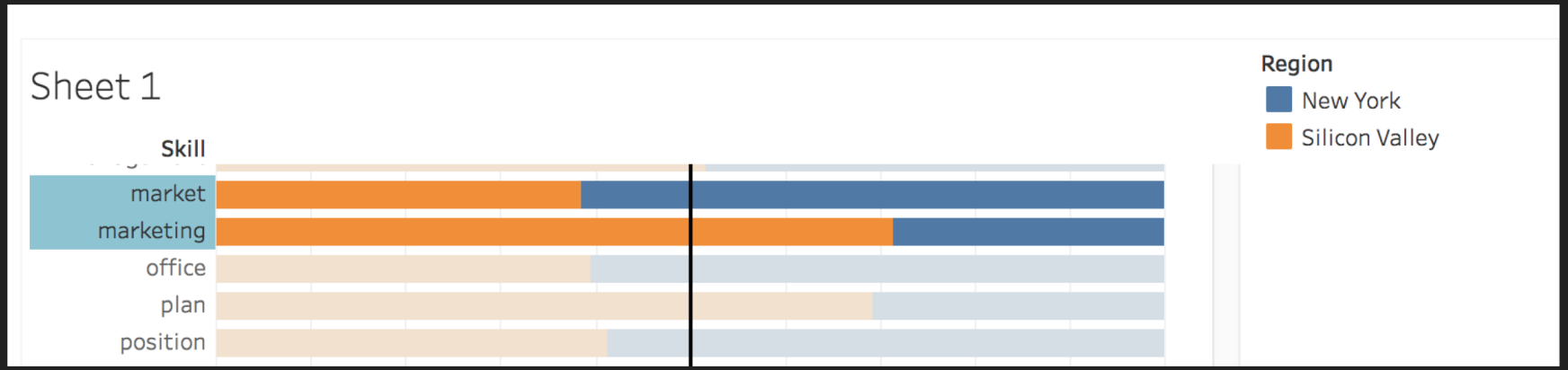
Tableau Link

https://public.tableau.com/profile/denis.vrdoljak#!/vizhome/SVvsNY_JobSkillsPercentCompare/Sheet3?publish=yes

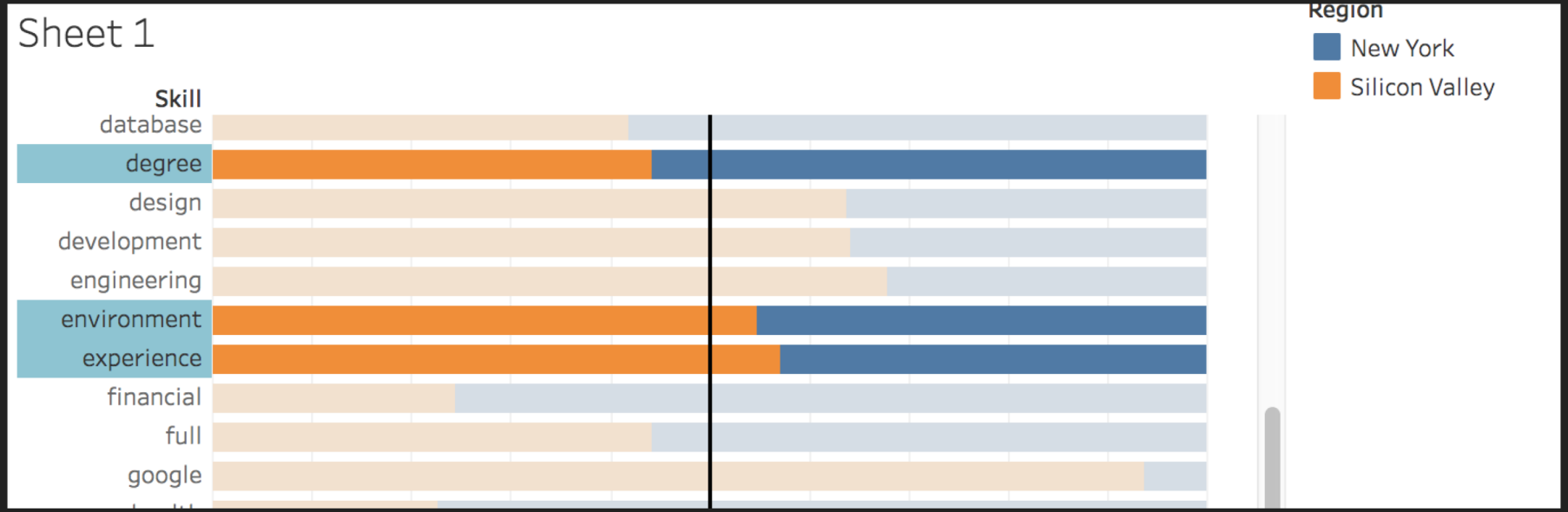
Who has Better Data Scientists?

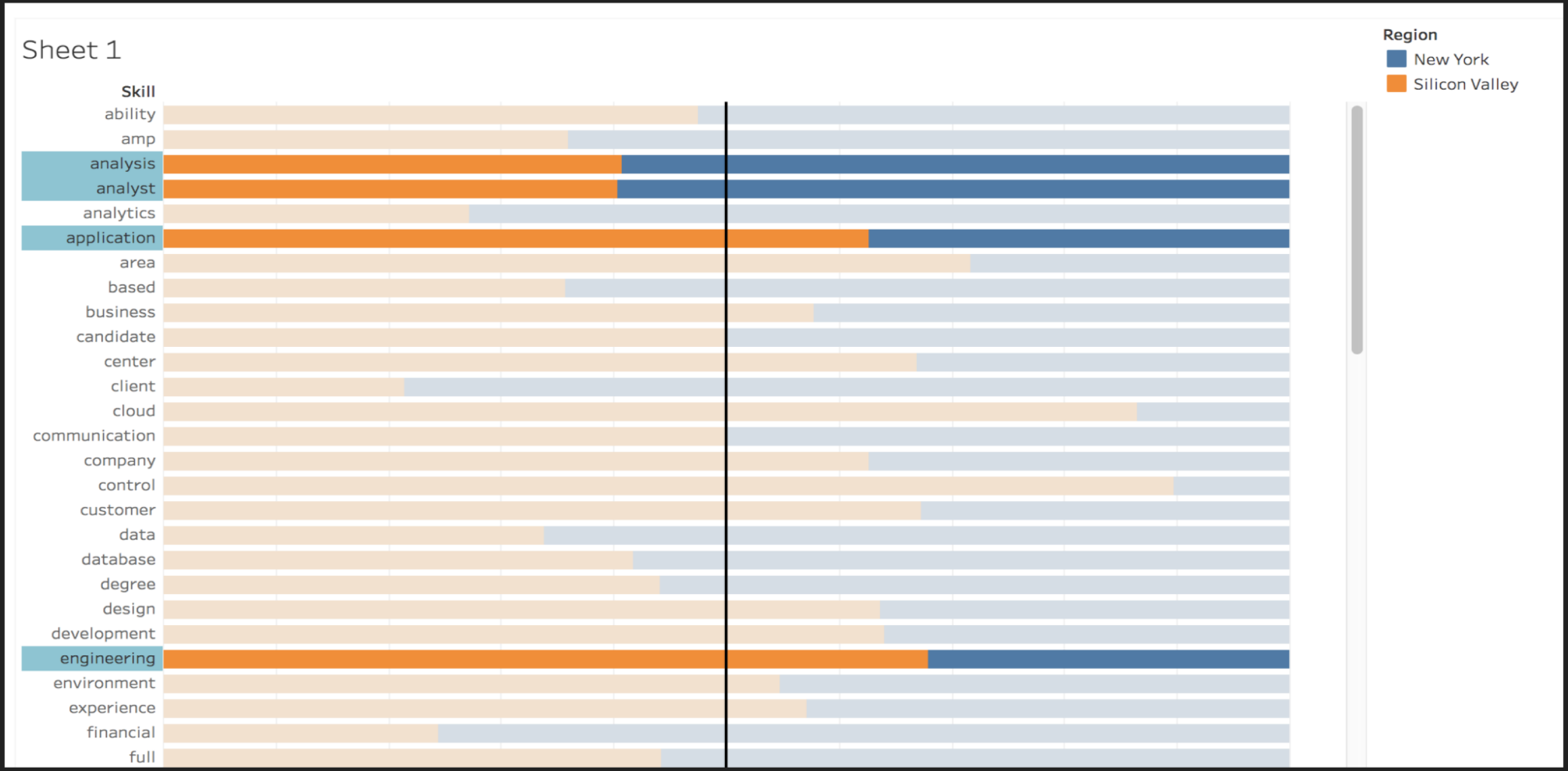


Who has Better Data Scientists?



Who has Better Data Scientists?




Sheet 1
Region
New York
Silicon Valley
Skill
ability
amp
analysis
analyst
analytics
application
area
based
business
candidate
center
client
cloud
communication
company
control
customer
data
database
degree
design
development
engineering
environment
experience
financial
full

…now let’s take a look at our very first project, and what we’ve done with it since we first started!

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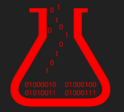
BioRevs:

Predicting Biotech IPO Rates through Collaboration Networks



Publications can be parsed into important data

Journal -

- Discipline
- Audience
- Impact

ANALYSIS

nature genetics

Understanding multicellular function and disease with human tissue-specific networks

Casey S Greene[1–3,13], Arjun Krishnan[4,13], Aaron K Wong[5,13], Emanuela Ricciotti[6,7], Rene A Zelaya[1], Daniel S Himmelstein[8], Ran Zhang[9], Boris M Hartmann[10], Elena Zaslavsky[10], Stuart C Sealfon[10], Daniel I Chasman[11], Garret A FitzGerald[6,7], Kara Dolinski[4], Tilo Grosser[6,7] & Olga G Troyanskaya[4,5,12]

Tissue and cell-type identity lie at the core of human physiology and disease. Understanding the genetic underpinnings of complex tissues and individual cell lineages is crucial for developing improved diagnostics and therapeutics. We present genome-wide functional interaction networks for 144 human tissues and cell types developed using a data-driven Bayesian methodology that integrates thousands of diverse experiments spanning tissue and disease states. Tissue-specific networks predict lineage-specific responses to perturbation, identify the changing functional roles of genes across tissues and illuminate relationships among diseases. We introduce NetWAS, which combines genes with nominally significant genome-wide association study (GWAS) *P* values and tissue-specific networks to identify disease-gene associations more accurately than GWAS alone. Our webserver, GIANT, provides an interface to human tissue networks through multi-gene queries, network visualization, analysis tools including NetWAS and downloadable networks. GIANT enables systematic exploration of the landscape of interacting genes that shape specialized cellular functions across more than a hundred human tissues and cell types.

The precise actions of genes are frequently dependent on their tissue context, and human diseases result from the disordered interplay of tissue- and cell lineage–specific processes[1–4]. These factors combine to make the understanding of tissue-specific gene functions, disease pathophysiology and gene-disease associations particularly challenging. Projects such as the Encyclopedia of DNA Elements (ENCODE)[5] and The Cancer Genome Atlas (TCGA)[6] provide comprehensive genomic profiles for cell lines and cancers, but the challenge of understanding human tissues and cell lineages in the multicellular context of a whole organism remains[7]. Integrative methods that infer functional gene interaction networks can capture the interplay of pathways, but existing networks lack tissue specificity[8].

Although direct assay of tissue-specific features remains infeasible in many normal human tissues, computational methods can infer these features from large data compendia. We recently found that even samples measuring mixed cell lineages contain extractable information related to lineage-specific expression[9]. In addition to tissue specificity, we[10–13] and others[14–17] have shown that heterogeneous genomic data contain functional information, for example, of gene expression regulation by protein-DNA, protein-RNA, protein-protein and metabolite-protein interactions. Here we develop and evaluate methods that simultaneously extract functional and tissue or cell-type signals to construct accurate maps of both where and how proteins act.

We build genome-scale functional maps of human tissues by integrating a collection of data sets covering thousands of experiments contained in more than 14,000 distinct publications. To integrate these data, we automatically assess each data set for its relevance to each of 144 tissue- and cell lineage–specific functional contexts. The resulting functional maps provide a detailed portrait of protein function and interactions in specific human tissues and cell lineages ranging from B lymphocytes to the renal glomerulus and the whole brain. This approach allows us to profile the specialized function of genes in a high-throughput manner, even in tissues and cell lineages for which no or few tissue-specific data exist.

In contrast with tissue-naive networks, which assume that the func-

[1]Department of Genetics, Geisel School of Medicine at Dartmouth, Hanover, New Hampshire, USA. [2]Dartmouth-Hitchcock Norris Cotton Cancer Center, Lebanon, New Hampshire, USA. [3]Institute for Quantitative Biomedical Sciences, Dartmouth College, Hanover, New Hampshire, USA. [4]Lewis-Sigler Institute for Integrative Genomics, Princeton University, Princeton, New Jersey, USA. [5]Department of Computer Science, Princeton University, Princeton, New Jersey, USA. [6]Department of Systems Pharmacology and Translational Therapeutics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, Pennsylvania, USA. [7]Institute for Translational Medicine and Therapeutics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, Pennsylvania, USA. [8]Biology and Medical Informatics, University of California, San Francisco, San Francisco, California, USA. [9]Department of Molecular Biology, Princeton University, Princeton,

Title -

- topic information

Collaborator list

- professional relationships

Company and institute

- workplace
- geographic location

Pubmed Database
The world's biomedical research

24,000,000

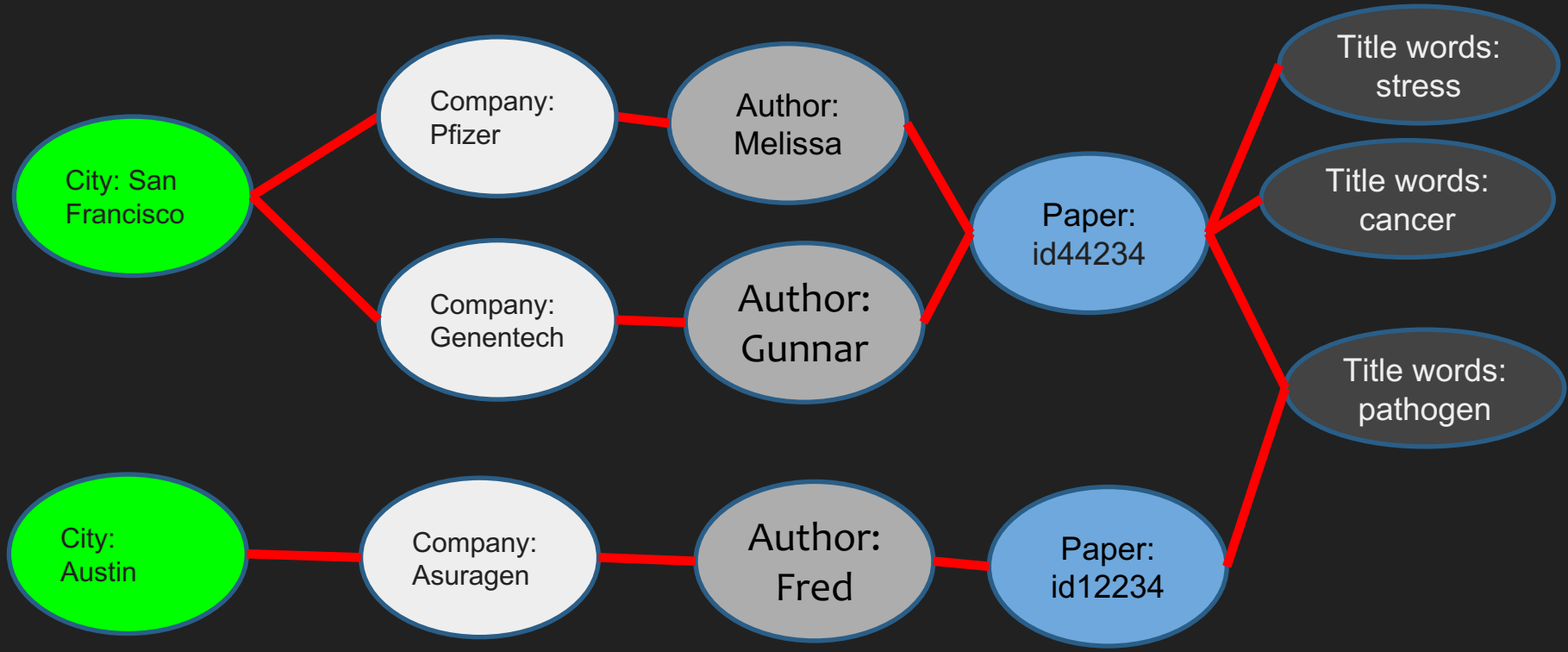
Full PubMed Dataset (all Biomedical literature)

~ 1.5 Million Open Source

PubMed Central (BioTech-open access subset)

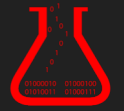
Data include: Publication Titles, Authors, and other Metadata

Publication and company data in a graph

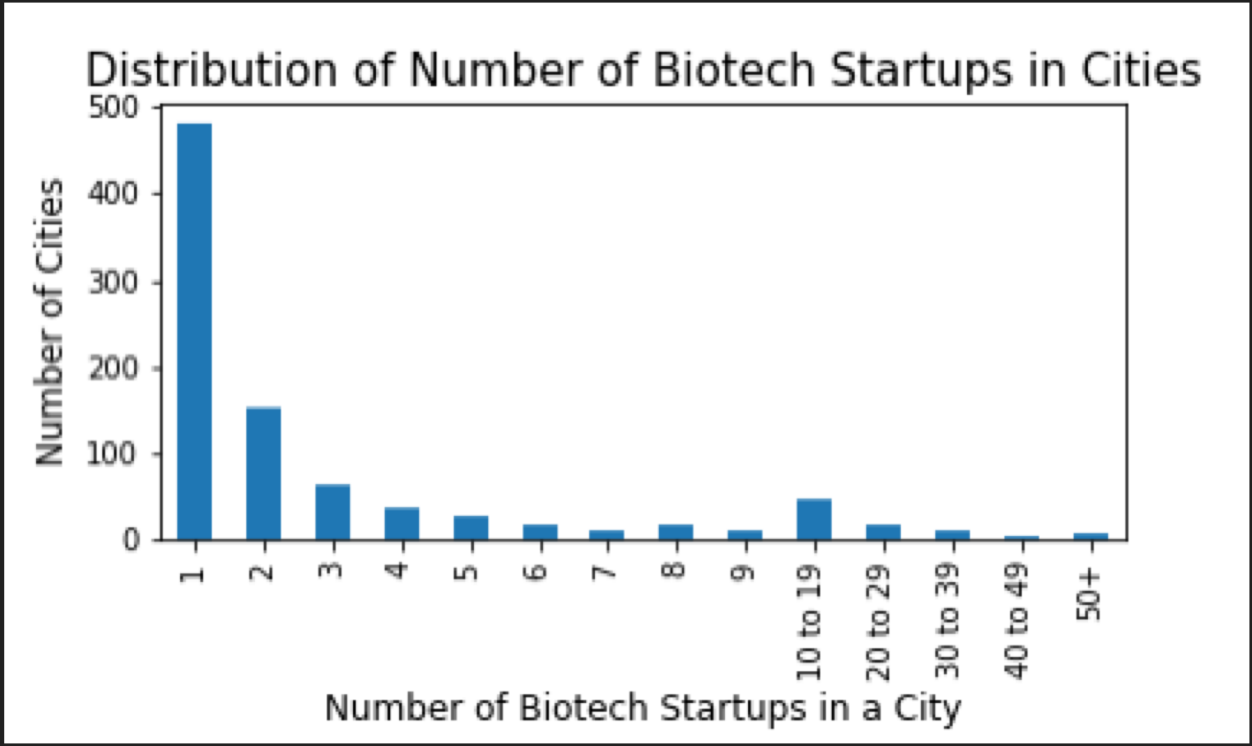


Conducting a job search in biotech

You could identify biotechnology hubs by counting companies



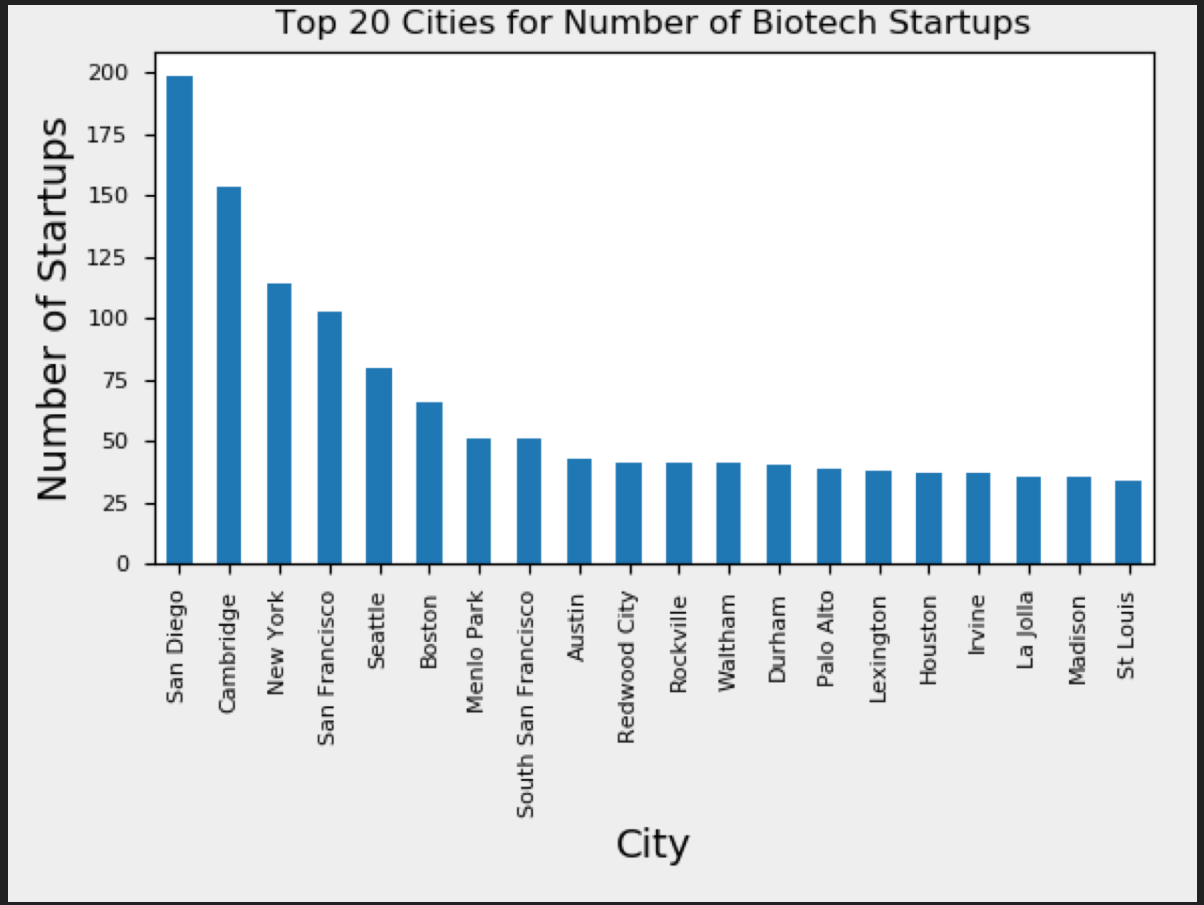
The Vast Majority of Cities have Few Biotech Startup Companies



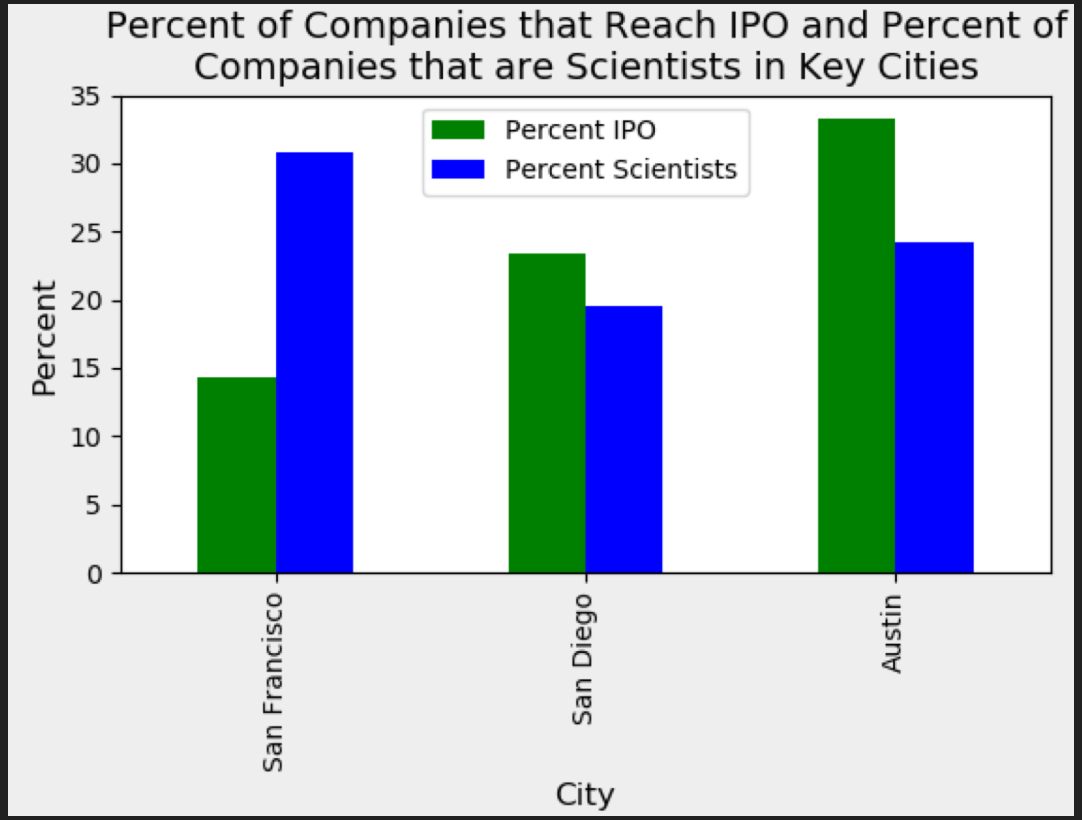
There are 899 US Cities that have at least one Biotech Company.

Most cities have very few companies.

We can focus on Some Biotech Hub Cities



Biotech hubs can be profiled by IPO and % scientists



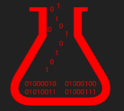
Percent IPO = % Companies reaching IPO in < 6000 days

National average is ~16% reach IPO.

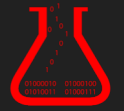
National average is ~21% Scientists.

You could even use public information to examine the how indexes of company quality

- percent scientists and
- likelihood of success (IPO)

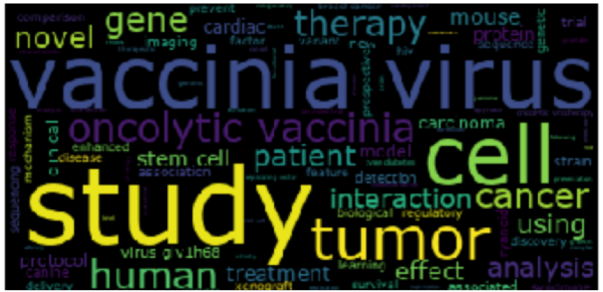


We can use a graph to get more

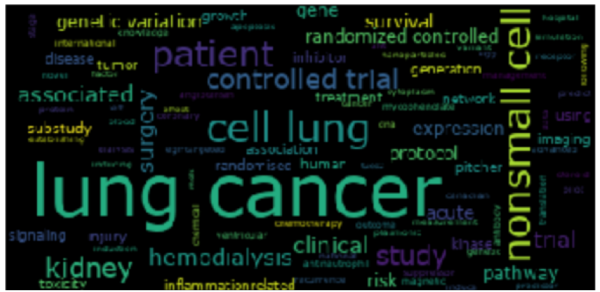


Cities Differ in Scientific Expertise

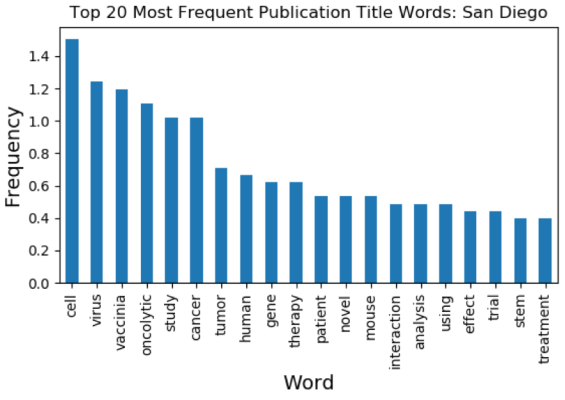
San Diego

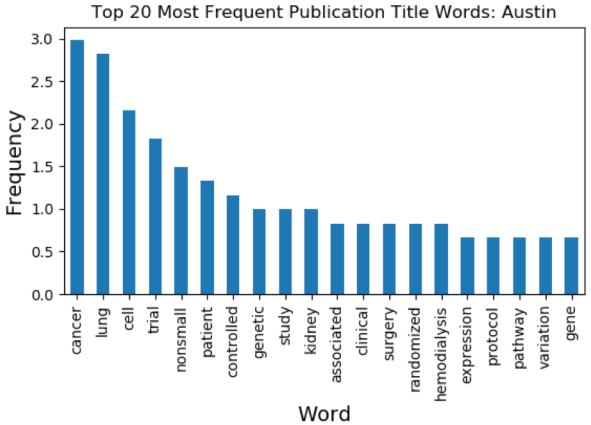


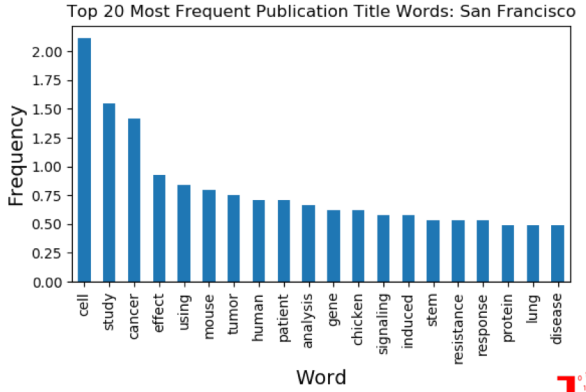
Austin



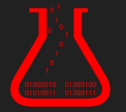
San Francisco



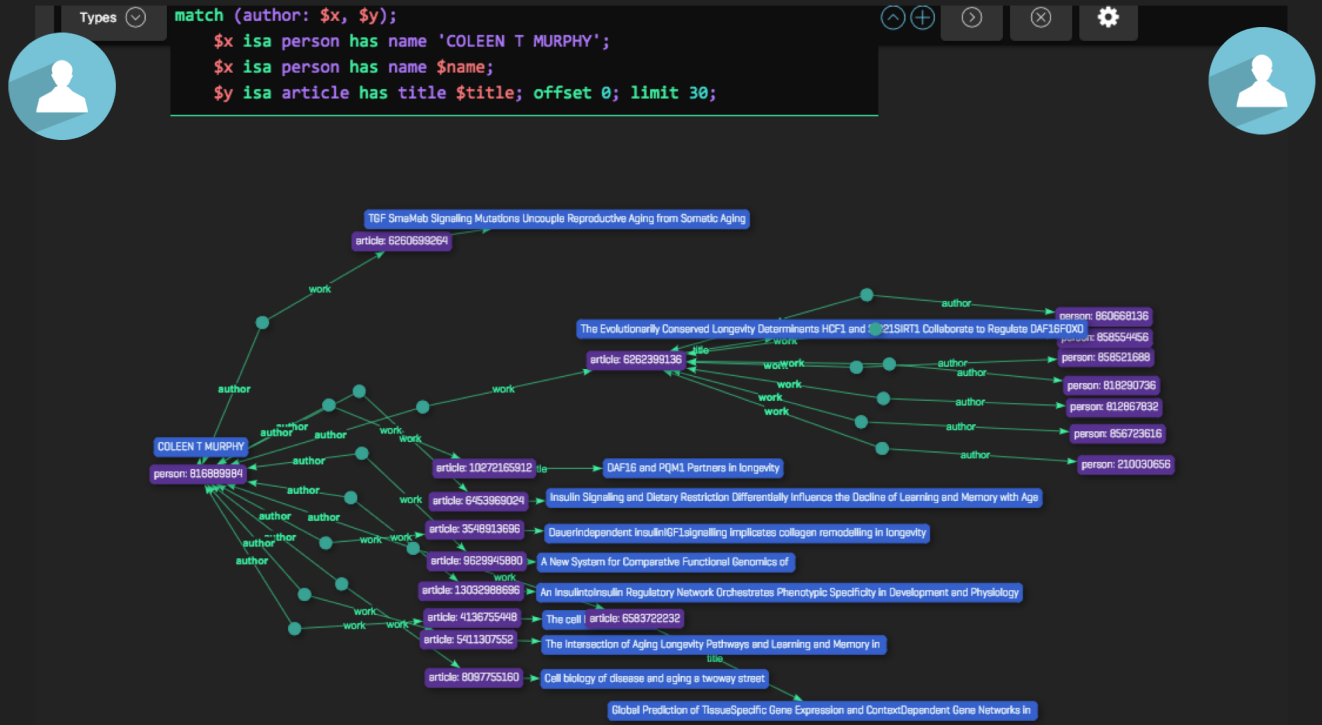




Quantification of science networks with collaboration graphs



We can get the collaboration network topology from the graph



Finding the top publishers

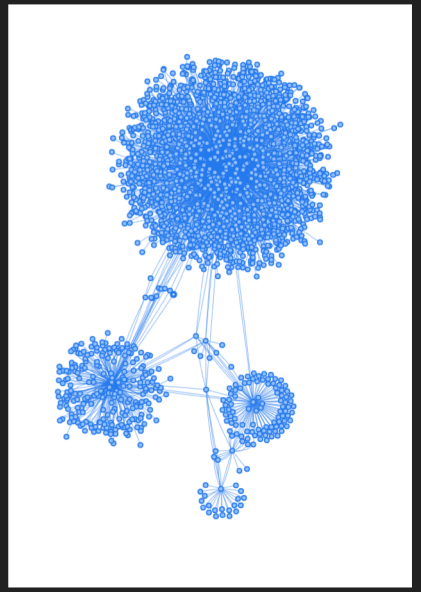
We identify the top publishers:

* Gunther Eysenbach
* Prof. Hoongkun Fun
* Seik Weng Ng

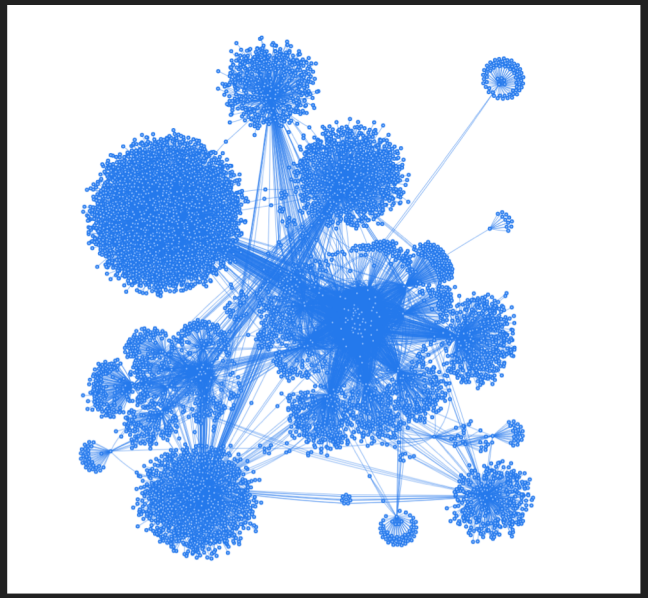
```
neo4j-sh (?)$ MATCH (n)-[r:AUTHORED]->(m)
> RETURN n, COUNT(r)
> ORDER BY COUNT(r) DESC
> LIMIT 10;
+-------------------------------------------------+
| n                                       | COUNT(r) |
+-------------------------------------------------+
| Node[487153]{name:"THE  "}              | 2671     |
| Node[865318]{name:"GUNTHER EYSENBACH"}  | 2055     |
| Node[78005]{name:"HOONGKUN FUN"}        | 1329     |
| Node[1520956]{name:"SEIK WENG NG"}      | 1233     |
| Node[12886]{name:"WEI WANG"}            | 1203     |
| Node[33084]{name:"WEI ZHANG"}           | 1029     |
| Node[148]{name:"YAN LI"}                | 829      |
| Node[6653]{name:"WEI LI"}               | 778      |
| Node[15555]{name:"JING WANG"}           | 737      |
| Node[20702]{name:"LI ZHANG"}            | 670      |
+-------------------------------------------------+
10 rows
24526 ms
```

Some typical publication patterns

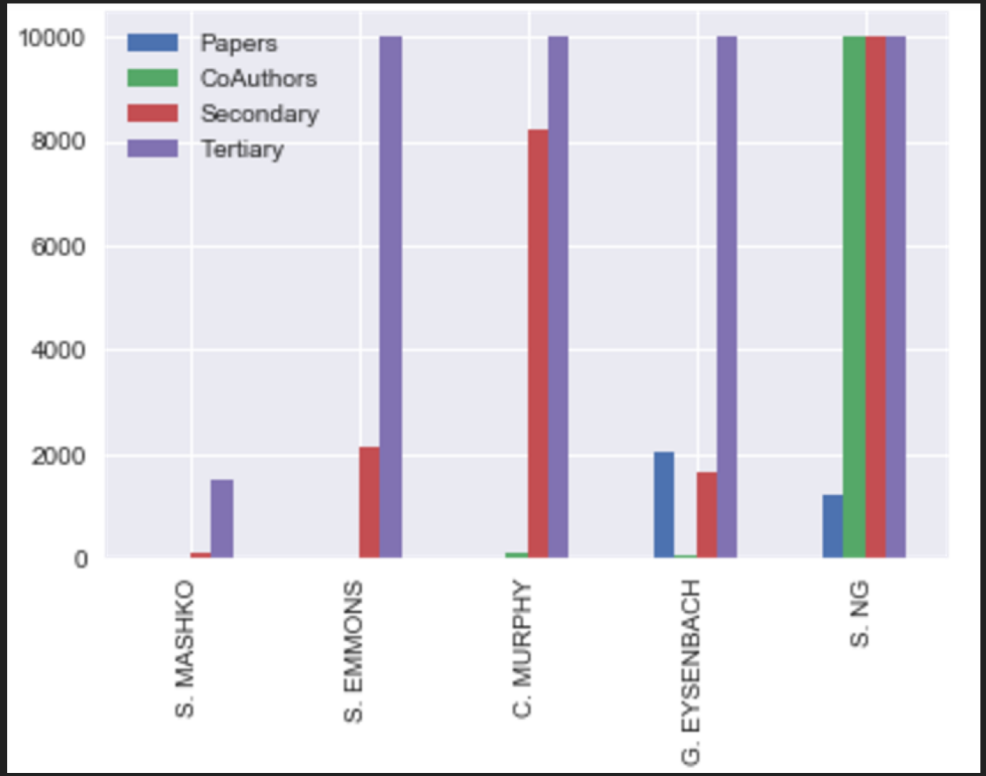
Scott Emmons' 2nd degree collaboration network



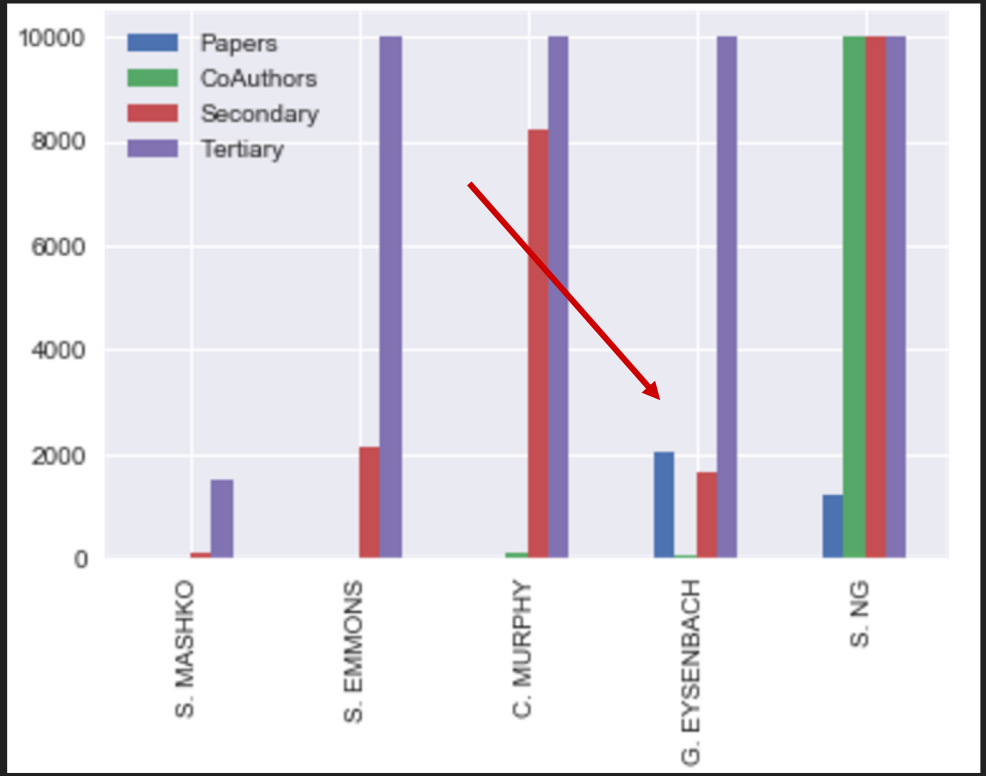
Coleen Murphy's 2nd degree collaboration network



Increasing node count with distance from author



We can see an outlier!



A big publisher with 2055 links!

“one of the most productive researchers, editors, and publishers in the online health field.”

in 2004 received the Janssen-Cilag Future Award, referred to as the German “health care nobel prize”.

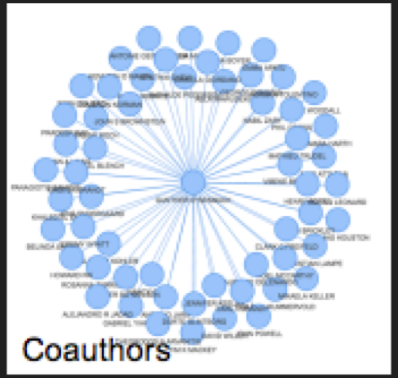
Founder of an academic field!
association between search engine queries and influenza incidence,
He coined the terms "infoveillance" and "infodemiology" for these kinds of approaches.

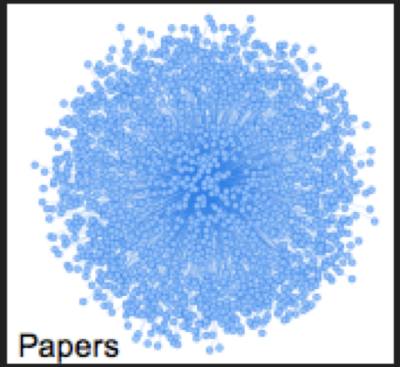
Few co-authors and many papers
Suspicious pattern

But he is only cited for 120 papers and 40 book chapters.

So what are those other 1900 links ?

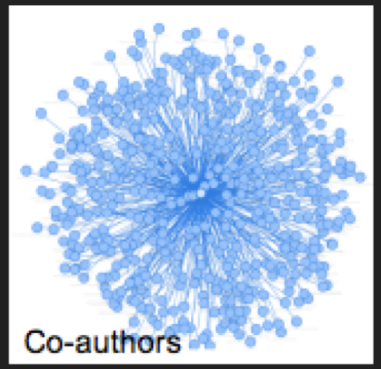
Probably editing jobs (false positives)

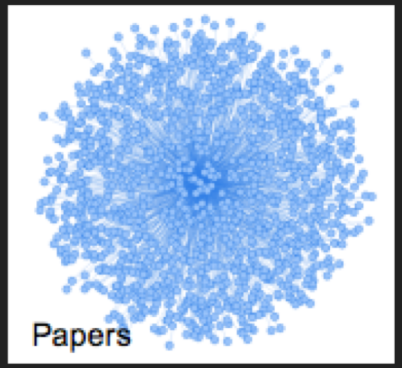




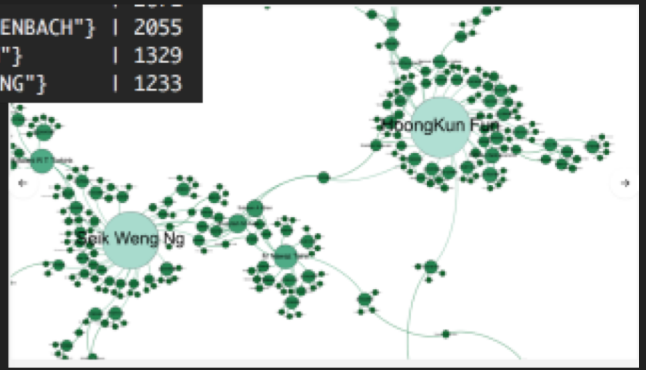
Prof. Kun has a pattern closer to what we expected

Many collaborators
and many publications



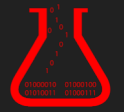


{name:"GUNTHER EYSENBACH"} | 2055
name:"HOONGKUN FUN"} | 1329
]{name:"SEIK WENG NG"} | 1233



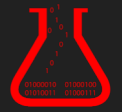
Intro
Background
Examples
Our Work

Graph Databases



Some Key Graph Databases

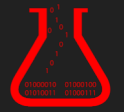
- Neo4J (well supported)
- Titan/Janus graph (distributed backend)
- AgensGraph (postgres compatible)
- Grakn (knowledge graph)



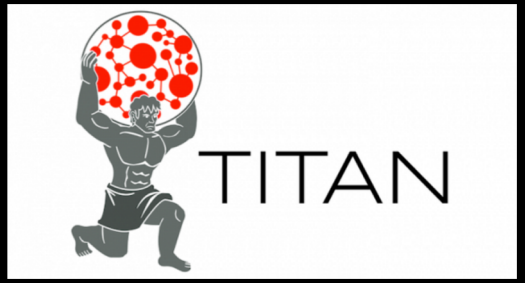
Neo4J

- Industry standard features
- Large userbase and developer community
- Built from the ground up as a graph database

https://neo4j.com/



Titan/Janus Graph



- Apache project
- Early adopter of distributed backend
- Elastic scalability
- Integration with Tinkerpop graph stack
- Multiple user access
- Real time updates

https://www.predictiveanalyticstoday.com/titan/

AgensGraph

- Highly performant graph database
- Hybrid database built on postgreSQL
- SQL and Cypher in the same query

http://bitnine.net/agensgraph/?ckattempt=1

GRAKN.AI

- Knowledge representation in graphs for AI purposes
  - Nodes represent “objects”, and edges are relationships between them.
- SQL-type query language, Graql, used to quickly and intuitively make queries in the knowledge graph
- Steadily growing technology

https://grakn.ai/

Thank You!

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