# GraphBLAS: A linear algebraic approach for high-performance graph algorithms

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## **OUTLINE**

- What makes graph computations difficult?
- The GraphBLAS standard
- Theoretical foundations of GraphBLAS
- Graph algorithms in GraphBLAS
- Graph processing in relational algebra
- GraphBLAS internals and API
- Further reading and libraries
- Summary



## **GRAPH PROCESSING CHALLENGES**

connectedness

the "curse of connectedness"

computer architectures

contemporary computer architectures are good at processing linear and hierarchical data structures, such as *Lists*, *Stacks*, or *Trees* 

caching and parallelization

a massive amount of random data access is required, CPU has frequent cache misses, and implementing parallelism is difficult



B. Shao, Y. Li, H. Wang, H. Xia (Microsoft Research), Trinity Graph Engine and its Applications, IEEE Data Engineering Bulleting 2017

## **GRAPH PROCESSING CHALLENGES**

What does it mean that graph algorithms have "a high communication to computation ratio"? [ICCS'15]

Most of the time is spent on chasing pointers.

Speedup with a CPU that has better arithmetic performance:

- machine learning → a lot
- relational query → some
- graph processing → very little

Standard latency hiding techniques break down:

pre-fetching and branch prediction provide little benefit

## DISTRIBUTED GRAPH PROCESSING

- Many recent works focused on computation models for distributed execution allowing systems to scale out.
  - o BSP (Bulk Synchronous Parallel) model by Leslie Valiant
  - MapReduce and Pregel models by Google
  - o Vertex-centric, Scatter-Gather, Gather-Apply-Scatter models
  - o Apache projects: Giraph, Spark GraphX, Flink Gelly, Hama
- Lots of research, summarized in survey/experiments papers



V. Kalavri et al.: *High-Level Programming Abstractions for Distributed Graph Processing*, TKDE 2018



K. Ammar, M.T. Özsu: *Experimental Analysis of Distributed Graph Systems*, VLDB 2018



O. Batarfi et al.: Large scale graph processing systems: survey and an experimental evaluation, Cluster 2015



M.T. Özsu: *Graph Processing: A Panaromic View and Some Open Problems,* VLDB 2019

## SCALING OUT VS. SCALING UP

- Distributed approaches are scalable but comparatively slow
  - large communication overhead
  - o load balancing issues due to irregular distributions
- Many systems struggle to outperform a single-threaded setup
  - COST = Configuration that Outperforms a Single Thread
- Alternatives:
  - o Partition-centric programming model (Blogel, etc.)
  - Linear algebra-based programming model



F. McSherry et al.: Scalability! But at what COST? HotOS 2015

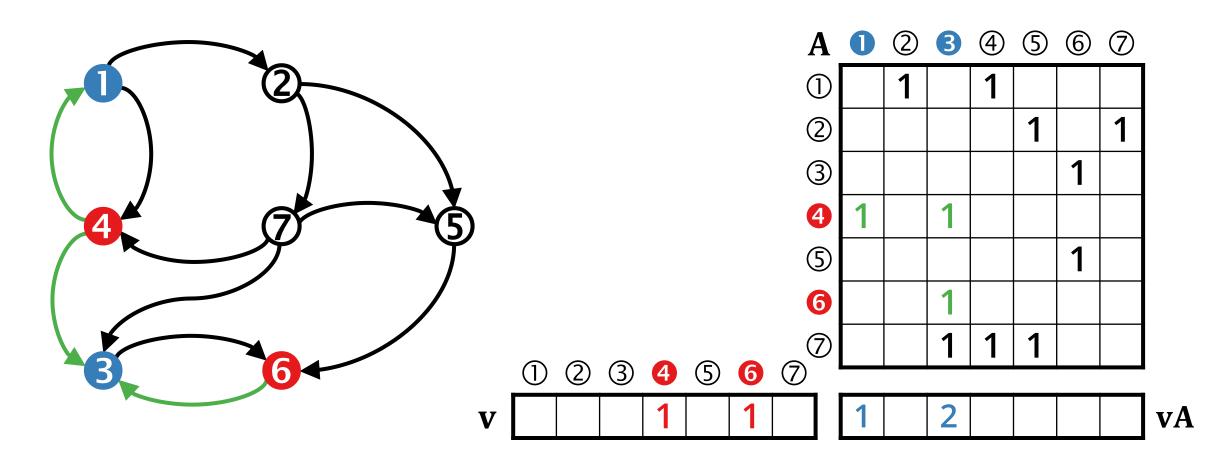


N. Satish et al.:

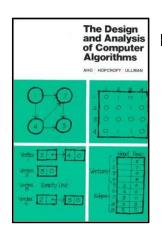
Navigating the Maze of Graph Analytics Frameworks using Massive Graph Datasets, SIGMOD 2014

## LINEAR ALGEBRA-BASED GRAPH PROCESSING

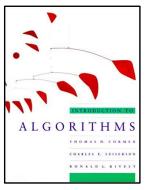
- Graphs are encoded as sparse adjacency matrices.
- Use vector/matrix operations to express graph algorithms.



#### TEXTBOOKS ON SEMIRING-BASED GRAPH PROCESSING



- 1974: Aho-Hopcroft-Ullman book
  - The Design and Analysis of Computer Algorithms
    - Sec. 5.6: Path-finding problems
    - Sec. 5.9: Path problems and matrix multiplication



- 1990: Cormen-Leiserson-Rivest book
  - Introduction to Algorithms
    - Sec. 26.4: A general framework for solving path problems in directed graphs



- 2011: GALLA book (edited by Kepner and Gilbert)
  - o Graph Algorithms in the Language of Linear Algebra

A lot of literature but few practical implementations.

# The GraphBLAS standard

#### THE GRAPHBLAS STANDARD

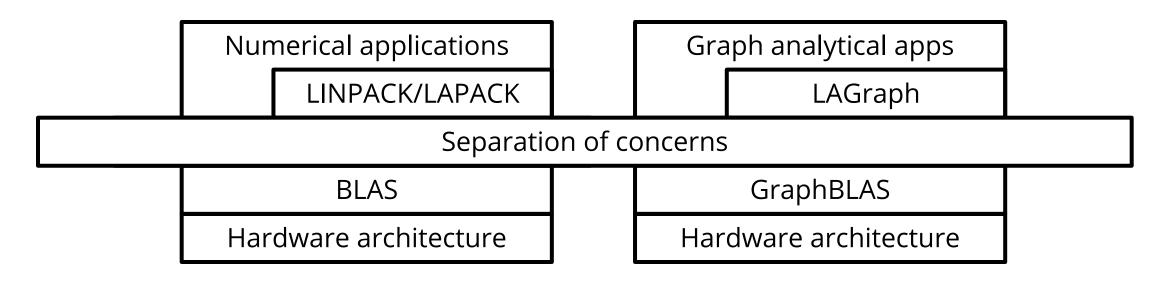
Goal: separate the concerns of the hardware/library/application designers.

1979: BLAS Basic Linear Algebra Subprograms

2001: Sparse BLAS an extension to BLAS (little uptake)

2013: GraphBLAS an effort to define standard building blocks

for graph algorithms in the language of linear algebra

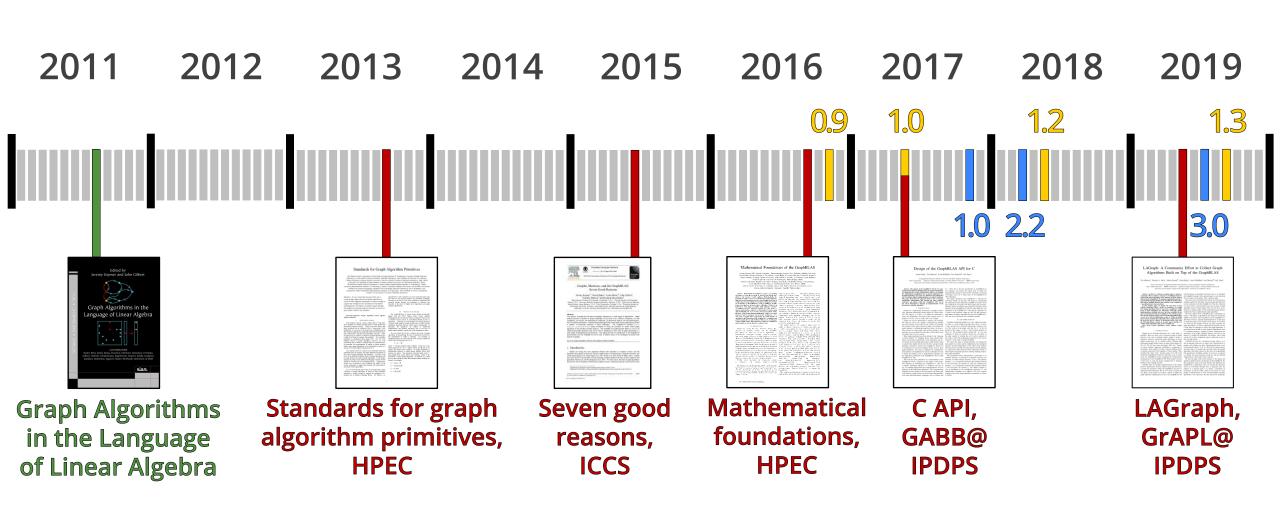




S. McMillan @ SEI Research Review (Carnegie Mellon University, 2015): *Graph algorithms on future architectures* 

#### **GRAPHBLAS TIMELINE**

Book — Papers — GraphBLAS standards — SuiteSparse:GraphBLAS releases



#### GRAPH ALGORITHMS IN LINEAR ALGEBRA

**Notation:** n = |V|, m = |E|. The complexity cells contain asymptotic bounds. **Takeaway:** The majority of common graph algorithms can be expressed efficiently in LA.

problem	algorithm	canonical complexity Θ	LA-based complexity Θ	
breadth-first search		m	m	
single source shortest naths	Dijkstra	$m + n \log n$	$n^2$	
single-source shortest paths	Bellman-Ford	mn	mn	
all-pairs shortest paths	Floyd-Warshall	$n^3$	$n^3$	
minimum channing troo	Prim	$m + n \log n$	$n^2$	
minimum spanning tree	Borůvka	$m \log n$	$m \log n$	
maximum flow	Edmonds-Karp	$m^2n$	$m^2n$	
maximal independent set	greedy	$m + n \log n$	$mn + n^2$	
maximal independent set	Luby	$m + n \log n$	$m \log n$	



Based on the table in J. Kepner: *Analytic Theory of Power Law Graphs,* SIAM Workshop for HPC on Large Graphs, 2008



See also L. Dhulipala, G.E. Blelloch, J. Shun: Theoretically Efficient Parallel Graph Algorithms Can Be Fast and Scalable, SPAA 2018

## Theoretical foundations of GraphBLAS

## MATRIX MULTIPLICATION

## Definition:

$$\mathbf{C} = \mathbf{A}\mathbf{B}$$

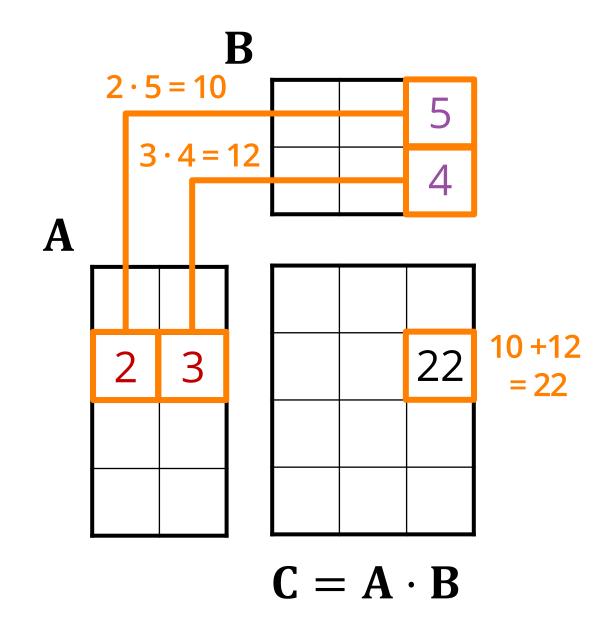
$$\mathbf{C}(i,j) = \sum_{k} \mathbf{A}(i,k) \cdot \mathbf{B}(k,j)$$

## Example:

$$C(2,3) = A(2,1) \cdot B(1,3) +$$

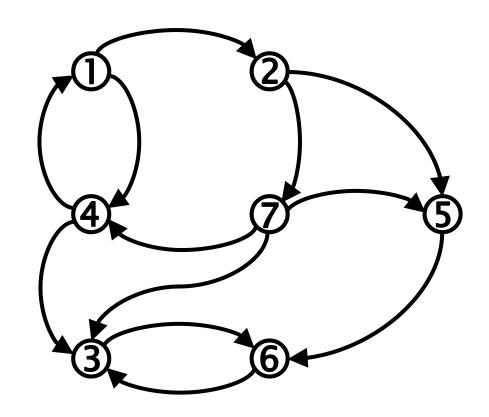
$$A(2,2) \cdot B(2,3)$$

$$= 2 \cdot 5 + 3 \cdot 4 = 22$$



## **ADJACENCY MATRIX**

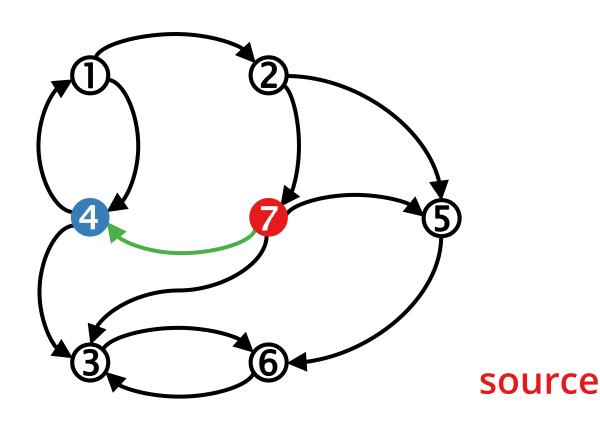
$$\mathbf{A}_{ij} = \begin{cases} 1 & \text{if } (v_i, v_j) \in E \\ 0 & \text{if } (v_i, v_j) \notin E \end{cases}$$



A	1	2	3	4	(5)	6	7
1		1		1			
2					1		1
3						1	
4	1		1				
(5)						1	
(i) (ii) (iii) (ii			1				
7			1	1	1		

## **ADJACENCY MATRIX**

$$\mathbf{A}_{ij} = \begin{cases} 1 & \text{if } (v_i, v_j) \in E \\ 0 & \text{if } (v_i, v_j) \notin E \end{cases}$$

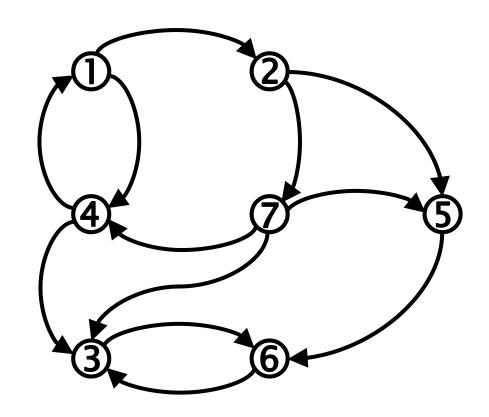


#### target

A	1	2	3	4	(5)	6	7
1		1		1			
① ② ③ ④					1		1
3						1	
4	1		1				
(5)						1	
(5) (6)			1				
7			1	1	1		

## **ADJACENCY MATRIX**

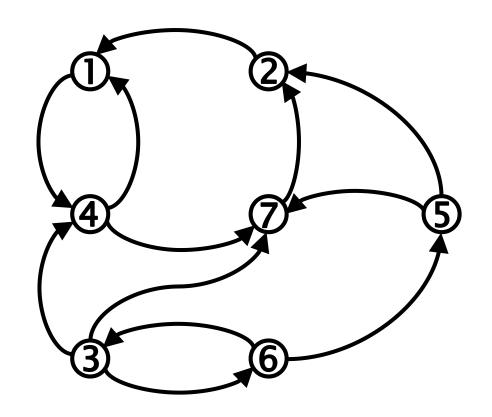
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A	1	2	3	4	(5)	6	7
1		1		1			
2					1		1
3						1	
4	1		1				
(5)						1	
(i) (ii) (iii) (ii			1				
7			1	1	1		

## **ADJACENCY MATRIX TRANSPOSED**

$$\mathbf{A}_{ij}^{\mathsf{T}} = \begin{cases} 1 & \text{if } (v_j, v_i) \in E \\ 0 & \text{if } (v_j, v_i) \notin E \end{cases}$$

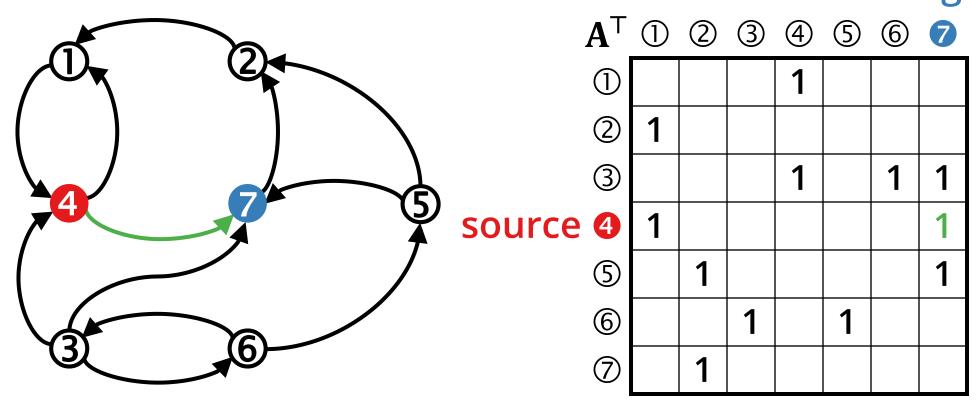


$\mathbf{A}^{T}$	1	2	3	4	(5)	6	7
1				1			
2	1						
<ul><li>의</li><li>의</li><li>의</li><li>⑤</li><li>⑥</li></ul>				1		1	1
4	1						1
(5)		1					1
6			1		1		
7		1					

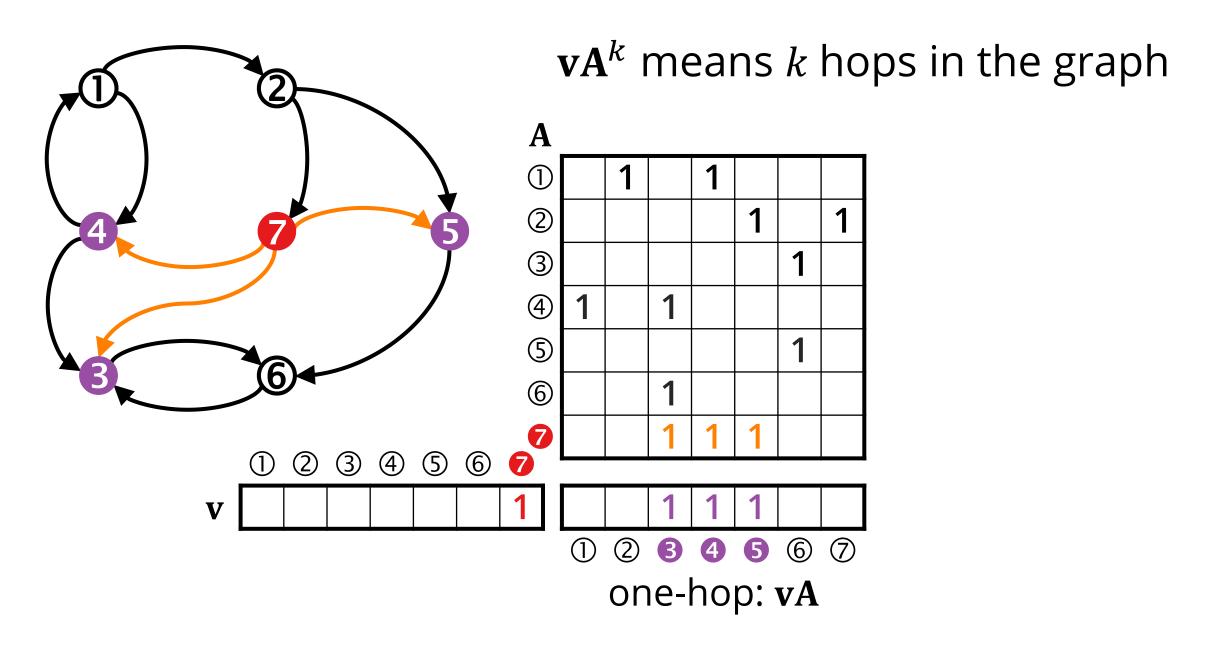
## **ADJACENCY MATRIX TRANSPOSED**

$$\mathbf{A}_{ij}^{\mathsf{T}} = \begin{cases} 1 & \text{if } (v_j, v_i) \in E \\ 0 & \text{if } (v_j, v_i) \notin E \end{cases}$$

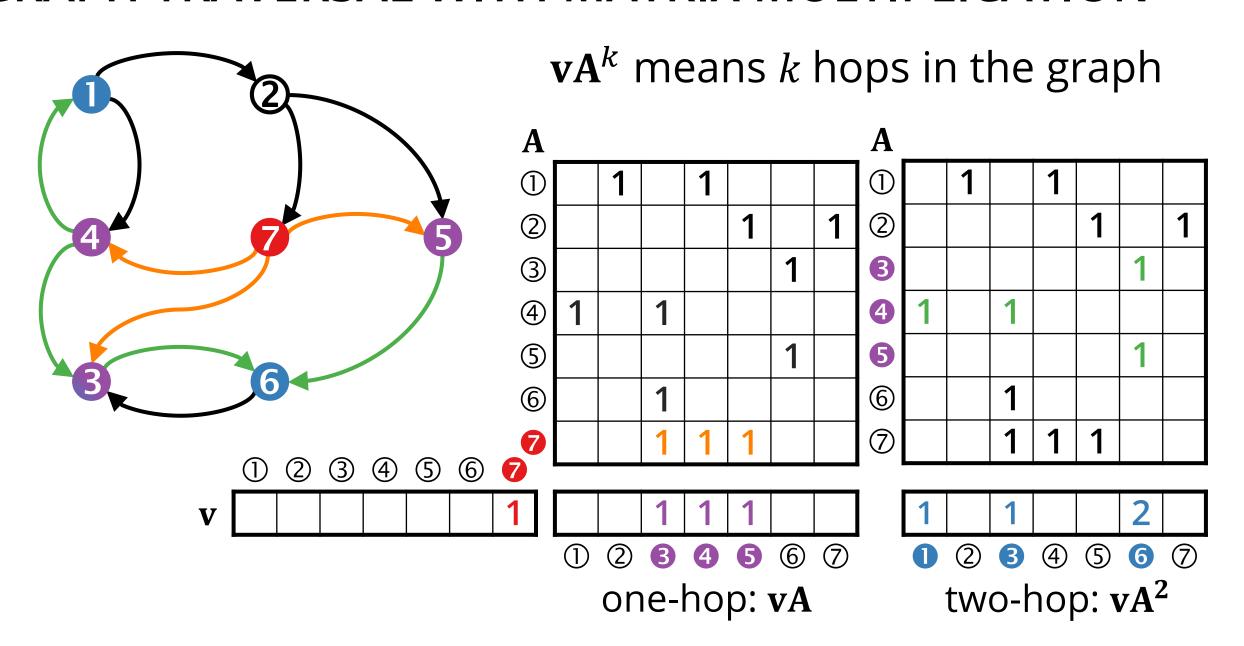




#### **GRAPH TRAVERSAL WITH MATRIX MULTIPLICATION**



#### **GRAPH TRAVERSAL WITH MATRIX MULTIPLICATION**



#### MATRIX MULTIPLICATION ON SEMIRINGS

Using the conventional semiring

$$\mathbf{C} = \mathbf{A}\mathbf{B}$$

$$\mathbf{C}(i,j) = \sum_{k} \mathbf{A}(i,k) \cdot \mathbf{B}(k,j)$$

Generalized formula\*

$$\mathbf{C} = \mathbf{A} \oplus . \otimes \mathbf{B}$$

$$\mathbf{C}(i,j) = \bigoplus_{k} \mathbf{A}(i,k) \otimes \mathbf{B}(k,j)$$

- A cornerstone of GraphBLAS: Use arbitrary semirings that override the  $\oplus$  addition and  $\otimes$  multiplication operators.
- \* Remark: Some definitions in the presentation are simplified. The full definitions are given at the end of the slideshow.

## **GRAPHBLAS SEMIRINGS\***

The  $\langle D, \bigoplus, \otimes, 0 \rangle$  algebraic structure is a GraphBLAS semiring if

- $\langle D, \bigoplus, 0 \rangle$  is a commutative monoid using the addition operation  $\bigoplus: D \times D \to D$ , where  $\forall a, b, c \in D$ :
  - $\circ$  Commutative  $a \oplus b = b \oplus a$
  - o Associative  $(a \oplus b) \oplus c = a \oplus (b \oplus c)$
  - o Identity  $a \oplus 0 = a$
- The multiplication operator is a closed binary operator  $\otimes: D \times D \to D$ .

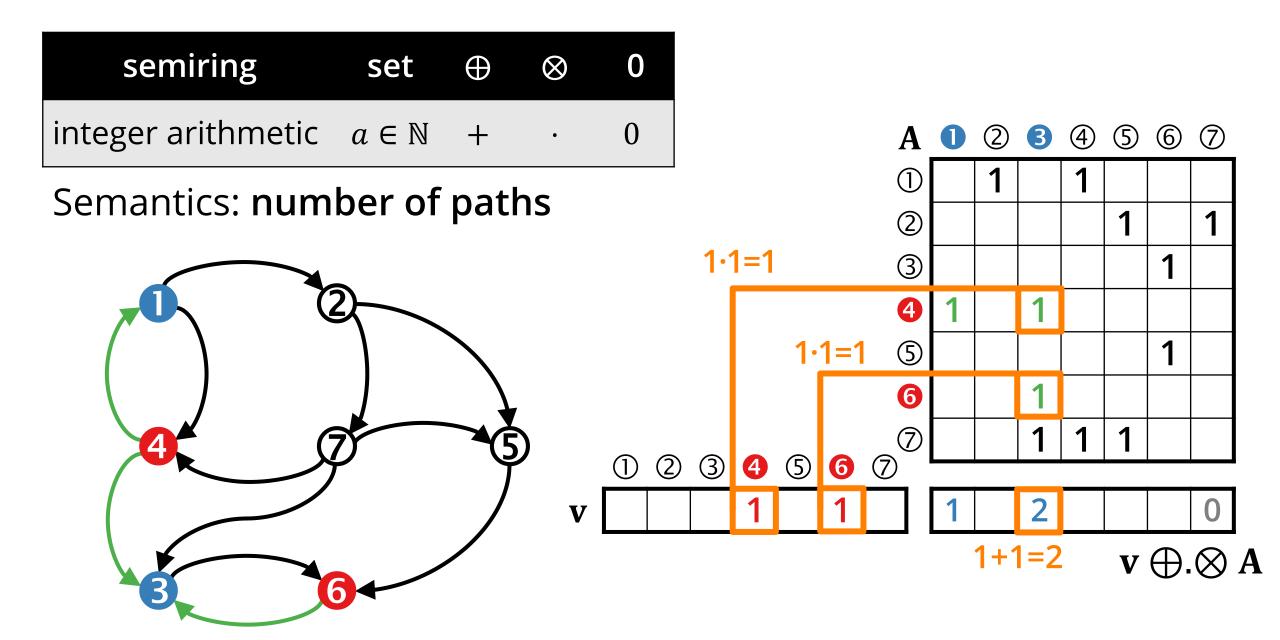
The mathematical definition of a semiring requires that  $\otimes$  is a monoid and distributes over  $\oplus$ . GraphBLAS omits these requirements.

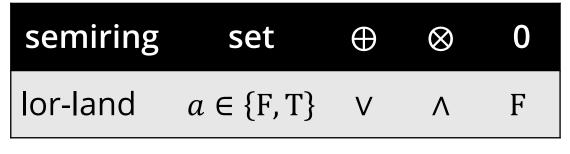
## **SEMIRINGS**

semiring	set	$\oplus$	$\otimes$	0	graph semantics
lor-land	$a \in \{F, T\}$	V	٨	F	connectivity
integer arithmetic	$a \in \mathbb{N}$	+	•	0	number of paths
real arithmetic	$a \in \mathbb{R}$	+	•	0	strength of all paths
min-plus	$a \in \mathbb{R} \cup \{+\infty\}$	min	+	+∞	shortest path
max-plus	$a \in \mathbb{R} \cup \{-\infty\}$	max	+	$-\infty$	graph matching

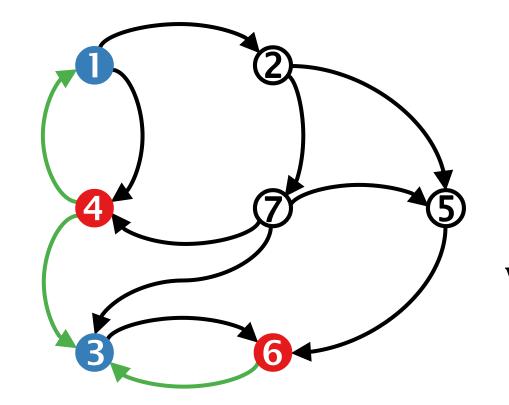
The default semiring is the conventional one:

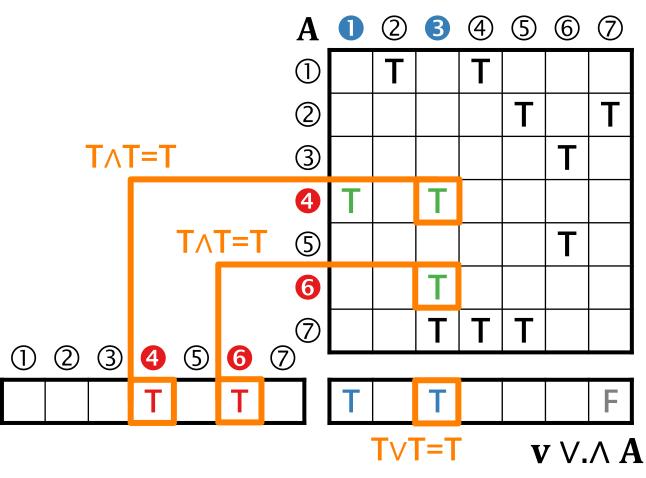
- Operator ⊗ defaults to floating point multiplication.
- Operator ⊕ defaults to floating point addition.

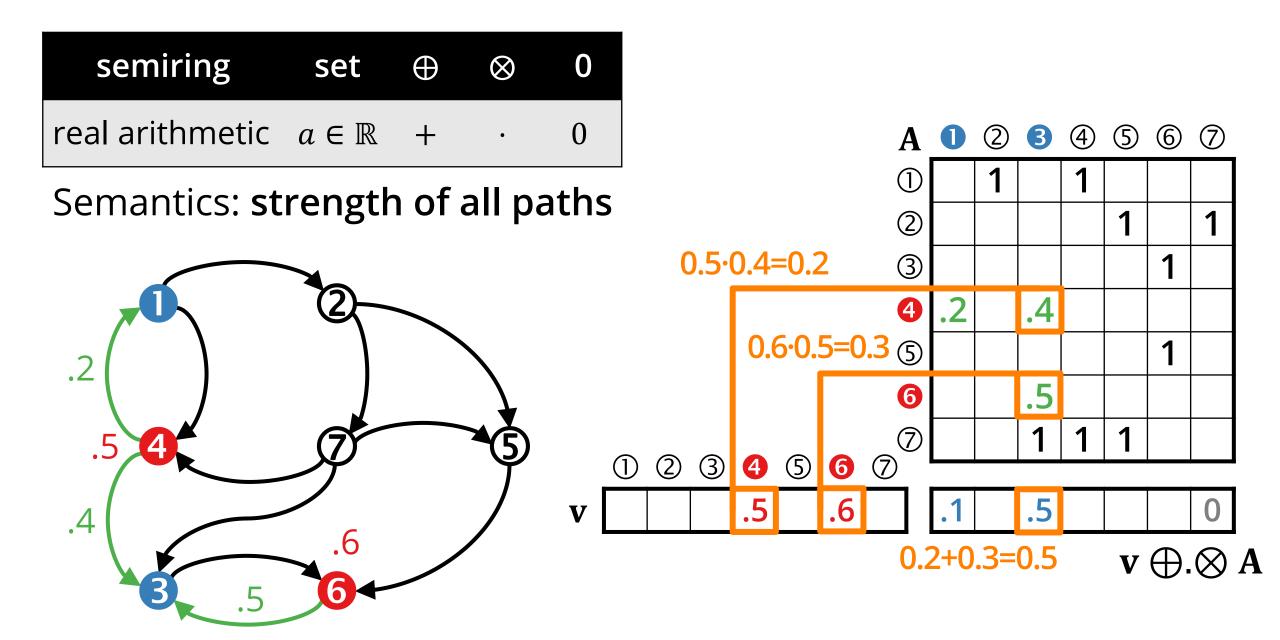


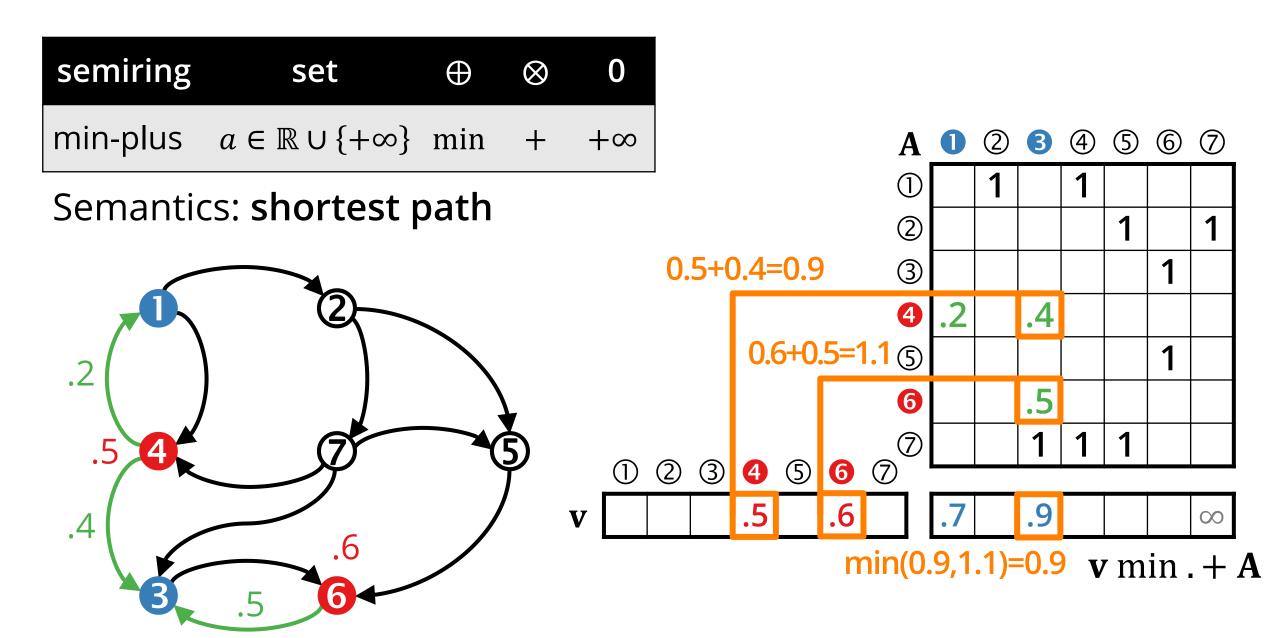


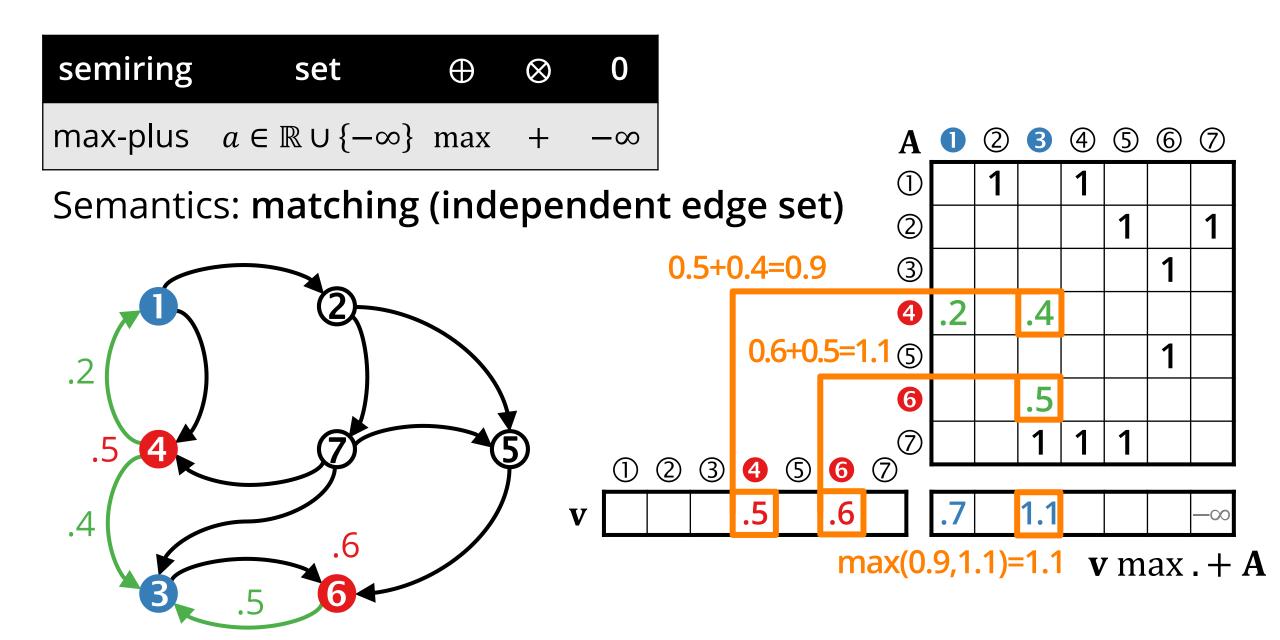
Semantics: reachability

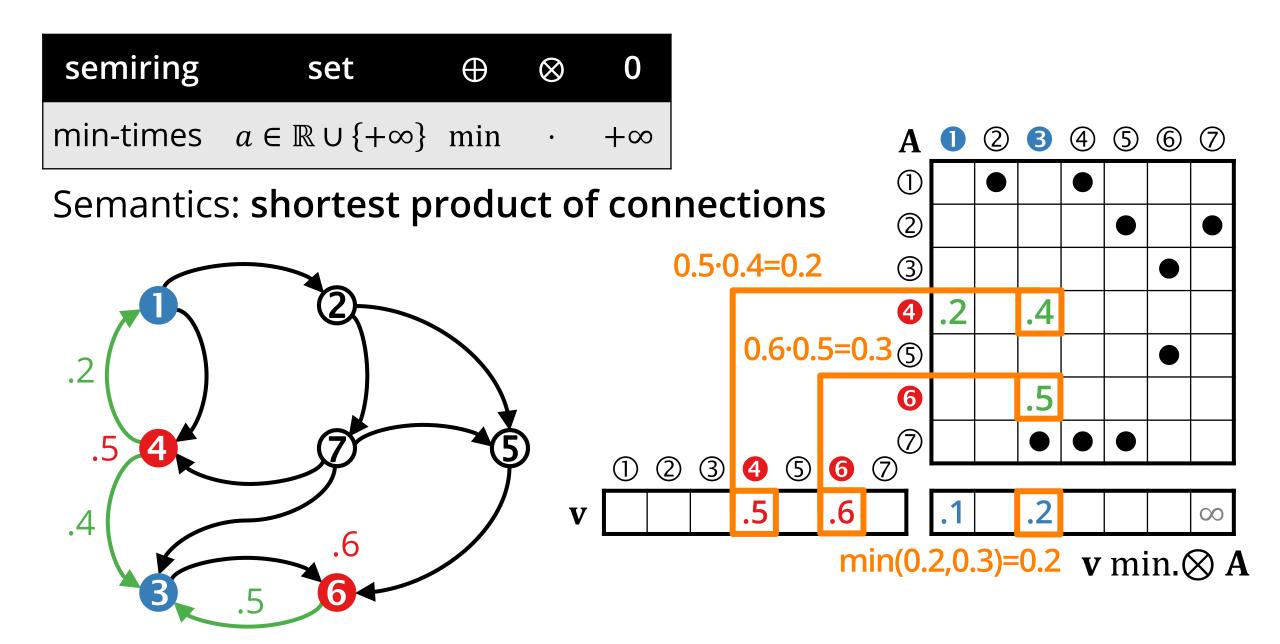


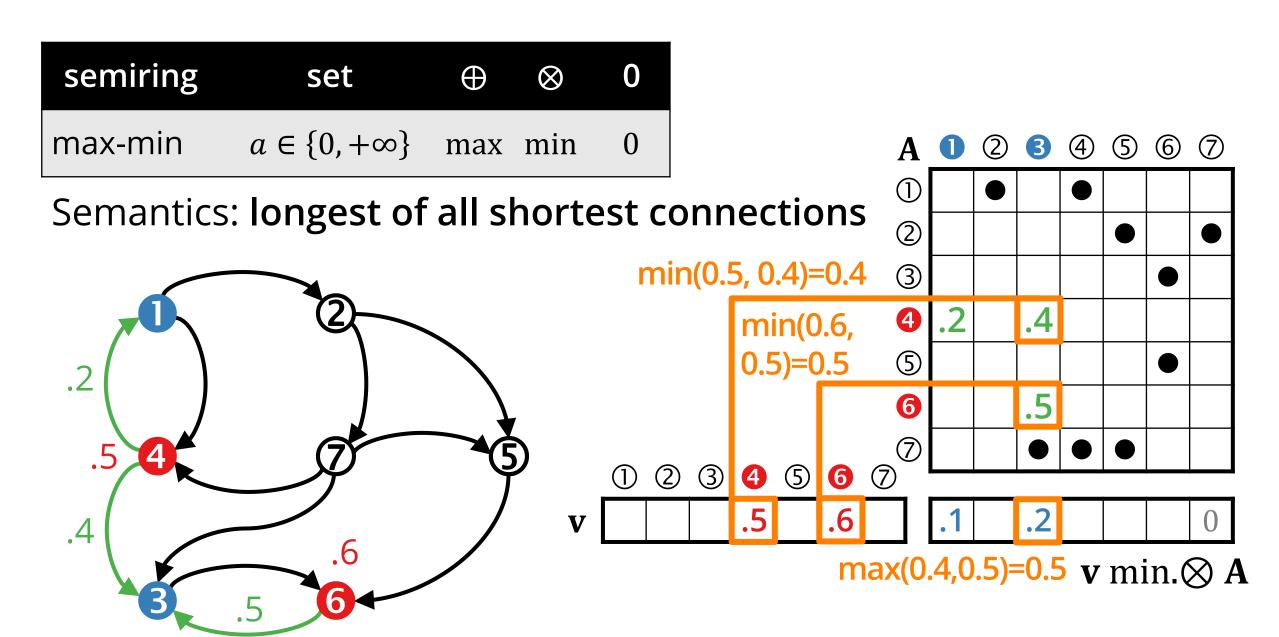




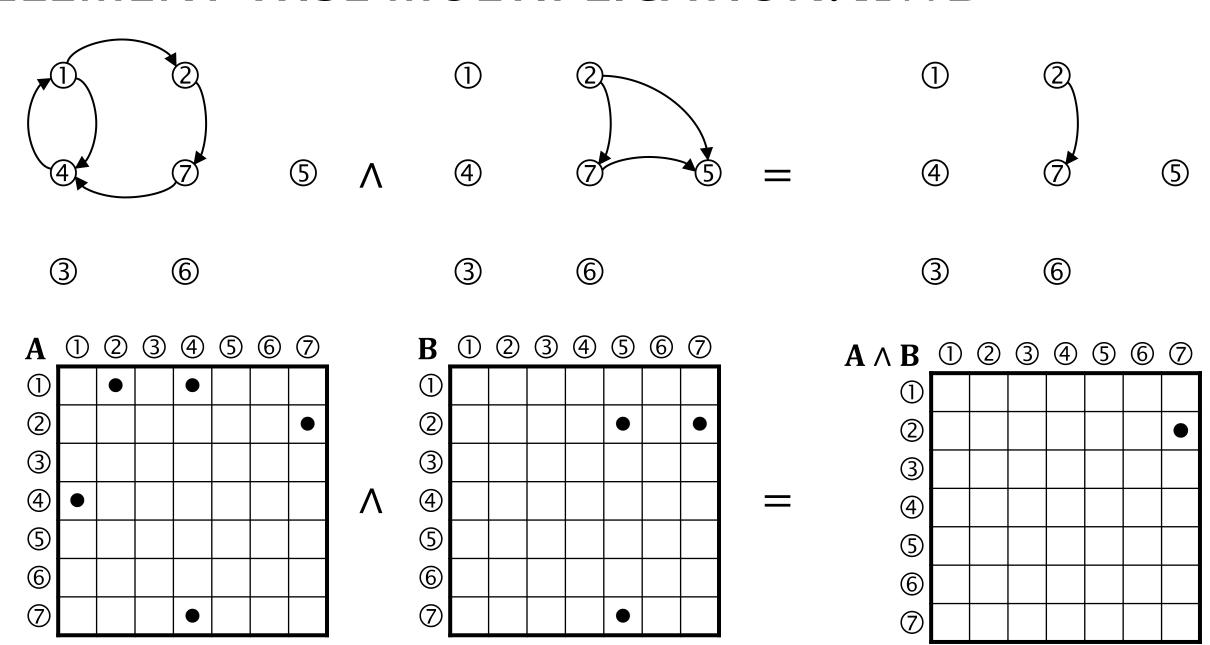




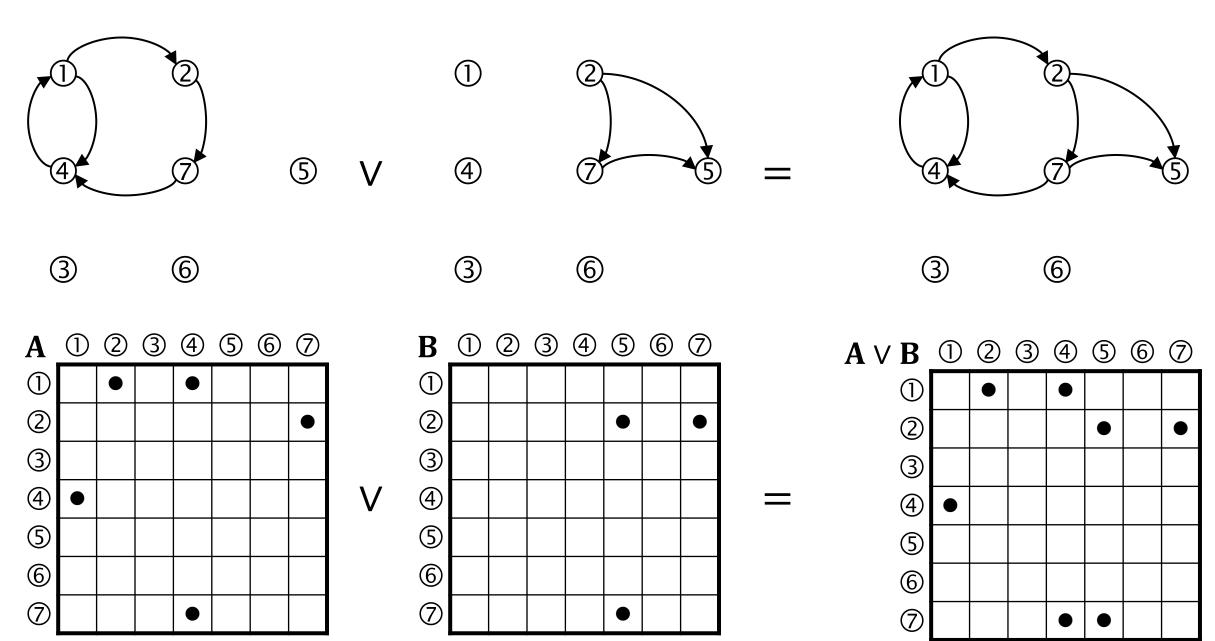




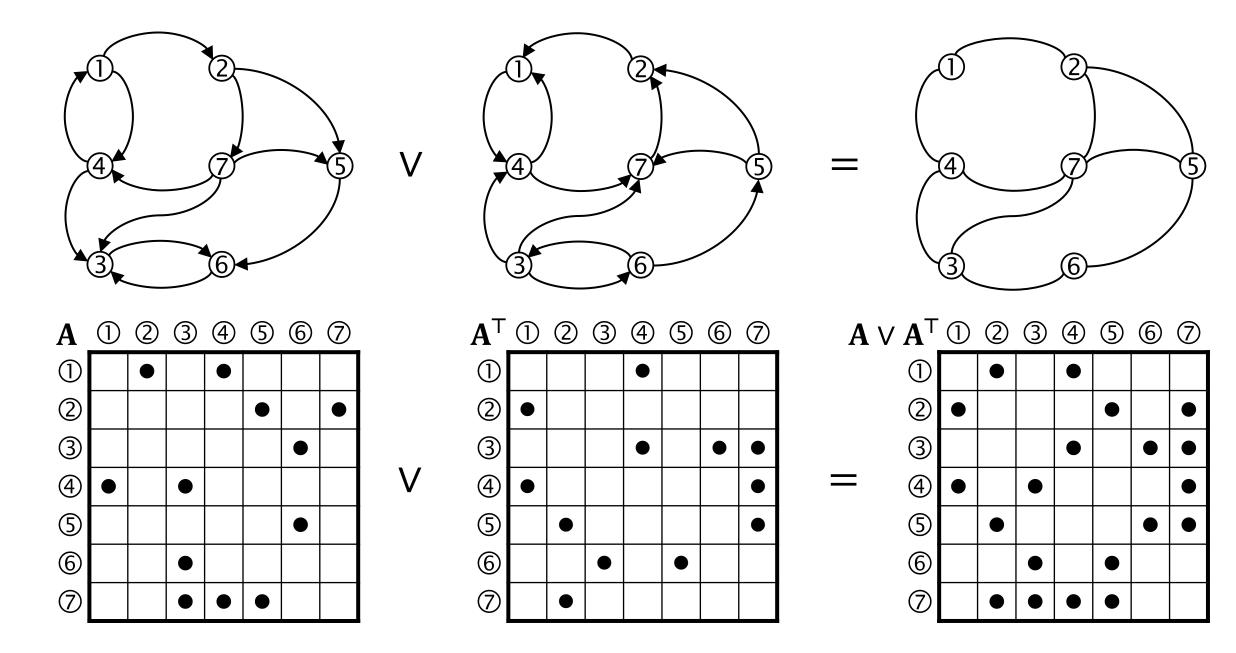
## **ELEMENT-WISE MULTIPLICATION: A ^ B**



## **ELEMENT-WISE ADDITION: A V B**



## TURNING A GRAPH INTO UNDIRECTED: $A \lor A^{\top}$



## **NOTATION\***

- Symbols:
  - **A**, **B**, **C**, **M** matrices
  - o u, v, w, m vectors
  - ∘ *s* scalar
  - $\circ$  *i, j* indices
  - $\circ \langle M \rangle, \langle m \rangle$  masks
- Operators:
  - ⊕ addition
  - ⊗ multiplication
  - o <sup>⊤</sup> transpose
  - Ø element-wise division

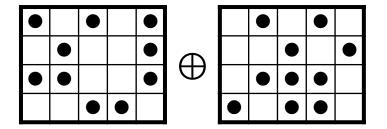
matrix-matrix multiplication $\mathbf{C}\langle\mathbf{M}\rangle = \mathbf{A} \oplus . \otimes \mathbf{I}$	
$\triangle \bigcirc \bigcirc$ vector matrix multiplication $\neg \neg \neg \neg \bigcirc \bigcirc \bigcirc$	_
$\oplus . \otimes$ vector-matrix multiplication $\mathbf{w} \langle \mathbf{m} \rangle = \mathbf{v} \oplus . \otimes A$	A
matrix-vector multiplication $\mathbf{w}\langle\mathbf{m}\rangle = \mathbf{A} \oplus . \otimes \mathbf{v}$	V
element-wise multiplication $\mathbf{C}\langle \mathbf{M} \rangle = \mathbf{A} \otimes \mathbf{B}$	
(set intersection of patterns) $\mathbf{w}\langle\mathbf{m}\rangle = \mathbf{u}\otimes\mathbf{v}$	
$\bigoplus \qquad \text{element-wise addition} \qquad \underline{\mathbf{C}\langle\mathbf{M}\rangle = \mathbf{A} \oplus \mathbf{B}}$	
(set union of patterns) $\mathbf{w}\langle\mathbf{m}\rangle = \mathbf{u} \oplus \mathbf{v}$	
$f = \text{apply upary operator} \qquad C\langle \mathbf{M} \rangle = f(\mathbf{A})$	
$f$ apply unary operator $\frac{\mathbf{w}\langle \mathbf{m}\rangle = f(\mathbf{v})}{\mathbf{w}\langle \mathbf{m}\rangle = f(\mathbf{v})}$	
reduce to vector $\mathbf{w}\langle\mathbf{m}\rangle = [\bigoplus_j \mathbf{A}(:$	,j)]
$[\bigoplus \cdots] {\text{reduce to scalar}} s = [\bigoplus_{ij} \mathbf{A}(i)]$	(i,j)
$\mathbf{A}^{T}$ transpose matrix $\mathbf{C}\langle\mathbf{M}\rangle = \mathbf{A}^{T}$	

Vectors can act as both column and row vectors.

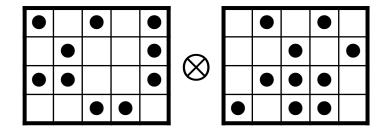
(Notation omitted for accumulator, selection, extraction, assignment...)

# LINEAR ALGEBRAIC PRIMITIVES FOR GRAPHS #1

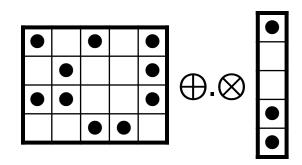
Element-wise addition: union of non-zero elements



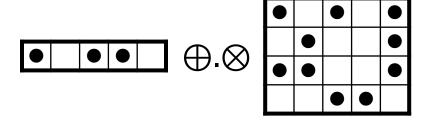
Element-wise multiplication: intersection of non-zero elements



Sparse matrix times sparse vector: process incoming edges

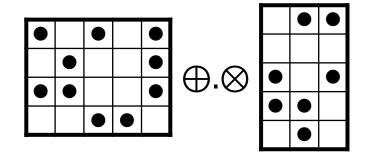


Sparse vector times sparse matrix: process outgoing edges

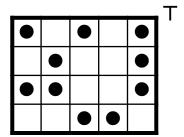


### LINEAR ALGEBRAIC PRIMITIVES FOR GRAPHS #2

Sparse matrix times sparse matrix: process connecting outgoing edges

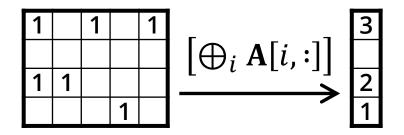


Matrix transpose: reverse edges

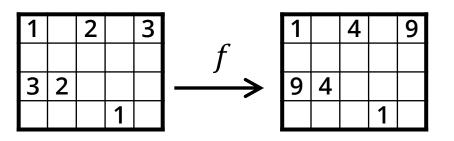


**Reduction:** 

aggregate values in each row



Apply: apply unary operator on all values



#### **ALGORITHMS**

- Breadth-first search
  - Levels
  - Parents
  - Multi-source
- Bellman-Ford
- PageRank
- Triangle count
  - Naïve
  - Masked
  - Cohen's algorithm
  - o Sandia

- o CMU
- Local clustering coefficient
- k-truss
- CDLP (Community Detection using Label Propagation)

Breadth-first search

# **BFS: BREADTH-FIRST SEARCH**

# • Algorithm:

- Start from a given vertex
- "Explore all neighbour vertices at the present level prior to moving on to the vertices at the next level" [Wikipedia]

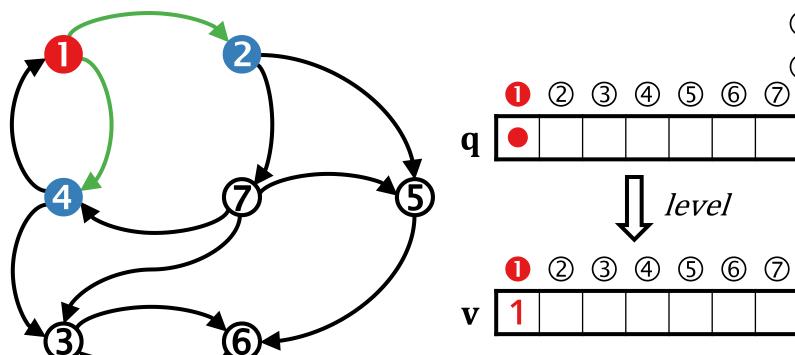
#### Variants:

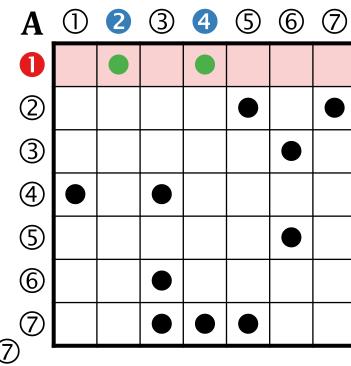
- Levels compute traversal level for each vertex
- o **Parents** compute parent for each vertex
- MSBFS start traversal from multiple source vertices

Breadth-first search / Levels

semiring	set	$\oplus$	$\otimes$	0
lor-land	$a \in \{F, T\}$	V	٨	F

level = 1



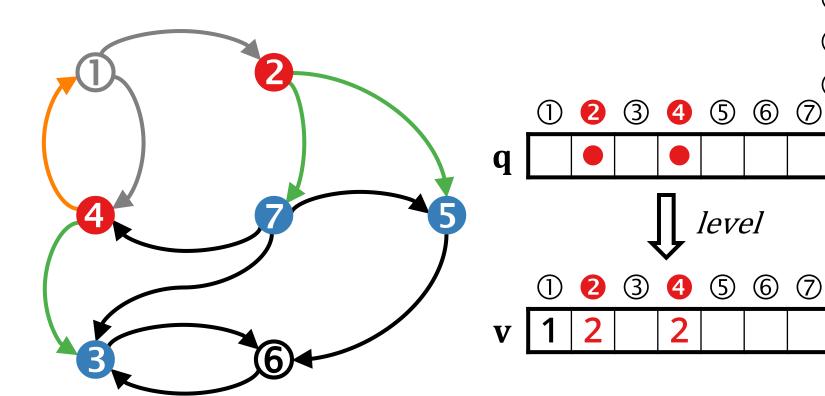


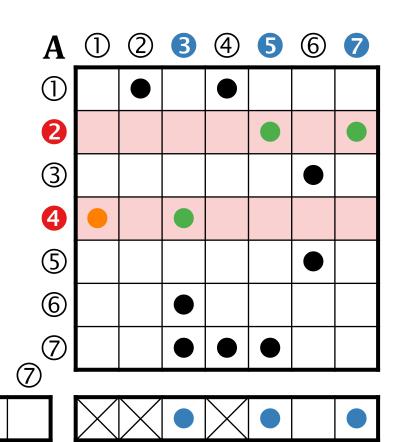


$$\mathbf{q}'\langle \overline{\mathbf{v}}\rangle = \mathbf{q} \lor . \land \mathbf{A}$$

semiring	set	$\oplus$	$\otimes$	0
lor-land	$a \in \{F, T\}$	V	٨	F

level = 2

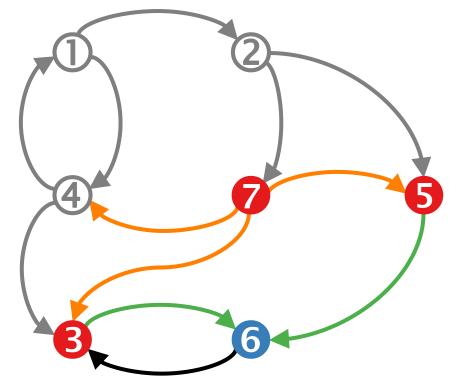


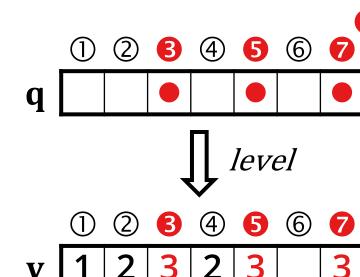


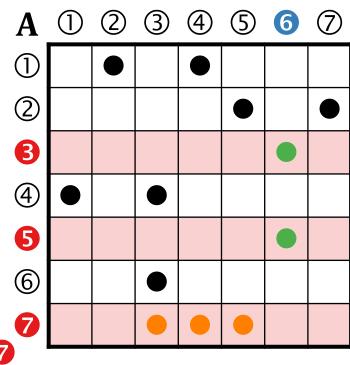
$$\mathbf{q}'\langle \overline{\mathbf{v}}\rangle = \mathbf{q} \vee . \wedge \mathbf{A}$$

semiring	set	$\oplus$	$\otimes$	0
lor-land	$a \in \{F, T\}$	V	٨	F

level = 3



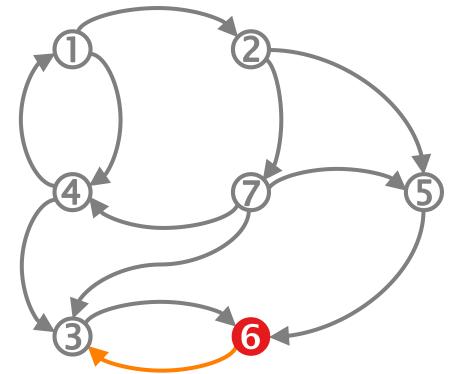


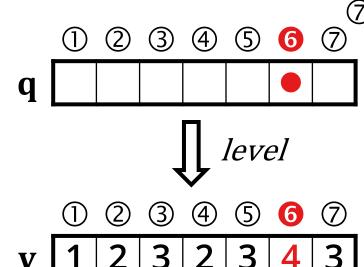


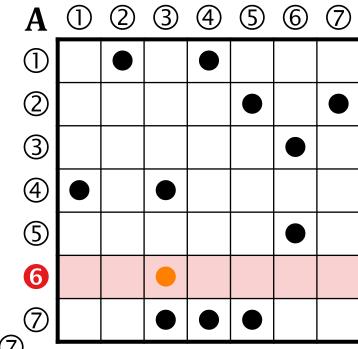
$$\mathbf{q}'\langle \overline{\mathbf{v}}\rangle = \mathbf{q} \lor . \land \mathbf{A}$$

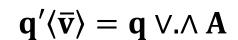
semiring	set	$\oplus$	$\otimes$	0
lor-land	$a \in \{F, T\}$	V	٨	F

level = 4









q' is empty → terminate

### **BFS – LEVELS: ALGORITHM**

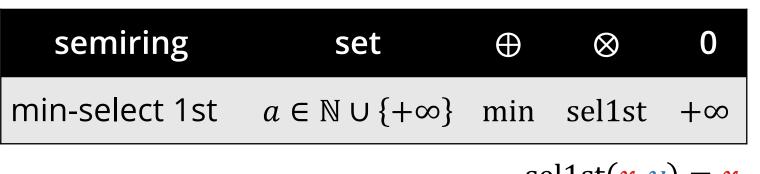


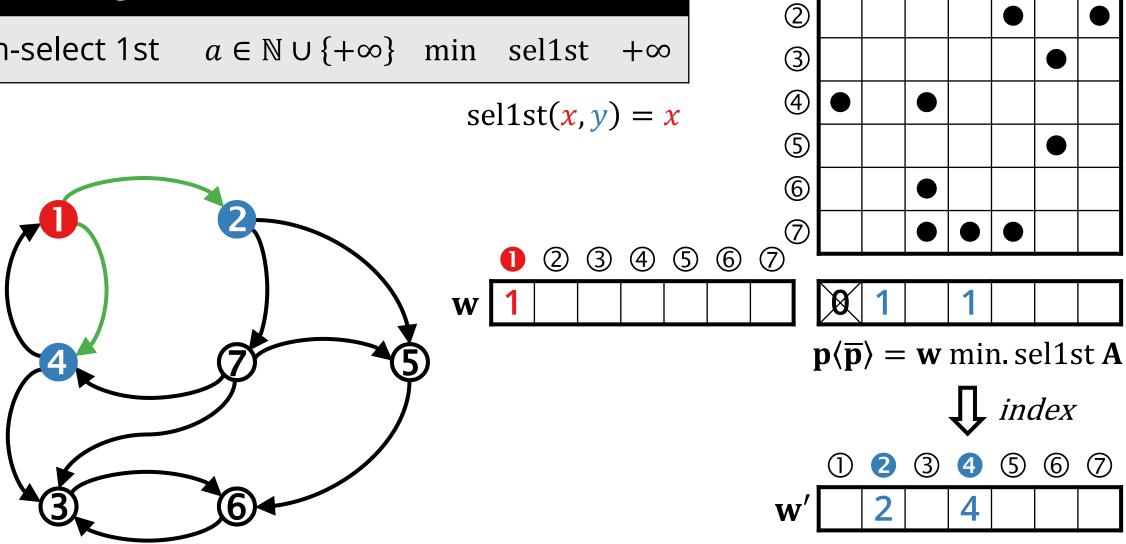
- Input: adjacency matrix **A**, source vertex *s*, #vertices *n*
- Output: vector of visited vertices v (integer)
- Workspace: queue vector q (Boolean)

- 1. q(s) = T
- 2. for level = 1 to n 1 \*terminate earlier if **q** is empty
- 3.  $\mathbf{v}\langle\mathbf{q}\rangle = level$  only change the values under the mask
- 4.  $clear(\mathbf{q})$  set all elements of  $\mathbf{q}$  to  $\mathbf{F}$
- 5.  $\mathbf{q}\langle \overline{\mathbf{v}} \rangle = \mathbf{q} \vee A$  use the lor-land semiring

Breadth-first search / Parents

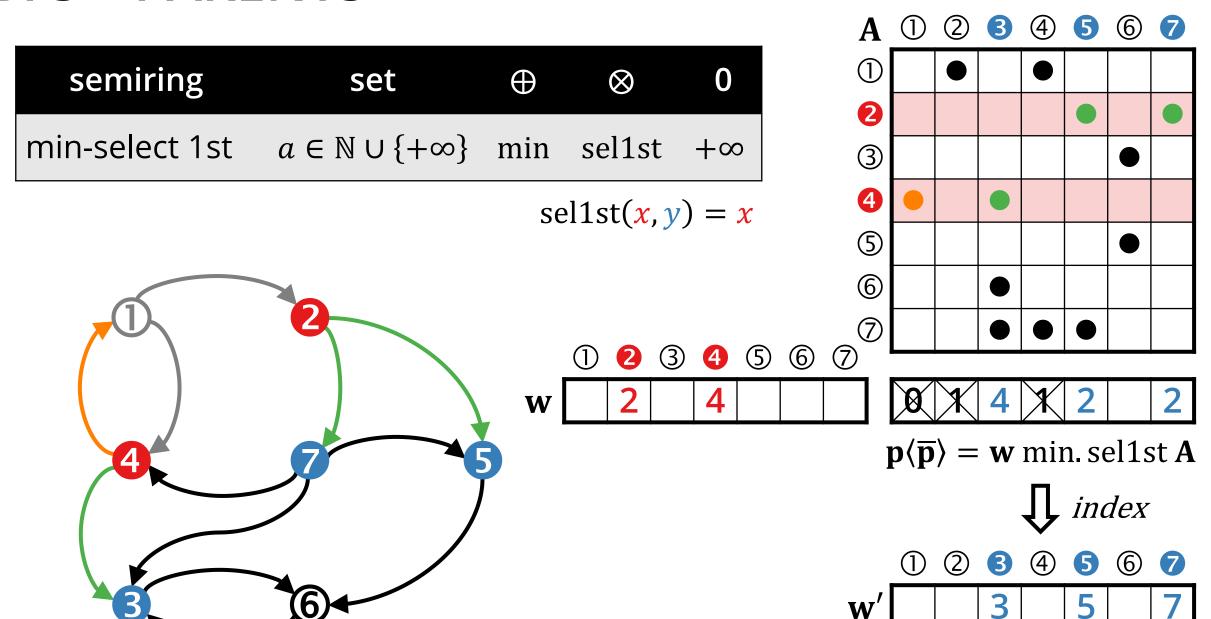
### **BFS – PARENTS**



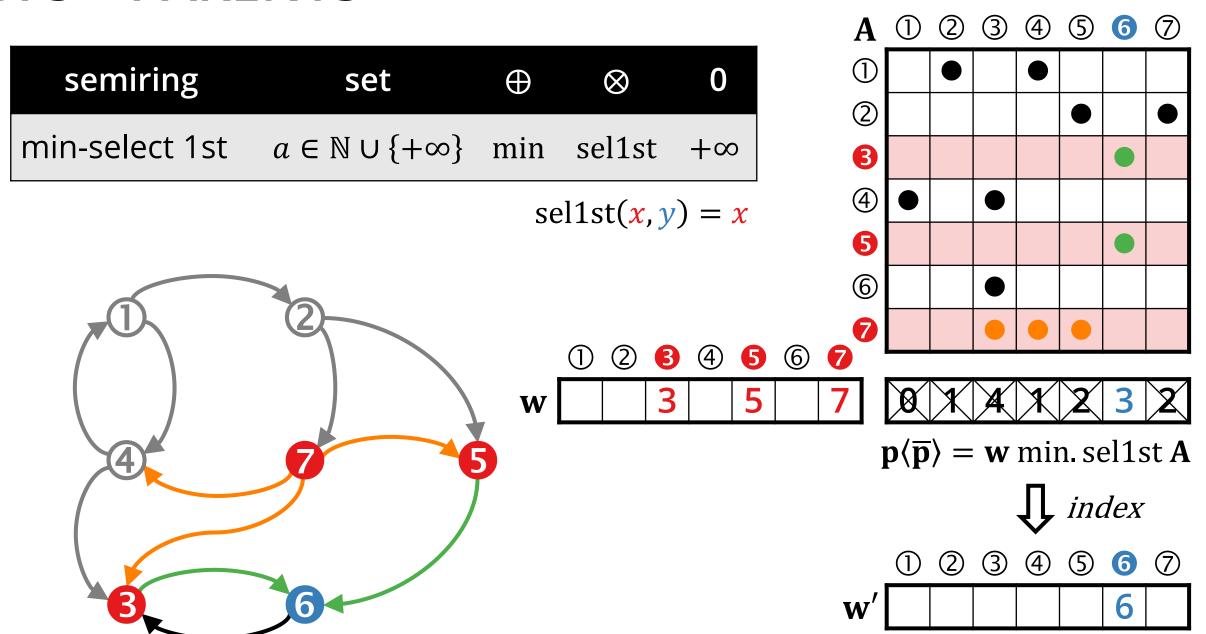


2 3 4 5 6 7

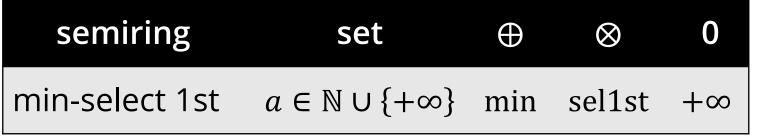
### **BFS - PARENTS**

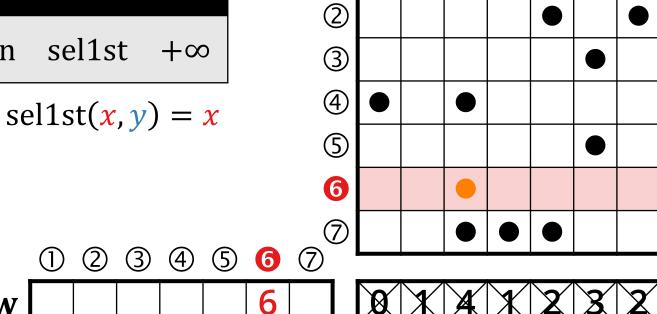


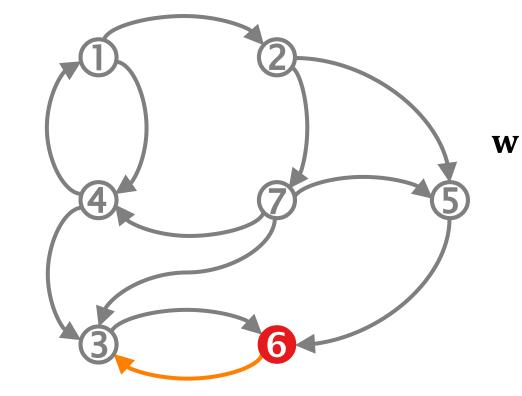
### **BFS - PARENTS**



### **BFS – PARENTS**



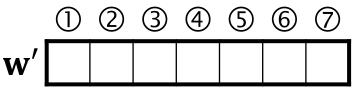




w' is empty → terminate



 $\mathbf{p}\langle \overline{\mathbf{p}}\rangle = \mathbf{w} \text{ min. sel1st } \mathbf{A}$ 



2 3 4 5

6 7

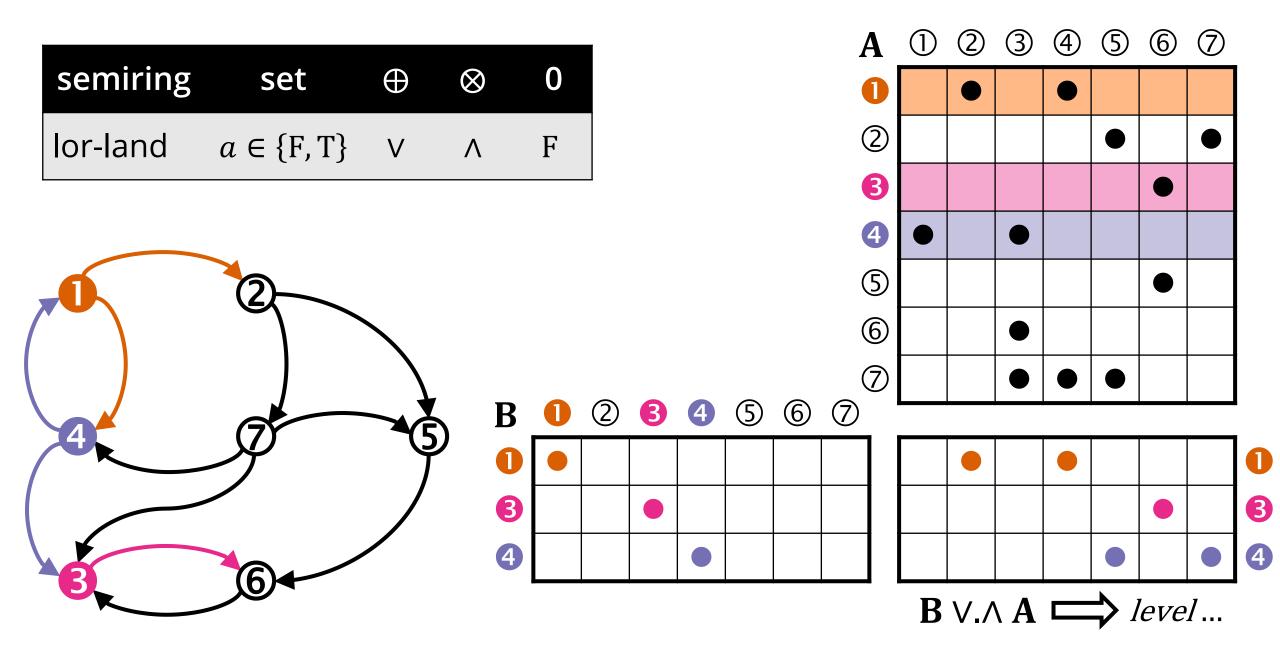
# **BFS - PARENTS: ALGORITHM**



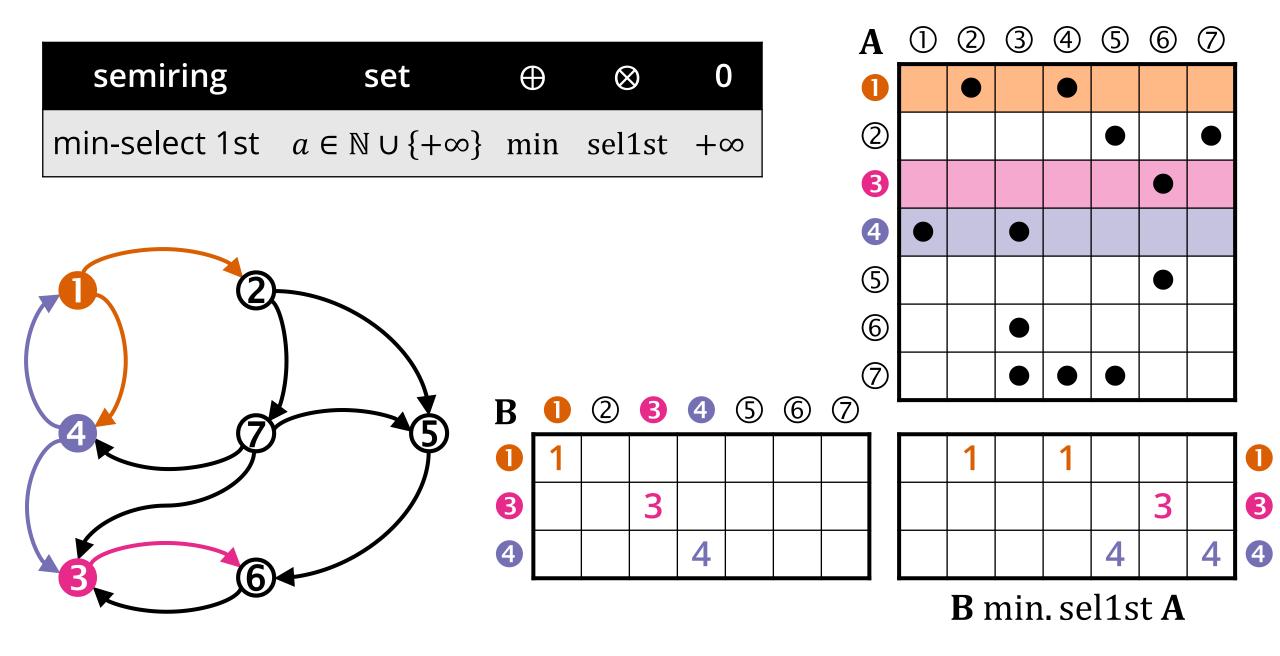
- Input: adjacency matrix **A**, source vertex *s*, #vertices *n*
- Output: parent vertices vector p (integer)
- Workspace: vertex index vector x (integer), wavefront vector w (integer), unvisited vertices vector u (Boolean)
- 1.  $\mathbf{x} = [1 \ 2 \ ... \ n]$
- 2. w(s) = s
- 3. for l = 1 to n 1 \*terminate earlier if we reach a fixed point
- 4.  $\mathbf{u} = \operatorname{pattern}(\overline{\mathbf{p}})$
- 5.  $\mathbf{p}\langle \mathbf{u}\rangle = \mathbf{w} \text{ min. sel1st } \mathbf{A}$
- 6.  $\mathbf{w}\langle \mathbf{u} \rangle = \operatorname{pattern}(\mathbf{p}) \otimes \mathbf{x}$

Multi-source BFS

### **MULTI-SOURCE BFS – LEVELS**



# **MULTI-SOURCE BFS – PARENTS**



### **BFS – PERFORMANCE**

- Naïve BFS impls are sometimes slow on real graphs with skewed distributions – further optimizations are needed.
- Direction-optimizing BFS was published in 2012.
  - $\circ$  Switches between push (vA) and pull (A<sup>T</sup>v) during execution:
    - Use the push direction when the frontier is small
    - Use the pull direction when the frontier becomes large
  - o Adopted to GraphBLAS in 2018



S. Beamer, K. Asanovic, D. Patterson: Direction-Optimizing Breadth-First Search, SC 2012



C. Yang: *High-performance linear algebra-based graph framework on the GPU,* PhD thesis, UC Davis, 2019



C. Yang, A. Buluç, J.D. Owens: *Implementing Push-Pull Efficiently in GraphBLAS*, ICPP 2018



A. Buluç: *GraphBLAS: Concepts, algorithms, and applications,* Scheduling Workshop, 2019

Single-source shortest path

### SSSP – SINGLE-SOURCE SHORTEST PATHS

#### Problem:

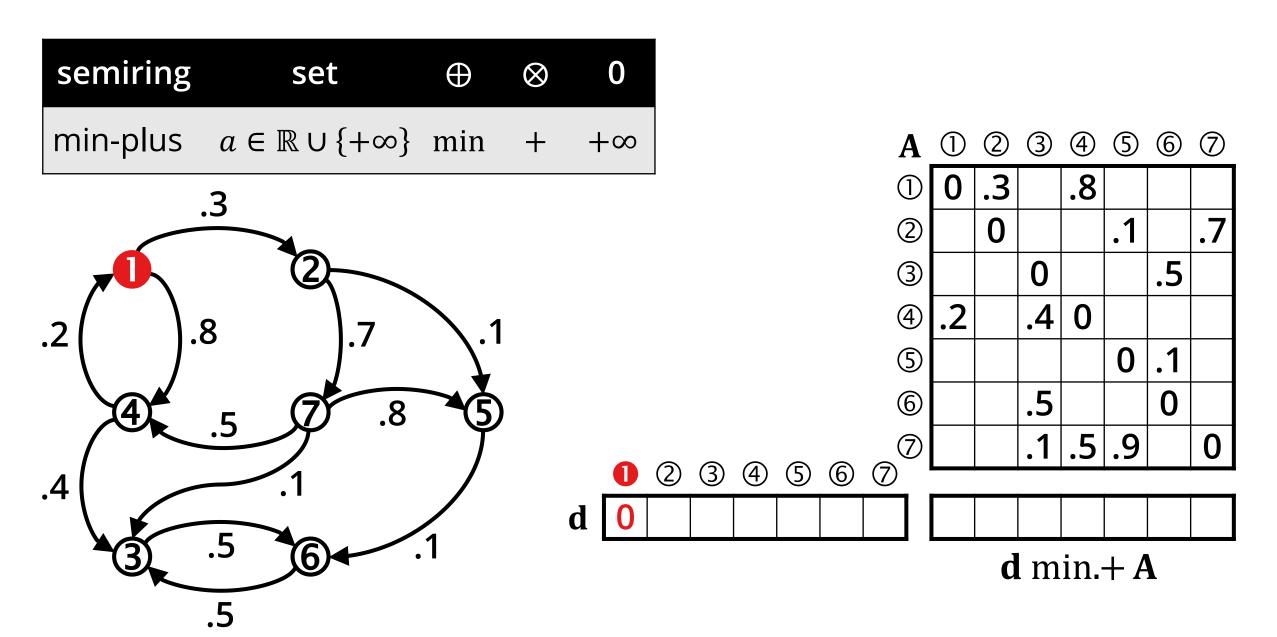
 From a given start vertex s, find the shortest paths to every other (reachable) vertex in the graph

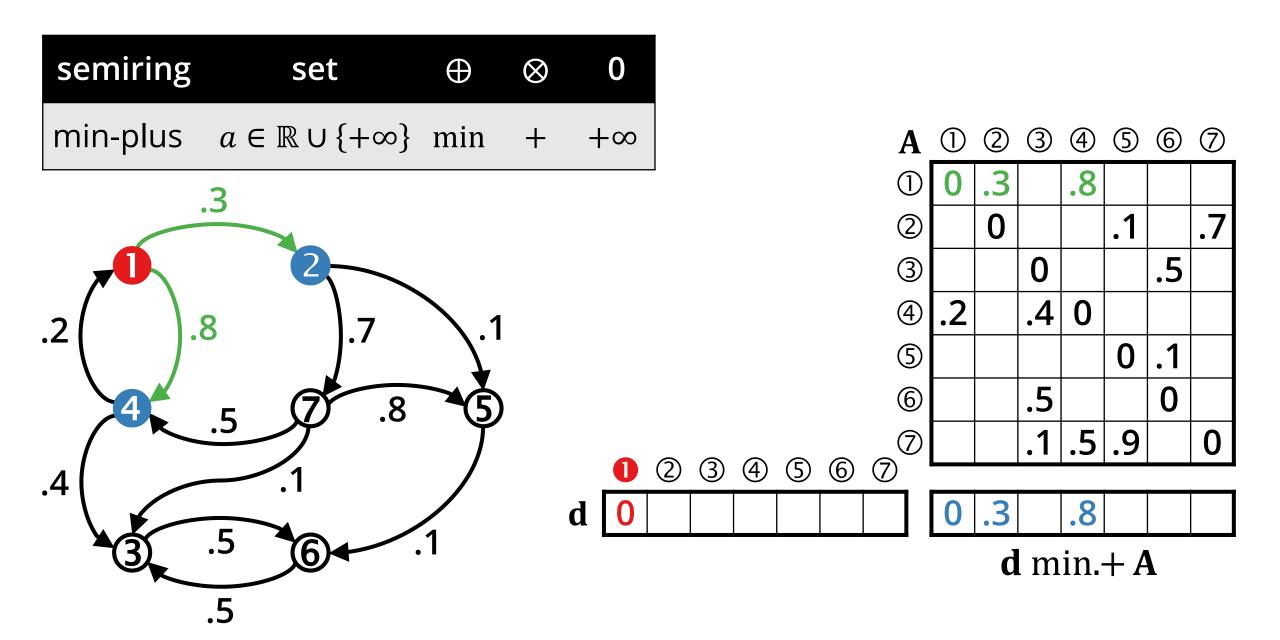
# Bellman-Ford algorithm:

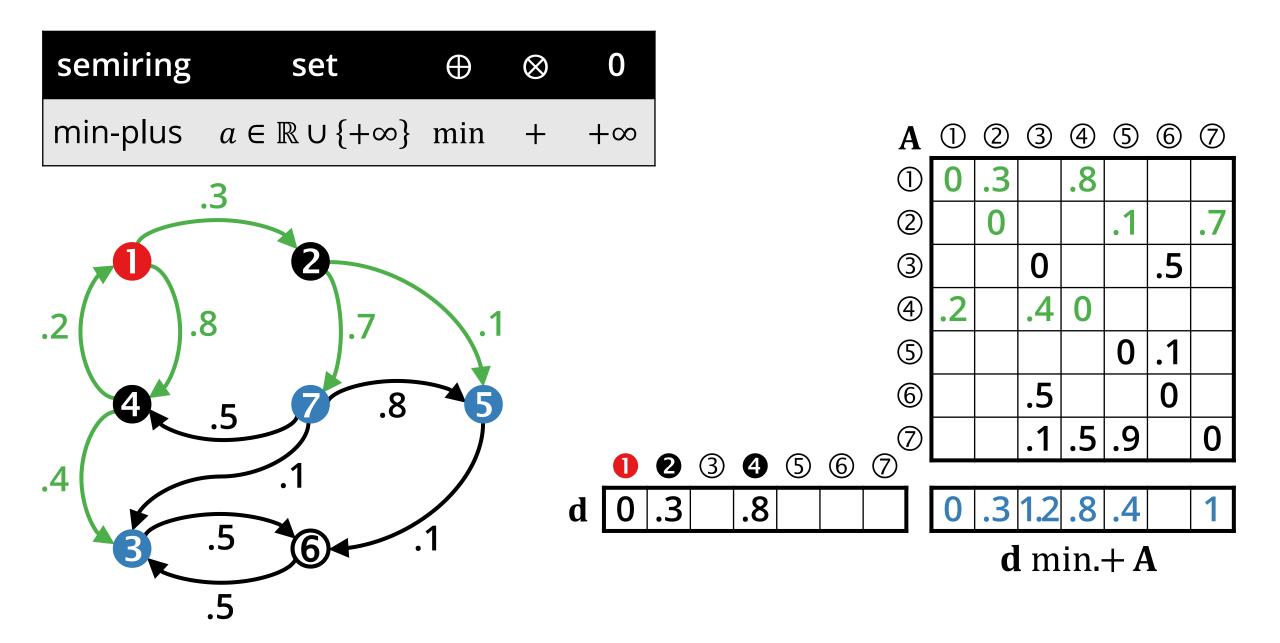
- Relaxes all edges in each step
- $\circ$  Guaranteed to find the shortest path using at most n-1 steps

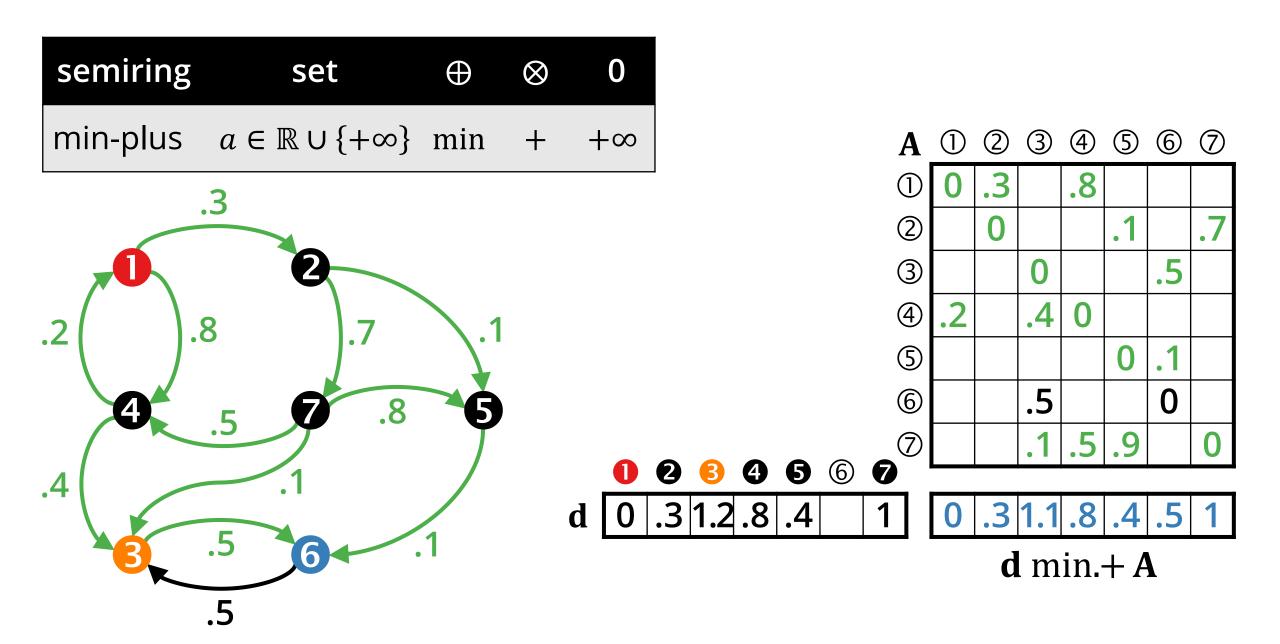
#### Observation:

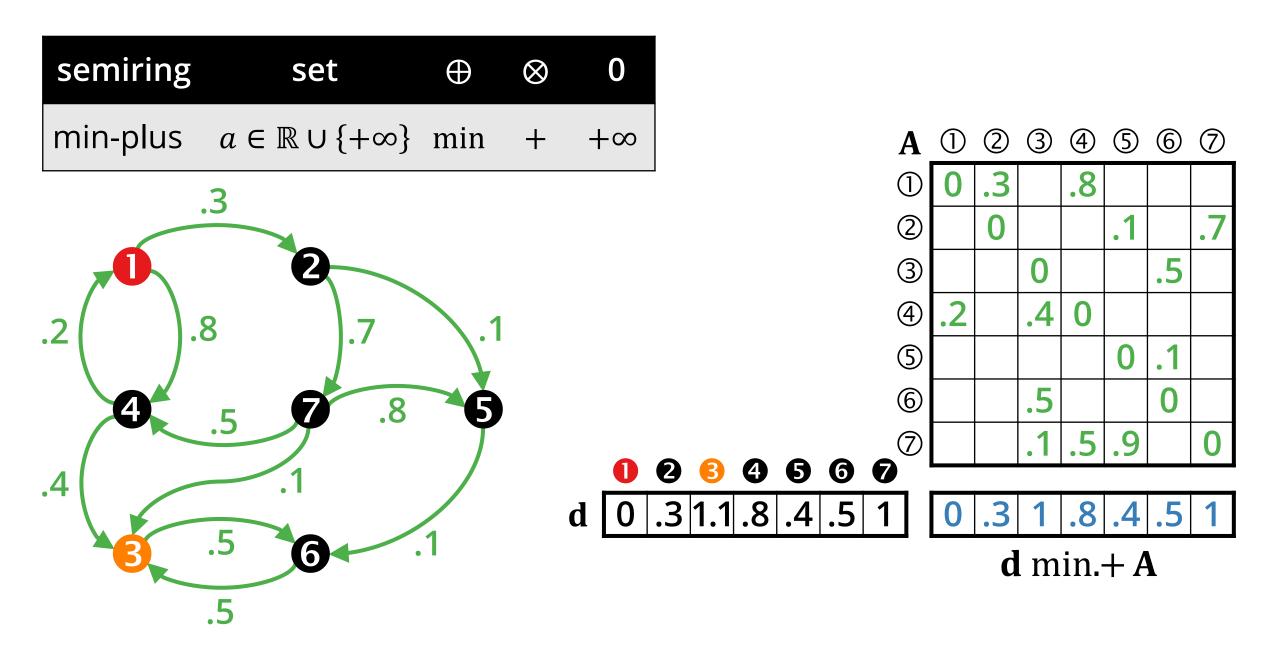
o The relaxation step can be captured using a VM multiplication











# SSSP - ALGEBRAIC BELLMAN-FORD ALGO.



**Input:** adjacency matrix  $\mathbf{A}$ , source vertex s, #vertices n

$$\mathbf{A}_{ij} = \begin{cases} 0 & \text{if } i = j \\ w(e_{ij}) & \text{if } e_{ij} \in E \\ \infty & \text{if } e_{ij} \notin E \end{cases}$$

Output: distance vector d (real)

- 1.  $\mathbf{d} = [\infty \infty ... \infty]$
- 2.  $\mathbf{d}(s) = 0$
- 3. for k = 1 to n 1 \*terminate earlier if we reach a fixed point
- 4.  $\mathbf{d} = \mathbf{d} \min + \mathbf{A}$

Optimizations for BFS (push/pull) also work here.

PageRank

# PAGERANK - DEFINITION (AS IN GRAPHALYTICS)

We use one of the simpler definitions. For k = 1 to t iterations:

$$\operatorname{PR}_0(v) = \frac{1}{n}, \quad \mathbf{d}(v) = \begin{cases} 1 & \text{if } \deg(v) \ge 1\\ 0 & \text{otherwise} \end{cases}$$

$$PR_{k}(v) = \frac{1 - \alpha}{n} + \alpha \cdot \sum_{u \in N_{\text{in}}(v)} \frac{PR_{k-1}(u)}{|N_{\text{out}}(u)|} + \frac{\alpha}{n} \cdot \sum_{w \in d} PR_{k-1}(w)$$
teleport influence dangling

 $\alpha$ : damping factor; d: dangling vertices,  $d = \{w \in V \mid |N_{\text{out}}| = 0\}$ 

There are dozens of PR definitions, some treat dangling vertices differently.

#### PAGERANK – IN LINEAR ALGEBRA

Initially:

$$\mathbf{pr}_0 = [1 \ 1 \ ... \ 1] \oslash n, \qquad \mathbf{d} = [\bigvee_j \mathbf{A}(:,j)]$$

In each iteration:

$$PR_k(v) = \frac{1-\alpha}{n} + \alpha \cdot \sum_{u \in N_{\text{in}}(v)} \frac{PR_{k-1}(u)}{|N_{\text{out}}(u)|} + \frac{\alpha}{n} \cdot \sum_{w \in d} PR_{k-1}(w)$$

$$\mathbf{pr}_{k} = \underbrace{\frac{1 - \alpha}{n}}_{\text{constant}} \oplus \alpha \otimes \left(\frac{\mathbf{pr}_{k-1}}{\mathbf{d}}\right) \oplus \otimes \mathbf{A} \oplus \underbrace{\frac{\alpha}{n} \otimes \left[\oplus_{i} \left(\mathbf{pr}_{k} \otimes \mathbf{d}\right)_{i}\right]}_{\text{element-wise sparse vector-}}$$

dense vector multiplication

# PAGERANK - ALGORITHM



**Input:** adjacency matrix **A**, damping factor  $\alpha$ , #iterations t, #vertices n

Output: PageRank pr (real)

Workspace: dangling vertices d (Boolean)

- 1.  $pr = [1 \ 1 \dots 1] \oslash n$
- 2.  $\mathbf{d} = \begin{bmatrix} \bigvee_{j} \mathbf{A}(:,j) \end{bmatrix}$
- 3. for k = 1 to t

4. 
$$\mathbf{pr} = \frac{1 - \alpha}{n} \oplus \alpha \otimes \left(\frac{\mathbf{pr}}{\mathbf{d}}\right) \oplus \otimes \mathbf{A} \oplus \frac{\alpha}{n} \otimes \left[\oplus_{i} (\mathbf{pr} \otimes \mathbf{d})_{i}\right]$$

PageRank variant using Markov models are more difficult to express.

Local clustering coefficient

# LCC: LOCAL CLUSTERING COEFFICIENT

$$LCC(v) = \frac{\text{\#edges between neighbours of } v}{\text{\#possible edges between neighbours of } v}$$

If 
$$|N(v)| \leq 1$$
, LCC $(v) = 0$ 

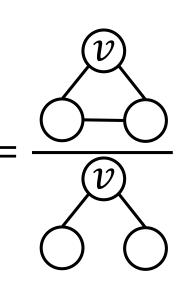
Important metric in social network analysis.

The numerator is the number of *triangles* in v, tri(v).

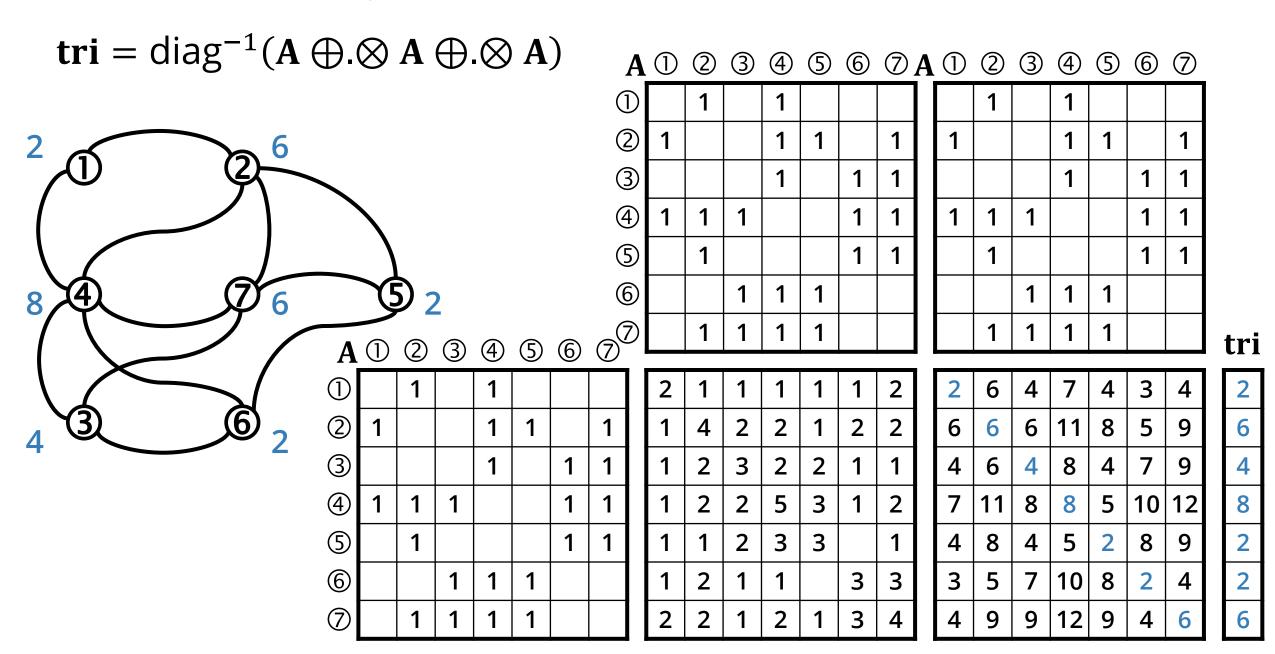
The denominator is the number of wedges in v, wed(v).

$$LCC(v) = \frac{tri(v)}{wed(v)}$$

The difficult part is tri(v).



## LCC EXAMPLE: NAÏVE APPROACH



#### LCC: NUMBER OF TRIANGLES IN EACH VERTEX

**Observation:** Matrix  $\mathbf{A} \oplus . \otimes \mathbf{A} \oplus . \otimes \mathbf{A}$  is not sparse.

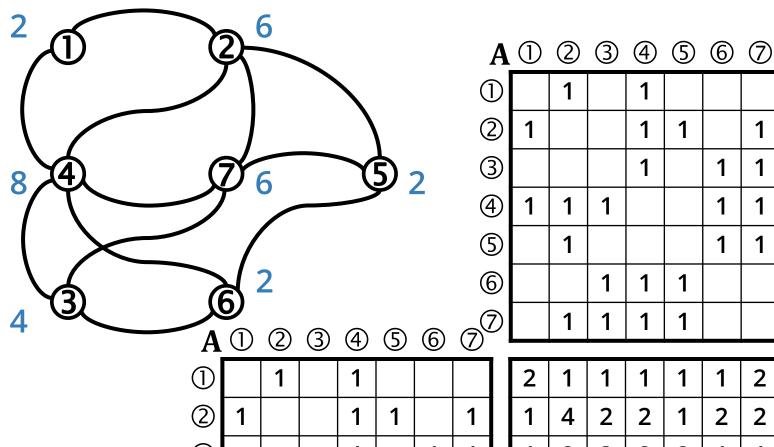
**Optimization:** Use element-wise multiplication ⊗ to close wedges into triangles:

$$TRI = A \oplus . \otimes A \otimes A$$

Then, perform a row-wise summation to get the number of triangles in each row:

$$\mathbf{tri} = \left[ \bigoplus_{j} \mathbf{TRI}(:,j) \right]$$

## LCC EXAMPLE: ELEMENT-WISE MULTIPLICATION



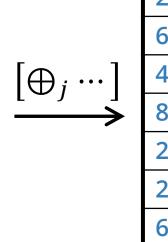
TRI = A	$A \oplus$	$A \otimes A$	$\otimes$ A
tri =	$\bigoplus_{i}$	TRI(:	,j)

$\mathbf{A}$	(1)	(2)	(3)	(4)	(5)	6	(7)
1		1		1			
2	1			1	1		1
3				1		1	1
(a) (b) (c) (d) (d) (d) (d) (e) (e) (e) (e) (e) (e) (e) (e) (e) (e	1	1	1			1	1
(5)		1				1	1
6			1	1	1		
7		1	1	1	1		

2	1	1	1	1	1	2
1	4	2	2	1	2	2
1	2	3	2	2	1	1
1	2	2	5	3	1	2
1	1	2	3	3		1
1	2	1	1		3	3
2	2	1	2	1	3	4

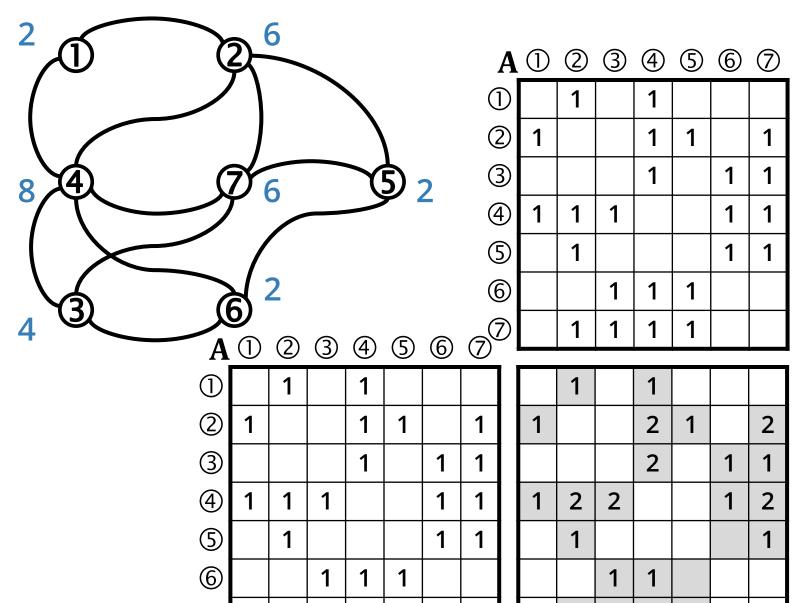
	1		1			
1			2	1		2
			2		1	1
1	2	2			1	2
	1					1
		1	1			
	2	1	2	1		

**TRI** 



tri

### LCC EXAMPLE: ELEMENT-WISE MULTIPLICATION

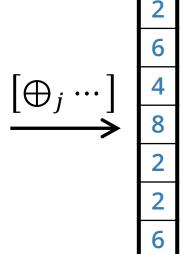


Masking limits where the operation is computed. Here, we use  $\mathbf{A}$  as a mask for  $\mathbf{A} \oplus . \otimes \mathbf{A}$ .

$$TRI\langle A \rangle = A \oplus . \otimes A$$

$$tri = \left[ \bigoplus_{j} TRI(:,j) \right]$$

$$tri$$



### LCC: NUMBER OF WEDGES IN EACH VERTEX

$$LCC(v) = \frac{tri(v)}{wed(v)}$$

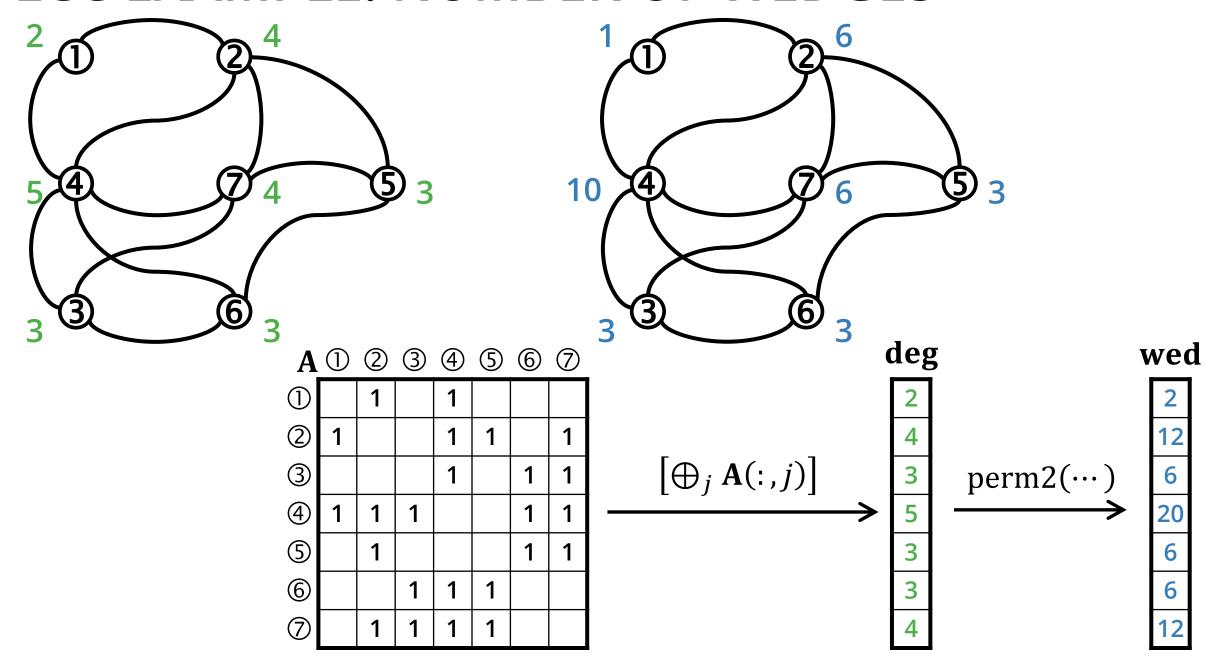
• For wed(v), we determine the #wedges for each vertex as the 2-permutation of its degree:

$$perm2(x) = x \cdot (x - 1)$$

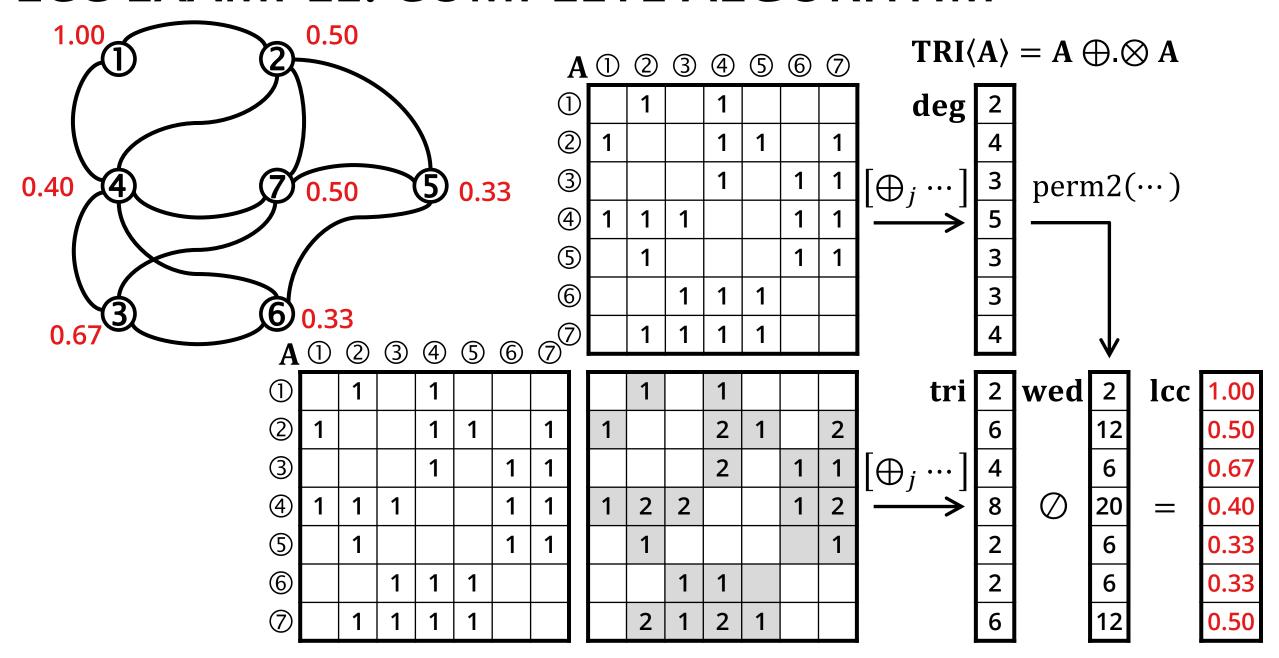
• Given the degrees  $deg = [\bigoplus_j A(:,j)]$ , we compute wed by applying a unary function on the elements of the vector:

$$wed = perm2(deg)$$

### LCC EXAMPLE: NUMBER OF WEDGES



### LCC EXAMPLE: COMPLETE ALGORITHM



### LCC: ALGORITHM



Input: adjacency matrix A

Output: vector lcc

Workspace: matrix TRI, vectors deg, lcc, and wed

- 1.  $TRI(A) = A \oplus . \otimes A$  triangle count matrix
- 2.  $\mathbf{tri} = \left[ \bigoplus_{i} \mathbf{TRI}(:,j) \right]$  triangle count vector
- 3.  $deg = [\bigoplus_{i} A(:,j)]$  vertex degree vector
- 4.  $\mathbf{wed} = \text{perm2}(\mathbf{deg})$  wedge count vector
- 5.  $lcc = tri \oslash wed$  LCC vector



M. Aznaveh, J. Chen, T.A. Davis, B. Hegyi, S.P. Kolodziej, T.G. Mattson, G. Szárnyas: *Parallel GraphBLAS with OpenMP,* Workshop on Combinatorial Scientific Computing 2020

### LCC: FURTHER OPTIMIZATIONS

Further optimization: use L, the lower triangular part of A.

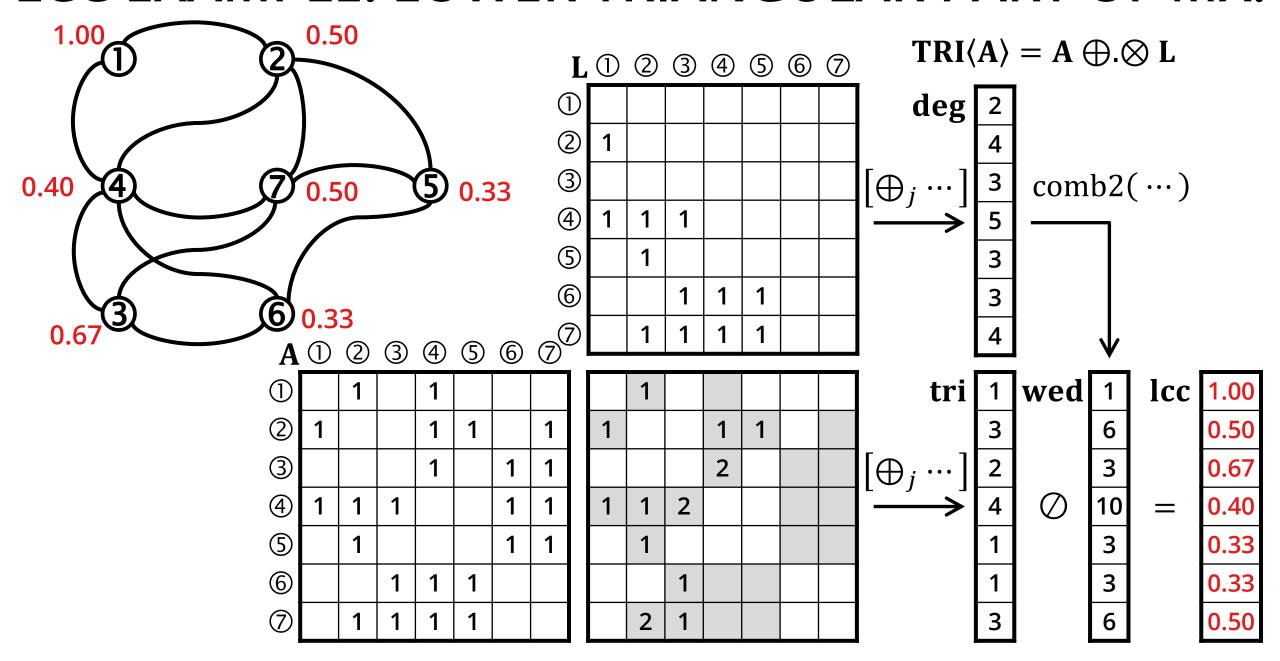
$$TRI\langle A \rangle = A \oplus . \otimes L$$

The number of wedges is now the 2-combination of deg.

$$comb2(x) = \frac{x \cdot (x-1)}{2}$$

Permuting the adjacency matrix allows further optimizations.

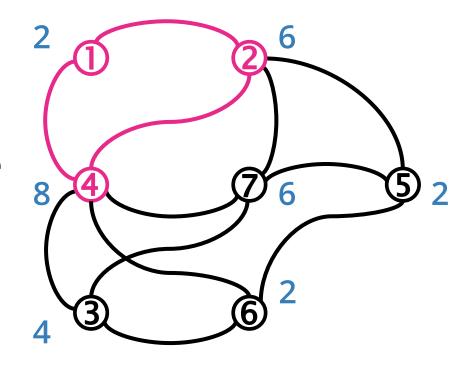
## LCC EXAMPLE: LOWER TRIANGULAR PART OF MX.



Triangle count / Definition

### TRIANGLE COUNT

- IEEE GraphChallenge: an annual competition at the HPEC conference
- The task of the 2017 GraphChallenge was triangle count: given a graph G, count the number of triangles.
- Triangle = "set of three mutually adjacent vertices in a graph"
- Many solutions employed a linear algebraic computation model



Number of unique triangles:

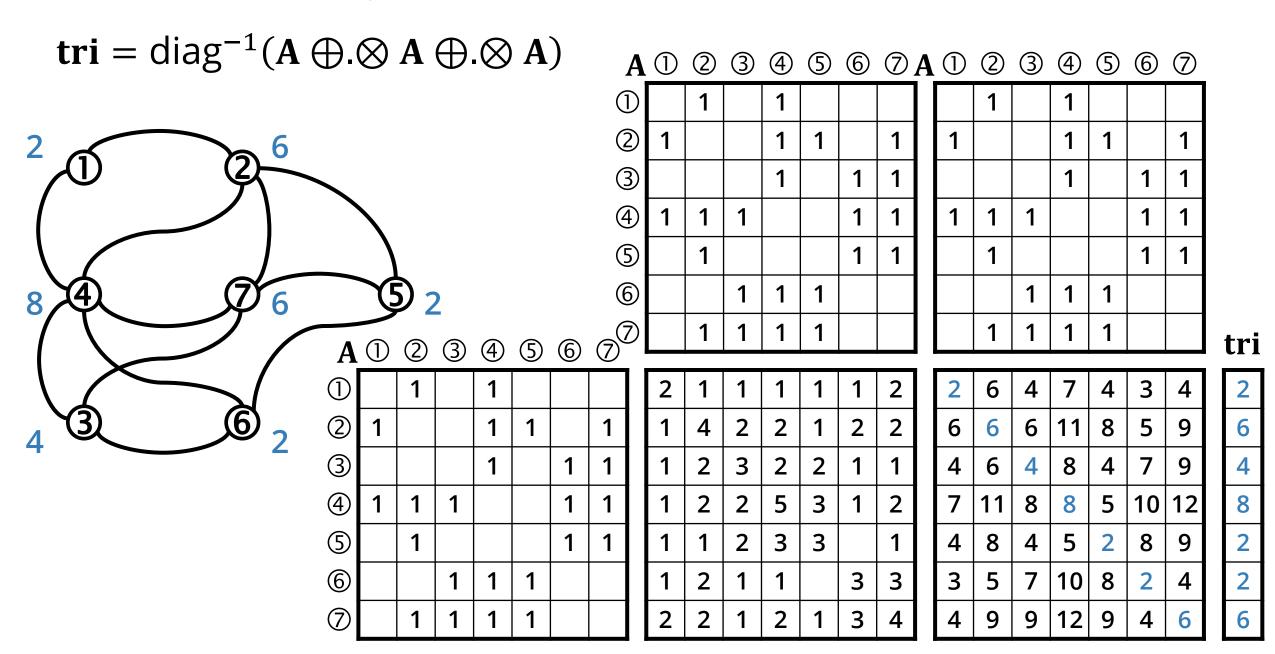
 $\frac{30}{6}$ 



GraphChallenge.org: Raising the Bar on Graph Analytic Performance, HPEC 2018

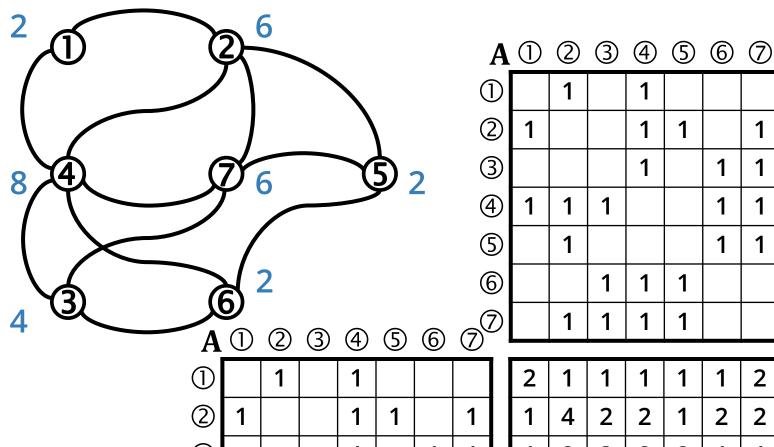
Triangle count / Naïve algorithm

## LCC EXAMPLE: NAÏVE APPROACH



Triangle count / Masked algorithm

## LCC EXAMPLE: ELEMENT-WISE MULTIPLICATION



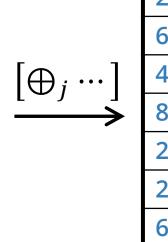
TRI = A	$A \oplus$	$A \otimes A$	$\otimes$ A
tri =	$\bigoplus_{i}$	TRI(:	,j)

$\mathbf{A}$	(1)	(2)	(3)	(4)	(5)	6	(7)
1		1		1			
2	1			1	1		1
3				1		1	1
(a) (b) (c) (d) (d) (d) (d) (e) (e) (e) (e) (e) (e) (e) (e) (e) (e	1	1	1			1	1
(5)		1				1	1
6			1	1	1		
7		1	1	1	1		

2	1	1	1	1	1	2
1	4	2	2	1	2	2
1	2	3	2	2	1	1
1	2	2	5	3	1	2
1	1	2	3	3		1
1	2	1	1		3	3
2	2	1	2	1	3	4

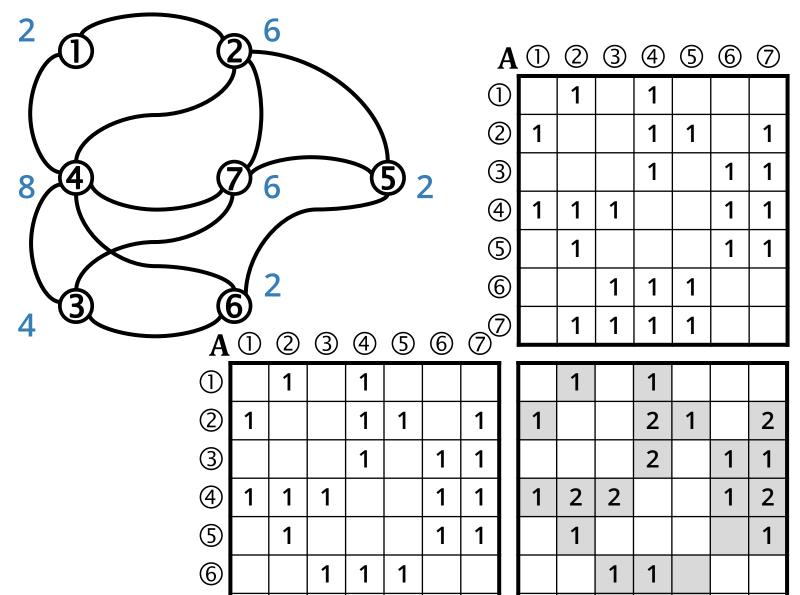
	1		1			
1			2	1		2
			2		1	1
1	2	2			1	2
	1					1
		1	1			
	2	1	2	1		

**TRI** 



tri

### LCC EXAMPLE: ELEMENT-WISE MULTIPLICATION

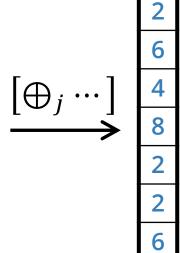


Masking limits where the operation is computed. Here, we use  $\mathbf{A}$  as a mask for  $\mathbf{A} \oplus . \otimes \mathbf{A}$ .

$$TRI\langle A \rangle = A \oplus . \otimes A$$

$$tri = \left[ \bigoplus_{j} TRI(:,j) \right]$$

$$tri$$



Triangle count / Cohen's algorithm

## **COHEN'S ALGORITHM: PSEUDOCODE**



Input: adjacency matrix A

Output: triangle count t

Workspace: matrices L, U, B, C

- 1.  $\mathbf{L} = \text{tril}(\mathbf{A})$
- 2.  $\mathbf{U} = \text{triu}(\mathbf{A})$
- 3.  $\mathbf{B} = \mathbf{L} \oplus . \otimes \mathbf{U}$
- 4.  $\mathbf{C} = \mathbf{B} \otimes \mathbf{A}$
- 5.  $t = \sum C/2$

extract the lower triangle from A

extract the upper triangle from A

multiply matrices L and U

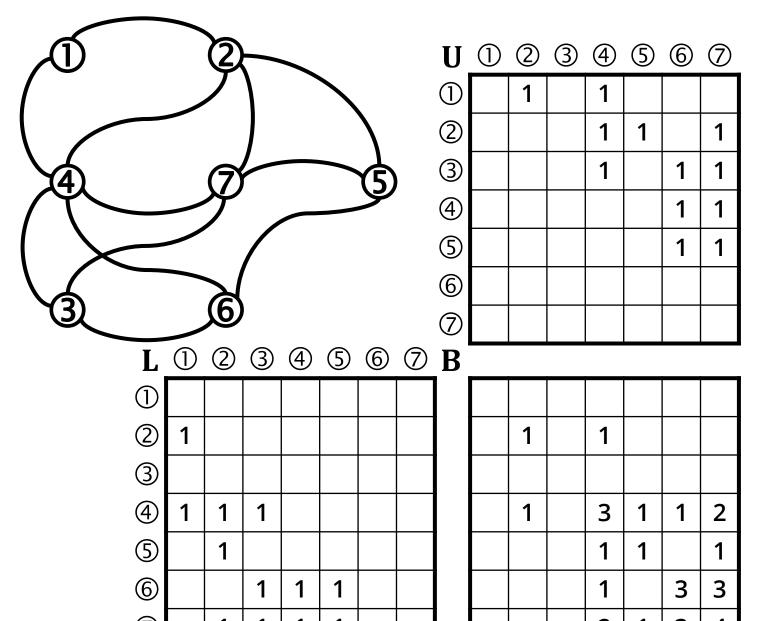
element-wise multiplication

sum the values in C and divide by 2

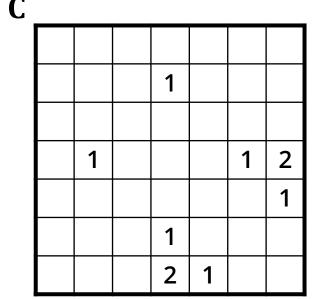


J. Cohen: *Graph Twiddling in a MapReduce World,* Comput. Sci. Eng. 2009

## **COHEN'S ALGORITHM**

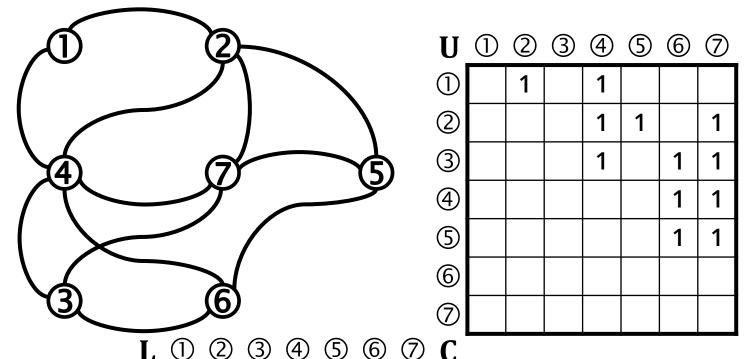


A	1	2	3	4	(5)	6	7
		1		1			
	1			1	1		1
				1		1	1
$\otimes$	1	1	1			1	1
		1				1	1
			1	1	1		
		1	1	1	1		



$$t = \sum C/2$$

## **COHEN'S ALGORITHM: MASKING**



L.	$\Box$		<u> </u>	$\Box$	<u> </u>	<u> </u>	$\underline{U}$
1							
2	1						
3							
	1	1	1				
(5)		1					
6			1	1	1		
(7)		1	1	1	1		

		1			
	1			1	2
					1
		1			
		2	1		

$$\mathbf{C}\langle \mathbf{A}\rangle = \mathbf{L} \oplus . \otimes \mathbf{U}$$
$$\mathbf{t} = \sum \mathbf{C}/2$$

Triangle count / Sandia algorithm

### SANDIA ALGORITHM



**Input:** adjacency matrix **A** 

Output: triangle count t

Workspace: matrices L, U, B, C

- 1.  $\mathbf{L} = \text{tril}(\mathbf{A})$
- 2.  $\mathbf{C}\langle \mathbf{L} \rangle = \mathbf{L} \oplus . \otimes \mathbf{L}$
- 3.  $t = \sum C$

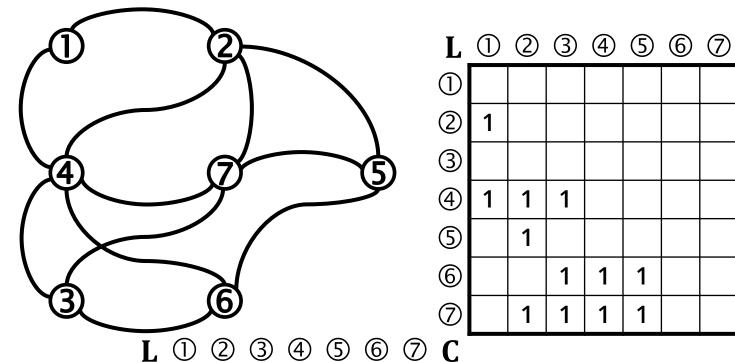
extract the lower triangle from A

multiply matrices L and L using mask L

sum the values in C



## **SANDIA ALGORITHM**



L	$\bigcirc$		(3)	4)	<u>(S)</u>	<u>(b)</u>	$\bigcirc$
1							
2	1						
3							
4	1	1	1				
(5)		1					
			1	1	1		
(7)		1	1	1	1		

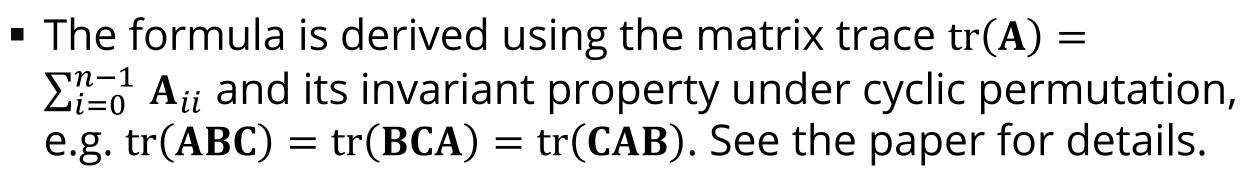
1				
		1		
	2	1		

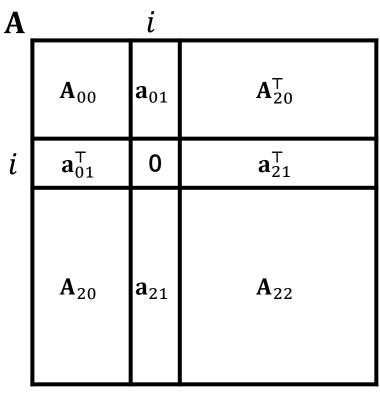
$$\mathbf{C}\langle\mathbf{L}\rangle = \mathbf{L} \oplus . \otimes \mathbf{L}$$
$$\mathbf{t} = \sum \mathbf{C}$$

Triangle count / CMU algorithm

## **CMU ALGORITHM**

- Iterates on the vertices of the graph, extracts corresponding submatrices and computes  $\mathbf{t} = \mathbf{t} + a_{10}^{\mathsf{T}} \oplus . \otimes A_{20} \oplus . \otimes a_{12}$
- Tradeoffs:
  - o does not require mxm, only vxm and mxv
  - o slower than mxm-based algorithms





T.M. Low et al. (Carnegie Mellon University):

### **CMU ALGORITHM: PSEUDOCODE**



**Input:** adjacency matrix **A** 

Output: triangle count t

Workspace: matrix  $\mathbf{A}_{20}$ ,  $\mathbf{a}_{10}$ ,  $\mathbf{a}_{12}^{\mathsf{T}}$ ,  $\mathbf{C}$ 

1. for 
$$i = 2$$
 to  $n - 1$ 

2. 
$$\mathbf{A}_{20} = \mathbf{A}[i+1:n,0:i-1]$$

3. 
$$\mathbf{a}_{10} = \mathbf{A}[0:i-1,i]$$

4. 
$$\mathbf{a}_{12} = \mathbf{A}[i, i+1:n]$$

5. 
$$\mathbf{t} = \mathbf{t} + a_{10}^{\mathsf{T}} \oplus \otimes A_{20} \oplus \otimes a_{12}$$

A		i	
	$\mathbf{A}_{00}$	$\mathbf{a}_{01}$	$\mathbf{A}_{20}^{T}$
i	$\mathbf{a}_{01}^{T}$	0	$\mathbf{a}_{21}^{T}$
	$\mathbf{A}_{20}$	<b>a</b> <sub>21</sub>	$\mathbf{A}_{22}$

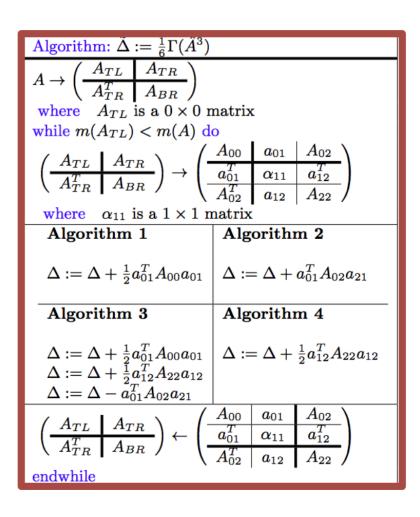


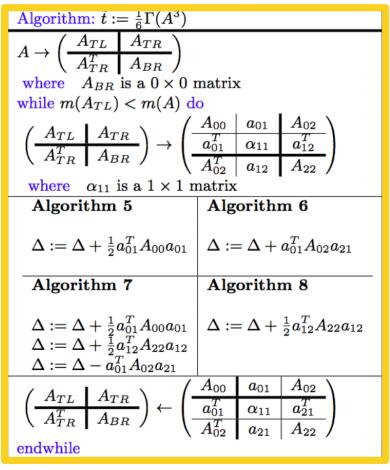
T.M. Low et al. (Carnegie Mellon University):

#### PROVABLY CORRECT ALGORITHMS

The "CMU algorithm" belongs to a family of algorithms which can be derived using the "FLAME approach".

There are 8 similar algorithms in total, the one presented here is Algorithm 2.







M. Lee, T.M. Low (Carnegie Mellon University): A family of provably correct algorithms for exact triangle counting, CORRECTNESS @ SC 2017

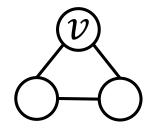


Source of the figure

Node-wise triangle count

### **NODE-WISE TRIANGLE COUNT**

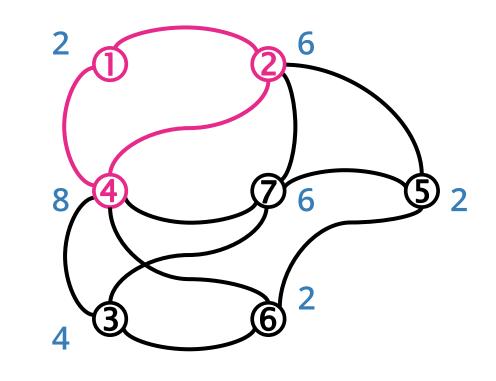
Triangle - Def 1: a set of three mutually adjacent nodes.



Def 2: a three-length closed path.

Usages:

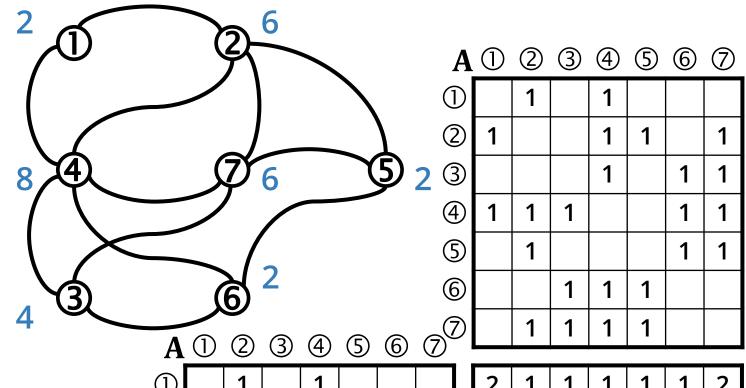
- Global clustering coefficient
- Local clustering coefficient
- Finding communities





GraphChallenge.org: Raising the Bar on Graph Analytic Performance, HPEC 2018

### TC: ELEMENT-WISE MULTIPLICATION



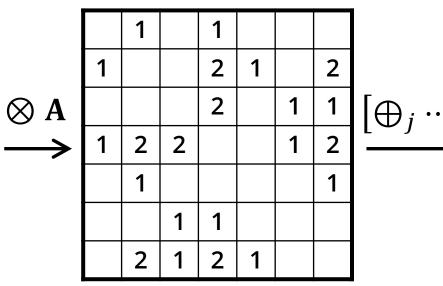
$TRI = \lambda$	$A \oplus . \otimes A \otimes A$
tri =	$\left[\bigoplus_{j} \mathbf{TRI}(:,j)\right]$

 $\mathbf{A} \oplus . \otimes \mathbf{A}$  is still very dense.

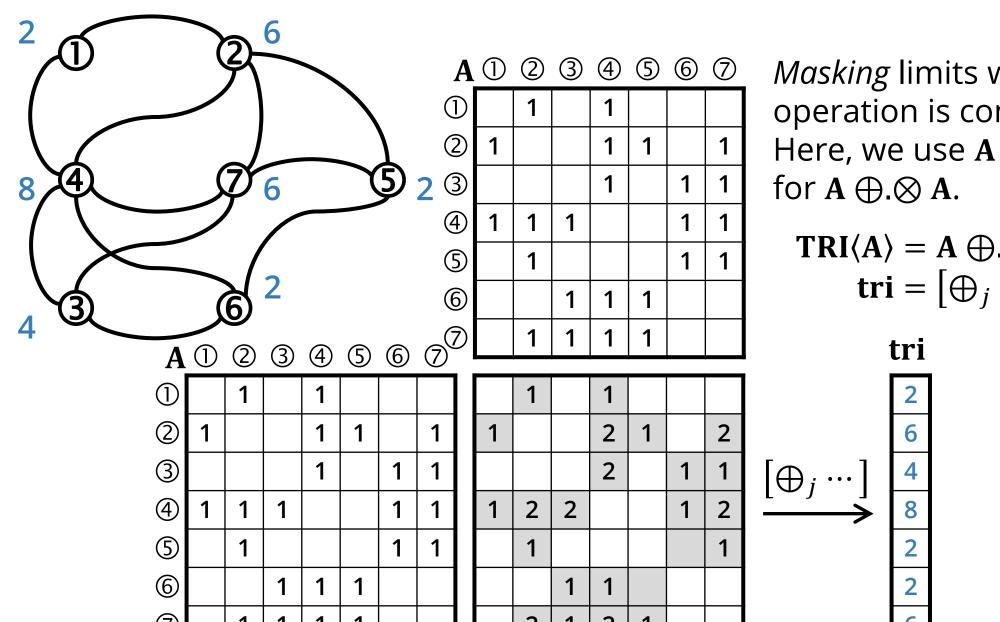
**TRI** 

1 N	•						
1		1		1			
2	1			1	1		1
3				1		1	1
	1	1	1			1	1
(5)		1				1	1
6			1	1	1		
7		1	1	1	1		

2	1	1	1	1	1	2
1	4	2	2	1	2	2
1	2	3	2	2	1	1
1	2	2	5	3	1	2
1	1	2	3	3		1
1	2	1	1		3	3
2	2	1	2	1	3	4

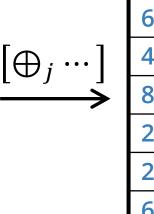


### TC: ELEMENT-WISE MULTIPLICATION



Masking limits where the operation is computed. Here, we use **A** as a mask

$$\mathbf{TRI}\langle \mathbf{A} \rangle = \mathbf{A} \oplus . \otimes \mathbf{A}$$
$$\mathbf{tri} = \left[ \bigoplus_{j} \mathbf{TRI}(:,j) \right]$$



#### TC: ALGORITHM



Input: adjacency matrix A

Output: vector tri

Workspace: matrix TRI

1.  $TRI\langle A \rangle = A \oplus . \otimes A$ 

- compute the triangle count matrix
- 2.  $\mathbf{tri} = \left[ \bigoplus_{j} \mathbf{TRI}(:,j) \right]$

compute the triangle count vector

Optimization: use **L**, the lower triangular part of **A** to avoid duplicates.  $\mathbf{TRI}\langle \mathbf{A}\rangle = \mathbf{A} \oplus . \otimes \mathbf{L}$ 

**Worst-case optimal joins:** There are deep theoretical connections between masked matrix multiplication and relational joins. It has been proven in 2013 that for the triangle query, binary joins always provide suboptimal runtime, which gave rise to new research on the family of worst-case optimal multi-way joins algorithms.

*k*-truss

### **K-TRUSS**

■ **Definition:** the k-truss is a subset of the graph with the same number of vertices, where each edge appears in at least k-2 triangles in the original graph.

#### K-TRUSS ALGORITHM



- Input: adjacency matrix **A**, scalar *k*
- Output: k-truss adjacency matrix C
- Helper:  $f(x, support) = x \ge support$

- 1. C = A
- 2. for i = 1 to n 1
- 3.  $\mathbf{C}\langle\mathbf{C}\rangle = \mathbf{C} \oplus . \wedge \mathbf{C}$  use the "plus-and" semiring
- 4.  $\mathbf{C} = f(\mathbf{C}, k 2)$  drop entries in  $\mathbf{C}$  less than k 2
- 5. terminate if the number of nonzero values in **C** did not change



T.A. Davis: Graph algorithms via SuiteSparse:GraphBLAS: triangle counting and k-truss, HPEC 2018

# Graph algorithms in GraphBLAS

Community detection using label propagation

#### CDLP: COMMUNITY DETECTION USING LABEL PROPAGATION

**Goal:** assign a label to each vertex representing the community it belongs to. The algorithm (originally published in network science) is slightly altered to ensure deterministic execution. Initially:

$$L_0(v) = v$$

In the  $k^{\text{th}}$  iteration:

$$L_k(v) = \min(\arg\max_l |u \in N(v)| L_{k-1}(u) = l|),$$

where N(v) is the set of neighbours of v.

Run for t iterations or until reaching a fixed point.



U.N. Raghavan, R. Albert, S. Kumara: *Near linear time algorithm to detect community structures in large-scale networks*, Phys. Rev. E, 2007

# IDEA: CAPTURE CDLP IN PURE GRAPHBLAS

- Define a semiring that operates over occurrence vectors
- operator: combines two occurrence vectors

$$0 \{6 \to 1, 9 \to 1\} \bigoplus \{6 \to 1, 7 \to 2\} = \{6 \to 2, 7 \to 2, 9 \to 1\}$$

Convert each element in a row to an occurrence vector

$$\circ \{6 \to 1\}, \{6 \to 1\}, \{7 \to 1\}, \{7 \to 1\}, \{9 \to 1\}$$

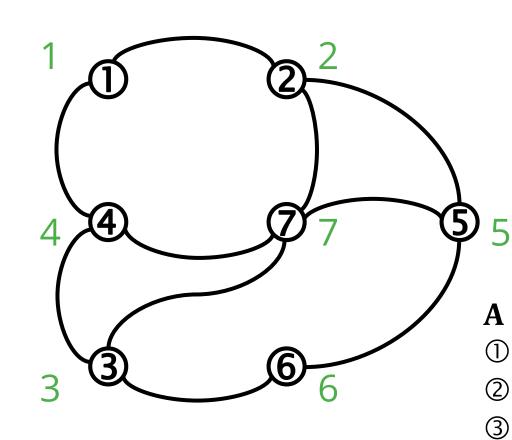
Reduce each row into a single occurrence vector:

$$\circ \{6 \rightarrow 2, 7 \rightarrow 2, 9 \rightarrow 1\}$$

- Select the min. mode element from the occurrence vector
   6
- Work on paper, but occurrence vectors need dynamic memory allocation, which leads to very poor performance

## CDLP IN LINEAR ALGEBRA

- Extract each row from F
  - Easy if the matrix is stored in CSR format
- Select the minimum mode value in each row
  - Sort elements using parallel merge sort
  - Pick the min value that has the longest run (done in a single pass)
- Sort each row r
- Use the sorted list to compute mode(r)

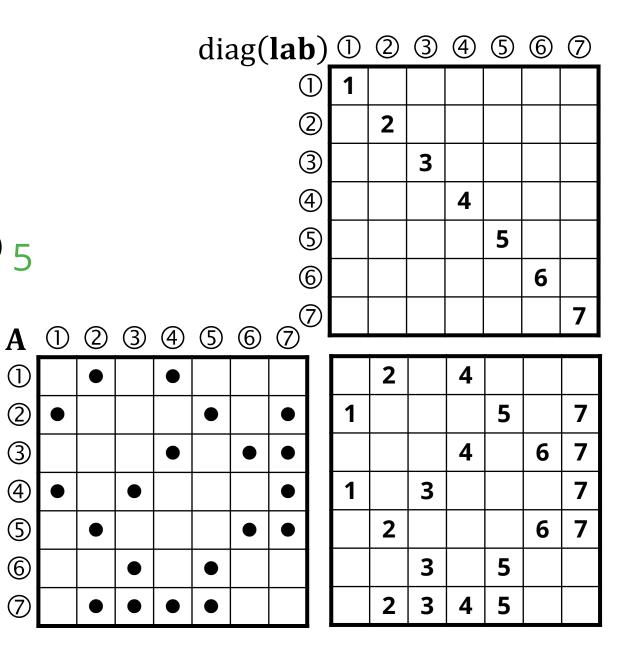


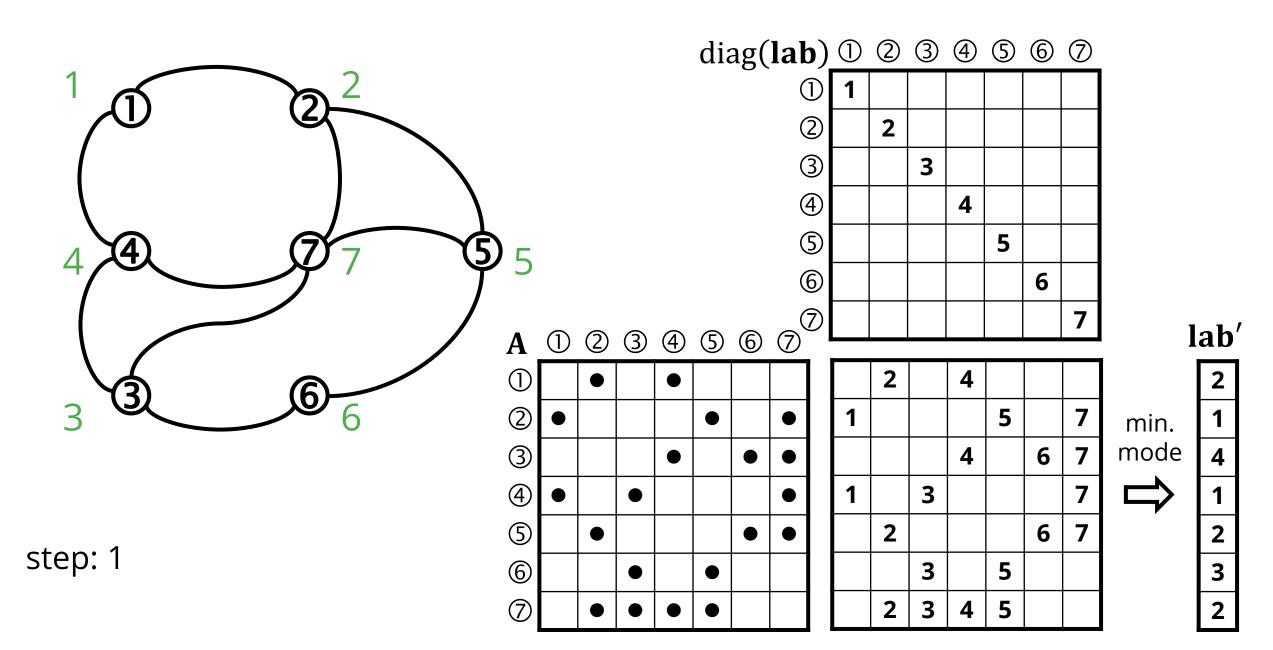
4

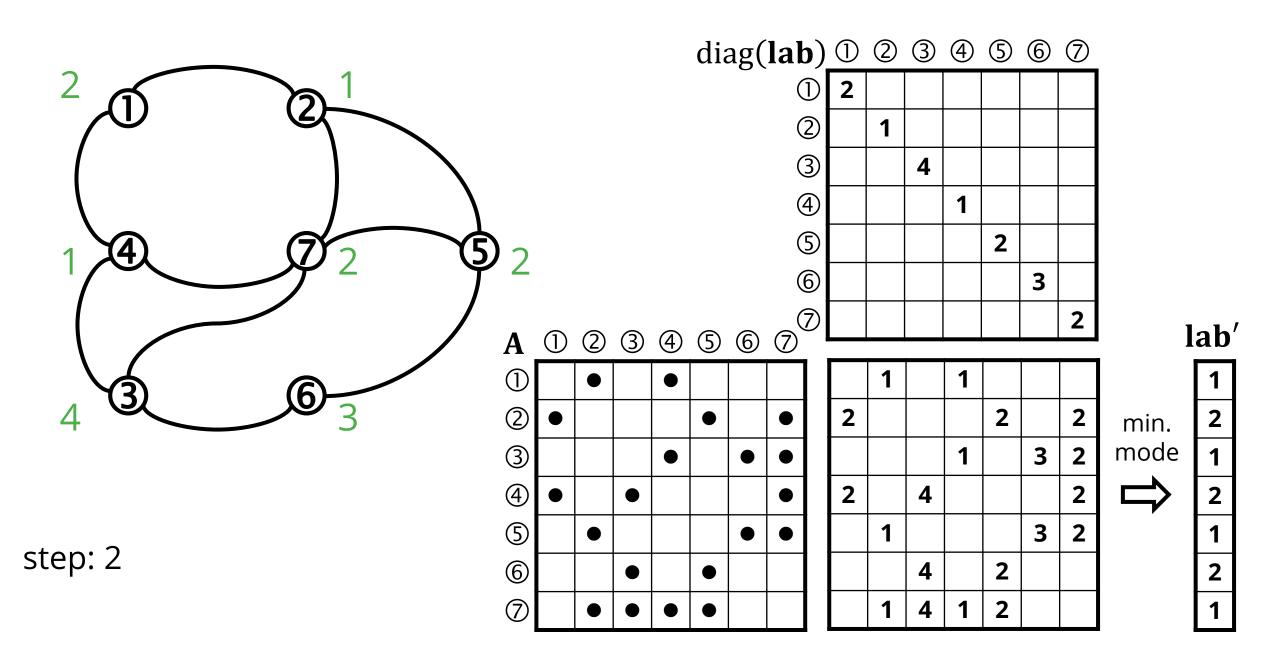
(5)

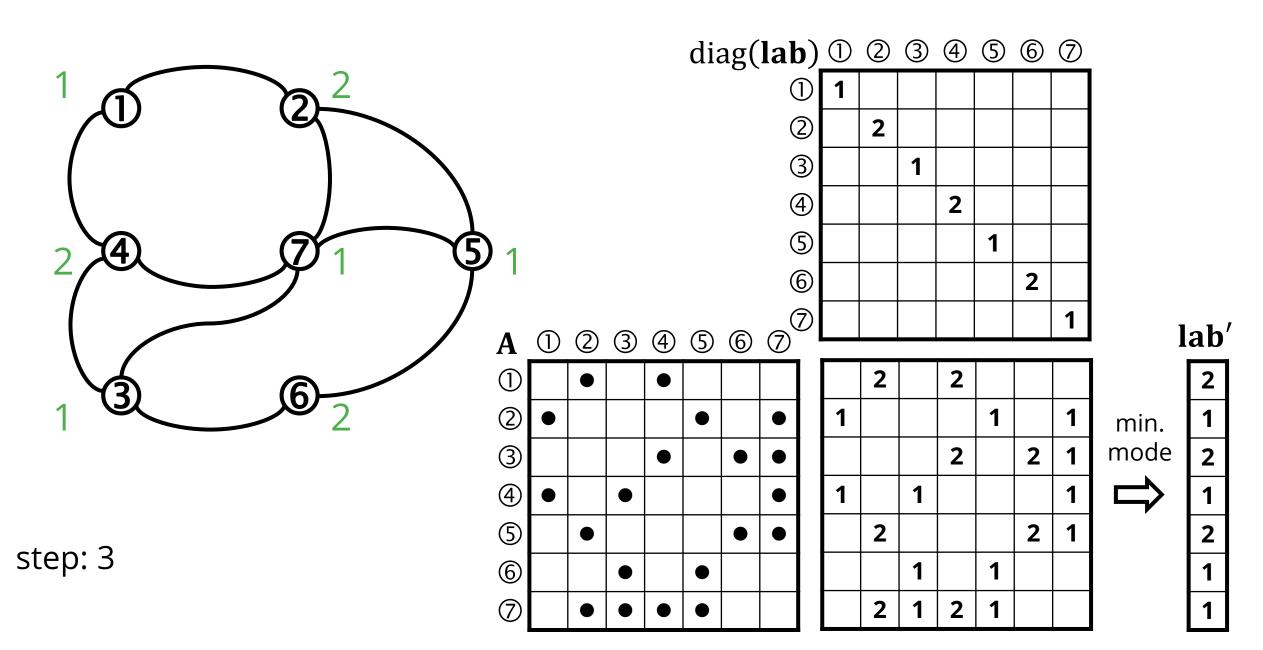
6

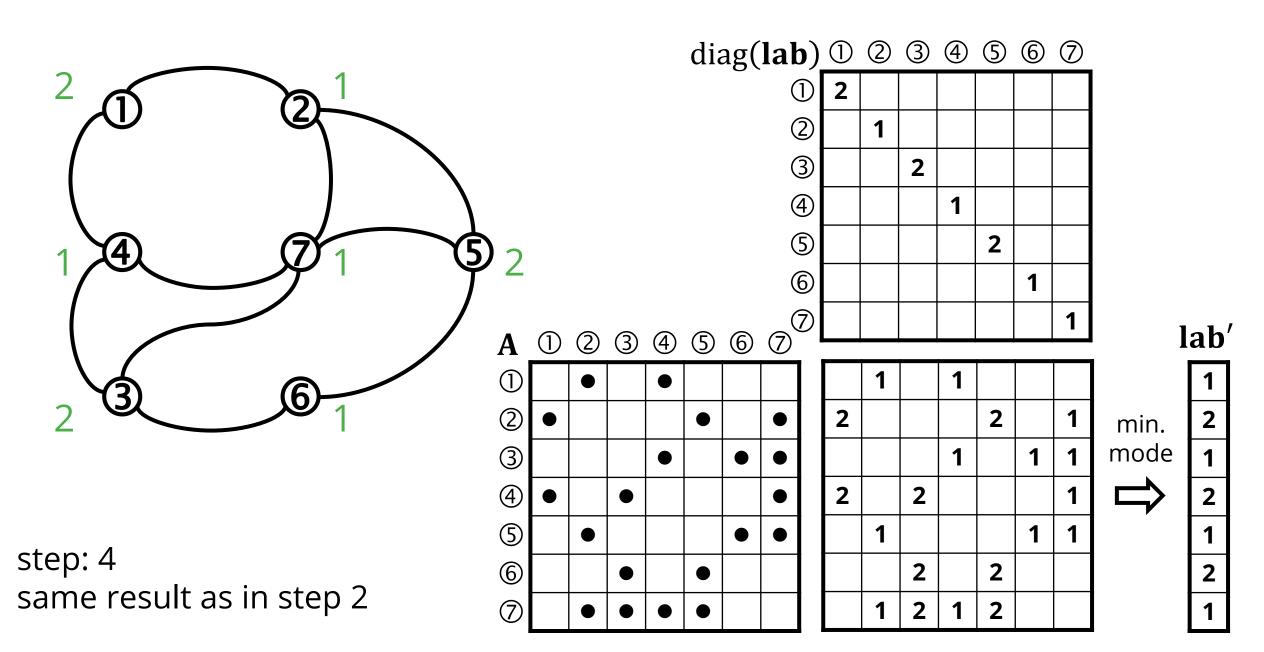
- Initially,  $lab = [1 \ 2 \ ... \ n]$
- Propagate labels to create a "frequency matrix":  $\mathbf{F} = \mathbf{A}$  any sel2nd diag( $\mathbf{lab}$ )











# **CDLP: ALGORITHM**



**Input:** adjacency matrix A, #vertices n, #iterations t

Output: vector lab

Workspace: matrix F, vector r

- 1.  $lab = [1 \ 2 \dots n]$
- 2. for k = 1 to t
- 3.  $\mathbf{F} = \mathbf{A}$  any sel2nd diag( $\mathbf{lab}$ )
- 4. for i = 1 to n
- 5.  $\mathbf{r} = \mathbf{F}(i,:)$
- 6.  $sort(\mathbf{r})$
- 7.  $L(i) = select_min_mode(r)$

Can be batched and parallelized

## **CDLP: ALGORITHM**



**Input:** adjacency matrix **A**, #vertices n, #iterations t

Output: vector lab

Workspace: matrix F, vector r, array of row indices I, array of values X

- 1.  $lab = [1 \ 2 \dots n]$
- 2. for k = 1 to t
- 3.  $\mathbf{F} = \mathbf{A}$  any.sel2nd diag( $\mathbf{lab}$ )
- 4.  $\langle I, \_, X \rangle = \text{extract\_tuples}(F)$
- 5.  $merge\_sort\_pairs(\langle I, X \rangle)$
- 6. lab = for each row in I, select min mode value from X

# CDLP ON DIRECTED GRAPHS

For directed graphs, we compute the labels  $L_k(v)$  as:

```
\min(\arg\max_{l} [|u \in N_{\text{in}}(v)| L_{k-1}(u) = l| + |u \in N_{\text{out}}(v)| L_{k-1}(u) = l|])
```

- In linear algebra, this can be expressed with two matrices:
  - $\circ$   $\mathbf{F}_{in} = \mathbf{A}$  any. sel2nd diag( $\mathbf{lab}$ )
  - $\circ \mathbf{F}_{\text{out}} = \mathbf{A}^{\mathsf{T}} \text{ any. sel2nd diag}(\mathbf{lab})$
- Simultaneously iterate over rows  $\mathbf{r_{in}}$  of  $\mathbf{F_{in}}$  and  $\mathbf{r_{out}}$  of  $\mathbf{F_{out}}$
- For each row pair, sort  $\mathbf{r}_{in} \cup \mathbf{r}_{out}$  and select the minimum mode value
- Batching also works:

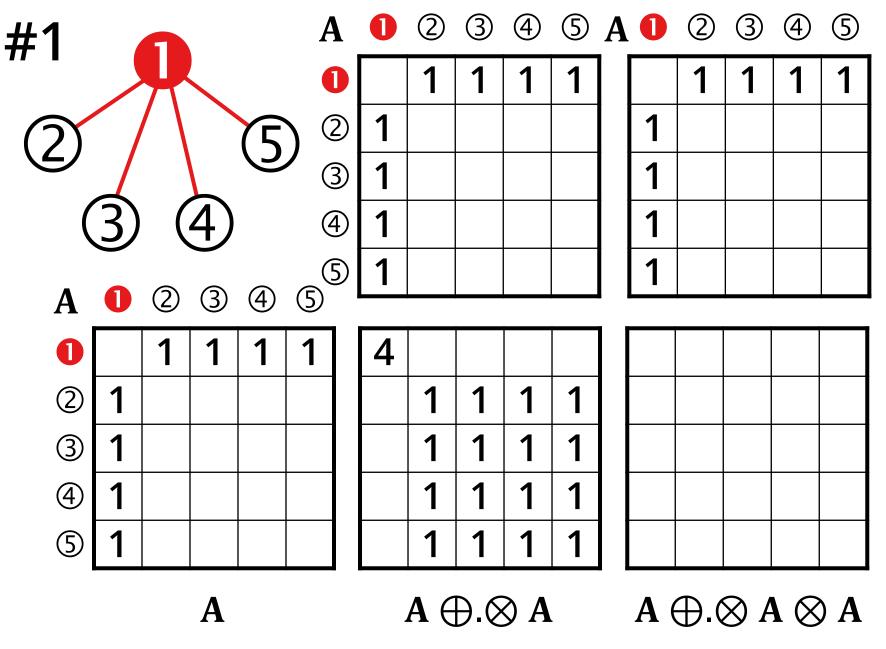
```
 \begin{array}{l} \circ \langle I_{in}, \_, X_{in} \rangle = \text{extract\_tuples}(F_{in}) \\ \circ \langle I_{out}, \_, X_{out} \rangle = \text{extract\_tuples}(F_{out}) \end{array} \right\} \text{merge\_sort\_pairs}(\langle I_{in} \cup I_{out}, X_{in} \cup X_{out} \rangle)
```

# Graph algorithms in GraphBLAS

The importance of masking

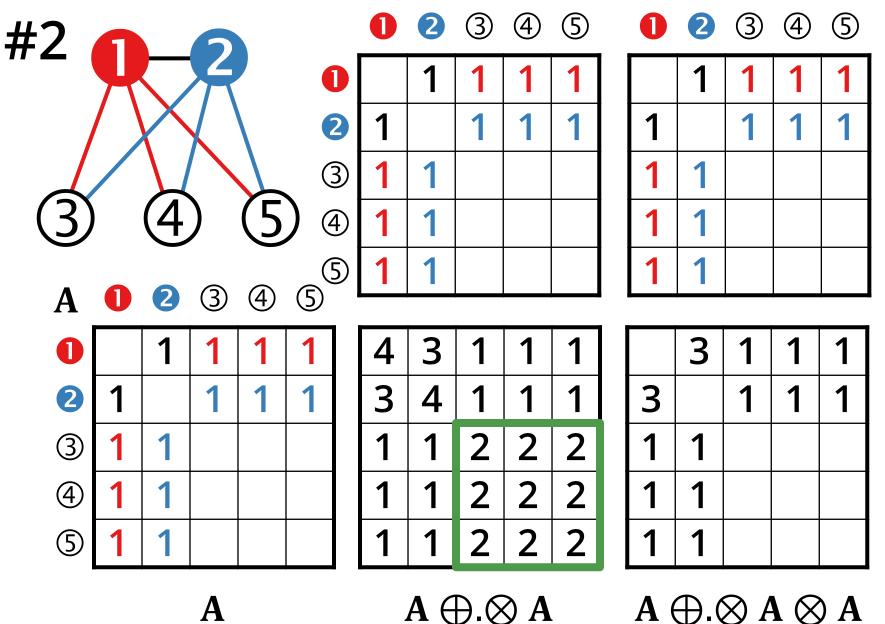
## THE IMPORTANCE OF MASKING

- **Q:** Is masking absolutely necessary?
- **A:** Yes, it can reduce the complexity of some algorithms. We demonstrate this with two examples.



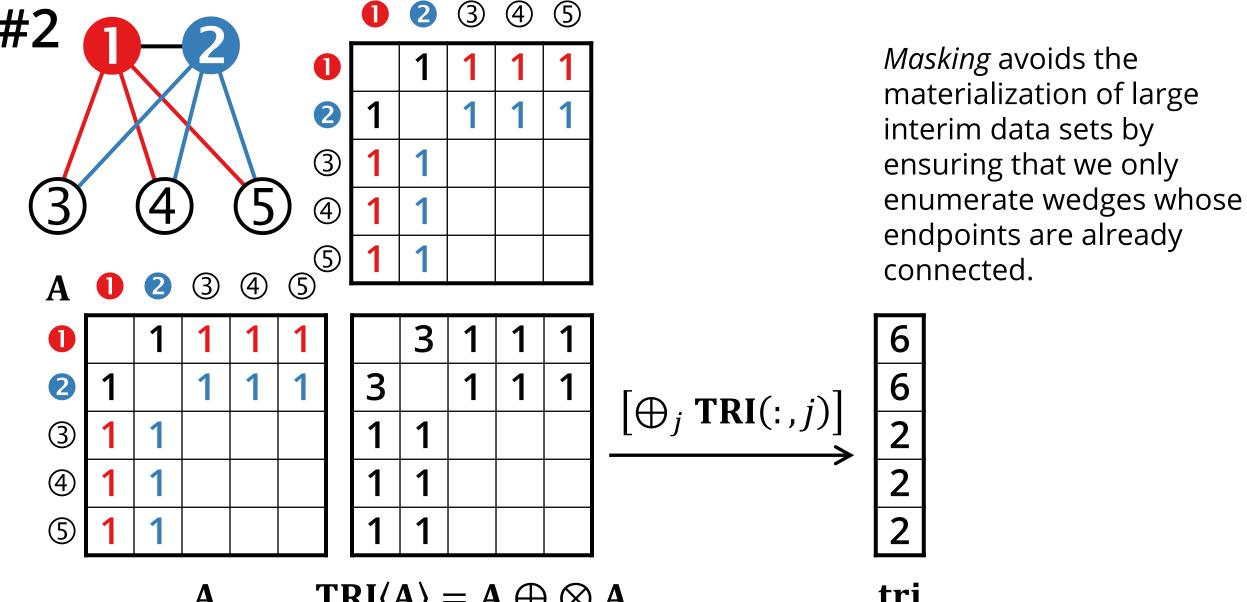
A simple corner case is the star graph: there are  $(n-1)^2$  wedges but none of them close into triangles.

We do quadratic work while it's clear that there are no triangles in the graph (it's a tree).



A full bipartite graph  $K_{2,3}$  with the vertices in the top partition connected.

A bipartite graph only has cycles of even length, so it's easy to see that all triangles will contain the two vertices in the top partition. Still,  $\mathbf{A} \oplus . \otimes \mathbf{A}$ enumerates all wedges starting and ending in the bottom partition, thus performing a lot of unnecessary work.



 $TRI\langle A \rangle = A \oplus . \otimes A$ A

tri

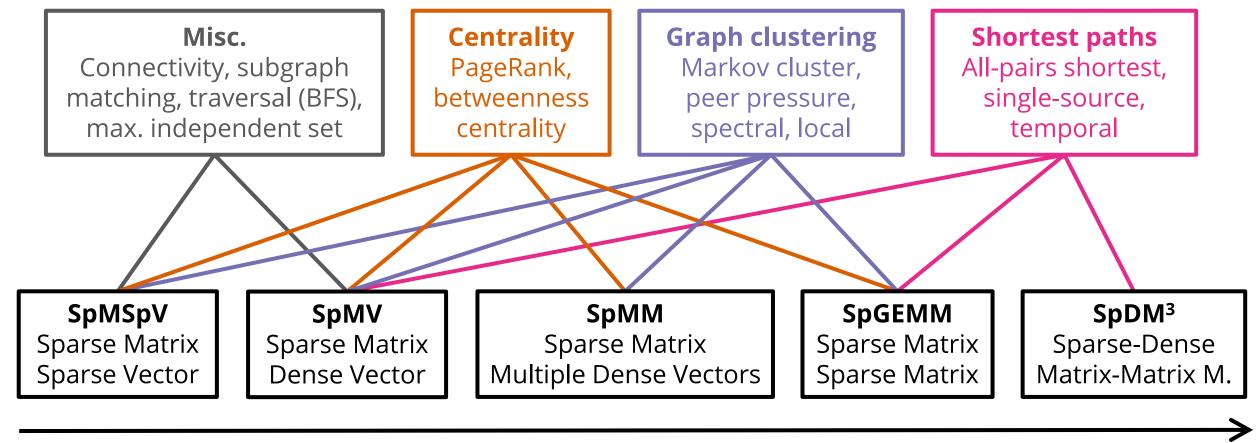
# Graph algorithms in GraphBLAS

Summary and other algorithms

# SUMMARY OF THE ALGORITHMS DISCUSSED

Algo.	Features demonstrated
BFS	lor-land and min-sel1st semirings, masked SpMV
SSSP	min-plus semiring
PR	real semiring, row-wise reduce
LCC	apply operation, masked matrix-market multiplication

# **GRAPH ALGORITHMS & GRAPHBLAS PRIMITIVES**



GraphBLAS primitives in increasing arithmetic intensity



Based on the figure in A. Buluç:

Graph algorithms, computational motifs, and GraphBLAS, ECP Meeting 2018

## OTHER ALGORITHMS IN GRAPHBLAS

Betweenness centrality: Brandes' algorithm



A. Buluç et al.: Design of the GraphBLAS C API, GABB@IPDPS 2017

**k-truss**: a subset of the graph with the same number of vertices, where each edge appears in at least k-2 triangles in the original graph.



T.A. Davis: Graph algorithms via SuiteSparse:GraphBLAS: triangle counting and k-truss, HPEC 2018

#### Maximal independent set: Luby's randomized algorithm



T.A. Davis: Algorithm 1000: SuiteSparse:GraphBLAS: graph algorithms in the language of sparse linear algebra, ACM TOMS, 2019

#### Sparse DNNs: represent sparse deep neural networks as graphs



J. Kepner et al.: *Enabling Massive Deep Neural Networks with the GraphBLAS*, HPEC 2017



T.A. Davis et al.: Write Quick, Run Fast: Sparse Deep Neural Network in 20 Minutes of Development Time via SuiteSparse:GraphBLAS, HPEC 2019

# Graph processing in relational algebra

# RELATIONAL ALGEBRA ON GRAPHS

Natural join:

 $A\bowtie B$ 

A natural join connects edges from A with an edge in B.

Semijoin:

 $A \ltimes B$ 

A semijoin keeps edges from A with a connecting edge in B.

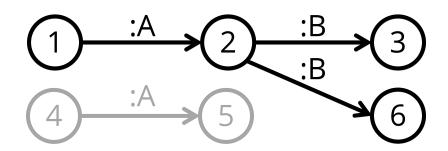
Antijoin:

 $A \ltimes B$ 

An antijoin keeps edges from A without a connecting edge in B.

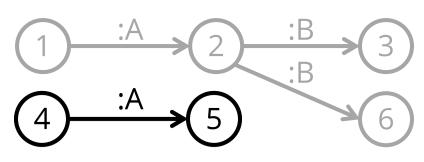
Left outer join:  $A\bowtie B$ 

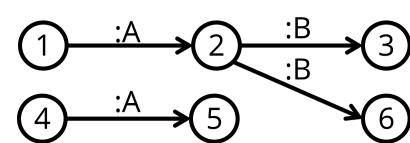
A left outer join keeps all edges from A with or without a connecting edge in *B*.



1	:A	<b>→</b> 2	:B :B 3	
4	:A	→5	36	

1)-	<u>:A</u>	<b>→</b> 2	:B :B	→3
4	:A	<b>→</b> 5		46





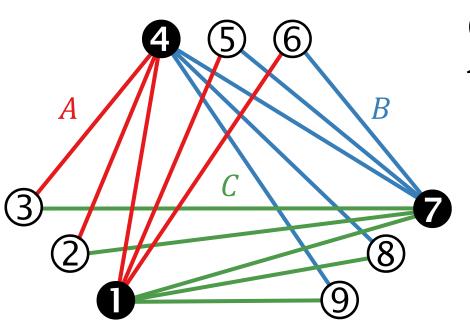
i	j	k
1	2	3
1	2	6

i	j
1	2

i	j
4	5

i	j	$\boldsymbol{k}$
1	2	3
1	2	6
4	5	null

# TRIANGLE QUERY



Given relations A(i, j), B(j, k), C(i, k)triangles can be enumerated with:

$$A \bowtie B \bowtie C$$

$\boldsymbol{A}$	$\bowtie$	E

i	j	$\boldsymbol{k}$
1	4	7
1	4	8
1	4	9
2	4	7
2	4	8
2	4	9

i	j
1	4
2	4
3	4
1	5
1	6

j	k
4	7
4	8
4	9
5	7
6	7

i	k
1	7
1	8
1	9
2	7
3	7

A	$\bowtie$	$B \triangleright$	$\triangleleft C$	i	j	$\boldsymbol{k}$
		_		1	4	7
i	$\boldsymbol{k}$			1	5	7
1	7			1	6	7
1	8			1	4	8
1	9			1	4	9
2	7			2	4	7

9

wedges that do not close into a triangle

<sup>\*</sup>Edges are stored in one direction: R[1] < R[2]

# **COMPLEXITY OF THE TRIANGLE QUERY**

For m edges, the AGM-bound of the triangle query is  $\mathcal{O}(m^{3/2})$ 

#### Theorem #1:

Any binary join plan for the triangle query takes  $\Omega(m^2)$  time.

To mitigate this, worst-case optimal join (WCOJ) algorithm use multi-way joins such as  $\bowtie (A, B, C)$ .

## Theorem #2:

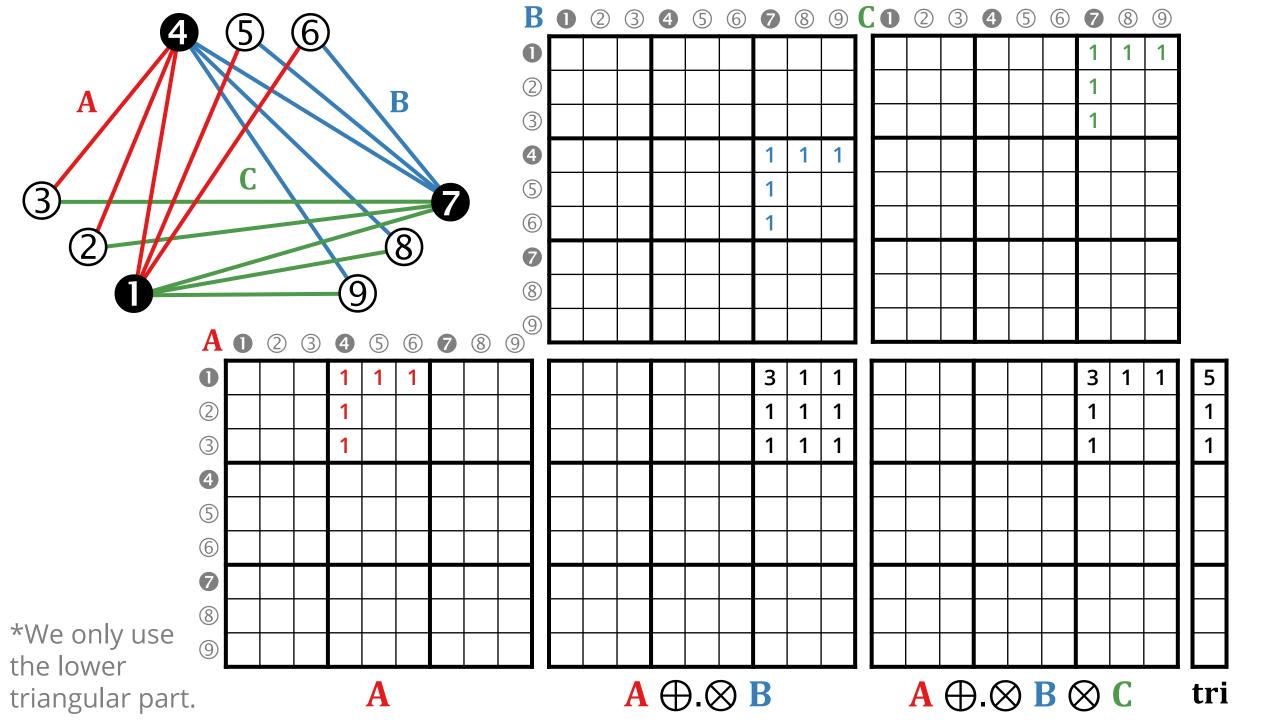
The worst-case complexity of the generic join algorithm (a WCOJ algorithm)  $\leq$  AGM bound.

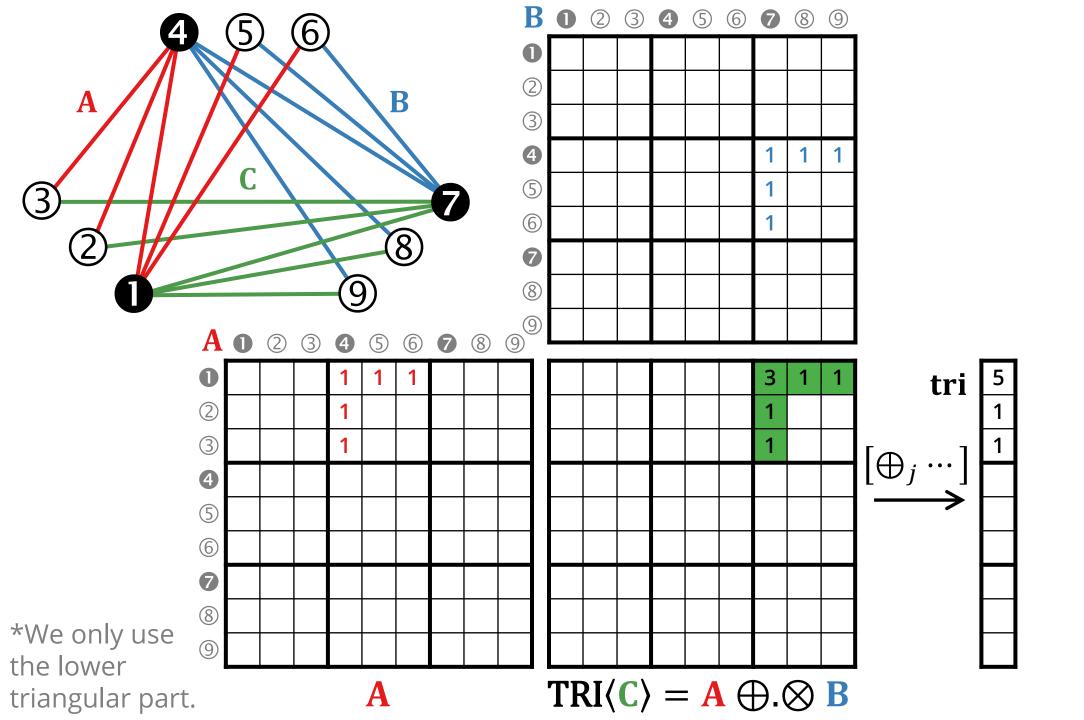


A. Atserias, M. Grohe, D. Marx, Size Bounds and Query Plans for Relational Joins, FOCS 2008



H.Q. Ngo et al.: *Skew strikes back: New developments in the theory of join algorithms,* SIGMOD Record 2013





## MASKING IN RELATIONAL ALGEBRA

Vertex-wise triangle count in linear algebra:

$$\mathbf{TRI}\langle \mathbf{C} \rangle = \mathbf{A} \oplus . \otimes \mathbf{B}$$
$$\mathbf{tri} = \left[ \bigoplus_{j} \mathbf{TRI}(:,j) \right]$$

Notice that in relational algebra, given A(i,j), B(j,k), C(i,k):

$$A \bowtie B \bowtie C \equiv (A \bowtie B) \bowtie C$$
 $A \bowtie B \bowtie C \equiv (B \bowtie C) \bowtie A \equiv (B \bowtie C) \bowtie A$ 
 $A \bowtie B \bowtie C \equiv (A \bowtie C) \bowtie B \equiv (A \bowtie C) \bowtie B$ 

Where the semijoin operator  $\ltimes$  is defined as:

$$R \bowtie S = \pi_{\operatorname{schema}(R)}(R \bowtie S) = R \bowtie \pi_{\operatorname{schema}(R) \cap \operatorname{schema}(S)}(S)$$

## MASKING IN RELATIONAL ALGEBRA

Given relational schemas A(i,j), B(j,k), C(i,k) and expression:  $A \bowtie B \bowtie C \equiv (A \bowtie B) \bowtie C$ 

The "masking" technique cannot be translated to relational algebra as a single operation – we have to use an outside loop to express it. Using relation T(i,k):

- 1. for all  $c \in C$  do
- 2.  $TRI = TRI \cup \pi_{i,k} ((A \ltimes \{c\}) \bowtie (B \ltimes \{c\}))$
- 3.  $tri = \gamma_{i,count(k) \to triCount}(TRI)$

i	triCount
1	5
2	1
3	1

Cf. 
$$TRI(C) = A \oplus . \otimes B$$
,  $tri = [\bigoplus_j TRI(:,j)]$ 

Relational algebra also allows triangle enumeration.

Given A(i,j), B(j,k), C(i,k), instead of the previous expression:

- 1. for all  $c \in C$  do
- 2.  $TRI = TRI \cup \pi_{i,k} ((A \ltimes \{c\}) \bowtie (B \ltimes \{c\}))$
- 3.  $tri = \gamma_{i,\text{count}(k) \to triCount}(TRI)$

### Compute:

- 1. for all  $c \in C$  do
- 2.  $TRI = TRI \cup ((A \ltimes \{c\}) \bowtie (B \ltimes \{c\}))$

2. 
$$TRI = TRI \cup ((A \ltimes \{c\}) \bowtie (B \ltimes \{c\}))$$

C	i	k	$\boldsymbol{A}$	i	j	B	j	k	$A \bowtie B \bowtie C$	i	j	k
	1	7		1	4		4	7		1	4	7
	1	8		2	4		4	8		1	5	7
	1	9		3	4		4	9		1	6	7
	2	7		1	5		5	7		1	4	8
	3	7		1	6		6	7		1	4	9
							2	4	7			
	$A \ltimes \{c\}  B \ltimes \{c\}$								3	4	7	

2. 
$$TRI = TRI \cup ((A \ltimes \{c\}) \bowtie (B \ltimes \{c\}))$$

C	i	k
	1	7
	1	8
	1	9
	2	7
	3	7

i	j	B	j	k			
1	4		4	7			
2	4		4	8			
3	4		4	9			
1	5		5	7			
1	6		6	7			
$A \times \{c\}  B \times \{c\}$							

$\triangleleft B \bowtie C$	i	j	k
	1	4	7
	1	5	7
	1	6	7
	1	4	8
	1	4	9
	2	4	7
	3	4	7

2. 
$$TRI = TRI \cup ((A \ltimes \{c\}) \bowtie (B \ltimes \{c\}))$$

1						ı			1
C	i	k	$\boldsymbol{A}$	i	j	B	j	$\boldsymbol{k}$	$A \bowtie B \bowtie$
	1	7		1	4		4	7	
	1	8		2	4		4	8	
	1	9		3	4		4	9	
	2	7		1	5		5	7	
	3	7		1	6		6	7	
$A \ltimes \{c\}  B \ltimes \{c\}$									

2. 
$$TRI = TRI \cup ((A \ltimes \{c\}) \bowtie (B \ltimes \{c\}))$$

C	i	$\boldsymbol{k}$	$\boldsymbol{A}$	i
	1	7		1
	1	8		2
	1	9		3
	2	7		1
	3	7		1
				1 D

	i	j	B	j	k			
	1	4		4	7			
	2	4		4	8			
	3	4		4	9			
	1	5		5	7			
	1	6		6	7			
F	$A \ltimes \{c\}$ $B \ltimes \{c\}$							

$\rtimes B \bowtie C$	i	j	k
	1	4	7
	1	5	7
	1	6	7
	1	4	8
	1	4	9
	2	4	7
	3	4	7

2. 
$$TRI = TRI \cup ((A \ltimes \{c\}) \bowtie (B \ltimes \{c\}))$$

C	i	k
	1	7
	1	8
	1	9
	2	7
	3	7

i	j	B
1	4	
2	4	
3	4	
1	5	
1	6	
4		5

	i	j	B	j	k			
	1	4		4	7			
	2	4		4	8			
	3	4		4	9			
	1	5		5	7			
	1	6		6	7			
$A \ltimes \{c\}$ $B \ltimes \{c\}$								

k	$A \bowtie B \bowtie C$	i	j	ļ
7		1	4	7
8		1	5	7
9		1	6	7
7		1	4	8
7		1	4	Ç
. ( .	7)	2	4	7
{ (		J	1	-

i	j	k
1	4	7
1	5	7
1	6	7
1	4	8
1	4	9
2	4	7
3	4	7

1. for all  $c \in C$  do

2. 
$$TRI = TRI \cup ((A \ltimes \{c\}) \bowtie (B \ltimes \{c\}))$$

C	i	k	A	i	j	B	j	k	$A\bowtie B\bowtie C$	i	j	$\boldsymbol{k}$
0	1	7		1	4		4	7		1	4	7
	1	8		2	4		4	8		1	5	7
	1	9		3	4		4	9		1	6	7
	2	7		1	5		5	7		1	4	8
	3	7		1	6		6	7		1	4	9
								2	4	7		
$A \ltimes \{c\}  B \ltimes \{c\}$									3	4	7	

Using semijoin pushdown on each tuple, we computed  $A \bowtie B \bowtie C$  without enumerating a quadratic-size interim relation. However, for efficient implementations, relations should also be sorted (see ref. for details).



H.Q. Ngo et al.: *Skew strikes back:*New developments in the theory of join algorithms, SIGMOD Record 2013

### TRIANGLE ENUMERATION IN LINEAR ALGEBRA

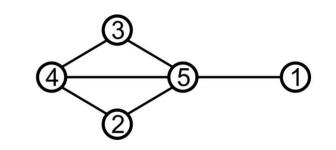
(Note that this work is yet to be ported to GraphBLAS.)

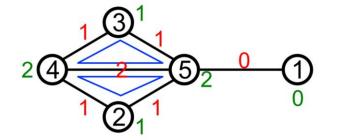
Triangle enumeration is possible by using triples as matrix elements and overloading " $\bigoplus$ . $\otimes$ " so that multiplying the adjacency matrix **A** with the incidence matrix **B** results in **C**:

$$C(i,j) = (i,x,y) \text{ iff } A(i,x) = A(i,y) = 1 \text{ and } B(x,j) = B(y,j) = 1$$



M.M. Wolf et al. *A task-based linear* algebra building blocks approach for scalable graph analytics, HPEC 2015





### MATRIX MULTIPLICATION IN RELATIONAL ALG.

	set	$\oplus$	$\otimes$	0
set relations	$R \subseteq D_1 \times \cdots \times D_k$	U	×	empty rel.
matrix relations	$R \subseteq D_1 \times D_2$	U	$\boxtimes$	empty rel.

#### **Observations:**

- a binary relation is analogous to a Boolean sparse matrix stored in coordinate list (COO) format
- a matrix multiplication is analogous to an equijoin on a binary relation that uses a single join attribute, and discards it after performing the join.

**Definition:** Given two binary relations R, S with a common attribute x, we define "multjoin" as:

$$R \boxtimes S = \pi_{R \cup S \setminus \{x\}} \left( R \bowtie_{R, x = S, x} S \right)$$

**Example:** 

 $A \boxtimes B$ 

## MM VS. MULTJOIN: REACHABILITY

### Matrices:

$$\mathbf{A} \in \mathbb{B}^{m \times n}$$
,  $\mathbf{B} \in \mathbb{B}^{n \times o}$ ,  $\mathbf{C} \in \mathbb{B}^{o \times p}$ 

For 
$$\mathbf{A} \vee A \otimes \mathbf{B}$$
:  $\langle \mathbf{A} \mathbf{B} \rangle_{ik} = \bigvee_{k} (\mathbf{A}_{ij} \wedge \mathbf{B}_{jk})$ 

#### For $\mathbf{A} \vee A \otimes \mathbf{B} \vee A \otimes \mathbf{C}$ :

$$\langle \mathbf{ABC} \rangle_{il} =$$

$$= \bigvee_{k} (\langle \mathbf{AB} \rangle_{ik} \wedge \mathbf{C}_{kl})$$

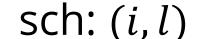
$$= \bigvee_{k} (\bigvee_{j} (\mathbf{A}_{ij} \wedge \mathbf{B}_{jk})) \wedge \mathbf{C}_{kl}$$

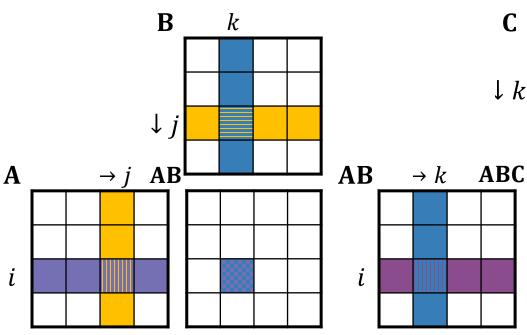
$$= \bigvee_{k} (\bigvee_{j} (\mathbf{A}_{ij} \wedge \mathbf{B}_{jk} \wedge \mathbf{C}_{kl}))$$

### **Relations:**

$$A \boxtimes B$$

$$A \boxtimes B \boxtimes C$$
 sch:  $(i, l)$ 





## MM VS. JOIN: COUNTING PATHS

### **Matrices:**

$$\mathbf{A} \in \mathbb{N}^{m \times n}$$
,  $\mathbf{B} \in \mathbb{N}^{n \times o}$ ,  $\mathbf{C} \in \mathbb{N}^{o \times p}$ 

$$\langle \mathbf{A}\mathbf{B} \rangle_{ik} = \sum_{i} \mathbf{A}_{ij} \otimes \mathbf{B}_{jk}$$

$$\langle \mathbf{ABC} \rangle_{il} = \sum_{k} (\sum_{j} \mathbf{A}_{ij} \otimes \mathbf{B}_{jk}) \otimes \mathbf{C}_{kl}$$
$$= \sum_{k} (\sum_{j} \mathbf{A}_{ij} \otimes \mathbf{B}_{jk} \otimes \mathbf{C}_{kl})$$

### **Relations:**

$$\gamma_{\operatorname{sum}(A_{va} \cdot B_{vb})}^{A.i,B.k}(A \bowtie B)$$

$$\gamma_{\operatorname{sum}(A_{va} \cdot B_{vb} \cdot C_{vc})}^{A.i,C.l}(A \bowtie B \bowtie C)$$

Enumerating triangles requires applying  $\sigma_{A.i=C.l}(...)$ 

## MATRIX MULTIPLICATION IN SQL: PATHS

```
\langle \mathbf{A} \mathbf{B} \rangle_{ik} = \sum_{j} \mathbf{A}_{ij} \otimes \mathbf{B}_{jk} \Rightarrow \gamma_{\Sigma(A_{va} \cdot B_{vb})}^{A.i,B.k} (A \bowtie B) select A.i, B.k, sum(A.va * B.vb) from A, B where A.j = B.j group by A.i, B.k;
```

```
 \langle \mathbf{ABC} \rangle_{il} = \sum_{k} (\sum_{j} \mathbf{A}_{ij} \otimes \mathbf{B}_{jk} \otimes \mathbf{C}_{kl}) \Rightarrow \gamma_{\Sigma(A_{va} \cdot B_{vb} \cdot C_{vc})}^{A.i,C.l} (A \bowtie B \bowtie C)  select A.i, C.l, sum(A.va * B.vb * C.vc) from A, B, C where A.j = B.j and B.k = C.k group by A.i, C.l;
```

## MATRIX MULTIPLICATION IN SQL: TRIANGLES

Relations A(i,j,va), B(j,k,vb), C(k,l,vc)  $\langle \mathbf{ABC} \rangle_{ii} = \sum_{k} (\sum_{j} \mathbf{A}_{ij} \otimes \mathbf{B}_{jk} \otimes \mathbf{C}_{kl}) \Rightarrow \gamma_{\Sigma(A_{va} \cdot B_{vb} \cdot C_{vc})}^{A.i,C.l} (\sigma_{A.i=C.l}(A \bowtie B \bowtie C))$ select A.i, C.l, sum(A.va \* B.vb \* C.vc) from A, B, C where A.j = B.j and B.k = C.k

and A.i = C.l

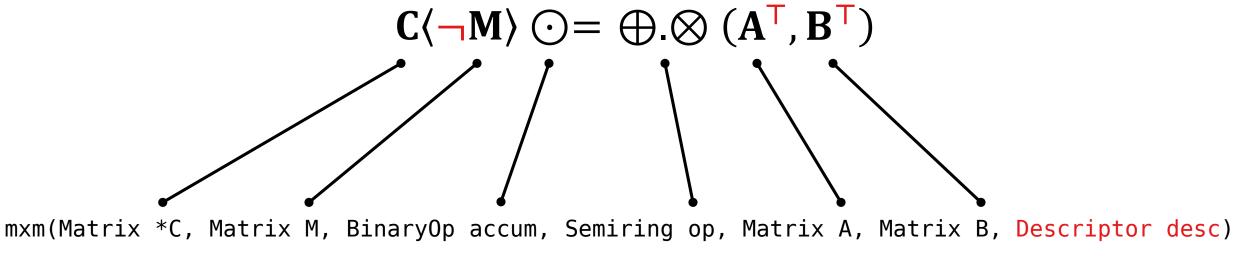
group by A.i, C.l;

Given relations A(i, j, va), B(j, k, vb), C(i, k, vc), we can simply use two natural joins:  $A \bowtie B \bowtie C$ .

## **GraphBLAS and SuiteSparse internals**

### **GRAPHBLAS C API**

- "A crucial piece of the GraphBLAS effort is to translate the mathematical specification to an API that
  - o is faithful to the mathematics as much as possible, and
  - o enables efficient implementations on modern hardware."

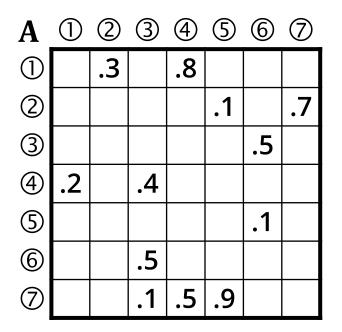




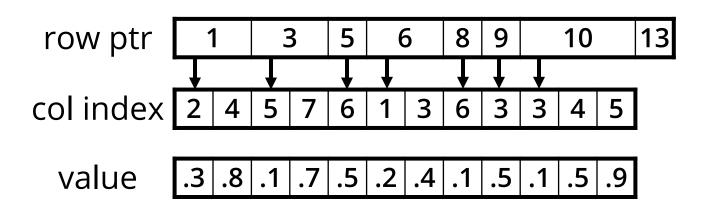
A. Buluç et al.: Design of the GraphBLAS C API, GABB@IPDPS 2017

## **GRAPHBLAS OBJECTS**

- GraphBLAS objects are opaque: the matrix representation can be adjusted to suit the data distribution, hardware, etc.
- The typical representations are compressed formats are:
  - CSR: Compressed Sparse Row (also known as CRS)
  - CSC: Compressed Sparse Column (also known as CCS)



CSR representation of **A**:



### SUITESPARSE: GRAPHBLAS INTERNALS

- Authored by Prof. Tim Davis at Texas A&M University, based on his SuiteSparse library (used in MATLAB).
- Design decisions, algorithms and data structures are discussed in the TOMS paper and in the User Guide.
- Extensions: methods and types prefixed with GxB.
- Sophisticated load balancer for multi-threaded execution.
- GPU implementation is a work-in-progress.



T.A. Davis: Algorithm 1000: SuiteSparse:GraphBLAS: graph algorithms in the language of sparse linear algebra, ACM TOMS, 2019

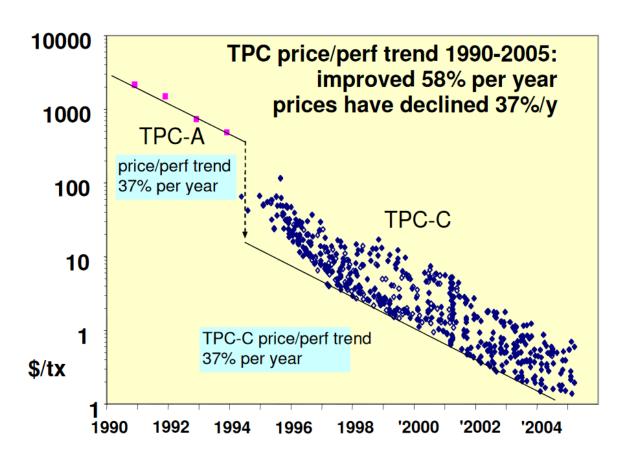


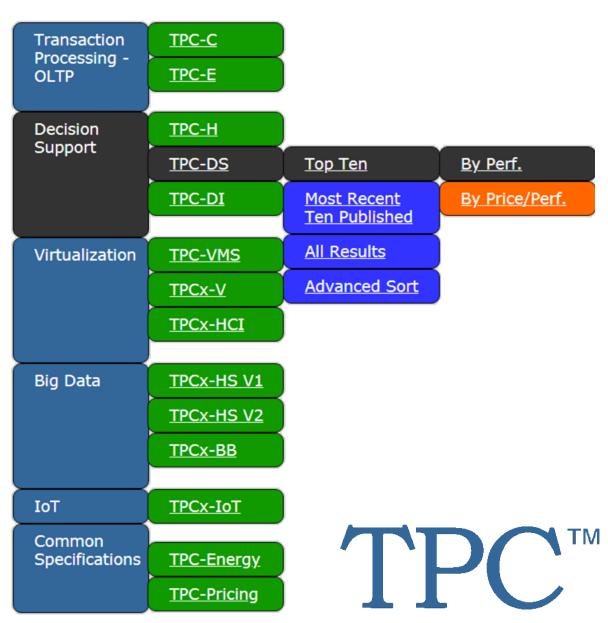
T.A. Davis: SuiteSparse:GraphBLAS: graph algorithms via sparse matrix operations on semirings, Sparse Days 2017

# **Graph benchmarks**

#### TPC: TRANSACTION PROCESSING PERFORMANCE COUNCIL

Standard specifications for benchmarking certain aspects of relational DBs





### LDBC: LINKED DATA BENCHMARK COUNCIL

- A non-profit academic & industrial organization
- Dedicated to define standard benchmarks for graph databases

### **EU FP7 project — Community meetings — Benchmark papers**



Social Network Benchmark Interactive workload SIGMOD 2015 Erling et al.





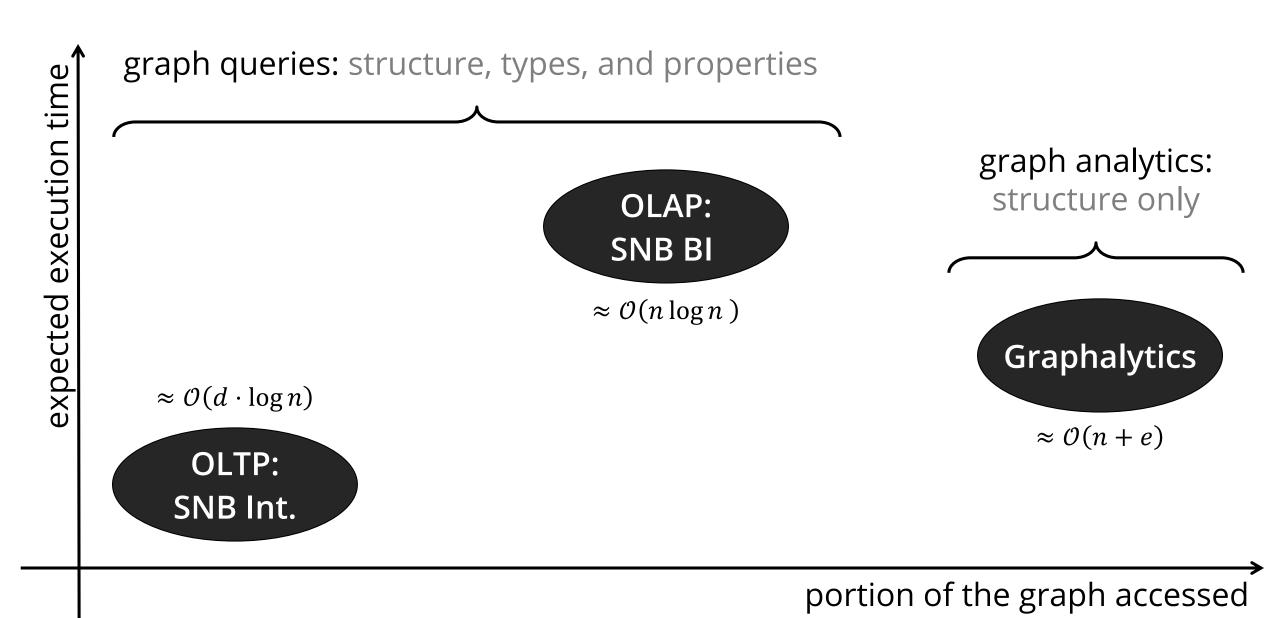


SNB
Business Intelligence
GRADES@SIGMOD 2018
Szárnyas et al.

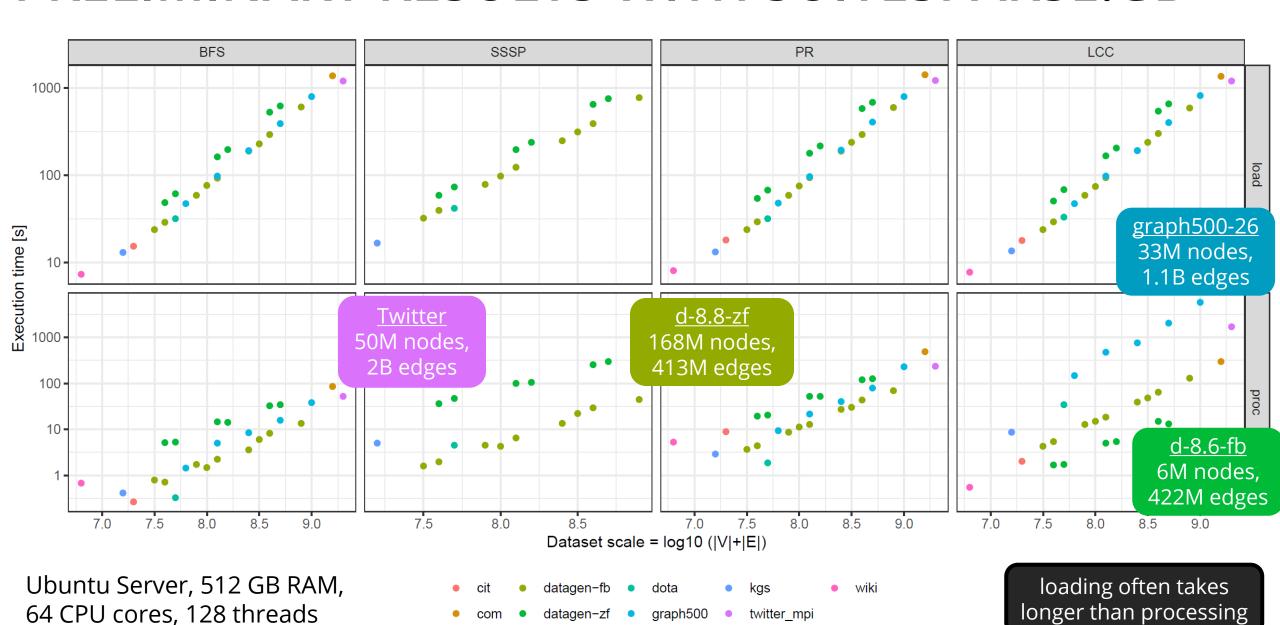
#### **Graphalytics**

VLDB 2016, losup et al.

### GRAPH PROCESSING CATEGORIES IN LDBC



### PRELIMINARY RESULTS WITH SUITESPARSE:GB



### THE GAP BENCHMARK SUITE

- Part of the Berkeley Graph Algorithm Platform project
- Same authors as the direction-optimizing BFS algorithm
- Six algorithms: BFS, SSSP, PageRank, connected components, betweenness centrality, triangle count
- Five data sets: Twitter, Web, Road, Kron, Urand
  - o 24M to 134M vertices, 68M to 2.1B edges
  - Weighted/unweighted, directed/undirected
- Very efficient baseline implementation in C++
- Maintained on arXiv v1: 2015, ..., v4: 2017



S. Beamer, K. Asanovic, D. Patterson: *The GAP Benchmark Suite,* arXiv, 2017



## Further reading and libraries

### **RESOURCES**

Presentations and tutorials for learning GraphBLAS along with a link to a collection of pointers.



J.R. Gilbert:

GraphBLAS: Graph Algorithms in the Language of Linear Algebra, Seminar talk since 2014



S. McMillan and T.G. Mattson:

A Hands-On Introduction to the GraphBLAS, Tutorial at HPEC since 2018



A. Buluç:

*GraphBLAS: Concepts, algorithms, and applications,* Scheduling Workshop, 2019



M. Kumar, J.E. Moreira, P. Pattnaik:

GraphBLAS: Handling performance concerns in large graph analytics, Computing Frontiers 2018



List of GraphBLAS-related books, papers, presentations, posters, software, etc. <a href="mailto:szarnyasg/graphblas-pointers">szarnyasg/graphblas-pointers</a>

### THE LAGRAPH LIBRARY

- Similar to the LAPACK library for BLAS
- Uses SuiteSparse:GraphBLAS
- Implementations of common algorithms
  - o BFS, SSSP, LCC, PageRank, Boruvka
  - Triangle count, k-truss
  - CDLP (community detection using label propagation)
  - Weakly connected components, Strongly Conn. Comps (draft)
  - Betweenness centrality
  - Deep neural network





### REQUIREMENTS BY GRAPH COMPUTATIONS

Libraries for linear-algebra based graph processing support the following features (prioritized):

- 1. Sparse matrices For reasonable performance
- 2. Arbitrary semirings For expressive power
- 3. Masking A big reduction in complexity for some algos
- 4. Parallel execution Constant speedup, ideally by #threads

Most matrix libraries only satisfy requirement #1:

- Intel MKL, Eigen, Boost uBLAS, MTL4, Armadillo, NIST Sparse BLAS, GMM++, CUSP (Thrust), Numpy, Efficient Java Matrix Library (EJML)
- The only exception is Julia's SparseArrays library, where arbitrary semirings can be used (#2) due to Julia's sophisticated type system

### **GRAPHBLAS PAPERS AND BOOKS**



- Standards for Graph Algorithm Primitives
  - o Position paper by 19 authors @ IEEE HPEC 2013



- Novel Algebras for Advanced Analytics in Julia
  - o Technical paper on semirings in Julia @ IEEE HPEC 2013



- Mathematical Foundations of the GraphBLAS
  - o Theory paper by 16 authors @ IEEE HPEC 2016

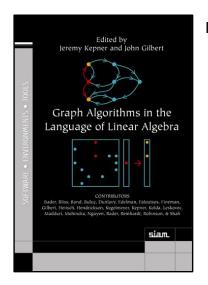


- Design of the GraphBLAS C API
  - Design decisions and overview of the C API @ GABB@IPDPS 2017

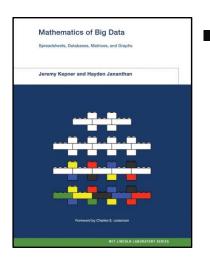


- Algorithm 1000: SuiteSparse:GraphBLAS: graph algorithms in the language of sparse linear algebra
  - o Algorithms in the SuiteSparse implementation @ ACM TOMS 2019

### **BOOKS**



- Graph Algorithms in the Language of Linear Algebra
  - o Edited by J. Kepner and J.R. Gilbert, published by SIAM in 2011
  - Algorithms for connected components, shortest paths, max-flow, betwenness centrality, spanning tree, graph generation, etc.
  - o Algorithms and data structure for fast matrix multiplication
  - o Predates GraphBLAS: preliminary notation, no API usage



- Mathematics of Big Data
  - Authored by Jananthan & Kepner, published by MIT Press in 2018
  - Generalizes the semiring-based approach for associative arrays
  - Contains reprints of papers, including the HPEC'16 paper above
  - Discusses D4M (Dynamic Distributed Dimensional Data Model)

### **GRAPHBLAS COMMUNITY**

Wiki: graphblas.org | Communication: mailing list, monthly telcos

#### **Annual events:**

- May: IEEE IPDPS conference
  - o GrAPL workshop (Graphs, Architectures, Programming and Learning), a merger of
    - GABB (Graph Algorithms Building Blocks)
    - GraML (Graph Algorithms and Machine Learning)
  - See <u>graphanalysis.org</u> for previous editions
- Sep: IEEE HPEC conference
  - GraphBLAS BoF meeting
- Nov: IEEE/ACM Supercomputing conference
  - GraphBLAS Working Group
  - IA<sup>3</sup> workshop (Workshop on Irregular Applications: Architectures and Algorithms)

Blog: AldenMath by Timothy Alden Davis

### **REDISGRAPH**

- Graph database built on top of Redis with partial (but extending) support for the Cypher language
- Uses SuiteSparse:GraphBLAS for graph operations
- Preliminary benchmark results show good performance on traversal-heavy workloads



R. Lipman, T.A. Davis: *Graph Algebra – Graph operations in the language of linear algebra* RedisConf 2018



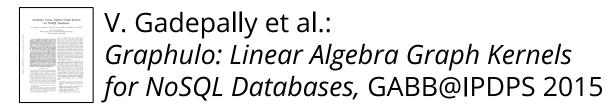
R. Lipman: RedisGraph internals RedisConf 2019

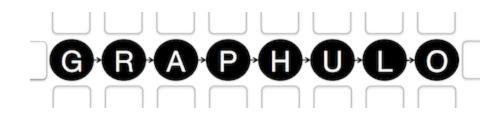
### **GRAPHBLAS IMPLEMENTATIONS**

- SuiteSparse:GraphBLAS
  - v1.0.0: Nov 2017 sequential
  - o v3.0.1: July 2019 parallel
  - o v3.1.0: Oct 2019 supports MATLAB bindings
- IBM GraphBLAS
  - Complete implementation in C++, released in May 2018
  - Concise but sequential
- GBTL (GraphBLAS Template Library): C++
  - v1.0: parallel but no longer maintained
  - o v2.0: sequential
- GraphBLAST: GPU implementation, based on GBTL

### **GRAPHULO**

- Build on top of the Accumulo distributed key-value store
- Written in Java
- Focus on scalability





### **COMBBLAS: COMBINATORIAL BLAS**

- "an extensible distributed memory parallel graph library offering a small but powerful set of linear algebra primitives"
- Not a GraphBLAS implementation but serves as an incubator for new ideas that may later find their way into GraphBLAS
- Scales to 250k+ CPU cores
  - Used on supercomputers such as Cray



# Learning GraphBLAS

### LEARNING GRAPHBLAS

- Challenging to get started need to have an understanding of:
  - Linear algebra (semirings, matrix multiplication, etc.)
  - Connection between linear algebra and graph operations (intuition)
  - Sizeable C API
- 200+ slides presenting algorithms in GraphBLAS
  - BFS variants, PageRank, Triangle count, k-truss
  - Community detection using label propagation
  - Luby's maximal independent set algorithm
  - o computing connected components on an overlay graph
  - o etc.

### PYGRAPHBLAS: PYTHON WRAPPER #1

- A Python wrapper
- See example code for SSSP and triangle count
- Close to pseudo-code
- Jupyter support

Added benefit: both Python and GraphBLAS use 0-based indexing

```
michelp/pygraphblas
```

```
def sssp(matrix, start):
    v = Vector.from_type(matrix.gb_type, matrix.nrows)
    v[start] = 0
    with min_plus, Accum(min_int64):
        for _ in range(matrix.nrows):
            w = Vector.dup(v)
            v @= matrix
            if w == v:
                break
        return v
 def sandia(A, L):
     return L.mxm(L, mask=L).reduce_int()
 sandia(M, M.tril())
```

### **GRBLAS: PYTHON WRAPPER #2**

- Goal: one-to-one mapping of the GraphBLAS API
  - less Pythonic
  - o comes with a Conda package
  - compiles user-defined functions to C



### TRADEOFFS OF GRAPHBLAS

- Updating CSR/CSC matrices is slow
  - SuiteSparse mitigates this to some extent by allowing incremental build before using the matrix but it still needs to rebuild the matrix before major operations such as mxv, mxm
  - o But: GraphBLAS objects are opaque and alternative formats can be used
    - Hornet [HPEC'18]
    - faimGraph [SC'18]
    - STINGER [HPEC'12]

# Summary

## VENUES ON GRAPH PROCESSING TECHNIQUES

- Database systems
- Database theory
- Information retrieval
- Operating systems
- High-perf. computing
- Distributed computing
- Parallel programming
- Algorithm design
- Software engineering
- Semantic web
- Graph transformation

- SIGMOD, VLDB, ICDE, EDBT, VLDB J., TKDE
- PODS, ICDT, TODS
- KDD, CIKM, WSDM, TKDD, DMKD J., & Big Data
- OSDI, SOSP, NSDI, ICPE, EuroSys
- SC, HPEC, HiPC, HPCC, HPDC, IPDPS
- PODC, DISC, ICDCS
- SPAA, ICPP, PLDI, PPoPP, ACM TOPC, Euro-Par
- TOMS, FOCS, STOC, SODA, SIAM J. Comput.
- ICSE, MODELS, FSE, ASE, FASE, OOPSLA, SoSyM
- WWW (TheWebConf), ISWC, WWW J., SWJ
- ICMT/ICGT, CAV, FMCAD, AGTIVE, ENTCS
- ...and many other mathematics and computer science venues.

### **SUMMARY**

- Linear algebra is a powerful abstraction
  - Good expressive power
  - Concise formulation of most graph algorithms
  - Very good performance
  - Still lots of ongoing research
- Trade-offs:
  - Learning curve (maths, C programming, GraphBLAS API)
  - Some algorithms are difficult to formulate in linear algebra
  - Only a few GraphBLAS implementations (yet)
- Overall: a very promising programming model for graph algorithms suited to the age of heterogeneous hardware

## SOME OPEN QUESTIONS

- What primitives should be added to GraphBLAS?
  - Sorting (CDLP)
  - Submatrix selection (k-truss)
  - Permutations (DFS)
- How to efficiently express SCC?
- How to implement GraphBLAS in a distributed system?



D.G. Spampinato et al.: Linear Algebraic Depth-First Search, ARRAYS@PLDI 2019



Y. Ahmad et al.: *LA3: A Scalable Link- and Locality-Aware Linear Algebra-Based Graph Analytics System,* VLDB 2018

- Incremental evaluation of SpMM/SpMV operations
  - Use an updatable matrix representation
  - $\circ$  Semirings  $\rightarrow$  rings  $\rightarrow$  additive inverse  $\rightarrow$  addition and removal
  - Incremental view maintenance techniques need rings (?)

### **ACKNOWLEDGEMENTS**

- Tim Davis and Tim Mattson for helpful discussions, members of GraphBLAS mailing list for their detailed feedback.
- The LDBC Graphalytics task force for creating the benchmark and assisting in the measurements.
- Master's students at BME for developing GraphBLAS-based algorithms: Bálint Hegyi, Márton Elekes, Petra Várhegyi, Lehel Boér

# "Nuances" - Some important adjustments to the definitions

### **GRAPHBLAS SEMIRINGS\***

The GraphBLAS specification defines semirings as follows:  $\langle D_{\text{out}}, D_{\text{in}_1}, D_{\text{in}_2}, \bigoplus, \otimes, 0 \rangle$  structure is a *GraphBLAS semiring* defined by

- $D_{\text{out}}$ ,  $D_{\text{in}_1}$ , and  $D_{\text{in}_2}$
- $\blacksquare$   $\bigoplus: D_{\text{out}} \times D_{\text{out}} \to D_{\text{out}}$
- $\blacksquare$   $\otimes: D_{\operatorname{in}_1} \times D_{\operatorname{in}_2} \to D_{\operatorname{out}}$
- $0 \in D_{\text{out}}$

three domains

an associative and commutative addition operation

a multiplicative operation

an identity element for ⊕

 $A = \langle D_{\text{out}}, \bigoplus, 0 \rangle$  is a commutative monoid.

 $F = \langle D_{\text{out}}, D_{\text{in}_1}, D_{\text{in}_2}, \otimes \rangle$  is a closed binary operator.

"It is expected that implementations will utilize IEEE-754 floating point arithmetic, which is not strictly associative." (C API specification)

### **MATRIX MULTIPLICATION\***

The simple formula of matrix multiplication

$$\mathbf{C} = \mathbf{A} \oplus . \otimes \mathbf{B}$$

$$\mathbf{C}(i,j) = \bigoplus_{j} \mathbf{A}(i,k) \otimes \mathbf{B}(k,j)$$

can lead to more complicated definitions. For example, what should the binary operator sel1st(x, y) = x return if y = 0?

$$sel1st(x, y) = \begin{cases} 0 & \text{if } y = 0 \\ x & \text{otherwise} \end{cases}$$

To simplify definitions, we use a generalized form of multiplication:

$$\mathbf{C}(i,j) = \bigoplus_{k \in \text{ind}(\mathbf{A}(i,:)) \cap \text{ind}(\mathbf{B}(:,j))} \mathbf{A}(i,k) \otimes \mathbf{B}(k,j)$$

where we only perform the multiplication in the intersection of the non-zero indices of  $\mathbf{A}$ 's ith row and  $\mathbf{B}$ 's jth column.

## **NOTATION\***

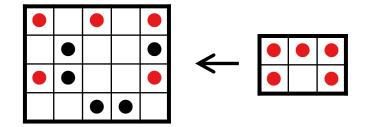
- Symbols:
  - **A**, **B**, **C**, **M** matrices
  - o **u**, **v**, **w**, **m** vectors
  - $\circ$  s, k scalar
  - $\circ$  *i, j* indices
  - $\circ \langle \mathbf{m} \rangle, \langle \mathbf{M} \rangle$  masks
- Operators:
  - $\circ \oplus$  addition
  - $\circ \otimes$  multiplication
  - T transpose Not included in the
  - o ⊙ accumulator → simplified table

This table contains all GrB and GxB (SuiteSparse-specific) operations.

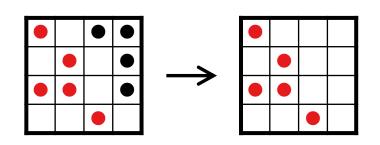
	symbol	operation	notation
	⊕.⊗	matrix-matrix multiplication	$C\langle M\rangle \odot = A \oplus . \otimes B$
		vector-matrix multiplication	$\mathbf{w}\langle\mathbf{m}\rangle\odot=\mathbf{v}\oplus.\otimes\mathbf{A}$
		matrix-vector multiplication	$\mathbf{w}\langle\mathbf{m}\rangle\odot=\mathbf{A}\oplus.\otimes\mathbf{v}$
	8	element-wise multiplication (set intersection of patterns)	$C\langle M\rangle\odot=A\otimes B$
			$\mathbf{w}\langle\mathbf{m}\rangle\odot=\mathbf{u}\otimes\mathbf{v}$
	$\oplus$	element-wise addition (set union of patterns)	$C\langle M\rangle\odot=A\oplus B$
			$\mathbf{w}\langle\mathbf{m}\rangle\odot=\mathbf{u}\oplus\mathbf{v}$
	f	apply unary operator	$\mathbf{C}\langle \mathbf{M}\rangle \odot = f(\mathbf{A})$
			$\mathbf{w}\langle\mathbf{m}\rangle\odot=f(\mathbf{v})$
	[⊕…]	reduce to vector	$\mathbf{w}\langle\mathbf{m}\rangle\bigcirc=\left[\bigoplus_{j}\mathbf{A}(:,j)\right]$
		reduce to scalar	$s \bigcirc = \left[ \bigoplus_{ij} \mathbf{A}(i,j) \right]$
	$\mathbf{A}^{T}$	transpose matrix	$C\langle M\rangle \bigcirc = A^{\top}$
	-	extract submatrix	$\mathbb{C}\langle M\rangle\bigcirc=A(i,j)$
			$\mathbf{w}\langle\mathbf{m}\rangle\odot=\mathbf{v}(\mathbf{i})$
	_	assign submatrix with submask for $C(I, J)$	$C\langle M\rangle(i,j)\odot=A$
			$\mathbf{w}\langle\mathbf{m}\rangle(\mathbf{i})\odot=\mathbf{v}$
	-	assign submatrix with mask for <b>C</b>	$C(i,j)\langle M\rangle\bigcirc=A$
			$w(i)\langle m\rangle\bigcirc=v$
	-	apply select operator (GxB)	$\mathbf{C}\langle\mathbf{M}\rangle\bigcirc=f(\mathbf{A},k)$
			$\mathbf{w}\langle\mathbf{m}\rangle\bigcirc=f(\mathbf{v},k)$
	-	Kronecker product	$C\langle M\rangle \bigcirc = \mathrm{kron}(A,B)$

### LINEAR ALGEBRAIC PRIMITIVES FOR GRAPHS #3\*

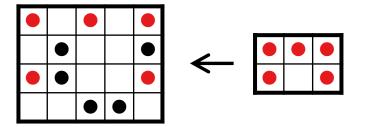
Sparse matrix extraction: induced subgraph



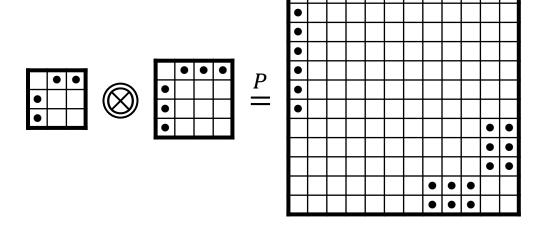
Sparse matrix selection (SuiteSparse): filtering edges



Sparse submatrix assignment: replace subgraph



Kronecker product: graph generation



### **MATRIX-VECTOR MULTIPLICATION\***

The operation  $\mathbf{v} \oplus . \otimes \mathbf{A}$  gives the vertices reachable from the ones in  $\mathbf{v}$ . However, GraphBLAS publications and implementations often use  $\mathbf{A}^{\mathsf{T}} \oplus . \otimes \mathbf{v}$  instead. The difference between these is that the former produces a row vector, while the latter produces a column vector:

$$\mathbf{v} \oplus . \otimes \mathbf{A} \equiv (\mathbf{A}^{\mathsf{T}} \oplus . \otimes \mathbf{v}^{\mathsf{T}})^{\mathsf{T}}$$

GraphBLAS does not distinguish row/column vectors, therefore the notations are (formally) equivalent:

$$\mathbf{v} \oplus . \otimes \mathbf{A} \equiv \mathbf{A}^{\mathsf{T}} \oplus . \otimes \mathbf{v}$$

In practice, the order of the operands can have a significant impact on performance. For example, if matrices are stored in CSR format, computing  $\mathbf{v} \oplus . \otimes \mathbf{A}$  is expensive compared to  $\mathbf{A}^{\mathsf{T}} \oplus . \otimes \mathbf{v}$ .



# Extra slides

#### THE CASE FOR LINEAR ALGEBRA-BASED GRAPH ALGORITHMS

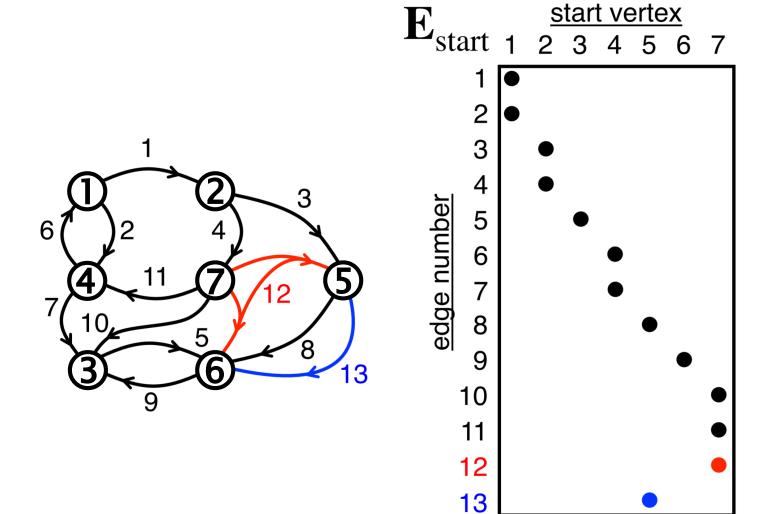
Many irregular applications contain coarse-grained parallelism that can be exploited by abstractions at the proper level.

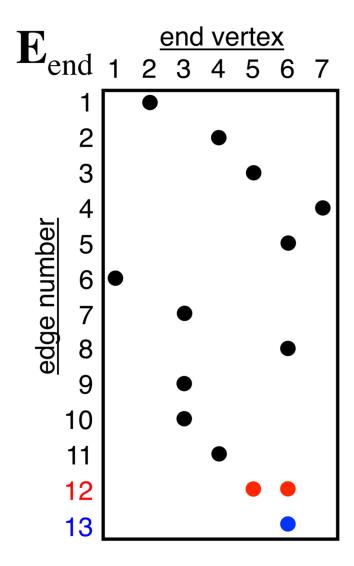
Traditional graph computation	Graphs in the language of linear algebra
Data-driven, unpredictable communication	Fixed communication patterns
Irregular and unstructured, poor locality of reference	Operations on matrix blocks exploit memory hierarchy
Fine-grained data accesses, dominated by latency	Coarse-grained parallelism, bandwidth-limited



D. Bader et al., *The GraphBLAS effort and its implications for Exascale,* SIAM Workshop on Exascale Applied Mathematics Challenges and Opportunities, 2014

### DIRECTED HYPERGRAPH EXAMPLE





# Graph algorithms in GraphBLAS

Weakly connected components

### WCC: WEAKLY CONNECTED COMPONENTS (SKETCH)

$$C = I \lor A \lor A^{2} \lor A^{3} \lor A^{4} \lor \cdots$$

$$D = I + A + A^{2} + A^{3} + A^{4} \lor \cdots \lor A^{K}$$

$$E \equiv (I - A)D$$

$$E = D - AD$$

$$= I + A + A^{2} + A^{3} + A^{4} + \cdots - A - A^{2} - A^{3} - A^{4} - \cdots$$

$$= I$$

$$= (I - A)D$$

$$D = (I - A)^{-1}$$



J. Kepner, J.R. Gilbert:

Graph Algorithms in the Language of Linear Algebra, Chapter 3, SIAM, 2011

### WCC: WEAKLY CONNECTED COMPONENTS

- The series for D does usually not converge. However, by replacing A with  $\alpha A$ , where  $\alpha$  is a sufficiently small positive number, the series converges. The derivation presented in the previous slide is still valid, resulting in  $D = (I \alpha A)^{-1}$ .
- While this trick ensures that the presented algorithm works correctly, this approach is still impractical as it computes the inverse of a sparse matrix which is dense in most cases.

### WCC: WEAKLY CONNECTED COMPONENTS

- Linear Algebraic Connected Components algorithm (LACC)
  - o Recent result, based on the Awerbuch-Shiloach algorithm.
  - Designed for supercomputers, scales to 250,000+ CPU cores.
  - "Distributed-memory LACC code that is used in our experiments is publicly available as part of the CombBLAS library. A simplified unoptimized serial GraphBLAS implementation is also committed to the LAGraph Library for educational purposes."
- See also FastSV.



A. Azad, A. Buluç: *LACC: A Linear-Algebraic Algorithm for Finding Connected Components in Distributed Memory,* IPDPS 2019

# Graph algorithms in GraphBLAS

Maximal independent set: Luby's algorithm

### **LUBY'S ALGORITHM**

To be done later.

# Notes

### **ABOUT THIS PRESENTATION**

- This presentation is intended to serve as an introduction to semiring-based graph processing and the GraphBLAS.
- Common graph algorithms (BFS, shortest path, PageRank, etc.) are used to demonstrate the features of GraphBLAS. Many of the algorithms presented are part of the LAGraph library.
- The presentation complements existing technical talks on GraphBLAS and can form a basis of anything from a short 20min overview to 2×90min lectures on the GraphBLAS.
- The slides contain numerous references to papers and talks.
- There are detailed textual explanations on some slides to make them usable as a learning material.

#### TECHNICAL DETAILS

- The slides were created with PowerPoint 2016 using the Open Sans and DejaVu Sans Mono font families (embedded in the presentation).
- The mathematical expressions are typeset with PowerPoint's built-in Equation Editor.
- The circled numbers (denoting graph vertices) are rendered using the standard Wingdings font.
- The text is written in Oxford English.
- The icons for referenced papers and talks are clickable and will lead to an open-access / preprint / author's copy version of the referred work (if such copy exists). The icons depict the first page of the cited document.

### **FUTURE WORK**

- Matrix representations
  - The 'typical' sparse matrix data structures: CSR, CRS
  - Basic updatable data structures: COO, LIL, DOK
  - Advanced updatable data structures: Hornet, faim
- Important algorithms
  - Matrix multiplication (dot, hash, heap, Gustavson)
- Advanced GraphBLAS features
  - o the accumulator
  - merge/replace
  - o submatrix extraction, assignment, Kronecker product