

Large Scale Graph Processing

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Ανάλυση και Επεξεργασία Δεδομένων

ΠΜΣ Ερευνητικές Κατευθύνσεις στην
Πληροφορική

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Molina



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Overview

1) Graphs

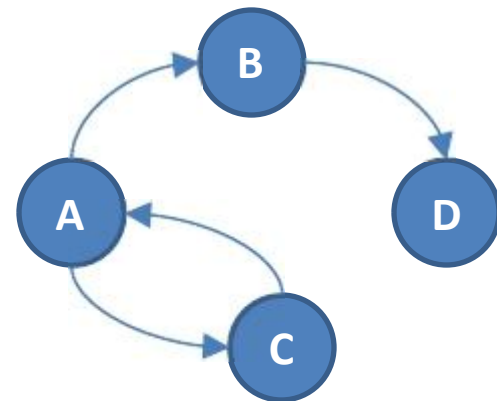
- 2) Graph processing with Hadoop/MapReduce
- 3) Google Pregel

Graphs

graph: abstract representation of a set of objects (**vertices**), where some pairs of these objects are connected by links (**edges**), which can be directed or undirected

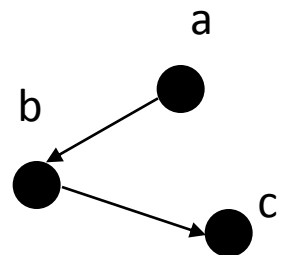
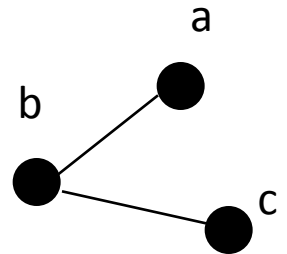
Graphs can be used to model arbitrary things like road networks, social networks, flows of goods, etc.

Majority of graph algorithms are iterative and traverse the graph in some way



What is a graph

- Formally: A finite graph $G(V, E)$ is a pair (V, E) , where V is a finite set and E is a *binary relation* on V .
 - Recall: A *relation* R between two sets X and Y is a subset of $X \times Y$.
 - For each selection of two distinct V 's, that pair of V 's is either in set E or not in set E .
- The elements of the set V are called *vertices* (or *nodes*) and those of set E are called *edges*.
- **Undirected graph:** The edges are unordered pairs of V (i.e. the binary relation is symmetric).
 - Ex: undirected $G(V, E)$; $V = \{a, b, c\}$, $E = \{\{a, b\}, \{b, c\}\}$
- **Directed graph** (digraph): The edges are ordered pairs of V (i.e. the binary relation is not necessarily symmetric).
 - Ex: digraph $G(V, E)$; $V = \{a, b, c\}$, $E = \{(a, b), (b, c)\}$

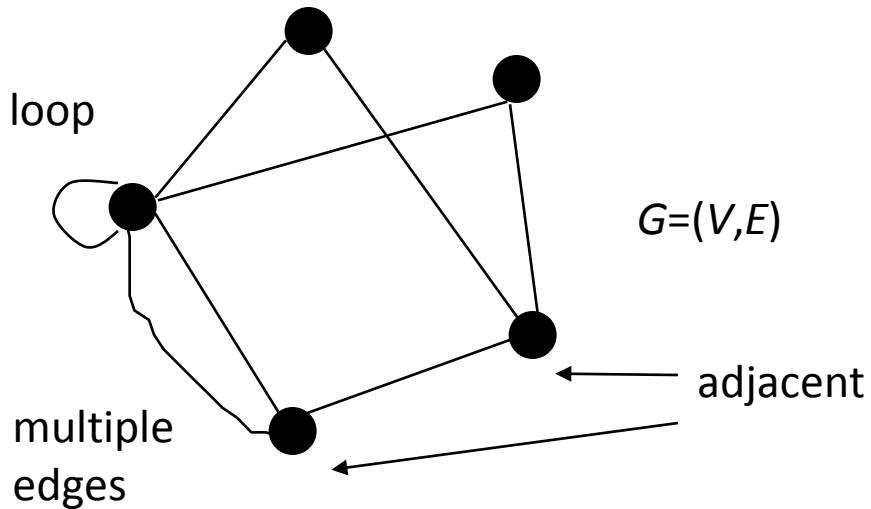


Why graphs?

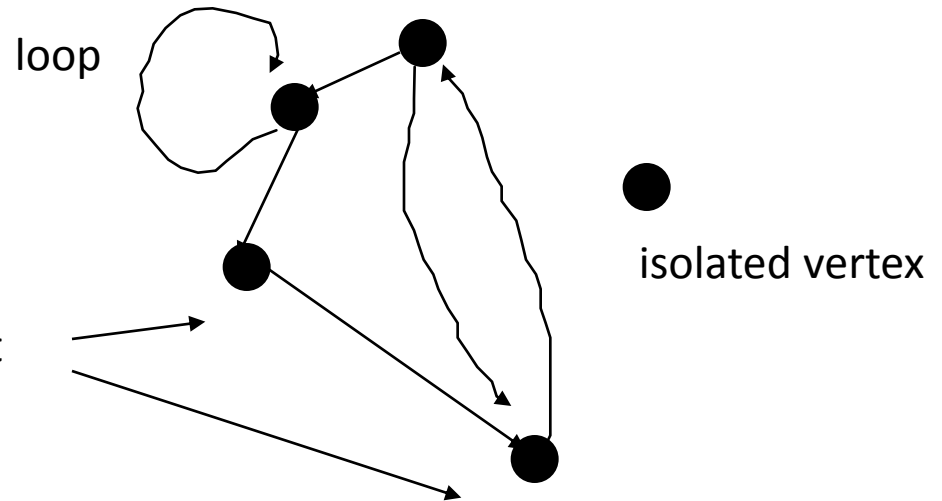
- Many problems can be stated in terms of a graph
- The properties of graphs are well-studied
 - Many algorithms exist to solve problems posed as graphs
 - Many problems are already known to be intractable
- By *reducing* an instance of a problem to a standard graph problem, we may be able to use well-known graph algorithms to provide an optimal solution
- Graphs are excellent structures for storing, searching, and retrieving large amounts of data
 - Graph theoretic techniques play an important role in increasing the storage/search efficiency of computational techniques.

Basic definitions

Undirected graph



Directed graph

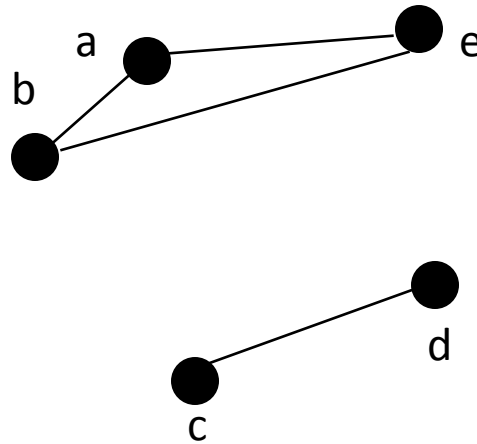
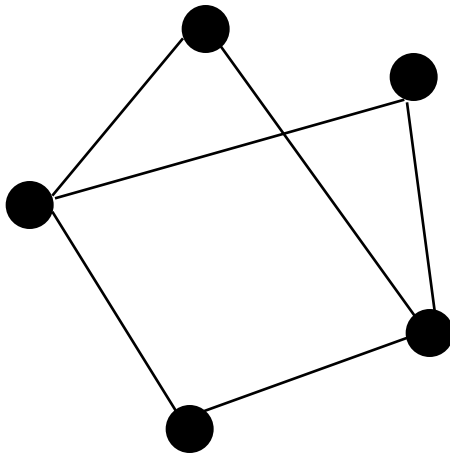


- **incidence**: an edge (directed or undirected) is incident to a vertex that is one of its end points.
- **degree** of a vertex: number of edges incident to it
 - Nodes of a digraph can also be said to have an **indegree** and an **outdegree**
- **adjacency**: two vertices connected by an edge are adjacent

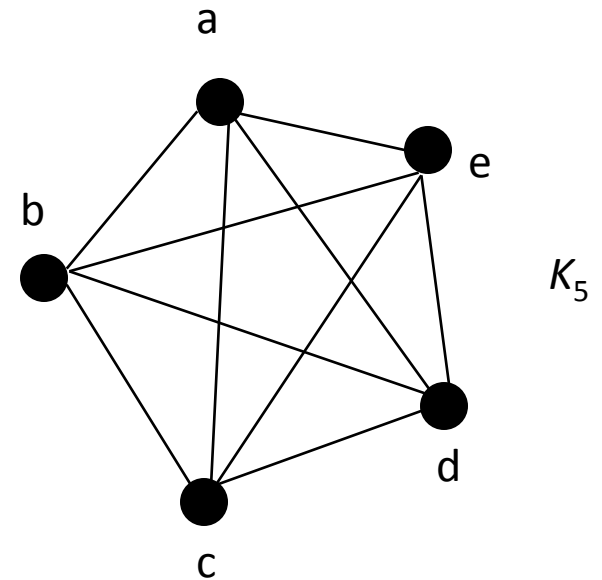
Types of graphs

- **simple graph:** an undirected graph with no loops or multiple edges between the same two vertices
- **multi-graph:** any graph that is not simple
- **connected graph:** all vertex pairs are joined by a path
- **disconnected graph:** at least one vertex pairs is not joined by a path
- **complete graph:** all vertex pairs are adjacent
 - K_n : the completely connected graph with n vertices

Simple graph

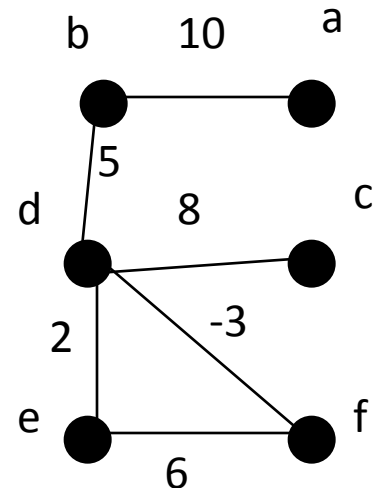
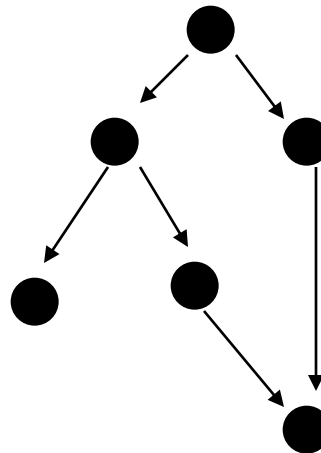
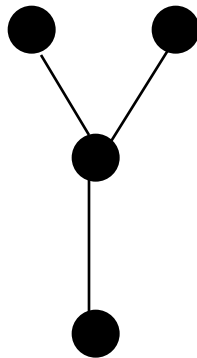
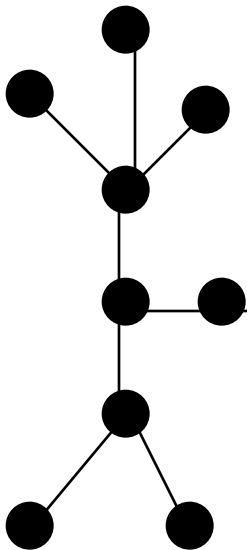


Disconnected graph
with two components



Types of graphs (2)

- **acyclic graph** (forest): a graph with no cycles
- **tree**: a connected, acyclic graph
- **rooted tree**: a tree with a “root” or “distinguished” vertex
 - **leaves**: the terminal nodes of a rooted tree
- **directed acyclic graph** (DAG): a digraph with no cycles
- **weighted graph**: any graph with weights associated with the edges (edge-weighted) and/or the vertices (vertex-weighted)



“Travel” in graphs



path: no vertex can be repeated

example path: a-b-c-d-e

trail: no edge can be repeated

example trail: a-b-c-d-e-b-d

walk: no restriction

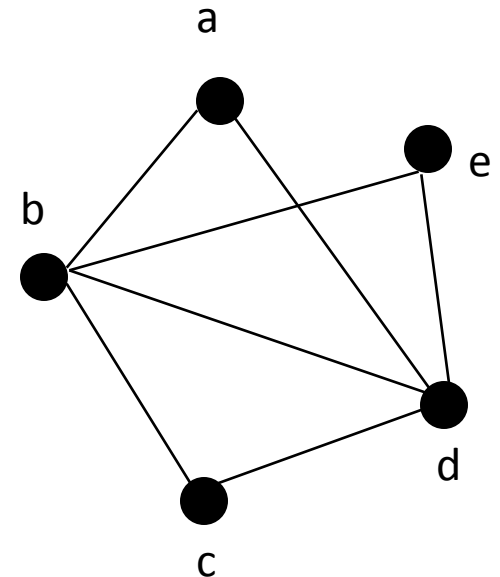
example walk: a-b-d-a-b-c

closed: if starting vertex is also ending vertex

length: number of edges in the path, trail, or walk

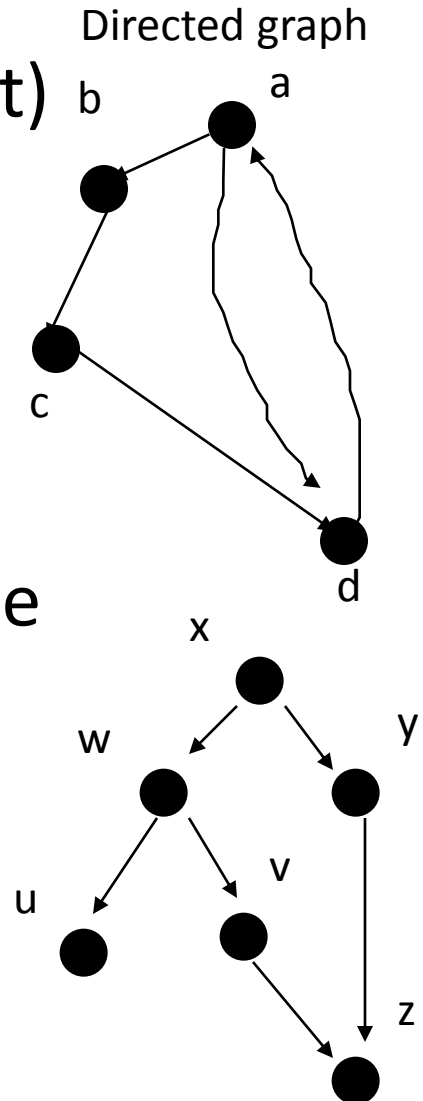
circuit: a closed trail (ex: a-b-c-d-b-e-d-a)

cycle: closed path (ex: a-b-c-d-a)



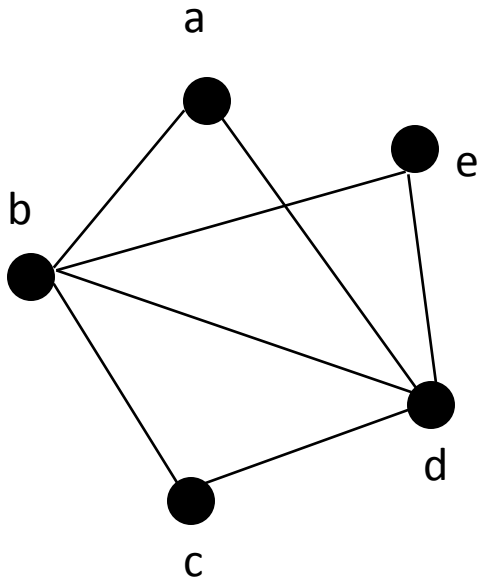
Digraph definitions

- **for digraphs only...**
- Every edge has a **head** (starting point) and a **tail** (ending point)
- Walks, trails, and paths can only use edges in the appropriate direction
- In a DAG, every path connects an **predecessor/ancestor** (the vertex at the head of the path) to its **successor/descendants** (nodes at the tail of any path).
- **parent:** direct ancestor (one hop)
- **child:** direct descendent (one hop)
- A descendent vertex is **reachable** from any of its ancestors vertices

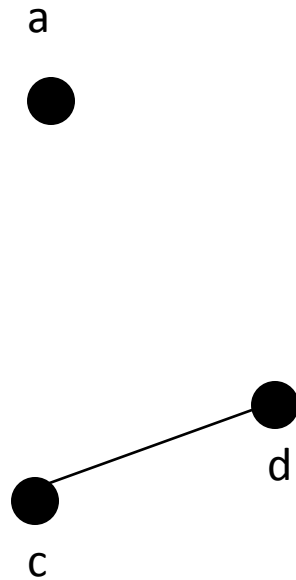


Subgraphs

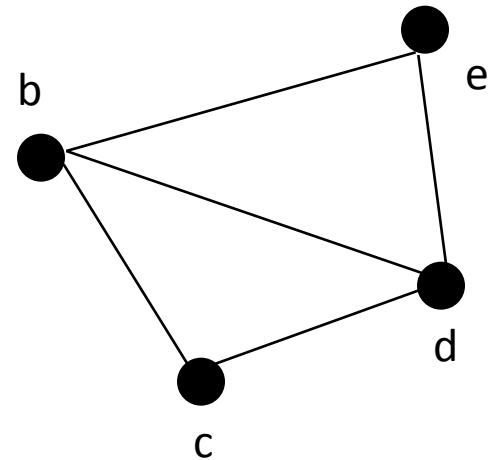
- $G'(V',E')$ is a **subgraph** of $G(V,E)$ if $V' \subseteq V$ and $E' \subseteq E$.
- **induced subgraph**: a subgraph that contains all possible edges in E that have end points of the vertices of the selected V'



$G(V,E)$



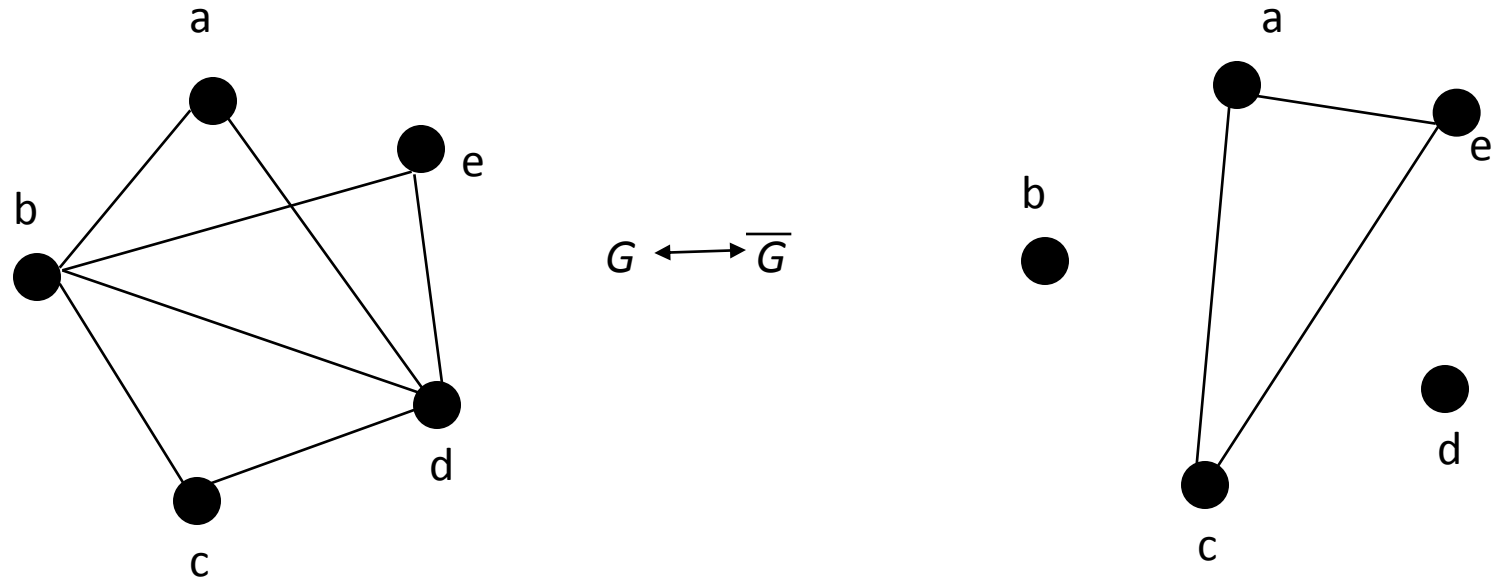
$G'(\{a,c,d\},\{\{c,d\}\})$



Induced subgraph of
 G with $V' = \{b,c,d,e\}$

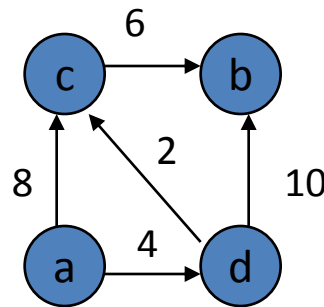
Complement of a graph

- The **complement** of a graph $G(V,E)$ is a graph with the same vertex set, but with vertices adjacent only if they were not adjacent in $G(V,E)$



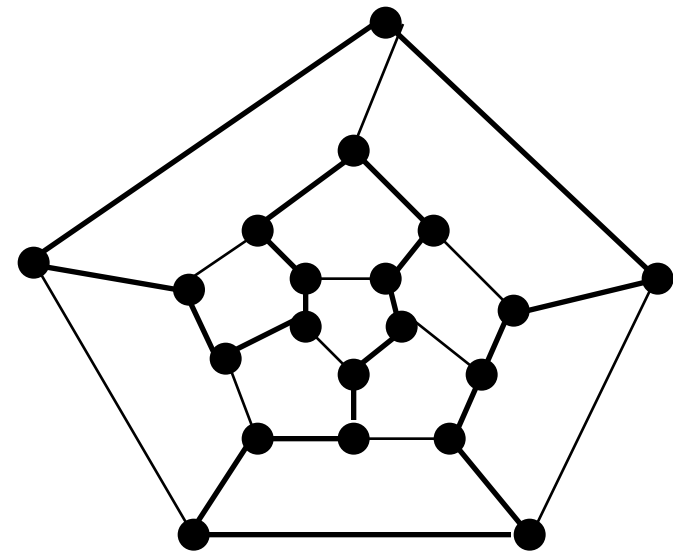
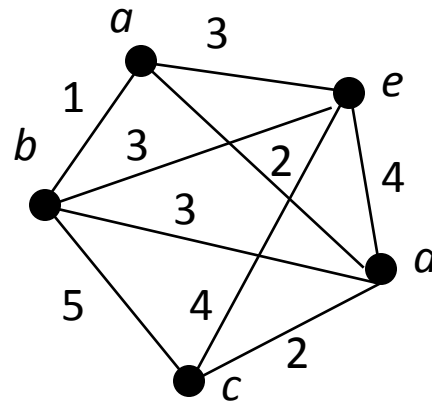
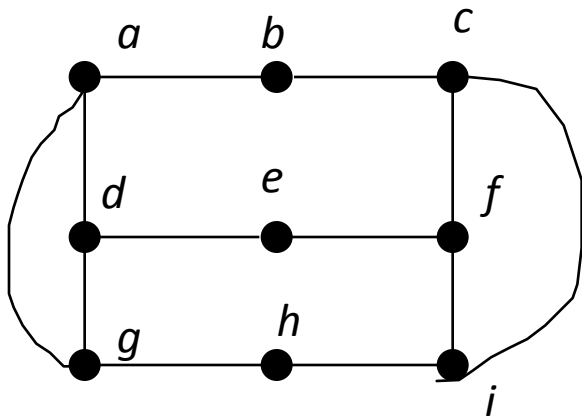
Famous problems: Shortest path

- Consider a weighted connected directed graph with a distinguished vertex
 - source:** a distinguished vertex with zero in-degree
- What is the path of total minimum weight from the source to any other vertex?
- Greedy strategy works for simple problems (no cycles, no negative weights)
- Longest path is a similar problem (complement weights)



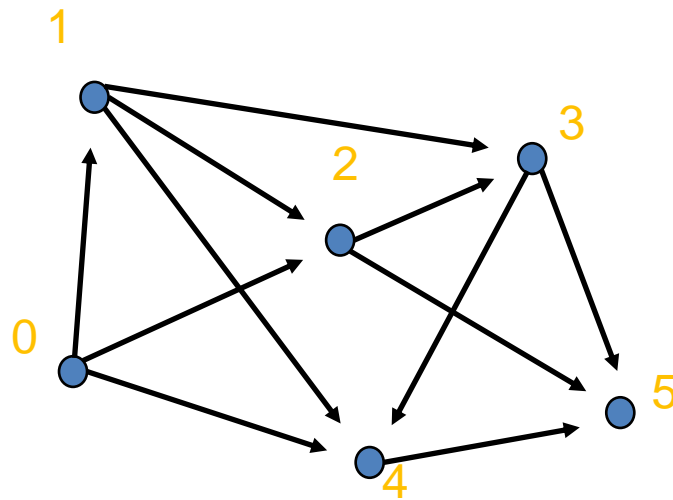
Famous problems: Hamilton & TSP

- **Hamiltonian path:** a path through a graph which contains every vertex exactly once
- Finding a Hamiltonian path is another NP-complete problem...
- **Traveling Salesmen Problem (TSP):** find a Hamiltonian path of minimum cost



Topological Sort

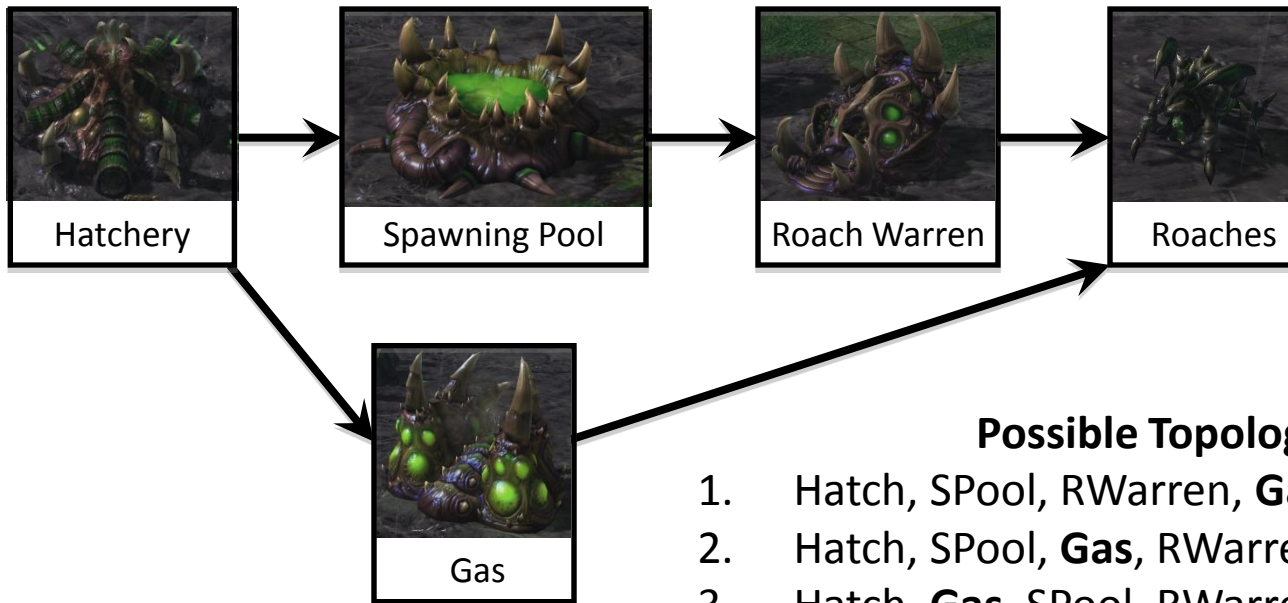
- We just computed a **topological sort** of the dag
 - This is a numbering of the vertices such that all edges go from lower- to higher-numbered vertices



- Useful in job scheduling with precedence constraints

Example of Topological Sort

- Starcraft II build order: Roach Rush



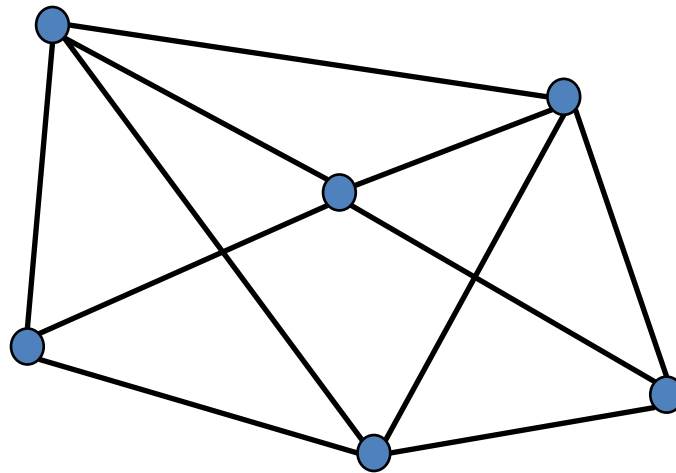
Possible Topological Sorts

1. Hatch, SPool, RWarren, **Gas**, Roaches
2. Hatch, SPool, **Gas**, RWarren, Roaches
3. Hatch, **Gas**, SPool, RWarren, Roaches



Graph Coloring

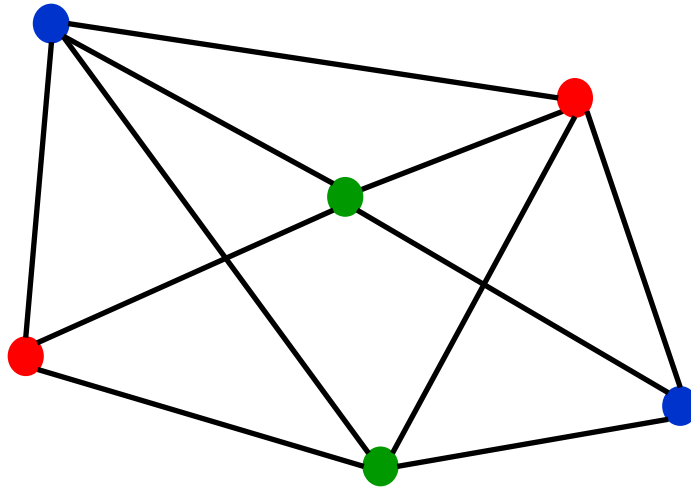
- A **coloring** of an undirected graph is an assignment of a color to each node such that no two adjacent vertices get the same color



- **chromatic number:** the smallest number of labels for a coloring of a graph
- How many colors are needed to color this graph?

Graph Coloring

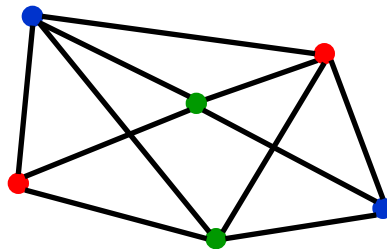
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- How many colors are needed to color this graph?

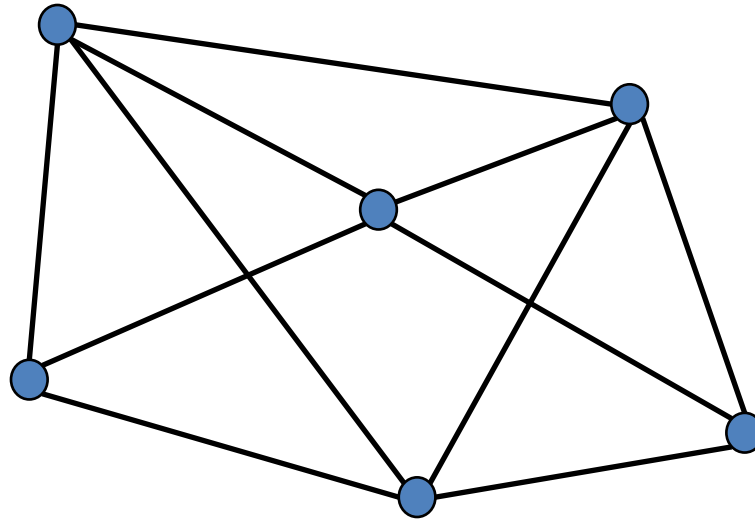
An Application of Coloring

- Vertices are jobs
- Edge (u,v) is present if jobs u and v each require access to the same shared resource, and thus cannot execute simultaneously
- Colors are time slots to schedule the jobs
- Minimum number of colors needed to color the graph = minimum number of time slots required



Planarity

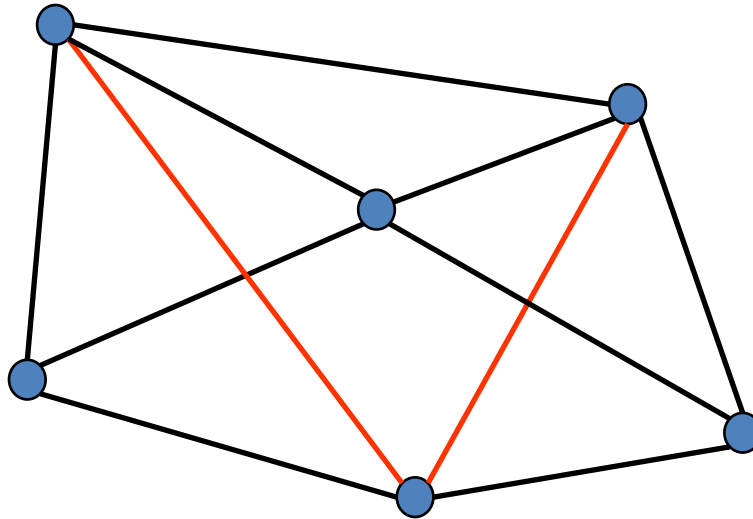
- A graph is **planar** if it can be embedded in the plane with no edges crossing



- Is this graph planar?

Planarity

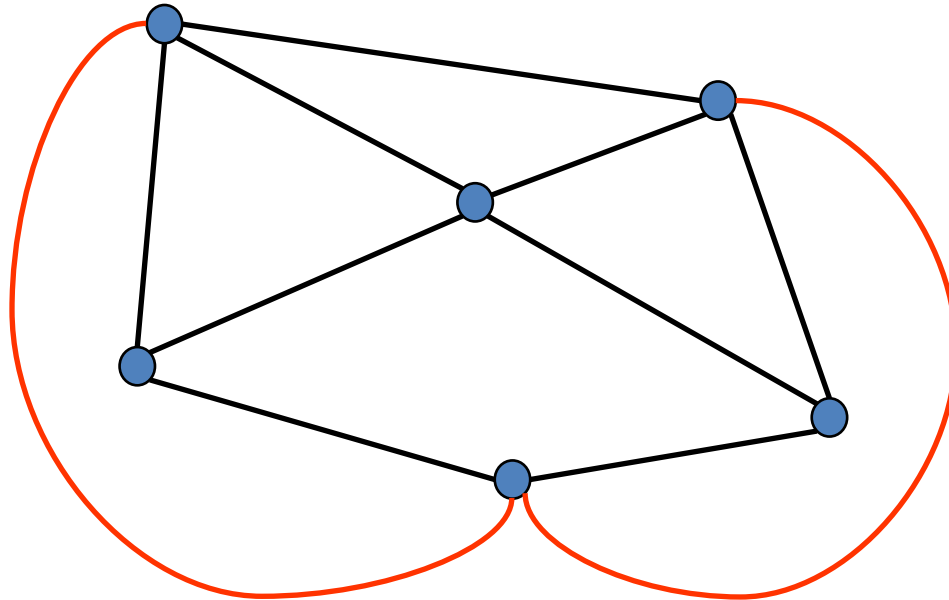
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 - Yes

Planarity

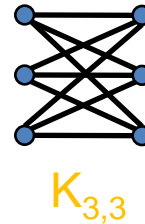
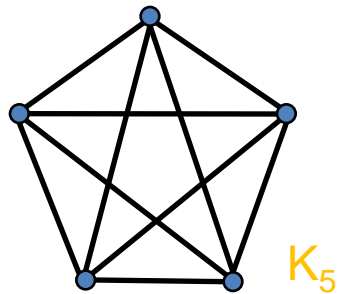
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- Is this graph planar?
 - Yes

Detecting Planarity

- Kuratowski's Theorem



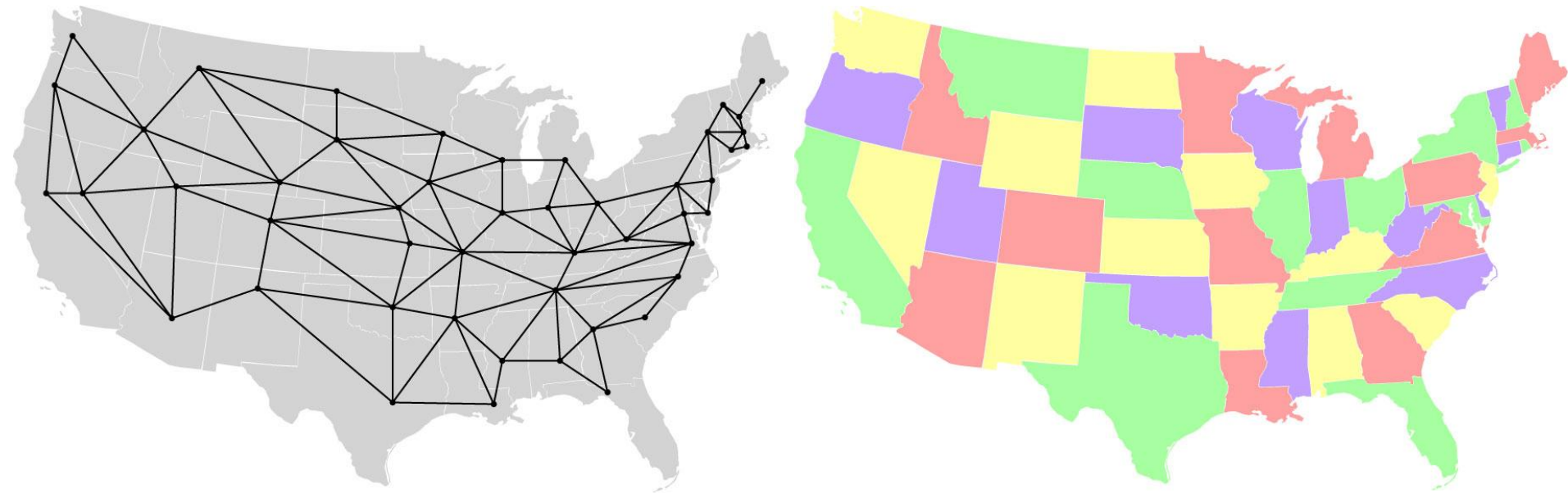
- A graph is planar if and only if it does not contain a copy of K_5 or $K_{3,3}$ (possibly with other nodes along the edges shown)

Four-Color Theorem: Every planar graph is 4-colorable.

(Appel & Haken, 1976)



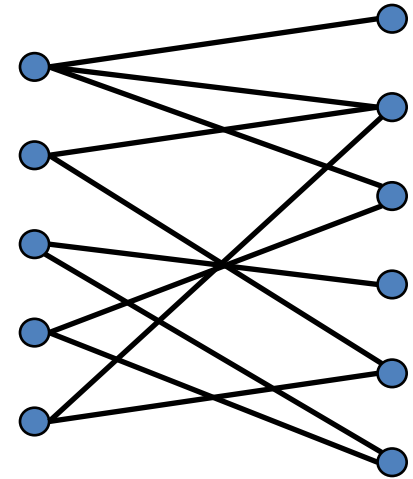
Another 4-colored planar graph



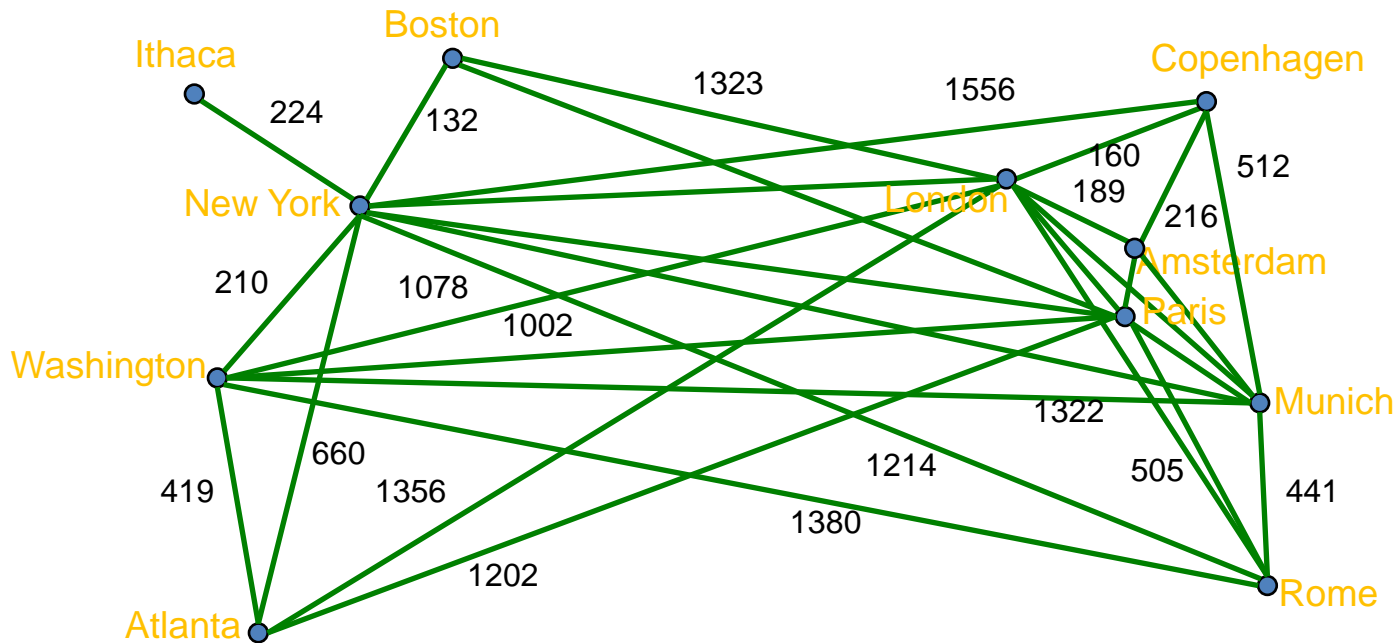
<http://www.cs.cmu.edu/~bryant/boolean/maps.html>

Bipartite Graphs

- A directed or undirected graph is **bipartite** if the vertices can be partitioned into two sets such that all edges go between the two sets
- The following are equivalent
 - G is bipartite
 - G is 2-colorable
 - G has no cycles of odd length



Traveling Salesperson



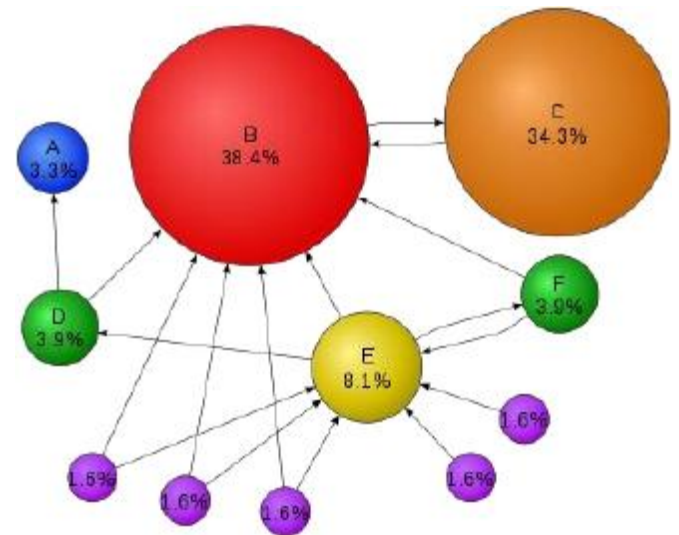
- Find a path of minimum distance that visits every city

The Web

- the World Wide Web itself can be seen as a huge graph, the so called **web graph**
 - **pages are vertices** connected by **edges that represent hyperlinks**
 - the web graph has **several billion vertices** and **several billion edges**
- the success of major internet companies such as Google is based on the ability to conduct computations on this huge graph

Google's PageRank

- success factor of Google's search engine:
 - much **better ranking of search results**
- ranking is based on **PageRank**, a graph algorithm computing the 'importance' of webpages
 - simple idea: **look at the structure of the underlying network**
 - important pages have a lot of links from other important pages
- major technical success factor of Google: ability to conduct **web scale graph processing**



Social Networks

- on facebook, twitter, LinkedIn, etc, the users and their interactions form a **social graph**
 - **users are vertices** connected by **edges that represent some kind of interaction** such as friendship, following, business contact
- fascinating research questions:
 - what is the structure of these graphs?
 - how do they evolve over time?
- analysis requires knowledge in both computer science and social sciences



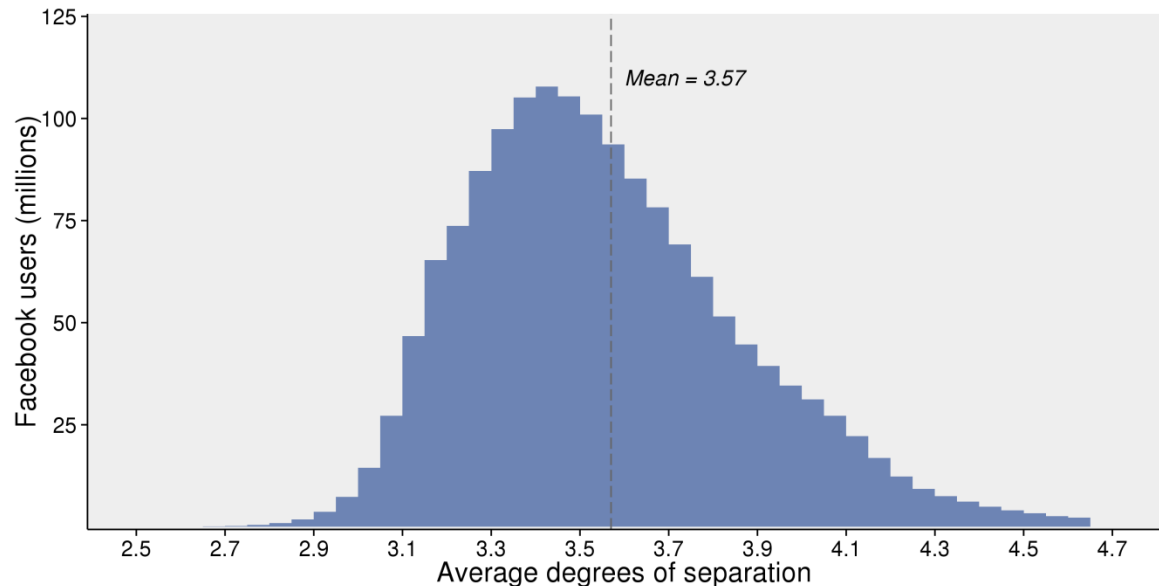
six degrees of separation

- **small world problem**
 - through how many social contacts do people know each other on average?
- **small world experiment** by Stanley Milgram
 - task: deliver a letter to a recipient whom you don't know personally
 - you may forward the letter only to persons that you know on a first-name basis
 - how many contacts does it take on average until the letter reaches the target?
- **results**
 - it took 5.5 to 6 contacts on average
 - confirmation of the popular assumption of **'six degrees of separation'** between humans
 - experiment criticised due to small number of participants, possibly biased selection



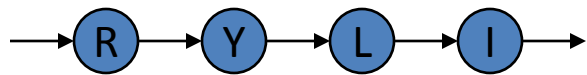
3.5 degrees of separation

- the small world problem as a graph problem in social network analysis
 - **what is the average distance between two users in a social graph?**
- In Feb 2016, a **world scale experiment** using the Facebook social graph
 - 1.6 billion users
 - result: average distance in Facebook is 3.57

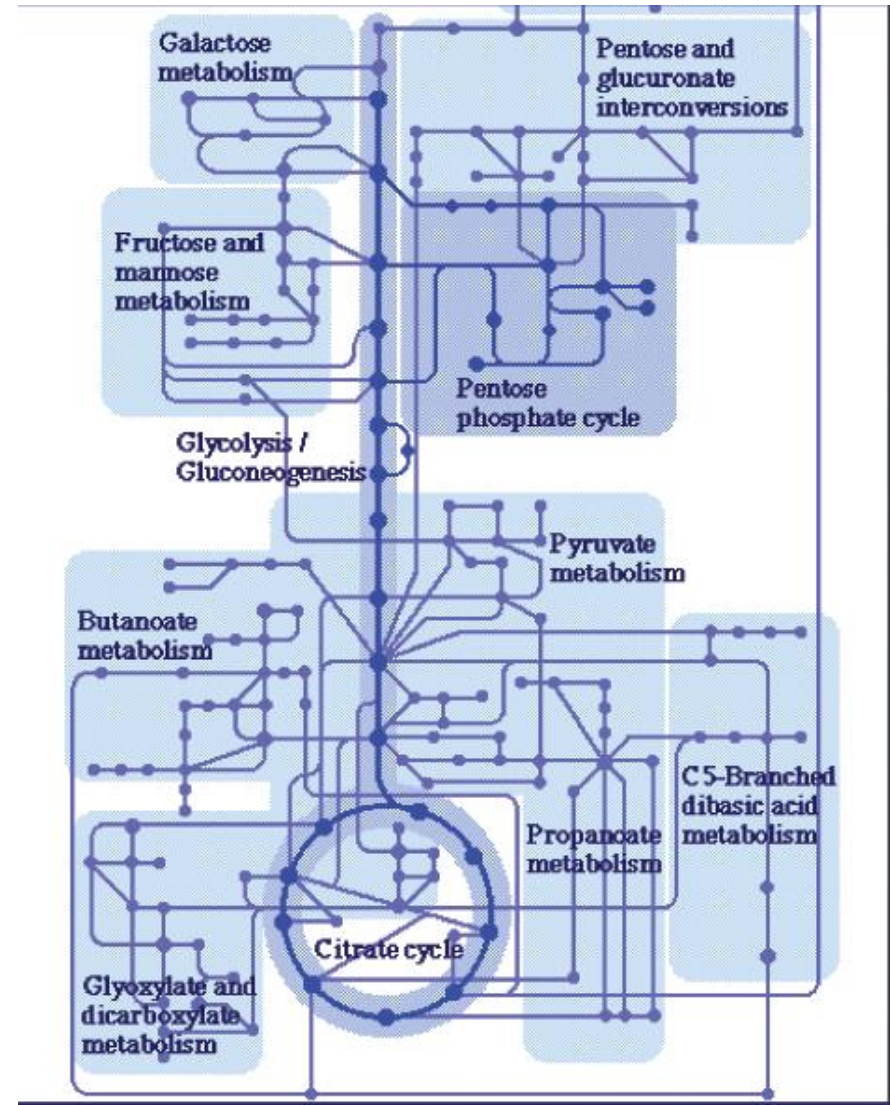
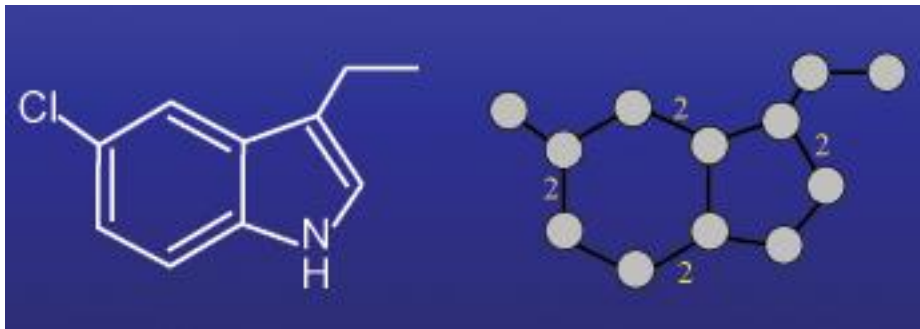


Graphs in bioinformatics

- Sequences
 - DNA, proteins, etc.

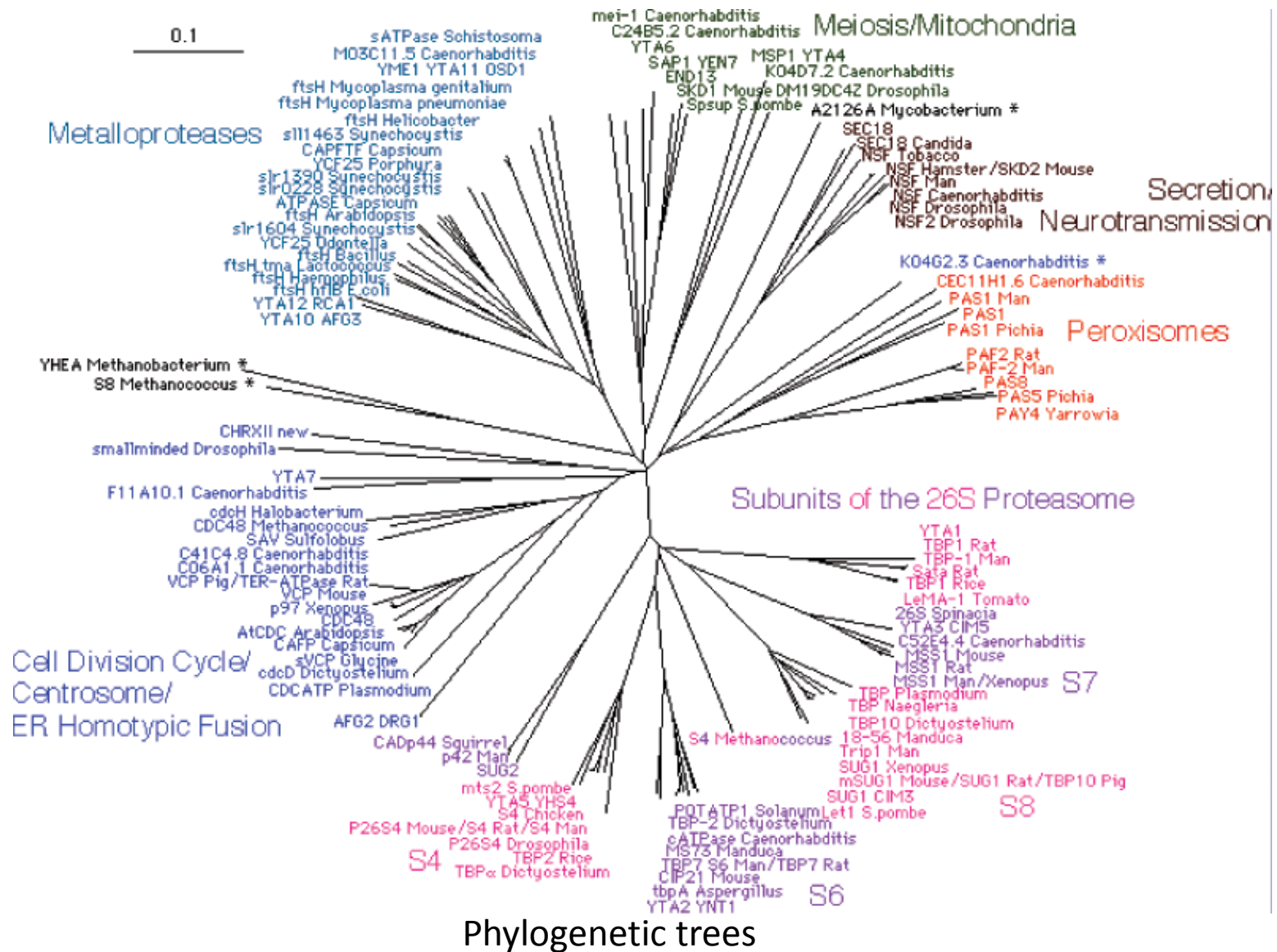


Chemical compounds



Metabolic pathways

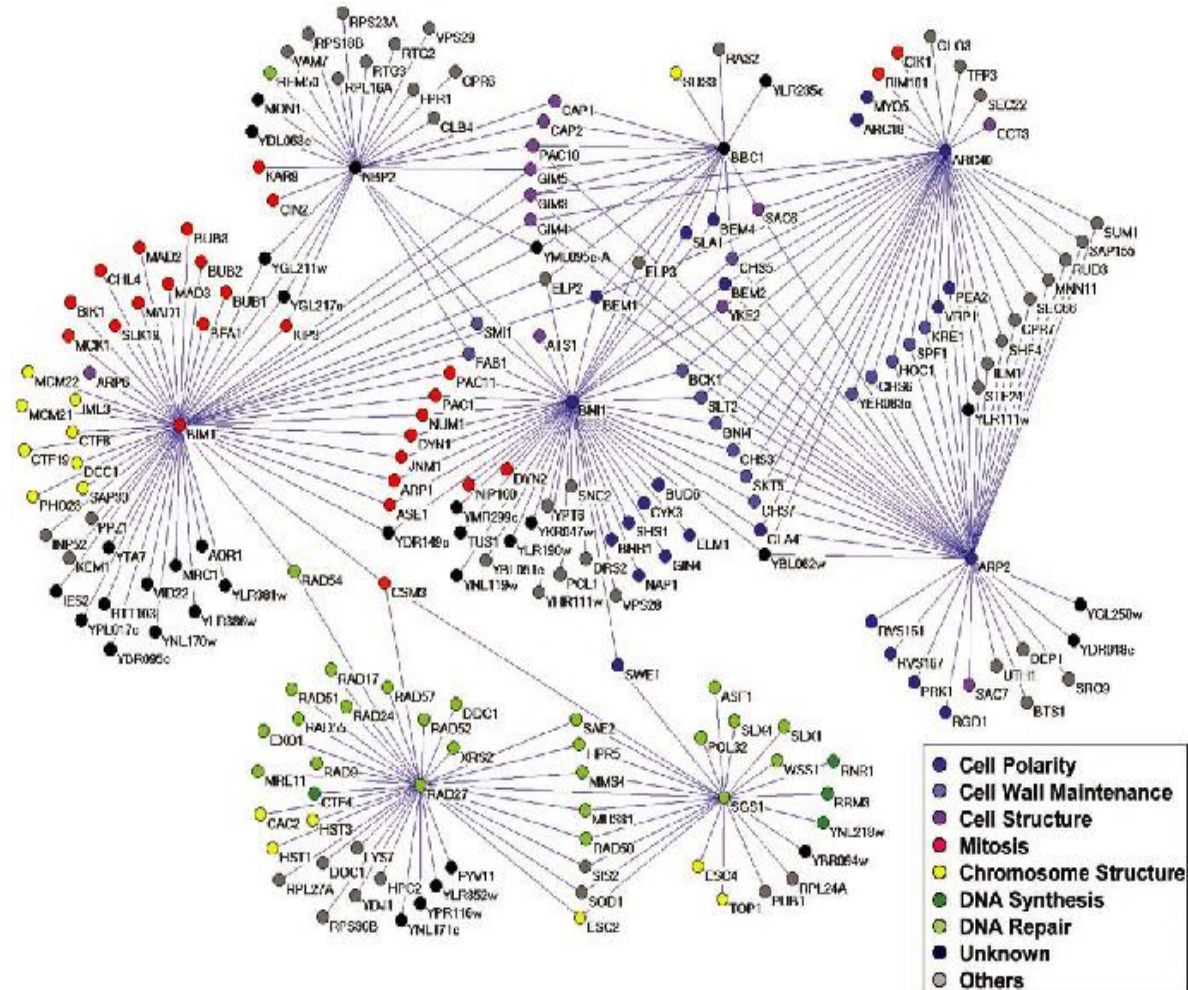
Graphs in bioinformatics



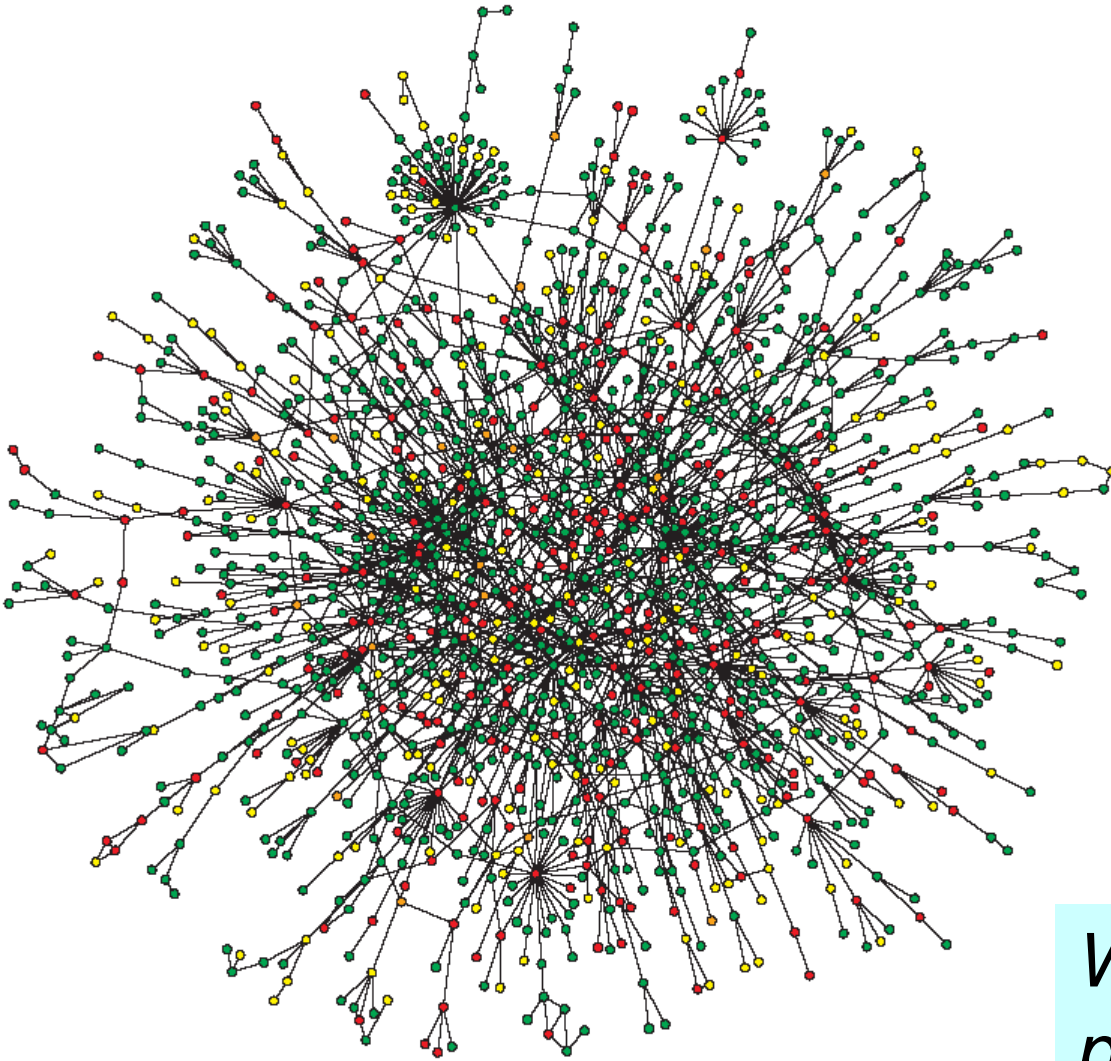
Genetic interactions: synthetic lethals and suppressors

Genetic Interactions:

- Widespread method used by geneticists to discover pathways in yeast, fly, and worm
- Implications for drug targeting and drug development for human disease
- Thousands are now reported in literature and systematic studies
- As with other types, the number of known genetic interactions is *exponentially increasing*...



Yeast protein-protein interaction network



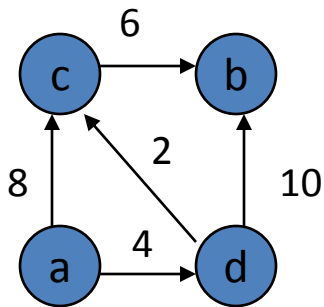
What are its network properties?

Applications of Graphs

- Communication networks; social networks
- Routing and shortest path problems
- Commodity distribution (network flow)
- Traffic control
- Resource allocation
- Numerical linear algebra (sparse matrices)
- Geometric modeling (meshes, topology, ...)
- Image processing (e.g., graph cuts)
- Computer animation (e.g., motion graphs)
- Systems biology
- ...

Computer representation

- **adjacency matrix:** a $|V| \times |V|$ array where each cell i,j contains the weight of the edge between v_i and v_j (or 0 for no edge)
- **adjacency list:** a $|V|$ array where each cell i contains a list of all vertices adjacent to v_i
- **incidence matrix:** a $|V|$ by $|E|$ array where each cell i,j contains a weight (or a defined constant HEAD for unweighted graphs) if the vertex i is the head of edge j or a constant TAIL if vertex i is the tail of edge j



	a	b	c	d
a			8	4
b				
c		6		
d		10	2	

adjacency
matrix

a	c (8), d (4)
b	
c	b (6)
d	c (2), b (10)

adjacency
list

	1	2	3	4	5
a		8			4
b	t			t	
c	6	t	t		
d			2	10	t

incidence
matrix

Overview

- 1) Graphs
- 2) Graph processing with Hadoop/MapReduce**
- 3) Google Pregel

Why not use MapReduce/Hadoop?

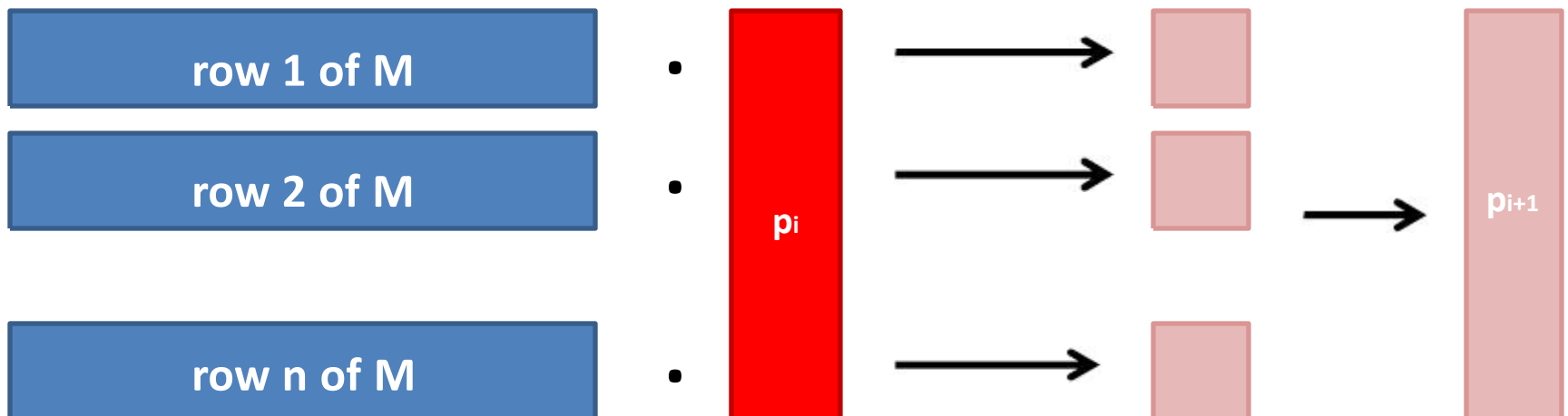
- MapReduce/Hadoop is a popular way to perform data-intensive computing, why not use it for graph processing?
- **Example: PageRank**
 - defined **recursively**
 - each vertex distributes its authority to its neighbors in equal proportions

$$p_i = \sum_{j \in \{(j,i)\}} \frac{p_j}{d_j}$$

Textbook approach to PageRank in MapReduce

- PageRank p is the **principal eigenvector** of the Markov matrix M defined by the **transition probabilities between web pages**
- it can be obtained by iteratively multiplying an initial PageRank vector by M (**power method**)

$$p_{i+1} = Mp_i$$



Drawbacks

- **Not intuitive:** only crazy scientists think in matrices and eigenvectors
- **Unnecessarily slow:** Each iteration is a single MapReduce job with lots of overhead
 - separately scheduled
 - the graph structure is read from disk
 - the intermediary result is written to HDFS
- **Hard to implement:** a join has to be implemented by hand, lots of work, best strategy is data dependent



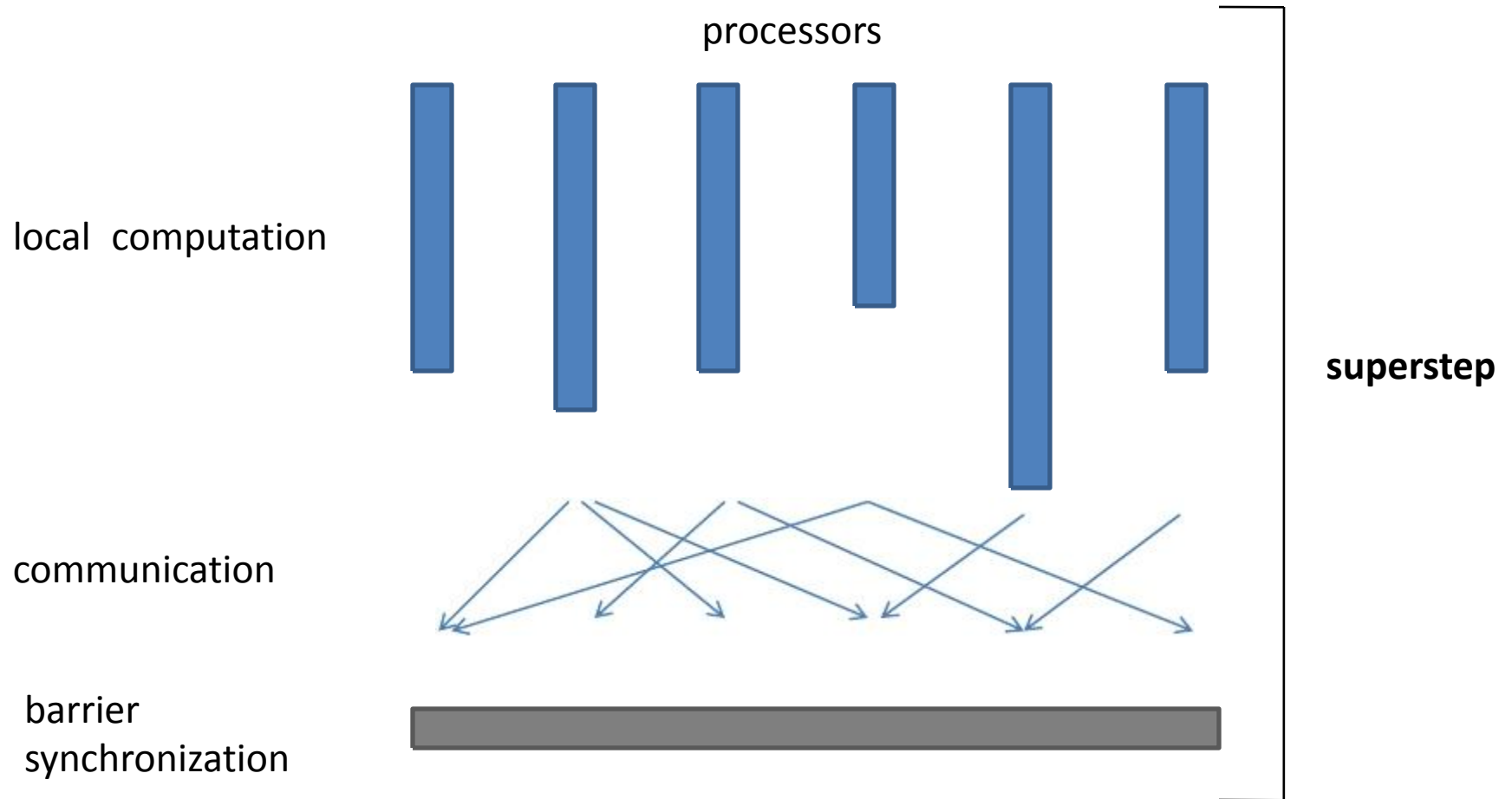
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Google Pregel

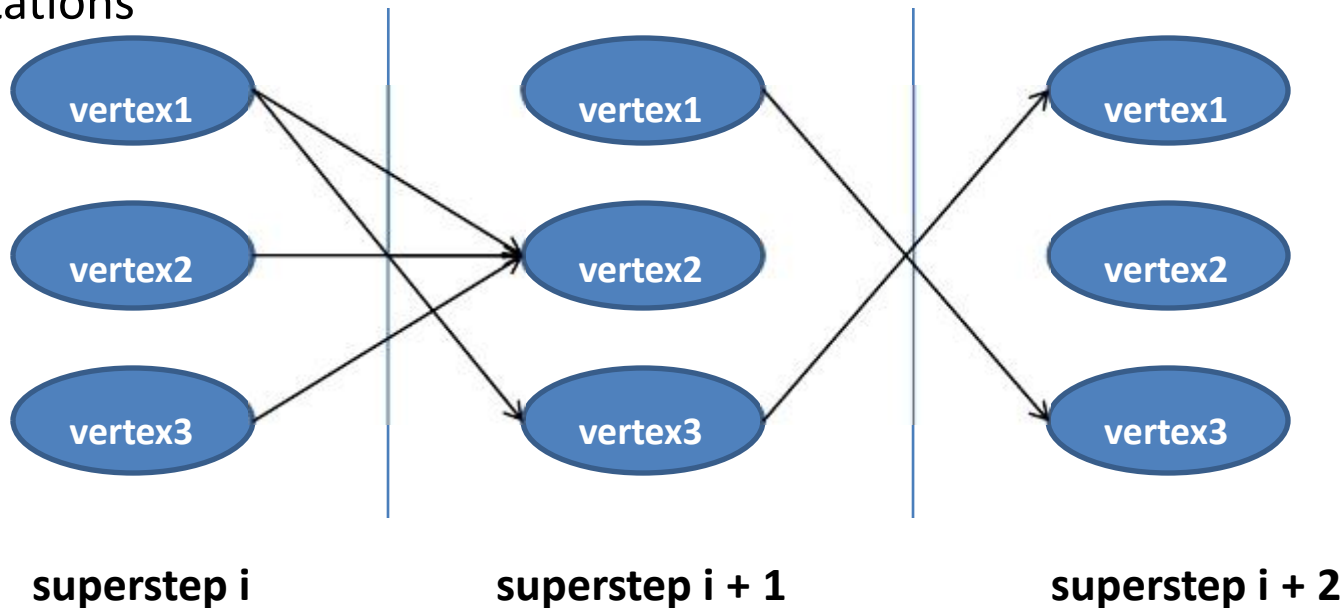
- distributed system especially developed for **large scale graph processing**
- intuitive API that let's you **,think like a vertex'**
- **Bulk Synchronous Parallel (BSP)** as execution model
- fault tolerance by **checkpointing**

Bulk Synchronous Parallel (BSP)

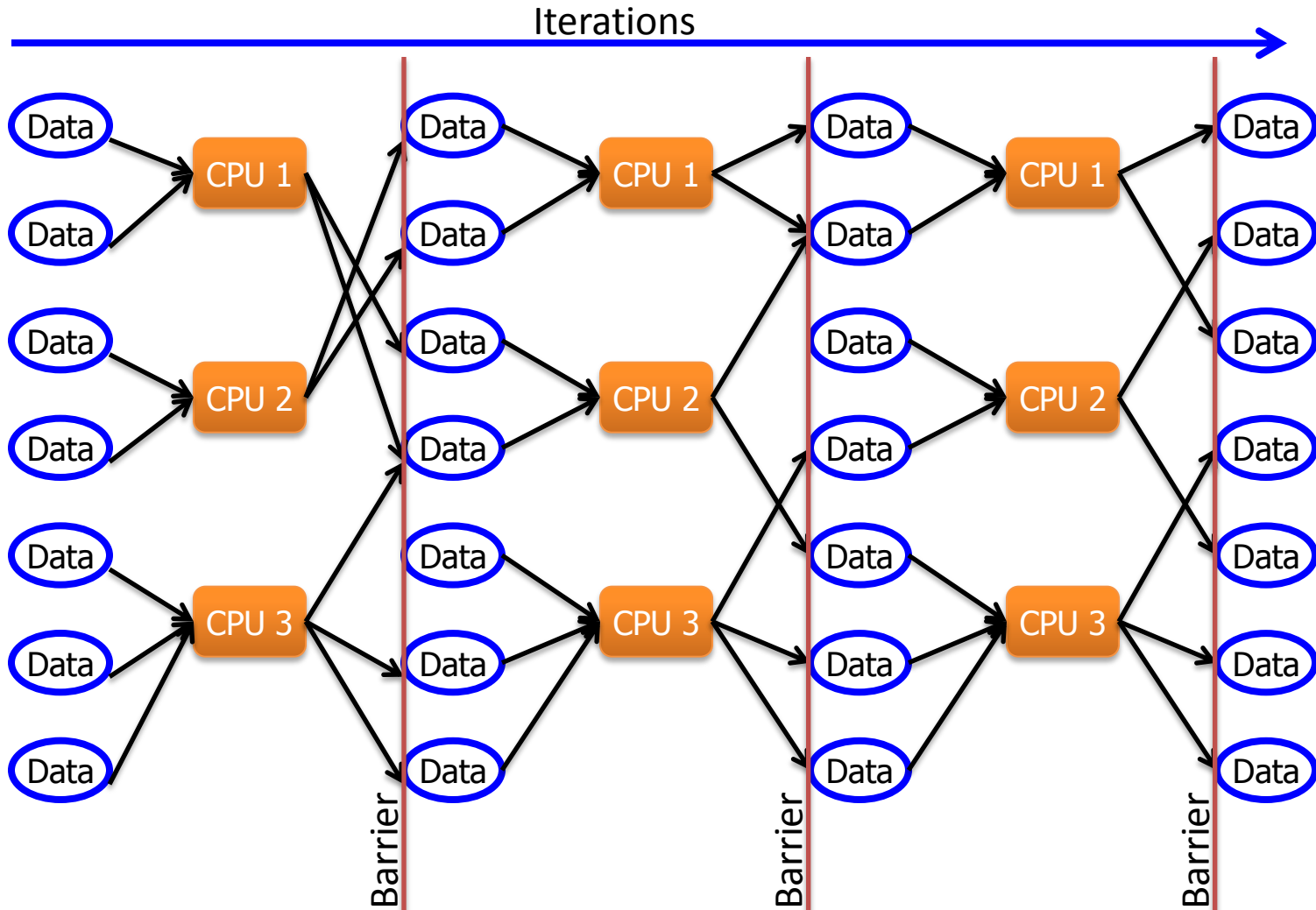


Vertex-centric BSP

- each vertex has an **id**, a **value**, a **list of its adjacent neighbor ids** and the corresponding **edge values**
- each vertex is invoked **in each superstep**, can **recompute its value** and **send messages to other vertices**, which are **delivered over superstep barriers**
- advanced features : **termination votes**, **combiners**, **aggregators**, **topology mutations**

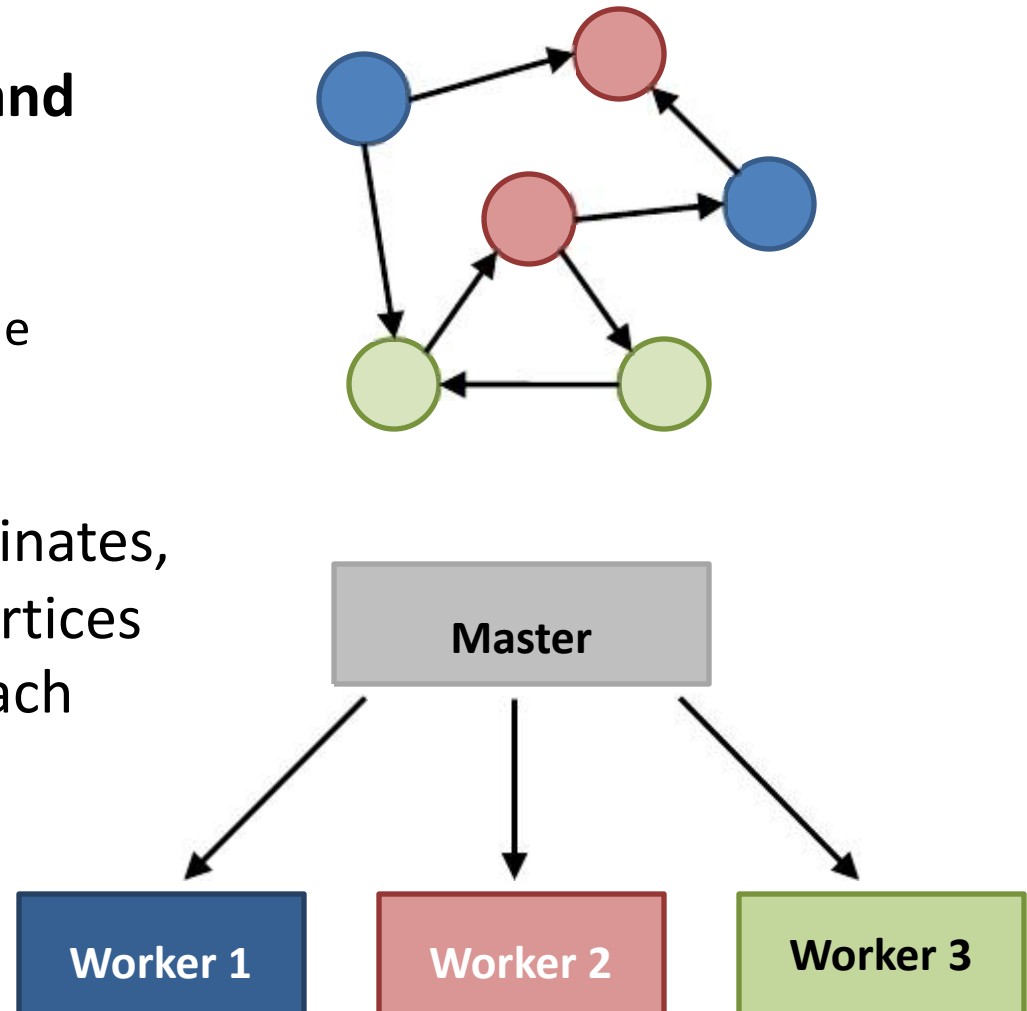


Bulk Synchronous Parallel Model



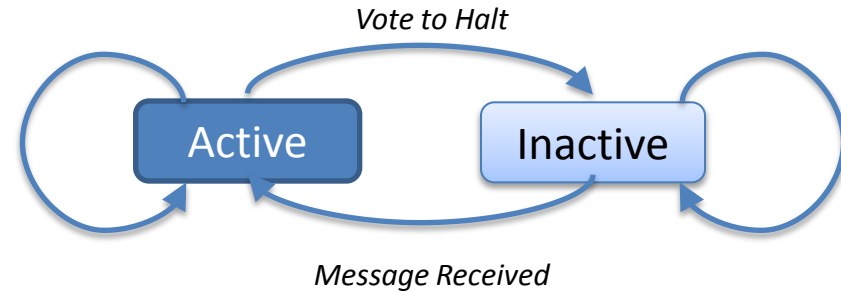
Master-slave architecture

- **vertices are partitioned and assigned to workers**
 - default: hash-partitioning
 - custom partitioning possible
- **master** assigns and coordinates, while **workers** execute vertices and communicate with each other



Algorithm Termination

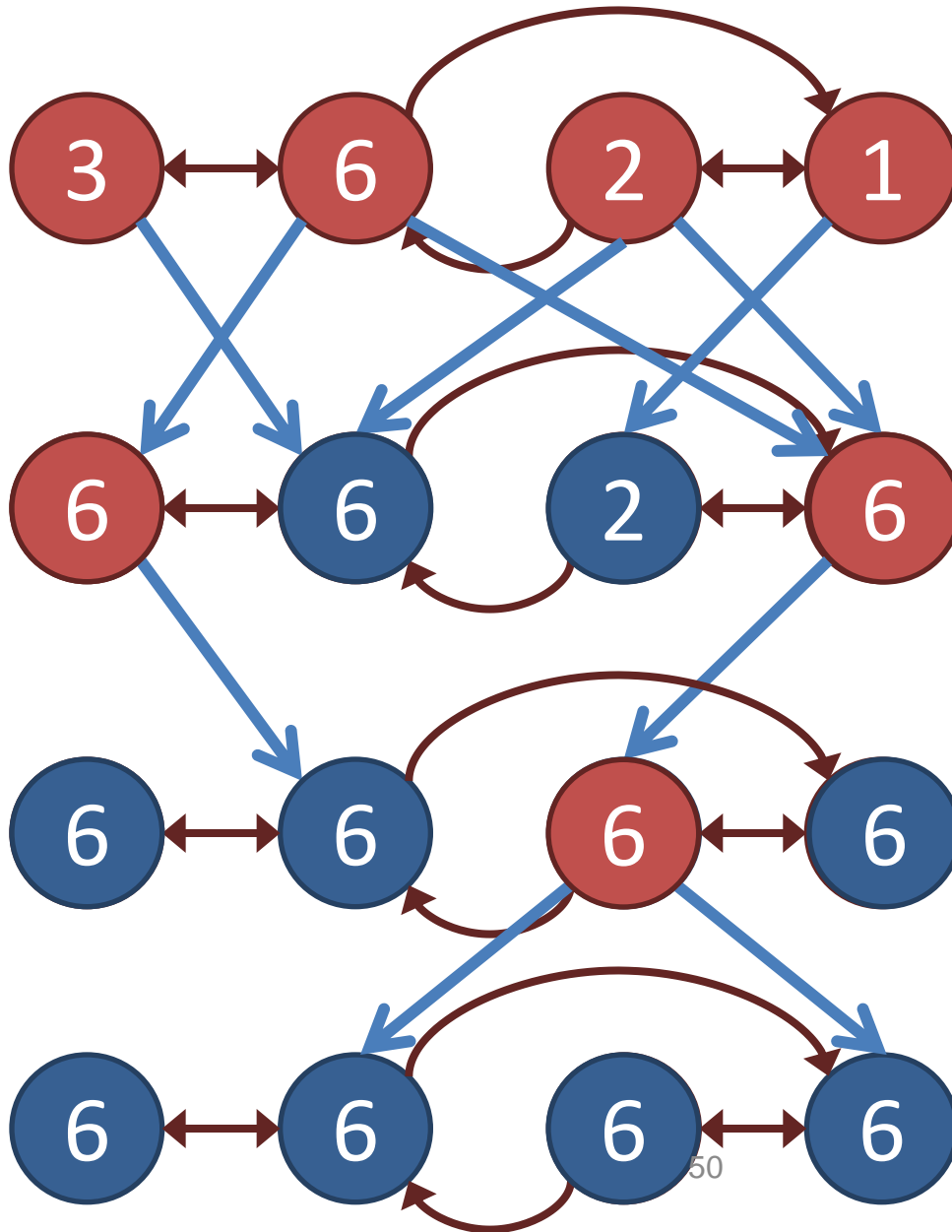
- Algorithm termination is based on every vertex voting to halt
 - In superstep 0, every vertex is active
 - All active vertices participate in the computation of any given superstep
 - A vertex deactivates itself by voting to halt and enters an inactive state
 - A vertex can return to active state if it receives an external message



Vertex State Machine

- Program terminates when all vertices are simultaneously inactive and there are no messages in transit

Finding the Max Value in a Graph

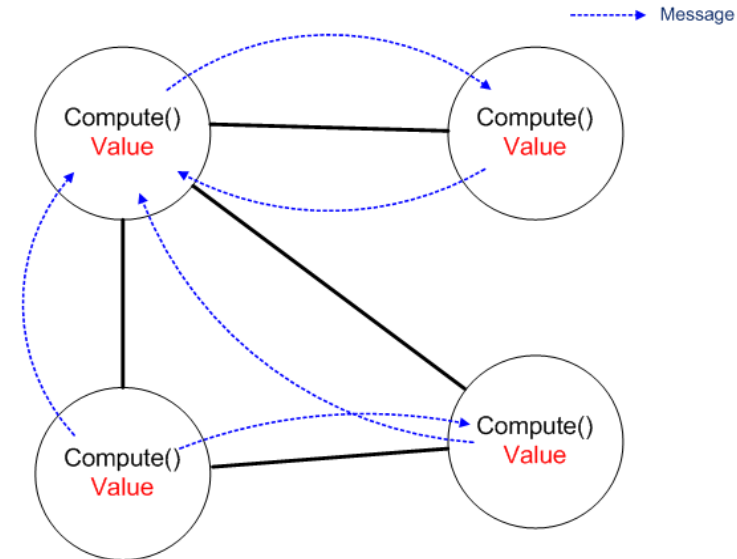


Blue Arrows
are messages

Blue vertices
have voted to
halt

Message Passing, Combiners, and Aggregators

- **Messages** can be passed from any vertex to any other vertex in the Graph
 - Any number of messages may be passed
 - Message order is not guaranteed
 - Messages will not be duplicated
- **Combiners** can be used to reduce the number of messages passed between supersteps
- **Aggregators** are available for reduction operations such as sum, min, max etc.

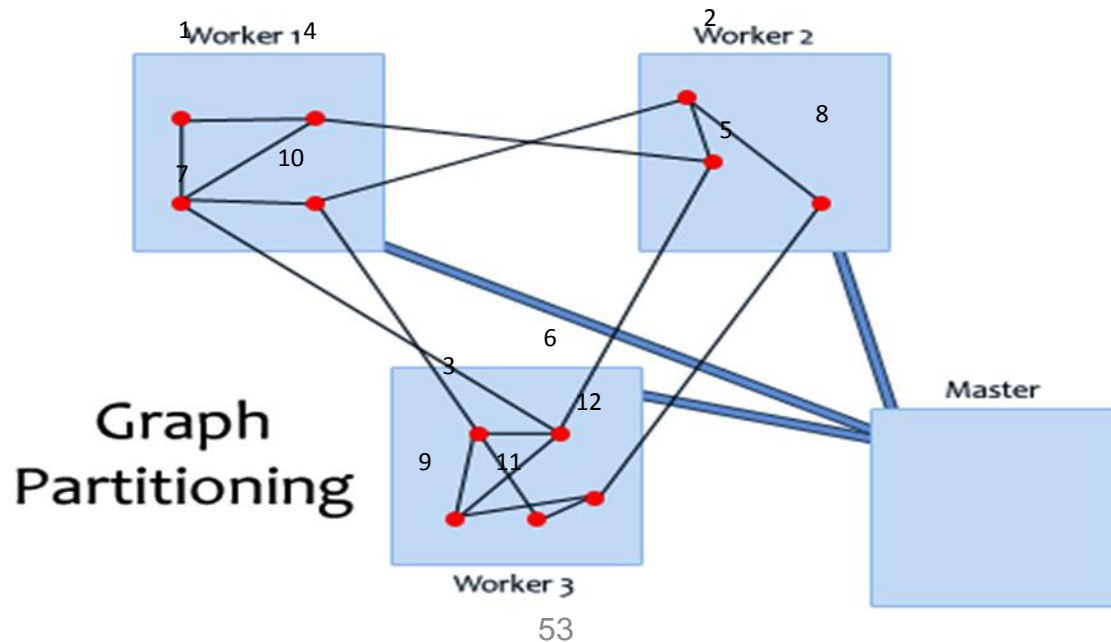


Topology Mutations, Input and Output

- The graph structure can be modified during any superstep
 - Vertices and edges can be added or deleted
 - Conflicts are handled using partial ordering of operations
 - User-defined handlers are also available to manage conflicts
- Flexible input and output formats
 - Text File
 - Relational Database
 - Bigtable Entries
- Interpretation of input is a “pre-processing” step separate from graph computation
 - Custom formats can be created by sub-classing the Reader and Writer classes

Graph Partitioning

- The input graph is divided into **partitions** consisting of vertices and outgoing edges
 - Default partitioning function is ***hash(ID) mod N***, where ***N*** is the # of partitions
 - It can be customized



Execution of a Pregel Program

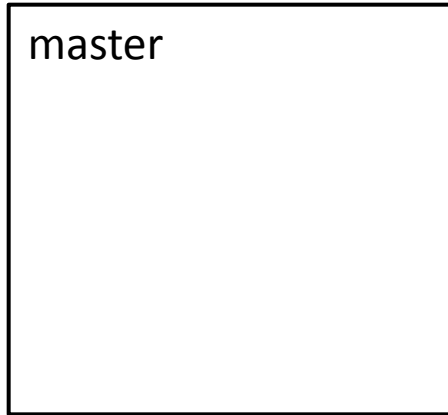
- **Steps of Program Execution:**

1. Copies of the program are distributed across all workers
 - 1.1 One copy is designated as a master
2. Master partitions the graph and assigns workers their respective partition(s) along with portions of the input
3. Master coordinates the execution of supersteps and delivers messages among vertices
4. Master calculates the number of inactive vertices after each superstep and signals workers to terminate if all vertices are inactive and no messages are in transit
5. Each worker may be instructed to save its portion of the graph

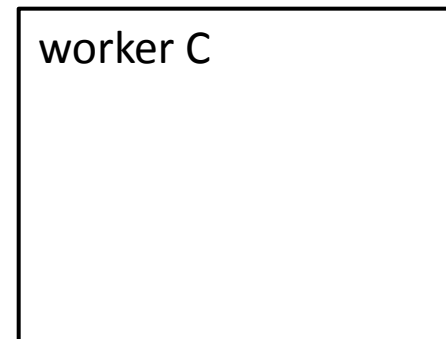
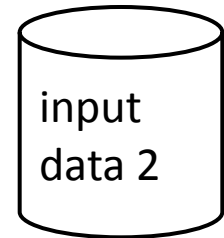
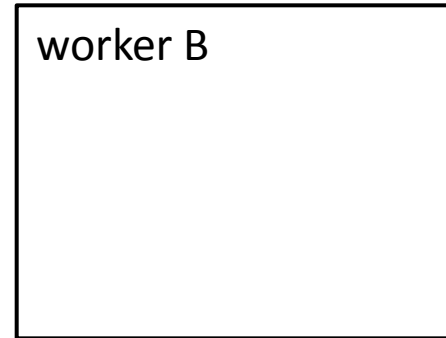
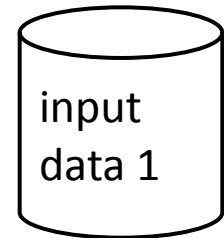
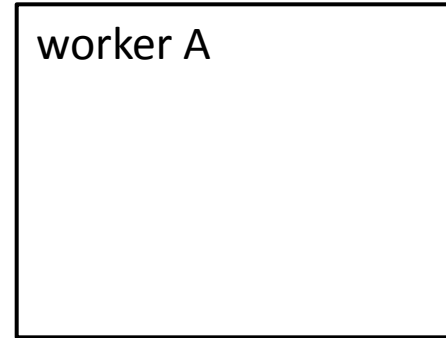
Fault Tolerance in Pregel

- Fault tolerance is achieved through **checkpointing**
 - At the start of every superstep the master may instruct the workers to save the state of their partitions in a stable storage
- Master uses *ping* messages to detect worker failures
- If a worker fails, the master reassigns corresponding vertices and input to another available worker and restarts the superstep
 - The available worker reloads the partition state of the failed worker from the most recent available checkpoint

Architecture

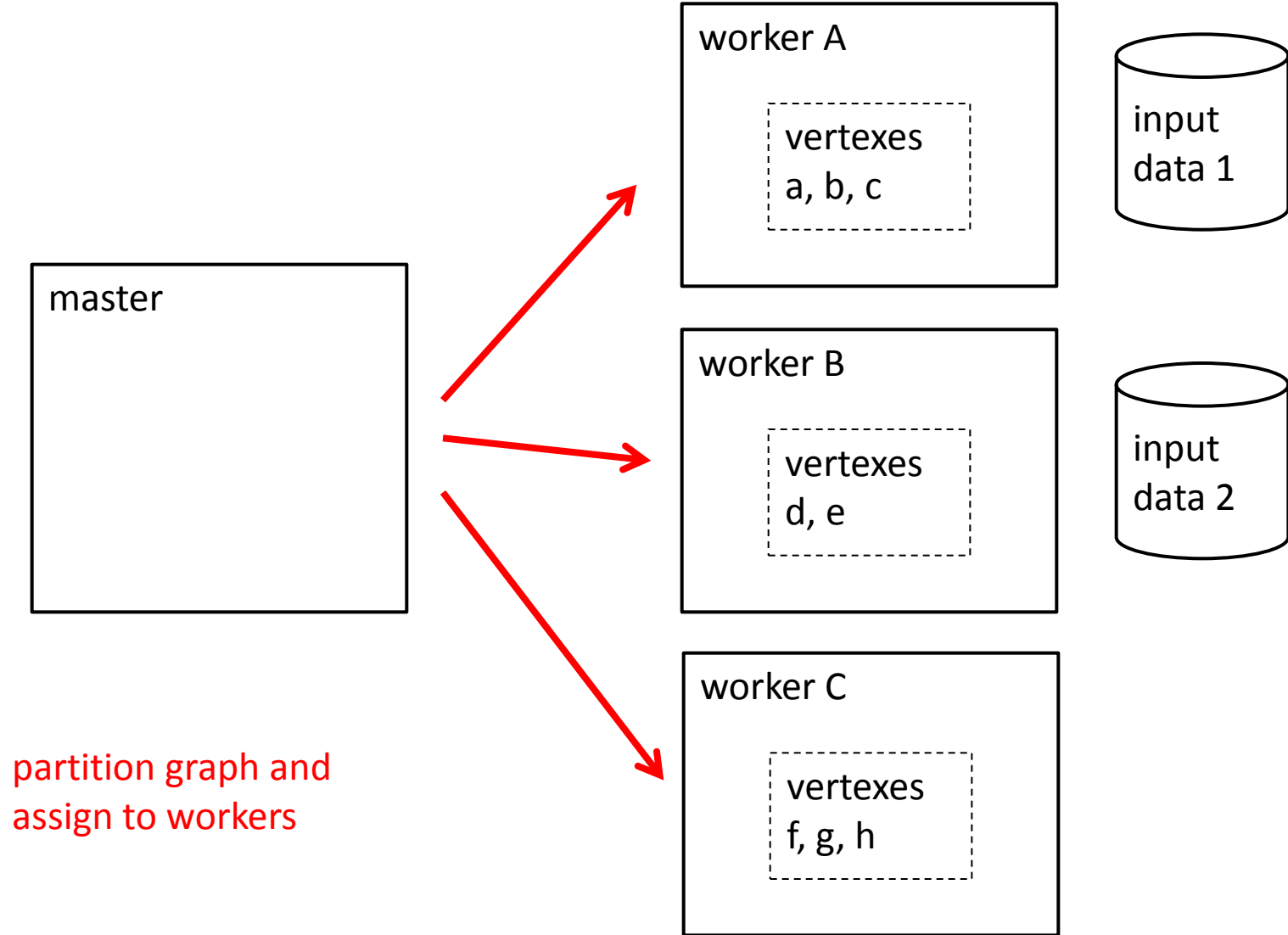


graph has nodes a,b,c,d...

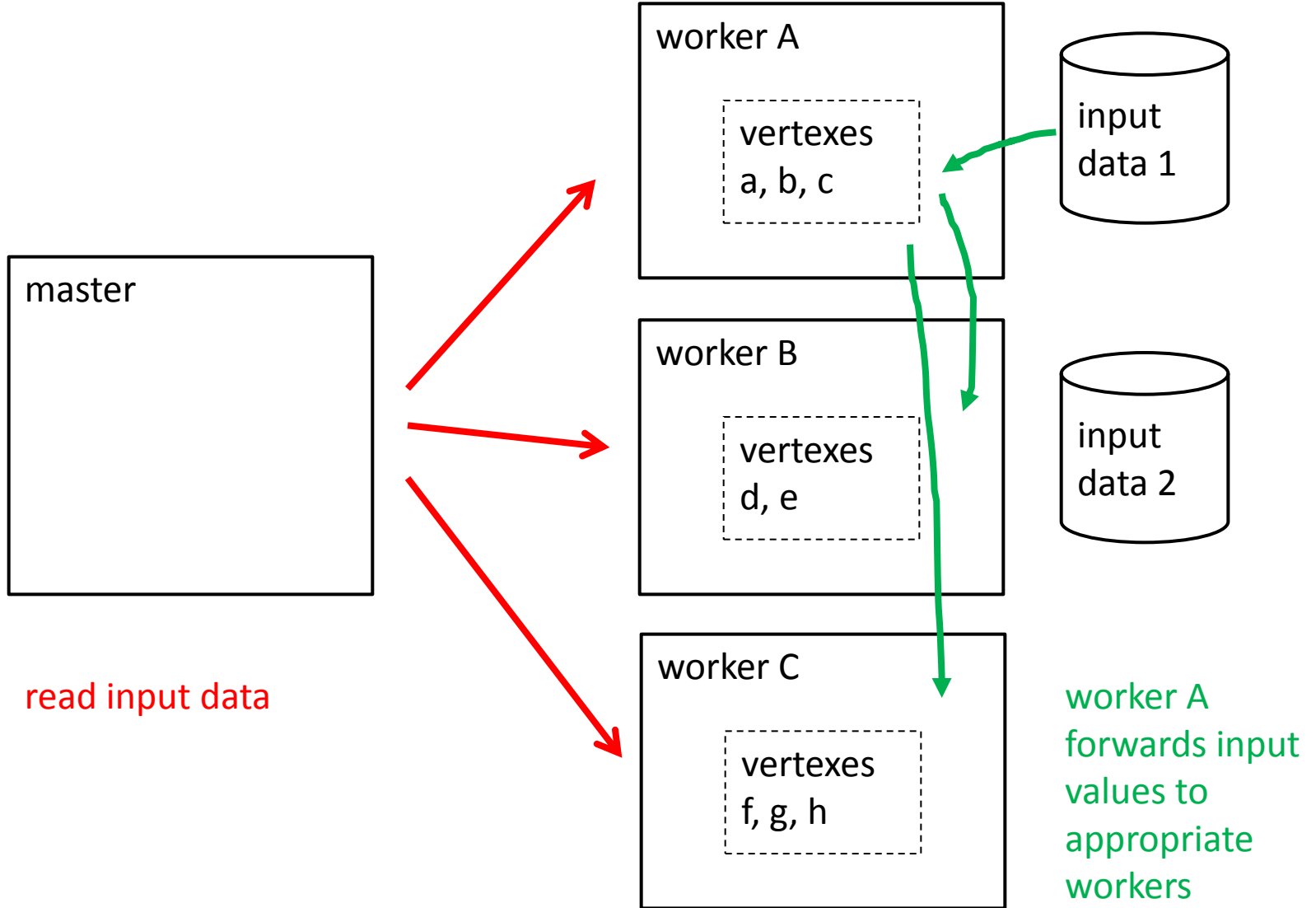


sample record:
[a, value]

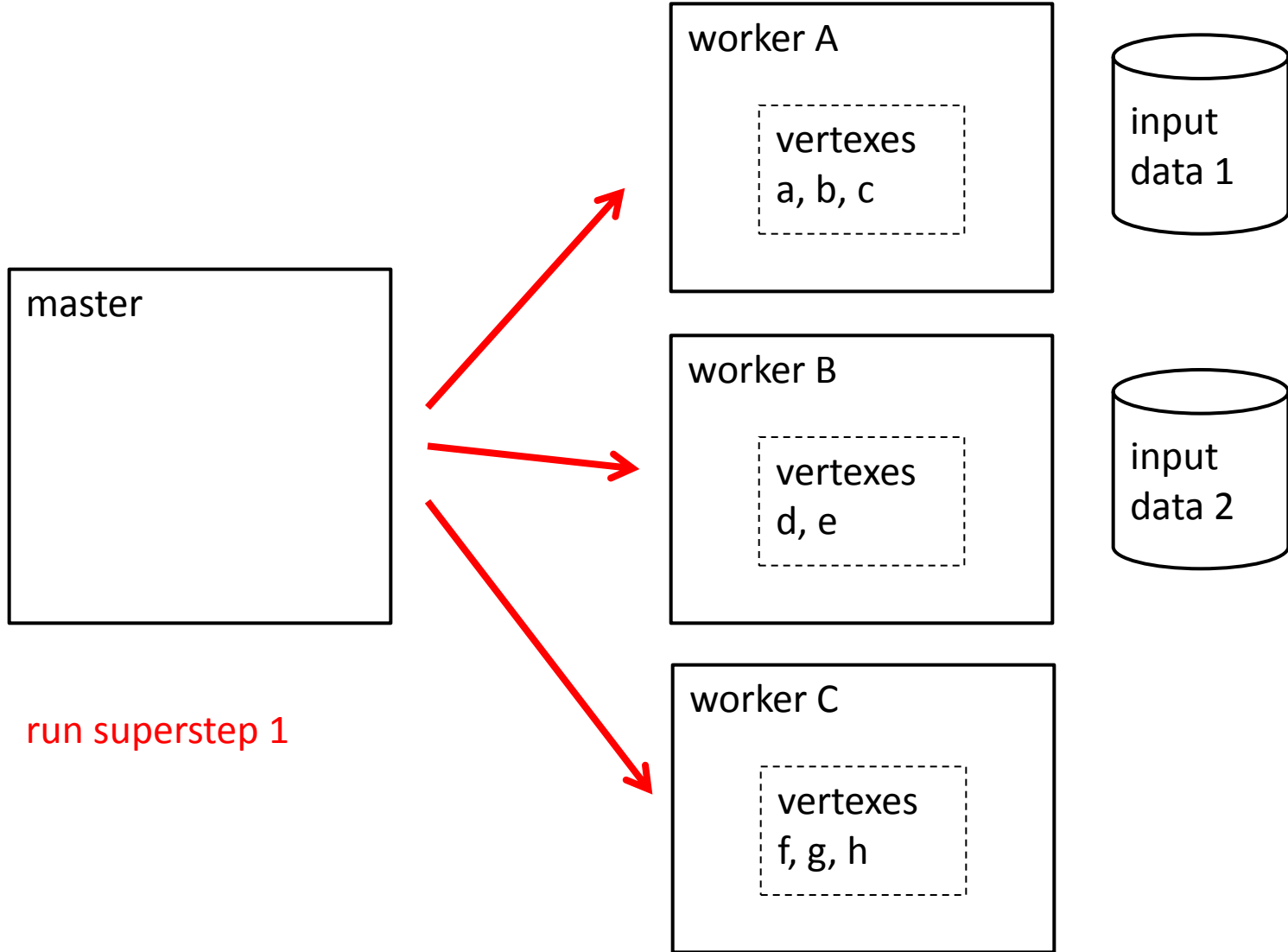
Architecture



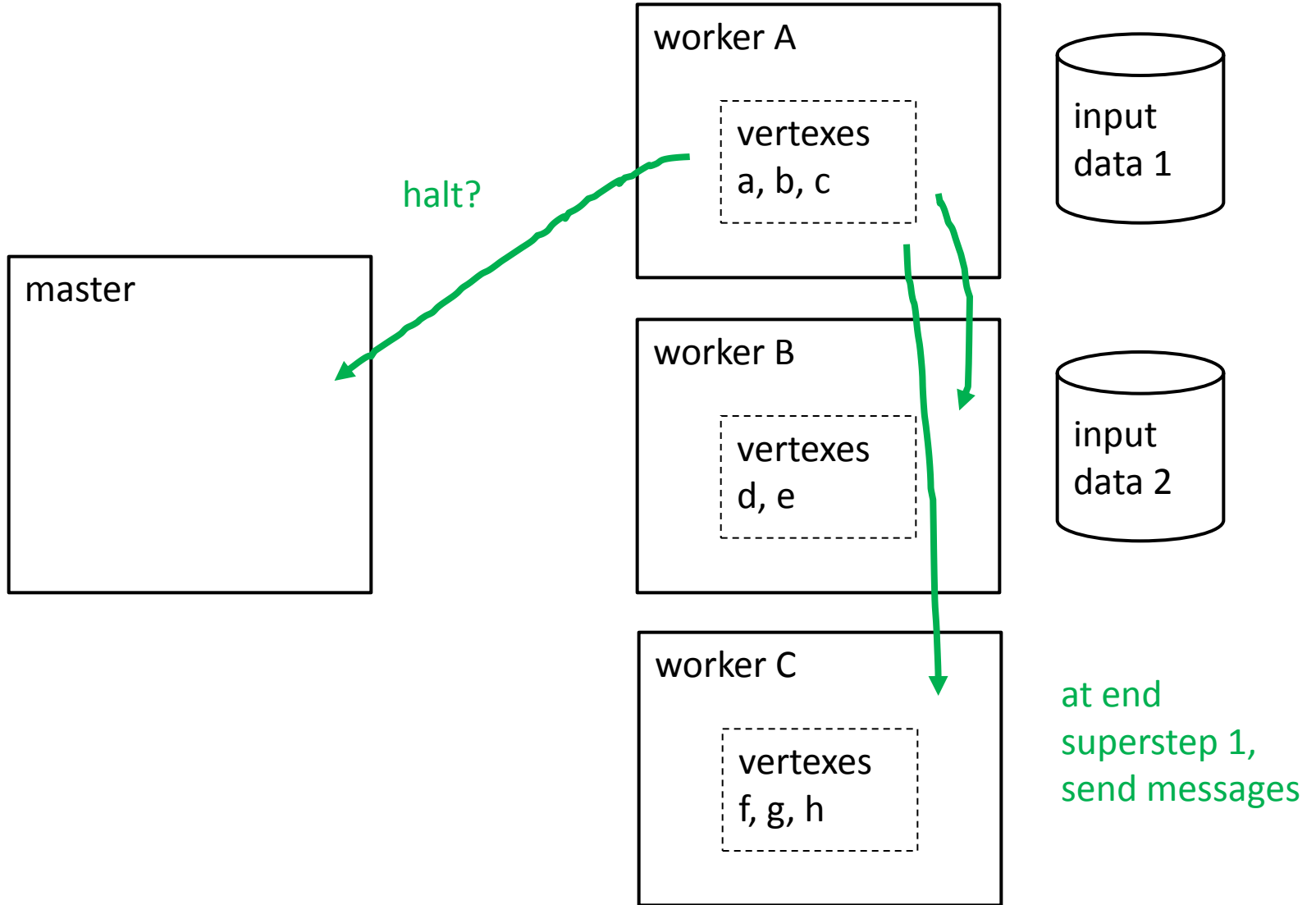
Architecture



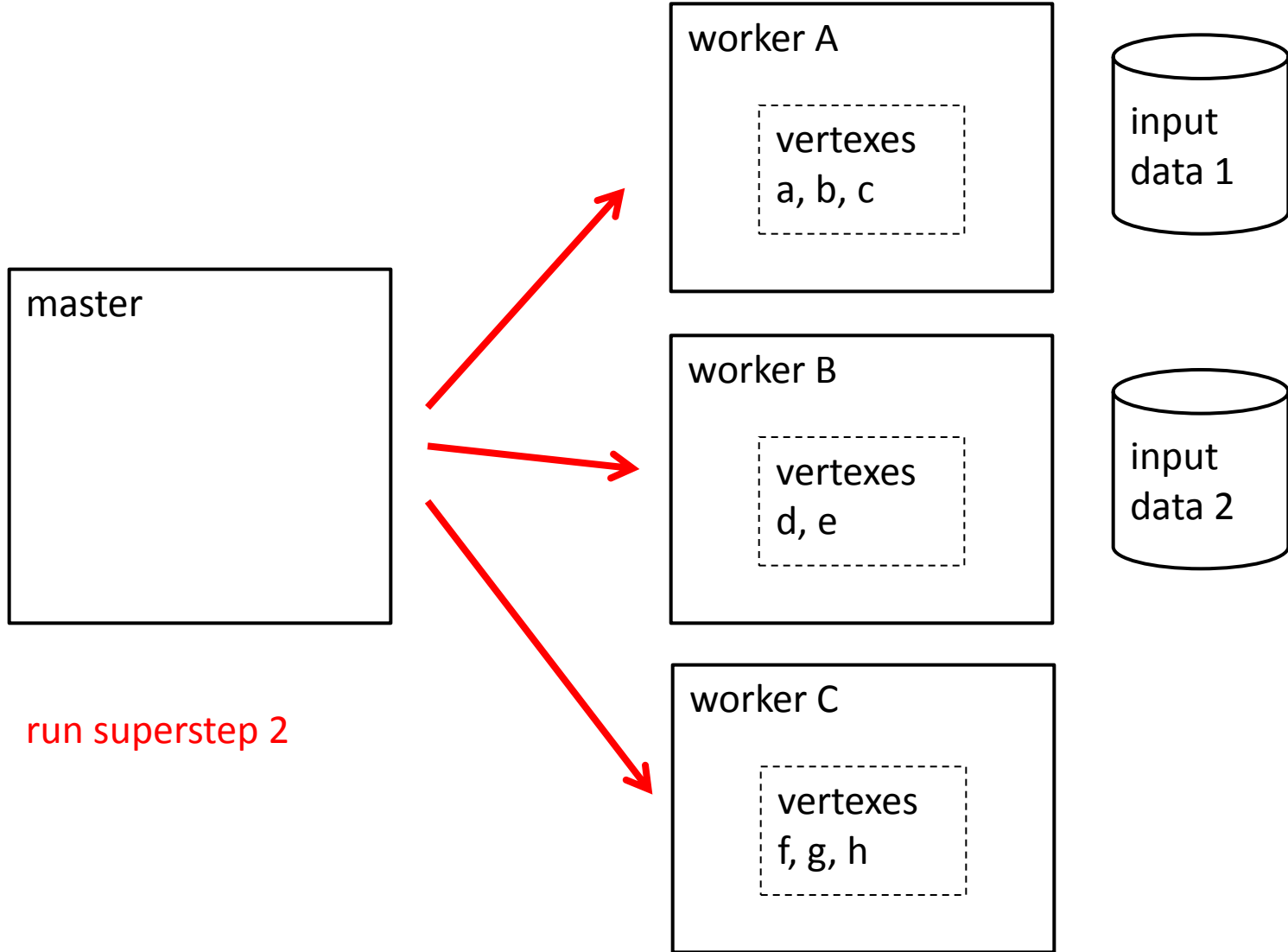
Architecture



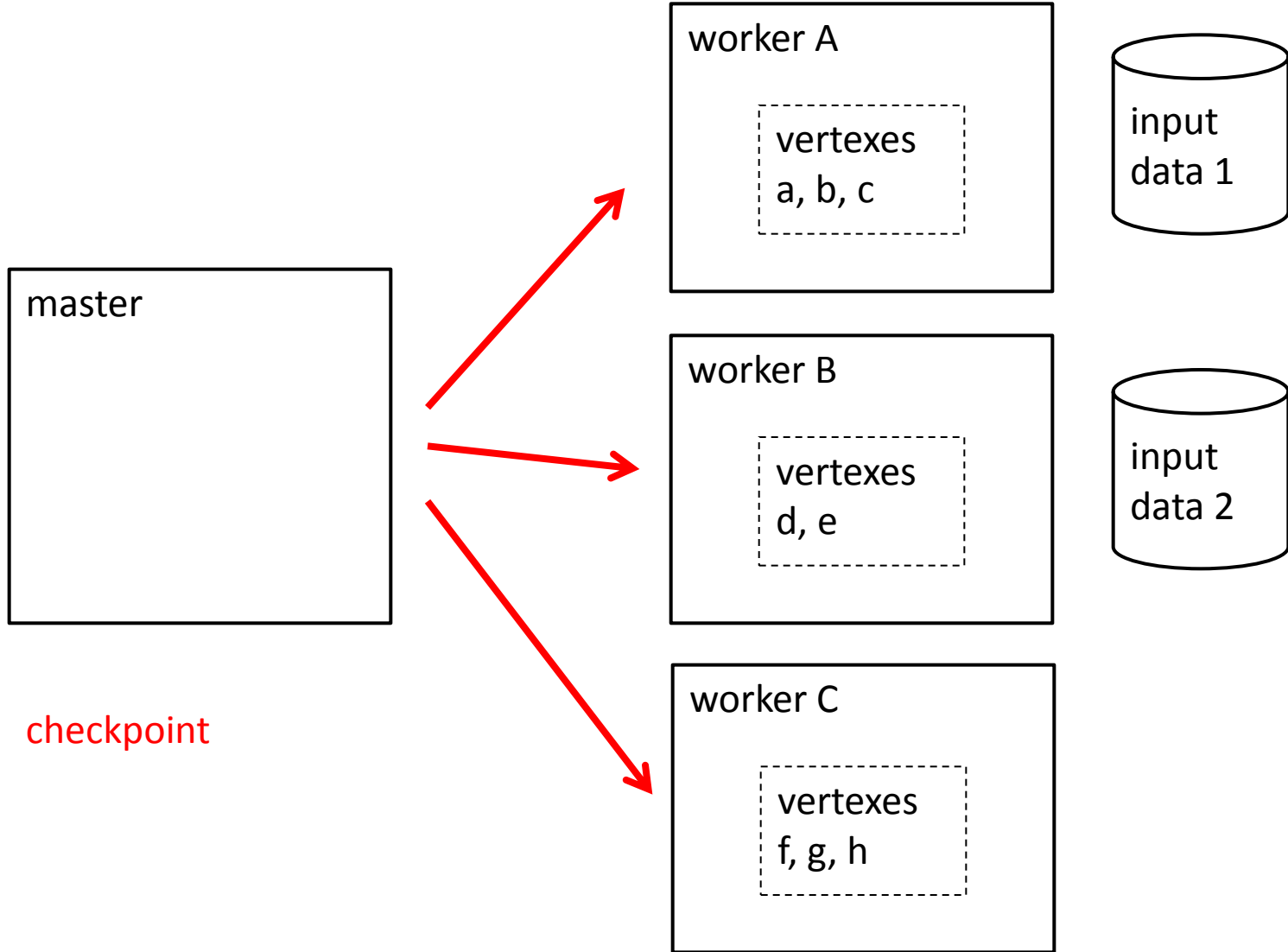
Architecture



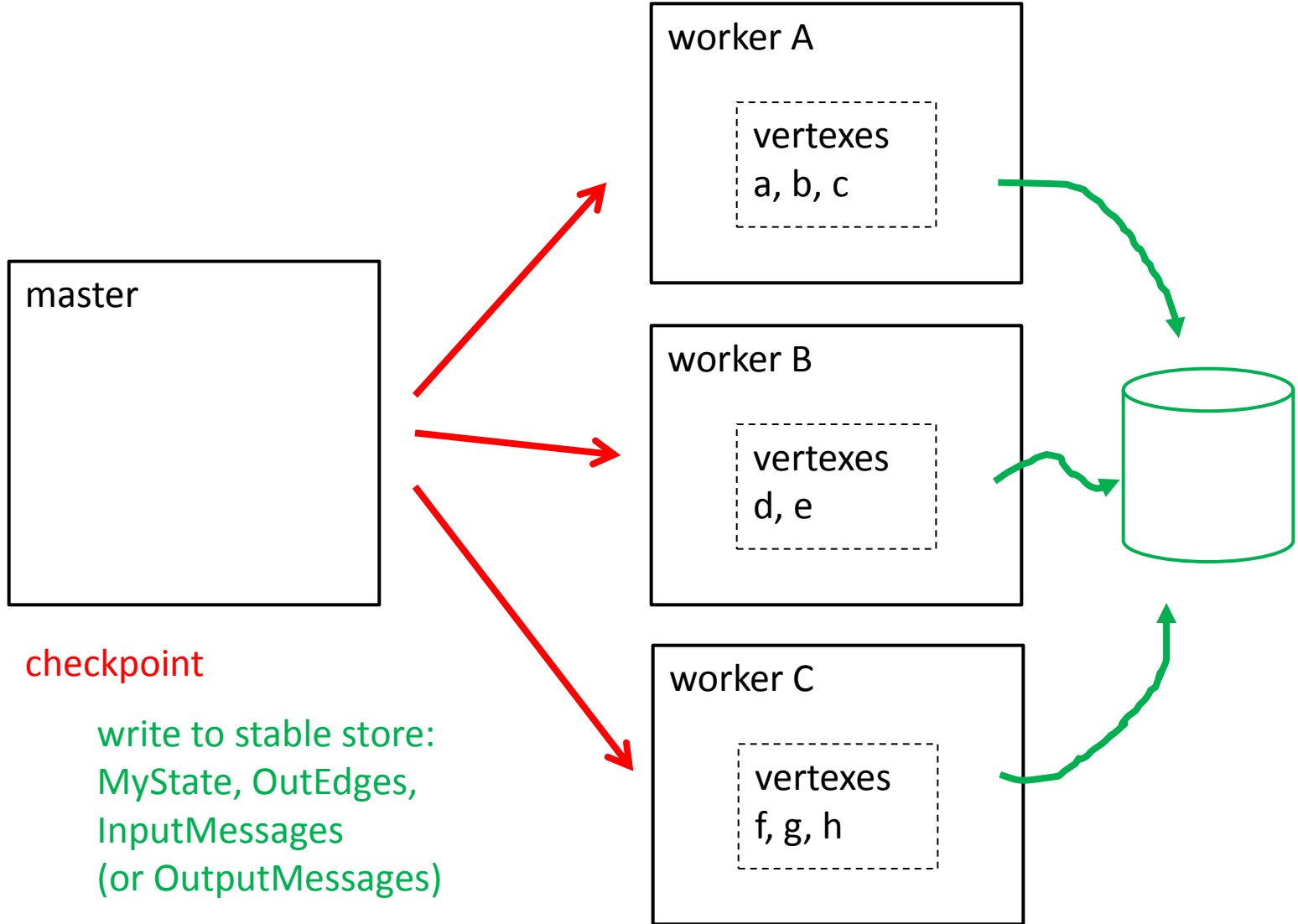
Architecture



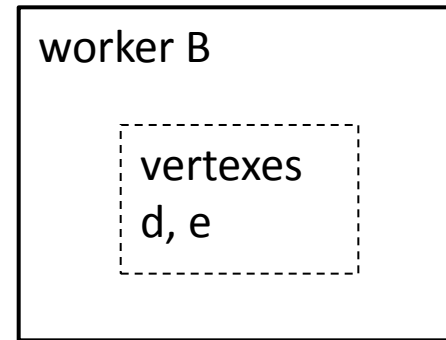
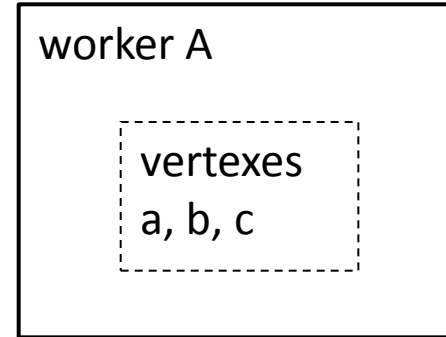
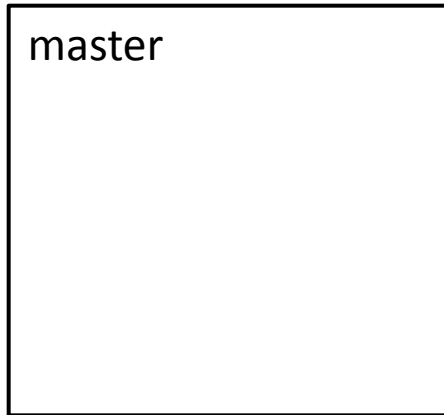
Architecture



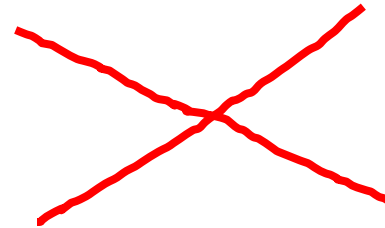
Architecture



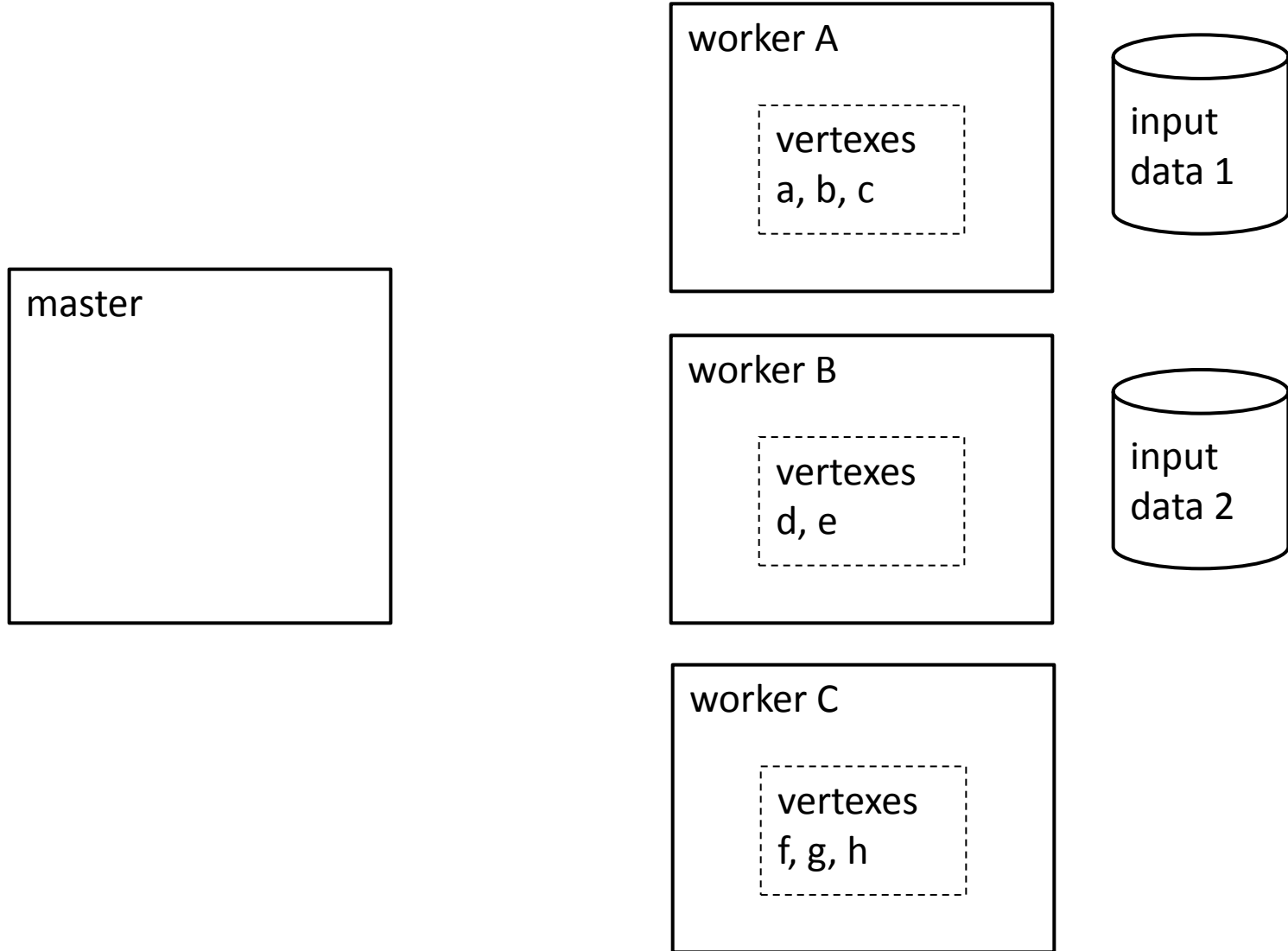
Architecture



if worker dies,
find replacement &
restart from
latest checkpoint



Architecture

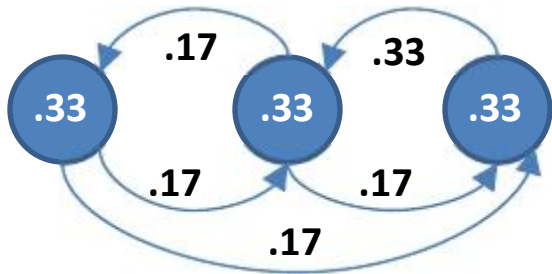


PageRank in Pregel

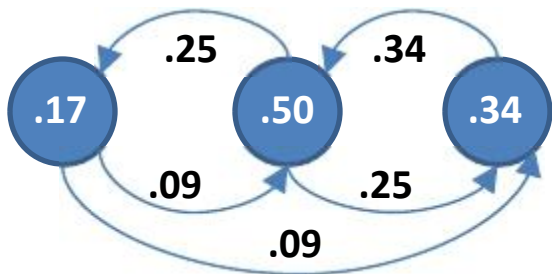
```
class PageRankVertex {  
  void compute(Iterator messages) {  
    if (getSuperstep() > 0) {  
      // recompute own PageRank from the neighborsmessages  
      pageRank = sum(messages);  
      setVertexValue(pageRank);  
    }  
  
    if (getSuperstep() < k) {  
      // send updated PageRank to each neighbor  
      sendMessageToAllNeighbors(pageRank / getNumOutEdges());  
    } else {  
      voteToHalt(); // terminate  
    }  
  }  
}
```

$$p_i = \sum_{j \in \{(j,i)\}} \frac{p_j}{d_j}$$

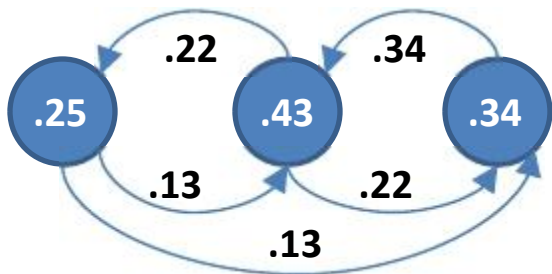
PageRank toy example



Superstep 0

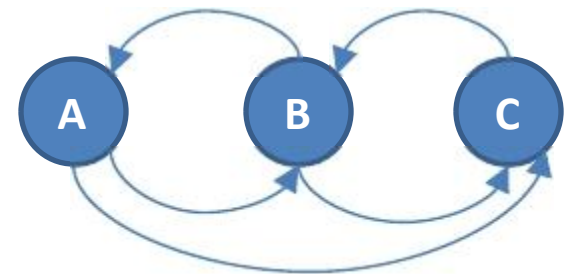


Superstep 1



Superstep 2

Input graph



Cool, where can I download it?

- Pregel is **proprietary**, but:
 - **Apache Giraph** is an open source implementation of Pregel
 - runs on **standard Hadoop infrastructure**
 - computation is executed **in memory**
 - can be a job in a **pipeline** (MapReduce, Hive)
 - uses **Apache ZooKeeper** for synchronization



NEO4J (Graph database)

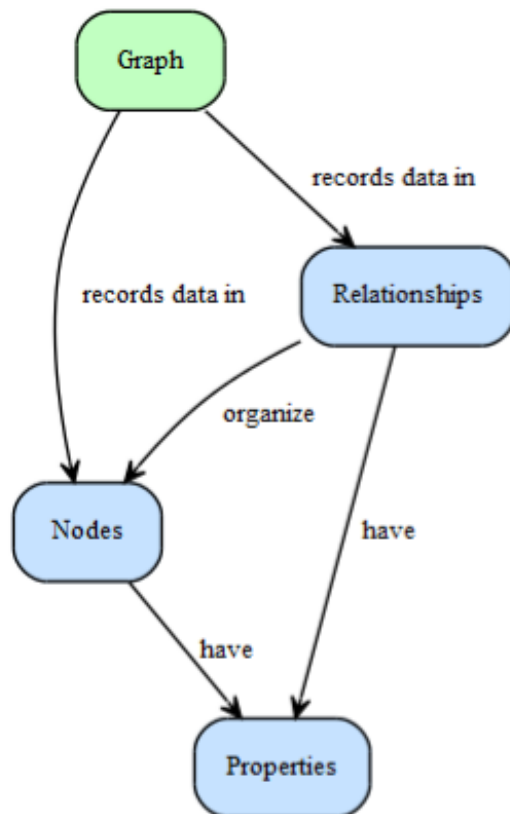
- A graph is a collection nodes (things) and edges (relationships) that connect pairs of nodes.
- Attach properties (key-value pairs) on nodes and relationships
- Relationships connect two nodes and both nodes and relationships can hold an arbitrary amount of key-value pairs.
- A graph database can be thought of as a key-value store, with full support for relationships.
- <http://neo4j.org/>

NEO4J

2.1.1. A Graph contains Nodes and Relationships

“A Graph —records data in→ Nodes —which have→ Properties”

The simplest possible graph is a single Node, a record that has named values referred to as Properties. A Node could start with a single Property and grow to a few million, though that can get a little awkward. At some point it makes sense to distribute the data into multiple nodes, organized with explicit Relationships.



NEO4J

2.1 Relationships organize the Graph

“Nodes —are organized by→ Relationships —which also have→ Properties”

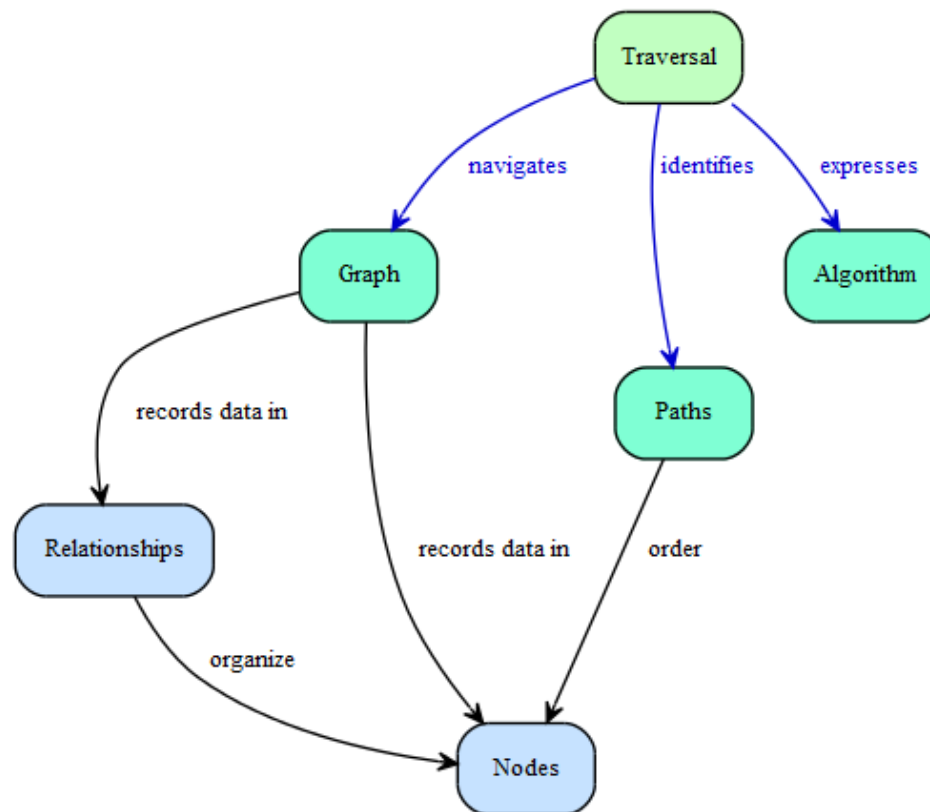
Relationships organize Nodes into arbitrary structures, allowing a Graph to resemble a List, a Tree, a Map, or a compound Entity - any of which can be combined into yet more complex, richly inter-connected structures.

NEO4J

Query a Graph with a Traversal

“A Traversal —navigates→ a Graph; it —identifies→ Paths —which order→ Nodes”

A Traversal is how you query a Graph, navigating from starting Nodes to related Nodes according to an algorithm, finding answers to questions like “what music do my friends like that I don’t yet own,” or “if this power supply goes down, what web services are affected?”

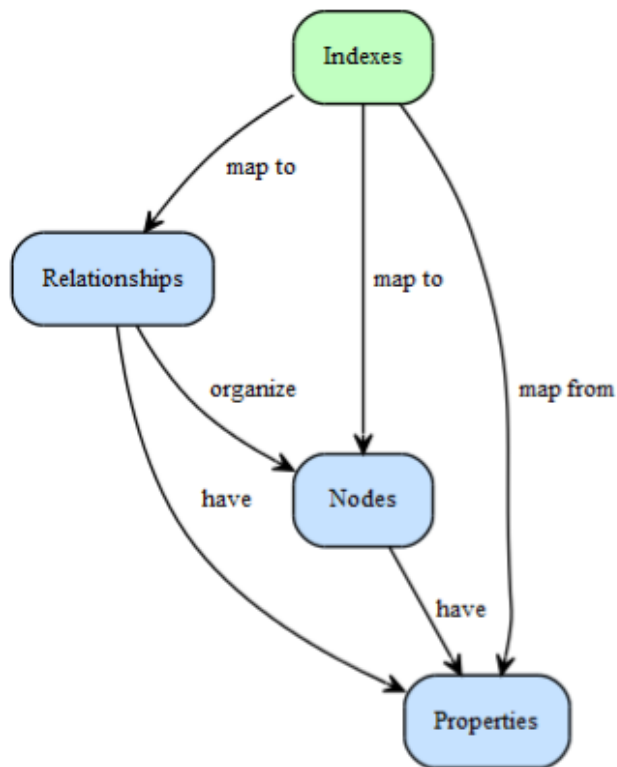


NEO4J

2.1.4. Indexes look-up Nodes or Relationships

“An Index maps from Properties to either Nodes or Relationships”

Often, you want to find a specific Node or Relationship according to a Property it has. Rather than traversing the entire graph, use an Index to perform a look-up, for questions like “find the Account for username master-of-graphs.”

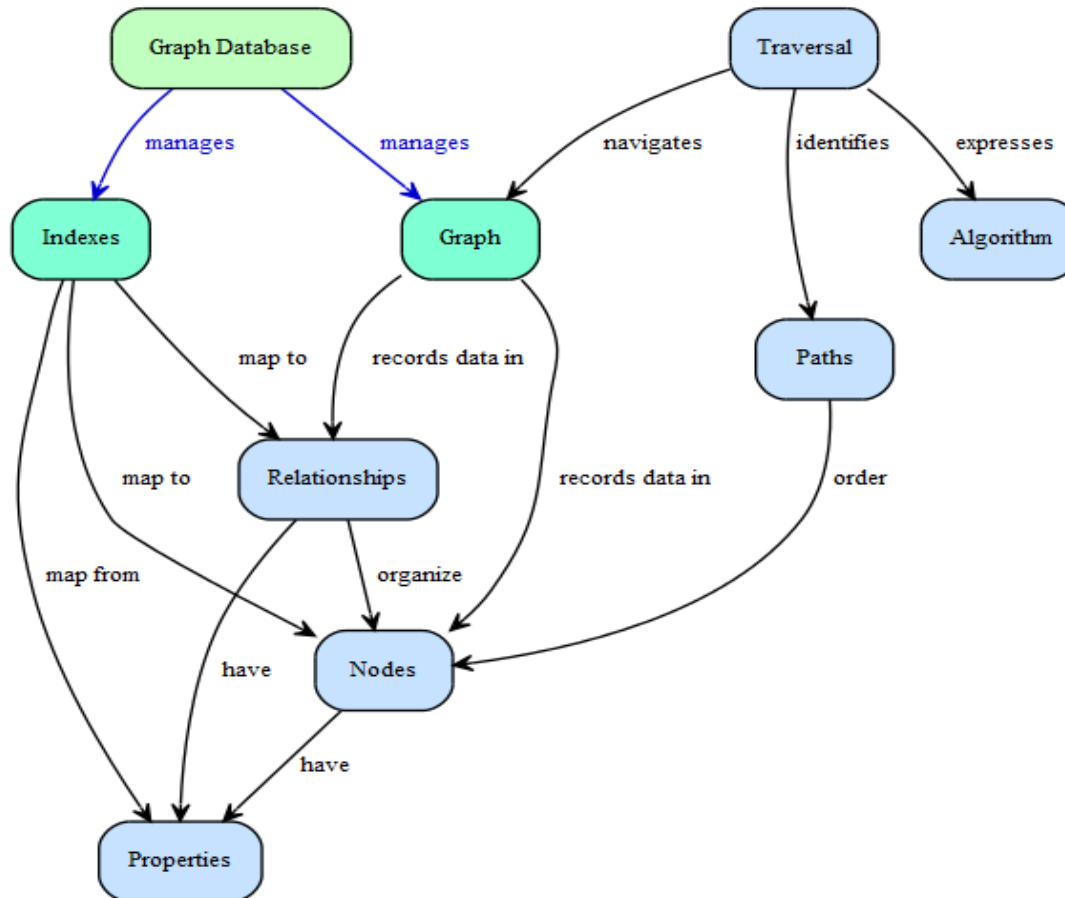


NEO4J

. Neo4j is a Graph Database

“A Graph Database —manages a→ Graph and —also manages related→ Indexes”

Neo4j is a commercially supported open-source graph database. It was designed and built from the ground-up to be a reliable database, optimized for graph structures instead of tables. Working with Neo4j, your application gets all the expressiveness of a graph, with all the dependability you expect out of a database.



NEO4J

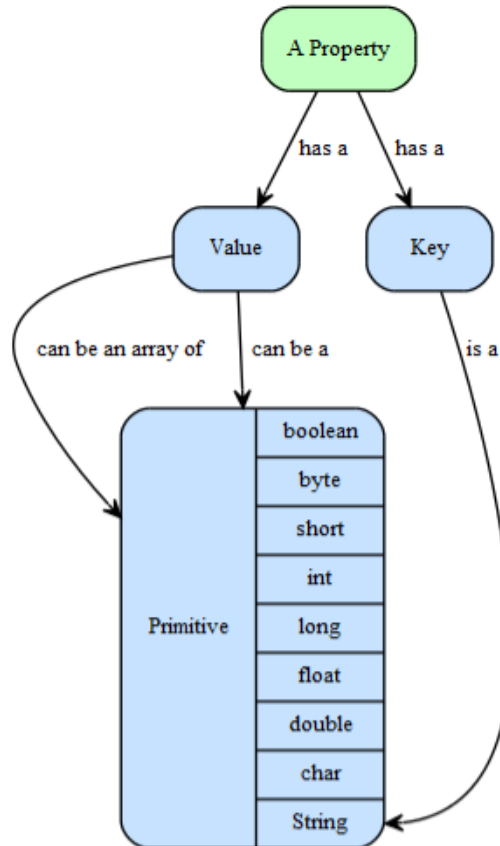
Properties

Properties are key-value pairs where the key is a string. Property values can be either a primitive or an array of one primitive type. For example `String`, `int` and `int[]` values are valid for properties.



Note

`null` is not a valid property value. Nulls can instead be modeled by the absence of a key.



NEO4J Features

- Dual license: open source and commercial
- Well suited for many web use cases such as tagging, metadata annotations, social networks, wikis and other network-shaped or hierarchical data sets
- Intuitive graph-oriented model for data representation. Instead of static and rigid tables, rows and columns, you work with a flexible graph network consisting of nodes, relationships and properties.
- Neo4j offers performance improvements on the order of 1000x or more compared to relational DBs.
- A disk-based, native storage manager completely optimized for storing graph structures for maximum performance and scalability
- Massive scalability. Neo4j can handle graphs of several billion nodes/relationships/properties on a single machine and can be sharded to scale out across multiple machines
- Fully transactional like a real database
- Neo4j traverses depths of 1000 levels and beyond at millisecond speed. (many orders of magnitude faster than relational systems)

Transactions

1. Debit 100 TL to Groceries Expense Account
2. Credit 100 to Checking Account

```
UPDATE account1 SET balance=balance-500;  
UPDATE account1 SET balance=balance+500;
```

- A transaction is simply a number of individual queries that are grouped together.
- Transactions provide an "all-or-nothing" proposition, stating that each work-unit performed in a database must either complete in its entirety or have no effect whatsoever.

Transactions

- four conditions (ACID) to which transactions need to adhere
1. Atomicity: The queries that make up the transaction must either all be carried out, or none at all should be carried out
 2. Consistency: Refers to the rules of the data. During the transaction, rules may be broken, but this state of affairs should never be visible from outside of the transaction.
 3. Isolation : Simply put, data being used for one transaction cannot be used by another transaction until the first transaction is complete.

```
Connection 1: SELECT balance FROM account1;
```

```
Connection 2: SELECT balance FROM account1;
```

```
Connection 1: UPDATE account1 SET balance = 900+100;
```

```
Connection 2: UPDATE account1 SET balance = 900-100;
```

4. Durability: Once a transaction has completed, its effects should remain, and not be reversible.