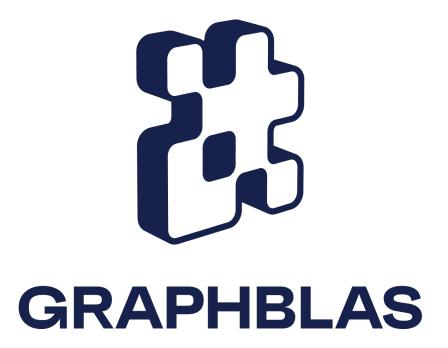
Introduction to GraphBLAS

A linear algebraic approach for concise, portable, and high-performance graph algorithms

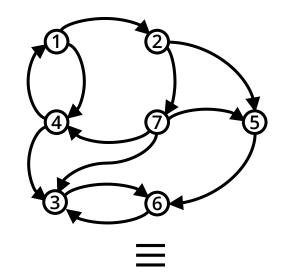
Gábor Szárnyas (CWI)

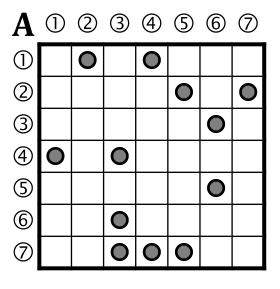


Motivation

GRAPHBLAS

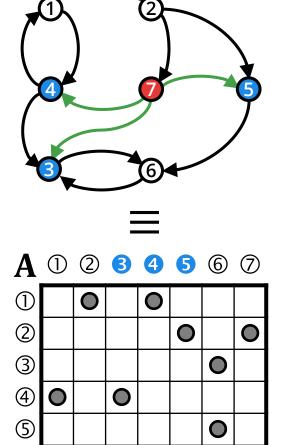
- Graph algorithms are challenging to program
 - irregular access patterns → poor locality
 - o caching and parallelization are difficult
- Optimizations often limit portability
- The GraphBLAS introduces an abstraction layer using the language of linear algebra
 - \circ graph \equiv sparse matrix
 - \circ traversal step \equiv vector-matrix multiplication

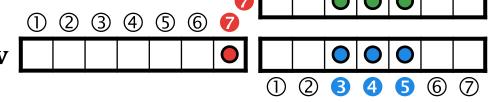




GRAPHBLAS

- Graph algorithms are challenging to program
 - irregular access patterns → poor locality
 - o caching and parallelization are difficult
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 - \circ traversal step \equiv vector-matrix multiplication







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

Graph algorithms have a high communication-to-computation ratio.

Speedup with a CPU that has better arithmetic performance:

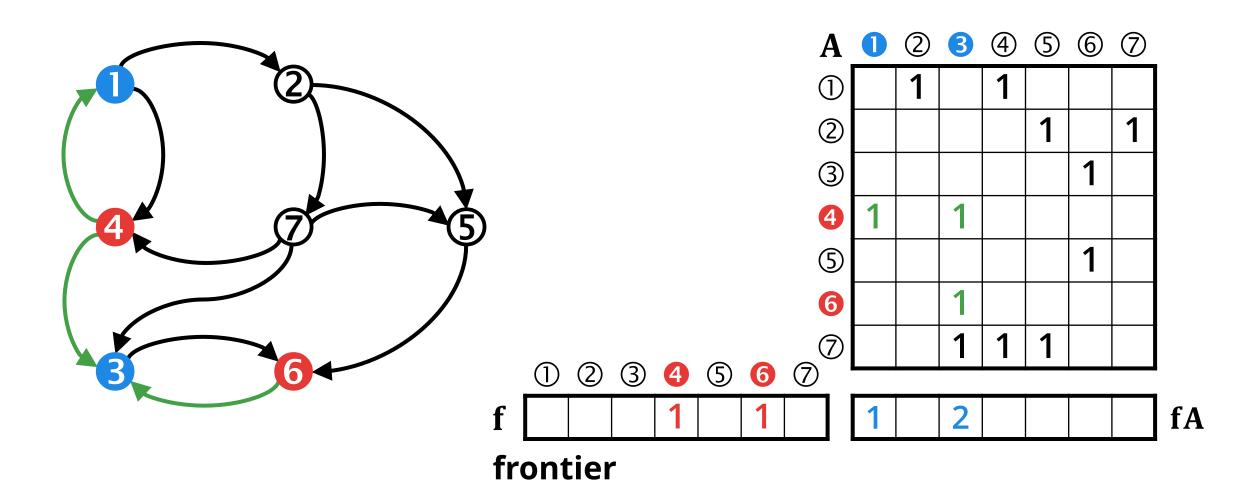
- machine learning → a lot
- relational queries → some
- graph processing → very little

Standard latency hiding techniques break down, e.g. pre-fetching and branch prediction provide little benefit.

Use a data representation and computation model which are expressive, machine-friendly, and portable.

LINEAR ALGEBRA-BASED GRAPH PROCESSING

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



The GraphBLAS standard

THE GRAPHBLAS STANDARD

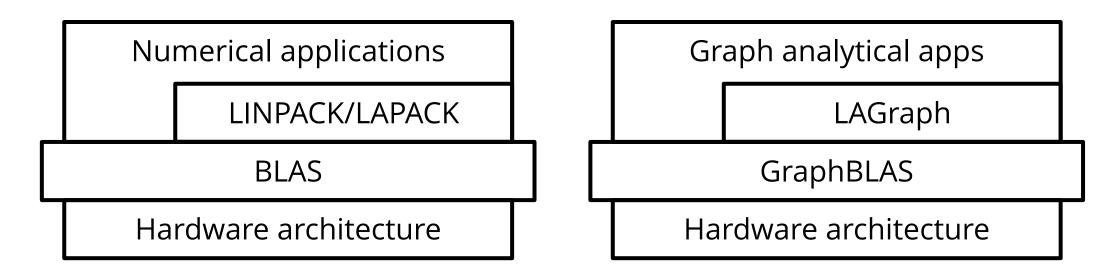
Goal: separate the concerns of the hardware, library, and application designers.

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

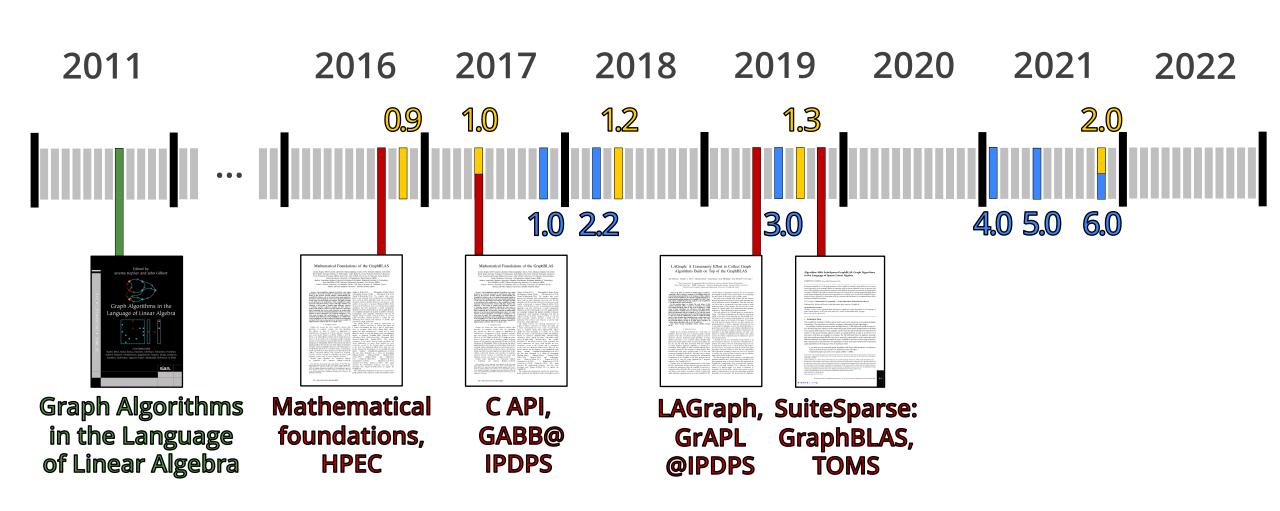




S. McMillan @ SEI Research Review (Carnegie Mellon University, 2015): *Graph algorithms on future architectures*

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 paths	Dijkstra	$m + n \log n$	n^2
single-source shortest patris	Bellman-Ford	mn	mn
all-pairs shortest paths	Floyd-Warshall	n^3	n^3
minimum spanning 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	$m + n \log n$	$mn + n^2$
maximai 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

KEY FEATURES OF GRAPHBLAS

Portable: supports x86, Arm (Apple M1); GPUs (WIP)

Efficient: within one order-of-magnitude compared to hand-tuned code

Concise: most textbook algorithms can be expressed with a few operations

Composable: the output of an algorithm can be used as an input of a subsequent algorithm

Flexible: can express algorithms on typed graphs and property graphs

Theoretical foundations of the GraphBLAS

DENSE MATRIX MULTIPLICATION

Definition:

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

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

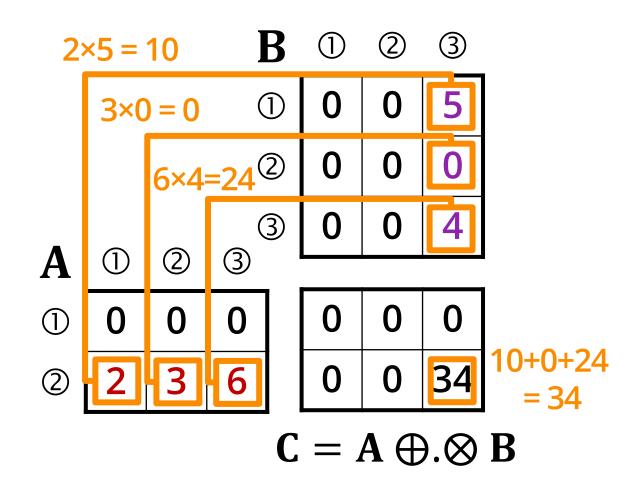
Example:

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

$$A(2,2) \times B(2,3) +$$

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

$$= 2 \times 5 + 3 \times 0 + 6 \times 4 = 34$$



SPARSE MATRIX MULTIPLICATION

Definition:

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

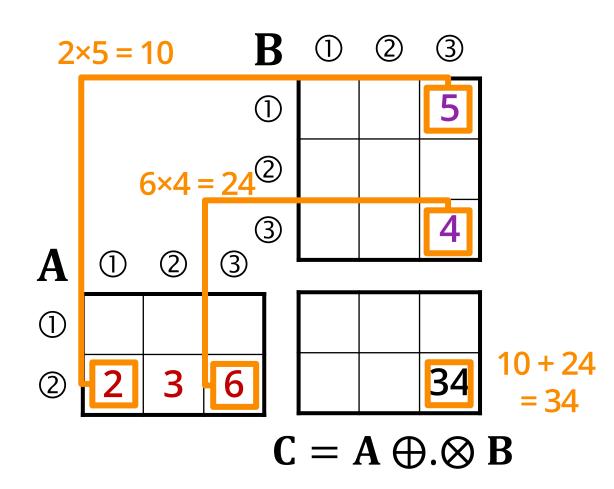
$$\mathbf{C}(i,j) = \bigoplus_{k \in \text{ind}(\mathbf{A}(i,:)) \cap \text{ind}(\mathbf{B}(:,j))} \mathbf{A}(i,k) \otimes \mathbf{B}(k,j)$$

Sparse matrix multiplication only evaluates the multiplication operator \otimes for positions where there is a non-zero element in both $\mathbf{A}(i,k)$ and $\mathbf{B}(k,j)$.

Example:

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

= $2 \times 5 + 6 \times 4 = 34$



MATRIX MULTIPLICATION $C = A \oplus . \otimes B$

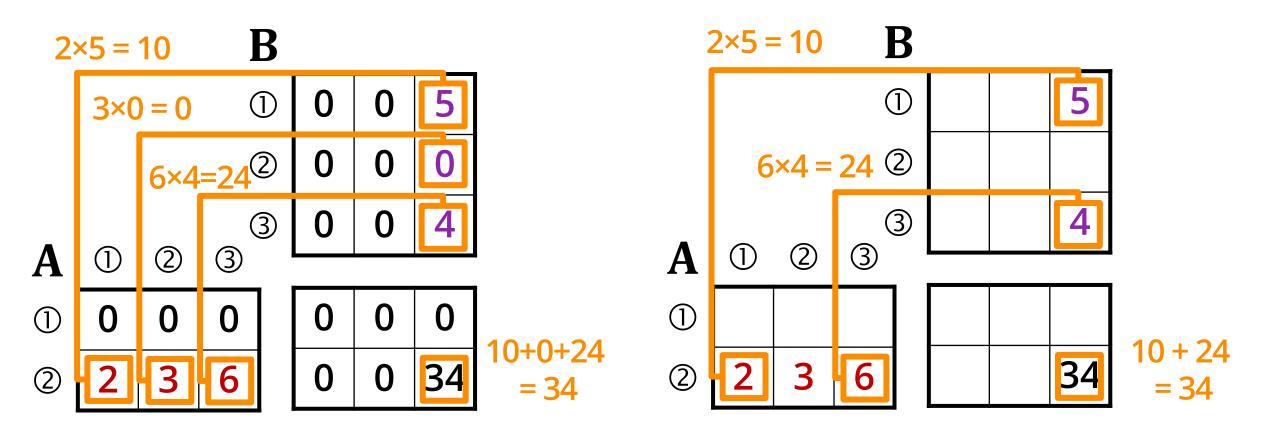
Multiplication on dense matrices

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

Multiplication on sparse matrices

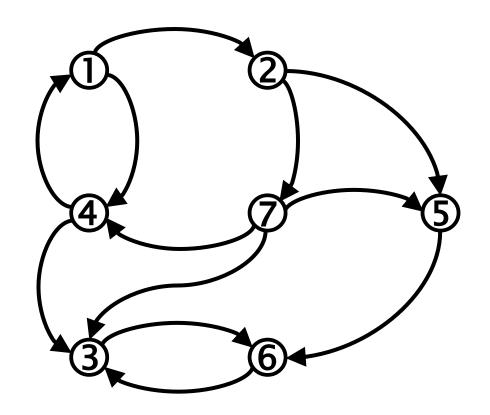
$$\mathbf{C}(i,j) = \bigoplus_{k \in \text{ind}(\mathbf{A}(i,:)) \cap \text{ind}(\mathbf{B}(:,j))} \mathbf{A}(i,k) \otimes \mathbf{B}(k,j)$$

Example: $C = A \oplus . \otimes B$



ADJACENCY MATRIX

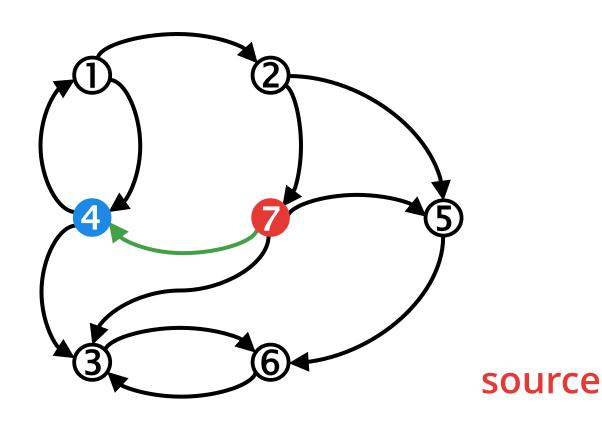
$$\mathbf{A}_{ij} = \begin{cases} 1 & \text{if } (v_i, v_j) \in E \\ 0 & \text{if } (v_i, v_j) \notin E \end{cases}$$



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

ADJACENCY MATRIX

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

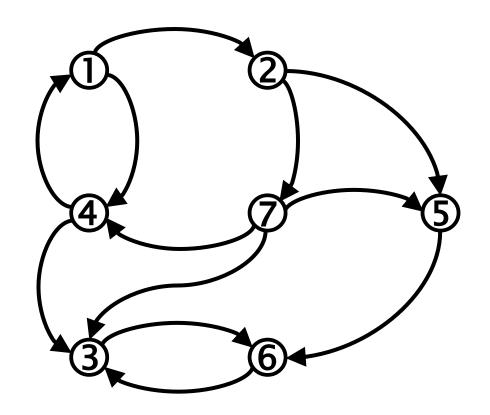


target

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

ADJACENCY MATRIX

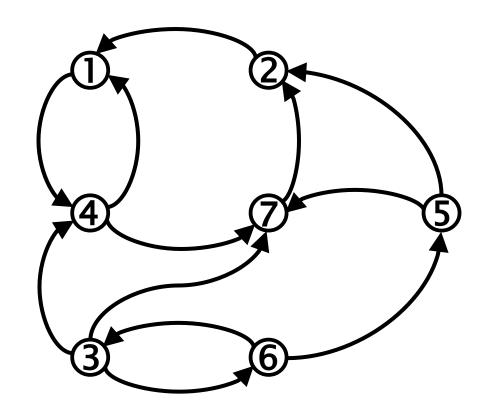
$$\mathbf{A}_{ij} = \begin{cases} 1 & \text{if } (v_i, v_j) \in E \\ 0 & \text{if } (v_i, v_j) \notin E \end{cases}$$



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

ADJACENCY MATRIX TRANSPOSED

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

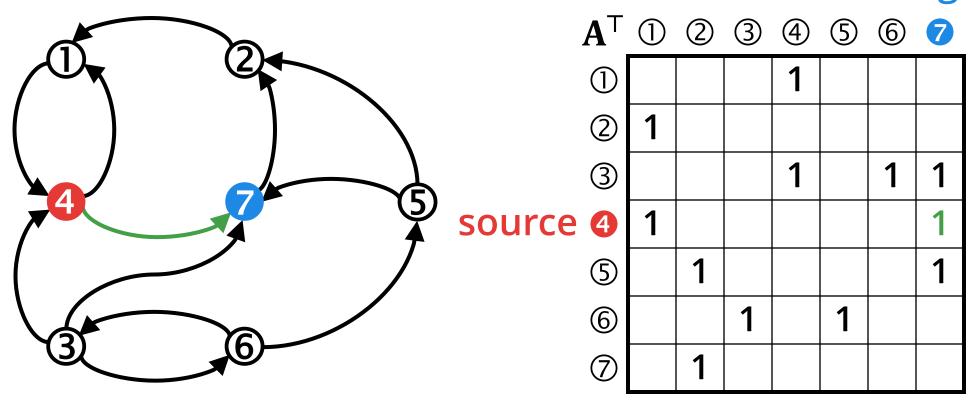


\mathbf{A}^{T}	1	2	3	4	(5)	6	7
1				1			
2	1						
3				1		1	1
③ ④	1						1
(5)		1					1
6			1		1		
7		1					

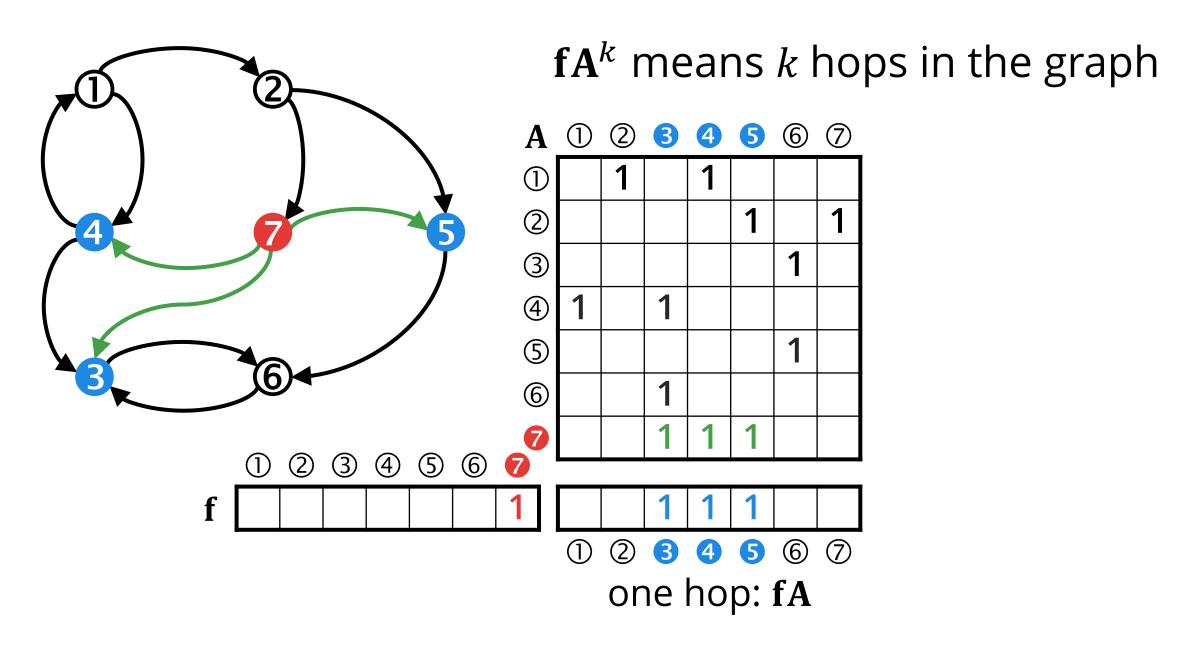
ADJACENCY MATRIX TRANSPOSED

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

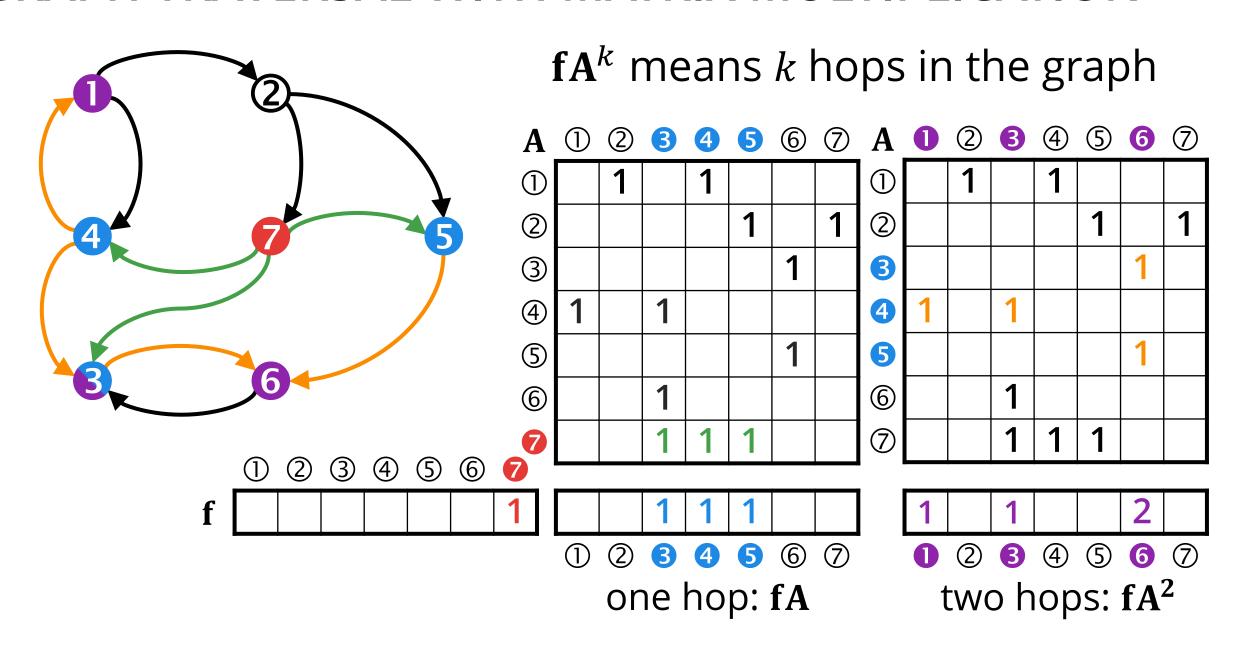
target



GRAPH TRAVERSAL WITH MATRIX MULTIPLICATION



GRAPH TRAVERSAL WITH MATRIX MULTIPLICATION



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 $\forall a, b, c \in D$, if the following hold:
 - \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.

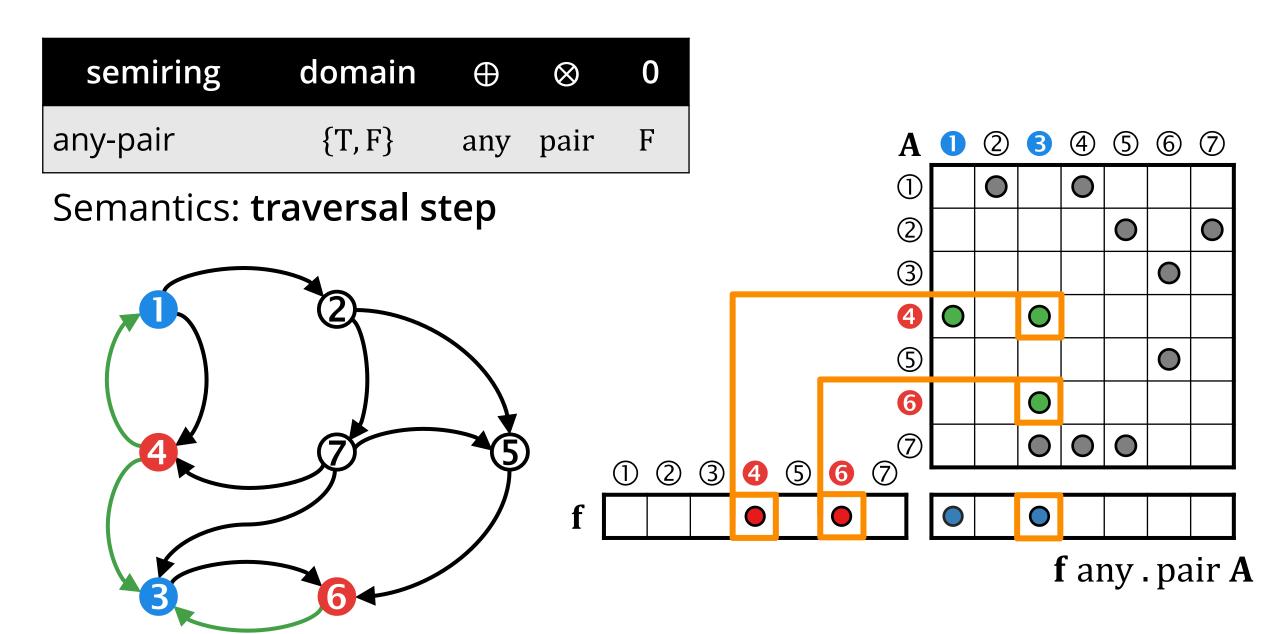
SEMIRINGS

semiring	domain	\oplus	\otimes	0	graph semantics
any-pair	{T, F}	any	pair	F	traversal step
integer arithmetic	N	+	×	0	number of paths
min-plus	ℝ ∪ {+∞}	min	+	+∞	shortest path

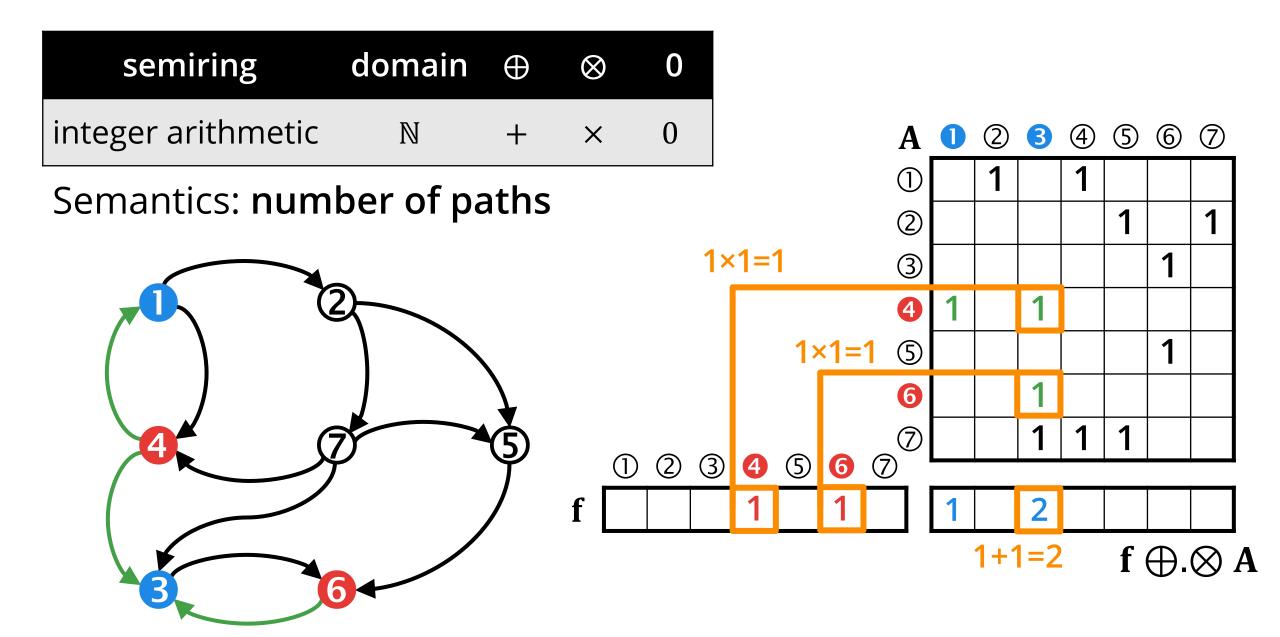
The default semiring is the conventional one:

- lacktriangledown \otimes defaults to the arithmetic multiplication operator.
- defaults to the arithmetic addition operator.

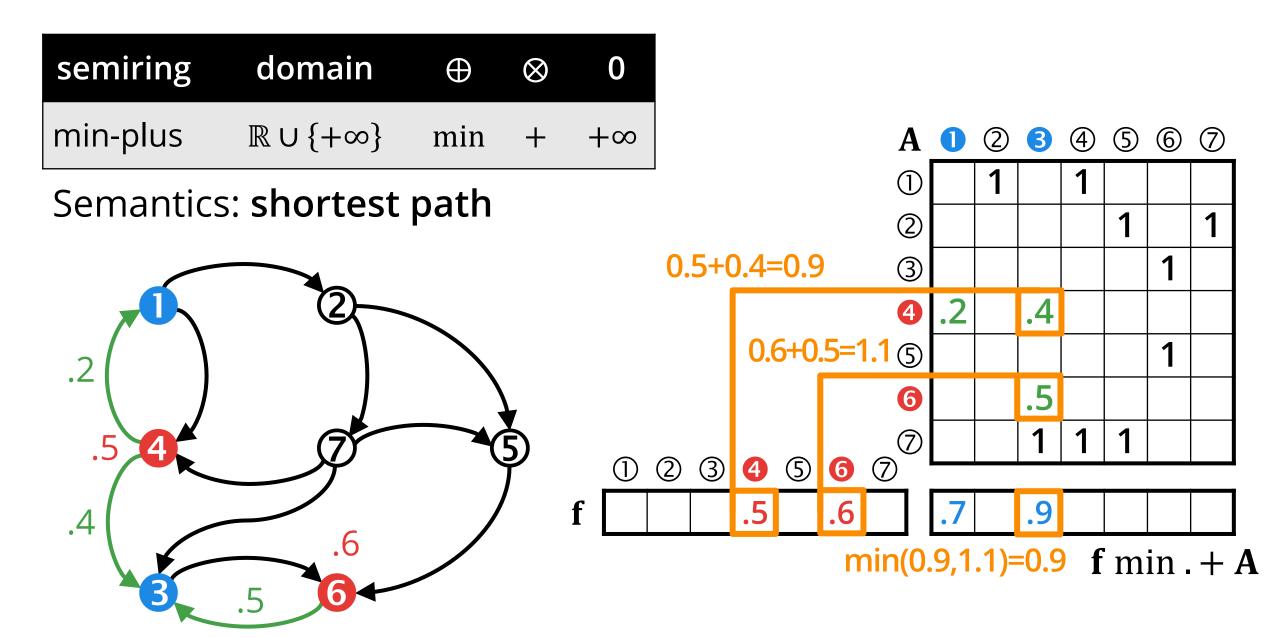
MATRIX-VECTOR MULTIPLICATION SEMANTICS



MATRIX-VECTOR MULTIPLICATION SEMANTICS

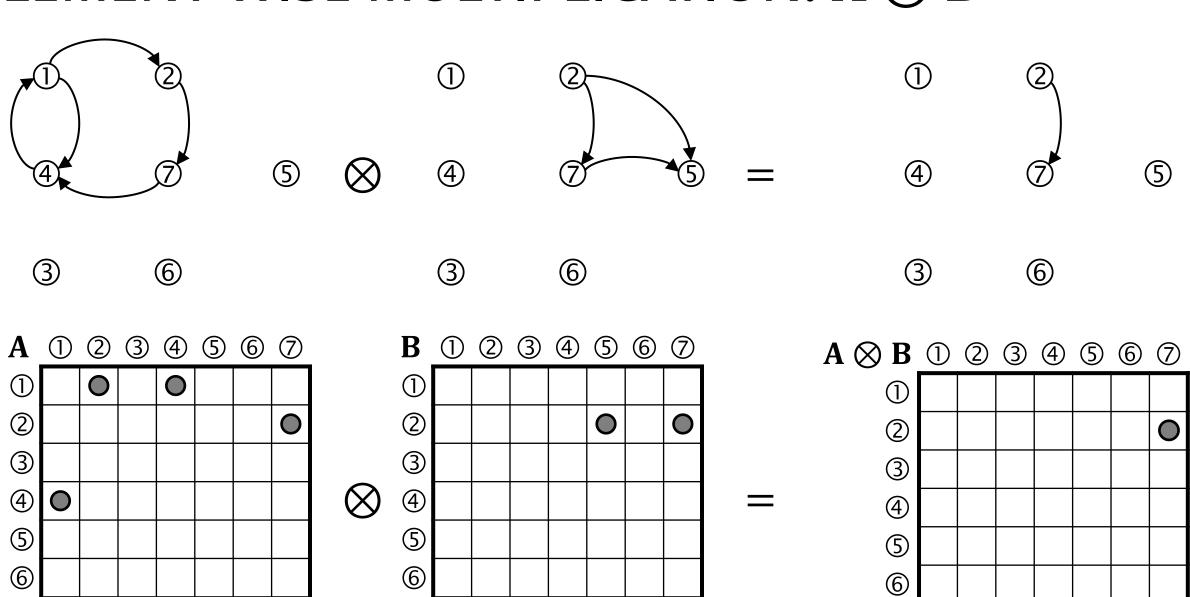


MATRIX-VECTOR MULTIPLICATION SEMANTICS

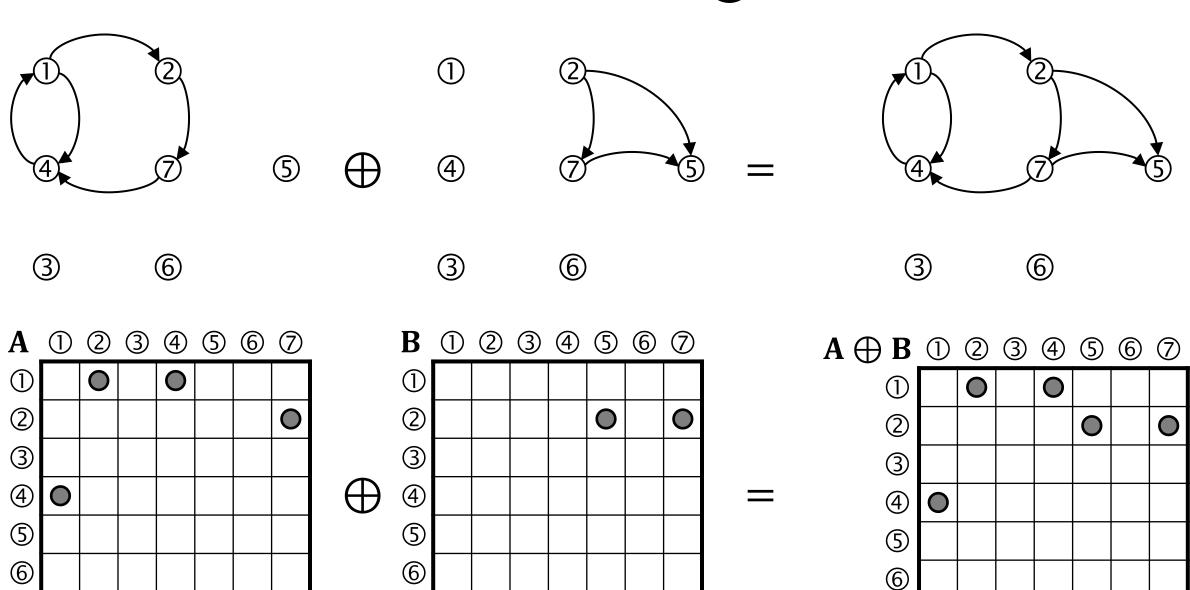


ELEMENT-WISE MULTIPLICATION: A \otimes B

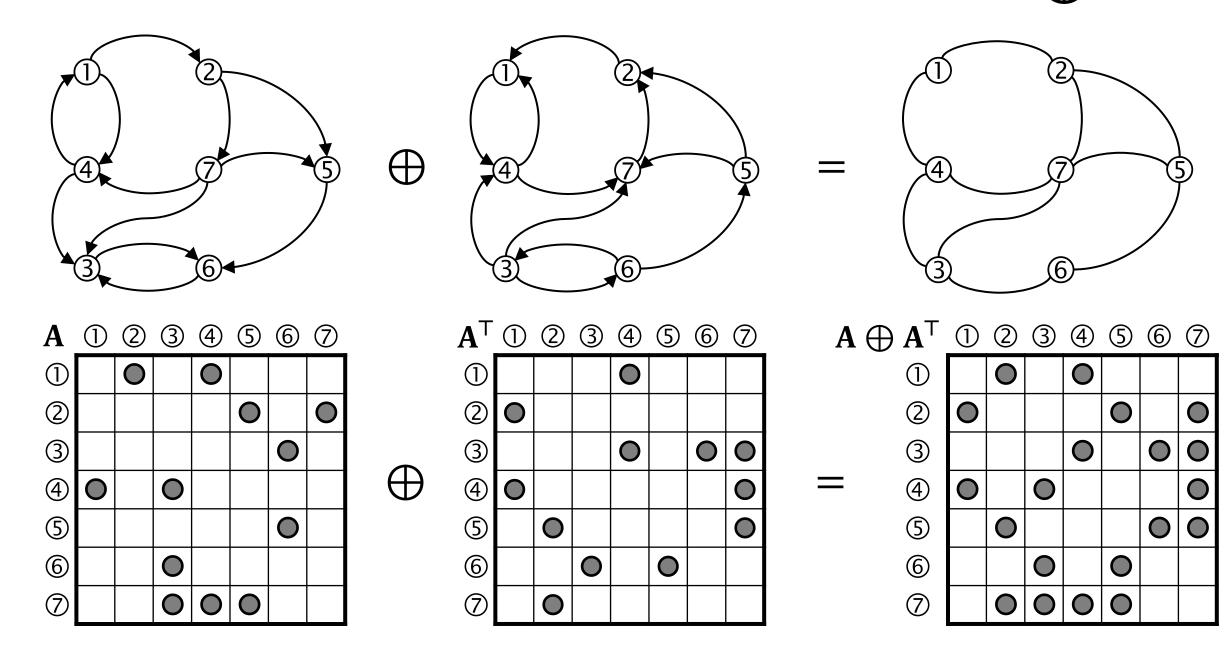
(7)



ELEMENT-WISE ADDITION: A B



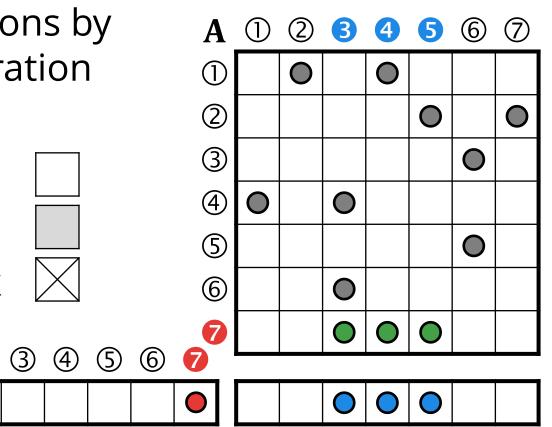
TURNING A GRAPH INTO UNDIRECTED: $A \oplus A^{T}$



MASKING

Prevent redundant computations by reducing the scope of an operation Operations can be executed

- without a mask
- with a regular mask
- with a complemented mask



 $\mathbf{w} = \mathbf{f} \oplus . \otimes \mathbf{A}$

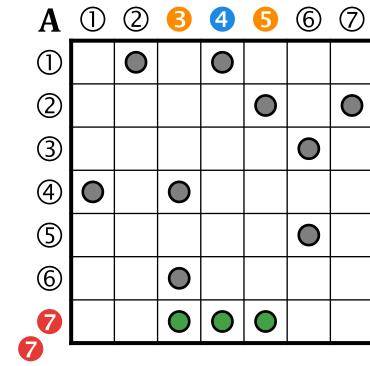
MASKING

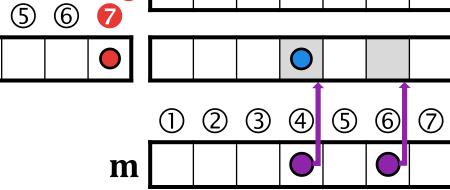
Prevent redundant computations by reducing the scope of an operation Operations can be executed

3

4

- without a mask
- with a regular mask
- with a complemented mask



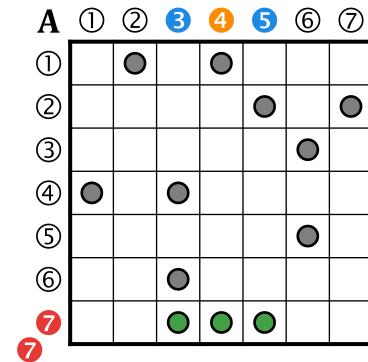


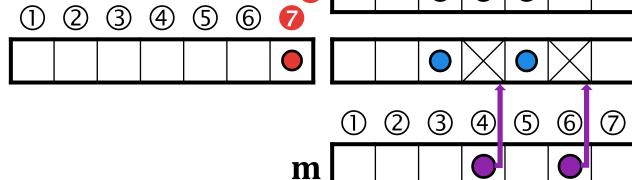
$$\mathbf{w}\langle \mathbf{m}\rangle = \mathbf{f} \oplus . \otimes \mathbf{A}$$

MASKING

Prevent redundant computations by reducing the scope of an operation Operations can be executed

- without a mask
- with a regular mask
- lacktriangle with a complemented mask igtimes





$$\mathbf{w}\langle \neg \mathbf{m} \rangle = \mathbf{f} \oplus . \otimes \mathbf{A}$$

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
 - Ø division
 - o [⊤] transpose

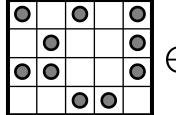
symbol	operation	notation
	matrix-matrix multiplication	$C\langle M\rangle = A \oplus . \otimes B$
⊕.⊗	vector-matrix multiplication	$\mathbf{w}\langle\mathbf{m}\rangle = \mathbf{v} \oplus . \otimes \mathbf{A}$
	matrix-vector multiplication	$\mathbf{w}\langle\mathbf{m}\rangle = \mathbf{A} \oplus . \otimes \mathbf{v}$
\otimes	element-wise multiplication	$C\langle M\rangle = A\otimes B$
	(set intersection of patterns)	$\mathbf{w}\langle\mathbf{m}\rangle = \mathbf{u} \otimes \mathbf{v}$
\oplus	element-wise addition	$C\langle M\rangle = A \oplus B$
Φ	(set union of patterns)	$\mathbf{w}\langle\mathbf{m}\rangle = \mathbf{u} \oplus \mathbf{v}$
$\int \int \partial u du d$	apply unary operator	$\mathbf{C}\langle\mathbf{M}\rangle = f(\mathbf{A})$
J	арріу штагу орегасог	$\mathbf{w}\langle\mathbf{m}\rangle = f(\mathbf{v})$
[]	reduce to vector	$\mathbf{w}\langle\mathbf{m}\rangle = \left[\bigoplus_{j} \mathbf{A}(:,j)\right]$
[⊕…]	reduce to scalar	$s = \left[\bigoplus_{ij} \mathbf{A}(i,j) \right]$
\mathbf{A}^{T}	transpose matrix	$\mathbf{C}\langle\mathbf{M}\rangle = \mathbf{A}^{T}$

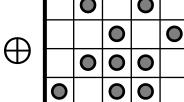
Vectors can act as both column and row vectors.

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

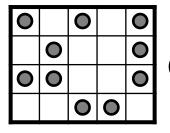
LINEAR ALGEBRAIC PRIMITIVES FOR GRAPHS #1

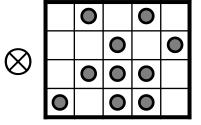
Element-wise addition: union of non-zero elements



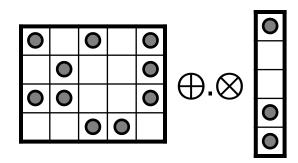


Element-wise multiplication: intersection of non-zero elements

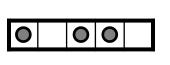




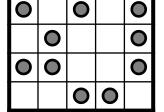
Sparse matrix times sparse vector: process incoming edges



Sparse vector times sparse matrix: process outgoing edges

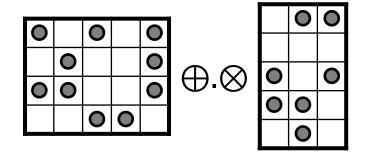




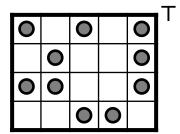


LINEAR ALGEBRAIC PRIMITIVES FOR GRAPHS #2

Sparse matrix times sparse matrix: process connecting outgoing edges

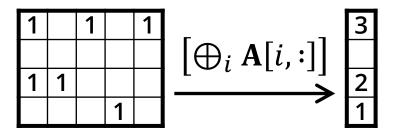


Matrix transpose: reverse edges



Reduction:

aggregate values in each row



Apply:

apply unary operator on all values

1		2		3		1		4		9
					$f(x) = x^2$					
3	2				\rightarrow	9	4			
			1						1	

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]

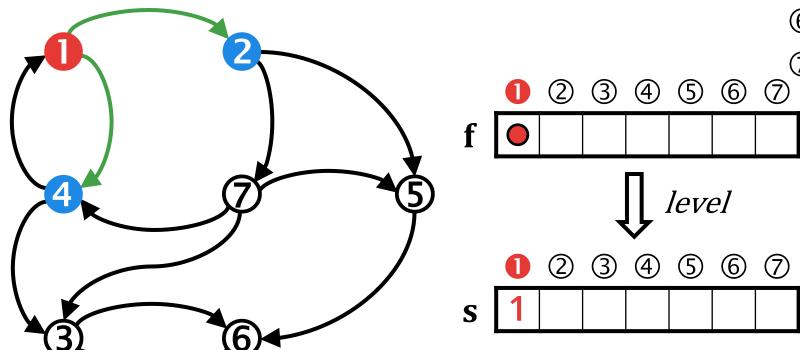
Variants:

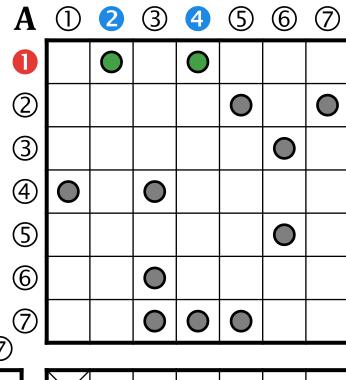
- Levels compute traversal level for each vertex
- Parents compute parent for each vertex
- MSBFS start traversal from multiple source vertices

Breadth-first search / Levels

semiring	domain	\oplus	\otimes	0
any-pair	{T, F}	any	pair	F

level = 1

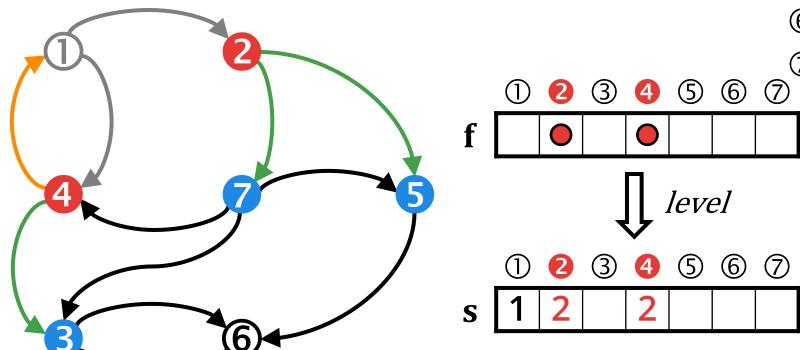


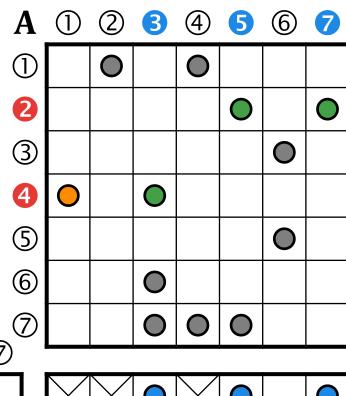


$$f(\neg s) = f$$
 any. pair A

semiring	domain	\oplus	\otimes	0
any-pair	{T, F}	any	pair	F

level = 2

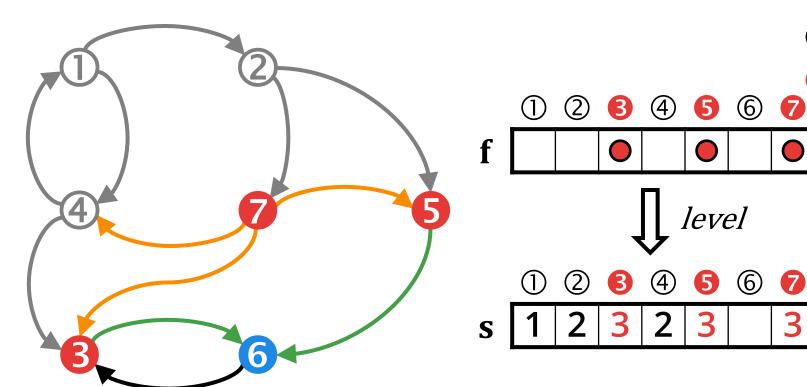


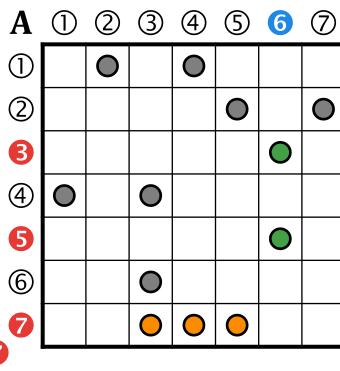


 $\mathbf{f}\langle \neg \mathbf{s} \rangle = \mathbf{f}$ any. pair \mathbf{A}

semiring	domain	\oplus	\otimes	0
any-pair	{T, F}	any	pair	F

level = 3

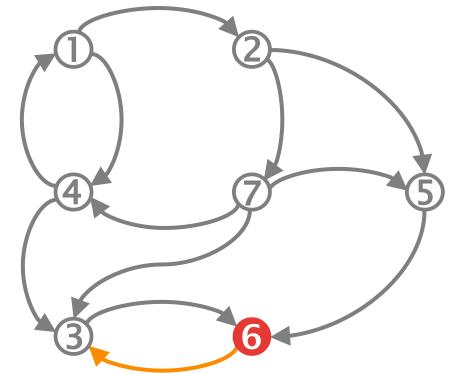


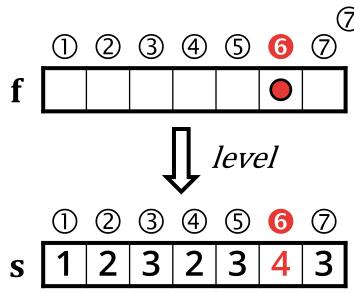


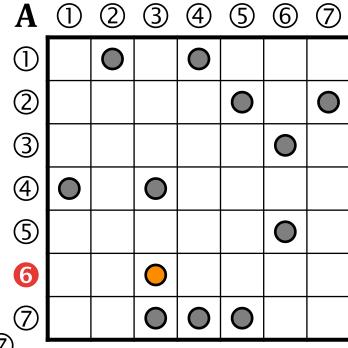
$$\mathbf{f}\langle \neg \mathbf{s} \rangle = \mathbf{f}$$
 any. pair \mathbf{A}

semiring	domain	\oplus	\otimes	0
any-pair	{T, F}	any	pair	F

level = 4







 $f(\neg s) = f$ any. pair A

f is empty
→ terminate

BFS - LEVELS: ALGORITHM

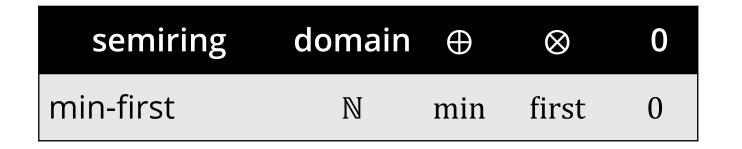


- Input: adjacency matrix **A**, source vertex *s*, #vertices *n*
- Output: vector of visited vertices v (integer)
- Workspace: frontier vector f (Boolean)

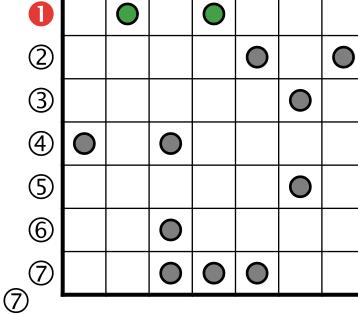
- 1. f(s) = T
- 2. for level = 1 to n 1 *terminate earlier if **f** is empty
- 3. $\mathbf{s}\langle\mathbf{f}\rangle = level$ assign the level value to the vertices in the frontier
- 4. clear(**f**) clear the frontier **f**
- 5. $\mathbf{f} \langle \neg \mathbf{s} \rangle = \mathbf{f}$ any pair **A** advance the frontier

Breadth-first search / Parents

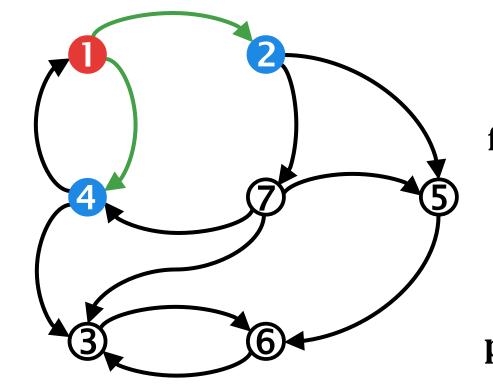
BFS – PARENTS

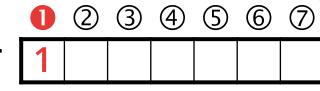


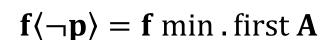
first(x, y) = x



A ① 2 3 4 5 6 7



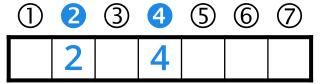




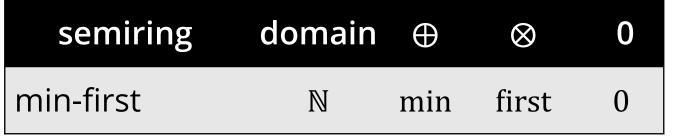
$$p\langle f\rangle = f$$

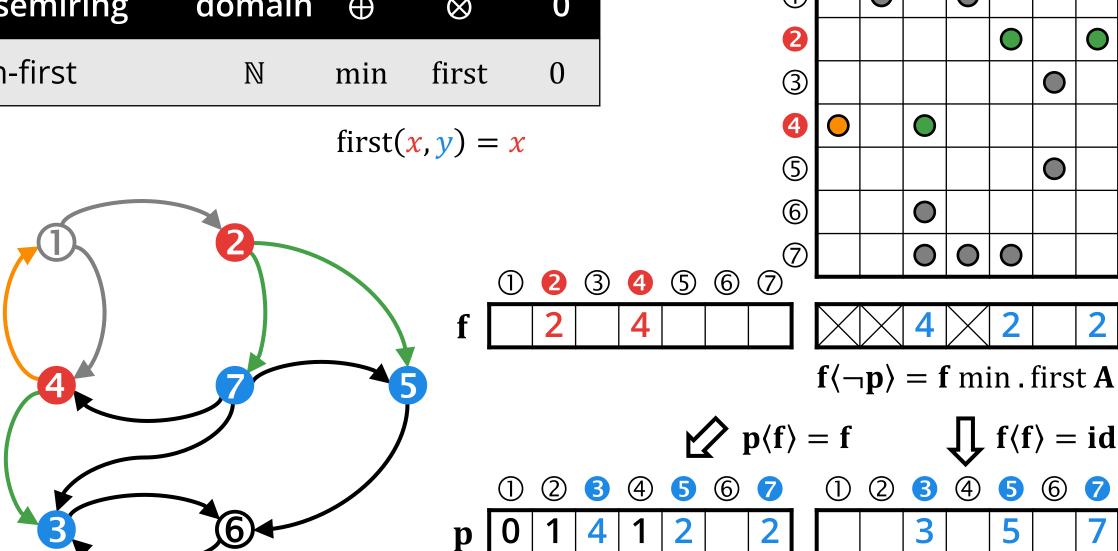






BFS – PARENTS

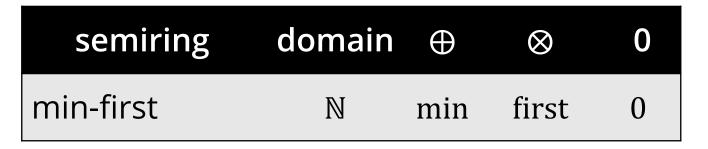




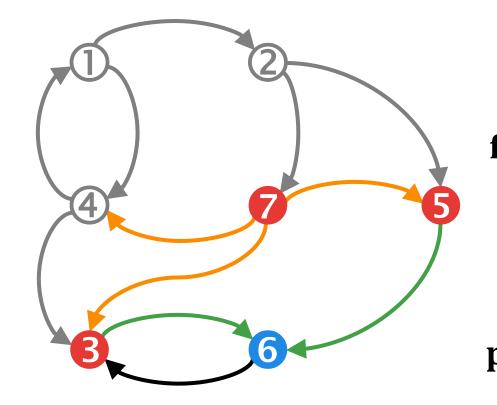
2 3 4 5

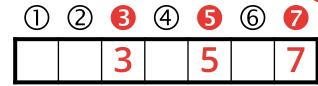
6 7

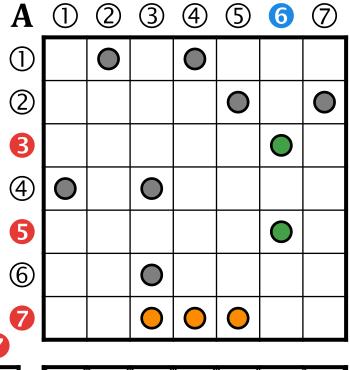
BFS - PARENTS





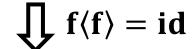




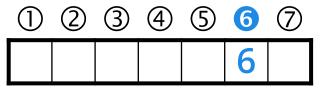


 $\mathbf{f}\langle \neg \mathbf{p} \rangle = \mathbf{f} \min. \text{ first } \mathbf{A}$

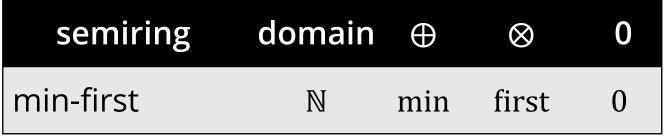
$$p\langle f\rangle = f$$

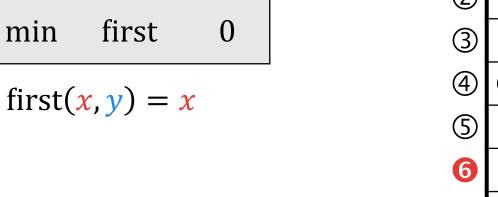


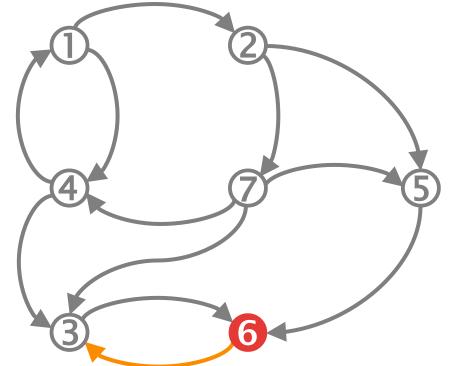


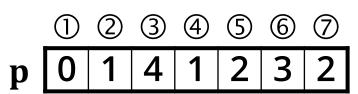


BFS – PARENTS



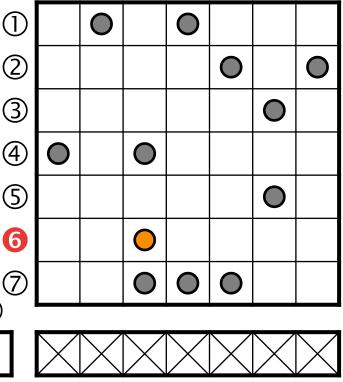






2 3 4 5 6

6



2 3 4 5 6 7

f is empty
→ terminate

 $\mathbf{f}\langle \neg \mathbf{p} \rangle = \mathbf{f} \text{ min. first } \mathbf{A}$

BFS - PARENTS: ALGORITHM



- Input: adjacency matrix **A**, source vertex *s*, #vertices *n*
- Output: parent vertices vector p (integer)
- Workspace: vertex index vector idx (integer), frontier vector
 f (integer)
- 1. $idx = [1 \ 2 \ ... \ n]$

we assume 1-based indexing here

- 2. f(s) = s
- 3. $\mathbf{p}(s) = 0$
- 4. for l = 1 to n 1

*terminate earlier if the frontier is empty

- 5. $\mathbf{f}(\neg \mathbf{p}) = \mathbf{f} \min. \text{ first } \mathbf{A} \text{ advance the frontier}$
- 6. $\mathbf{p}\langle\mathbf{f}\rangle=\mathbf{f}$

assign parent ids to the frontier's vertices

7. $f\langle f\rangle = idx$

assign vertex ids $\mathbf{f}(i) = i$

BFS - PARENTS: OPTIMIZATIONS

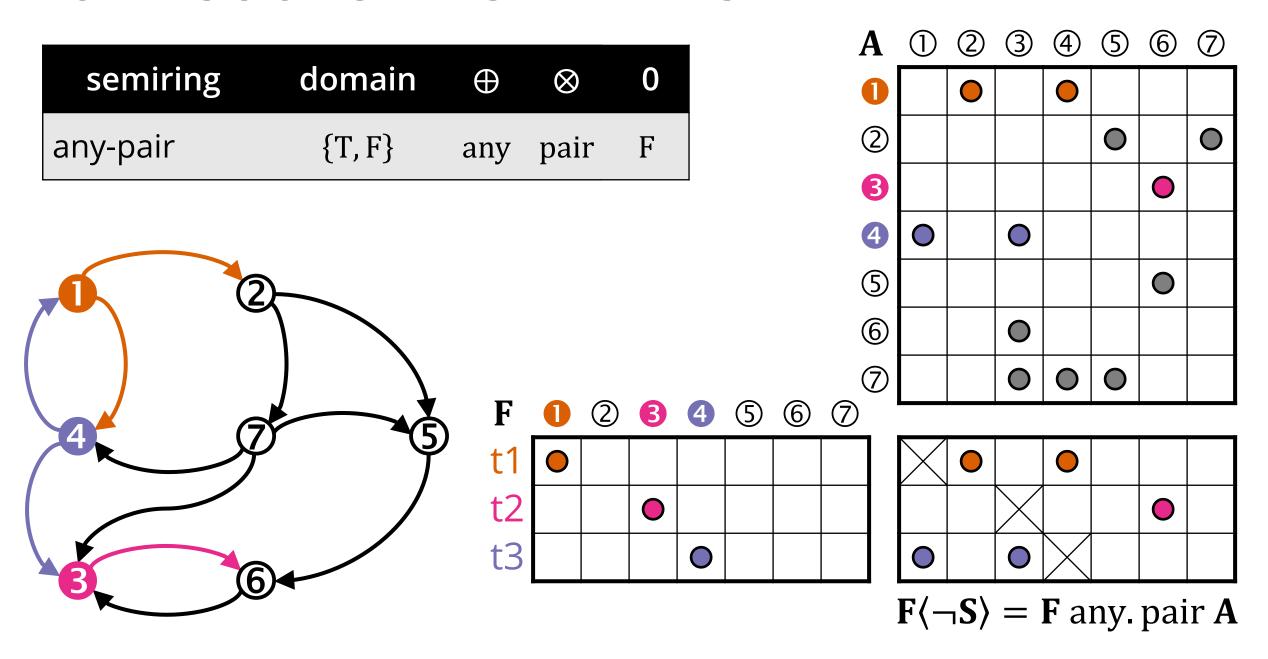
- If getting deterministic results is not a requirement (i.e. any parent vertex can be returned), instead of min. sel1st, one can use the any. first semiring.
- This optimization is allowed by the GAP Benchmark Suite.
- Direction-optimizing traversal (push/pull) can be exploited.
- The secondi (note the "i") semiring can be used to express the BFS Parent algorithm. When using this semiring, one does not even have to look at the values in either A of f.

This algorithm is described in:

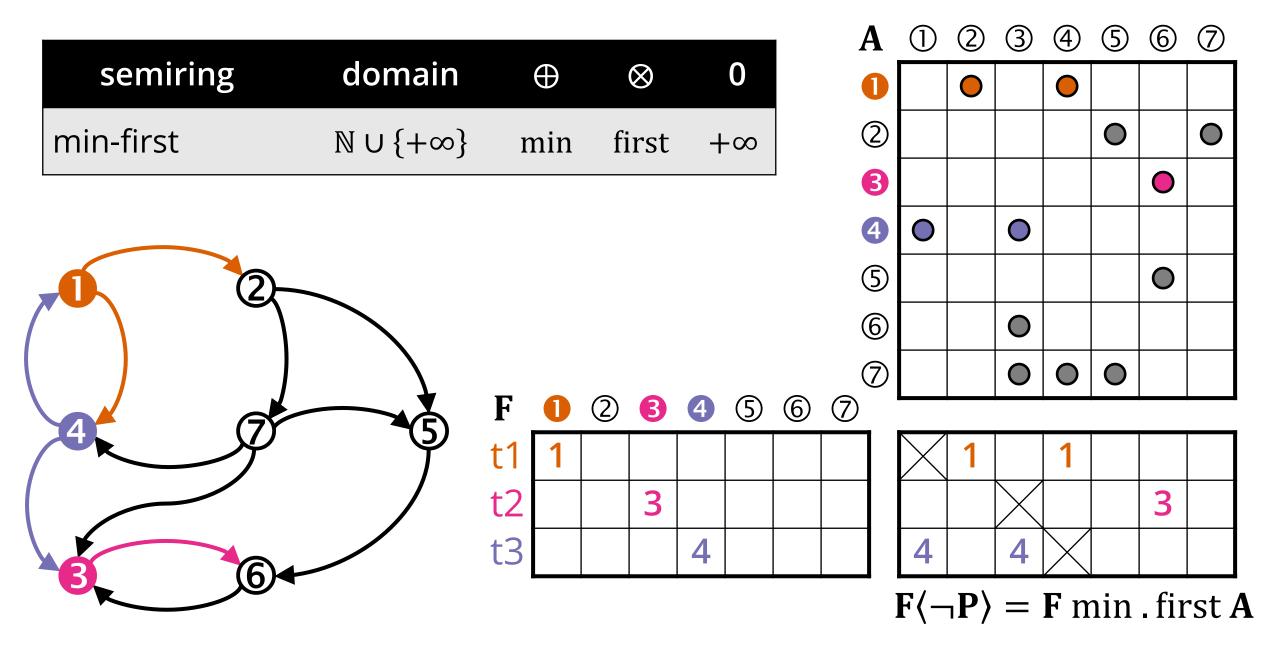
Evaluation of Graph Analytics Frameworks Using the GAP Benchmark Suite, IISWC 2020

Multi-source BFS

MULTI-SOURCE BFS – LEVELS



MULTI-SOURCE BFS – PARENTS



BFS – PERFORMANCE

- Naïve BFS impls can be 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^Tv) during execution:
 - Use the push direction when the frontier is small
 - Use the pull direction when the frontier becomes large
 - Adopted to GraphBLAS in 2018 (Yang et al.'s ICPP paper)



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 paths

SSSP – SINGLE-SOURCE SHORTEST PATHS

Problem:

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

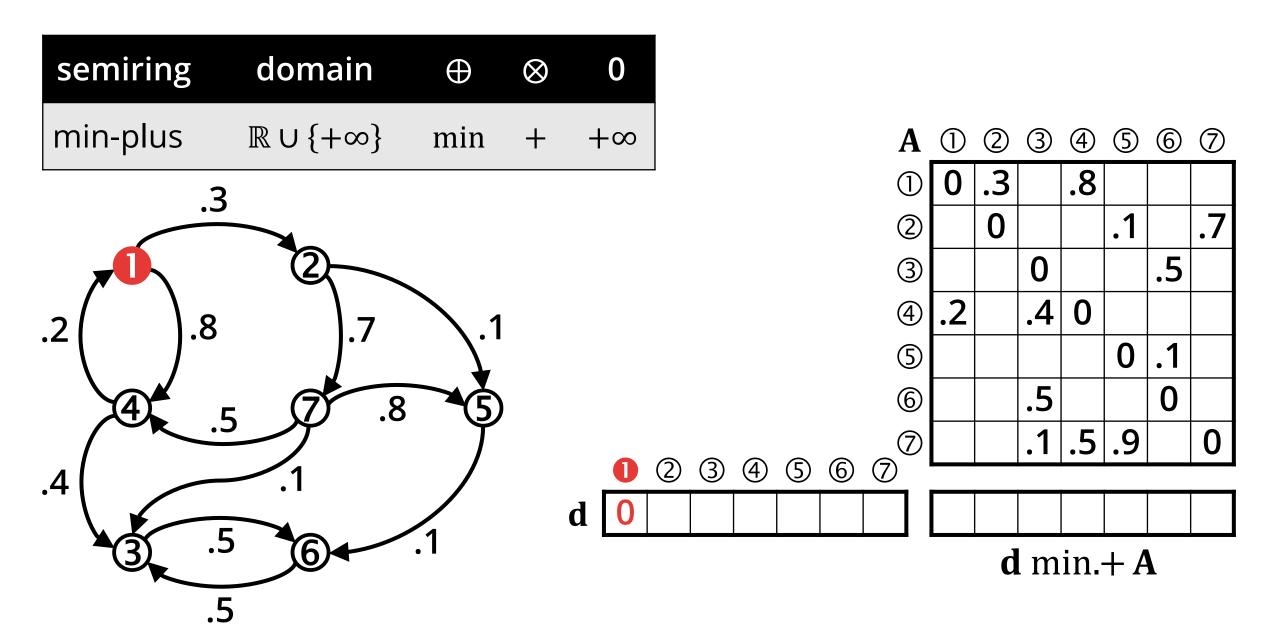
Bellman-Ford algorithm:

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

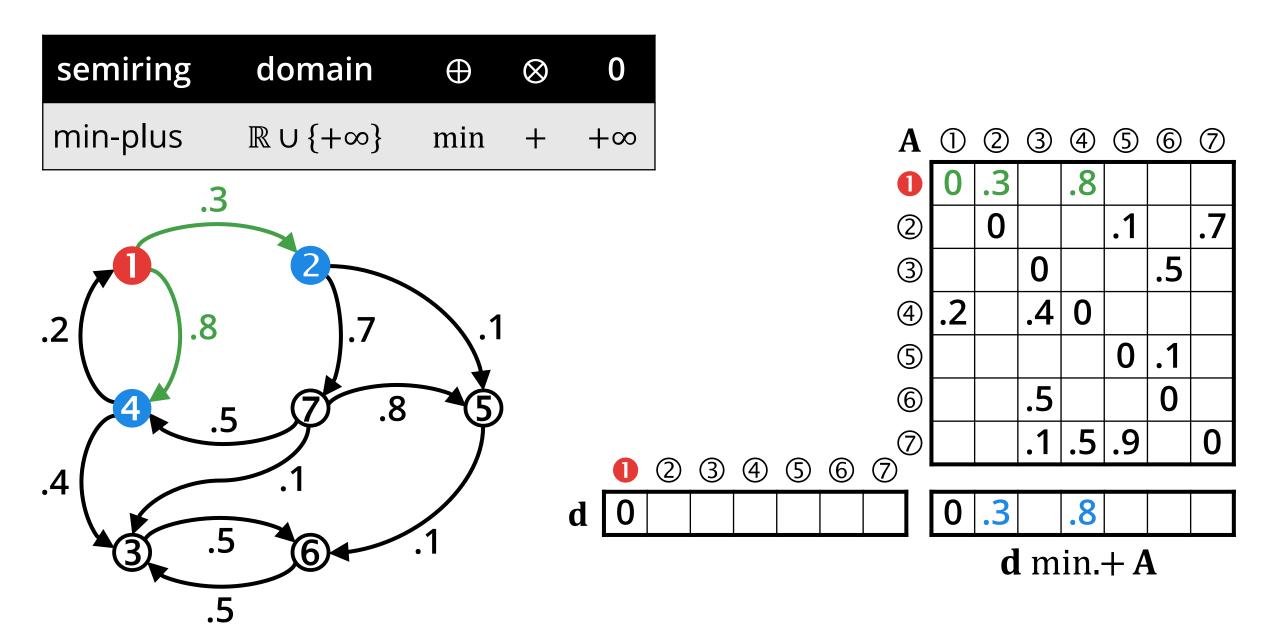
Observation:

- The relaxation step can be captured using a VM multiplication
- Unlike in BFS, there is no masking here, as revisiting edges that have been visited previously can be useful.

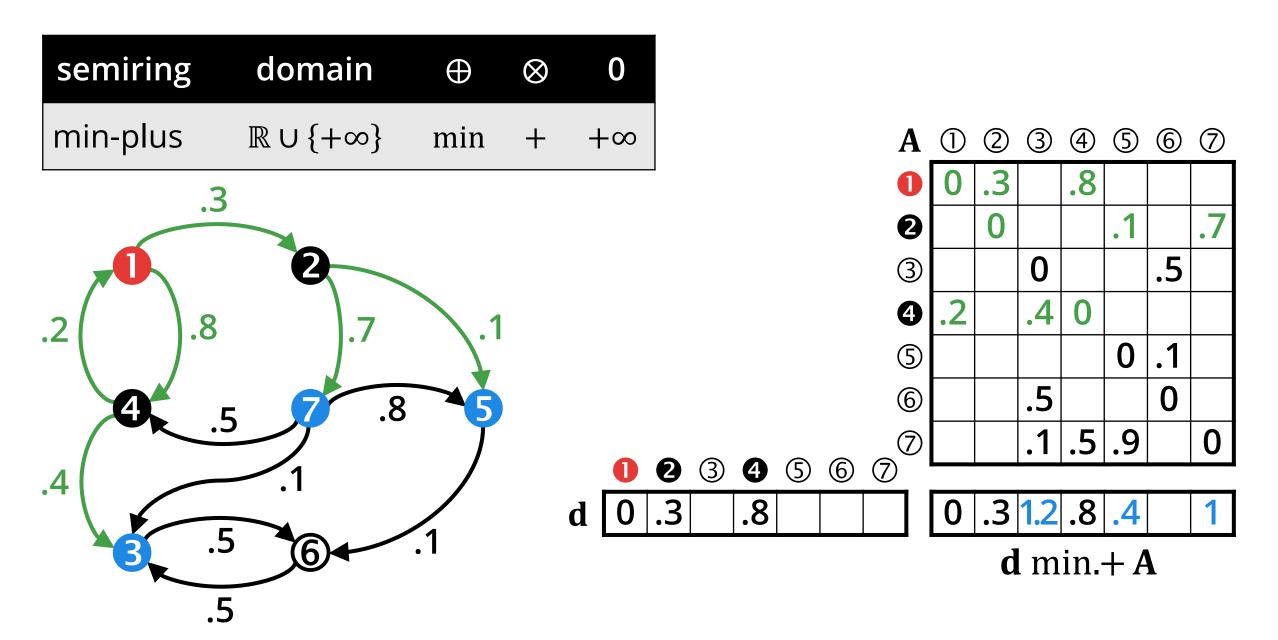
SSSP – ALGEBRAIC BELLMAN-FORD



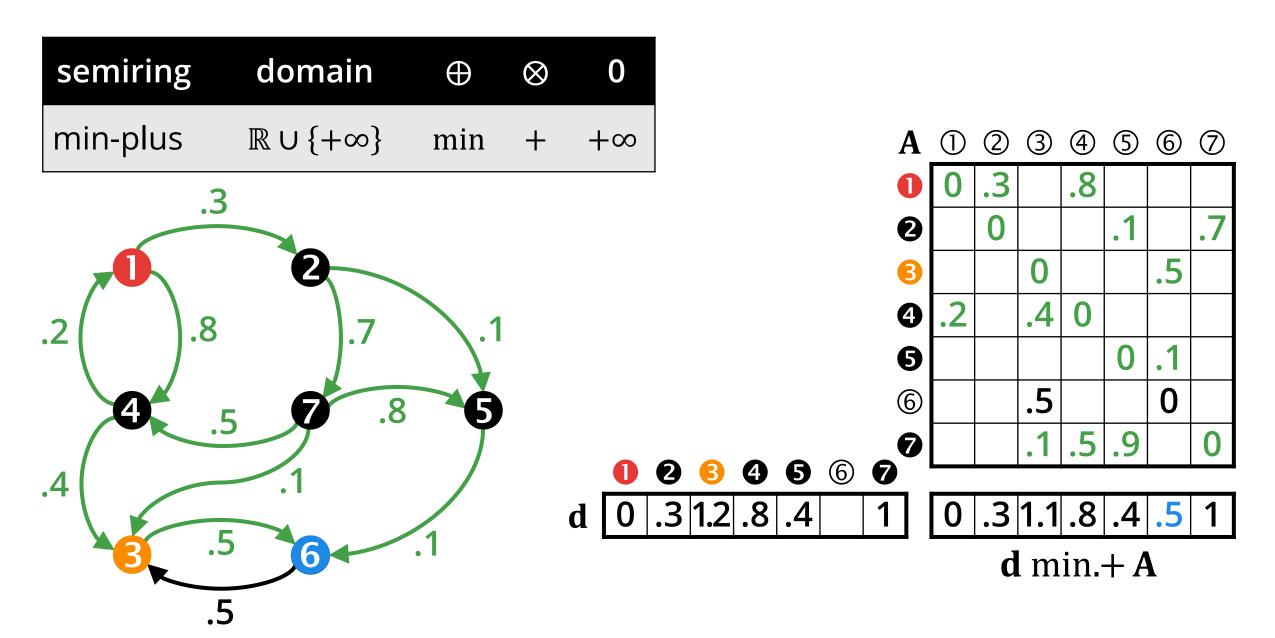
SSSP – ALGEBRAIC BELLMAN-FORD



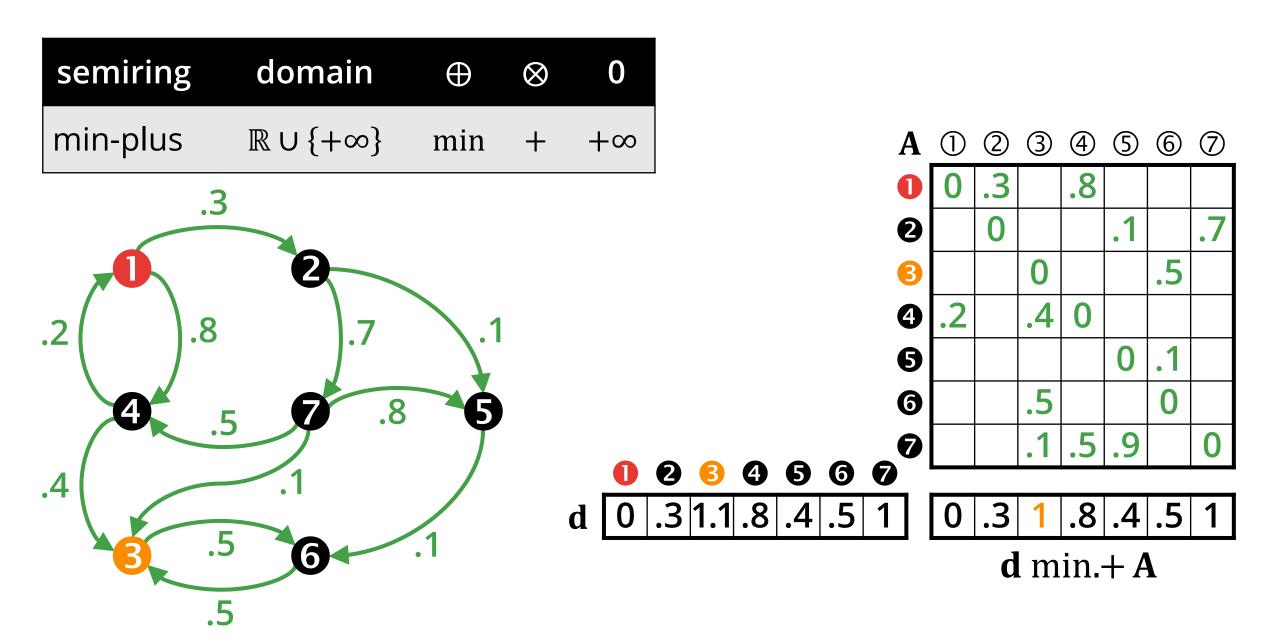
SSSP - ALGEBRAIC BELLMAN-FORD



SSSP – ALGEBRAIC BELLMAN-FORD



SSSP – ALGEBRAIC BELLMAN-FORD



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)

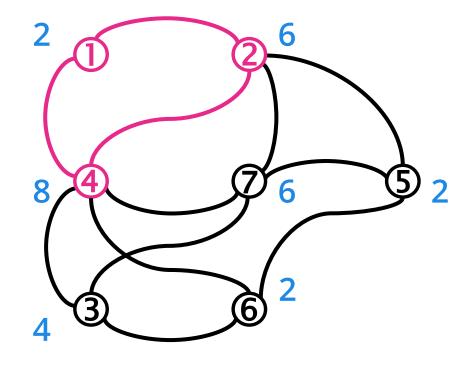
- 1. $\mathbf{d} = [\infty \infty ... \infty]$
- 2. d(s) = 0
- 3. for k = 1 to n 1 *terminate earlier if we reach a fixed point
- 4. $\mathbf{d} = \mathbf{d} \min + \mathbf{A}$

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

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:

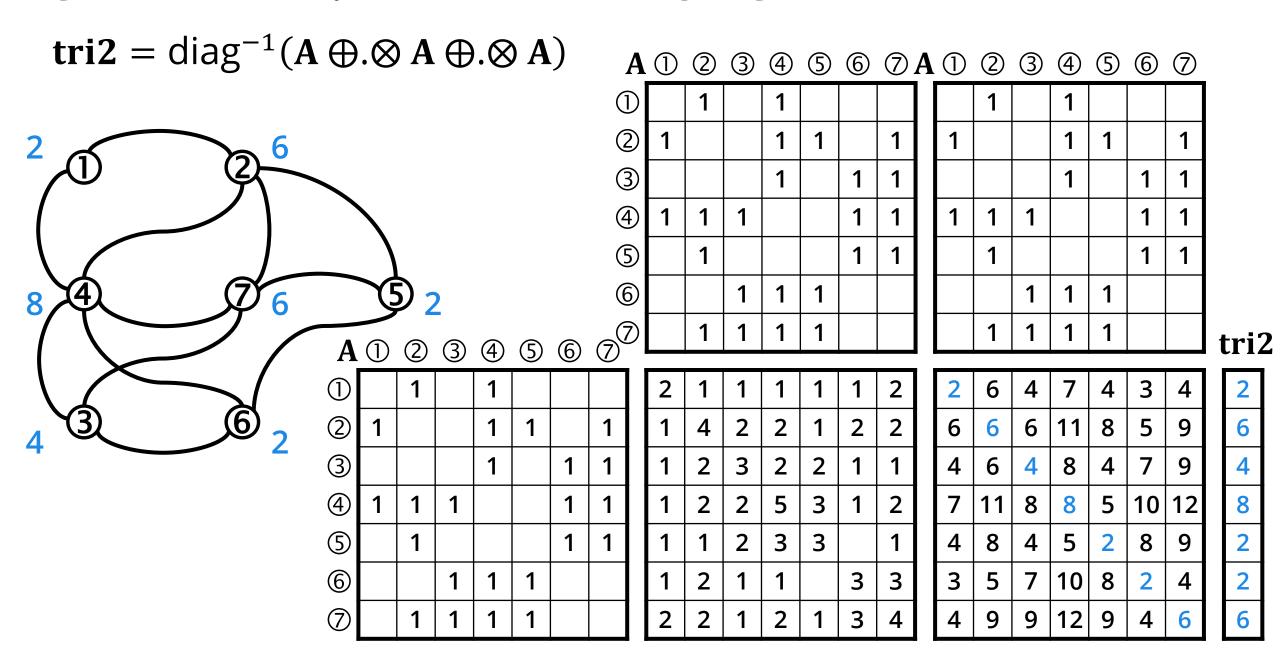
 $\frac{30}{6}$



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

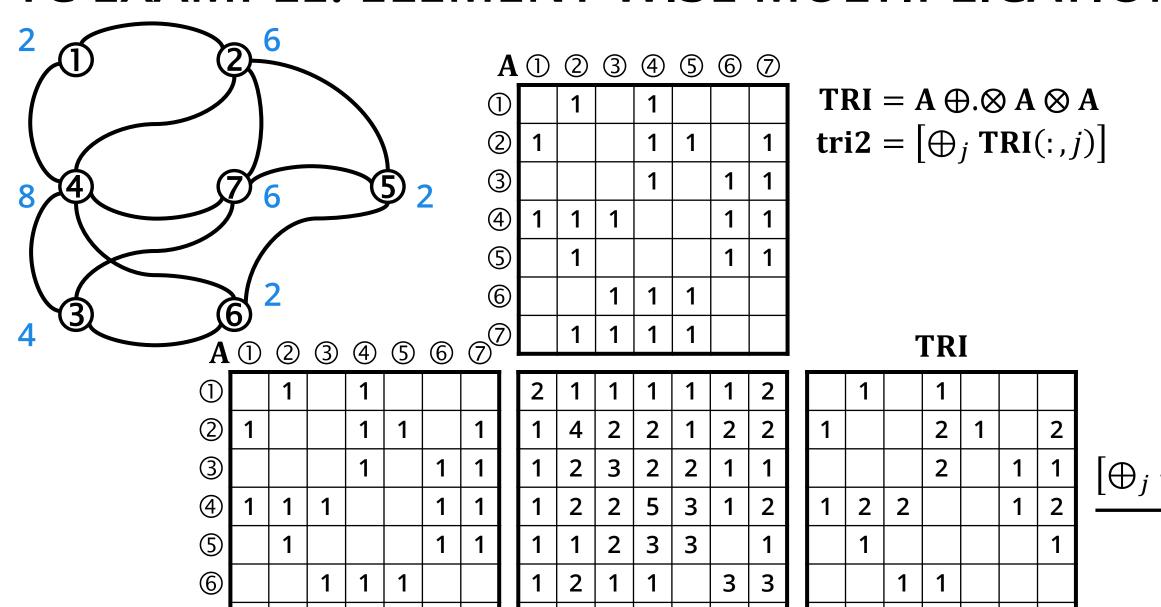
Triangle count / Naïve algorithm

TC EXAMPLE: NAÏVE APPROACH



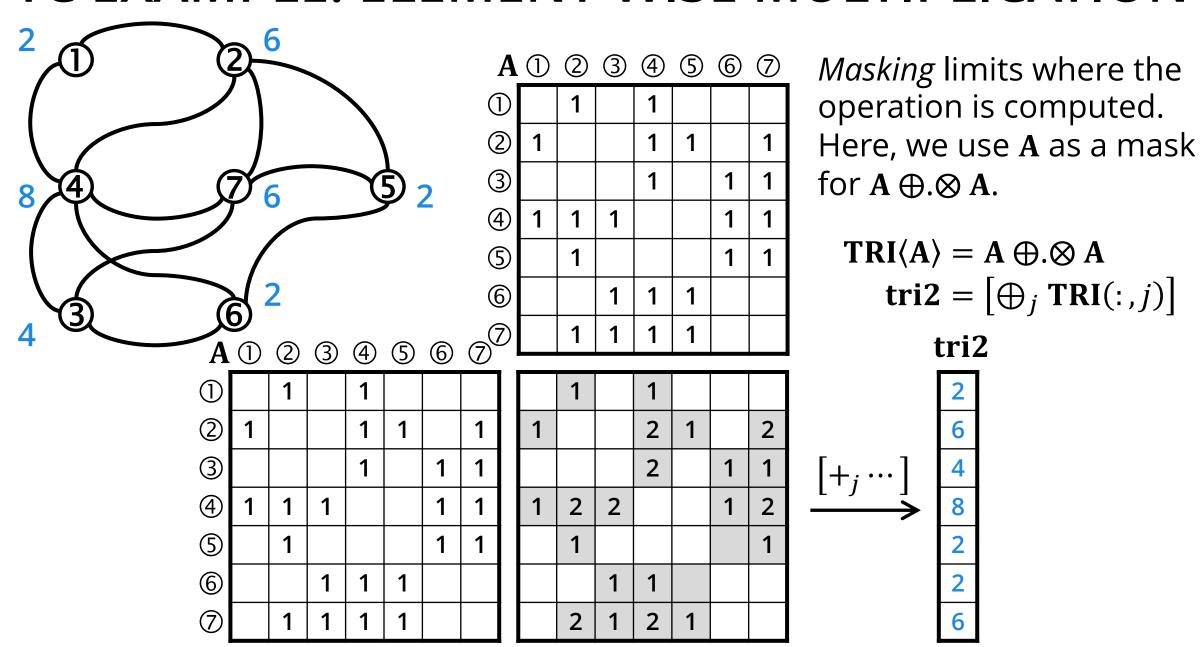
Triangle count / Masked algorithm

TC EXAMPLE: ELEMENT-WISE MULTIPLICATION



tri2

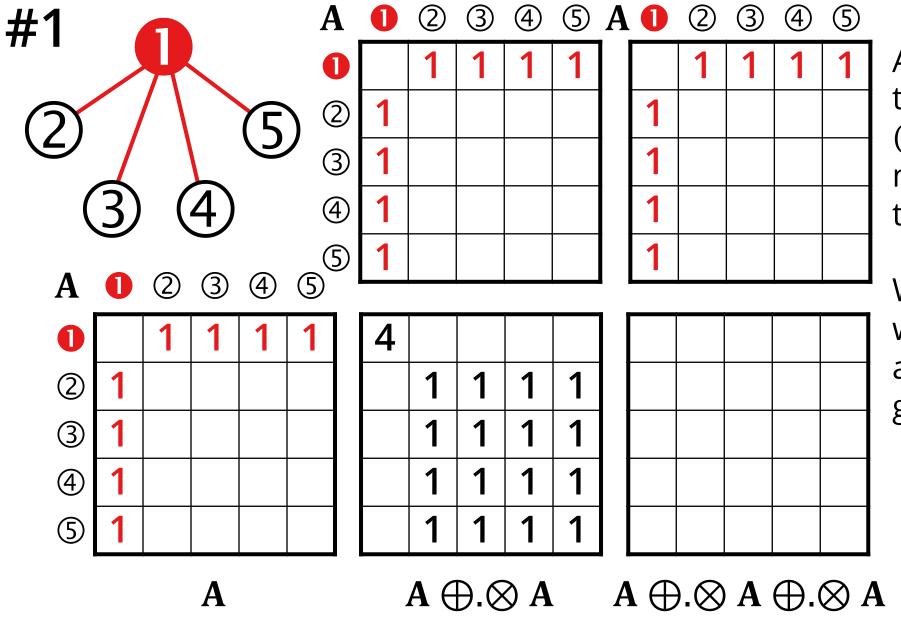
TC EXAMPLE: ELEMENT-WISE MULTIPLICATION



The importance of masking

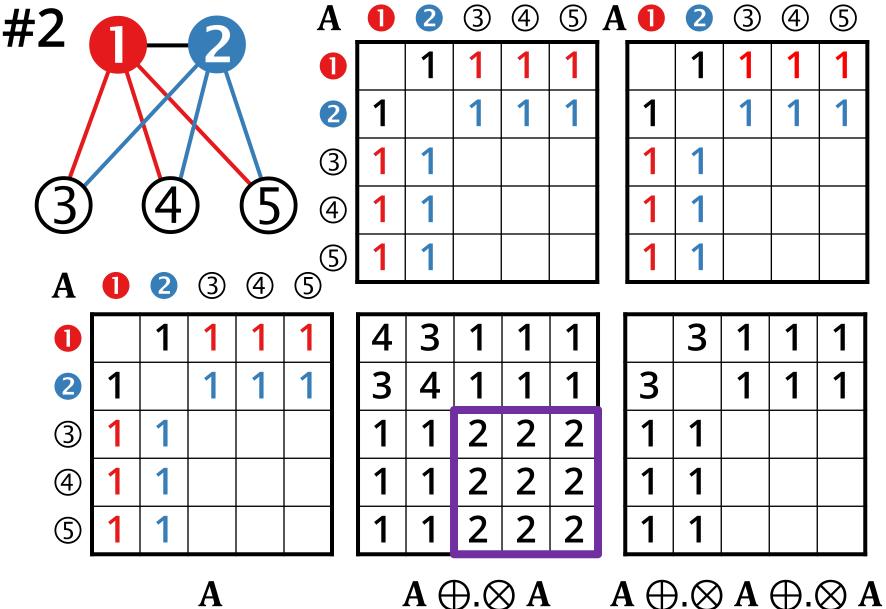
THE IMPORTANCE OF MASKING

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



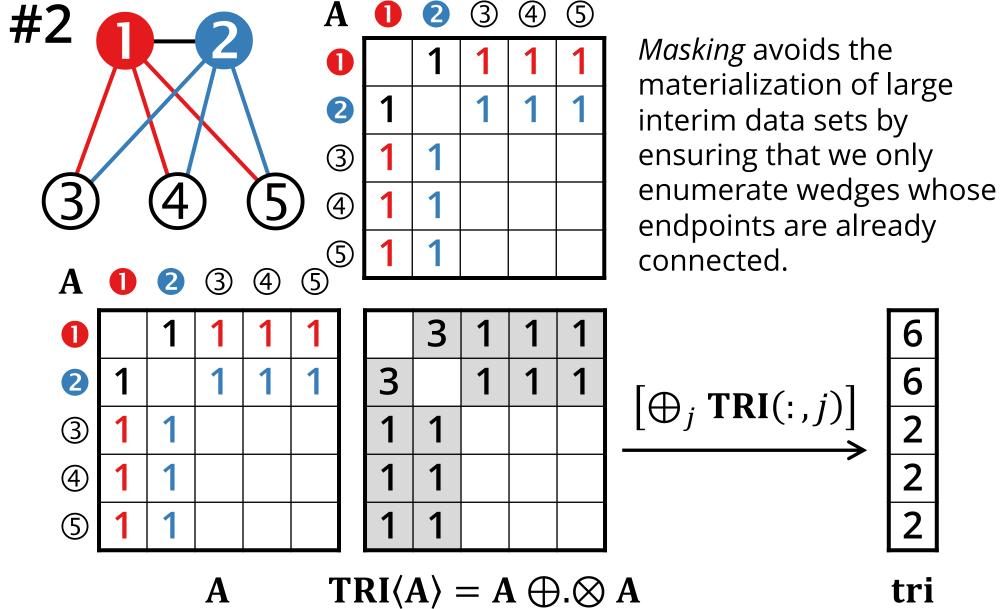
A simple corner case is the star graph: there are $(n-1)^2$ wedges but none of them close into triangles.

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, **A** ⊕.⊗ **A** enumerates all wedges starting and ending in the bottom partition, thus performing a lot of unnecessary work.



$$\mathbf{A} \qquad \mathbf{TRI}\langle \mathbf{A} \rangle = \mathbf{A} \oplus . \otimes \mathbf{A}$$

Triangle count / Cohen's algorithm

COHEN'S ALGORITHM: PSEUDOCODE



Input: adjacency matrix A

Output: triangle count *t*

Workspace: matrices L, U, B, C

1. $\mathbf{L} = \text{tril}(\mathbf{A})$

extract the lower triangle from A

2. $\mathbf{U} = \text{triu}(\mathbf{A})$

extract the upper triangle from A

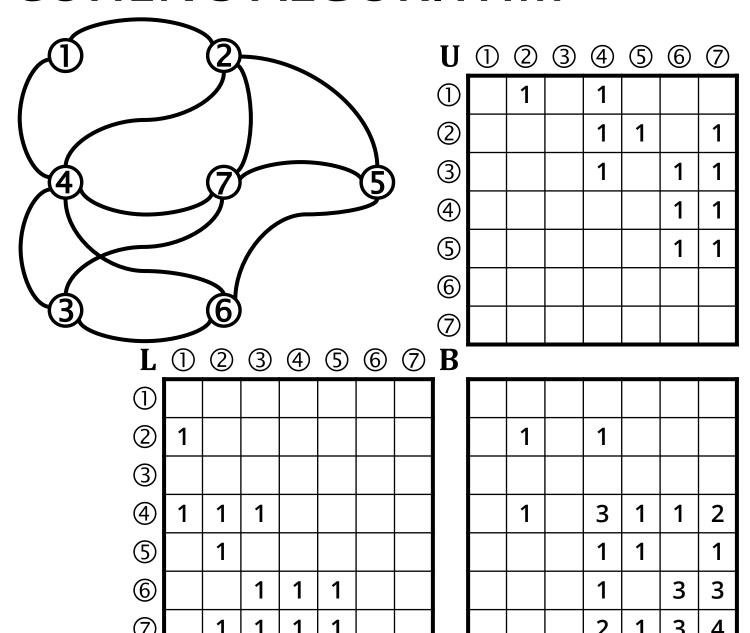
- 3. $\mathbf{B} = \mathbf{L} \oplus . \otimes \mathbf{U}$
- 4. $\mathbf{C} = \mathbf{B} \otimes \mathbf{A}$
- 5. $t = \sum C/2$

sum the values in C and divide by 2

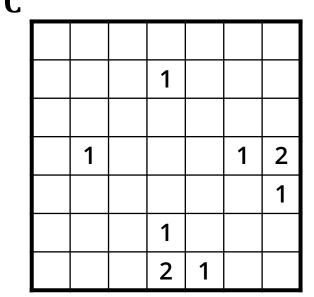


J. Cohen: Graph Twiddling in a MapReduce World, Comput. Sci. Eng. 2009

COHEN'S ALGORITHM

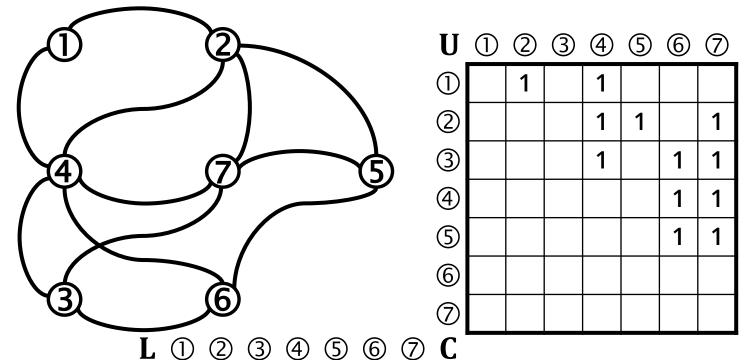


A	1	2	3	4	(5)	6	7
		1		1			
	1			1	1		1
				1		1	1
\otimes	1	1	1			1	1
		1				1	1
			1	1	1		
	·	1	1	1	1		



$$t = \sum \mathbf{C}/2$$

COHEN'S ALGORITHM: MASKING



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

	1			
1			1	2
				1
	1			
	2	1		

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

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. $t = \sum \mathbf{C}$

extract the lower triangle from A

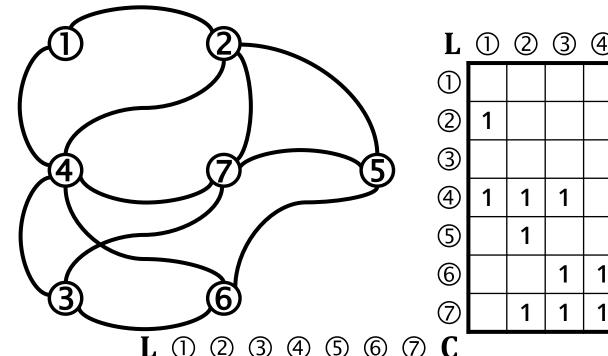
multiply matrices L and L using mask L

sum the values in C



M.M. Wolf et al. (Sandia National Laboratories):

SANDIA ALGORITHM



L	1	2	3	4	(5)	6	7
1							
2	1						
① ② ③							
4	1	1	1				
456		1					
6			1	1	1		
\bigcirc		1	1	1	1		

<u>ы</u> .	\Box		<u> </u>	4	$\overline{\mathcal{O}}$	<u> </u>	\bigcirc
1							
2	1						
3							
4	1	1	1				
(5)		1					
			1	1	1		
7		1	1	1	1		

1				
		1		
	2	1		

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

Triangle count / CMU algorithm

CMU ALGORITHM

- Iterates on the vertices of the graph, extracts corresponding submatrices and computes $t = t + a_{10}^{\mathsf{T}} \oplus . \otimes A_{20} \oplus . \otimes a_{12}$
- Tradeoffs:
 - o does not require mxm, only vxm and mxv
 - o requires efficient subgraph extraction
- The formula is derived using the matrix trace $tr(A) = \sum_{i=0}^{n-1} A_{ii}$ and its invariant property under cyclic permutation, e.g. tr(ABC) = tr(BCA) = tr(CAB). See the paper for details.

 $\mathbf{A}_{20}^{\mathsf{T}}$

 $\mathbf{a}_{21}^{\mathsf{T}}$

 \mathbf{A}_{00}

 \mathbf{A}_{20}



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

CMU ALGORITHM: PSEUDOCODE



Input: adjacency matrix A

Output: triangle count *t*

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

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

A		i	
	\mathbf{A}_{00}	a ₀₁	\mathbf{A}_{20}^{T}
i	\mathbf{a}_{01}^{T}	0	\mathbf{a}_{21}^{T}
	\mathbf{A}_{20}	a ₂₁	\mathbf{A}_{22}

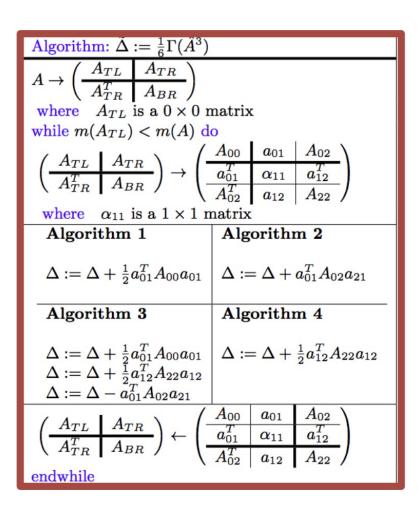


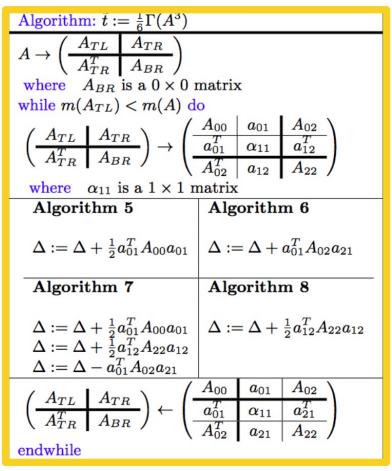
T.M. Low et al. (Carnegie Mellon University):

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

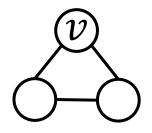


Source of the figure

Vertex-wise triangle count

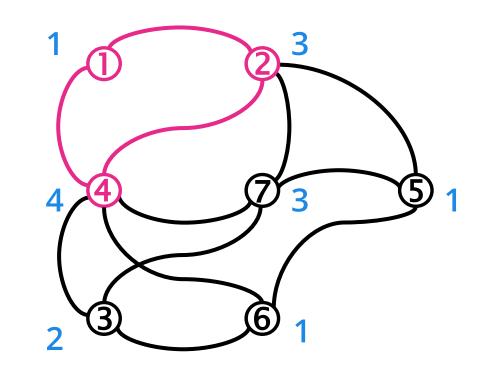
VERTEX-WISE TRIANGLE COUNT

Triangle: a set of three mutually adjacent vertices.



Usages:

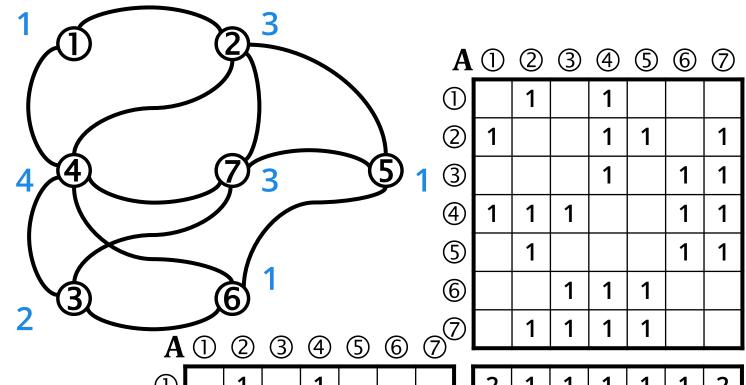
- Global clustering coefficient
- Local clustering coefficient (transitivity)
- Finding communities





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

TC: ELEMENT-WISE MULTIPLICATION



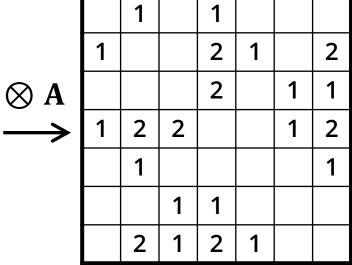
 $TRI = A \oplus . \otimes A \otimes A$ $tri = [\bigoplus_{j} TRI(:,j)]/2$

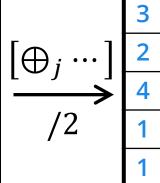
 $\mathbf{A} \oplus . \otimes \mathbf{A}$ is still very dense.

TRI

	<u>.</u>	<u> </u>	<u> </u>	<u>.</u>	<u> </u>	<u> </u>	<u> </u>
1		1		1			
2	1			1	1		1
3				1		1	1
4	1	1	1			1	1
(5)		1				1	1
			1	1	1		
7		1	1	1	1		

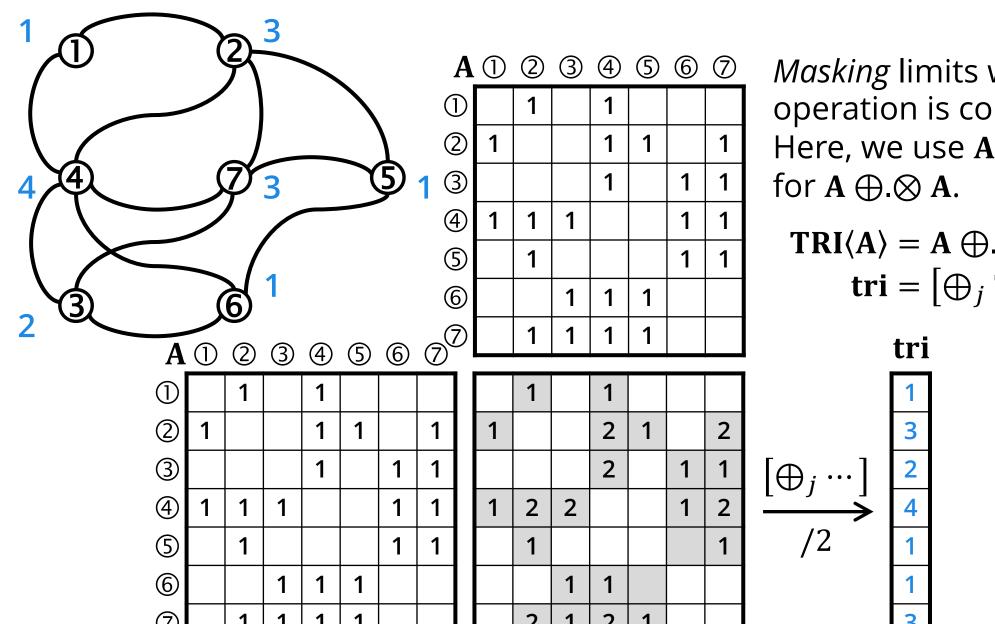
2	1	1	1	1	1	2
1	4	2	2	1	2	2
1	2	3	2	2	1	1
1	2	2	5	3	1	2
1	1	2	3	3		1
1	2	1	1		3	3
2	2	1	2	1	3	4





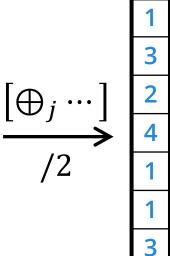
tri

TC: ELEMENT-WISE MULTIPLICATION



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

$$\mathbf{TRI}\langle \mathbf{A} \rangle = \mathbf{A} \oplus . \otimes \mathbf{A}$$
$$\mathbf{tri} = \left[\bigoplus_{j} \mathbf{TRI}(:,j) \right] / 2$$



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. $\mathbf{tri} = \left[\bigoplus_{j} \mathbf{TRI}(:,j) \right] / 2$ 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.

Local clustering coefficient (transitivity)

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 $(v) = 0$

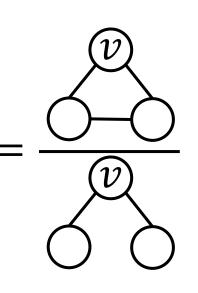
Important metric in social network analysis.

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: NUMBER OF WEDGES IN EACH VERTEX

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

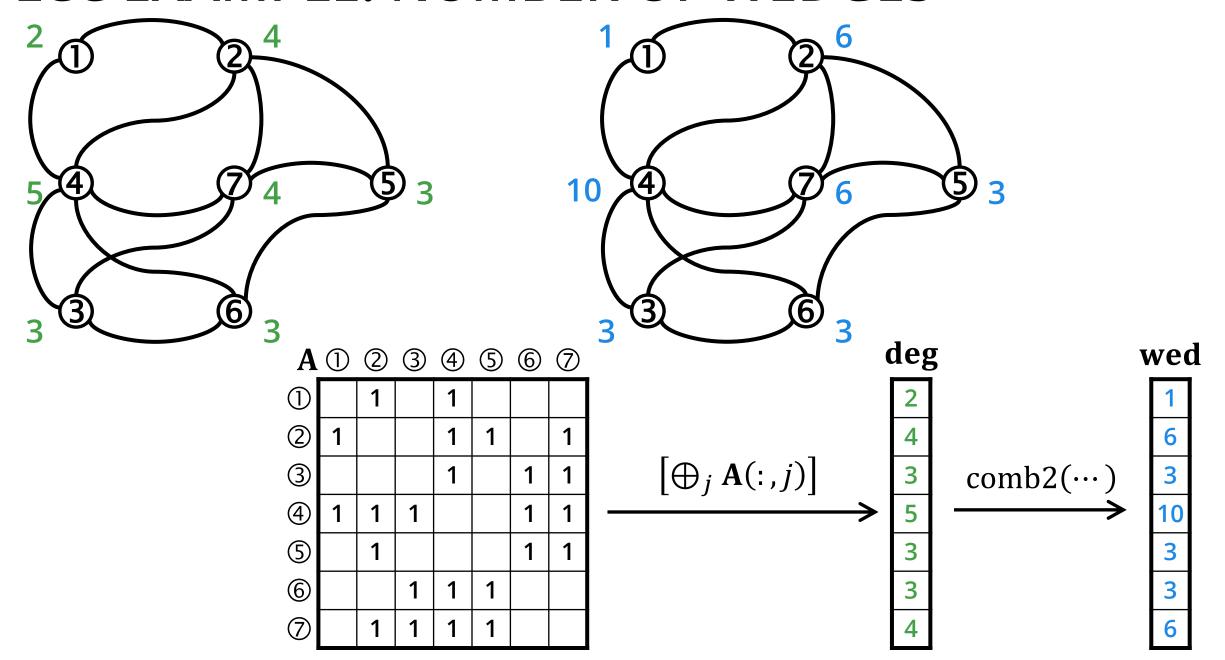
• For wed(v), we determine the #wedges for each vertex as the 2-combination of its degree:

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

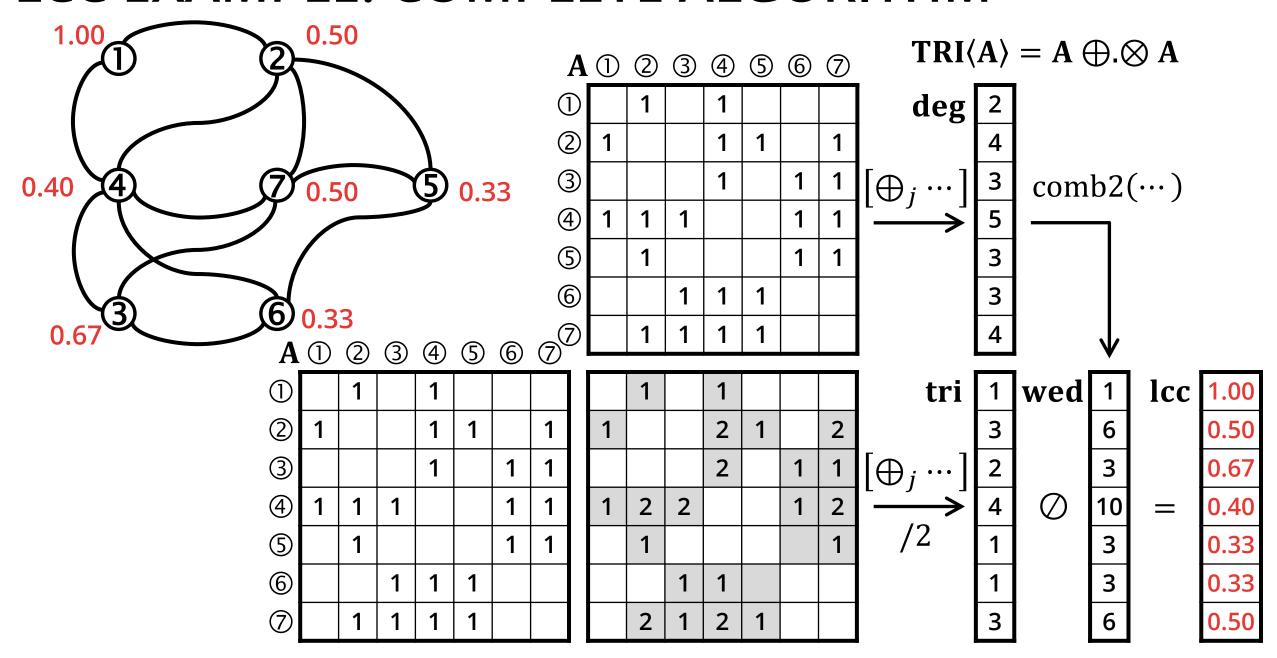
• Given the degrees $deg = [\bigoplus_j A(:,j)]$, we compute wed by applying a unary function on the elements of the vector:

$$wed = comb2(deg)$$

LCC EXAMPLE: NUMBER OF WEDGES



LCC EXAMPLE: COMPLETE ALGORITHM



LCC: ALGORITHM



Input: adjacency matrix **A**

Output: vector lcc

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

- 1. $TRI(A) = A \oplus . \otimes A$ compute triangle count matrix
- 2. $\mathbf{tri} = [\bigoplus_{i} \mathbf{TRI}(:,j)]/2$ reduce to triangle count vector
- 3. $\mathbf{deg} = [\bigoplus_j \mathbf{A}(:,j)]$ reduce to vertex degree vector
- 4. $\mathbf{wed} = \mathbf{comb2(deg)}$ apply comb2 to get 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.

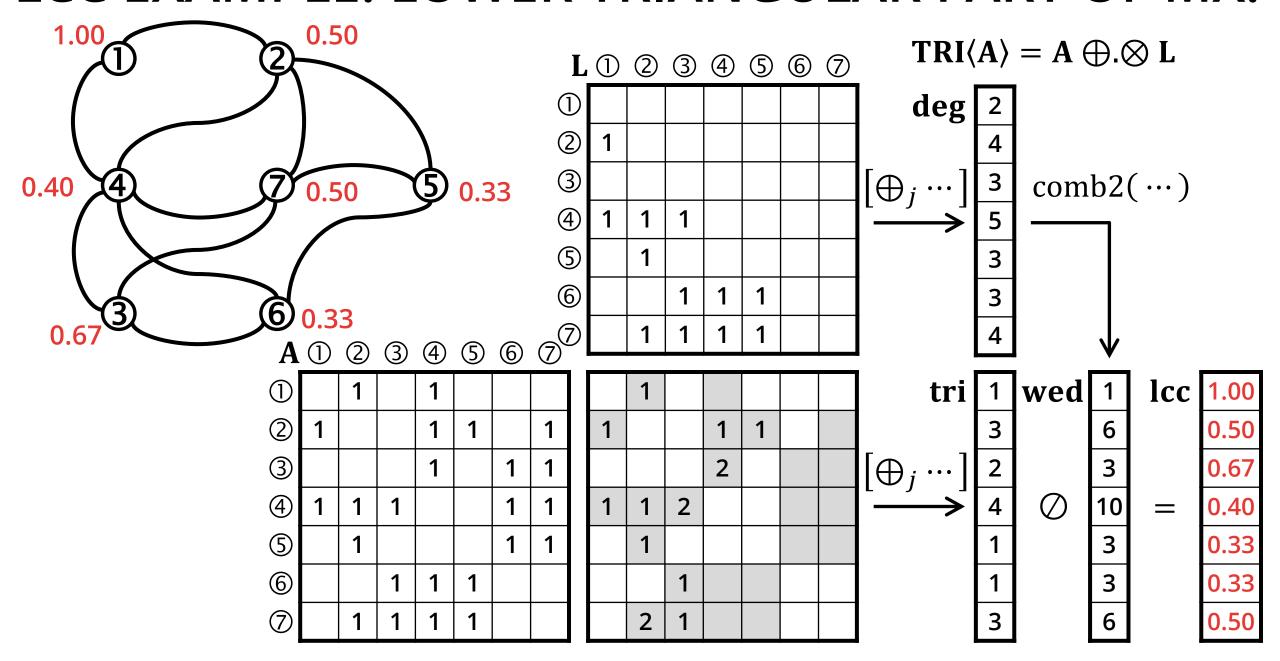
$$TRI\langle A \rangle = A \oplus . \otimes L$$

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.



PageRank

PAGERANK - DEFINITION (LDBC GRAPHALYTICS)

For k = 1 to t iterations:

$$PR_0(v) = \frac{1}{n}$$

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

 α : damping factor

dng: dangling vertices, $dng = \{w \in V : |N_{out}(w)| = 0\}$

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

PAGERANK – IN LINEAR ALGEBRA

Initially:

$$\mathbf{pr}_0 = [1 \ 1 \dots 1] \oslash n, \quad \mathbf{outd} = [\bigoplus_j \mathbf{A}(:,j)]$$

In each iteration:

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

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

element-wise sparse vectordense vector multiplication

PAGERANK - ALGORITHM



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

Output: PageRank vector pr (real); Workspace: vectors (real)

- 1. $\mathbf{pr} = [1 \ 1 \dots 1] \oslash n$
- 2. **outdegrees** = $[\bigoplus_j \mathbf{A}(:,j)]$
- 3. for k = 1 to t
- 4. importance = $\alpha \otimes (pr \oslash outdegrees) \oplus \otimes A$
- 5. **danglingVertexRanks** $\langle \neg outdegrees \rangle = pr(:)$
- 6. $totalDanglingRank = \frac{\alpha}{n} \otimes [\bigoplus_i \mathbf{danglingVertexRanks}(i)]$
- 7. $\mathbf{pr} = \frac{1-\alpha}{n} \oplus totalDanglingRank \oplus \mathbf{importance}$

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.
$$\mathbf{C}\langle\mathbf{C}\rangle = \mathbf{C} \oplus A \mathbf{C}$$
 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 non-zero 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^{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

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

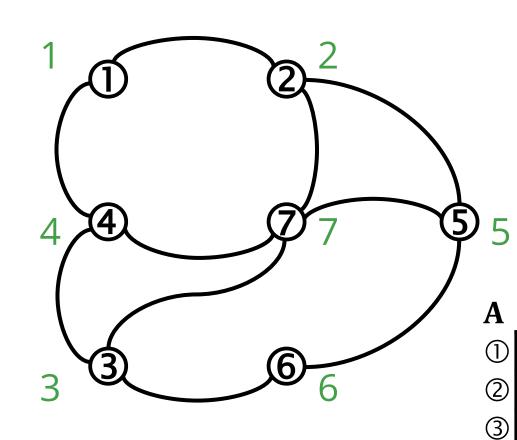
Reduce each row into a single occurrence vector:

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

- Select the min. mode element from the occurrence vector: 6
- Works on paper, but occurrence vectors need dynamic memory allocation, which leads to poor performance with the current GraphBLAS API

CDLP IN LINEAR ALGEBRA: FASTER ALGORITHM

- 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)
- The matrix multiplications are always performed with a diagonal matrix as the second operand so we never need the addition operator. Therefore, we set it to $\bigoplus \equiv$ any.

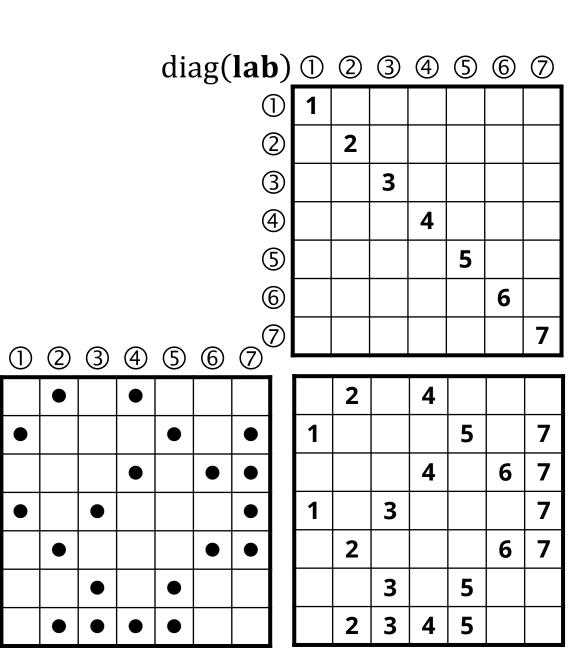


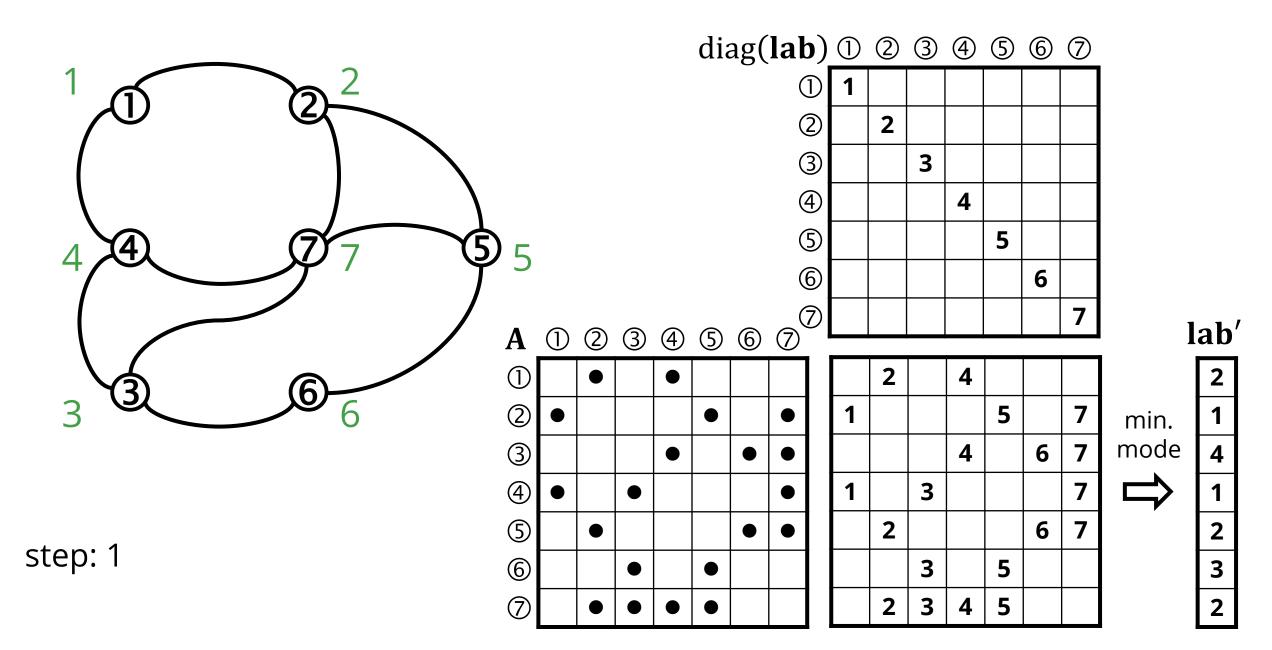
4

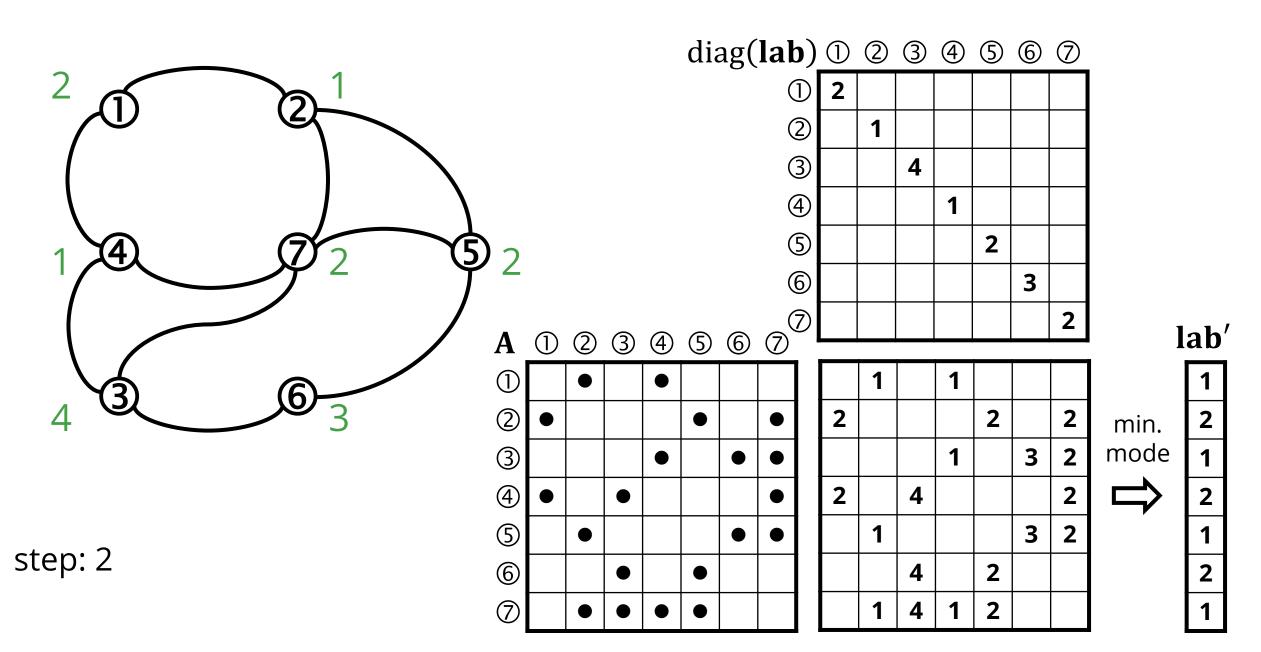
(5)

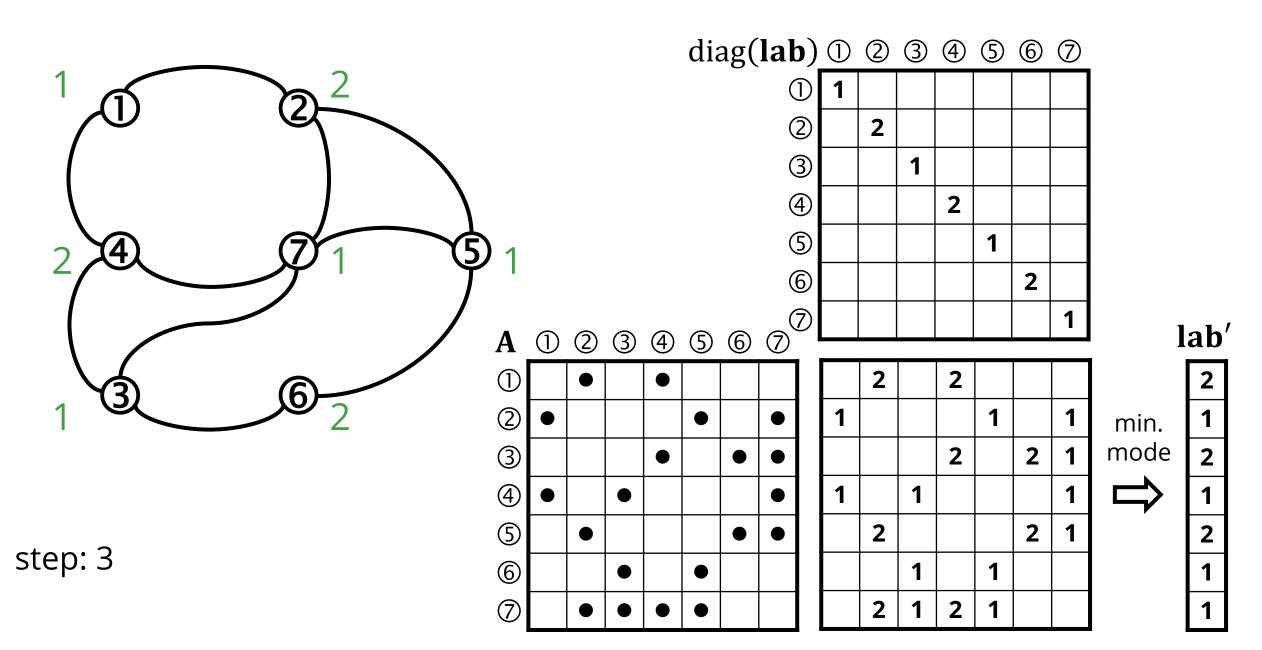
6

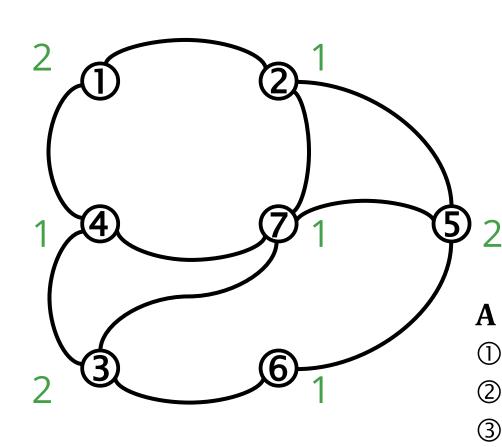
- Initially, $lab = [1 \ 2 \ ... \ n]$
- Propagate labels to create a "frequency matrix":
 F = A any . sel2nd diag(lab)











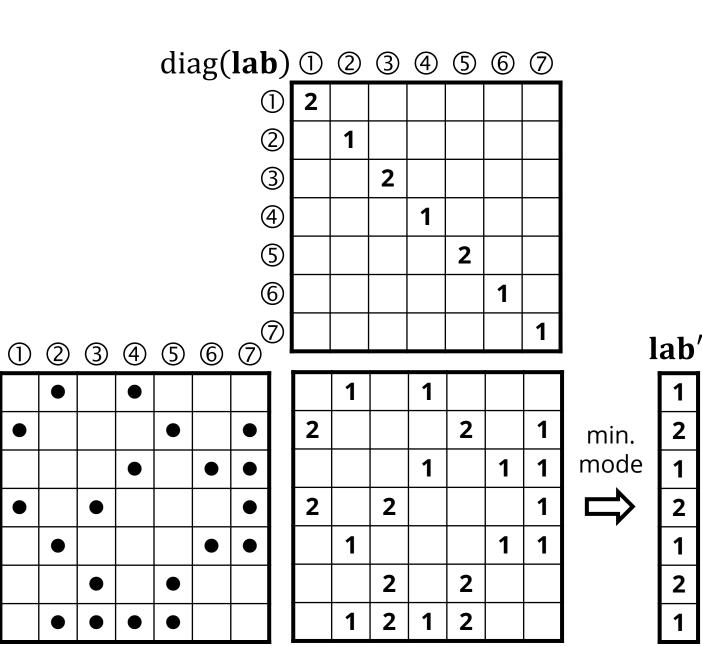
step: 4 – same result as in step 2 The original non-deterministic variant of the algorithm is better at avoiding such oscillations.

4

(5)

6

(7)



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. $lab(i) = select_min_mode(r)$

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} \left[ |\{u \in N_{\text{in}}(v): L_{k-1}(u) = l\}| + |\{u \in N_{\text{out}}(v): L_{k-1}(u) = l\}| \right])
```

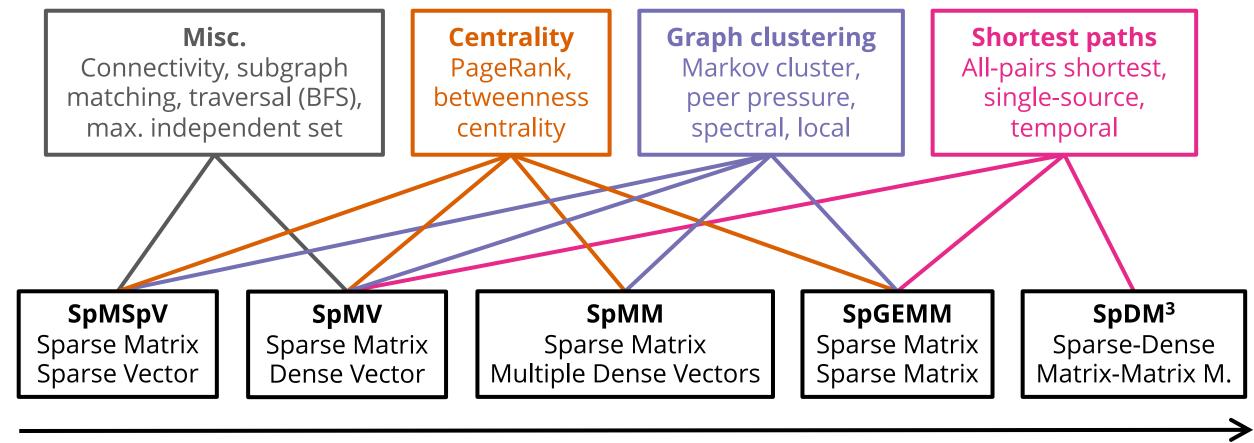
- In linear algebra, this can be expressed with two matrices:
 - \circ $\mathbf{F}_{in} = \mathbf{A}$ any. sel2nd diag(\mathbf{lab})
 - $\circ \mathbf{F}_{\text{out}} = \mathbf{A}^{\mathsf{T}}$ any. sel2nd diag(**lab**)
- Simultaneously iterate over rows $\mathbf{r_{in}}$ of $\mathbf{F_{in}}$ and $\mathbf{r_{out}}$ 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 = extract\_tuples(F_{in}) \\ \circ \; \langle I_{out}, \_, X_{out} \rangle = extract\_tuples(F_{out}) \end{array} \right\} \; merge\_sort\_pairs(\langle I_{in} \cup I_{out}, X_{in} \cup X_{out} \rangle) \\ \end{array}
```

Graph algorithms in GraphBLAS

Graph algorithms & GraphBLAS primitives

GRAPH ALGORITHMS & GRAPHBLAS PRIMITIVES



GraphBLAS primitives in increasing cost

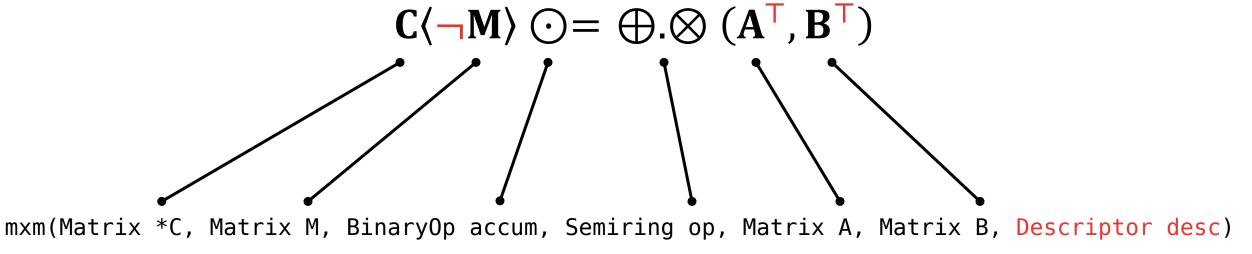


Based on the figure in A. Buluç: *Graph algorithms, computational motifs, and GraphBLAS,* ECP Meeting 2018

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."

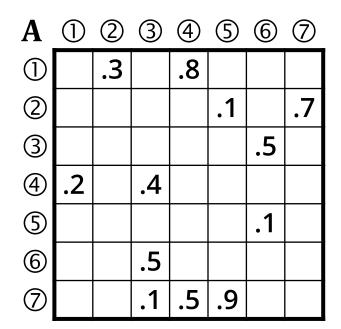




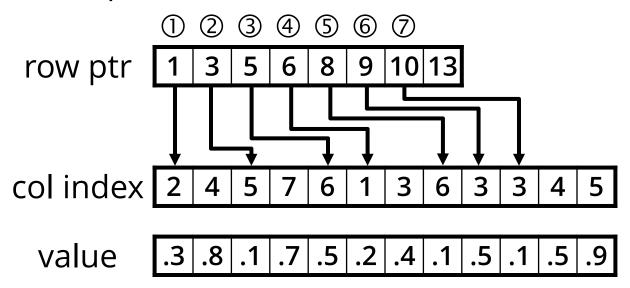
A. Buluç et al.: *Design of the GraphBLAS C API,* GABB@IPDPS 2017

GRAPHBLAS OBJECTS

- GraphBLAS objects are opaque: the matrix representation can be adjusted to suit the data distribution, hardware, etc.
- The typical representations 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.
- A GPU implementation is 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

Further reading and libraries

RESOURCES

Presentations and tutorials for learning GraphBLAS:



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. szarnyasg/graphblas-pointers

THE LAGRAPH LIBRARY

- Similar to the LAPACK library for BLAS
- Uses SuiteSparse:GraphBLAS
- Implementations of common algorithms
 - o BFS, SSSP, LCC, PageRank, Borůvka
 - Triangle count, k-truss
 - CDLP (community detection using label propagation)
 - Weakly connected components, Strongly Connected Components
 - 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 libraries **only satisfy requirement #1:** Intel MKL, Eigen, Boost uBLAS, MTL4, Armadillo, NIST Sparse BLAS, GMM++, CUSP, Numpy

Exceptions are the Efficient Java Matrix Library (EJML) and Julia's SparseArrays library, where arbitrary semirings can be used.

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

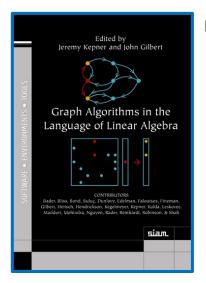


- Design of the GraphBLAS C API
 - Design decisions and overview of the C API @ GABB@IPDPS 2017

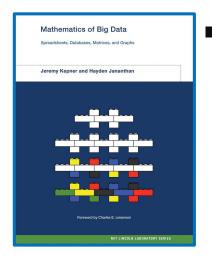


- Algorithm 1000: SuiteSparse:GraphBLAS: graph algorithms in the language of sparse linear algebra
 - o Algorithms in the SuiteSparse implementation @ ACM TOMS 2019

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 important papers, including the HPEC'16 paper above
 - Discusses D4M (Dynamic Distributed Dimensional Data Model)

GRAPHBLAS COMMUNITY

Wiki: graphblas.org | Communication: primarily mailing list

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
 - o IA³ workshop (Workshop on Irregular Applications: Architectures and Algorithms)

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



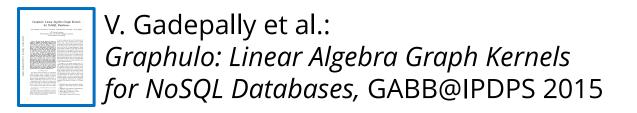
R. Lipman: RedisGraph internals RedisConf 2019

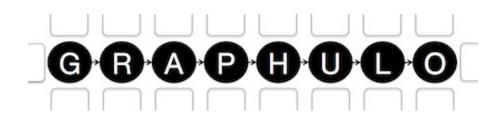
GRAPHBLAS IMPLEMENTATIONS

- SuiteSparse:GraphBLAS
 - v1.0.0: Nov 2017 sequential
 - o v3.0.1: July 2019 parallel
 - o v4.0.1draft: Dec 2020 many optimizations, incl. bitmap format
- 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, v3.0: 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



PYGRAPHBLAS: PYTHON WRAPPER

- Goal: Pythonic
 GraphBLAS wrapper,
 close to pseudo-code
- See example code for SSSP and triangle count
- Comes with Jupyter notebooks

```
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())
```

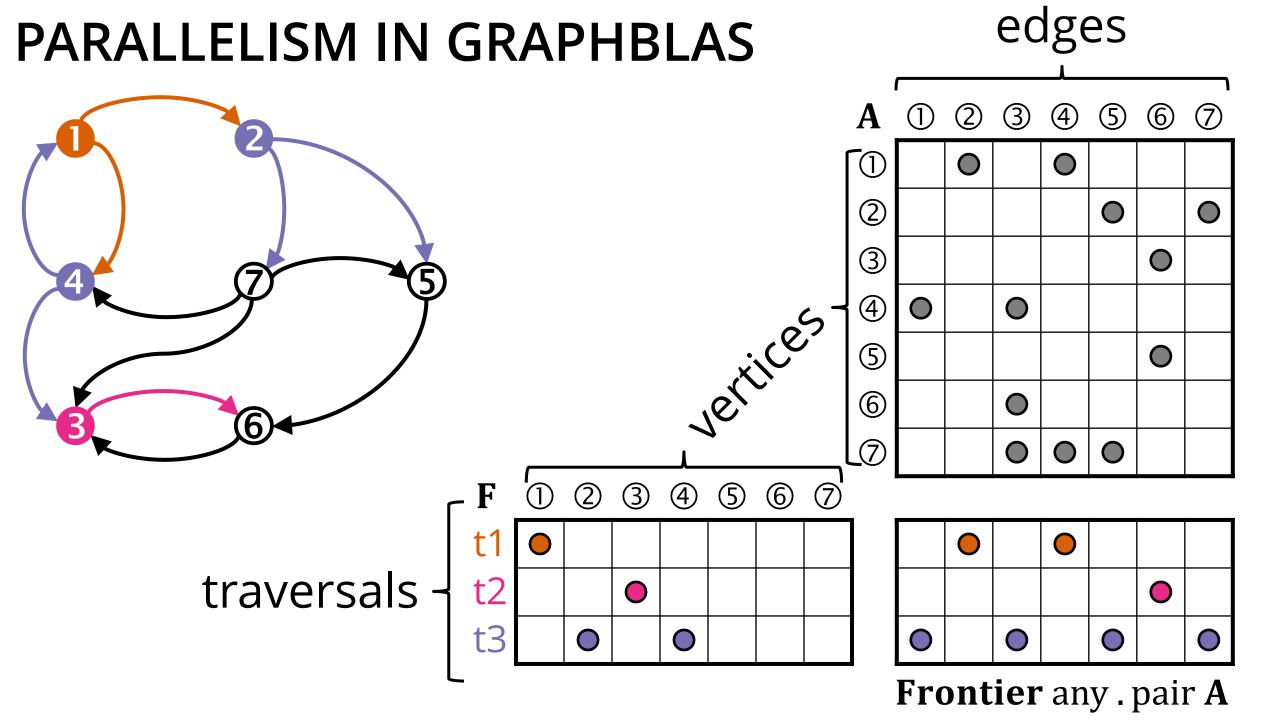


GRBLAS: PYTHON WRAPPER

- Goal: wrapper with an almost 1-to-1 mapping to the GrB API
 - Comes with a Conda package
 - Compiles user-defined functions to C
 - Supports visualization

```
M(mask, accum) << A.mxm(B, semiring) # mxm
w(mask, accum) << A.mxv(v, semiring) # mxv
w(mask, accum) << v.vxm(B, semiring) # vxm
M(mask, accum) << A.ewise_add(B, binaryop) # eWiseAdd
M(mask, accum) << A.ewise_mult(B, binaryop) # eWiseMult
M(mask, accum) << A.kronecker(B, binaryop) # kronecker
M(mask, accum) << A.T # transpose</pre>
```

Parallelism in GraphBLAS



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

Summary

SUMMARY

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

"Nuances" - Some important adjustments to the definitions

GRAPHBLAS SEMIRINGS*

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

- D_{out} , D_{in_1} , and D_{in_2} three domains
- $\bigoplus: D_{\text{out}} \times D_{\text{out}} \to D_{\text{out}}$ an associative and commutative addition operation
- $\otimes: D_{\text{in}_1} \times D_{\text{in}_2} \to D_{\text{out}}$ a multiplicative operation
- $0 \in D_{\text{out}}$ an identity element for \bigoplus

 $A = \langle D_{\text{out}}, \bigoplus, 0 \rangle$ 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)

NOTATION*

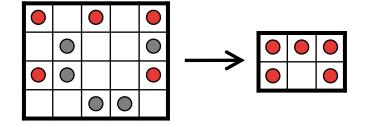
- Symbols:
 - A, B, C, M matrices
 - u, v, w, m vectors
 - \circ s, k scalar
 - \circ *i, j* indices
 - $\circ \langle \mathbf{m} \rangle, \langle \mathbf{M} \rangle$ masks
- Operators:
 - $\circ \oplus$ addition
 - $\circ \otimes$ multiplication, \oslash division
 - T transpose Not included in the
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

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

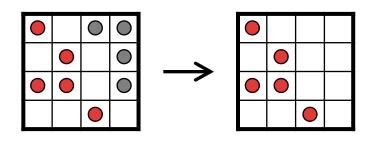
	symbol	operation	notation
	⊕.⊗	matrix-matrix multiplication	$C\langle M\rangle \bigcirc = A \oplus . \otimes B$
		vector-matrix multiplication	$\mathbf{w}\langle\mathbf{m}\rangle\odot=\mathbf{v}\oplus.\otimes\mathbf{A}$
		matrix-vector multiplication	$\mathbf{w}\langle\mathbf{m}\rangle\odot=\mathbf{A}\oplus.\otimes\mathbf{v}$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

LINEAR ALGEBRAIC PRIMITIVES FOR GRAPHS #3*

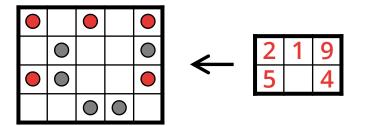
Sparse matrix extraction: induced subgraph



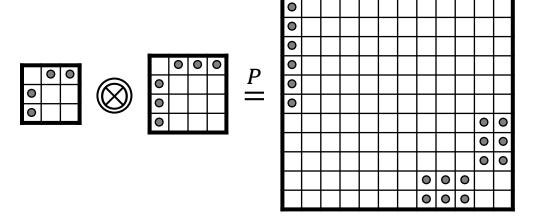
Sparse matrix selection: filtering edges



Sparse submatrix assignment: replace subgraph



Kronecker product: graph generation



0|0|0|0

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:

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

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

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

ELEMENT-WISE SUBTRACTION

Element-wise subtraction can be defined as an element-wise addition on the INT64_MINUS monoid. It has the following semantics $\mathbf{C} = \mathbf{A} \ominus \mathbf{B}$ is computed on the union of the patterns of the input matrices \mathbf{A} and \mathbf{B} .

For cells where only one input matrix has a non-zero value but the other does not (e.g. $\mathbf{B}[0,0] = 1$ but $\mathbf{A}[0,0]$ is empty), the result is the non-zero value: $\mathbf{C}[0,0] = 1$.

$$\begin{array}{c|ccccc}
\mathbf{A} & \mathbf{B} & \mathbf{C} \\
\hline
 & 1 & 1 \\
\hline
 & 1 & 1
\end{array}$$

$$\begin{array}{c|ccccc}
\mathbf{B} & \mathbf{C} \\
\hline
 & 1 & 1 \\
\hline
 & 1 & 1
\end{array}$$

This might come across as counter-intuitive first but it confirms the specification:

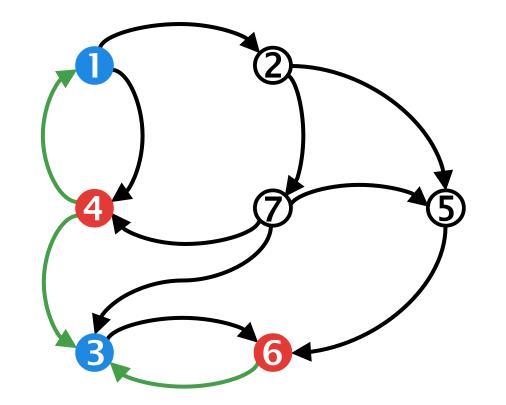
```
The intermediate matrix \widetilde{\mathbf{T}} = \langle \mathbf{D}_{out}(\mathsf{op}), \mathbf{nrows}(\widetilde{\mathbf{A}}), \mathbf{ncols}(\widetilde{\mathbf{A}}), \{(i,j,T_{ij}) : \mathbf{ind}(\widetilde{\mathbf{A}}) \cap \mathbf{ind}(\widetilde{\mathbf{B}}) \neq \emptyset \} \rangle
is created. The value of each of its elements is computed by

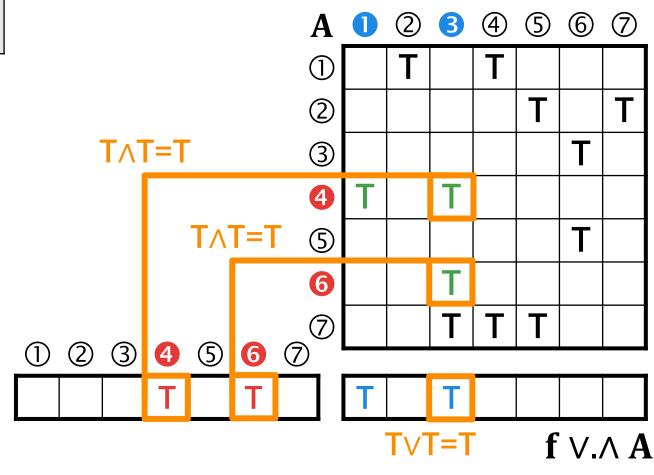
T_{ij} = (\widetilde{\mathbf{A}}(i,j) \oplus \widetilde{\mathbf{B}}(i,j)), \forall (i,j) \in \mathbf{ind}(\widetilde{\mathbf{A}}) \cap \mathbf{ind}(\widetilde{\mathbf{B}})
T_{ij} = \widetilde{\mathbf{A}}(i,j), \forall (i,j) \in (\mathbf{ind}(\widetilde{\mathbf{A}}) - (\mathbf{ind}(\widetilde{\mathbf{B}}) \cap \mathbf{ind}(\widetilde{\mathbf{A}})))
T_{ij} = \widetilde{\mathbf{B}}(i,j), \forall (i,j) \in (\mathbf{ind}(\widetilde{\mathbf{B}}) - (\mathbf{ind}(\widetilde{\mathbf{B}}) \cap \mathbf{ind}(\widetilde{\mathbf{A}})))
where the difference operator in the previous expressions refers to set difference.
```

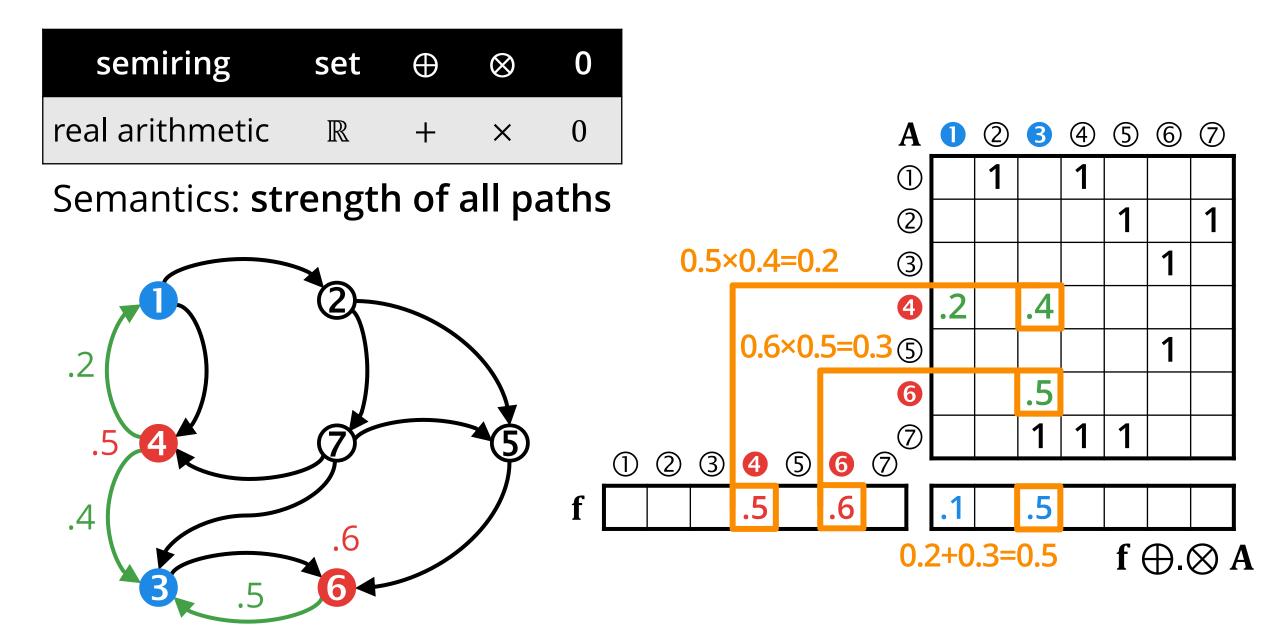
More semirings

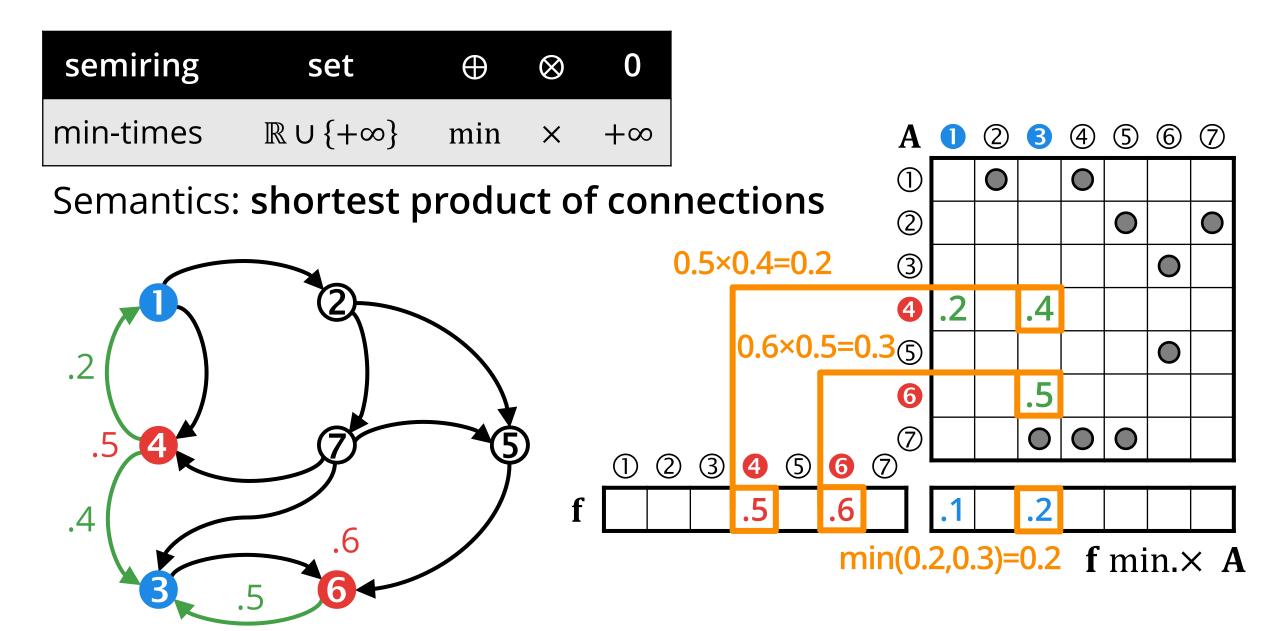


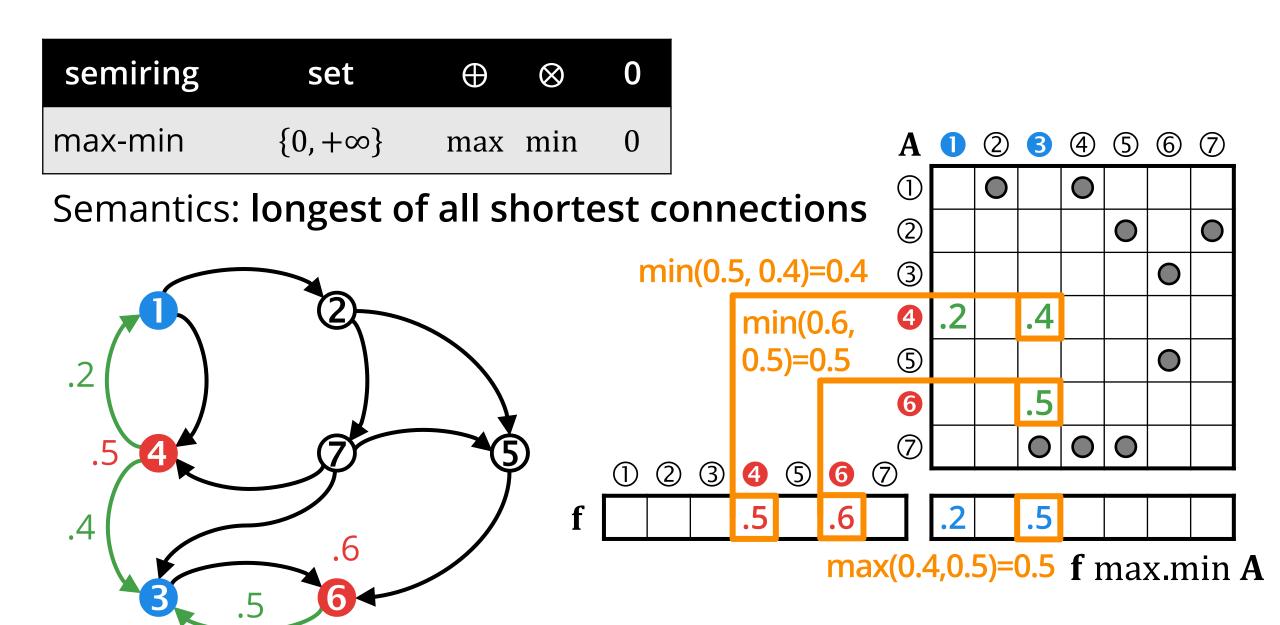
Semantics: reachability

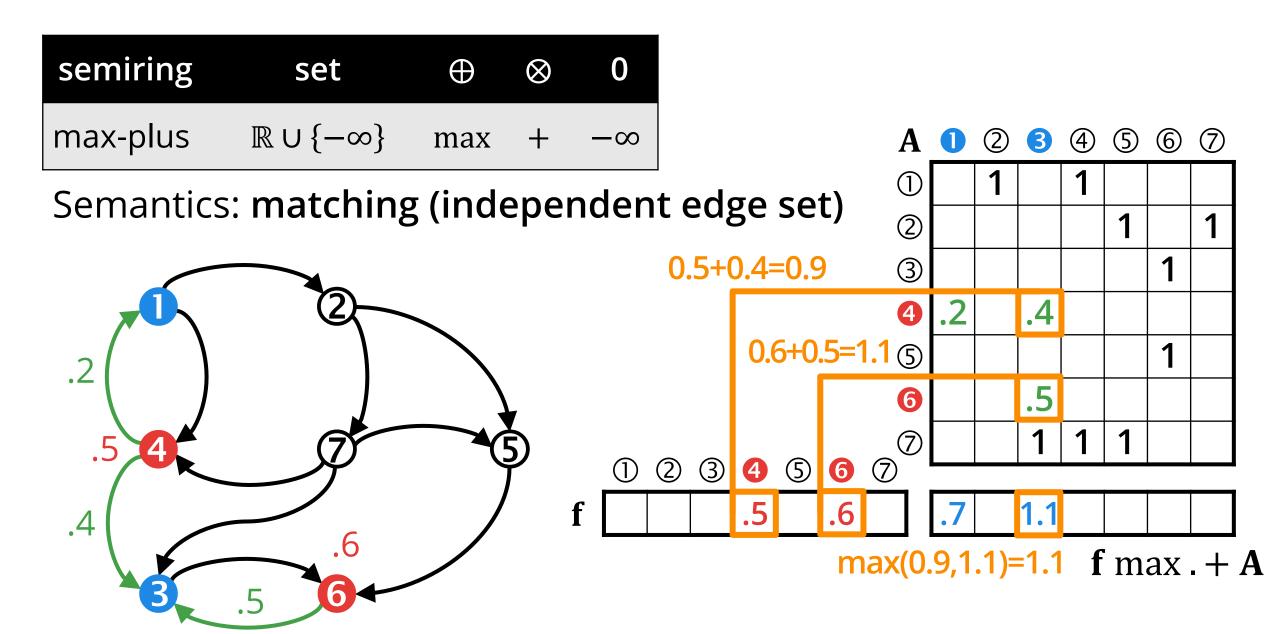












Case study: SIGMOD 2014 Contest

Overview

SIGMOD 2014 PROGRAMMING CONTEST

Annual contest

- Teams compete on database-related programming tasks
- Highly-optimized C++ implementations

2014 event

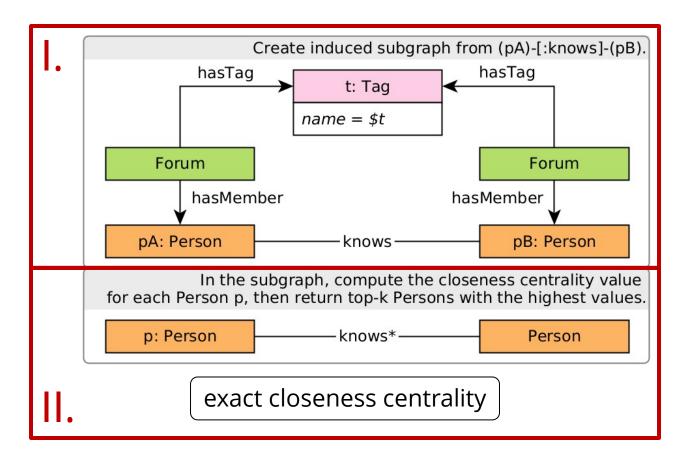
- Tasks on the LDBC social network graph
 - Benchmark data set for property graphs
 - o People, forums, comments, hashtags, etc.

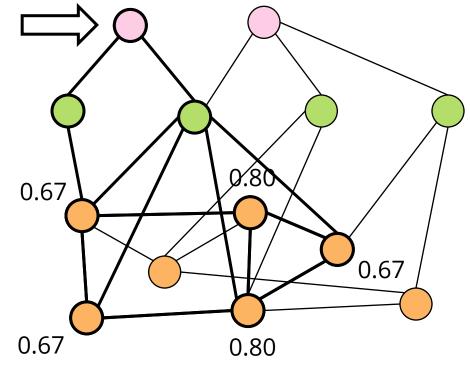


- 4 queries
 - Mix of filtering operations and graph algorithms

QUERY TEMPLATE

- I. Compute an induced subgraph over Person-knows-Person
- II. Run the graph algorithm on the subgraph

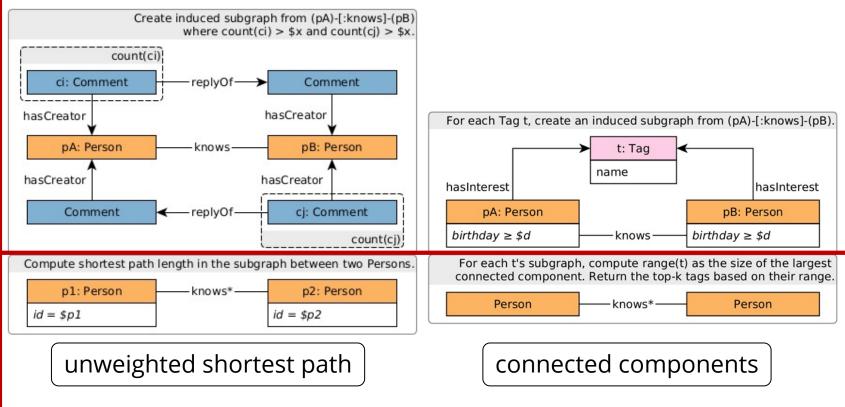


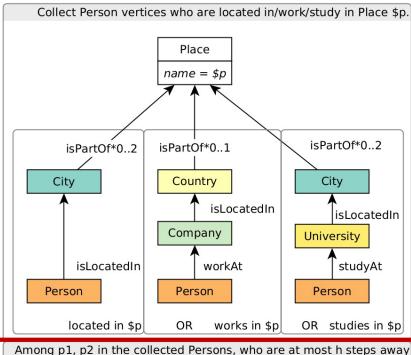


key kernel: all-source BFS

OVERVIEW OF QUERIES 1, 2, 3

I. Filter the induced subgraph(s)





hasInterest

t: Tag

hasInterest

p1: Person

knows*1..h

p2: Person

pairwise reachability

II. Run the graph algorithm

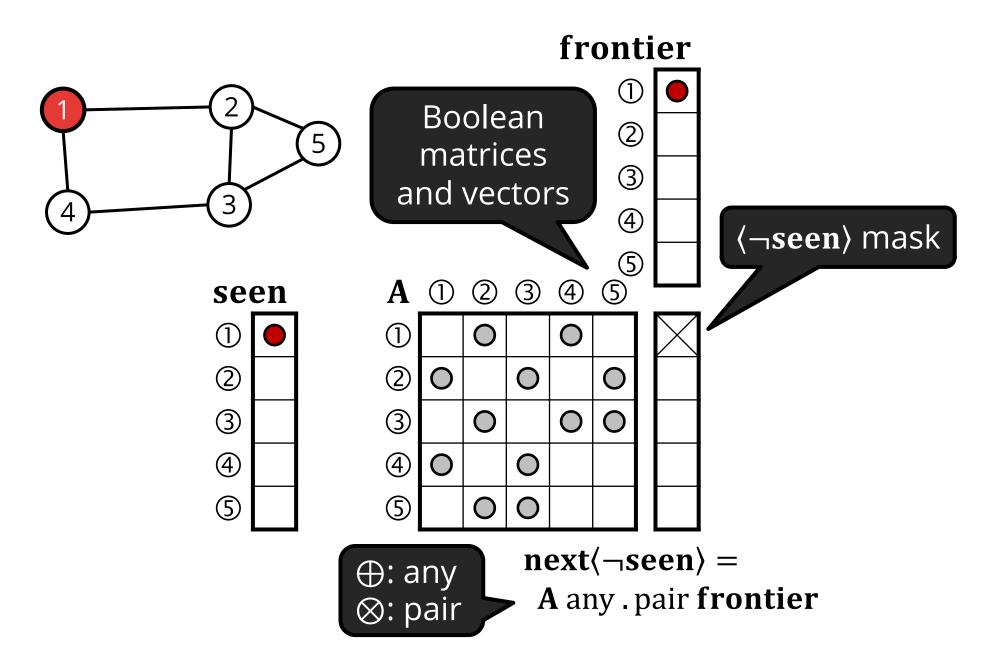
GRAPHBLAS SOLUTION OF THE QUERIES

- Loading includes relabelling UINT64 vertex IDs to a contiguous sequence 0 ... N — 1.
- Filtering the induced subgraph from the property graph is mostly straightforward and composable with the algorithms.
- The algorithms can be concisely expressed in GraphBLAS:
 - Connected components ✓ → FastSV [<u>Zhang et al., PPSC'20</u>]
 - o BFS ✓
 - Bidirectional BFS
 - All-source BFS + bitwise optimization
 - Multi-source bidirectional BFS

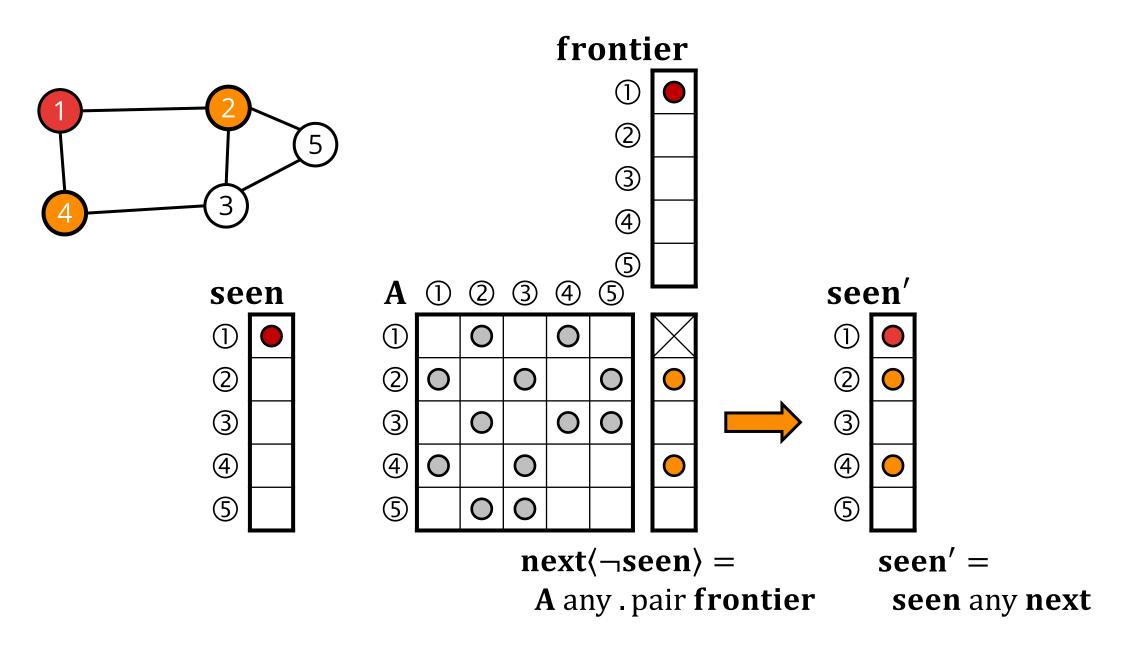
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BFS

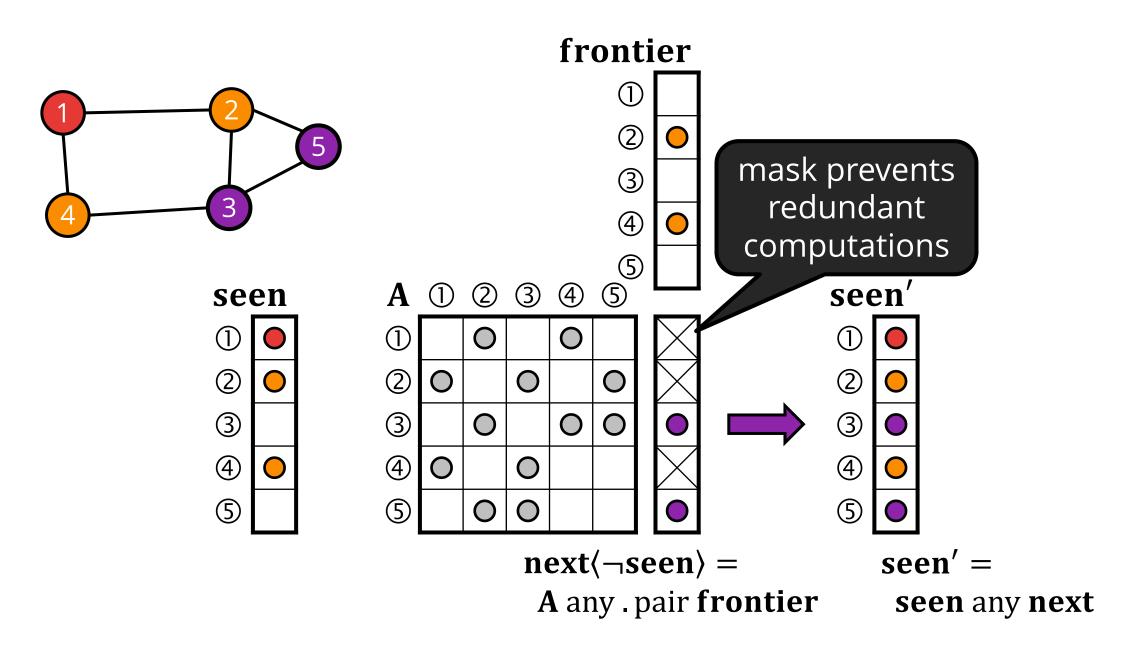
BFS: BREADTH-FIRST SEARCH



BFS: BREADTH-FIRST SEARCH



BFS: BREADTH-FIRST SEARCH



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All-source BFS

Q4: CLOSENESS CENTRALITY VALUES

Q4 computes the top-*k* Person vertices based on their exact closeness centrality values:

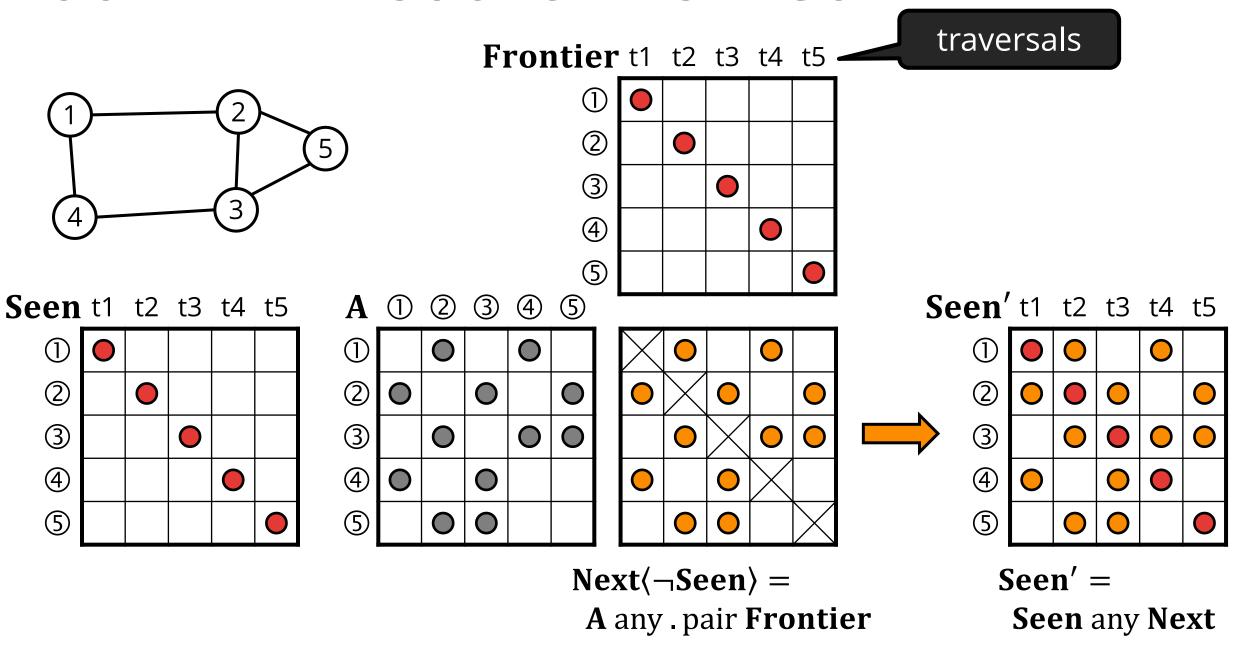
$$CCV(p) = \frac{(C(p) - 1)^2}{(n - 1) \cdot s(p)}$$

where

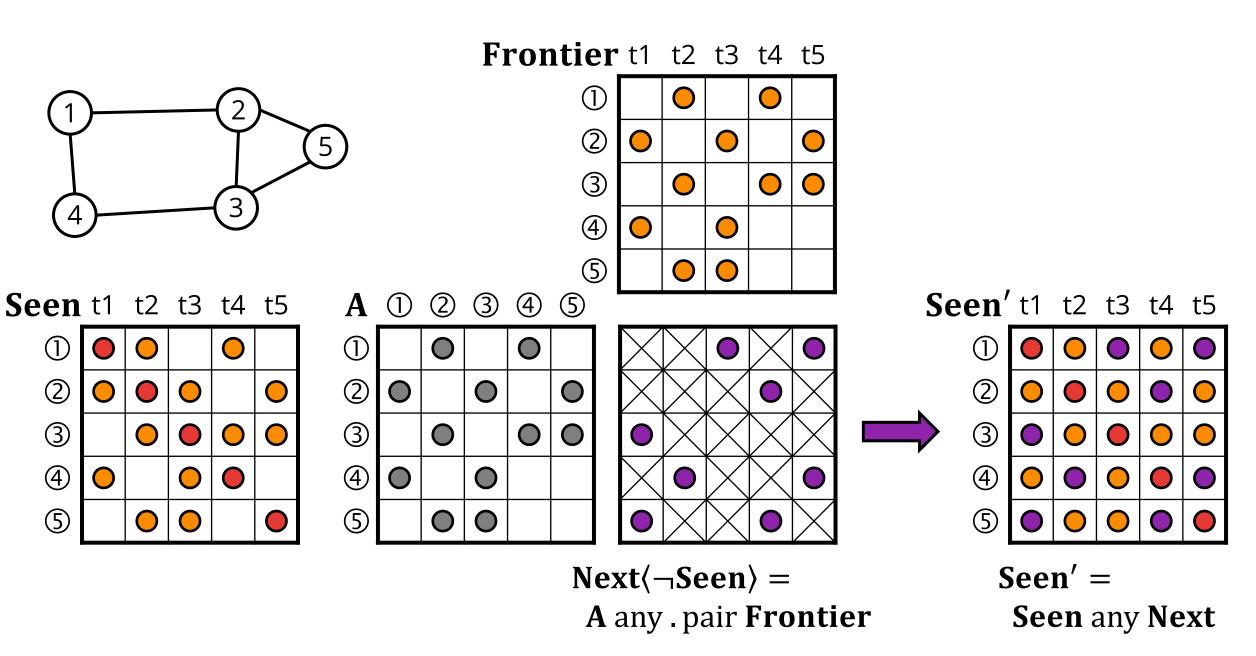
- C(p) is the size of the connected component of vertex p,
- lacktriangleright n is the number of vertices in the induced graph,
- s(p) is the sum of geodesic distances to all other reachable persons from p.

s(p) is challenging: needs unweighted all-pairs shortest paths.

BOOLEAN ALL-SOURCE BFS ALGORITHM



BOOLEAN ALL-SOURCE BFS ALGORITHM



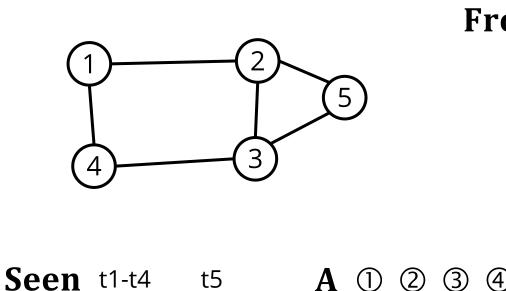
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Bitwise all-source BFS

BITWISE ALL-SOURCE BFS ALGORITHM

- For large graphs, the all-source BFS algorithm might need to run 500k+ traversals
- Two top-ranking teams used bitwise operations to process traversals in batches of 64 [<u>Then et al., VLDB'15</u>]
- This idea can be adopted in the GraphBLAS algorithm by
 - using UINT64 values
 - o performing the multiplication on the bor second semiring, where bor is "bitwise or" and second(x, y) = y
- 5-10x speedup compared to the Boolean all-source BFS

BITWISE ALL-SOURCE BFS ALGORITHM



t5

0000

0000

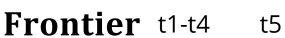
1000

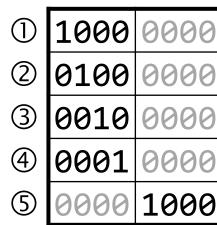
0001

0100 0000

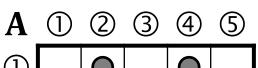
0010 0000

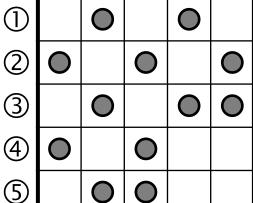
0000 1000



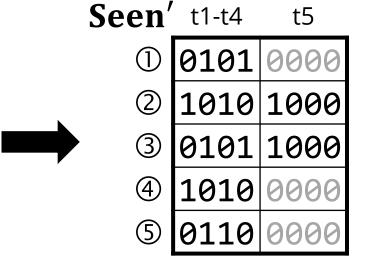


Using UINT4s here





0101	0000
1010	1000
0101	1000
1010	0000
0110	0000



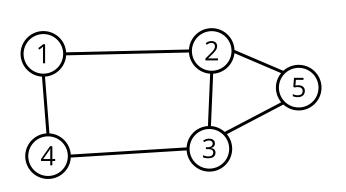
Seen' =

Next =

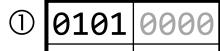
A bor second Frontier

Seen bor Next

BITWISE ALL-SOURCE BFS ALGORITHM



Frontier t1-t4 t5



- 2 1010 1000
- 3 |0101 | 1000
- **4 | 1010 | 0000**
 - 0 | 0110 | 0000

Full VLDB paper on this algorithm

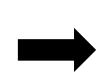
VS.

9 GrB operations

	t1-t4	
1	0101 1010 0101 1010	0000
2	1010	1000
3	0101	1000
4	1010	0000
(5)	0110	0000

A	\bigcirc		(3)	4)	<u>(5)</u>
1		0		0	
① ②	0		0		0
3		0		0	0
4	0		0		
(5)		0	0		

0010	1000
0001	0000
1000	0000
0100	1000
1001	0000



een	t1-t4	<u>t5</u>
1	1111	
2	1111	
3	1111	
4	1111	1000
(5)	1111	1000

Seen' =

Next =

A bor . second Frontier

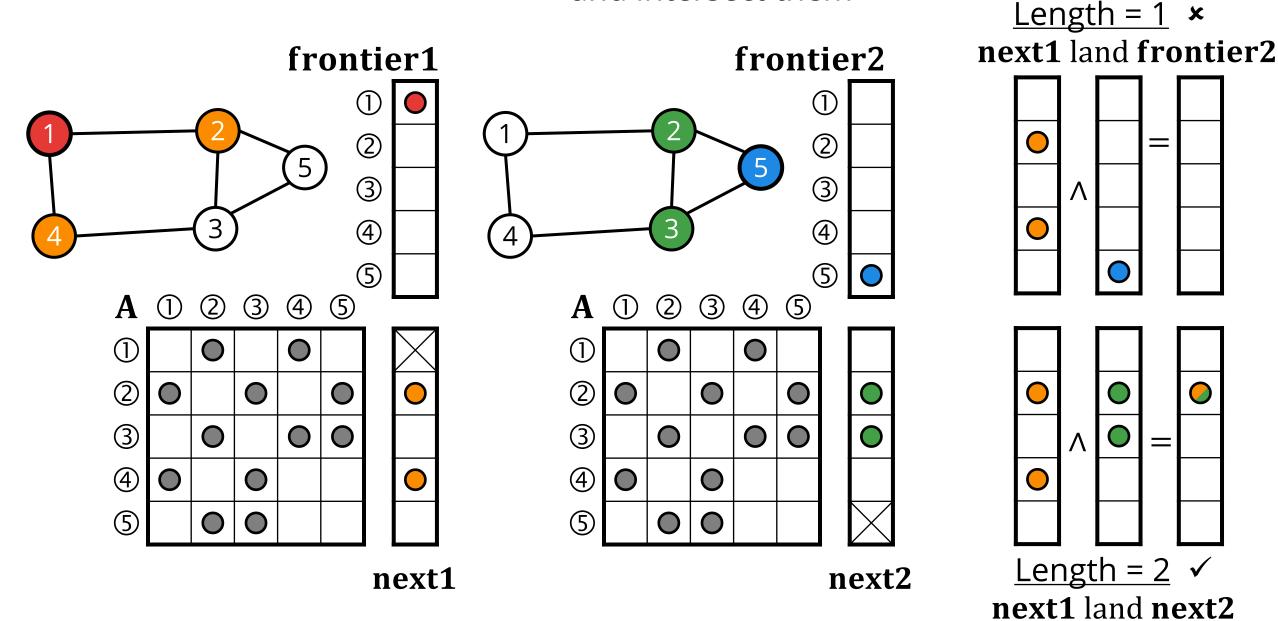
Seen bor Next

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Bidirectional BFS

BIDIRECTIONAL BFS

Advance frontiers alternately and intersect them



Case study: SIGMOD 2014 Contest

Bidirectional MSBFS

BIDIRECTIONAL MSBFS ALGORITHM

Pairwise reachability problem:

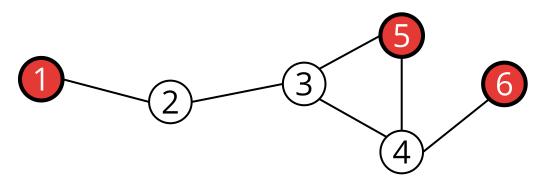
From a given set of k vertices, which pairs of vertices are reachable from each other with at most h hops?

Naïve solution:

Run a k-source MSBFS for h steps and check reachability. The frontiers get large as they grow exponentially.

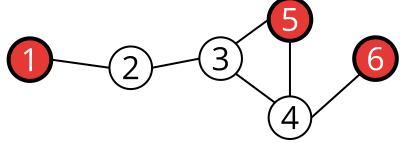
Better solution:

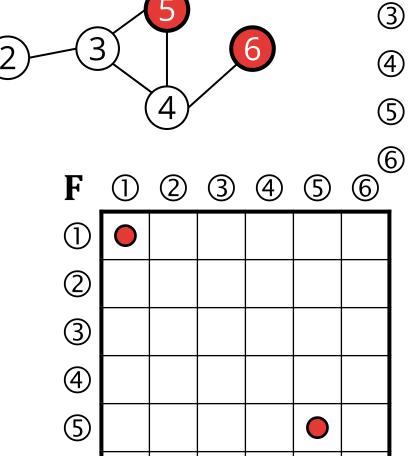
Advance all frontiers simultaneously for $\lceil h/2 \rceil$ iterations.

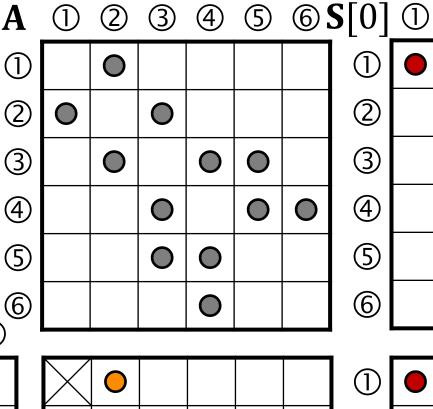


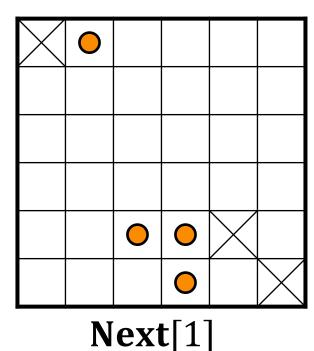
BIDIRECTIONAL MSBFS

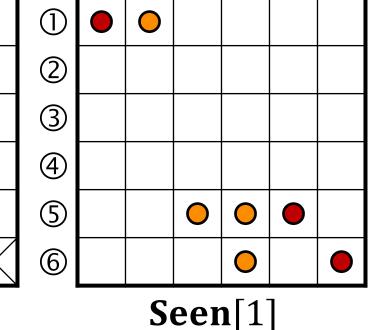
Seen[1]: reachability with ≤ 1 hops







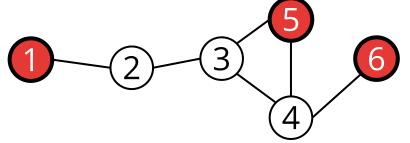




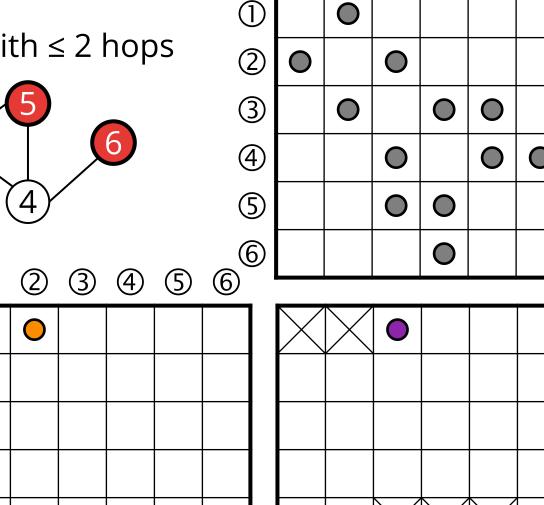
(5)

BIDIRECTIONAL MSBFS

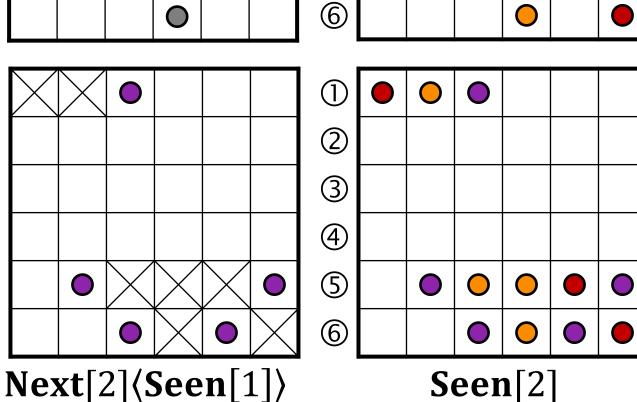
Seen[2]: reachability with \leq 2 hops



(5)

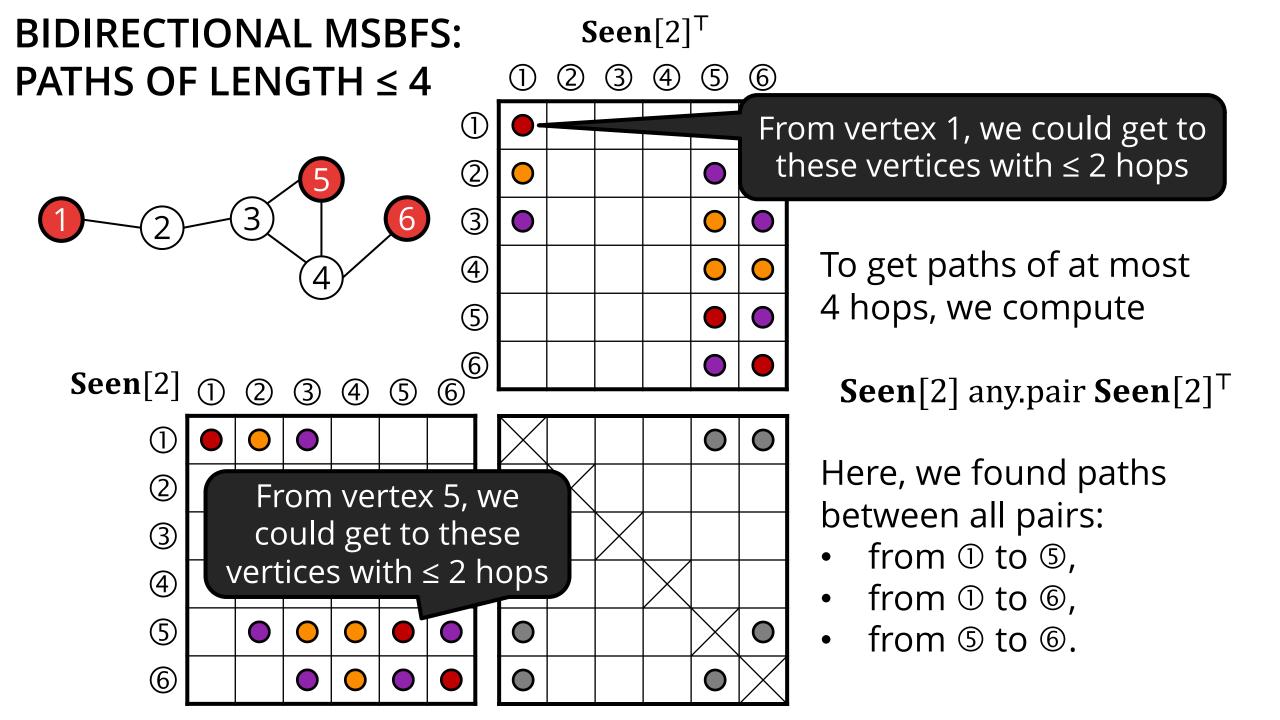


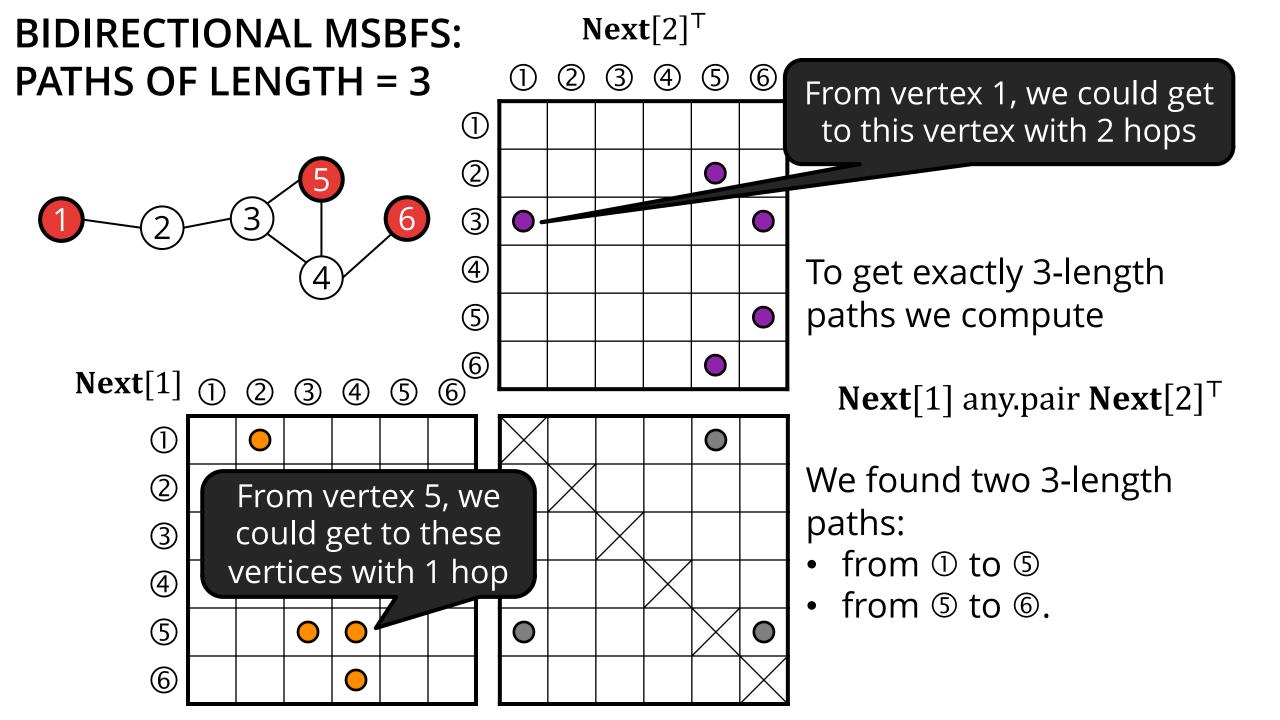
(5)



S[1] **1**

(5)



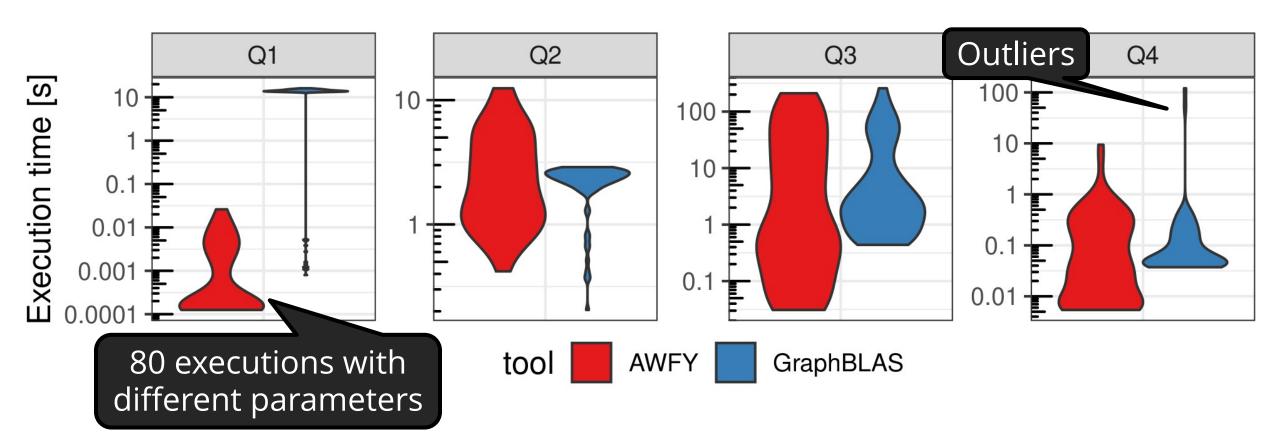


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Results

BENCHMARK RESULTS

- The top solution of AWFY vs. SuiteSparse:GraphBLAS v3.3.3
- AWFY's solution uses SIMD instructions → difficult to port
- GraphBLAS load times are slow (see details in paper)



SUMMARY

An interesting case study, see <u>technical report</u>



- GraphBLAS can capture mixed workloads
 - Induced subgraph computations are simple to express
 - o Algorithms are concise, bitwise optimizations can be adopted
 - o Performance is *sometimes* on par with specialized solutions
- Future optimizations
 - Q1: filter the induced subgraph on-the-fly
 - Q4: use more sophisticated unweighted shortest path algorithms



ACKNOWLEDGEMENTS

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- Thanks to the LDBC Graphalytics task force for creating the benchmark and assisting in the measurements.
- Thanks to the Master's students at BME for exploring the area of GraphBLAS: Bálint Hegyi, Petra Várhegyi, Lehel Boér

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.