Architecture of Enterprise Applications 20
Neo4J & Graph Computing

Haopeng Chen

***RE**liable, **IN**telligent and **S**calable Systems Group (**REINS**)*
Shanghai Jiao Tong University
Shanghai, China
http://reins.se.sjtu.edu.cn/~chenhp
e-mail: chen-hp@sjtu.edu.cn

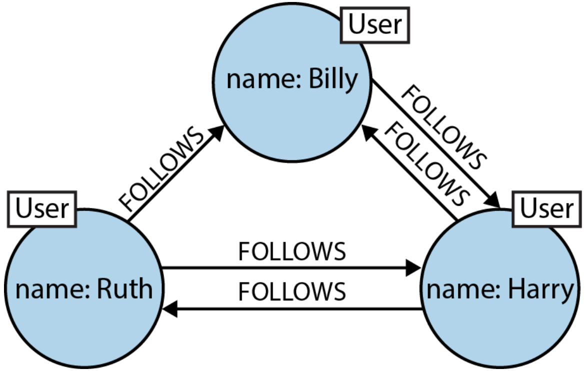
Contents and Objectives

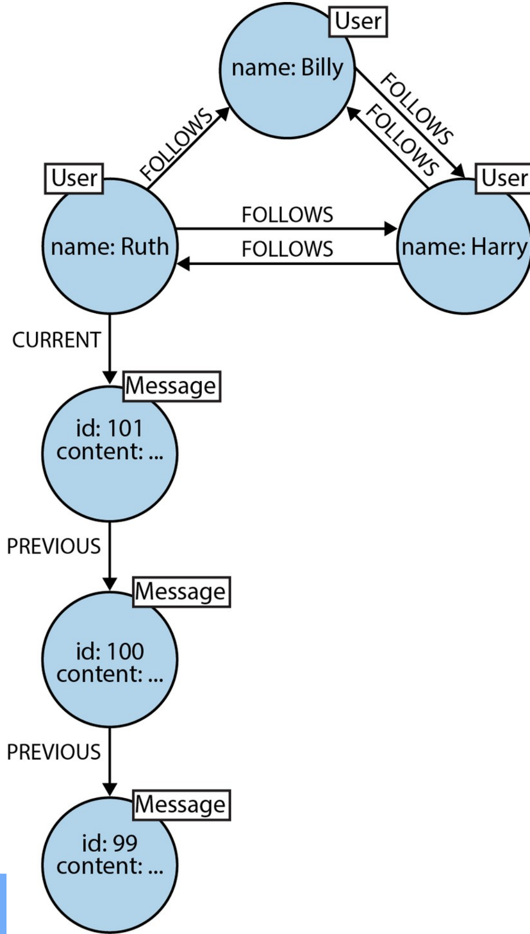
- Contents
  - Neo4J
  - Graph Database
  - Options for Storing Connected Data
  - Data Modeling with Graphs
  - Building a Graph Database Application
  - Graph Database Internals

- Objectives
  - 能够根据数据特性和数据访问模式，识别适合图数据库存储的数据，设计并实现其在图数据库中的存储和访问方案

What is a Graph?

- Formally, a graph is just a collection of *vertices* and *edges*
  - or, in less intimidating language, a set of *nodes* and the *relationships* that connect them.
  - Graphs represent entities as nodes and the ways in which those entities relate to the world as relationships.



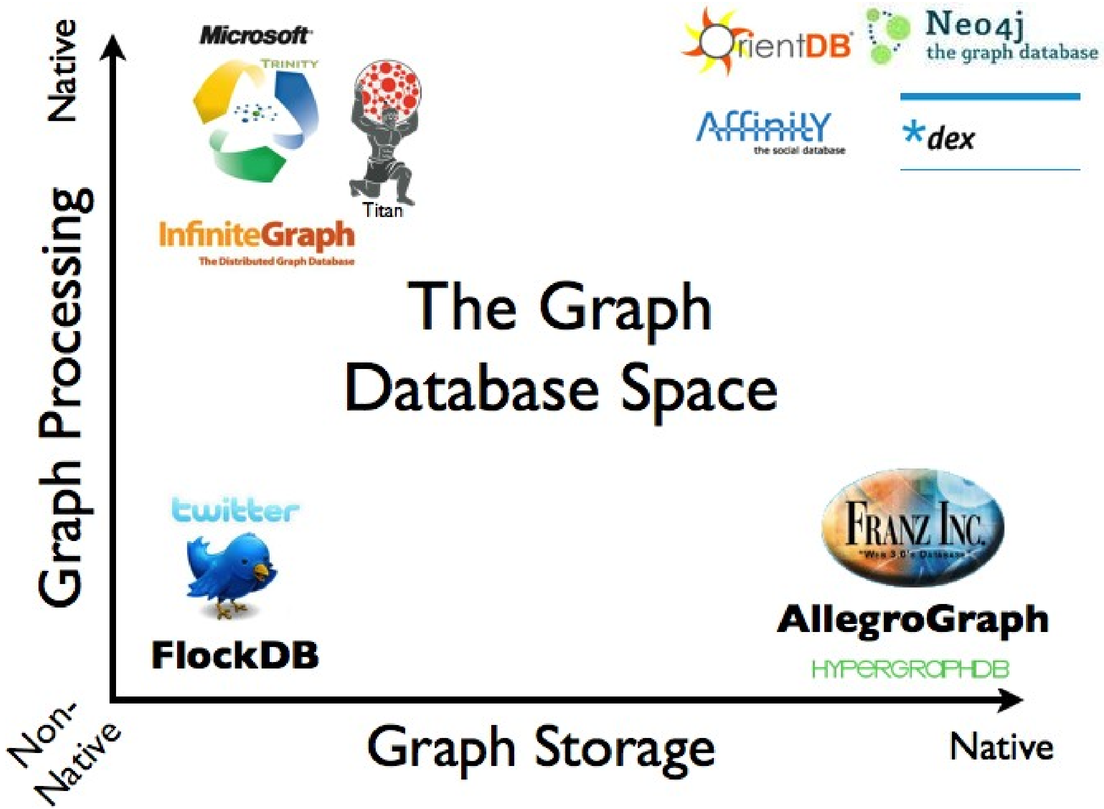


Graph Databases

- A *graph database management system* (henceforth, a *graph database*) is
  - an online database management system with Create, Read, Update, and Delete (CRUD) methods that expose a graph data model.
  - Graph databases are generally built for use with transactional (OLTP) systems.
  - Accordingly, they are normally optimized for transactional performance, and engineered with transactional integrity and operational availability in mind.

- There are two properties of graph databases we should consider when investigating graph database technologies:
  - *The underlying storage*
  - *The processing engine*

Graph Databases



Options for Storing Connected Data

- **Relational Databases Lack Relationships**

User

UserID	User	Address	Phone	Email	Alternate
1	Alice	123 Foo St.	12345678	alice@example.org	alice@neo4j.org
2	Bob	456 Bar Ave.		bob@example.org	
…	…	…	…	…	…
99	Zach	99 South St.		zach@example.org	

Order

OrderID	UserID
1234	1
5678	1
…	…
5588	99

LineItem

OrderID	ProductID	Quantity
1234	765	2
1234	987	1
…	…	…
5588	765	1

Product

ProductID	Description	Handling
321	strawberry ice cream	freezer
765	potatoes	
…	…	
987	dried spaghetti	

Options for Storing Connected Data

- **Relational Databases Lack Relationships**

Person	
ID	Person
1	Alice
2	Bob
…	…
99	Zach

PersonFriend	
PersonID	FriendID
1	2
2	1
2	99
…	…
99	1

Example 1. Bob’s friends

```
SELECT p1.Person
FROM Person p1 JOIN PersonFriend
     ON PersonFriend.FriendID = p1.ID
JOIN Person p2
     ON PersonFriend.PersonID = p2.ID
WHERE p2.Person = 'Bob’
```

Example 2-2. Who is friends with Bob?

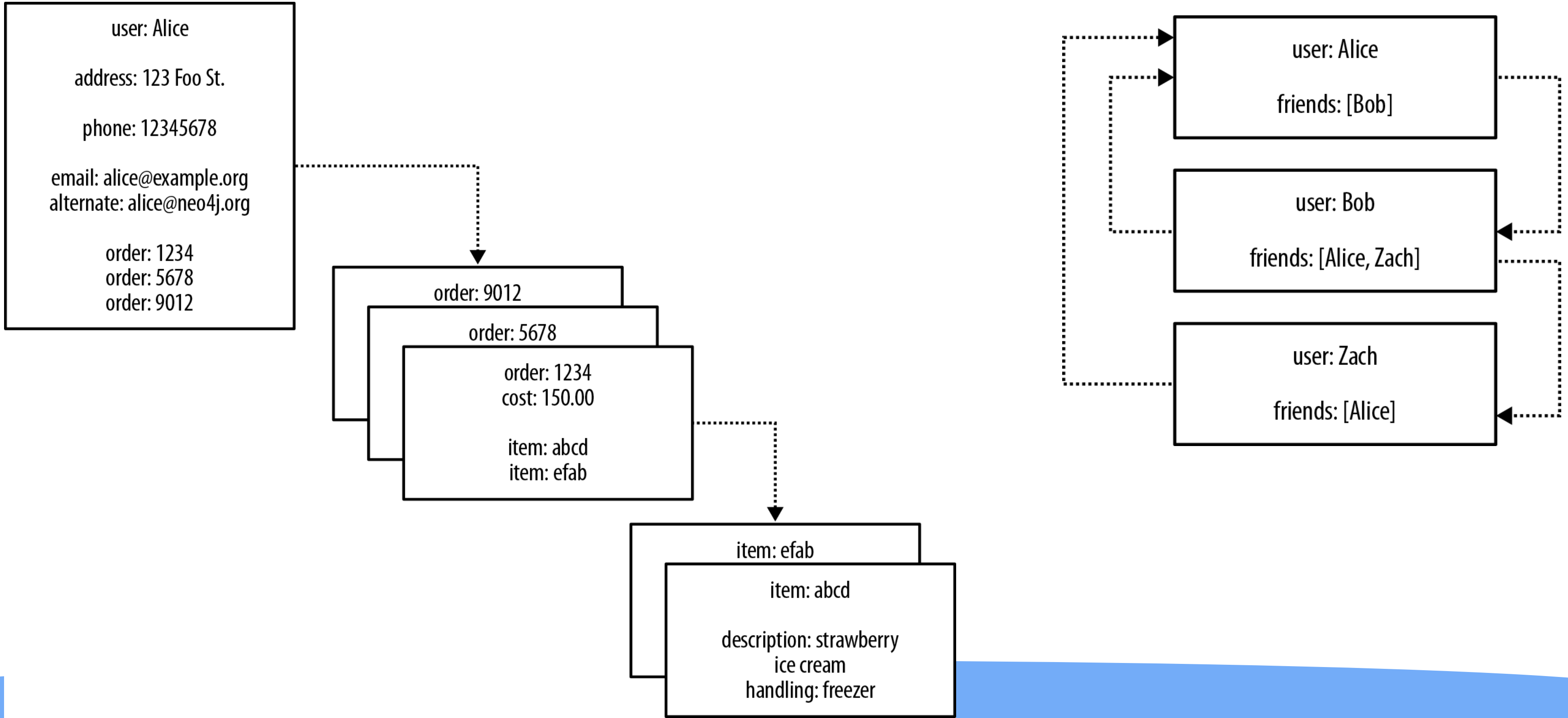
```
SELECT p1.Person
FROM Person p1 JOIN PersonFriend
     ON PersonFriend.PersonID = p1.ID
JOIN Person p2
     ON PersonFriend.FriendID = p2.ID
WHERE p2.Person = 'Bob’
```

Example 3. Alice’s friends-of-friends

```
SELECT p1.Person AS PERSON,
          p2.Person AS FRIEND_OF_FRIEND
FROM PersonFriend pf1 JOIN Person p1
   ON pf1.PersonID = p1.ID
JOIN PersonFriend pf2
   ON pf2.PersonID = pf1.FriendID
JOIN Person p2
   ON pf2.FriendID = p2.ID
WHERE p1.Person = 'Alice' AND pf2.FriendID <> p1.ID
```

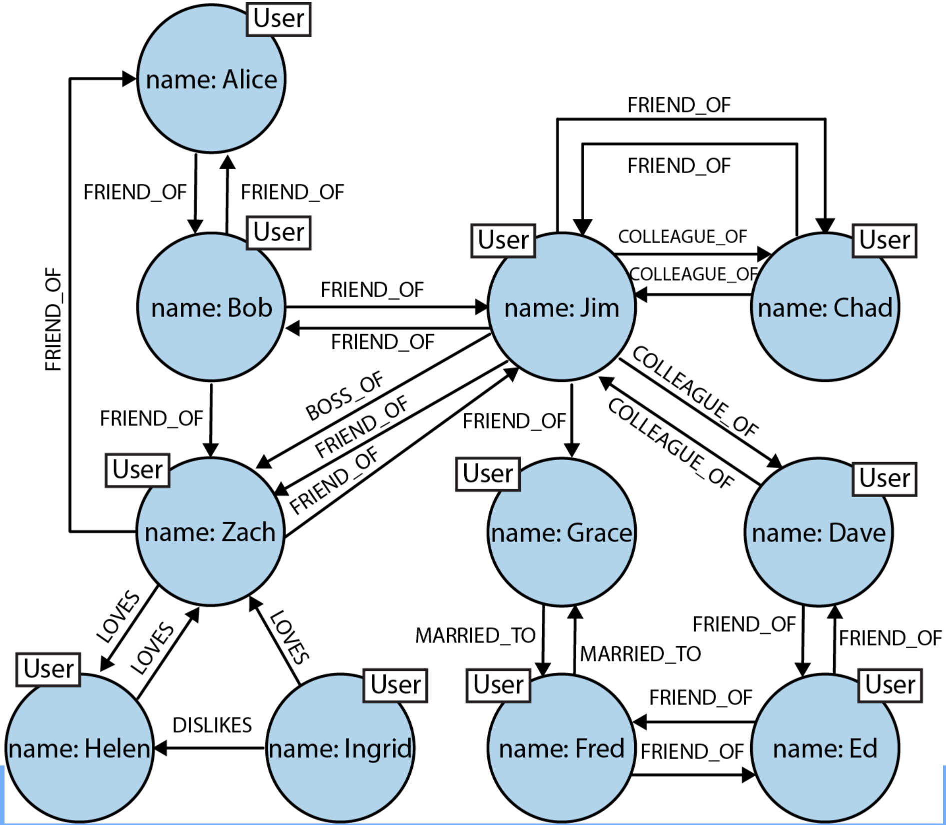
Options for Storing Connected Data

- **NOSQL Databases Also Lack Relationships**

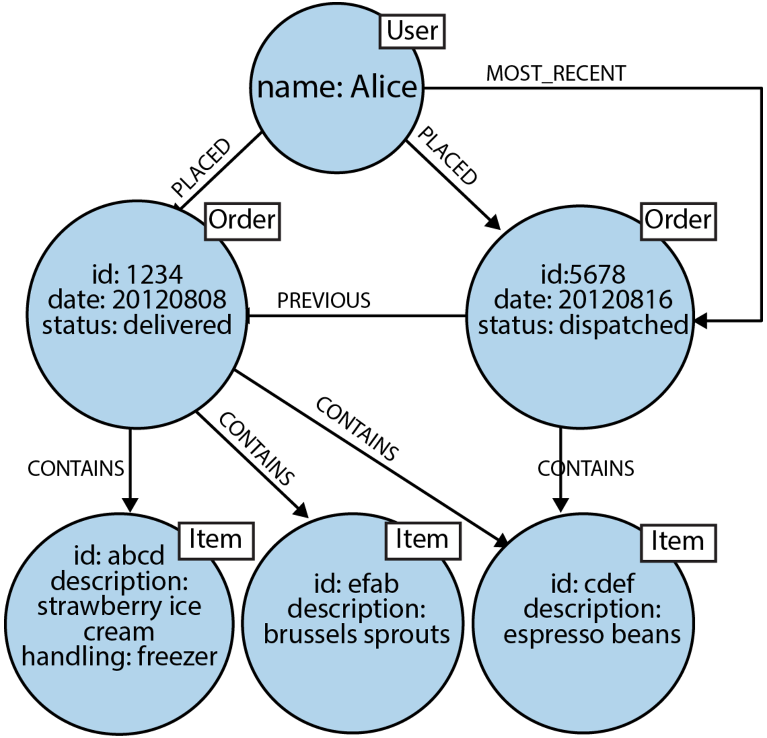


Options for Storing Connected Data

- **Graph Databases Embrace Relationships**



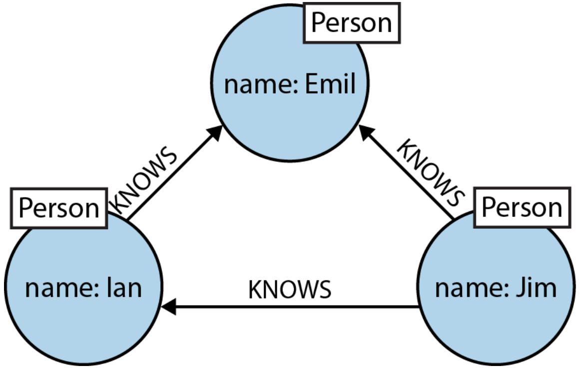
- **Graph Databases Embrace Relationships**



- **The Labeled Property Graph Model**
- A *labeled property graph* is made up of *nodes*, *relationships*, *properties*, and *labels*.
  - Nodes contain properties. Think of nodes as documents that store properties in the form of arbitrary key-value pairs. In Neo4j, the keys are strings and the values are the Java string and primitive data types, plus arrays of these types.
  - Nodes can be tagged with one or more labels. Labels group nodes together, and indicate the roles they play within the dataset.
  - Relationships connect nodes and structure the graph. A relationship always has a direction, a single name, and a *start node* and an *end node*—there are no dangling relationships. Together, a relationship's direction and name add semantic clarity to the structuring of nodes.

Data Modeling with Graphs

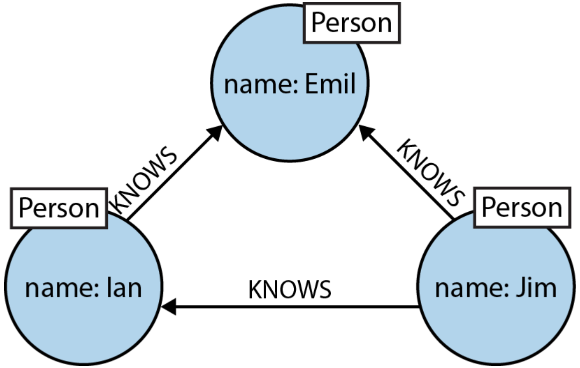
- **Querying Graphs: Cypher**
  - Cypher is an expressive (yet compact) graph database query language.



- Here's the equivalent ASCII art representation in Cypher:

  (emil:Person {name:'Emil'}) <-[:KNOWS]-(jim:Person {name:'Jim'}) -[:KNOWS]->(ian:Person {name:'Ian'}) -[:KNOWS]->(emil)

- **Querying Graphs: Cypher**
  - Cypher is an expressive (yet compact) graph database query language.



- Match:

```
MATCH (a:Person)-[:KNOWS]->(b)-[:KNOWS]->(c), (a)-[:KNOWS]->(c)
WHERE a.name = 'Jim'
RETURN b, c
```

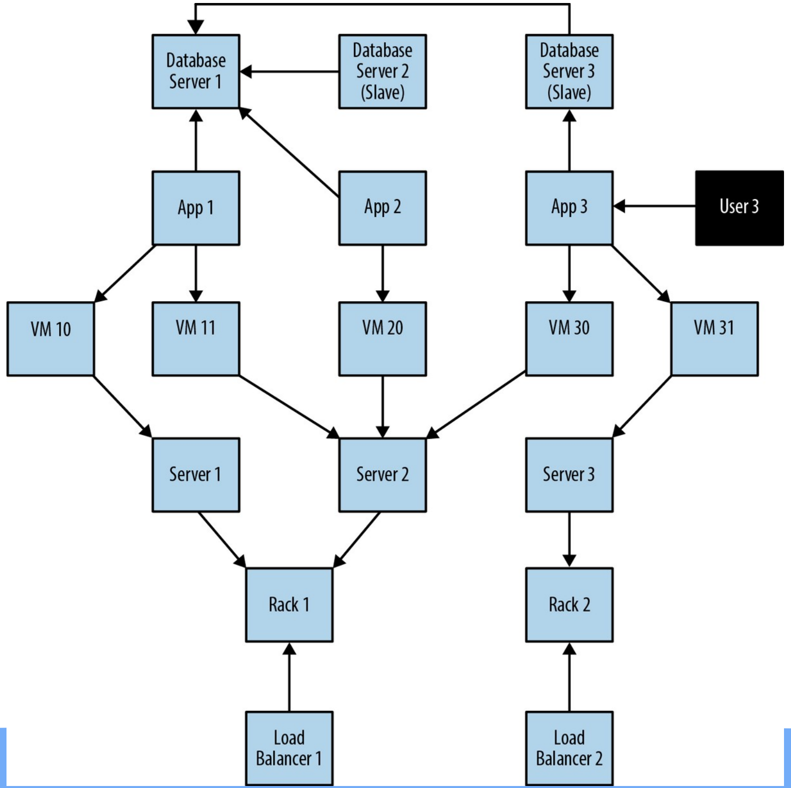
Data Modeling with Graphs

REliable, INtelligent & Scalable Systems

- **Querying Graphs: Cypher**
- The other clauses we can use in a Cypher query include:
  - WHERE
    - Provides criteria for filtering pattern matching results.
  - CREATE and CREATE UNIQUE
    - Create nodes and relationships.
  - MERGE
    - Ensures that the supplied pattern exists in the graph, either by reusing existing nodes and relationships that match the supplied predicates, or by creating new nodes and relationships.
  - DELETE
    - Removes nodes, relationships, and properties.
  - SET
    - Sets property values
  - FOREACH
    - Performs an updating action for each element in a list.
  - UNION
    - Merges results from two or more queries.
  - WITH
    - Chains subsequent query parts and forwards results from one to the next. Similar to piping commands in Unix.
  - START
    - Specifies one or more explicit starting points—nodes or relationships—in the graph.

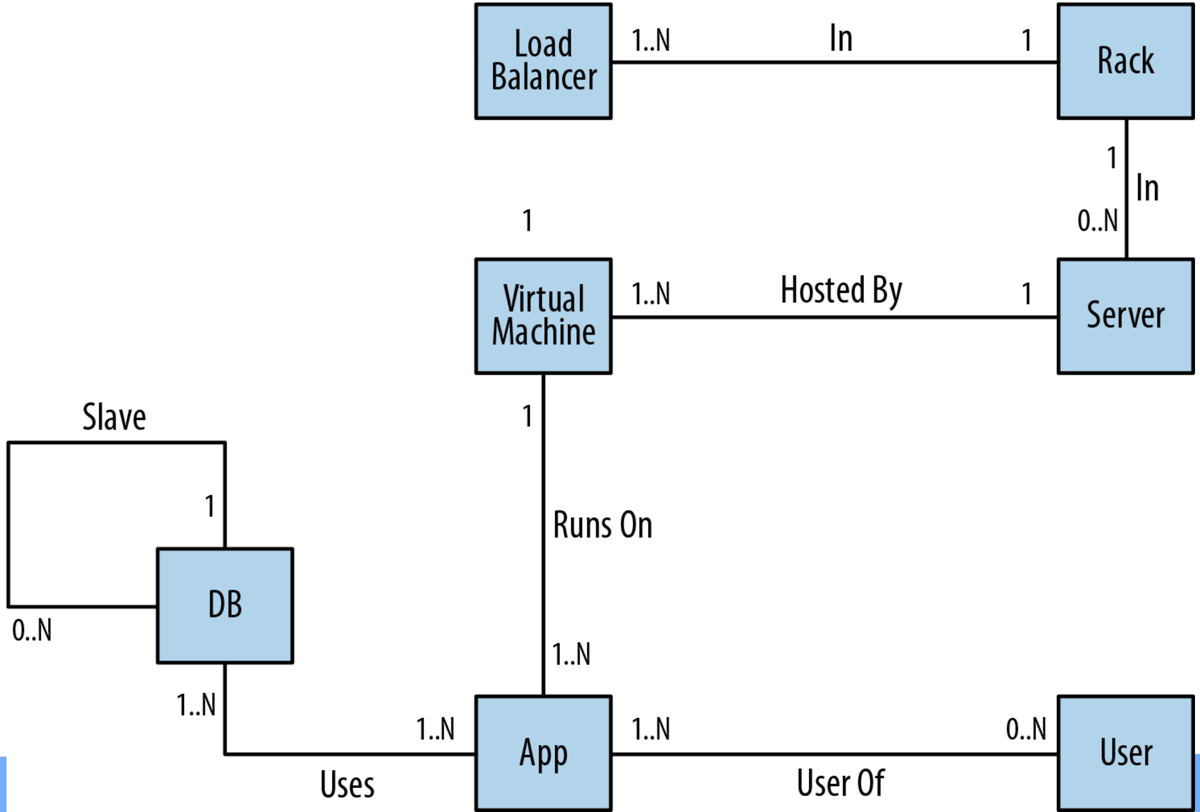
Data Modeling with Graphs

- **A Comparison of Relational and Graph Modeling**
  - To facilitate this comparison, we'll examine a simple data center management domain.



Data Modeling with Graphs

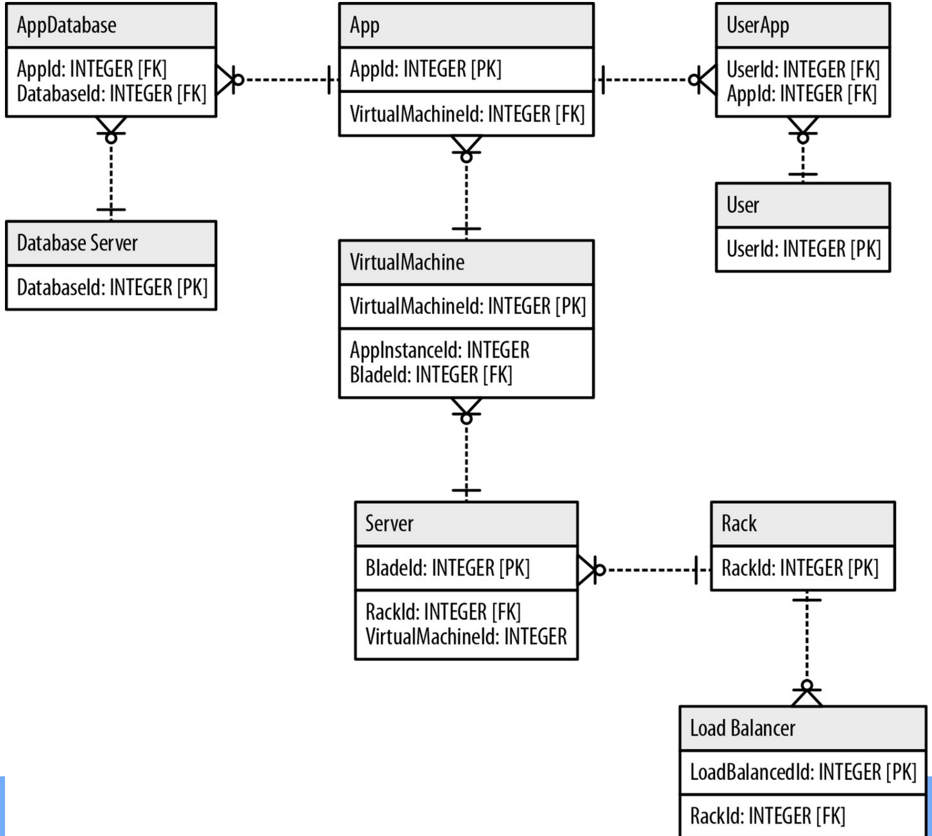
- **Relational Modeling in a Systems Management Domain**



Data Modeling with Graphs

REliable, INtelligent & Scalable Systems

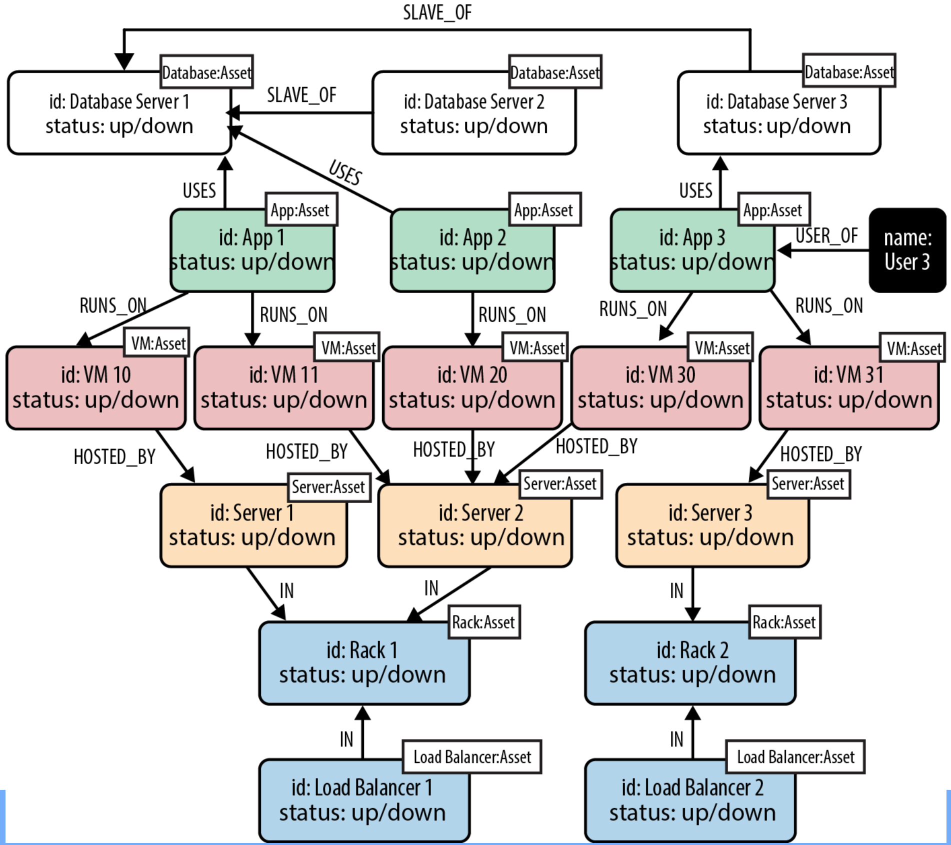
- **Relational Modeling in a Systems Management Domain**



Data Modeling with Graphs

REliable, INtelligent & Scalable Systems

- **Graph Modeling in a Systems Management Domain**



Data Modeling with Graphs

- **Test Graph Model**
  - When a user reports a problem, we can limit the physical fault-finding to problematic network elements between the user and the application and the application and its dependencies.

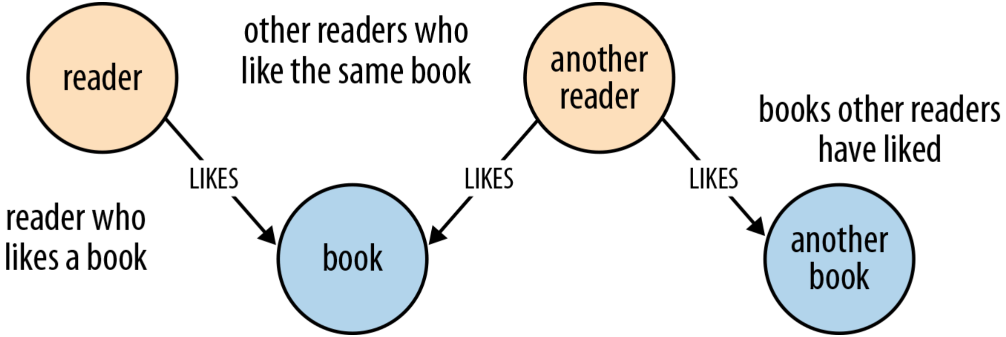
  - In our graph we can find the faulty equipment with the following query:
    - **MATCH** (user:User)-[*1..5]-(asset:Asset)
      WHERE user.name = 'User 3' AND asset.status = 'down' **RETURN DISTINCT** asset

  - This allows us to match paths such as:

    (user)-[:USER_OF]->(app)
    (user)-[:USER_OF]->(app)-[:USES]->(database)
    (user)-[:USER_OF]->(app)-[:USES]->(database)-[:SLAVE_OF]->(another-database)
    (user)-[:USER_OF]->(app)-[:RUNS_ON]->(vm)
    (user)-[:USER_OF]->(app)-[:RUNS_ON]->(vm)-[:HOSTED_BY]->(server)
    (user)-[:USER_OF]->(app)-[:RUNS_ON]->(vm)-[:HOSTED_BY]->(server)-[:**IN**]->(rack)
    (user)-[:USER_OF]->(app)-[:RUNS_ON]->(vm)-[:HOSTED_BY]->(server)-[:**IN**]->(rack) <-[:**IN**]-(load-balancer)

Building a Graph Database Application

- **Describe the Model in Terms of the Application's Needs**
- Here's an example of a user story for a book review web application:
  - **AS A** reader who likes a book, **I WANT** to know which books other readers who like the same book have liked, **SO THAT** I can find other books to read.



  - since *Alice likes Dune, find books that others who like Dune have enjoyed*:

    MATCH (:Reader {name:'Alice'})-[:LIKES]->(:Book {title:'Dune'})<-[:LIKES]-(:Reader)-[:LIKES]->(books:Book)

    RETURN books.title

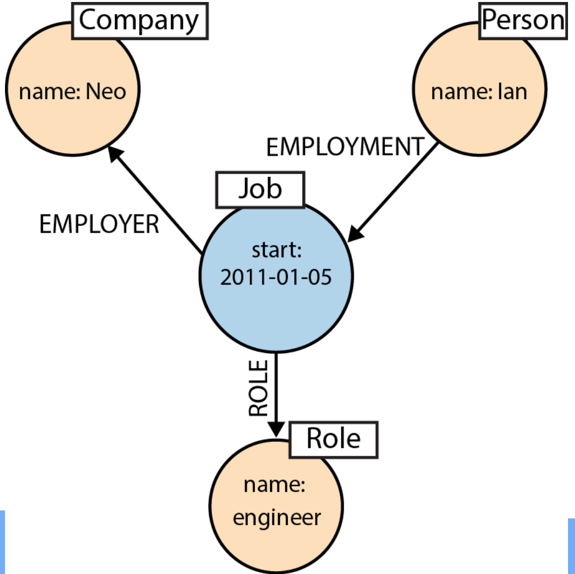
Building a Graph Database Application

- **Nodes for Things, Relationships for Structure**
  - Use nodes to represent entities—that is, the *things* in our domain that are of interest to us, and which can be labeled and grouped.
  - Use relationships both to express the *connections* between entities and to establish semantic context for each entity, thereby structuring the domain.
  - Use relationship direction to further clarify relationship semantics. Many relationships are asymmetrical, which is why relationships in a property graph are always directed. For bidirectional relationships, we should make our queries ignore direction, rather than using two relationships.
  - Use node properties to represent entity attributes, plus any necessary entity metadata, such as timestamps, version numbers, etc.
  - Use relationship properties to express the strength, weight, or quality of a relationship, plus any necessary relationship metadata, such as timestamps, version numbers, etc.

Building a Graph Database Application

- **Model Facts as Nodes**
- **Employment**
  - The Figure shows how the fact of Ian being employed by Neo Technology in the role of engineer can be represented in the graph.

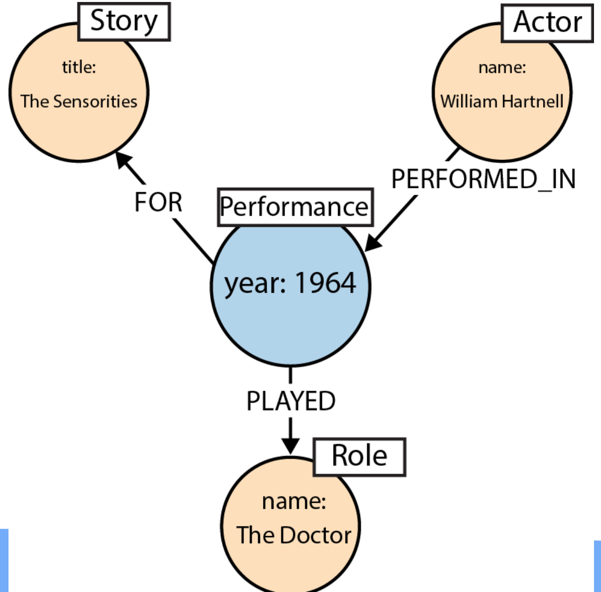
```
CREATE (:Person {name:'Ian'})-[:EMPLOYMENT]-> (employment:Job {start_date:'2011-01-05'}) -
[:EMPLOYER]->(:Company {name:'Neo'}),
(employment)-[:ROLE]->(:Role {name:'engineer'})
```



REliable, INtelligent & Scalable Systems

- **Model Facts as Nodes**
- **Performance**
  - The Figure shows how the fact that William Hartnell played The Doctor in the story *The Sensorites* can be represented in the graph.

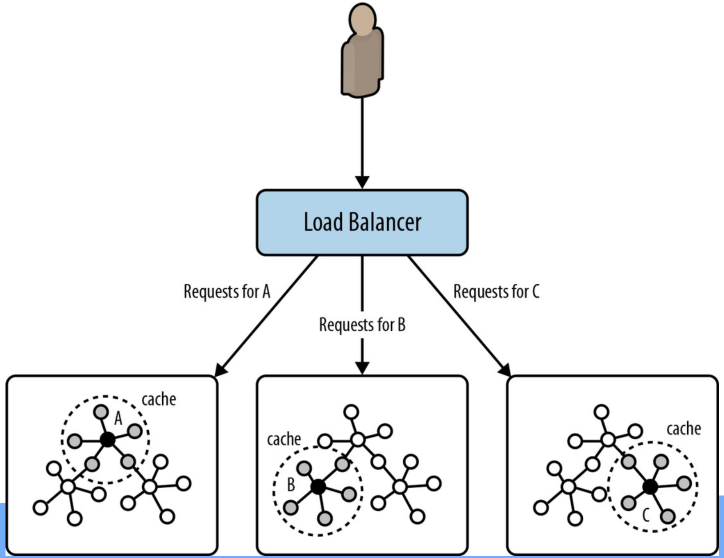
```
CREATE (:Actor {name:'William Hartnell'})-[:PERFORMED_IN]-> (performance:Performance {year:1964})-
[:PLAYED]-> (:Role {name:'The Doctor'}),
(performance)-[:FOR]->(:Story {title:'The Sensorites'})
```

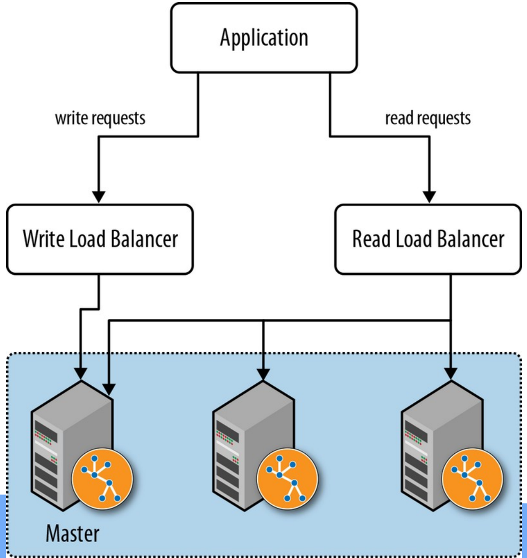


Building a Graph Database Application

- **Embedded versus Server**
  - Most databases today run as a server that is accessed through a client library. Neo4j is somewhat unusual in that it can be run in embedded as well as server mode.
  - In embedded mode, Neo4j runs in the same process as our application.
  - Running Neo4j in server mode is the most common means of deploying the database today.

- **Cluster**

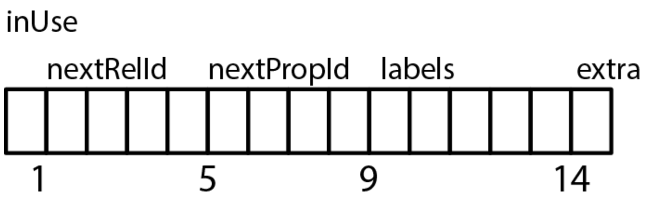




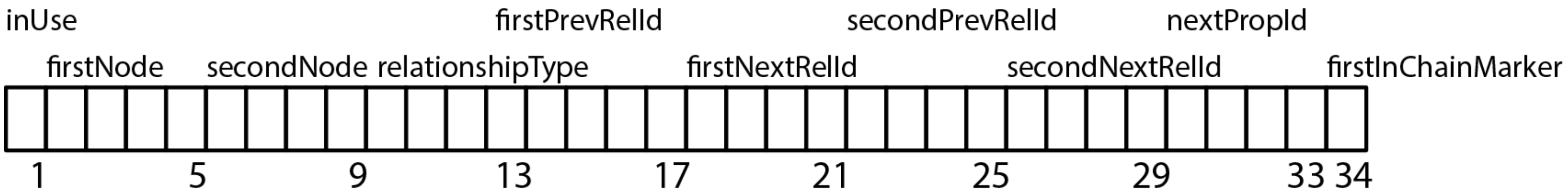
Graph Database Internals

- Neo4j stores graph data in a number of different *store files*.
  - Each store file contains the data for a specific part of the graph (e.g., there are separate stores for nodes, relation- ships, labels, and properties).

Node (15 bytes)



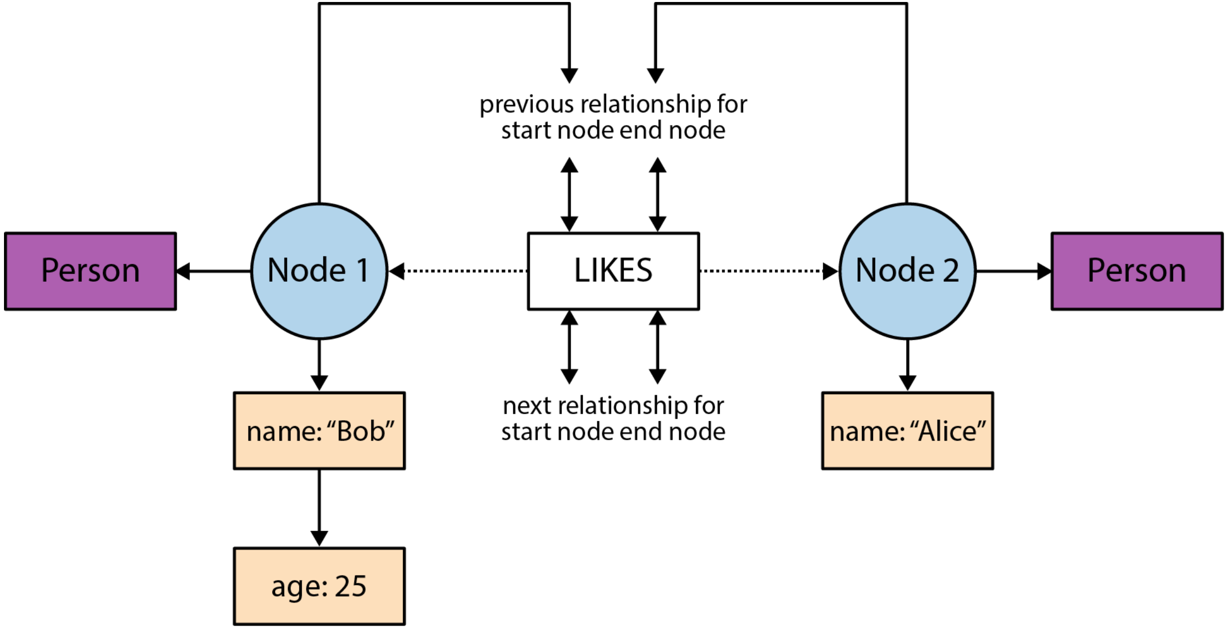
Relationship (34 bytes)



Graph Database Internals

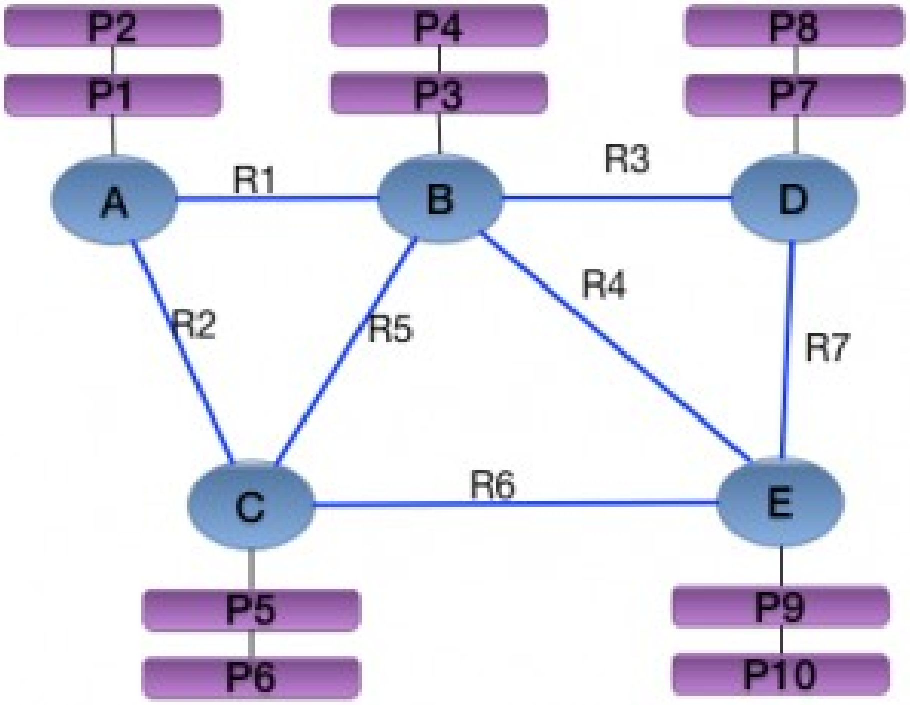
REliable, INtelligent & Scalable Systems

- Neo4j stores graph data in a number of different *store files*.
  - Doubly Linked Lists in the Relationship Store



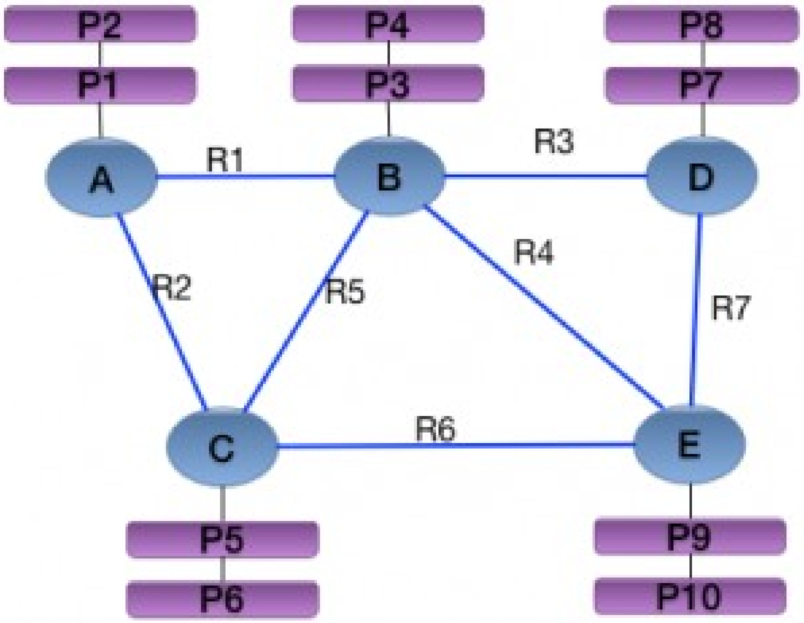
Graph Database Internals

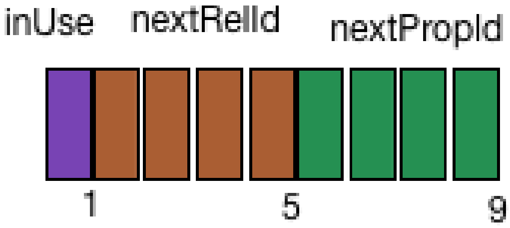
- Neo4j stores graph data



Graph Database Internals

- Neo4j stores graph data
  - Node

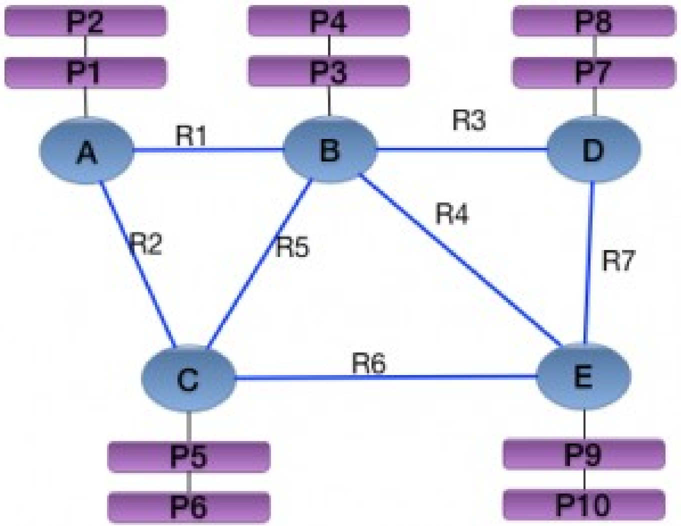


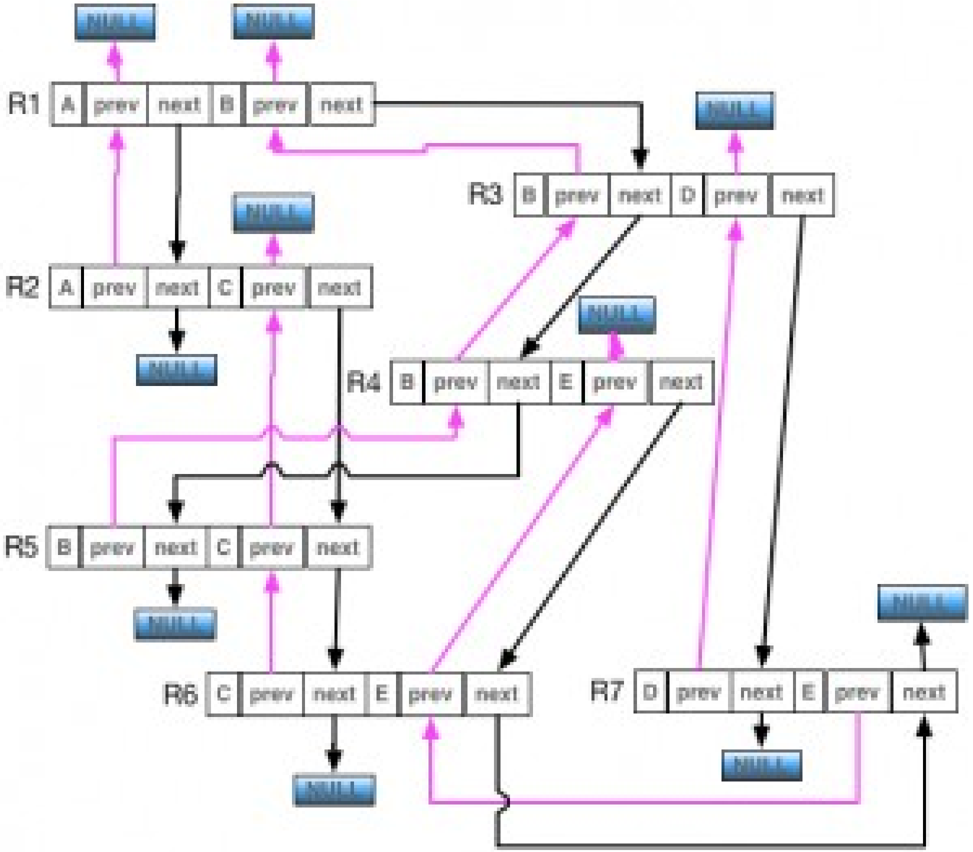


A:	1	R1	P1
B:	1	R1	P3
C:	1	R2	P5
D:	1	R3	P7
E:	1	R4	P9

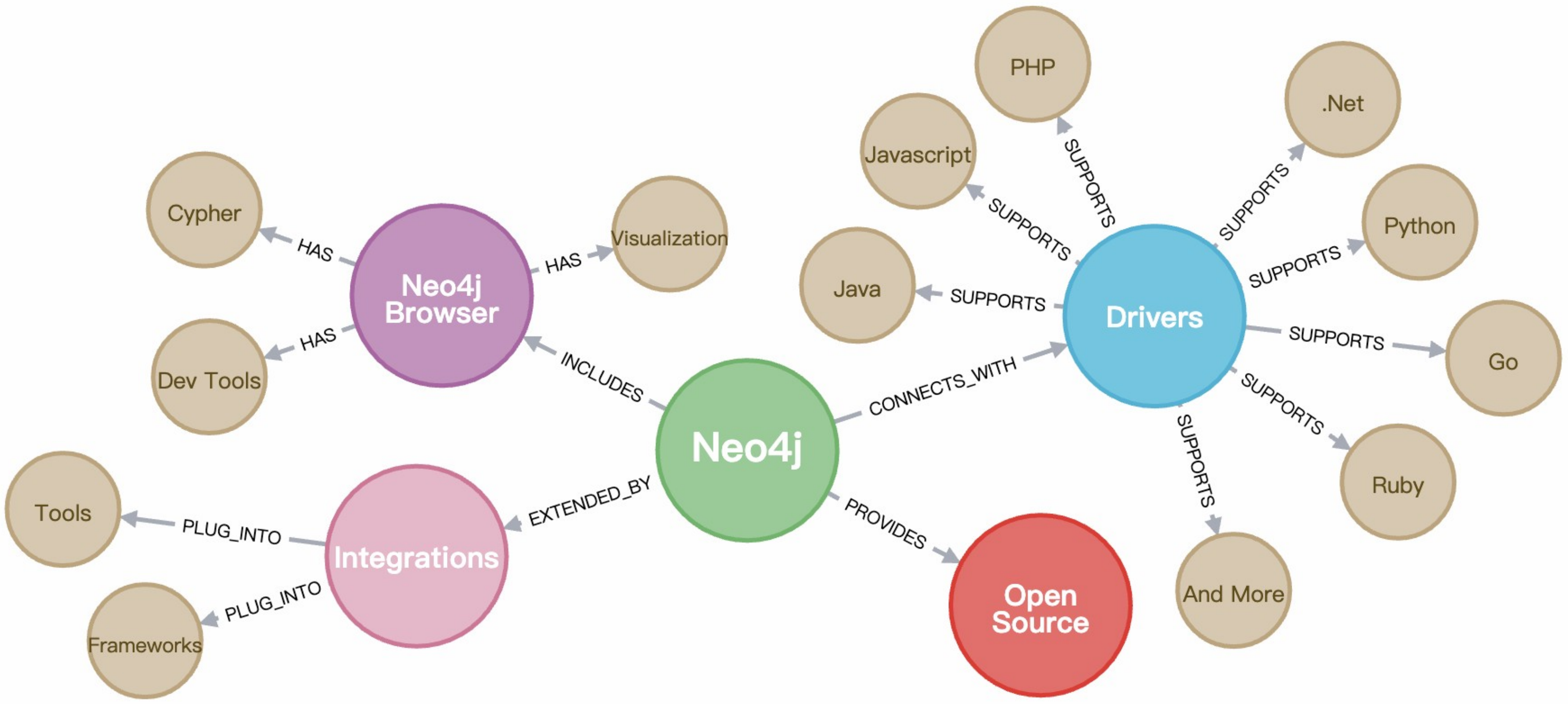
Graph Database Internals

- Neo4j stores graph data
  - relationship





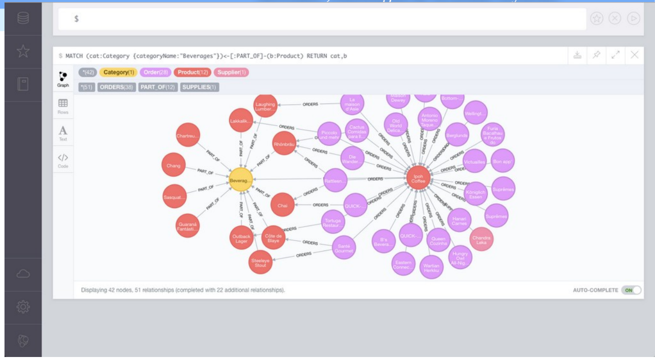
Neo4j



Neo4j
Neo4j Browser
Cypher
Visualization
Dev Tools
HAS
HAS
HAS
INCLUDES
Integrations
Tools
Frameworks
PLUG_INTO
PLUG_INTO
EXTENDED_BY
CONNECTS_WITH
Drivers
PHP
Javascript
.Net
Python
Java
Go
Ruby
And More
SUPPORTS
PROVIDES
Open Source

Install and Run Neo4j

REliable, INtelligent & Scalable Systems



1. Open up your terminal/shell.
2. Extract the contents of the archive, using:
   tar -xf <filecode>.
   For example,
   tar -xf neo4j-community-4.3.3-unix.tar.gz
3. Place the extracted files in a permanent home on your server. The top level directory is referred to as NEO4J_HOME.
   – To run Neo4j as a console application, use:
     <NEO4J_HOME>/bin/neo4j console
   – To run Neo4j in a background process, use:
     <NEO4J_HOME>/bin/neo4j start
4. Visit http://localhost:7474 in your web browser.
5. Connect using the username 'neo4j' with default password 'neo4j'. You'll then be prompted to change the password.

Sample

- pom.xml

```xml
<dependencies>
    <dependency>
        <groupId>org.springframework.boot</groupId>
        <artifactId>spring-boot-starter-data-neo4j</artifactId>
    </dependency>

    <dependency>
        <groupId>org.springframework.boot</groupId>
        <artifactId>spring-boot-starter-test</artifactId>
        <scope>test</scope>
        <exclusions>
            <exclusion>
                <groupId>org.junit.vintage</groupId>
                <artifactId>junit-vintage-engine</artifactId>
            </exclusion>
        </exclusions>
    </dependency>
</dependencies>
```

Sample

REliable, INtelligent & Scalable Systems

- Person.java

```
@NodeEntity
public class Person {

    @Id @GeneratedValue
    private Long id;
    private String name;

    private Person() {
        // Empty constructor required as of Neo4j API 2.0.5
    };
    public Person(String name) {
        this.name = name;
    }

    @Relationship(type = "TEAMMATE", direction = Relationship.UNDIRECTED)
    public Set<Person> teammates;

    public void worksWith(Person person) {
        if (teammates == null) {
            teammates = new HashSet<>();
        }
        teammates.add(person);
    }
```

Sample

- Person.java

```
public String toString() {

    return this.name + "'s teammates => "
            + Optional.ofNullable(this.teammates).orElse(
            Collections.emptySet()).stream()
            .map(Person::getName)
            .collect(Collectors.toList());
}

public String getName() {
    return name;
}

public void setName(String name) {
    this.name = name;
}
}
```

Sample

- PersonRepository.java

```
package com.example.accessingdataneo4j;

import java.util.List;
import org.springframework.data.neo4j.repository.Neo4jRepository;

public interface PersonRepository extends Neo4jRepository<Person, Long> {

   Person findByName(String name);
   List<Person> findByTeammatesName(String name);
}
```

Sample

REliable, INtelligent & Scalable Systems

- AccessingDataNeo4jApplication.java

```
@SpringBootApplication
@EnableNeo4jRepositories
public class AccessingDataNeo4jApplication {

   private final static Logger log = LoggerFactory.getLogger(AccessingDataNeo4jApplication.class);

   public static void main(String[] args) throws Exception {
      SpringApplication.run(AccessingDataNeo4jApplication.class, args);
      System.exit(0);
   }

   @Bean
   CommandLineRunner demo(PersonRepository personRepository) {
      return args -> {
         personRepository.deleteAll();

         Person greg = new Person("Greg");
         Person roy = new Person("Roy");
         Person craig = new Person("Craig");

         List<Person> team = Arrays.asList(greg, roy, craig);
```

Sample

REliable, INtelligent & Scalable Systems

- AccessingDataNeo4jApplication.java

```
List<Person> team = Arrays.asList(greg, roy, craig);

log.info("Before linking up with Neo4j...");

team.stream().forEach(person -> log.info("\t" + person.toString()));

personRepository.save(greg);
personRepository.save(roy);
personRepository.save(craig);

greg = personRepository.findByName(greg.getName());
greg.worksWith(roy);
greg.worksWith(craig);
personRepository.save(greg);

roy = personRepository.findByName(roy.getName());
roy.worksWith(craig);
// We already know that roy works with greg
personRepository.save(roy);
```

Sample

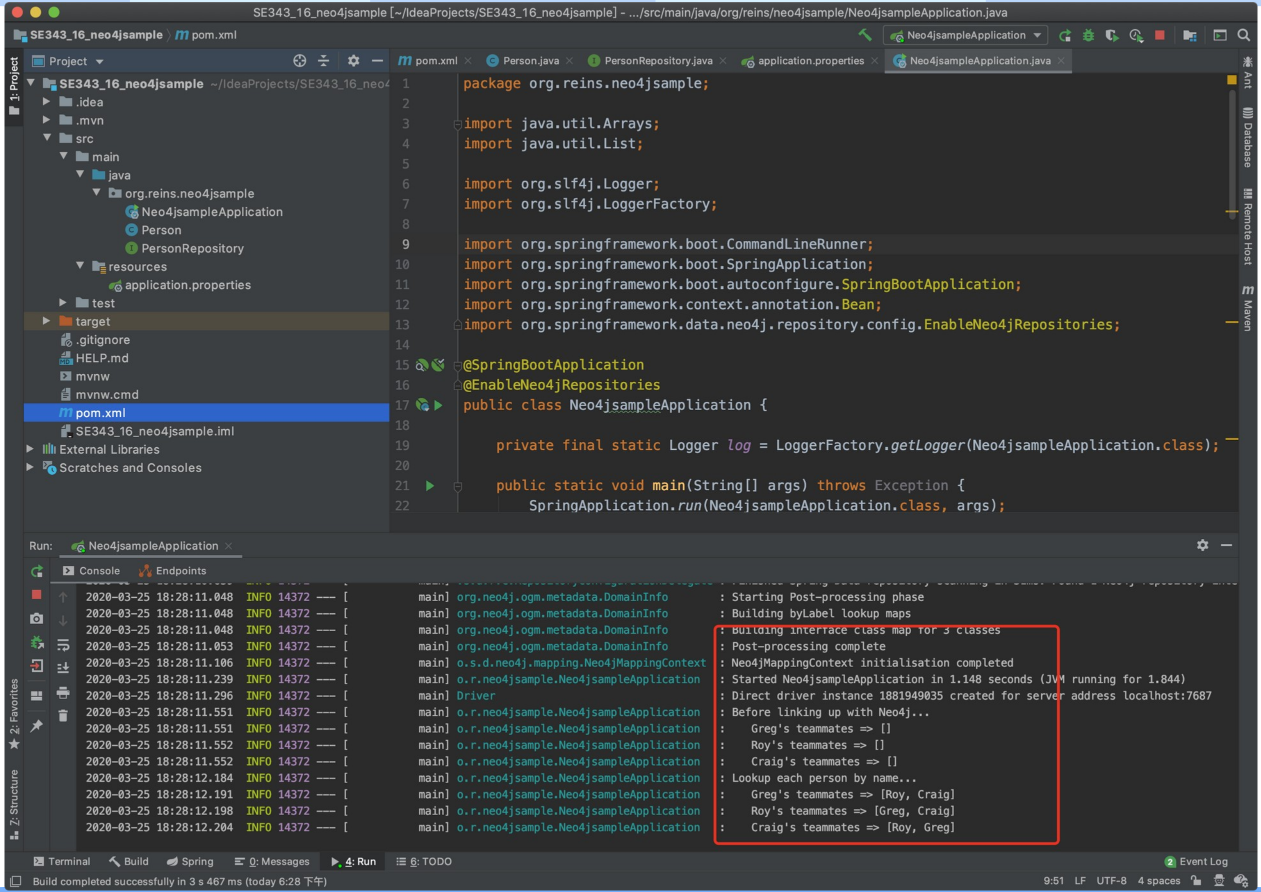
REliable, INtelligent & Scalable Systems

- AccessingDataNeo4jApplication.java

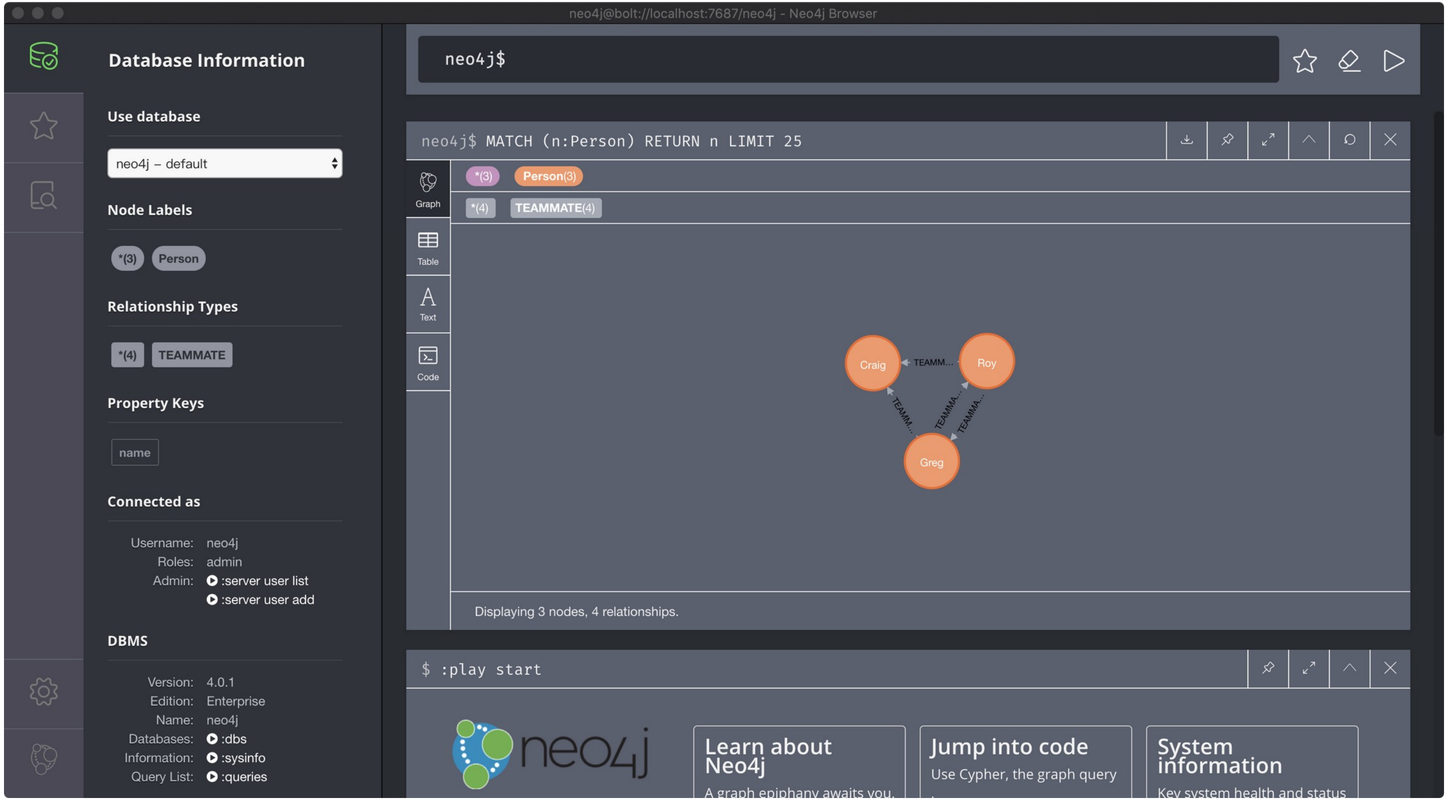
```
        // We already know craig works with roy and greg

        log.info("Lookup each person by name...");
        team.stream().forEach(person -> log.info(
              "\t" + personRepository.findByName(person.getName()).toString()));

        List<Person> teammates = personRepository.findByTeammatesName(greg.getName());
        log.info("The following have Greg as a teammate...");
        teammates.stream().forEach(person -> log.info("\t" + person.getName()));
      };
    }

}
```

Sample

REliable, INtelligent & Scalable Systems

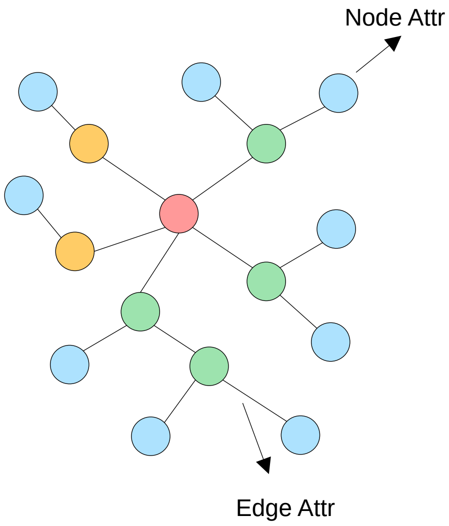


Sample


neo4j@bolt://localhost:7687/neo4j - Neo4j Browser
Database Information
Use database
neo4j – default
Node Labels
*(3)
Person
Relationship Types
*(4)
TEAMMATE
Property Keys
name
Connected as
Username: neo4j
Roles: admin
Admin: :server user list
:server user add
DBMS
Version: 4.0.1
Edition: Enterprise
Name: neo4j
Databases: :dbs
Information: :sysinfo
Query List: :queries
neo4j$
neo4j$ MATCH (n:Person) RETURN n LIMIT 25
*(3) Person(3)
*(4) TEAMMATE(4)
Graph
Table
Text
Code
Craig
Roy
Greg
TEAMM...
Displaying 3 nodes, 4 relationships.
$:play start
neo4j
Learn about Neo4j
A graph epiphany awaits you.
Jump into code
Use Cypher, the graph query
System information
Key system health and status

图计算概论

- 图数据上的分类问题
  - 图粒度 vs. 节点粒度
  - 节点特征 vs. 边特征
- 应用场景：
  - 应用对象：社交网络、交易网络（边特征敏感）
  - 应用任务：用户分类、异常行为检测…
- 图神经网络：
  - 传统图神经网络未考虑边特征对于分类结果的影响
    - 谱图理论： Graph Convolutional Network (GCN)
    - 图注意力： Graph Attention Network (GAT)
  - 仅有少数研究考虑了 GNN 在边特征上的拓展
    - 仅可处理标签化的边特征（ R-GCN)
    - 仅将边特征视为权重进行处理（ EGNN ）



边特征映射

- 边特征的集合形式 → 邻接形式

$$\vec{e}_p \to \vec{e}_{ij}$$

- 边映射矩阵　$\mathbf{M}_E$
  - 维度大小为 $N \times N \times M$
  - 第三维度： one-hot 编码
  - 可以预先构造

- 高维矩阵乘法

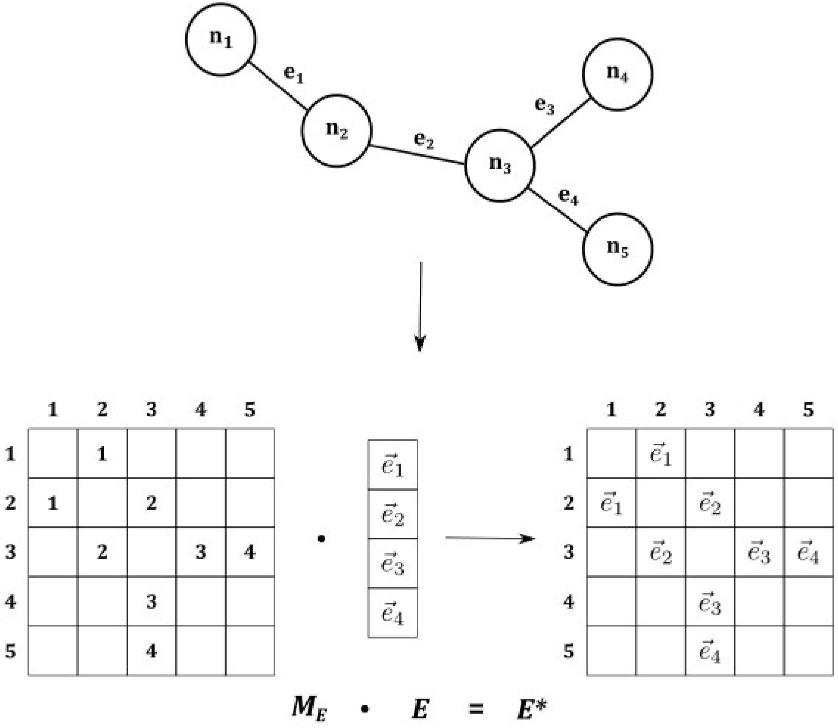


图 3–3 图上的边特征映射变换举例

节点注意力模块

- 节点特征的聚合（参与后续迭代）

$$\vec{h}_i' = \sigma(\sum_{j \in \mathcal{N}_i} \alpha_{ij} \vec{h}_j)$$

$$\sum_{j \in \mathcal{N}_i} \alpha_{ij} = 1$$

- 带有边特征的聚合（仅于融合层使用）

$$\vec{m}_i = \sigma(\sum_{j \in \mathcal{N}_i} \alpha_{ij} (\vec{h}_j \| \vec{e}_{ij}))$$

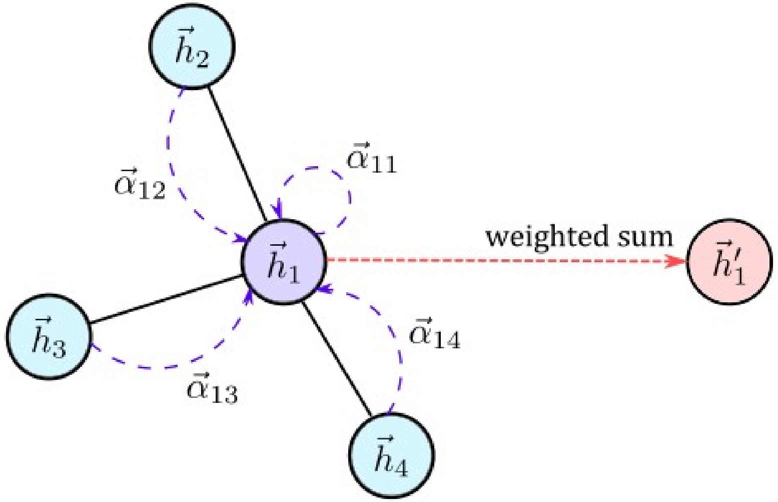


图 3–5 节点注意力模块中的节点特征聚合举例

注意力权重计算

- 带有边特征的注意力权重计算

$$w_{ij} = a(\vec{h}_i, \vec{h}_j, \vec{e}_{ij})$$

- 权重标准化（softmax）

$$\alpha_{ij} = \mathrm{softmax_j}(w_{ij}) = \frac{\exp(w_{ij})}{\sum_{k\in\mathcal{N}_i}\exp(w_{ik})}$$

- 展开

$$\alpha_{ij} = \frac{\exp(\mathrm{LeakyReLU}(\vec{\mathbf{a}}^T[\vec{h}_i \| \vec{h}_j \| \vec{e}_{ij}]))}{\sum_{k\in\mathcal{N}_i}\exp(\mathrm{LeakyReLU}(\vec{\mathbf{a}}^T[\vec{h}_i \| \vec{h}_k \| \vec{e}_{ik}]))}$$

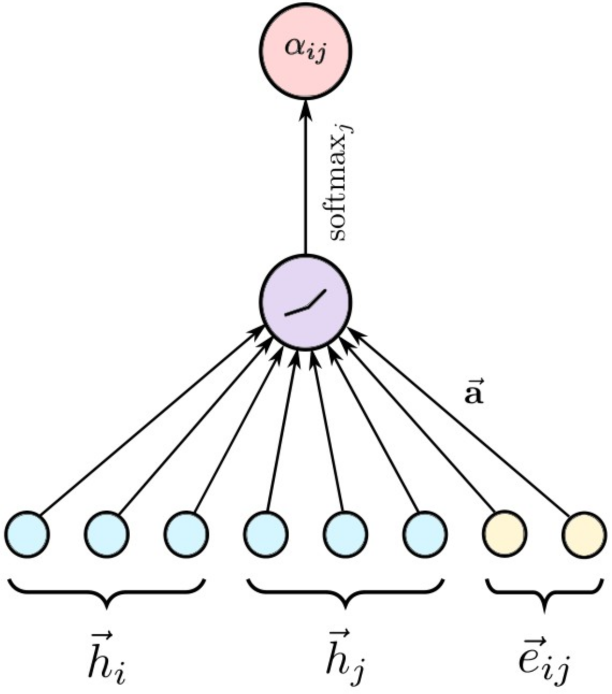


图 3–4 标准化注意力权重计算方式举例

边注意力模块

- 边特征迭代的必要性
  - 节点与边特征在迭代上的一致性
  - 模型的对称性

- 点边互换策略
  - 反转图
  - 边邻接矩阵、节点映射矩阵

$$\beta_{pq} = \frac{\exp(\text{LeakyReLU}(\vec{\mathbf{b}}^T[\vec{e}_p \| \vec{e}_q \| \vec{h}_{pq}]))}{\sum_{k\in\mathcal{N}_p}\exp(\text{LeakyReLU}(\vec{\mathbf{b}}^T[\vec{e}_p\|\vec{e}_k\|\vec{h}_{pk}]))}$$

$$\vec{e}'_p = \sigma\Big(\sum_{q\in\mathcal{N}_p}\beta_{pq}\vec{e}_q\Big)$$

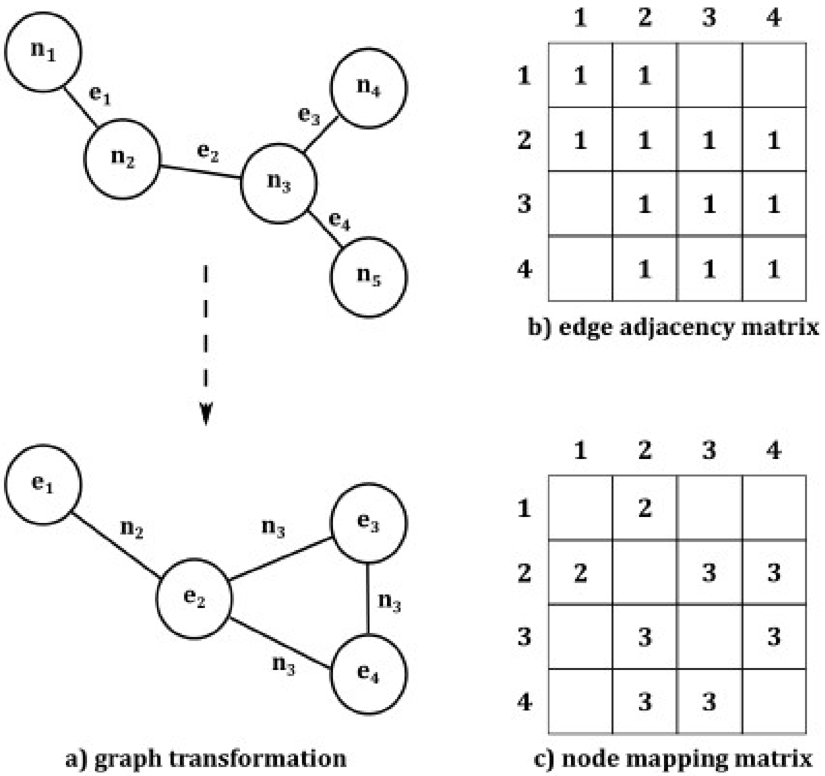


图 3-7 边特征迭代相关的图转换过程及相关矩阵图示

融合层

- 多尺度的特征融合策略

$$\vec{h}_i^* = \mathop{\Big\|}_{l=1}^{L} m_i^l$$

- 粗粒度的 multi-head attention

$$\vec{h}_i^* = \mathop{\Big\|}_{k=1}^{K} \Big(\mathop{\Big\|}_{l=1}^{L} m_i^{l,k} \Big)$$

- 维度压缩

$$\vec{h}_i^f = \mathrm{LeakyReLU}(\mathbf{W}\vec{h}_i^*)$$

- softmax

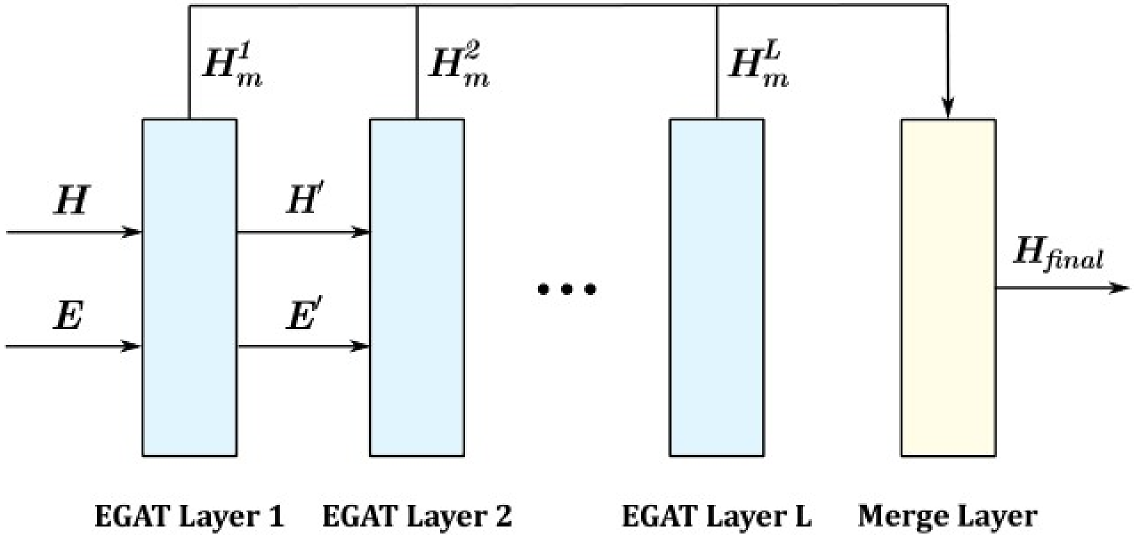


图 3–8 EGAT 融合层及与其相关的输入输出实例

稀疏矩阵表示

- 邻接矩阵 & 映射矩阵
  - 维度大小 ~ 图规模关系的非线性
  - 内存与显存的局限性 & 计算的复杂性
- 稀疏矩阵表示
  - 空元素数量 >> 非空元素数量
  - 高维映射矩阵的初次压缩

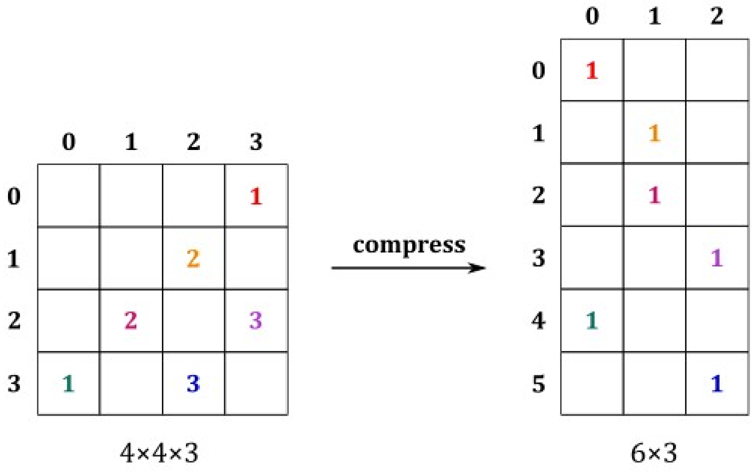


图 4–2 映射矩阵维度压缩示意图

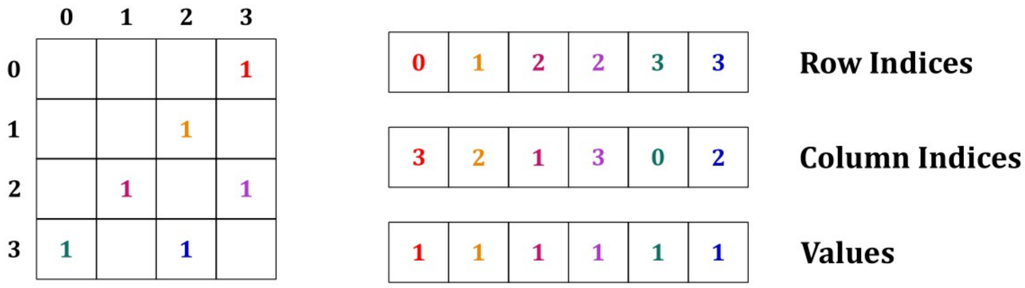
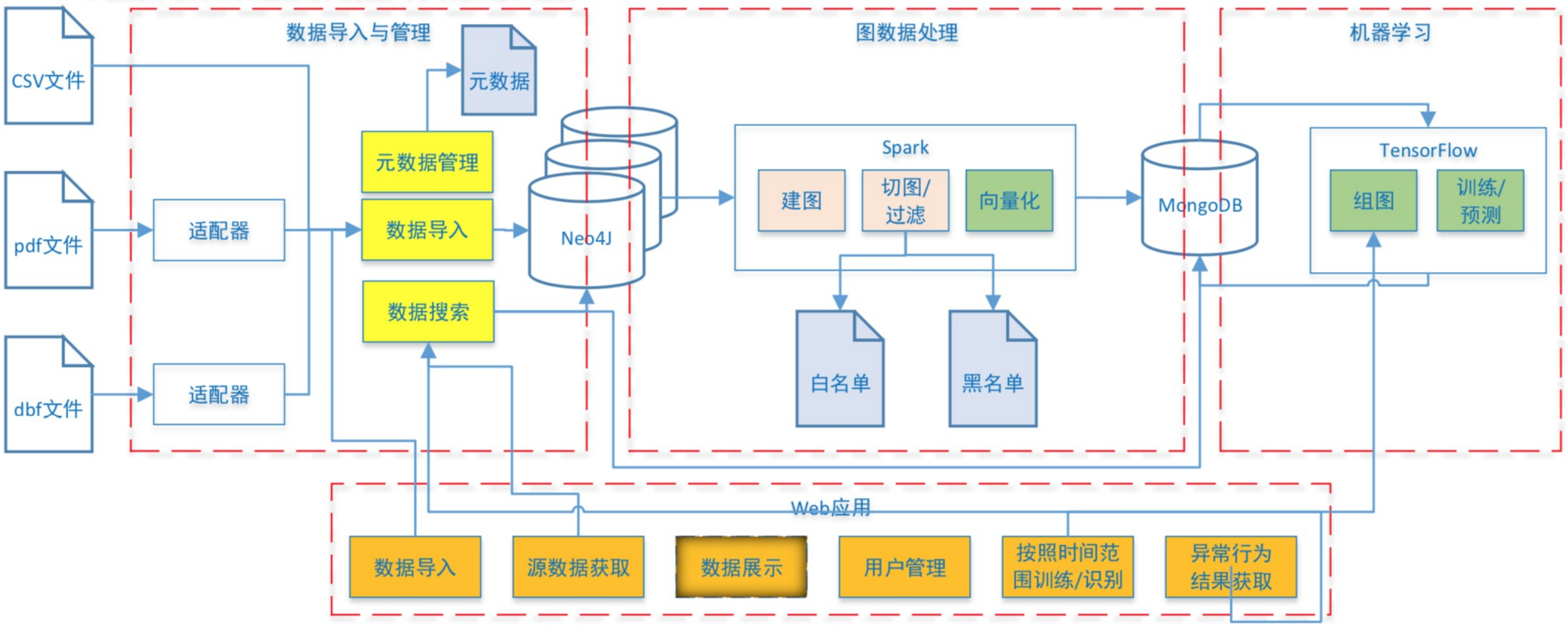


图 4–1 COO 格式下稀疏矩阵表示形式举例

总体流程与架构设计

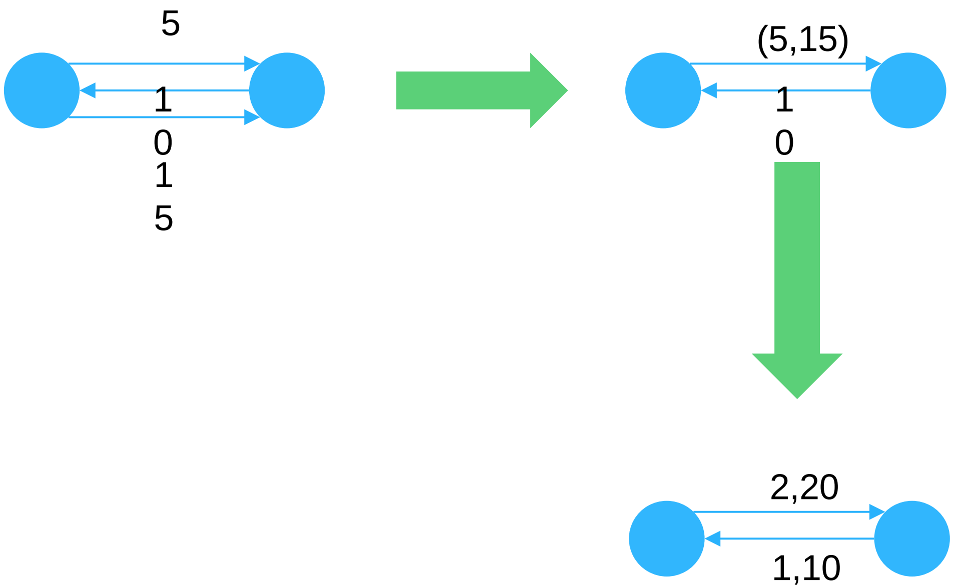
REliable, INtelligent & Scalable Systems

- 根据实体关联数据构建图 -> 根据样例学习图中的模式 -> 发现符合预期模式的数据，进行预警



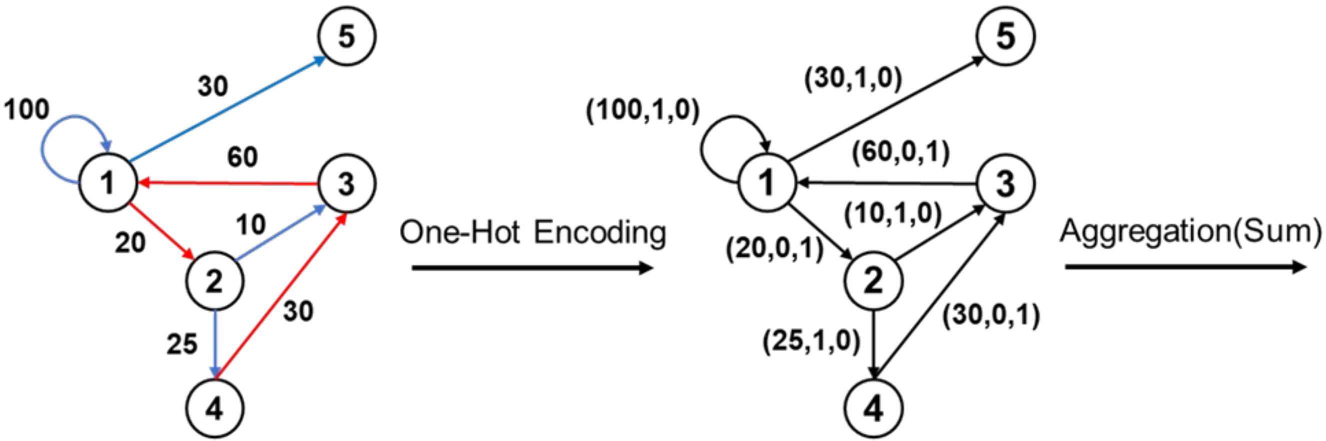
边属性合并

- Multi-Graph 多边合并



边属性合并

- 边属性 -> 节点属性



	In	Out	Self-loop
1	(60,0,1)	(50,1,1)	(100,1,0)
2	(20,0,1)	(35,2,0)	(0,0,0)
3	(40,1,1)	(60,0,1)	(0,0,0)
4	(25,1,0)	(30,0,1)	(0,0,0)
5	(30,1,0)	(0,0,0)	(0,0,0)

图向量化

- Graph -> Vector

```
data = {
  time: 2019-01,
  type: train,
  data:
  [
     {
       id: 1,
       label: 1,
       neighbors: [{
           id: 1,
           attr: {
               layer: 0,
               origin: [1.0, 1.0],
               summable: [1.0, 2.0]
           },
           …
       }]
     },
     …
  ]
}
```

时间

数据类型

数据

中心节点ID

中心节点标签

邻居节点

邻居节点ID

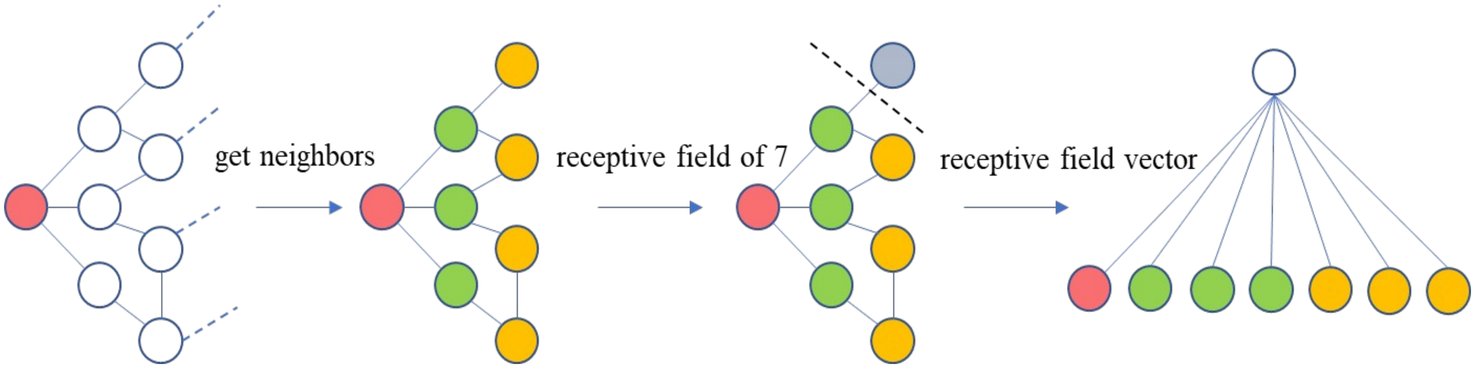
距中心节点距离

邻居节点原始属性

邻居节点可加属性（边合并属性）

图向量化

- GraphX (Pregel 迭代计算)
- 设置传播层数上限
- 固定的邻居数量（ Fixed-Size)
- 结果存储到 MongoDB 中 （ Hiding Processing Latency ）



References

- Graph Databases: NEW OPPORTUNITIES FOR CONNECTED DATA
  - http://graphdatabases.com/?ref=blog&_ga=2.114598147.542116335.1524369358-1583480045.1524187154

- Neo4j 图数据库简介和底层原理
  - https://blog.csdn.net/bluejoe2000/article/details/72978478
- Neo4j install
  - https://neo4j.com/download-thanks/?edition=community&release=4.3.3&flavour=unix
- Accessing Data with Neo4j
  - https://spring.io/guides/gs/accessing-data-neo4j/

Thank You!