

# A Hands-On Introduction to GraphBLAS: The Python Edition

<http://graphblas.org>

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... and the other members of the GraphBLAS specification group:  
**Aydın Buluç (UC Berkeley/LBNL)**, **Jose Moreira (IBM)**, and **Ben Brock (UC Berkeley)**.

With a special thank you to **Tim Davis (Texas A&M)** for GraphBLAS support in SuiteSparse and **Michel Pelletier (Graphegon)** for creating pygraphblas.

To get course materials onto your laptop:

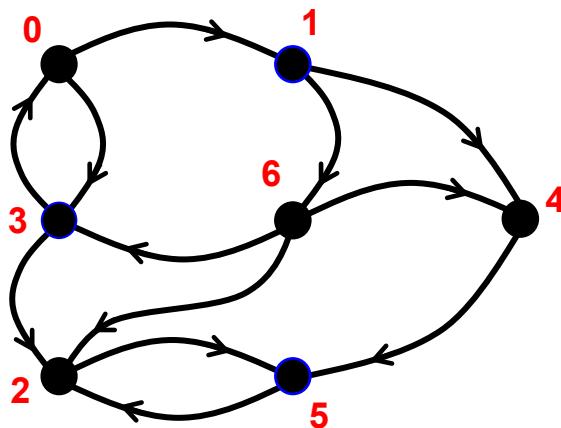
```
$ git clone https://github.com/GraphBLAS-Tutorials/HPEC21-Tutorial.git
```

# Outline

- ➡ • Graphs and Linear Algebra
- The GraphBLAS API and Adjacency Matrices
- GraphBLAS Operations
- Pygraphblas and modifying the behavior of operations.
- Graph Algorithms expressed with GraphBLAS
  - Breadth-First Traversal
  - Connected Components
  - Triangle Counting
  - PageRank

# Understanding relationships between items

- Graph: A visual representation of a set of vertices and the connections between them (edges).



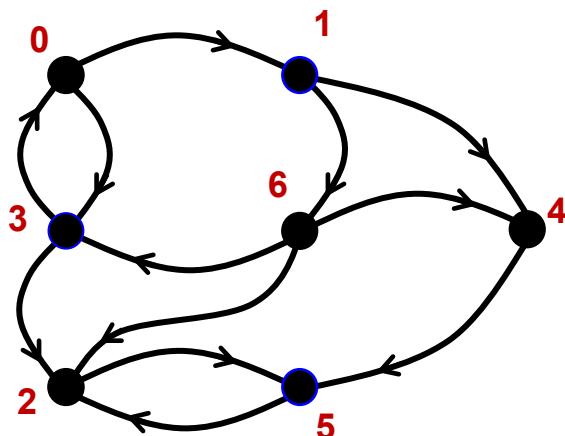
- Graph: Two sets, one for the vertices ( $v$ ) and one for the edges ( $e$ )

$$v \in [0, 1, 2, 3, 4, 5, 6]$$

$$e \in [(0,1), (0,3), (1,4), (1,6), (2,5), (3,0), (3,2), (4,5), (5,2), (6,2), (6,3), (6,4)]$$

# A graph as a matrix

- Adjacency Matrix: A square matrix (usually sparse) where rows and columns are labeled by vertices and non-empty values are edges from a row vertex to a column vertex



To vertex  
(columns)

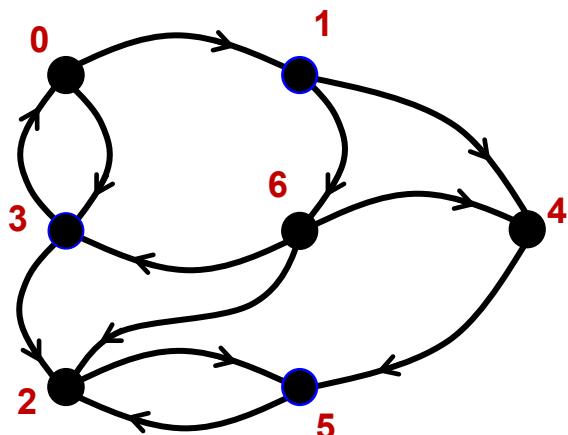
From vertex  
(rows)

$$A = \begin{bmatrix} & \star & & \star & & \\ - & - & - & - & \star & - & \star \\ - & - & - & - & - & \star & - \\ \star & - & \star & - & - & - & - \\ - & - & - & - & - & - & \star \\ - & - & \star & - & - & - & - \\ - & - & \star & \star & \star & - & - \end{bmatrix}$$

By using a matrix, I can turn algorithms working with graphs into linear algebra.

# A Directed graph as a matrix

- Adjacency Matrix: A square matrix (usually sparse) where rows and columns are labeled by vertices and non-empty values are edges from a row vertex to a column vertex

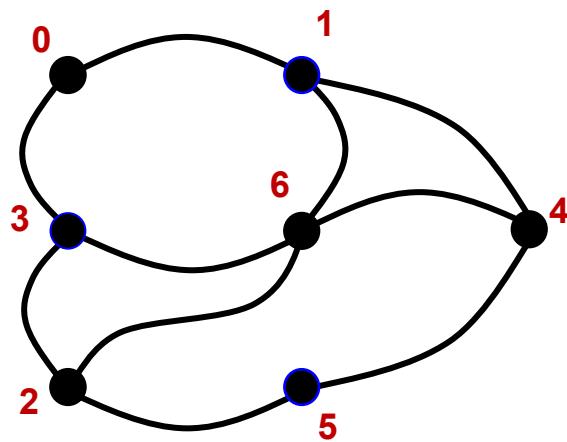


		To vertex (columns)					
		-	-	-	-	-	-
From vertex (rows)	-	-	★	-	★	-	-
		★	-	★	-	-	-
-	-	-	-	-	-	★	-
		-	-	★	-	-	-
-	-	-	-	★	-	-	-
		-	-	★	★	★	-

This is a directed graph  
(the edges have arrows)

# An Undirected graph as a matrix

- Adjacency Matrix: A square matrix (usually sparse) where rows and columns are labeled by vertices and non-empty values are edges from a row vertex to a column vertex

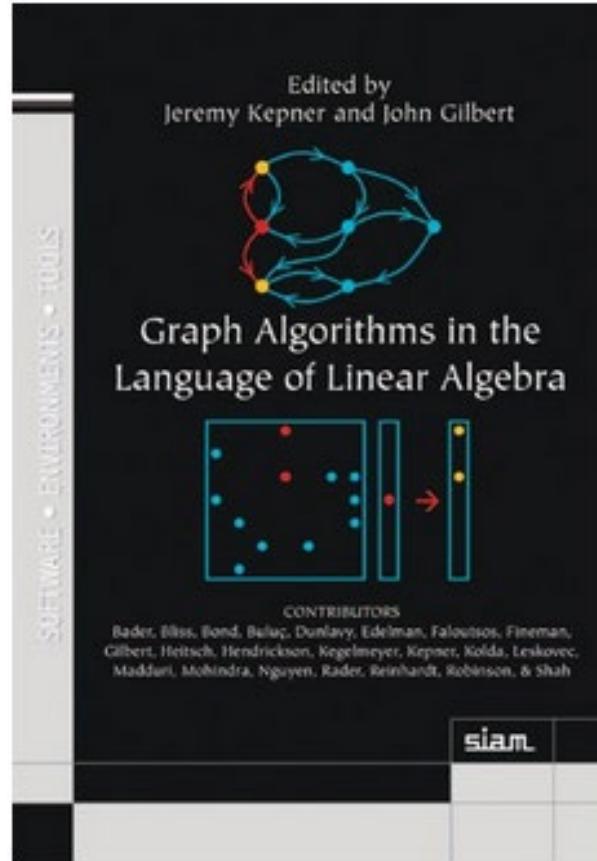


		To vertex (columns)					
		-	-	-	-	-	-
A =	From vertex (rows)	-	★	-	★	-	-
		-	★	-	★	-	★
		-	★	-	★	-	★
		-	★	-	★	-	★
		-	★	-	★	-	★
		-	★	★	★	★	-
		-	★	★	★	★	-

This is an undirected graph (no arrows on the edges)  
and the Adjacency matrix is symmetric

# Graph Algorithms and Linear Algebra

- Most common graph algorithms can be represented in terms of linear algebra.
  - This is a mature field ... it even has a book.
- Benefits of graphs as linear algebra
  - Well suited to memory hierarchies of modern microprocessors
  - Can utilize decades of experience in distributed/parallel computing from linear algebra in supercomputing.
  - Easier to understand ... for some people.



# How do linear algebra people write software?

- They do so in terms of the BLAS:
  - The **Basic Linear Algebra Subprograms**: low-level building blocks from which any linear algebra algorithm can be written

BLAS 1	Vector/vector	Lawson, Hanson, Kincaid and Krogh, 1979	LINPACK
BLAS 2	Matrix/vector	Dongarra, Du Croz, Hammarling and Hanson, 1988	LINPACK on vector machines
BLAS 3	Matrix/matrix	Dongarra, Du Croz, Hammarling and Hanson, 1990	LAPACK on cache-based machines

- The BLAS supports a separation of concerns:
  - HW/SW optimization experts tuned the BLAS for specific platforms.
  - Linear algebra experts build software on top of the BLAS ... high performance “for free”.
- It is difficult to over-state the impact of the BLAS ... they revolutionized the practice of computational linear algebra.

# GraphBLAS: building blocks for graphs as linear algebra

- Basic objects
  - Matrix, vector, algebraic structures, and “control objects”
- Fundamental operations over these objects

Matrix multiplication

$$\begin{bmatrix} \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \end{bmatrix} \times \begin{bmatrix} \bullet & \bullet \\ \bullet & \bullet \\ \bullet & \bullet \\ \bullet & \bullet \end{bmatrix}$$

Element-wise operations  
(eWiseAdd,  
eWiseMult)

$$\begin{bmatrix} \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \end{bmatrix} \cdot * \begin{bmatrix} \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \end{bmatrix}$$

Matrix-vector multiplication  
(vxm, mxv)

$$\begin{bmatrix} \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \end{bmatrix} \times \begin{bmatrix} \bullet \\ \bullet \\ \bullet \\ \bullet \\ \bullet \end{bmatrix}$$

Extract (and  
Assign)  
submatrices

$$\begin{bmatrix} \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \end{bmatrix} \leftarrow \begin{bmatrix} \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \end{bmatrix}$$

...plus reduction, transpose, and application of a function to each element of a matrix or vector

# GraphBLAS References

## Mathematical Foundations of the GraphBLAS

Jeremy Kepner (MIT Lincoln Laboratory Supercomputing Center), Peter Aaltonen (Indiana University),  
David Bader (Georgia Institute of Technology), Aydin Buluç (Lawrence Berkeley National Laboratory),  
Franz Franchetti (Carnegie Mellon University), John Gilbert (University of California, Santa Barbara),  
Dylan Hutchison (University of Washington), Manoj Kumar (IBM),  
Andrew Lumsdaine (Indiana University), Henning Meyerhenke (Karlsruhe Institute of Technology),  
Scott McMillan (CMU Software Engineering Institute), Jose Moreira (IBM),  
John D. Owens (University of California, Davis), Carl Yang (University of California, Davis),  
Marcin Zalewski (Indiana University), Timothy Mattson (Intel)

IEEE HPEC 2016

## Design of the GraphBLAS API for C

Aydin Buluç<sup>†</sup>, Tim Mattson<sup>‡</sup>, Scott McMillan<sup>§</sup>, José Moreira<sup>¶</sup>, Carl Yang<sup>\*,†</sup>

<sup>†</sup>*Computational Research Division, Lawrence Berkeley National Laboratory*

<sup>‡</sup>*Intel Corporation*

<sup>§</sup>*Software Engineering Institute, Carnegie Mellon University*

<sup>¶</sup>*IBM Corporation*

<sup>\*</sup>*Electrical and Computer Engineering Department, University of California, Davis, USA*

GABB@IPDPS 2017

The official GraphBLAS C spec can be found at: [www.graphblas.org](http://www.graphblas.org)

# GraphBLAS Implementations

SuiteSparse library (Texas A&M): First fully conforming GraphBLAS release

- <http://faculty.cse.tamu.edu/davis/suitesparse.html>

GraphBLAS C (IBM): the second fully conforming release

- <https://github.com/IBM/ibmgraphblas>

GBTL: GraphBLAS Template Library (CMU/SEI/IU/PNNL): GraphBLAS C++ implementation

- <https://github.com/cmu-sei/gbtl>

GraphBLAST: A C++ implementation for GraphBLAS for GPUs (UC Davis)

- <https://github.com/gunrock/graphblast>

Python bindings:

- PyGB: A python wrapper around GBTL (UW/PNNL/CMU)
  - <https://github.com/jessecoleman/gbtl-python-binding>
- pygraphblas: A python wrapper around SuiteSparse GraphBLAS
  - <https://github.com/michelp/pygraphblas>
- grblas: Anaconda's python wrapper around SuiteSparse GraphBLAS
  - <https://github.com/metagraph-dev/grblas>

pggraphblas: A PostgreSQL wrapper around Suite Sparse GraphBLAS

- <https://github.com/michelp/pggraphblas>

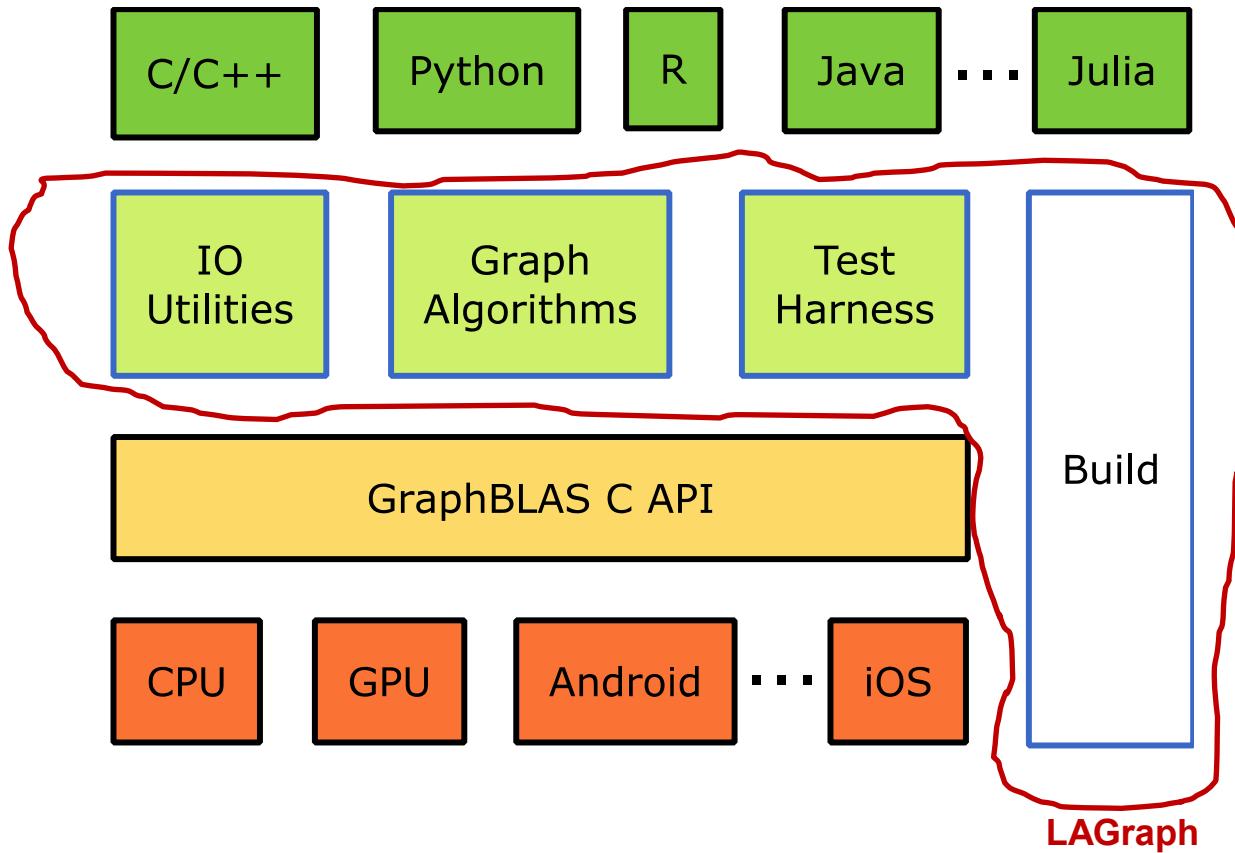
Julia wrapper around SuiteSparse

- SuiteSparseGraphBLAS.jl

Matlab and Julia wrappers around SuiteSparse GraphBLAS

- <https://aldenmath.com>

# The GraphBLAS Vision



# LAGraph: A curated collection of high level Graph Algorithms

Graph Algorithms built on top of the GraphBLAS.

## LAGraph: A Community Effort to Collect Graph Algorithms Built on Top of the GraphBLAS

Tim Mattson<sup>‡</sup>, Timothy A. Davis<sup>◦</sup>, Manoj Kumar<sup>¶</sup>, Aydin Buluç<sup>†</sup>, Scott McMillan<sup>§</sup>, José Moreira<sup>¶</sup>, Carl Yang<sup>\*,†</sup>

<sup>‡</sup>*Intel Corporation* <sup>†</sup>*Computational Research Division, Lawrence Berkeley National Laboratory*

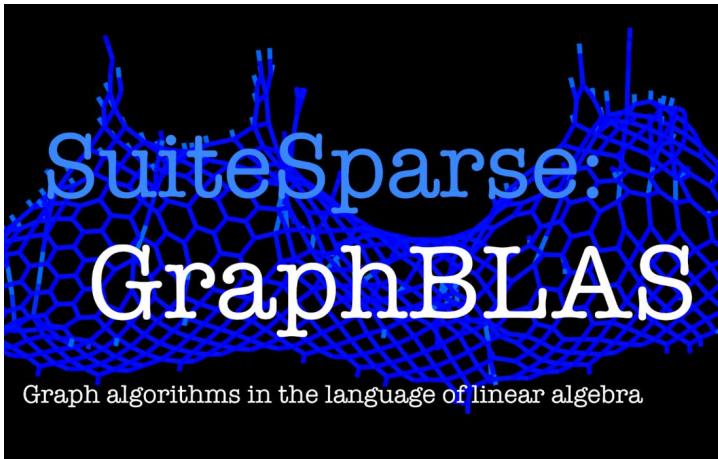
<sup>◦</sup>*Texas A&M University* <sup>¶</sup>*IBM Corporation* <sup>§</sup>*Software Engineering Institute, Carnegie Mellon University*

<sup>\*</sup>*Electrical and Computer Engineering Department, University of California, Davis*

GrAPL 2019

Official release of LAGraph library v1.0 later in 2021

# SuiteSparse: C libraries for GraphBLAS and LAGraph



Tim Davis  
Texas A&M  
University

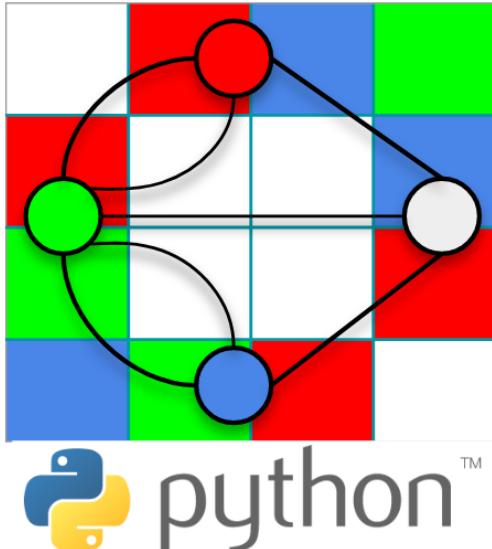


**SuiteSparse:GraphBLAS** : open-source GraphBLAS library with OpenMP (Apache 2.0)

- high performance, internal parallelism, allows for easy-to-code fast graph algorithms
- fully compliant with v1.3 C API
- MATLAB interface, many overloaded operators and functions ( $C(M)=A*B$ , etc)
- GxB extensions: ANY monoid, import/export, positional ops in semirings, scalars, float and double complex, select operation, PAIR operator, type query, subassign, ...
- matrix data structures: sparse (CSR/CSC) / hypersparse / bitmap / full
- <https://people.engr.tamu.edu/davis/GraphBLAS.html>

logo: mathematical art by T. D. <http://www.notesartstudio.com/sincere.html>

# Graphegon



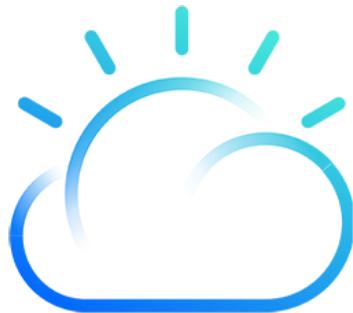
- pygraphblas is developed by Graphegon.
- Open-source package using the SuiteSparse:GraphBLAS library.
- Specializing in GraphBLAS solutions using C, Python and PostgreSQL.
- <https://github.com/Graphegon/pygraphblas>

Pygraphblas Documentation at: <https://graphegon.github.io/pygraphblas/pygraphblas/index.html>

*Your personalized*



*container powered by*



# IBM Cloud

“You log into the cloud by ssh and magic happens that causes little people floating in the cloud to create an account for you that runs on fairy dust and makes a container float up from the ether to respond to your every whim.”

# GraphBLAS in the cloud: Setting up your session

- SSH into the host `graphblas.tk` with the username `user` and password `graphblastutorial2021`.
- You should see output similar to the following:

```
$ ssh user@graphblas.tk  
user@graphblas.tk's password:
```

```
[I 21:42:32.806 NotebookApp] Writing notebook server cookie secret to /home/jovyan/.local/share/jupyter/runtime/notebook_cookie_secret  
[I 21:42:33.440 NotebookApp] JupyterLab extension loaded from /opt/conda/lib/python3.9/site-packages/jupyterlab  
[I 21:42:33.440 NotebookApp] JupyterLab application directory is /opt/conda/share/jupyter/lab  
[I 21:42:33.443 NotebookApp] Serving notebooks from local directory: /home/jovyan/tutorial-workspace/HPEC21-Tutorial/notebook-workspace  
[I 21:42:33.443 NotebookApp] Jupyter Notebook 6.1.6 is running at:  
...  
Your Jupyter Notebook should now be ready:  
=====  
http://graphblas.tk:98765/?token=1234567890abcdef1234567890abcdef1234567890abcdef  
=====  
****SAVE THIS URL!**** You will need in case you close your browser window.
```

If you do not see a URL, or there otherwise appears to be an error, please alert the tutorial staff.  
Connection to graphblas.tk closed.

- To access the notebook, open this file in a browser (Chrome or Firefox recommended):  
<file:///home/jovyan/.local/share/jupyter/runtime/nbserver-7-open.html>
- Or copy and paste the **graphblas.tk URL** (above) into your browser. This will open up a Jupyter Notebook running inside a Docker container created just for you in the IBM cloud.
- **Bookmark or save your URL**. You can reconnect to same instance throughout the tutorial.

# Exercise 1: Running a GraphBLAS program

- Launch the GraphBLAS container in the cloud

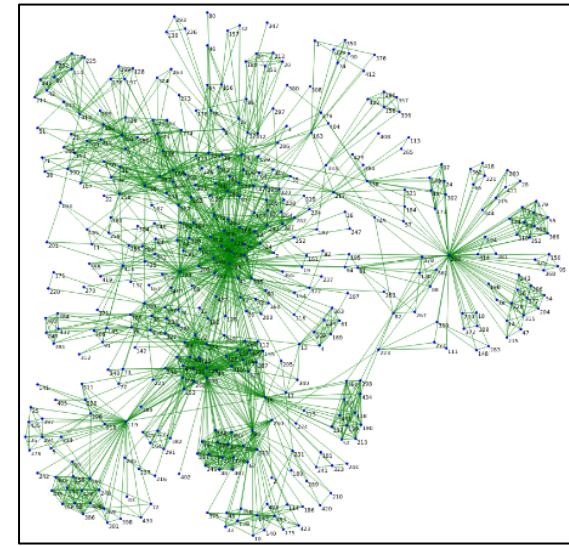
```
$ ssh user@graphblas.tk
```

- It will ask for a password

```
graphblastutorial2021
```

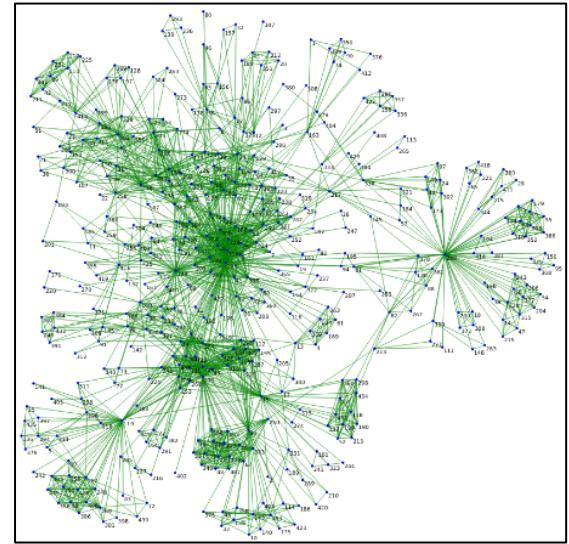
- Cut-and-paste the returned URL in your browser  
(Save this URL so you can reconnect to the container later).

- Launch the AnalyzeGraph notebook and run-all from the cells menu to find the “2-hop” neighborhood of one author in the HPEC papers graph and then perform PageRank and draw a visualization of this reduced neighborhood [*this visualization could take a few minutes to render*].
- If all goes well, we will have confirmed that everything is working ... that you have a container you can access through Jupyter notebook.



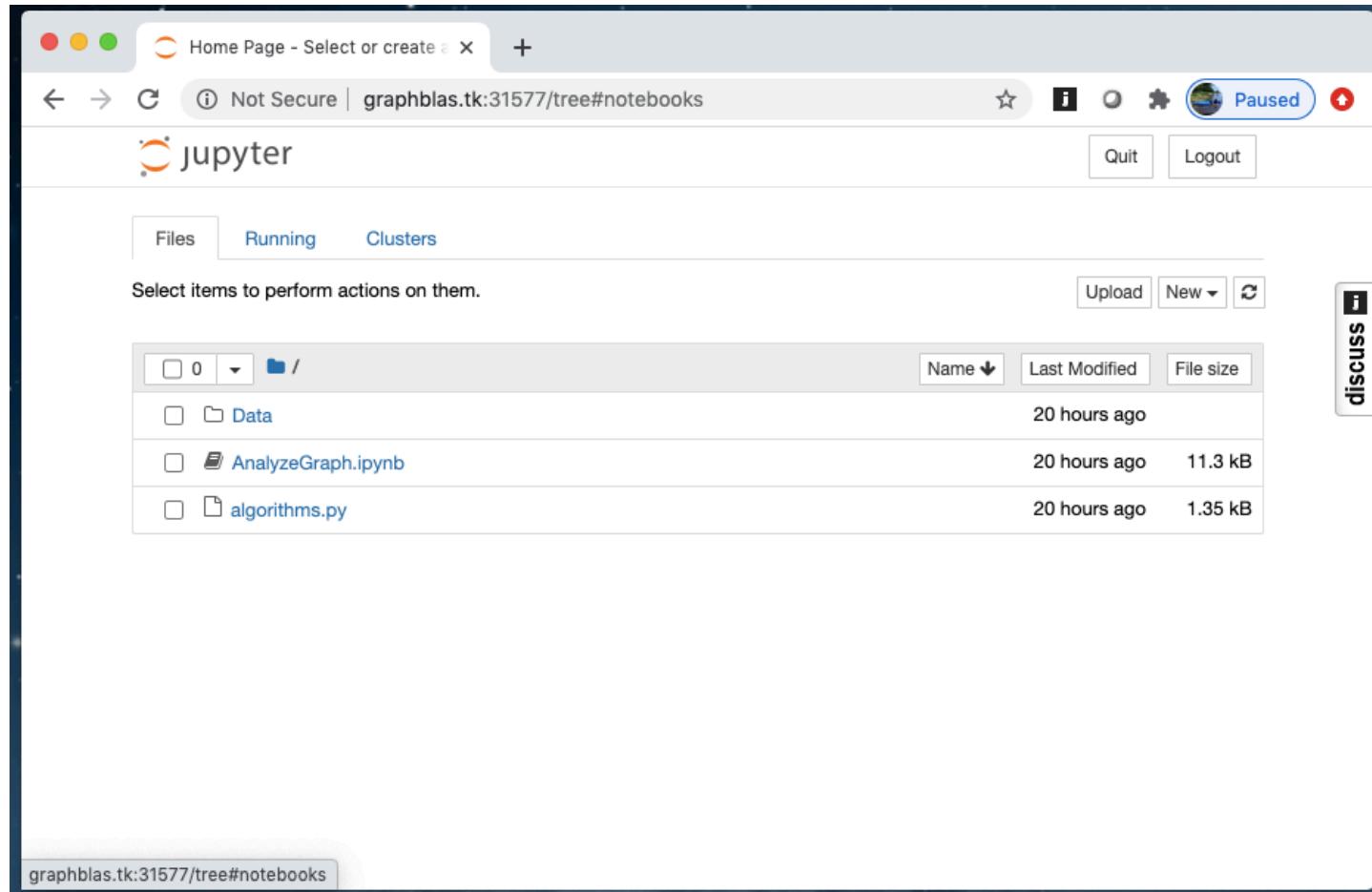
# HPEC Authors Dataset

- Data represents all pairs of HPEC\* authors that have coauthored papers. The edge value represents how many papers the pair have coauthored.
- Graph (undirected):
  - 1,747 vertices (unique authors)
  - 10,072 edges (coauthor count)
- Data directory contains index tables containing the mapping between vertex ID and author name, the raw publication data, and python scripts to perform various queries



\*HPEC: IEEE High Performance Extreme Computing Conference, held each September where many Graph People gather each year.

# The jupyter session exposed by the container



# The AnalyzeGraph Notebook

The screenshot shows a Jupyter Notebook interface with the title "AnalyzeGraph" in the header. The notebook contains two code cells:

**In [1]:**

```
import time
import pygraphblas as grb
import algorithms
from pygraphblas.gviz import draw, draw_graph_op as draw_op
from pygraphblas.gviz import draw_cy
```

**Step 1: load a graph from a matrix market file**

Nodes are authors of papers and abstracts published at IEEE HPEC through 2019. Edges connect coauthors of papers.

**In [2]:**

```
pathname = './Data/hpec_coauthors.mtx'

with open(pathname, 'r') as f:
    t0 = time.time()
    M = grb.Matrix.from_mm(f, grb.types.UINT64)
    t1 = time.time()
    print("## Step 1: Elapsed time: %s sec." % (t1 - t0))
```

\*\*\* Step 1: Elapsed time: 0.038427114486694336 sec.

**Step 2: compute some basic statistics on the graph**

# Run all the cells in the notebook

The screenshot shows a Jupyter Notebook interface with the title "jupyter AnalyzeGraph (unsaved changes)". The "Cell" menu is open, with the "Run All" option circled in red. The code in cell [1] imports time, pygraphblas, and algorithms from pygraphblas. The code in cell [2] opens a matrix market file, measures the elapsed time, and prints the result.

In [1]:

```
import time
import pygraphblas
import algorithms
from pygraphblas import *
from pygraphblas import algorithms
```

Step 1: load a graph from a matrix market file

Nodes are authors of papers and abstracts published at IEEE HPEC through 2019. Edges connect coauthors of papers.

In [2]:

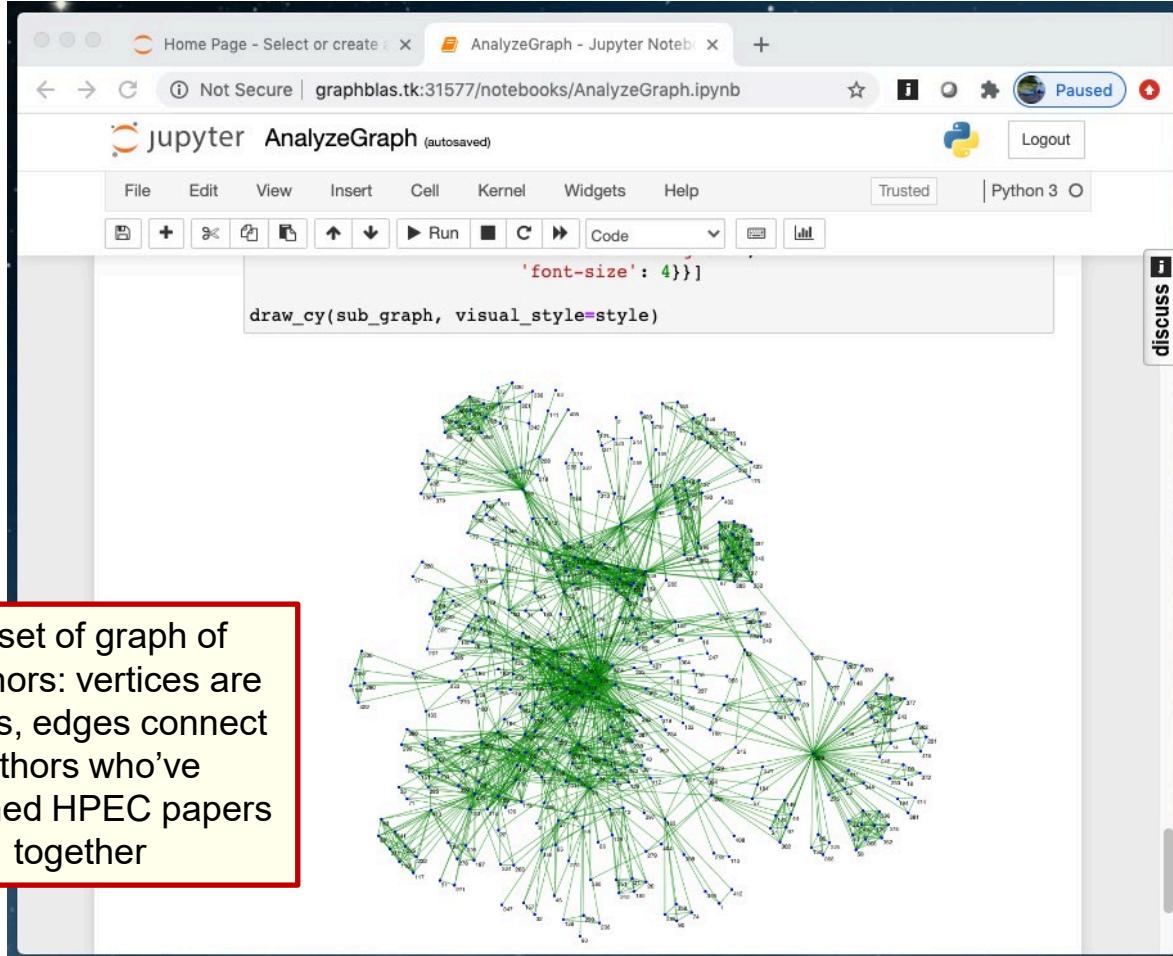
```
pathname = './Data/hpec_coauthors.mtx'

with open(pathname, 'r') as f:
    t0 = time.time()
    M = grb.Matrix.from_mm(f, grb.types.UINT64)
    t1 = time.time()
    print("*** Step 1: Elapsed time: %s sec." % (t1 - t0))

*** Step 1: Elapsed time: 0.038427114486694336 sec.
```

Step 2: compute some basic statistics on the graph

# The result (after a few minutes)



# Outline

- Graphs and Linear Algebra
- The GraphBLAS API and Adjacency Matrices
- GraphBLAS Operations
- Pygraphblas and modifying the behavior of operations.
- Graph Algorithms expressed with GraphBLAS
  - Breadth-First Traversal
  - Connected Components
  - Triangle Counting
  - PageRank

# The GraphBLAS API: Maps Math Spec onto the C programming language

- **Opaque object:** An object manipulated strictly through the GraphBLAS API whose implementation is not defined by the GraphBLAS specification.

`GrB_Matrix` → A 2D sparse array, row indices, column indices and values

`GrB_Vector` → A 1D sparse array

- **Method:** Any function that manipulates a GraphBLAS opaque object.
- **Domain:** the set of available values used for the elements of matrices, the elements of vectors, and when defining operators.
  - Examples are `GrB_UINT64`, `GrB_INT32`, `GrB_BOOL`, `GrB_FP32`
- **Operation:** a method that corresponds to an operation defined in the GraphBLAS math spec.  
<http://www.mit.edu/~kepner/GraphBLAS/GraphBLAS-Math-release.pdf>

```
GrB_mxm(C, GrB_NULL, GrB_NULL, GrB_LOR LAND BOOL, A, B, GrB_NULL);
```

```
GrB_mxv(w, GrB_NULL, GrB_NULL, GrB_LOR LAND BOOL, A, v, GrB_NULL);
```

```
GrB_eWiseAdd(C, GrB_NULL, GrB_NULL, GrB_LOR, A, B, GrB_NULL);
```

# The GraphBLAS API: pygraphblas

## Maps the C API onto Python

- **Opaque object:** An object manipulated strictly through the GraphBLAS API whose implementation is not defined by the GraphBLAS specification.

`Matrix.sparse` → A 2D sparse array, row indices, column indices and values

`Vector.sparse` → A 1D sparse array

- **Method:** Any function that manipulates a GraphBLAS opaque object.
- **Domain:** the set of available values used for the elements of matrices, the elements of vectors, and when defining operators.
  - Examples are `UINT64`, `INT32`, `BOOL`, `FP32`
- **Operation:** a method that corresponds to an operation defined in the GraphBLAS math spec.  
<http://www.mit.edu/~kepner/GraphBLAS/GraphBLAS-Math-release.pdf>

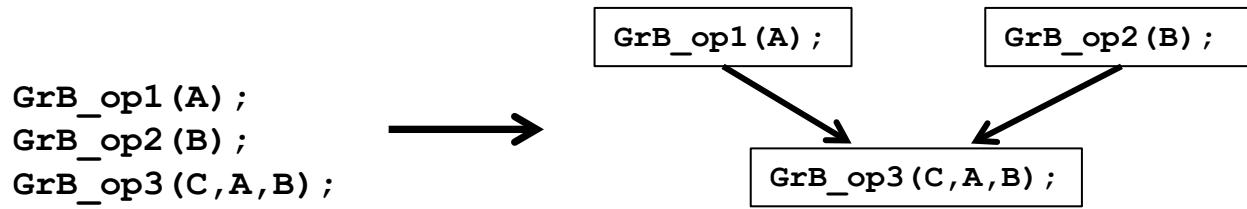
`Matrix multiply`     $C = A \odot B$      $C = A.mxm(B)$     or    `A.mxm(B, out=C)`

`Matrix Vector`     $w = A @ v$      $w = A.mxv(v)$     or    `A.mxv(v, out=w)`

`Element-wise add`     $C = A + B$      $C = A.eadd(B)$     or    `A.eadd(B, out=C)`

# GraphBLAS Execution modes

- A GraphBLAS program defines a DAG of operations.
- Objects are defined by the sequence of GraphBLAS method calls, but the value of the object is not assured until a GraphBLAS method queries its state.
- This gives an implementation flexibility to optimize the execution (fusing methods, replacing method sequences by more efficient ones, etc.)



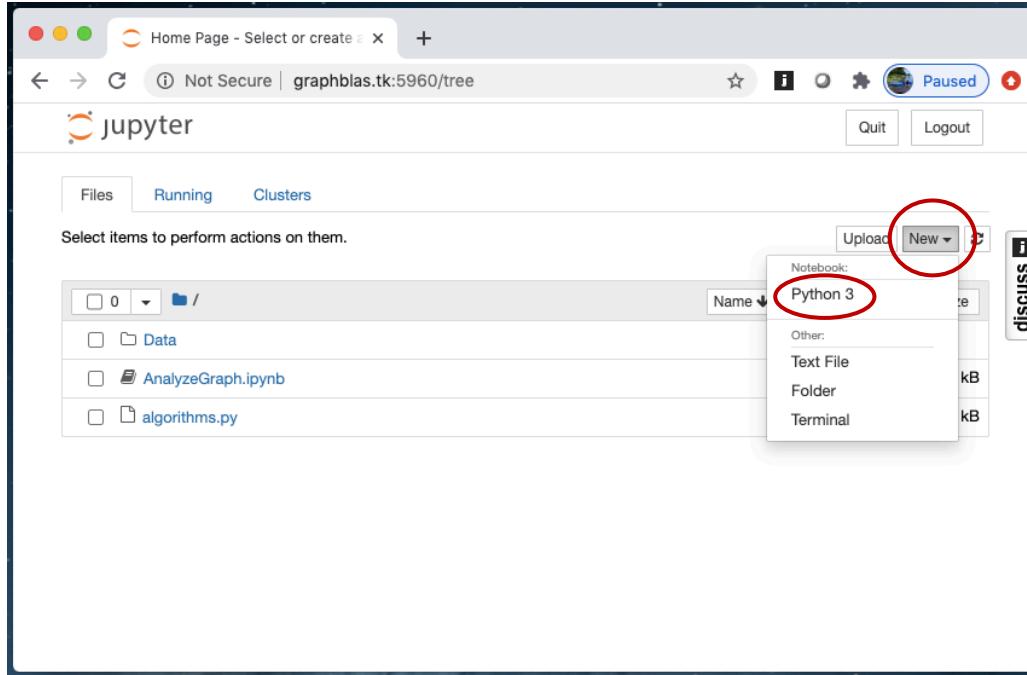
- An execution of a GraphBLAS program defines a context for the library.
- The execution runs in one of two modes:
  - Blocking mode ... executes methods in program order with each method completing before the next is called
  - Non-Blocking mode ... methods launched in order. Complete in any order consistent with the DAG. Objects **may** not exit in fully defined state until queried.
- **Pygraphblas uses non-blocking mode**

# Creating a matrix

- Matrices in real problems are imported into a program from a file or an external application.
- We can also build a matrix, element by element
  - Import pygraphblas        `import pygraphblas as grb`
  - Set size of matrix        `n = 3`
  - Build a square matrix:    `A = grb.Matrix.sparse(grb.UINT64, n, n)`
  - Set a value in the matrix `A[1, 2] = 4`
  - Look at the matrix        `print(A)`

# Exercise 2: Your first pygraphblas program

- Open a new jupyter notebook with Python 3.
- Create a matrix, set a few values, and print the result.
- Play around to make sure you are comfortable with the environment



```
import pygraphblas as grb
A = grb.Matrix.sparse(grb.type, n, n)
A[row,col] = val
some common types are UINT64, BOOL, FP32, INT8, FP64
print(A)
```

# Exercise 2: Your first pygraphblas program

- Open a new jupyter notebook with Python 3.
- Create a matrix, set a few values, and print the result.
- Play around to make sure you are comfortable with the environment

The screenshot shows a Jupyter Notebook window titled "Untitled". The toolbar includes "File", "Edit", "View", "Insert", "Cell", "Kernel", "Widgets", and "Help". The status bar indicates "Trusted" and "Python 3". The code cell (In [7]) contains the following Python code:

```
import pygraphblas as grb
A = grb.Matrix.sparse(grb.UINT64, 4, 4)
A[1,1] = 2
A[0,3] = 3
A[3,2] = 4
print(A)
```

The output of the code is a sparse matrix represented as a table:

	0	1	2	3	
0				3	0
1			2		1
2					2
3			4		3
	0	1	2	3	

```
import pygraphblas as grb
A = grb.Matrix.sparse(grb.type, n, n)
A[row,col] = val
some common types are UINT64, BOOL, FP32, INT8, FP64
print(A)
```

# Creating a matrix

- Matrices in real problems are imported into the program from a file or an external application.

- We can build Matrices from lists:

- Import pygraphblas:      `import pygraphblas as grb`
- List of row indices:      `ri = [0, 2, 4, 5]`
- List of column indices:    `ci = [1, 3, 5, 5]`
- List of Values:            `val = [True]*len(ri)` ← A list of True as long as ri
- Build the matrix:          `A = grb.Matrix.from_lists(ri, ci, val)`
- Number of columns:        `NUM_NODES = A.ncol`

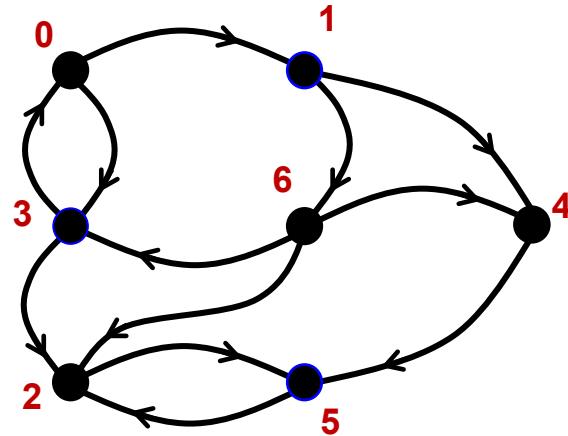
- We can look at a matrix as a matrix (with print) or as a graph:

```
from pygraphblas.gviz import draw_graph as draw
draw(A)
```

# Exercise 3: Adjacency matrix

- Look at the matrix from Exercise 2 as a graph using `draw_graph()`.
- Experiment with setting different elements until you are comfortable with the connection between a graph and an adjacency matrix.
- Create the adjacency matrix of the “GraphBLAS logo graph” from lists
- Items you will need from the `pygraphblas`

```
import pygraphblas as grb
from pygraphblas.gviz import draw_graph as draw
A = grb.Matrix.from_lists(rowList, columnList, valueList)
A = grb.Matrix.sparse(grb.type, n, n)
print(A)
draw(A)
some common types are UINT64, BOOL, FP32, INT8, FP64
```



# Exercise 3: Adjacency matrix

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Not Secure | graphblas.tk:5960/notebooks/Untitled.ipynb?kernel\_name=python3

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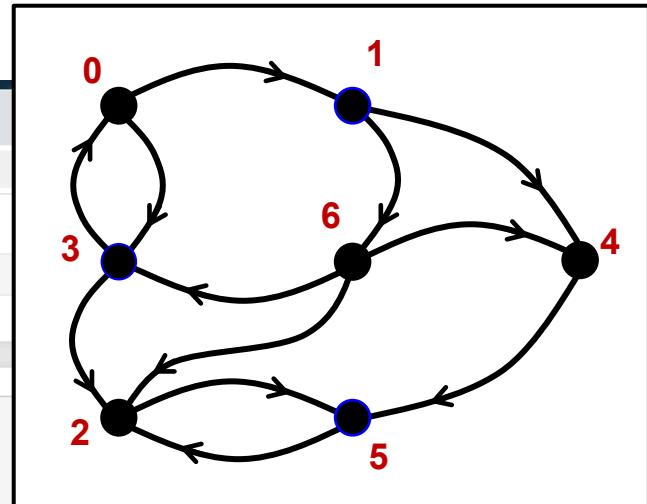
Code

```
In [20]: import pygraphblas as grb
from pygraphblas.gviz import draw_graph as draw
rowInd = [0,0,1,1,2,3,3,4,5,6,6,6]
colInd = [1,3,4,6,5,0,2,5,2,2,3,4]
values = [True]*len(rowInd)
A = grb.Matrix.from_lists(rowInd,colInd,values)
draw(A)
```

Out[20]:

```
graph LR; 0((0)) -- True --> 1((1)); 0((0)) -- True --> 3((3)); 1((1)) -- True --> 0((0)); 1((1)) -- True --> 2((2)); 1((1)) -- True --> 4((4)); 1((1)) -- True --> 6((6)); 2((2)) -- True --> 0((0)); 2((2)) -- True --> 3((3)); 2((2)) -- True --> 5((5)); 3((3)) -- True --> 0((0)); 3((3)) -- True --> 2((2)); 3((3)) -- True --> 4((4)); 4((4)) -- True --> 1((1)); 4((4)) -- True --> 3((3)); 4((4)) -- True --> 5((5)); 5((5)) -- True --> 2((2)); 5((5)) -- True --> 4((4)); 6((6)) -- True --> 1((1)); 6((6)) -- True --> 4((4));
```

In [ ]:



# Outline

- Graphs and Linear Algebra
- The GraphBLAS API and Adjacency Matrices
- ➡ • GraphBLAS Operations
  - Pygraphblas and modifying the behavior of operations.
  - Graph Algorithms expressed with GraphBLAS
    - Breadth-First Traversal
    - Connected Components
    - Triangle Counting
    - PageRank

# GraphBLAS vectors and matrices

- Let's review our Matrix and Vector Objects.
- They are opaque ... the structure is not defined in the spec so implementors have maximum flexibility to optimize their implementation
- pygraphblas defines a number of static methods to use when working with matrices and vectors

We've seen  
these already

```
import pygraphblas as grb
#Create a sparse matrix with Nrows and Ncols
A = grb.Matrix.sparse(type, Nrows, Ncols)

#Create a sparse matrix from index and value lists
A = grb.Matrix.from_lists(rowInd, colInd, valList)
```

The vector case  
is analogous to  
the matrix case

```
#Create a sparse vector of size N
v = grb.Vector.sparse(type, N)

#Create a sparse vector from index and value lists
v = grb.Vector.from_lists(indList, valList)
```

# GraphBLAS Operations (from the Math Spec\*)

Operation Name	Mathematical Notation		
mxm	$\mathbf{C}\langle\mathbf{M}, r\rangle$	=	$\mathbf{C} \odot \mathbf{A} \oplus . \otimes \mathbf{B}$
mxv	$\mathbf{w}\langle\mathbf{m}, r\rangle$	=	$\mathbf{w} \odot \mathbf{A} \oplus . \otimes \mathbf{u}$
vxm	$\mathbf{w}^T\langle\mathbf{m}^T, r\rangle$	=	$\mathbf{w}^T \odot \mathbf{u}^T \oplus . \otimes \mathbf{A}$
eWiseMult	$\mathbf{C}\langle\mathbf{M}, r\rangle$	=	$\mathbf{C} \odot \mathbf{A} \otimes \mathbf{B}$
	$\mathbf{w}\langle\mathbf{m}, r\rangle$	=	$\mathbf{w} \odot \mathbf{u} \otimes \mathbf{v}$
eWiseAdd	$\mathbf{C}\langle\mathbf{M}, r\rangle$	=	$\mathbf{C} \odot \mathbf{A} \oplus \mathbf{B}$
	$\mathbf{w}\langle\mathbf{m}, r\rangle$	=	$\mathbf{w} \odot \mathbf{u} \oplus \mathbf{v}$
extract	$\mathbf{C}\langle\mathbf{M}, r\rangle$	=	$\mathbf{C} \odot \mathbf{A}(i, j)$
	$\mathbf{w}\langle\mathbf{m}, r\rangle$	=	$\mathbf{w} \odot \mathbf{u}(i)$
assign	$\mathbf{C}\langle\mathbf{M}, r\rangle(i, j)$	=	$\mathbf{C}(i, j) \odot \mathbf{A}$
	$\mathbf{w}\langle\mathbf{m}, r\rangle(i)$	=	$\mathbf{w}(i) \odot \mathbf{u}$
reduce (row)	$\mathbf{w}\langle\mathbf{m}, r\rangle$	=	$\mathbf{w} \odot [\oplus_j \mathbf{A}(:, j)]$
reduce (scalar)	$s$	=	$s \odot [\oplus_{i,j} \mathbf{A}(i, j)]$
	$s$	=	$s \odot [\oplus_i \mathbf{u}(i)]$
apply	$\mathbf{C}\langle\mathbf{M}, r\rangle$	=	$\mathbf{C} \odot f_u(\mathbf{A})$
	$\mathbf{w}\langle\mathbf{m}, r\rangle$	=	$\mathbf{w} \odot f_u(\mathbf{u})$
apply(indexop)	$\mathbf{C}\langle\mathbf{M}, r\rangle$	=	$\mathbf{C} \odot f_i(\mathbf{A}, \text{ind}(\mathbf{A}), s)$
	$\mathbf{w}\langle\mathbf{m}, r\rangle$	=	$\mathbf{w} \odot f_i(\mathbf{u}, \text{ind}(\mathbf{u}), s)$
select	$\mathbf{C}\langle\mathbf{M}, r\rangle$	=	$\mathbf{C} \odot \mathbf{A}\langle f_i(\mathbf{A}, \text{ind}(\mathbf{A}), s) \rangle$
	$\mathbf{w}\langle\mathbf{m}, r\rangle$	=	$\mathbf{w} \odot \mathbf{u}\langle f_i(\mathbf{u}, \text{ind}(\mathbf{u}), s) \rangle$
transpose	$\mathbf{C}\langle\mathbf{M}, r\rangle$	=	$\mathbf{C} \odot \mathbf{A}^T$
kronecker	$\mathbf{C}\langle\mathbf{M}, r\rangle$	=	$\mathbf{C} \odot \mathbf{A} \otimes \mathbf{B}$

We use  $\odot$ ,  $\oplus$ , and  $\otimes$  since we can change the operators mapped onto those symbols.

**mxv()**

$w \odot= A \oplus . \otimes u$

Multiply a matrix times a vector to produce a vector

$$w(i) = w(i) \odot \sum_{k=0}^N A(i, k) \otimes u(k)$$

$$w \in S^M \quad u \in S^N \quad A \in S^{M \times N}$$

Definitions:

- $S$  is the domain of the objects  $w$ ,  $u$ , and  $A$
- $\odot$  is an optional accumulation operator (a binary operator)
- $\otimes$  and  $\oplus$  are multiplication and addition (or generalizations thereof)
- $\sum$  uses the  $\oplus$  operator

**mxv()**

$w \odot= A \oplus . \otimes u$

Multiply a matrix times a vector to produce a vector

$$w(i) = w(i) \odot \sum_{k \in \text{ind}(A(i,:)) \cap \text{ind}(u)} A(i, k) \otimes u(k)$$

The summation is over the intersection of the existing elements in the  $i^{\text{th}}$  row of  $A$  with  $u$  ... which avoids exposing how empty elements (i.e. “zeros”) are represented. This becomes important when we change the semiring between operations

$$w \in S^M \quad u \in S^N \quad A \in S^{M \times N}$$

Definitions:

- $S$  is the domain of the objects  $w$ ,  $u$ , and  $A$
- $\odot$  is an optional accumulation operator (a binary operator)
- $\otimes$  and  $\oplus$  are multiplication and addition (or generalizations thereof)
- $\sum$  uses the  $\oplus$  operator
- $\text{ind}(u)$  returns the indices of the stored values of  $u$

# Matrix vector multiplication: mxv()      $w \odot= A \oplus . \otimes u$

- The operators used are an accumulator ( $\odot$ ) and the algebraic semiring operators ( $\oplus$  and  $\otimes$ ). We will say a great deal more about semirings later ... for now we'll use the default case for Boolean data, the LOR\_LAND semiring (i.e., logical OR for  $\oplus$ , Logical AND for  $\otimes$ ).

```
import pygraphblas as grb

# A's type taken from values
A = grb.Matrix.from_lists(rowInd, colInd, values)
N = A.ncols

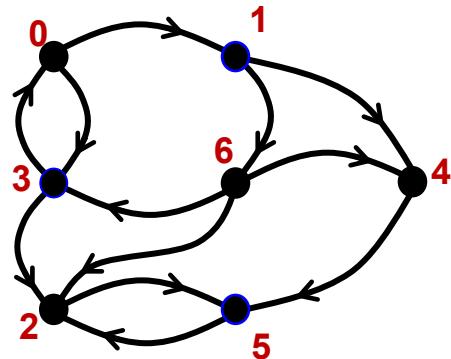
# Create a vector of length N and type BOOL
u = grb.Vector.sparse(grb.BOOL, N)
u[ind] = True      # set the value

w = A.mxv(u)
w = A @ u
A.mxv(u, out=w)
```

These three compute the same result in w.  
The third reuses an existing w.

# Exercise 4: Matrix Vector Multiplication

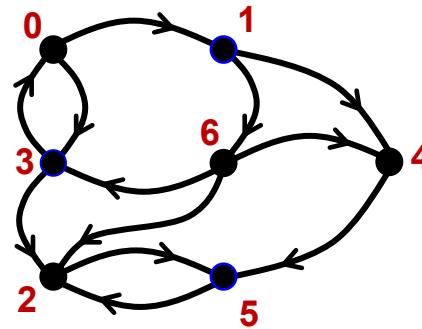
- Use the adjacency matrix from exercise 3 and a vector with a single value to select one of the nodes in the graph.
- Find the product  $mxv$ , print the result, and interpret its meaning.
- You'll need the following from pygraphblas:



```
import pygraphblas as grb
from pygraphblas.gviz import draw_graph as draw
A = grb.Matrix.from_lists(rowList, columnList, values)
u = grb.Vector.sparse(grb.BOOL, N)
w = A.mxv(u)
A.mxv(u, out=w)    # reuse a w that already exists
w = A @ u
print(A), print(w)
draw(A)
```

# Solution to exercise 4

```
NODES = 7  
u = grb.Vector.sparse(grb.BOOL, NODES)  
u[2] = True  
w = A @ u  
print(w)
```

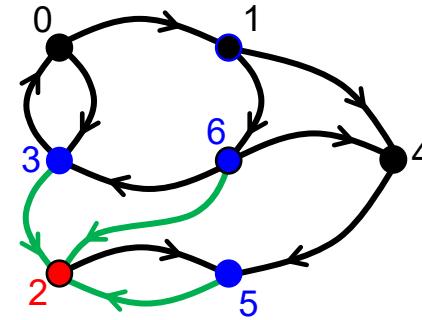


w		A		u
		0 1 2 3 4 5 6		
0		0  t t	0	
1		1  t t	1	
2		2  t t	2  t	
3  t	=	3  t t	3	
4		4  t t	4	
5  t		5  t t	5	
6  t		6  t t t	6	
		0 1 2 3 4 5 6		

@

# Solution to exercise 4

```
NODES = 7  
u = grb.Vector.sparse(grb.BOOL, NODES)  
u[2] = True  
w = A @ u  
print(w)
```



w	A	u
0	0  t t   0	0
1	1  t t   1	1
2	2  t t   2	2  t
3  t	3  t t   3	@ 3
4	4  t t   4	4
5  t	5  t t   5	5
6  t	6  t t t   6	6
	0 1 2 3 4 5 6	

The stored elements of the adjacency matrix,  $A(i,j)$  indicate an edge **from** vertex  $i$  **to** vertex  $j$

So, the matrix vector product scans over a row (from) to find when an edge lands at the destination.

# Finding neighbors

- A more common operation is to input a vector selecting a source and find all the neighbors one hop away from that vertex.
- Using `mxv()`, how would you do this?

# Finding neighbors

- A more common operation is to input a vector selecting a source and find all the neighbors one hop away from that vertex.
- Using `mxv()`, how would you do this?
  - The adjacency matrix elements indicate edges
    - **From** a vertex (row index)
    - **To** another vertex (columns index)
  - Then the **transpose** of the adjacency matrix indicates edges
    - **To** a vertex (row index)
    - **From** other vertices (column index)
- Therefore, we can find the neighbors of a vertex (marked by the non-empty elements of `v`)
$$\text{neighbors} = A^T \oplus . \otimes v$$

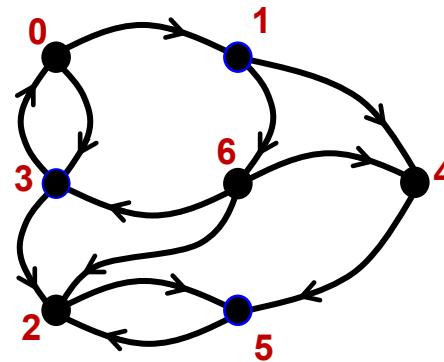
```
neighbors = A.T @ v
```

```
neighbors = A.mxv(v, desc=grb.descriptor.T0)
```

Two ways to do a transpose with pygraphblas

## Exercise 5: Find one hop neighbors

- This is a really quick exercise.
- Go back to your code for exercise 4 and verify that you can use the transpose to find the one hop neighbors of a source vertex.



```
import pygraphblas as grb
from pygraphblas.gviz import draw_graph as draw
A = grb.Matrix.from_lists(rowList, columnList, values)
u = grb.Vector.sparse(grb.BOOL, N)
Atrans = A.T
w = A.mxv(u)
A.mxv(u, out=w)
w = A @ u
print(A)
draw(A)
```

# Solution to exercise 5: Find one-hop neighbors

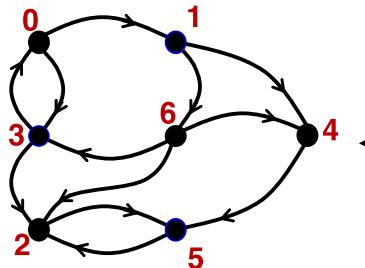
```
NODES = 7
```

```
u = grb.Vector.sparse(grb.BOOL, NODES)
```

```
u[6] = True
```

```
w = A.T @ u
```

```
print(w)
```



A

	0	1	2	3	4	5	6	
0	t							0
1		t						1
2						t		2
3				t		t		3
4					t			4
5						t		5
6							t	6

w

$$\begin{array}{l}
 \begin{array}{l}
 \begin{array}{l}
 0| \\
 1| \\
 2| t \\
 3| t \\
 4| t \\
 5| \\
 6|
 \end{array} = \begin{array}{l}
 0| \\
 1| t \\
 2| \\
 3| t \\
 4| t \\
 5| \\
 6|
 \end{array} @ \begin{array}{l}
 0| \\
 1| \\
 2| \\
 3| \\
 4| \\
 5| \\
 6| t
 \end{array}
 \end{array}
 \end{array}$$

$$\begin{array}{ccccccccc}
 & & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\
 & & | & & & t & | & 0 & | \\
 & & 1 & | & t & & | & 1 & | \\
 & & | & t & & t & | & 2 & | \\
 & & 2 & | & & t & | & 3 & | \\
 & & | & t & & & | & 4 & | \\
 & & 3 & | & t & & | & 5 & | \\
 & & | & t & & t & | & 6 & | \\
 & & 4 & | & & & | & & \\
 & & | & t & & & | & & \\
 & & 5 & | & t & & | & & \\
 & & | & & & t & | & & \\
 & & 6 & | & & & | & & \\
 & & | & & & & | & & \\
 & & 0 & 1 & 2 & 3 & 4 & 5 & 6
 \end{array}$$

# The GraphBLAS Operations

Operation Name	Mathematical Notation		
mxm	$C \langle M, r \rangle =$	$C \odot A \oplus . \otimes B$	
mxv	$w \langle m, r \rangle =$	$w \odot A \oplus . \otimes u$	
vxm	$w^T \langle m^T, r \rangle =$	$w^T \odot u^T \oplus . \otimes A$	
eWiseMult	$C \langle M, r \rangle =$	$C \odot A \otimes B$	
	$w \langle m, r \rangle =$	$w \odot u \otimes v$	
eWiseAdd	$C \langle M, r \rangle =$	$C \odot A \oplus B$	
	$w \langle m, r \rangle =$	$w \odot u \oplus v$	
extract	$C \langle M, r \rangle =$	$C \odot A(i, j)$	
	$w \langle m, r \rangle =$	$w \odot u(i)$	
assign	$C \langle M, r \rangle(i, j) =$	$C(i, j) \odot A$	
	$w \langle m, r \rangle(i) =$	$w(i) \odot u$	
reduce (row)	$w \langle m, r \rangle =$	$w \odot [\oplus_j A(:, j)]$	
reduce (scalar)	$s =$	$s \odot [\oplus_{i,j} A(i, j)]$	
	$s =$	$s \odot [\oplus_i u(i)]$	
apply	$C \langle M, r \rangle =$	$C \odot f_u(A)$	
	$w \langle m, r \rangle =$	$w \odot f_u(u)$	
apply(indexop)	$C \langle M, r \rangle =$	$C \odot f_i(A, \text{ind}(A), s)$	
	$w \langle m, r \rangle =$	$w \odot f_i(u, \text{ind}(u), s)$	
select	$C \langle M, r \rangle =$	$C \odot A \langle f_i(A, \text{ind}(A), s) \rangle$	
	$w \langle m, r \rangle =$	$w \odot u \langle f_i(u, \text{ind}(u), s) \rangle$	
transpose	$C \langle M, r \rangle =$	$C \odot A^T$	
kronecker	$C \langle M, r \rangle =$	$C \odot A \otimes B$	

$\langle M, m \rangle$ : write masks  
(Matrix or vector).

$\langle r \rangle$ : selects “replace or combine” for elements not selected by the mask.

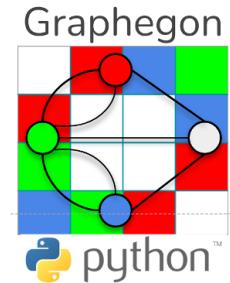
We've only covered mxv, so far, but the same conventions are used across all operations, so we'll have no problem later when we use the others

# Outline

- Graphs and Linear Algebra
- The GraphBLAS API and Adjacency Matrices
- GraphBLAS Operations
- ➡ • Pygraphblas and modifying the behavior of operations.
- Graph Algorithms expressed with GraphBLAS
  - Breadth-First Traversal
  - Connected Components
  - Triangle Counting
  - PageRank

# pygraphblas:

- We've been using pygraphblas for a while now. Let's pause a moment and take a closer look at some of the details behind this system.
  - pygraphblas is a python wrapper around the SuiteSparse GraphBLAS library.
    - Brought to us by Michel Pelletier and his company Graphegon.
  - pygraphblas uses CFFI to automate much of the process of generating an interface to SuiteSparse GraphBLAS library ... thus helping pygraphblas to closely track new releases of SuiteSparse.
  - Open-Source release ... also provided as docker containers:
    - Minimal: an Ipython interpreter-only
    - Notebook: Includes a Jupyter notebook server
  - Documentation for pygraphblas (with lots of examples) can be found here:
    - <https://graphegon.github.io/pygraphblas/pygraphblas/index.html>



# pygraphblas: Matrix and Vector part 1

- Matrix constructors ... commonly used cases:

- `sparse(typ, nrows=None, ncols=None)`
- `dense(typ, nrows, ncols, fill=None, sparsity=None)`
- `from_lists(I, J, V, nrows=None, ncols=None, typ=None)`
- `dup(A)`
- `random(typ, nrows, ncols, nvals, make_pattern=False, make_symmetric=False, make_skew_symmetric=False, make_hermitian=True, no_diagonal=False, seed=None)`

Common types (typ) are: BOOL, FP64, FP32, INT64, INT32, INT16, INT8, UINT64, UINT32, UINT16, UINT8

- Vector constructors ... commonly used cases:

- `sparse(typ, size=None)`
- `from_lists(I, V, size=None, typ=None)`
- `from_1_to_n(n)`
- `dense(typ, size, fill=None)`
- `dup(v)`

For arguments with default value **None**, if the argument is not provided, pygraphblas will infer what it needs from the other arguments

```
import pygraphblas as grb
N = 8
Nval = 16
graph = grb.Matrix.random(grb.INT8, N, N, Nval, make_symmetric=True)
g2 = graph.dup()
vec = grb.Vector.from_1_to_n(N)
res = g2@vec
```

# pygraphblas: Matrices and Vectors part 2

- The Matrix type includes instance attributes and properties ... a few of which are:
  - **nrows**
  - **ncols**
  - **nvals**
  - **T** ← take the transpose of the matrix
  - **M** ← create a bool matrix, true where a defined element exists
  - **get(i,j,default=None)**
- The Vector type includes instance attributes and properties ... a few of which are:
  - **size**
  - **nvals**
  - **Indexes**
  - **get(i, ,default=None)**

```
import pygraphblas as grb
g2 = grb.Matrix.from_lists([1,1,2],[1,2,0],[4,-5,0])
gm = g2.M
g4 = g2.Matrix.mxm(g2.T, mask=gm) ←
NUM_NODES = g2.nrows
vec = grb.Vector.from_1_to_n(NUM_NODES)
for i in vec.indexes: ←
    do_something(i)
jj = vec.size/2
print(vec.get(jj,default=10)) ←
```

Uses a write-mask to select elements of the product to store

Using an iterator over the vector

Extract element jj. If there is no element jj, then return the default value 10 (the default default is None)

# Changing the behavior of a GraphBLAS operation

- Most GraphBLAS operations take an argument that is an opaque object called a “**descriptor**”.
- The descriptor controls the behavior of the method and how objects are handled inside the method.
- The descriptor controls:
  - Do you *transpose input matrices*?
    - T0     $\leftarrow$  transpose first argument
    - T1     $\leftarrow$  transpose second argument
  - Does the computation *replace existing values in the output object* or combine with them when a mask is used?
  - Take the *structure* and/or *complement* of the *mask* object (swap empty/false  $\leftrightarrow$  filled/true values in a sparse object).

They can be combined:  
T0T1  $\leftarrow$  transpose both args

....To be discussed later

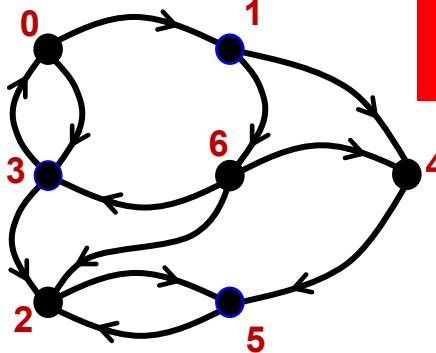
Descriptor example: `Hop = A.mxm(B, desc = grb.descriptor.T0)`

A pygraphblas descriptor is a distinct module so you must specify it as such when used.  
In this example, T0 transposes A. T1 would transpose B

# Exercise 6: find one hop neighbors (again)

Due to a lack of time, we'll skip this and go straight to my solution

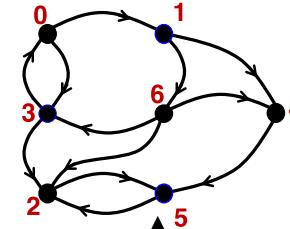
- This is a really quick exercise.
- Go back to your code for exercise 5 and verify that you can specify a descriptor to use the transpose to find the one hop neighbors of a source vertex.



```
import pygraphblas as grb
from pygraphblas.gviz import draw_graph as draw
A = grb.Matrix.from_lists(rowList, columnList, values)
u = grb.Vector.sparse(grb.BOOL, N)
Atrans = A.T
w = A.mxv(u, desc = ??)
A.mxv(u, out=w, desc = ??)
print(A)
draw(A)
```

# Solution to exercise 6: Find one-hop neighbors

```
NODES = 7
u = grb.Vector.sparse(grb.BOOL, NODES)
u[6] = True
w = A.mxv(u, desc = grb.descriptor.T0)
print(w)
```



A	0   0 1 2 3 4 5 6	0   0
	1   t	1   1
	2   t	2   2
	3   t	3   3
	4   t	4   4
	5	5   5
	6   t	6   t

$$\begin{array}{c}
 \mathbf{w} \\
 \begin{array}{ccccccc}
 & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\
 0 | & 0 | & & t & & & | & 0 \\
 1 | & 1 | & t & & & & | & 1 \\
 2 | & t & & t & t & t | & 2 \\
 3 | & t & & & t & | & 3 \\
 4 | & t & & t & & t | & 4 \\
 5 | & & & t & t & & | & 5 \\
 6 | & t & & & & & | & 6 \\
 & 0 & 1 & 2 & 3 & 4 & 5 & 6
 \end{array}
 \end{array}
 \quad
 \begin{array}{c}
 \mathbf{u} \\
 \begin{array}{c}
 @ \\
 0 | \\
 1 | \\
 2 | \\
 3 | \\
 4 | \\
 5 | \\
 6 | t
 \end{array}
 \end{array}$$

$\mathbf{A}^T$

=

## Matrix vector multiplication: mxv()

$$w \odot = A \oplus . \otimes u$$

- The operators in GraphBLAS operations are:
  - Accumulator  $\odot$
  - Addition  $\oplus$
  - Multiplication  $\otimes$
- The operators are implied by type.

It's time to say more about these operators

Pygraphblas type	$\odot$	$\oplus$	$\otimes$
types.BOOL	LOR	LOR	LAND
types.INT32	32 bit int add	32 bit int add	32 bit int multiply
types.FP32	32 bit float add	32 bit float add	32 bit float multiply

```
import pygraphblas as grb

# Matrix A and vectors w and u defined elsewhere.
# Assume they are of type INT32
A.mxv(u, accum=grb.INT32.PLUS, out=w)
```

Implicit  $\oplus$  and  $\otimes$  based on type of A, u, and/or w.  $\odot$  defined explicitly

$\oplus . \otimes$  are considered together as part of an algebraic semiring (our next topic)

# Algebraic Semirings

- Semiring: An Algebraic structure that generalizes real arithmetic by replacing  $(\oplus, \otimes)$  with binary operations (Op1, Op2)
  - Op1 and Op2 have identity elements sometimes called 0 and 1
  - Op1 and Op2 are associative.
  - Op1 is commutative, Op2 distributes over Op1 from both left and right
  - The Op1 identity is an Op2 annihilator.

# Algebraic Semirings

- Semiring: An Algebraic structure that generalizes real arithmetic by replacing  $(\oplus, \otimes)$  with binary operations (Op1, Op2)
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$(R, +, *, 0, 1)$ Real Field	Standard operations in linear algebra
---------------------------------	---------------------------------------

Notation:  $(R, +, *, 0, 1)$

Scalar type	Op1	Op2	Identity Op1	Identity Op2
-------------	-----	-----	--------------	--------------

# Algebraic Semirings

- Semiring: An Algebraic structure that generalizes real arithmetic by replacing  $(\oplus, \otimes)$  with binary operations (Op1, Op2)
  - Op1 and Op2 have identity elements sometimes called 0 and 1
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  - The Op1 identity is an Op2 annihilator.

$(R, +, *, 0, 1)$ Real Field	Standard operations in linear algebra
$(R \cup \{\infty\}, \min, +, \infty, 0)$ Tropical semiring	Shortest path algorithms
$(\{0,1\},  , \&, 0, 1)$ Boolean Semiring	Graph traversal algorithms
$(R \cup \{\infty\}, \min, *, \infty, 1)$	Selecting a subgraph or contracting nodes to form a quotient graph.

# Working with semirings

- In Graph Algorithms, changing semirings multiple times inside a single algorithm is quite common. Hence, the semiring (and implied accumulator  $\oplus$  by default) can be directly manipulated.
- We can do this using python's "with" statement

```
with grb.BOOL.LOR_LAND:  
    w += A@v  
  
with grb.BOOL.LOR_LAND:  
    w = A.mxv(u, accum=grb.BOOL.LOR)
```

Matrix vector product of A and v accumulating the result with the existing elements of w using:

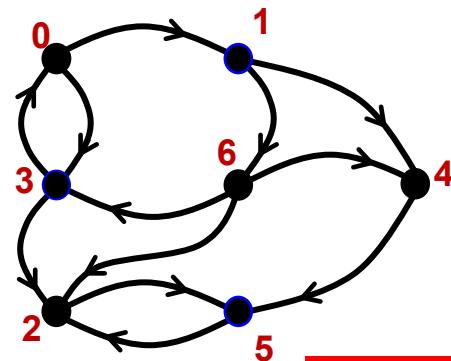
- $\oplus = \odot$  = Logical OR
- $\otimes$  = Logical AND

- Common semirings include (though pygraphblas has MANY more)

$(R, +, *, 0, 1)$ Real Field	Standard operations in linear algebra	<b>FP64.PLUS_TIMES</b>
$(R \cup \{\infty\}, \min, +, \infty, 0)$ Tropical semiring	Shortest path algorithms	<b>FP64.MIN_PLUS</b>
$(\{0,1\},  , \&, 0, 1)$ Boolean Semiring	Graph traversal algorithms	<b>BOOL.LOR_LAND</b>
$(R \cup \{\infty\}, \min, *, \infty, 1)$	Selecting a subgraph or contracting nodes to form a quotient graph.	<b>FP64.MIN_TIMES</b>

## Exercise 7: find one hop neighbors (again)

- This is a really quick exercise.
- Go back to your code for exercise 6 and verify that you can specify the semiring to find the one hop neighbors of a source vertex.



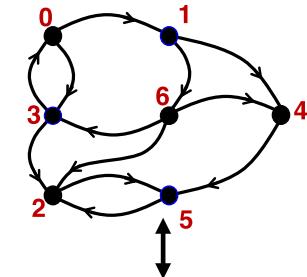
```
import pygraphblas as grb
from pygraphblas.gviz import draw_graph as draw
A = grb.Matrix.from_lists(rowList, columnList, values)
u = grb.Vector.sparse(grb.BOOL, N)
Atrans = A.T
with grb.<type>.<semiring>:
    w = A.mxv(u, desc = ??)
    A.mxv(u, out=w, desc = ??)
print(A)
draw(A)
```

Due to a lack of time, we'll skip this exercise and go straight to my solution

# Solution to exercise 7: Find one-hop neighbors

NODES = 7

```
u = grb.Vector.sparse(grb.BOOL, NODES)
u[6] = True
with grb.BOOL.LOR_LAND:
    w = A.mxv(u, desc = grb.descriptor.T0)
print(w)
```



	0	1	2	3	4	5	6	
0		t		t				0
1			t					1
2	t			t	t	t	2	2
3	t				t	t	3	3
4	t					t	4	4
5				t	t		5	5
6				t		t	6	6
	0	1	2	3	4	5	6	

$$\begin{array}{c}
 \mathbf{w} \\
 \begin{array}{ccccccccc}
 & & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\
 \begin{array}{|l} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{array} & = & \begin{array}{|l} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{array} & & \mathbf{A}^T & & \mathbf{u} \\
 & & & & & & & @ & \\
 & & & & & & & & \begin{array}{|l} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{array}
 \end{array}
 \end{array}$$

# Pygraphblas Documentation

- We have only covered a small portion of the GraphBLAS.
- Pygraphblas has much more to offer.
- Documentation is available at:

<https://graphegon.github.io/pygraphblas/pygraphblas/index.html>

- The pygraphblas documentation describes:
  - Numerous additional semirings organized by type.
  - Numerous binary and unary functions so you can choose your own accumulators or build custom semirings.
  - The ability to create custom binary and unary operators using a JIT decorator.
  - Options to control multithreading and other internal features of the SuiteSparse GraphBLAS library
  - The pygraphblas.gviz sub-module which includes methods for looking at small graphs but also a binding to the Cytoscape module for working with large complex graphs

# pygraphblas API Reference

~| GraphBLAS.org | [Github](#) | SuiteSparse::GraphBLAS User Guide |~

discuss

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GxB\_SPEC

### ► Functions

binary\_op  
unary\_op  
select\_op  
options\_set  
options\_get

### ► Types

► Matrix  
► Vector  
► Scalar

# pygraphblas

## Installation

pygraphblas requires the SuiteSparse::GraphBLAS library. The easiest way currently to install pygraphblas on Linux is to use pip:

```
pip install pygraphblas
```

This is currently only supported on Linux but Windows and MacOS binary packages are currently a work in progress.

To install from source, first install SuiteSparse, then run:

```
python setup.py install
```

There are two ways to download precompiled binaries of pygraphblas with SuiteSparse included. One way is to use `pip install pygraphblas` on an Intel Linux machine. This will download a package compatible with most modern linux distributions. This also works in a Docker container on Mac.

There are also pre-build docker images based on Ubuntu 20.04 that have a pre-compiled SuiteSparse and pygraphblas installed. These come in two flavors `minimal` which is the Ipython interpreter-only, and `notebook` which comes with a complete Jupyter Notebook server. These containers also work on Mac.

An installation script for Ubuntu 18.04 is provided in the `install-ubuntu.sh` file.

NOTE: DO NOT USE THESE PRE-COMPILED BINARIES FOR BENCHMARKING SUITESPARSE. These binaries are not guaranteed to be ideally compiled for your environment.

pygraphblas API documentation +

graphegon.github.io/pygraphblas/pygraphblas/index.html#header-classes

Summary

Introduction to Graphs and Matrices

Using the API

► Global variables

- GxB\_INDEX\_MAX
- GxB\_IMPLEMENTATION
- GxB\_SPEC

► Functions

- binary\_op
- unary\_op
- select\_op
- options\_set
- options\_get

► Types

- Matrix
- Vector
- Scalar
- Accum
- BOOL
- FP64
- FP32
- FC64
- FC32
- INT64
- INT32
- INT16
- INT8
- UINT64
- UINT32
- UINT16
- UINT8

## ► Types

```
class Matrix (matrix, typ=None)
```

GraphBLAS Sparse Matrix

This is a high-level wrapper around the GrB\_Matrix C type using the [cffi](#) library.

A Matrix supports many possible operations according to the GraphBLAS API. Many of those operations have overloaded operators.

Operator	Description	Default
A @ B	Matrix Matrix Multiplication	type default PLUS_TIMES semiring
v @ A	Vector Matrix Multiplication	type default PLUS_TIMES semiring
A @ v	Matrix Vector Multiplication	type default PLUS_TIMES semiring
A @= B	In-place Matrix Matrix Multiplication	type default PLUS_TIMES semiring
v @= A	In-place Vector Matrix Multiplication	type default PLUS_TIMES semiring
A @= v	In-place Matrix Vector Multiplication	type default PLUS_TIMES semiring
A   B	Matrix Union	type default SECOND combiner
A  = B	In-place Matrix Union	type default SECOND combiner
A & B	Matrix Intersection	type default SECOND combiner
A &= B	In-place Matrix Intersection	type default SECOND combiner
A + B	Matrix Element-Wise Union	type default PLUS combiner
A += B	In-place Matrix Element-Wise Union	type default PLUS combiner
A - B	Matrix Element-Wise Union	type default MINUS combiner
A -= B	In-place Matrix Element-Wise Union	type default MINUS combiner
A * B	Matrix Element-Wise Intersection	type default TIMES combiner
A *= B	In-place Matrix Element-Wise Intersection	type default TIMES combiner
A / B	Matrix Element-Wise Intersection	type default DIV combiner
A /= B	In-place Matrix Element-Wise Intersection	type default DIV combiner
A == B	Compare Element-Wise Union	type default EQ operator
A != B	Compare Element-Wise Union	type default NE operator
A < B	Compare Element-Wise Union	type default LT operator
A > B	Compare Element-Wise Union	type default GT operator
A <= B	Compare Element-Wise Union	type default LE operator
A >= B	Compare Element-Wise Union	type default GE operator

Note that all the above operator syntax is merely sugar over various combinations of calling [Matrix.mxm\(\)](#), [Matrix.mxv\(\)](#), [Vector.vxm\(\)](#), [Matrix.eadd\(\)](#), and [Matrix.emult\(\)](#).

discuss

# Outline

- Graphs and Linear Algebra
- The GraphBLAS API and Adjacency Matrices
- GraphBLAS Operations
- Pygraphblas and modifying the behavior of operations.
- Graph Algorithms expressed with GraphBLAS
  - ➡ – Breadth-First Traversal
    - Connected Components
    - Triangle Counting
    - PageRank

# Breadth First Traversal (aka BFS)

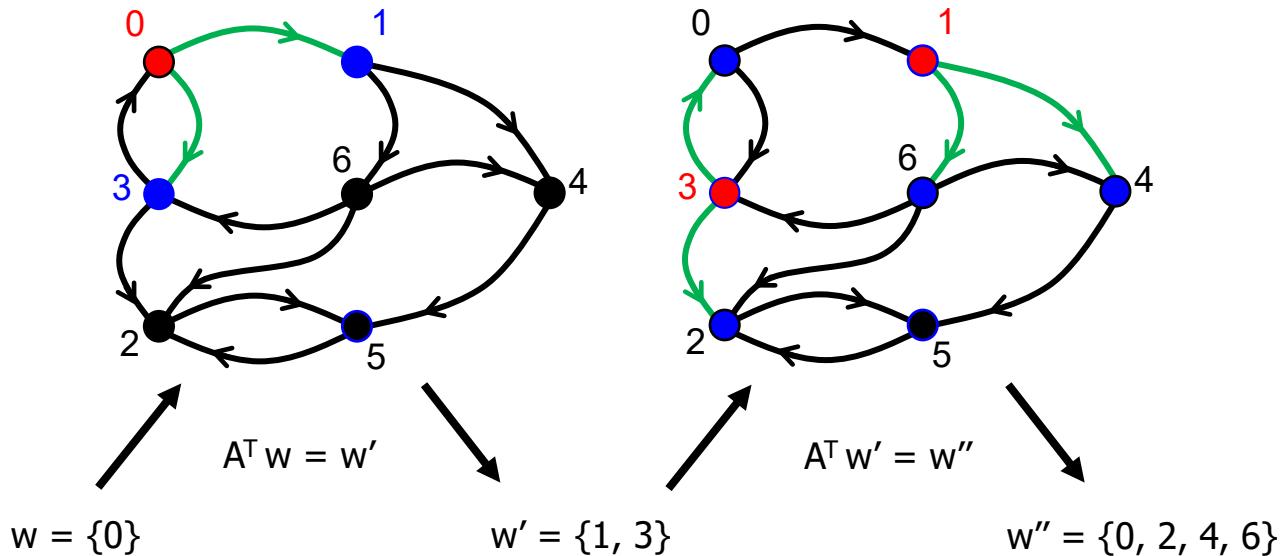
- The Breadth First Traversal:
  - Start from one or more initial vertices
  - Visit all accessible one hop neighbors
  - Visit all accessible unique two hop neighbors
  - Continue until there are no more unique vertices to visit
  - Note: Need to keep track of vertices visited so you don't visit the same vertex more than once
- Breadth first traversal is a common pattern used in a variety of graph algorithms
  - Build a spanning tree that contains all vertices and minimal number of edges
  - Search for accessible vertices with certain properties.
  - Find shortest paths between vertices.
  - Other more advanced algorithms such as maxflow and betweenness centrality

# Our Breadth First Traversal plan

- We will build up this algorithm using the GraphBLAS through a series of exercises:
  - Wavefronts and how to move from one wavefront to the next.
  - Iteration across wavefronts
  - Track which vertices have been visited
  - Avoid revisiting vertices
- \*\*\* At this point you have a basic BFS algorithm. \*\*\*
- Use this to construct a Connected Components algorithm

# Wavefronts

- A subset of vertices accessed at one stage in a breadth first search pattern ...  
for example ....
  - “You tell two friends, and they tell two friends...”



**Red**=current wavefront and visited, **Blue**=next wavefront, **Black**=unvisited

$A$  = Adjacency Matrix       $w$  = wavefront vectors

## Exercise 8: Traverse the graph

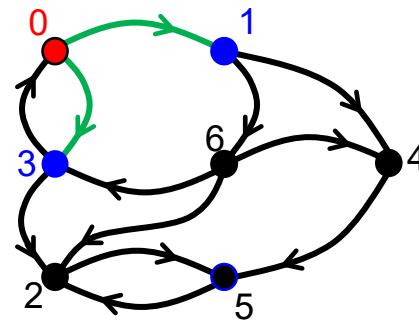
- Modify your code from Exercises 5/6/7 to iterate from one waveform to the next.
- Output each waveform
- How long before you get a repeating pattern?
- You may need the following statements, objects and methods from pygraphblas:

```
import pygraphblas as grb
from pygraphblas.gviz import draw_graph as draw
A = grb.Matrix.from_lists(rowList, columnList, values)
u = grb.Vector.sparse(grb.<type>, N)
Atrans = A.T
with grb.<type>.<semiring>:
    w = A.mxv(u, desc = ??)
    A.mxv(u, out=w, desc = ??)
print(A)
draw(A)
```

# Solution to exercise 8

```
NUM_NODES = 7
w = grb.Vector.sparse(grb.BOOL, NUM_NODES)
w[0] = True # 1st wavefront has one node set.
print(w)

with grb.BOOL.LOR_LAND:
    for i in range(NUM_NODES):
        graph.mxv(w, out=w, desc=grb.descriptor.T0)
        print(w)
```

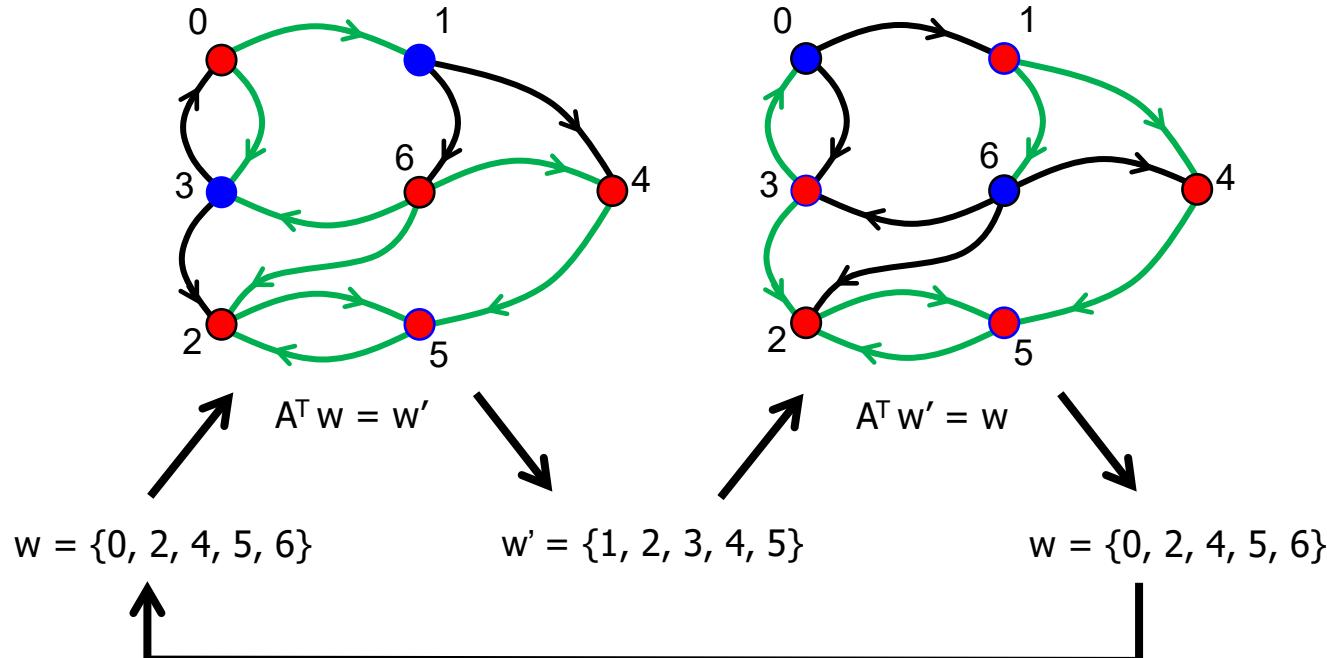


Init	i=0	i=1	i=2	i=3	i=4	i=5	i=6
.	0	0  t	0	0  t	0	0  t	0
0  t	1  t	1	1  t	1	1  t	1	1  t
1	2	2  t	2  t	2  t	2  t	2  t	2  t
2	3  t	3	3  t	3	3  t	3	3  t
3	4	4  t	4  t	4  t	4  t	4  t	4  t
4	5	5	5  t	5  t	5  t	5  t	5  t
5	6	6  t	6	6  t	6	6  t	6
6							

The same vector can be used for both input and output.  
Starts repeating after only a few iterations. Why?

# Solution to exercise 8: wavefronts

- “We tell a bunch, and they tell bunch...(rinse and repeat)”



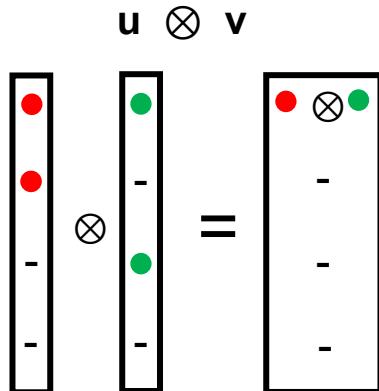
**Red**=current wavefront and visited, **Blue**=next wavefront, **Black**=unvisited

## Visited lists

- Breadth-first traversal requires that we only need to visit each node once.
- Next step is to keep track of visited nodes.
- You can do this by accumulating the wavefronts.
  - Use element-wise “addition” with logical-OR.

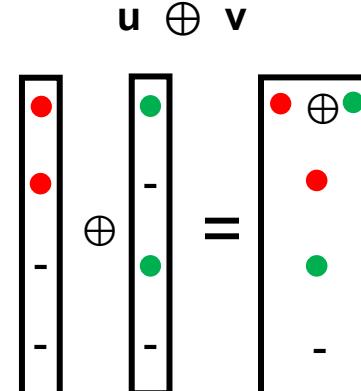
# Element-wise Operations: Mult and Add

- $\otimes$  assumes unstored values (-) are the binary operator's *annihilator*:



Examples:  $(x, 0)$ , (and, false),  $(+, \infty)$

- $\oplus$  assumes unstored values (-) are the binary operator's *identity*:



Examples:  $(+, 0)$ , (or, false),  $(\min, \infty)$

\*What if we define  $\oplus$  to be subtraction?

The rules for element-wise addition also apply to the accumulation operator,  $\odot$

# Element-wise Multiplication $w \otimes= (u \otimes v)$

- Compute the element-wise “multiplication” of two GraphBLAS vectors.
- Performs the implicit or explicit “multiply” operator (`mult_op`) on the **intersection** of the sparse entries in each input vector,  $u$  and  $v$ .
- `emult` defined as a member function of Vector class (also Matrix class)

```
import pygraphblas as grb
u = grb.Vector.sparse(grb.BOOL, NODES);
v = grb.Vector.sparse(grb.BOOL, NODES);

# using an implicit operator (LAND)
v *= u           ← In-place element-wise multiplication.
w = u * v
w = u.emult(v)  } These three compute the same result in w.
u.emult(v, out=w) } The third reuses an existing w.

# using an explicit operator (LAND)
w = u.emult(v, mult_op=grb.BOOL.LAND)

# using a context manager
with grb.BOOL.LAND:
    w = u.emult(v)
    u.emult(v, out=w)
```

The code illustrates four ways to perform element-wise multiplication on two Boolean vectors  $u$  and  $v$ . The first three methods are grouped by a brace and annotated with red text: "In-place element-wise multiplication.", "These three compute the same result in w.", and "The third reuses an existing w.". The fourth method is grouped by a brace and annotated with red text: "These three compute the same result in w, too.".

# Element-wise Addition

$$w \cancel{\oplus} = (u \oplus v)$$

- Compute the element-wise “**addition**” of two GraphBLAS vectors.
- Performs the implied or explicit “addition” operator (`add_op`) on the **union** of the sparse entries in each input vector,  $u$  and  $v$ .
- `eadd` defined as a member function of Vector class (also Matrix class)

```
import pygraphblas as grb
u = grb.Vector.sparse(grb.BOOL, NODES);
v = grb.Vector.sparse(grb.BOOL, NODES);

# using an implicit operator (LOR)
v += u ← In-place element-wise addition.
w = u + v
w = u.eadd(v) These three compute the same result in w.
u.eadd(v, out=w) The third reuses an existing w.

# using an explicit operator (LOR)
w = u.eadd(v, add_op=grb.BOOL.LOR)

# using a context manager
with grb.BOOL.LOR:
    w = u.eadd(v)
    u.eadd(v, out=w) These three compute the same result in w, too.
```

## Exercise 9: Keep track of ‘visited’ nodes

- Modify code from Exercise 8 to compute the visited set as you iterate.
- You may need the following statements, objects and methods from pygraphblas:

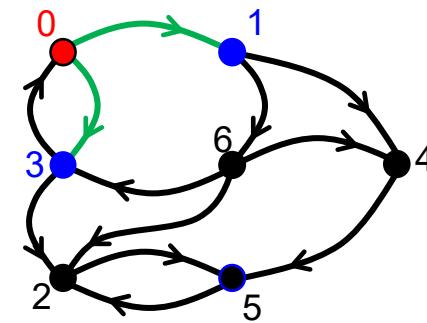
```
import pygraphblas as grb
from pygraphblas.gviz import draw_graph as draw
A = grb.Matrix.from_lists(rowList, columnList, values)
u = grb.Vector.sparse(grb.BOOL, N)
Atrans = A.T
with grb.<type>.<semiring>:
    w = A.mxv(u, desc = ??)
    v = w.eadd(v)
    v += w
    A.mxv(u, out=w, desc = ??)
print(A)
draw(A)
```

# Solution to exercise 9

```
NODES = 7;
v = grb.Vector.sparse(grb.BOOL, NODES);
w = grb.Vector.sparse(grb.BOOL, NODES);
w[0] = True # 1st wavefront has one node set.
```

```
with grb.BOOL.LOR_LAND:
    for i in range(NUM_NODES):
        v.eadd(w, out=v, add_op=grb.BOOL.LOR)           # v += w
        print(v)
    graph.mxv(w, out=w, desc=grb.descriptor.T0) # w = graph.T @ w
    print(w)
```

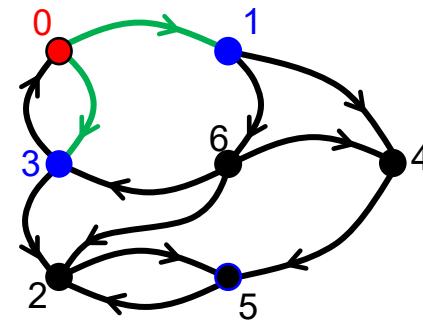
	i=0	i=1	i=2	i=3	i=4	i=5	i=6
v	0  t	0  t	0  t	0  t	0  t	0  t	0  t
	1	1  t	1  t	1  t	1  t	1  t	1  t
	2	2	2  t	2  t	2  t	2  t	2  t
	3	3  t	3  t	3  t	3  t	3  t	3  t
	4	4	4  t	4  t	4  t	4  t	4  t
	5	5	5  t	5  t	5  t	5  t	5  t
	6	6	6  t	6  t	6  t	6  t	6  t
w	0	0  t	0	0  t	0	0  t	0
	1  t	1	1  t	1	1  t	1	1  t
	2	2  t	2  t	2  t	2  t	2  t	2  t
	3  t	3	3  t	3	3  t	3	3  t
	4	4  t	4  t	4  t	4  t	4  t	4  t
	5	5	5  t	5  t	5  t	5  t	5  t
	6	6  t	6	6  t	6	6  t	6



# Solution to exercise 9

```
NODES = 7;  
v = grb.Vector.sparse(grb.BOOL, NODES);  
w = grb.Vector.sparse(grb.BOOL, NODES);  
w[0] = True # 1st wavefront has one node set.
```

```
with grb.BOOL.LOR_LAND:  
    for i in range(NUM_NODES):  
        v.eadd(w, out=v, add_op=grb.BOOL.LOR) # v += w  
        print(v)  
    graph.mxv(w, out=w, desc=grb.descriptor.T0) # w = graph.T @ w  
    print(w)
```



What should the exit condition be?

	i=0	i=1					i=6
v	0  t	0  t	2  t	2  t	2  t	2  t	t
w	1  t	1  t	3  t	3  t	3  t	3  t	0  t
	2  t	2  t	2  t	2  t	2  t	2  t	1  t
	4  t	4  t	4  t	4  t	4  t	4  t	2  t
	5  t	5  t	5  t	5  t	5  t	5  t	3  t
	6  t	6  t	6  t	6  t	6  t	6  t	4  t
							5  t
							6  t

## mxv() revisited

$w \leftarrow s(m), r \otimes = A \oplus . \otimes u$

- We now need to go back and introduce more notation that will support more efficient graph operations.
- Every GraphBLAS operation that produces a Vector or Matrix result supports an optional **write mask**.
- Three new descriptor flags can be used to affect mask behavior.

```
import pygraphblas as grb

grb.descriptor.R    # REPLACE flag,      'r'
grb.descriptor.S    # mask STRUCTURE,   's(.)'
grb.descriptor.C    # mask COMPLEMENT, '¬(.)'

A.mxv(u, out=w, mask=m, desc=grb.descriptor.[R][S][C])
```

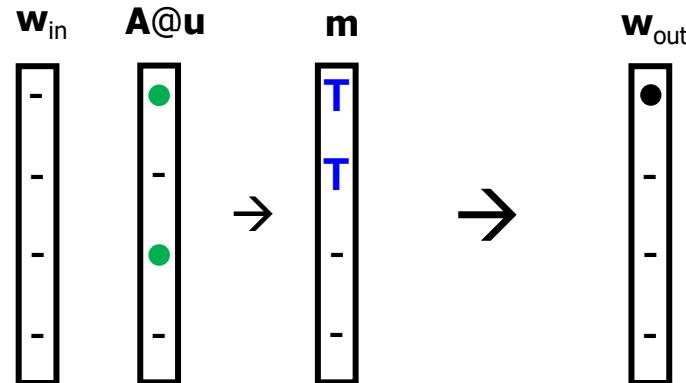
It's time to explain masking and REPLACE in GraphBLAS operations.

# Masking

A mask,  $\mathbf{m}$ , is interpreted as a logical ‘stencil’ that controls which elements of the result can be written to the output

- Any location in the mask that evaluates to ‘true’ can be written
- Same size as output object (mask Vectors or mask Matrices)
- Any location in the mask that evaluates to ‘true’ can be written in the output object

$$\mathbf{w}(\mathbf{m}) = \mathbf{A} \oplus \cdot \otimes \mathbf{u}$$

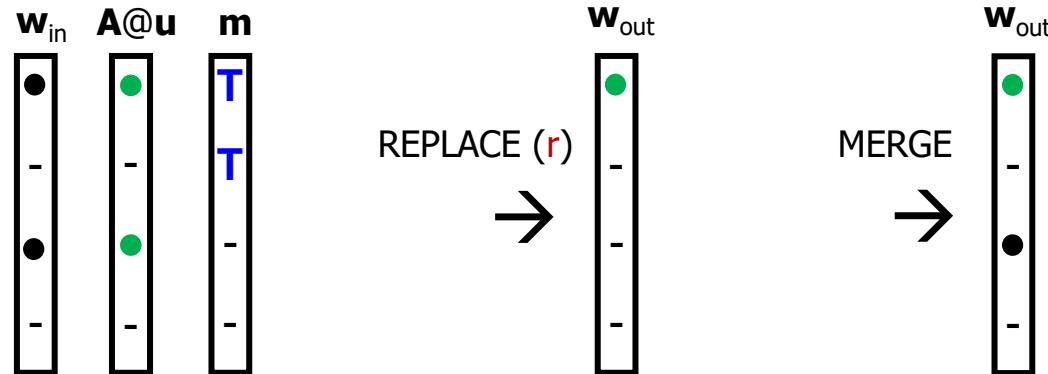


`A.mxv(u, out=w, mask=m)`

# REPLACE vs. “MERGE”

- When a mask is used and the output container is not empty when the operation is called...what do you do to the “masked out” elements?
  - REPLACE (r): all unwritten locations are cleared (zeroed out).
  - MERGE: all unwritten locations are left unchanged.

$$w \langle m, r \rangle = A \oplus . \otimes u$$



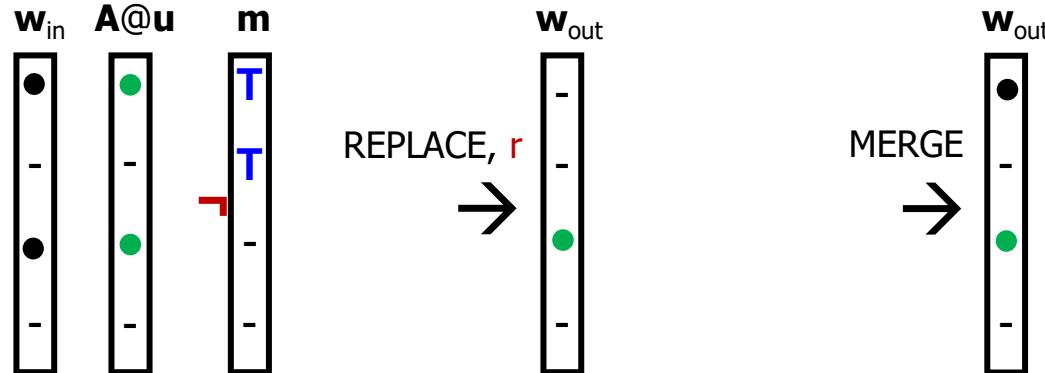
- Behavior defaults to MERGE; otherwise, use a `descriptor.R`:

```
A.mxv(u, out=w, mask=m, [desc=grb.descriptor.R])
```

# Complement (mask)

- Specified with a descriptor: `grb.descriptor.C`
- Inverts the logic of mask (write enabled on false)

$$\mathbf{w} \langle \neg \mathbf{m}, r \rangle = \mathbf{A} \oplus_{\cdot} \otimes \mathbf{u}$$

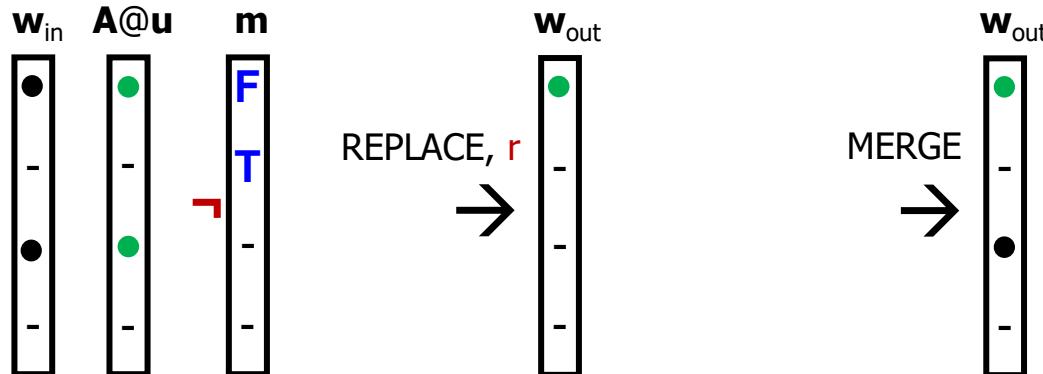


```
A.mxv(u, out=w, mask=m, desc=grb.descriptor.RC) # REPLACE  
A.mxv(u, out=w, mask=m, desc=grb.descriptor.C) # MERGE
```

# Structure only (mask)

- Specified with a descriptor: `grb.descriptor.S`
- Writes are enabled by the pattern of stored values (not the values themselves)

$$\mathbf{w}\langle \mathbf{s}(\mathbf{m}), \mathbf{r} \rangle = \mathbf{A} \oplus.\otimes \mathbf{u}$$

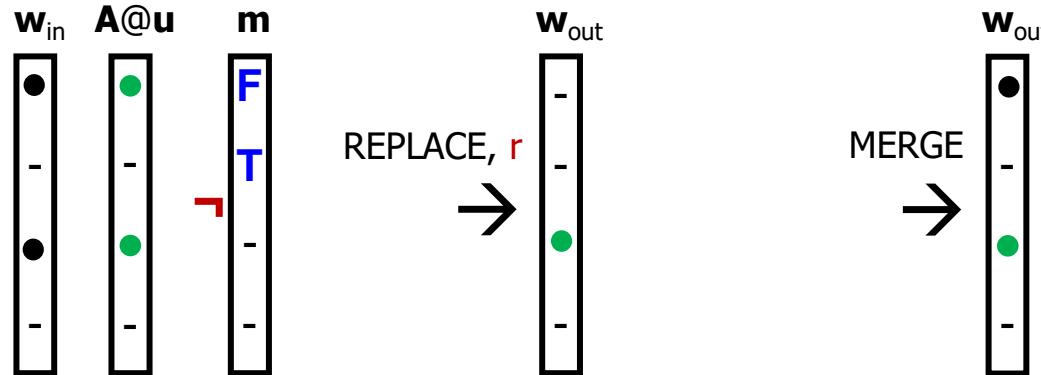


```
A.mxv(u, out=w, mask=m, desc=grb.descriptor.RS) # REPLACE  
A.mxv(u, out=w, mask=m, desc=grb.descriptor.S) # MERGE
```

# Complement the Structure of a mask

- Specified with a descriptor: `grb.descriptor.SC`
- Writes are enabled by the pattern of stored values (not the values themselves)...where values are NOT stored

$$\mathbf{w} \langle \neg S(\mathbf{m}), r \rangle = \mathbf{A} \oplus . \otimes \mathbf{u}$$



```
A.mxv(u, out=w, mask=m, desc=grb.descriptor.RSC) # REPLACE  
A.mxv(u, out=w, mask=m, desc=grb.descriptor.SC)   # MERGE
```

# Using Descriptors (summary)

- All of the possible flags for `grb.descriptor`:
  - R: Replace flag (only used when masks are present)
  - S: Structure of a mask
  - C: Complement the mask (structure or otherwise)
  - T0: Transpose the first operand (only when it is a Matrix)
  - T1: Transpose the second operand (only when it is a Matrix)
- All 31 combinations of flags are predefined in a set order:
  - `grb.descriptor. [R] [S] [C] [T0] [T1]`

# Exercise 10: Avoid revisiting

- Use the visited list as a mask prevent revisiting previous nodes
- Exit the loop when there is no more ‘work’ to be done
- You will need the following statements, objects and methods from pygraphblas:

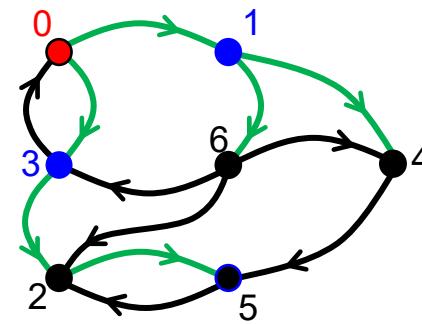
```
import pygraphblas as grb
from pygraphblas.gviz import draw_graph as draw
A = grb.Matrix.from_lists(rowList, columnList, values)
v = grb.Vector.sparse(grb.BOOL, N)
Atrans = A.T
with grb.<type>.<semiring>:
    w = A.mxv(u, desc=??)
    v = w.eadd(v)
    v += w
    v.nvals
    v.size
    A.mxv(u, out=w, mask=u, desc = ??)
    grb.descriptor.[R][S][C][T0][T1]
    print(A)
    draw(A)
```

# Solution to exercise 10

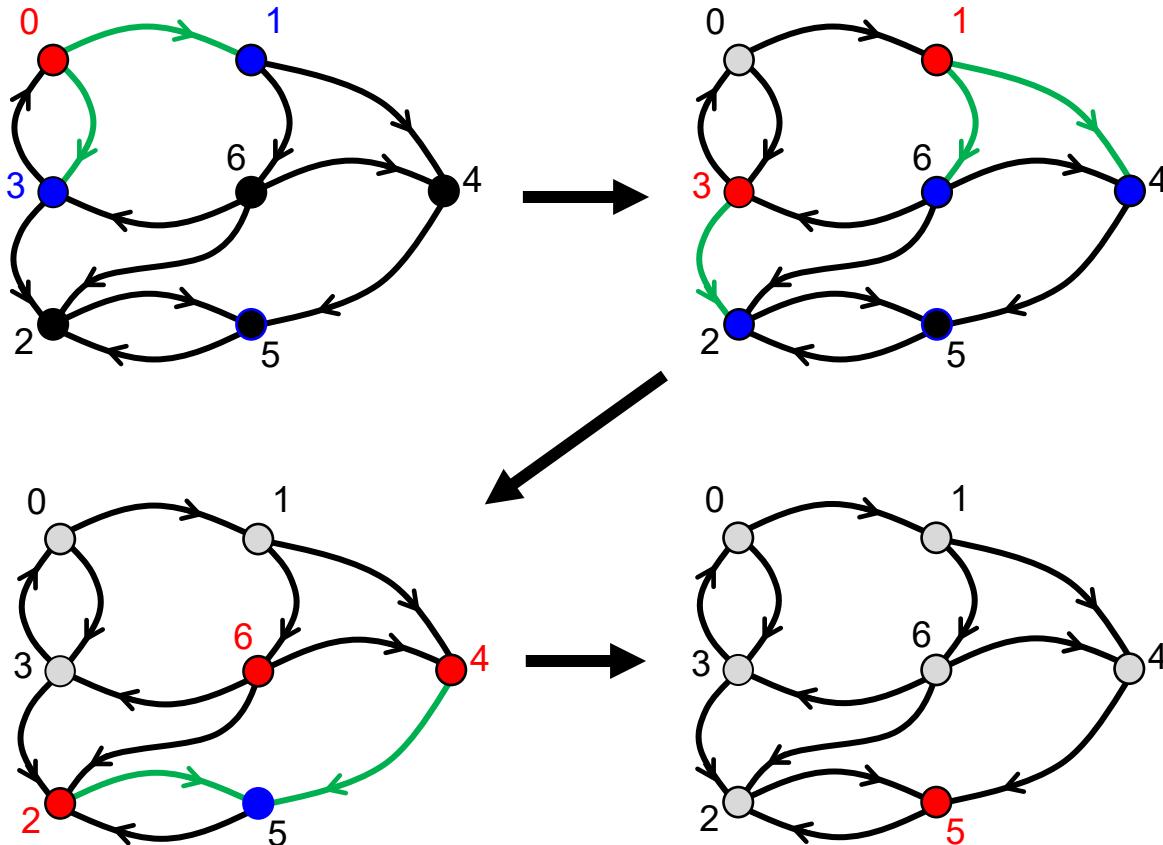
```
NODES = 7;
v = grb.Vector.sparse(grb.BOOL, NODES);
w = grb.Vector.sparse(grb.BOOL, NODES);
w[0] = True # 1st wavefront has one node set.
```

```
with grb.BOOL.LOR_LAND:
    while w.nvals > 0:
        v.eadd(w, out=v, add_op=grb.BOOL.LOR) # v += w
        print(v)
        # w<!v, r> = graph.T @ w
        graph.mxv(w, mask=v, out=w, desc=grb.descriptor.RCT0)
        print(w)
```

	i=0	i=1	i=2	i=3
v	0  t	0  t	0  t	0  t
	1	1	1  t	1  t
	2	2	2	2  t
	3	3	3  t	3  t
	4	4	4  t	4  t
	5	5	5	5  t
	6	6	6	6  t
w	0  t	0  t	0	0
	1	1  t	1	1
	2	2	2  t	2
	3	3  t	3	3
	4	4	4  t	4
	5	5	5	5
	6	6	6  t	6



# Breadth-First Traversal



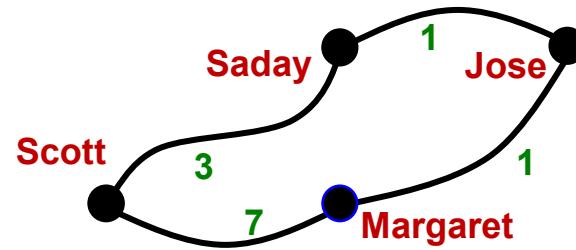
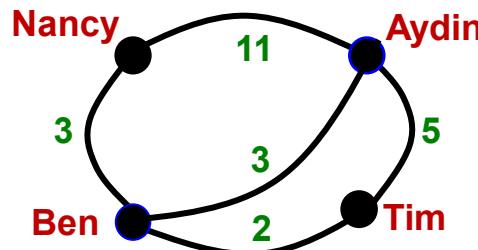
**Red**=current wavefront and visited, **Blue**=next wavefront, **Gray**=visited, **Black**=unvisited

# Outline

- Graphs and Linear Algebra
- The GraphBLAS API and Adjacency Matrices
- GraphBLAS Operations
- Pygraphblas and modifying the behavior of operations.
- Graph Algorithms expressed with GraphBLAS
  - Breadth-First Traversal
  - Connected Components
  - Triangle Counting
  - PageRank

# Connected Components

- Connected Components
  - Identify groups of vertices with paths to one another.
  - Identify how many of these groups (components) exist in the data.
  - Goal: **assign** all vertices within a component with the same unique ID.
  - For this exercise, the graph will consist of undirected edges
  - Note: applying this to directed graphs by converting to undirected is called “weakly connected components.”



# assign(), et al.

- There are several variants of assign

- Standard vector assignment: `w.assign(u, index=I)`
- Standard matrix assignment: `c.assign_matrix(A, rindex=I, cindex=J)`

$$\mathbf{w}(i) \odot= \mathbf{u} \qquad \qquad \mathbf{C}(i,j) \odot= \mathbf{A}$$

- Assign a vector to the elements of column  $c_j$  of a matrix: `c.assign_col(..)`
- Assign a vector to the elements of row  $r_i$  of a matrix: `c.assign_row(..)`

$$\mathbf{C}(i, c_j) \odot= \mathbf{u} \qquad \mathbf{C}(r_i, j) \odot= \mathbf{u}^T$$

- Assign a constant to a subset of a vector: `w.assign_scalar(..)`
- Assign a constant to a subset of a matrix: `c.assign_scalar(..)`

$$\mathbf{w}(i) \odot= c \qquad \qquad \mathbf{C}(i,j) \odot= c$$

**A** and **C** are GraphBLAS matrices.   **u** and **w** are GraphBLAS vectors    $i$  and  $j$  are index arrays

# Vector.assign\_scalar()

$$\mathbf{w}(i) \odot= c$$

```
def assign_scalar(self, value, index = None, mask = None, ...)
```

```
w = grb.Vector.sparse(grb.INT32, 5)
```

- Assign a constant to a list of indices:

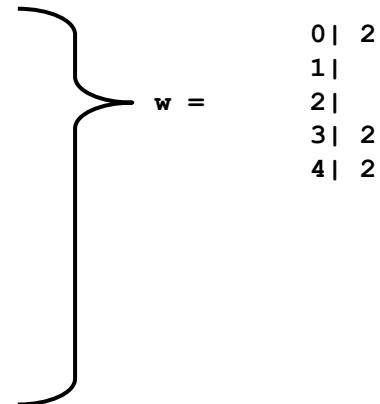
```
w.assign_scalar(2, [0,3,4])
```

- Assign a constant to a subset of the output with a mask:

```
m = grb.Vector.from_lists([0,3,4],[True]*3,size=5)
w.assign_scalar(2, mask=m)
```

- Alternative form using masking:

```
w[m] = 2
```



# Vector.assign\_scalar()

$$\mathbf{w}(i) \odot= c$$

```
def assign_scalar(self, value, index = None, mask = None, ...)
```

```
w = grb.Vector.sparse(grb.INT32, 5)
```

- Assign a constant to a list of indices:

```
w.assign_scalar(2, [0,3,4])
```

- Assign a constant to a subset of the output with a mask:

```
m = grb.Vector.from_lists([0,3,4], [True]*3, size=5)
w.assign_scalar(2, mask=m)
```

- Alternative form using masking:

```
w[m] = 2
```

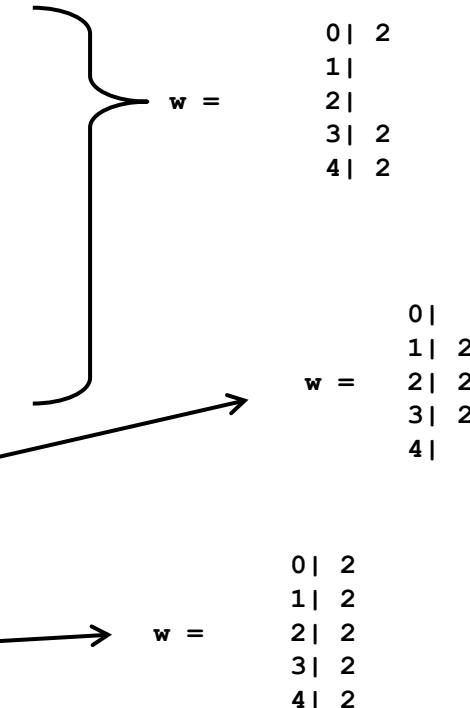
- Colon notation is also supported: w[begin:end]:

```
w[1:4] = 2
```

- Equivalent ways to fill a Vector (index=None):

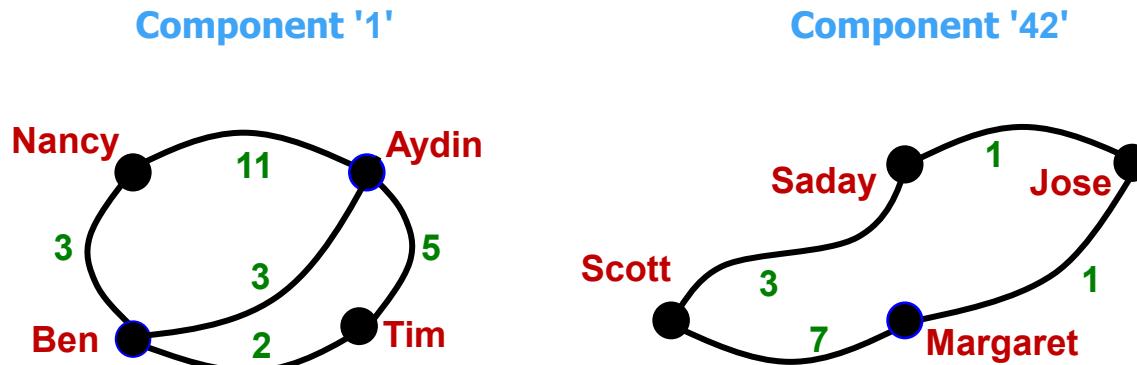
```
w[:] = 2
```

```
w.assign_scalar(2)
```



# Our Connected Components plan

- Strategy:
  - Create a new vector and Initialize all vertex IDs to “unassigned”
  - While there are unassigned vertices:
    - Pick an unassigned vertex
    - Perform BFS marking all reachable vertices
    - Assign all reachable vertices with a unique '**component number**'.



# Our Connected Components plan

- We need an undirected graph with disconnected components to play with:

```
row_ind = [0, 0, 0, 1, 1, 2, 3, 3, 4, 4, 5, 5, 6, 7, 7, 8, 8, 8]
col_ind = [1, 4, 8, 0, 8, 6, 5, 7, 0, 8, 3, 7, 2, 3, 5, 0, 1, 4]
values   = [1, 2, 1, 1, 3, 4, 1, 2, 2, 5, 1, 2, 4, 2, 2, 1, 3, 5]
```

Matrix: GRAPH =

	0	1	2	3	4	5	6	7	8		
0		1			2					1	0
1		1								3	1
2						4					2
3					1		2				3
4		2						5		4	
5				1			2				5
6			4								6
7				2	2						7
8	1	3			5						8
	0	1	2	3	4	5	6	7	8		

# Our Connected Components plan

- We need an undirected graph with disconnected components to play with:

```
row_ind = [0, 0, 0, 1, 1, 2, 3, 3, 4, 4, 5, 5, 6, 7, 7, 8, 8, 8]
col_ind = [1, 4, 8, 0, 8, 6, 5, 7, 0, 8, 3, 7, 2, 3, 5, 0, 1, 4]
values   = [1, 2, 1, 1, 3, 4, 1, 2, 2, 5, 1, 2, 4, 2, 2, 1, 3, 5]
```

Matrix: GRAPH =

	0	1	2	3	4	5	6	7	8	
0		1			2					1   0
1		1						3   1		
2						4			1   2	
3					1		2		1   3	
4		2						5   4		
5			1				2		1   5	
6			4						1   6	
7				2	2				1   7	
8	1	3			5				1   8	
	0	1	2	3	4	5	6	7	8	

How many  
components  
are there?

# Exercise 11: Connected Components

- Wrap the code from Exercise 10 in a function called BFS:

```
def BFS(graph, src_node): # Adjacency Matrix, vertex ID  
    ...  
    return v # Boolean Vector with reachable nodes set to True
```

- Call BFS to compute the membership of each connected component (CC):

- Create a Vector of size NUM\_NODES to hold CC ID for each node.
- Each CC consists of all reachable (visited) nodes from a given root.
- Iterate over the visited list finding unreached nodes to start a BFS
- Use the following undirected, weighted graph, **with multiple components**:

```
row_ind = [0, 0, 0, 1, 1, 2, 3, 3, 4, 4, 5, 5, 6, 7, 7, 8, 8, 8]  
col_ind = [1, 4, 8, 0, 8, 6, 5, 7, 0, 8, 3, 7, 2, 3, 5, 0, 1, 4]  
values = [1, 2, 1, 1, 3, 4, 1, 2, 2, 5, 1, 2, 4, 2, 2, 1, 3, 5]
```

- Challenge: use `Vector.assign_scalar()` to assign component IDs

```
import pygraphblas as grb  
from pygraphblas.gviz import draw_graph as draw  
A = grb.Matrix.from_lists(rInd, cInd, vals)  
v = grb.Vector.sparse(grb.BOOL, N)  
v.assign_scalar(val, index=None, mask=None)  
v.get(index)
```

```
w = A.mxv(u, desc=???)  
v = w.eadd(v), v += w  
A.mxv(u, out=w, desc = ???)  
grb.descriptor.[R][S][C][T0][T1]  
with grb.<type>.<semiring>:  
Atrans = A.T
```

```
v.nvals  
v.size  
A.nvals  
A.nrows  
print(A)  
draw(A)
```

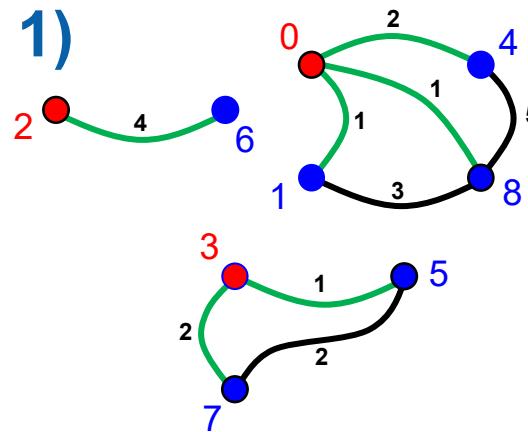
# Solution to exercise 11 (part 1)

```
def BFS(graph, src_node):
    NODES = graph.nrows;
    v = grb.Vector.sparse(grb.BOOL, NODES);
    w = grb.Vector.sparse(grb.BOOL, NODES);
    w[src_node] = True # 1st wavefront

    with grb.BOOL.LOR_LAND:
        while w.nvals > 0:
            #v.eadd(w, out=v, add_op=grb.BOOL.LOR) # v += w
            v.assign_scalar(True, mask=w)           # v[w] = True

            # w<!v, r> = graph.T @ w
            graph.mxv(w, mask=v, out=w, desc=grb.descriptor.RCT0)

    return v
```



Mostly the same as Exercise 10:

- Need to get the number of nodes from matrix properties, i.e., nrows
- This illustrates another way to accumulate the visited list using assign

# Solution to exercise 11 (part 2)

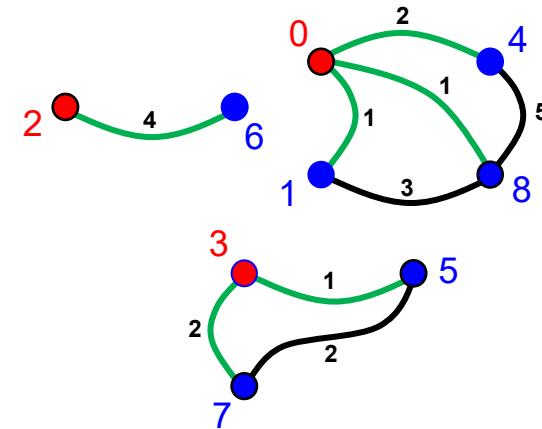
```
def CC(graph):
    NUM_NODES = graph.nrows
    cc_ids     = grb.Vector.sparse(grb.UINT64, NUM_NODES)
    num_ccs    = 0

    for src_node in range(NUM_NODES):
        if cc_ids.get(src_node) is None:
            print("Processing node", src_node)

            # find all nodes reachable from src_node
            visited = BFS(graph, src_node)

            cc_ids.assign_scalar(num_ccs, mask=visited) # cc_ids[visited]=num_ccs
            num_ccs += 1

    return num_ccs, cc_ids
```



Notes:

- If `cc_ids.get(index)` returns `None`, there is no stored value at that location (it has not been visited yet).
- Using `assign_scalar` to assign component IDs to visited vertices
- Not shown: opportunity for early exit when `cc_ids.nvals == NUM_NODES`

# Solution to exercise 11 (part 3)

```
def BFS(graph, src_node):
    ...
    return v

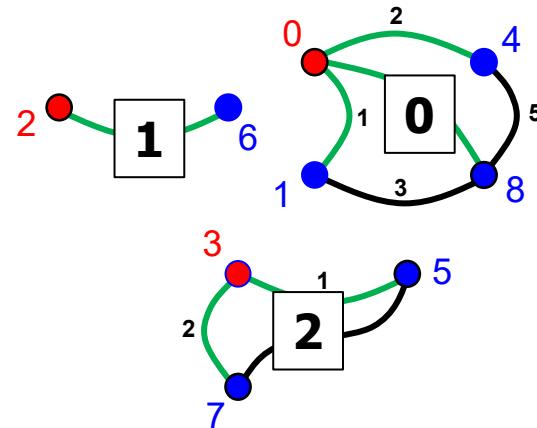
def CC(graph):
    ...
    return num_ccs, cc_ids

row_ind = [0, 0, 0, 1, 1, 2, 3, ...]
col_ind = [1, 4, 8, 0, 8, 6, 5, ...]
values   = [1, 2, 1, 1, 3, 4, 1, ...]
graph = grb.Matrix.from_lists(row_ind, col_ind, values)

num_ccs, cc_ids = CC(graph)

print("\nFound", num_ccs, "components.")
print(cc_ids)

draw(graph)
draw(graph, label_vector = cc_ids)
```



Output:

Processing node 0
Processing node 2
Processing node 3
Found 3 components.
0  0
1  0
2  1
3  2
4  0
5  2
6  1
7  2
8  0

# Putting it all together...

- Copying CC algorithm to AnalyzeGraph notebook...

```
.  
. .  
.  
*** Step 3a: Running Tutorial connected components  
algorithm.  
Largest component #0 (size = 822)  
*** Step 3a: Elapsed time: 0.0222051 sec*  
Found 246 components
```

- Check out the LAGraph repository for *significantly* more efficient algorithms\*\* written in C for the GraphBLAS (coming soon to python)
  - <https://github.com/GraphBLAS/LAGraph>

\*On one core of i9-9900 @ 3.10GHz

\*\*Azad, Buluç. "LACC: a linear-algebraic algorithm for finding connected components in distributed memory" (IPDPS 2019).

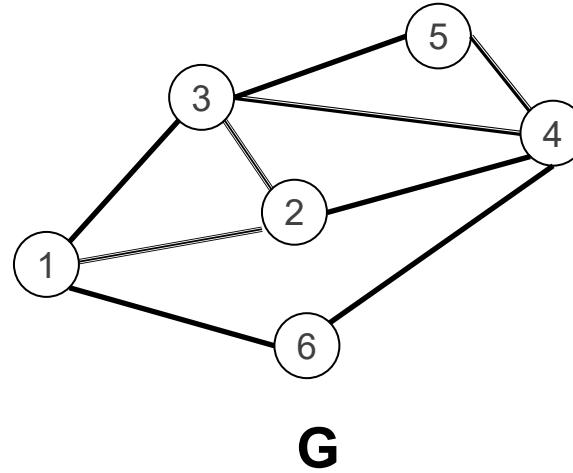
\*\*Zhang, Azad, Hu. "FastSV: FastSV: A Distributed-Memory Connected Component Algorithm with Fast Convergence" (SIAM PP20).

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  - – Triangle Counting
  - PageRank

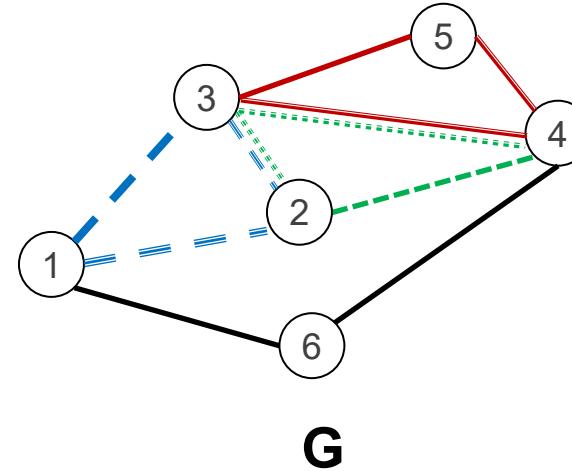
# Triangle Counting

- A triangle is a structure in a graph where three vertices are mutually adjacent.
- Can you identify the triangles in Graph, G?



# Triangle Counting

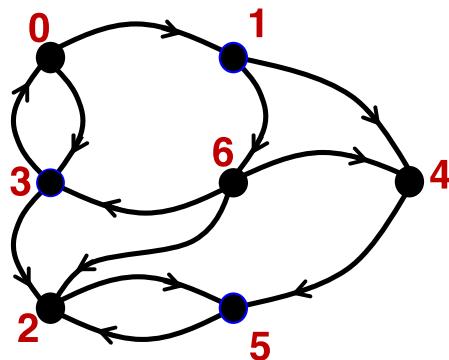
- A triangle is a structure in a graph where three vertices are mutually adjacent.
- Can you identify the triangles in Graph, G?



- Triangles are one of many ways to help characterize the communities in a graph.
- Triangles define vertices connected by transitivity relations
- Counting Triangles is also a common benchmark for Graph frameworks.

# Triangles and undirected graphs

- While we can define triangle counting for directed graphs, it is typically used with *undirected, unweighted* graphs with *no self-loops*.
- We'll work with our GraphBLAS logo graph ... which is a directed graph.



- How can we convert any arbitrary graph into an unweighted, undirected graph with no self-loops?

The screenshot shows a web browser displaying the `pygraphblas API documentation` at [graphegon.github.io/pygraphblas/pygraphblas/index.html](https://graphegon.github.io/pygraphblas/pygraphblas/index.html). The page title is `pygraphblas API Reference`. Below the title, there are links to `GraphBLAS.org`, `Github`, and `SuiteSparse::GraphBLAS User Guide`. A sidebar on the left contains a navigation menu with sections like `Index`, `Installation` (with `Docker`), `Tests`, `Summary`, `Introduction to Graphs and Matrices`, `Using the API`, `Global variables` (listing `GxB_INDEX_MAX`, `GxB_IMPLEMENTATION`, `GxB_SPEC`), `Functions` (listing `binary_op`, `unary_op`, `select_op`, `options_set`, `options_get`), and `Types` (listing `Matrix`, `Vector`, `Scalar`). The main content area starts with a large `pygraphblas` logo, followed by the `Installation` section. This section includes instructions to install SuiteSparse, a command-line instruction for running setup.py, and text about downloading precompiled binaries or using Docker images. A callout box highlights the text: "Let's use this as a chance to practice finding what we need from the pygraphblas documentation". At the bottom, there is a note about using pre-compiled binaries for benchmarking.

pygraphblas API Reference

~| GraphBLAS.org | Github | SuiteSparse::GraphBLAS User Guide |~

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Docker

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Summary

Introduction to Graphs and Matrices

Using the API

▶ Global variables

`GxB_INDEX_MAX`  
`GxB_IMPLEMENTATION`  
`GxB_SPEC`

▶ Functions

`binary_op`  
`unary_op`  
`select_op`  
`options_set`  
`options_get`

▶ Types

`Matrix`  
`Vector`  
`Scalar`

# pygraphblas

## Installation

pygraphblas requires the SuiteSparse:GraphBLAS library. To install SuiteSparse, then run:

```
python setup.py install
```

There are two ways to download precompiled binaries. One way is to use `pip install pygraphblas` on an interlinux machine. This will download a package compatible with most modern linux distributions. This also works in a Docker container on Mac.

There are also pre-build docker images based on Ubuntu 20.04 that have a pre-compiled SuiteSparse and pygraphblas installed. These come in two flavors `minimal` which is the Ipython interpreter-only, and `notebook` which comes with a complete Jupyter Notebook server. These containers also work on Mac.

An installation script for Ubuntu 18.04 is provided in the `install-ubuntu.sh` file.

NOTE: DO NOT USE THESE PRE-COMPILED BINARIES FOR BENCHMARKING SUITESPARSE. These binaries are not guaranteed to be ideally compiled for your environment. You must build your own binaries on your own platforms if you intend to do ANY valid benchmarking.

discuss

pygraphblas API documentation

graphon.github.io/pygraphblas/pygraphblas/index.html#pygraphblas.Matrix

## ► Types

- ▼ Matrix
  - M
  - T
  - apply
  - apply\_first
  - apply\_second
  - assign\_col
  - assign\_matrix
  - assign\_row
  - assign\_scalar
  - cast
  - clear
  - cols
  - dense
  - diag
  - dup
  - eadd
  - emult
  - extract\_col
  - extract\_matrix
  - extract\_row
  - format
  - from\_binfile
  - from\_lists
  - from\_mm
  - from\_tsv
  - gb\_type
  - get
  - hyper\_switch
  - identity
  - iseq
  - isne
  - kronecker

## ► Types

**class Matrix (matrix, typ=None)**

GraphBLAS Sparse Matrix

This is a high-level wrapper around the GrB\_Matrix C type using the [cffi](#) library.

A Matrix supports many possible operations according to the GraphBLAS API. Many of those operations have overloaded operators.

**Operat or**

<b>Operat or</b>	<b>Description</b>	<b>Default</b>
A @ B	Matrix Matrix Multiplication	type default PLUS_TIMES semiring
v @ A	Vector Matrix Multiplication	type default PLUS_TIMES semiring
A @ v	Matrix Vector Multiplication	type default PLUS_TIMES semiring
A @= B	In-place Matrix Matrix Multiplication	type default PLUS_TIMES semiring
v @= A	In-place Vector Matrix Multiplication	type default PLUS_TIMES semiring
A @=		type default PLUS_TIMES semiring
A & B	Matrix Intersection	type default SECOND combiner
A &= B	In-place Matrix Intersection	type default SECOND combiner
A + B	Matrix Element-Wise Union	type default PLUS combiner
A += B	In-place Matrix Element-Wise Union	type default PLUS combiner
A - B	Matrix Element-Wise Union	type default MINUS combiner
A -= B	In-place Matrix Element-Wise Union	type default MINUS combiner

You'll find what you need from the list of methods associated with the matrix type

**discuss**

pygraphblas API documentation

graphon.github.io/pygraphblas/pygraphblas/index.html#pygraphblas.Matrix

max  
min  
mmx  
mxv  
ncols  
nonzero  
nrows  
nvals  
offdiag  
pattern  
print  
random  
reduce\_bool  
reduce\_float  
reduce\_int  
reduce\_vector  
resize  
rows  
select  
shape  
sparse  
sparsity  
sparsity\_status  
square  
ssget  
to\_arrays  
to\_binfile  
to\_html\_table  
to\_lists  
to\_markdown\_table  
to\_mm  
to\_numpy  
to\_scipy\_sparse  
to\_string  
transpose

## ► Types

**class Matrix (matrix, typ=None)**

GraphBLAS Sparse Matrix

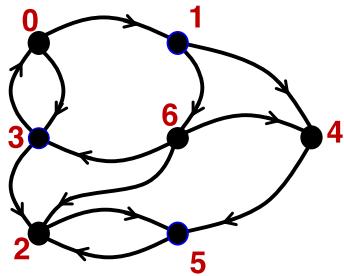
This is a high-level wrapper around the GrB\_Matrix C type using the [cffi](#) library.

A Matrix supports many possible operations according to the GraphBLAS API. Many of those operations have overloaded operators.

**discuss**

Operator or	Description	Default
$A @ B$	Matrix Matrix Multiplication	type default PLUS_TIMES semiring
$v @ A$	Vector Matrix Multiplication	type default PLUS_TIMES semiring
$A @ v$	Matrix Vector Multiplication	type default PLUS_TIMES semiring
$A @= B$	In-place Matrix Matrix Multiplication	type default PLUS_TIMES semiring
$v @= A$	In-place Vector Matrix Multiplication	type default PLUS_TIMES semiring
$A @= v$	In-place Matrix Vector Multiplication	type default PLUS_TIMES semiring
$A   B$	Matrix Union	type default SECOND combiner
$A  = B$	In-place Matrix Union	type default SECOND combiner
$A & B$	Matrix Intersection	type default SECOND combiner
$A &= B$	In-place Matrix Intersection	type default SECOND combiner
$A + B$	Matrix Element-Wise Union	type default PLUS combiner
$A += B$	In-place Matrix Element-Wise Union	type default PLUS combiner
$A - B$	Matrix Element-Wise Union	type default MINUS combiner
$A -= B$	In-place Matrix Element-Wise Union	type default MINUS combiner

## Exercise 12: Convert a directed graph into an undirected graph

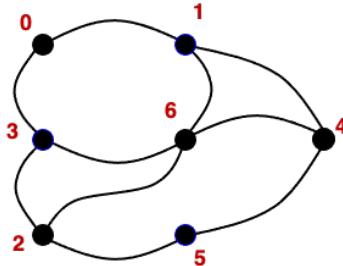


- The GraphBLAS “logo graph” you’ve been using since exercise 2 is a directed graph.

	0	1	2	3	4	5	6	
0		1		1				0
1					1		1	1
2						1		2
3			1		1			3
4						1		4
5				1				5
6	0	1	2	3	4	5	6	

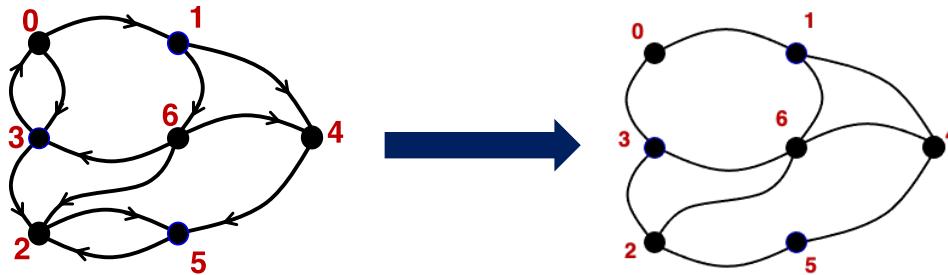
- Look at the methods available with the **Matrix type** from the online pygraphblas documentation and write a python function to convert a directed graph into an unweighted, undirected graph of type uint64 with no self loops

<https://graphegon.github.io/pygraphblas/pygraphblas/index.html>



	0	1	2	3	4	5	6	
0		1		1				0
1	1				1		1	1
2				1		1	1	2
3	1		1			1		3
4		1				1	1	4
5			1		1			5
6	0	1	1	1	1			6

## Exercise 12: Hint



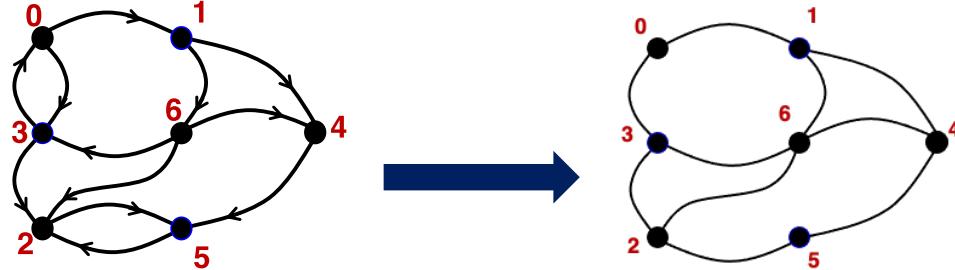
- Three steps:
  - Convert from input type to uint64 (but with the same pattern)
  - Remove self loops (i.e., the diagonal elements)
  - An undirected graph corresponds to a symmetric matrix. How do you take any matrix of values set to one (i.e., identify of uint64) and make it symmetric with values set to the identify of uint64? ← remember: you can control the operators used in GraphBLAS

<https://graphegon.github.io/pygraphblas/pygraphblas/index.html>

Note: The operation (directed-graph → undirected-graph) is used quite often.

For example, the weakly connected components (CCs) of a directed graph are the CCs of the undirected graph generated from the directed graph.

## Exercise 12: Solution



```
def UndirUnweight(G):
    G_unw = G.pattern(typ = grb.UINT64) # replace weights with UINT64 identity
    G_nl = G_unw.offdiag() # make sure there are no self-loops

    # make symmetric by adding (OR-ing) the matrix with its transpose
    G_nl.eadd(G_nl, add_op=grb.UINT64.LOR, desc=grb.descriptor.T1,
               out=G_nl)
    return G_nl
```

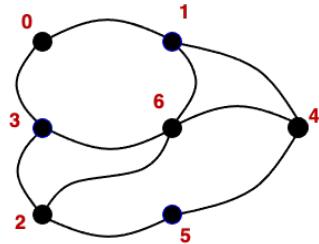
	0	1	2	3	4	5	6	
0	1		1				0	
1				1	1		1	
2					1		2	
3	1		1			3		
4					1		4	
5		1				5		
6		1	1	1		6		
	0	1	2	3	4	5	6	

	0	1	2	3	4	5	6	
0	1		1				0	
1		1					1	
2				1	1	1	1	2
3	1		1			1		3
4					1		1	4
5		1				1		5
6		1	1	1	1	1	1	6
	0	1	2	3	4	5	6	

# Counting Triangles

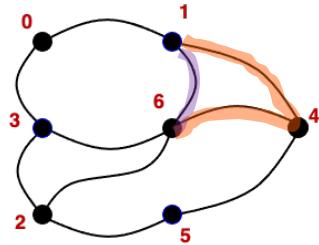
- Our goal is to count the number of triangles in an unweighted, undirected graph that has no self-edges.
- Consider our undirected “logo” graph



- There are two triangles:  $(2,3,6)$  and  $(1,4,6)$
- Think of the problem in terms of hops over edges between vertices. In terms of hops, how would you define a triangle?

# Counting Triangles

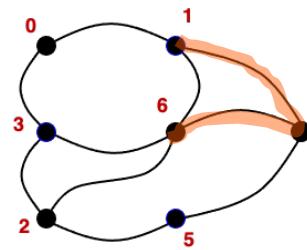
- Our goal is to count the number of triangles in an unweighted, undirected graph that has no self-edges.
- Consider our undirected “logo” graph



- There are two Triangles: (2,3,6) and (1,4,6)
- Think of the problem in terms of hops over edges between vertices. In terms of hops, how would you define a triangle?
  - A triangle occurs when a node is connected to another node in two ways:
    1. A two-hop “wedge”, ↗
    2. A direct edge (i.e. one hop) ↘

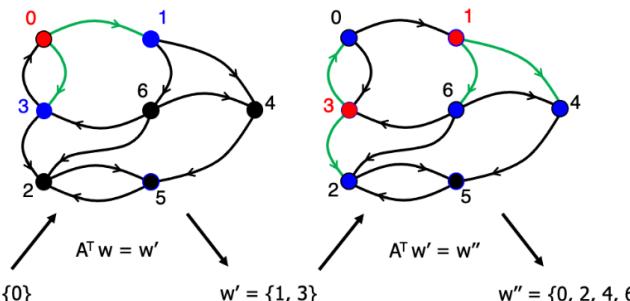
# Finding wedges

- How do we find all the “wedges” in a graph?
- Or put in other terms ... how do we find all the two hop paths between nodes in a Graph?
- Remember in Exercise 8 ... we learned to think of multiplication by an adjacency matrix as advancing a wavefront as you traverse a graph?



## Wavefronts

- A subset of vertices accessed at one stage in a breadth first search pattern ... for example ....
  - “You tell two friends, and they tell two friends...”



Red=current wavefront and visited, Blue=next wavefront, Black=unvisited

A = Adjacency Matrix      w = wavefront vectors  
Distribution Statement A: Approved for public release and unlimited distribution.

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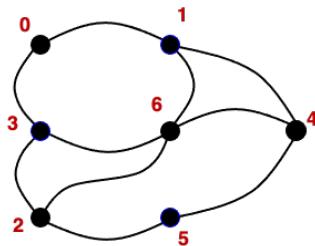
With this perspective on mxv, what does mxm for our undirected graph mean?

# Matrix Multiplication

- Matrix multiplication over our adjacency matrices ... let's look at the result for our undirected graph.

$$\begin{array}{c|cccccc} & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\ \hline 0 & & 1 & & 1 & & & \\ 1 & 1 & & & 1 & & 1 & \\ 2 & & 1 & & 1 & 1 & & \\ 3 & 1 & 1 & & 1 & 1 & & \\ 4 & & 1 & & 1 & 1 & & \\ 5 & & 1 & 1 & 1 & & & \\ 6 & 1 & 1 & 1 & 1 & & & \end{array} \oplus \otimes \begin{array}{c|cccccc} & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\ \hline 0 & & 1 & & 1 & & & \\ 1 & 1 & & & 1 & & 1 & \\ 2 & & 1 & & 1 & 1 & & \\ 3 & 1 & 1 & & 1 & 1 & & \\ 4 & & 1 & & 1 & 1 & & \\ 5 & & 1 & 1 & 1 & & & \\ 6 & 1 & 1 & 1 & 1 & & & \end{array} = \begin{array}{c|cccccc} & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\ \hline 0 & 2 & & 1 & & 1 & & 2 \\ 1 & & 3 & 1 & 2 & 1 & 1 & 1 \\ 2 & 1 & 1 & 3 & 1 & 2 & 1 & 1 \\ 3 & 2 & 1 & 3 & 1 & 1 & 1 & 1 \\ 4 & 1 & 1 & 2 & 1 & 3 & & 1 \\ 5 & 1 & & 1 & 1 & & 2 & 2 \\ 6 & 2 & 1 & 1 & 1 & 1 & 2 & 4 \end{array}$$

- What does the product  $A \oplus \otimes A = A^2$  tell you?

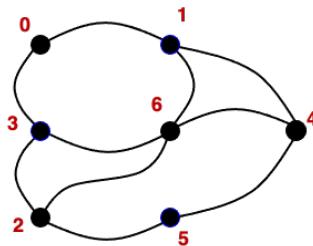


# Matrix Multiplication

- Matrix multiplication over our adjacency matrices ... let's look at the result for our undirected graph.

$$\begin{array}{c|cccccc} & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\ \hline 0 & & 1 & & 1 & & & \\ 1 & 1 & & & 1 & & 1 & \\ 2 & & 1 & & 1 & 1 & & \\ 3 & 1 & 1 & & 1 & & 1 & \\ 4 & & 1 & & 1 & 1 & & \\ 5 & & 1 & 1 & 1 & & & \\ 6 & 1 & 1 & 1 & 1 & & & \end{array} \oplus \otimes \begin{array}{c|cccccc} & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\ \hline 0 & & 1 & & 1 & & & \\ 1 & 1 & & & 1 & & 1 & \\ 2 & & 1 & & 1 & 1 & & \\ 3 & 1 & 1 & & 1 & & 1 & \\ 4 & & 1 & & 1 & 1 & & \\ 5 & & 1 & 1 & 1 & & & \\ 6 & 1 & 1 & 1 & 1 & & & \end{array} = \begin{array}{c|cccccc} & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\ \hline 0 & 2 & & 1 & & 1 & & 2 \\ 1 & & 3 & 1 & 2 & 1 & 1 & 1 \\ 2 & 1 & 1 & 3 & 1 & 2 & & 1 \\ 3 & 2 & 1 & 3 & 1 & 1 & 1 & 1 \\ 4 & 1 & 1 & 2 & 1 & 3 & & 1 \\ 5 & 1 & & 1 & 1 & & 2 & 2 \\ 6 & 2 & 1 & 1 & 1 & 1 & 2 & 4 \end{array}$$

- What does the product  $A \oplus \otimes A = A^2$  tell you?
  - It tells you all the two hop paths between nodes in the graphs



## Matrix Matrix multiplication: mxm()

$$C \odot= A \oplus . \otimes B$$

- The operators in GraphBLAS operations are:

- Accumulator  $\odot$
- Addition  $\oplus$
- Multiplication  $\otimes$

- The operators are implied by type.

Pygraphblas type	$\odot$	$\oplus$	$\otimes$
grb.BOOL	LOR	LOR	LAND
grb.INT32	32 bit int add	32 bit int add	32 bit int multiply
grb.FP32	32 bit float add	32 bit float add	32 bit float multiply

- Pygraphblas gives you multiple ways to do matrix multiplication

```
import pygraphblas as grb
# A, B and C are graphBLAS matrices defined elsewhere
D = A.mxm(B, mask=A) # creates a new D, uses A as a mask
A.mxm(B, semiring=grb.UINT64.PLUS_TIMES, out=C) # uses existing C
E = A@B      # uses default semiring based on types and creates a new E
```

With grb.UINT64.PLUS\_TIMES:

F=A@A

# From wedges to triangles

- We now know how to find all the wedges.
- How do we keep only the wedges that are part of a triangle?
  - There is more than one way to do this .... We leave it as an exercise for you to figure this out (hint: it uses GraphBLAS concepts we have already covered)
- So after you solve that problem, you have a graphBLAS matrix with all the triangles. How do you count them?
- Reduction to scalar: sum together all the elements of a matrix

```
Trimat.reduce_int(grb.UINT64.PLUS_MONOID)
```

The matrix  
that is  
being  
reduced

The name  
of the  
graphBLAS  
operation

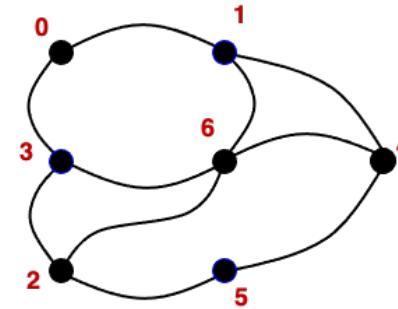
The type and  
operator used in  
the reduction

# Exercise 13: Counting Triangles

- Write a function that will count the triangles in an undirected, unweighted graph that has no self-loops.
- Use the graph you generated in Exercise 13.

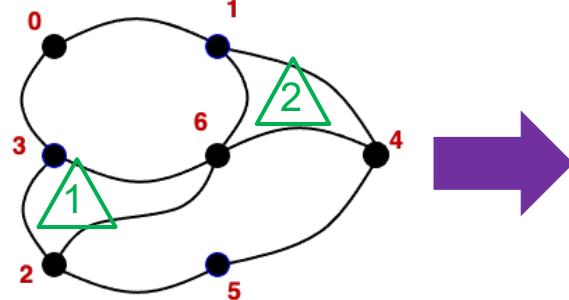
- Hints:

- There are multiple ways to close wedges to find triangles. Think hard ... we've shown you how to do this already.
  - Ask yourself ... how many times are you counting each triangle? Is overcounting an issue?



<https://graphegon.github.io/pygraphblas/pygraphblas/index.html>

# Exercise 13: First solution



	0	1	2	3	4	5	6	
0	0	1	1	1	2	1	0	0
1	1	0	1	1	1	1	1	1
2	1	1	0	1	2	1	2	2
3	2	1	3	1	1	1	3	3
4	1	1	2	1	3	1	4	4
5	1		1	2	2	2	5	5
6	2	1	1	1	1	2	4	6
	0	1	2	3	4	5	6	

```
def TriCount1(inGraph):
    out = inGraph.mxm(inGraph, semiring=grb.UINT64.PLUS_TIMES)
    tri = out.emult(inGraph)
    red = tri.reduce_int(grb.UINT64.PLUS_MONOID)

    return red/6 ← Overcount by 6 ... once for each vertex (3) in each direction (x2) for 6 total
```

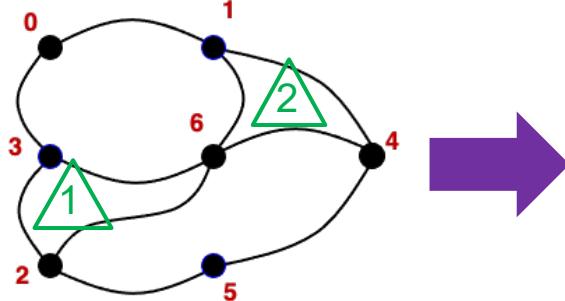
	0	1	2	3	4	5	6	
0	2	1	1	1	2	1	0	0
1	3	1	2	1	1	1	1	1
2	1	1	3	1	2	1	2	2
3	2	1	3	1	1	1	3	3
4	1	1	2	1	3	1	4	4
5	1		1	2	2	2	5	5
6	2	1	1	1	1	2	4	6
	0	1	2	3	4	5	6	

Counts of all the two-hop paths (wedges)

	0	1	2	3	4	5	6	
0	0	1	1	1	1	1	0	0
1	1	0	1	1	1	1	1	1
2	2		0	1	1	1	1	2
3	3		1	0	1	1	1	3
4	4		1	1	0	1	1	4
5	5		1	1	1	0	1	5
6	6		1	1	1	1	0	6
	0	1	2	3	4	5	6	

Keep wedges with an edge to close them

# Exercise 13: Second solution



	0	1	2	3	4	5	6	
0		1	1	1				0
1		1			1	1	1	1
2			1		1	1	1	2
3		1		1				3
4			1			1	1	4
5				1	1	1		5
6		1	1	1	1			6
	0	1	2	3	4	5	6	

```
def TriCount2(inGraph):
    out=inGraph.mxm(inGraph,semiring=grb.UINT64.PLUS_TIMES,mask=inGraph)
    red=out.reduce_int(grb.UINT64.PLUS_MONOID)

    return red/6 ← Overcount by 6 ... once for each vertex (3) in each direction (x2) for 6 total
```

	0	1	2	3	4	5	6	
0								0
1				1		1		1
2			1			1		2
out = 3		1				1		3
4		1				1		4
5								5
6	1	1	1	1				6
	0	1	2	3	4	5	6	

All the two-hop paths (wedges)

Only keep wedges with a closing edge in the original graph (using the mask)

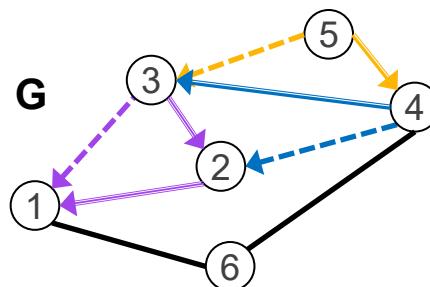
## Exercise 13: Third solution – work with lower triangular matrices only

```
def TriCount3(inGraph):
    L = inGraph.tril(-1)
    T = L.mm(L, semiring=grb.UINT64.PLUS_TIMES, mask=L)
    red = T.reduce_int(grb.UINT64.PLUS_MONOID)
    return red
```

← Counts each triangle once (hi-mid-lo wedge closed by hi-lo edge)

$$\left( \begin{array}{cccccc} 1 & 2 & 3 & 4 & 5 & 6 \\ 1 & & & & & \\ 2 & 1 & & & & \\ 3 & 1 & 1 & & & \\ 4 & & 1 & 1 & & \\ 5 & & & 1 & 1 & \\ 6 & 1 & & & 1 & \\ \end{array} \right) \times \left( \begin{array}{cccccc} 1 & 2 & 3 & 4 & 5 & 6 \\ 1 & & & & & \\ 2 & 1 & & & & \\ 3 & 1 & 1 & & & \\ 4 & & 1 & 1 & & \\ 5 & & & 1 & 1 & \\ 6 & 1 & & & 1 & \\ \end{array} \right) \circ \left( \begin{array}{cccccc} 1 & 2 & 3 & 4 & 5 & 6 \\ 1 & & & & & \\ 2 & 1 & & & & \\ 3 & 1 & 1 & & & \\ 4 & & 1 & 1 & & \\ 5 & & & 1 & 1 & \\ 6 & 1 & & & 1 & \\ \end{array} \right) = \left( \begin{array}{cccccc} 1 & 2 & 3 & 4 & 5 & 6 \\ 1 & & & & & \\ 2 & 1 & & & & \\ 3 & 1 & 1 & & & \\ 4 & & 1 & & & \\ 5 & & & 1 & & \\ 6 & 1 & & & 1 & \\ \end{array} \right)$$

$L$        $L$        $L$        $T$



$$\left( \begin{array}{cccccc} 1 & 2 & 3 & 4 & 5 & 6 \\ 1 & & & & & \\ 2 & 1 & & & & \\ 3 & & 1 & & & \\ 4 & & & 1 & 1 & \\ 5 & & & & 1 & 1 \\ 6 & & & & & 1 & \\ \end{array} \right)$$

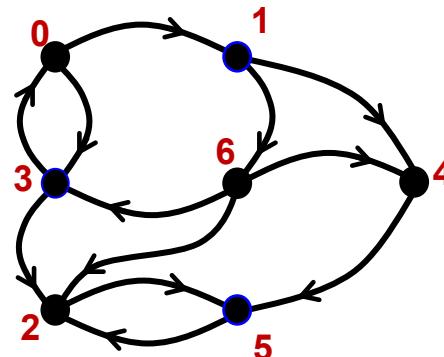
$L^2$

# Outline

- Graphs and Linear Algebra
- The GraphBLAS API and Adjacency Matrices
- GraphBLAS Operations
- Pygraphblas and modifying the behavior of operations.
- Graph Algorithms expressed with GraphBLAS
  - Breadth-First Traversal
  - Connected Components
  - Triangle Counting
  - – PageRank

# PageRank

- PageRank algorithm
  - Given a set of webpages (vertices), each page containing hyperlinks (edges) to other pages, the PageRank algorithm gives a measure of the *importance* of each page
  - The intuition is that (1) more important pages will receive more links from other pages and (2) links from more important pages count more than links from less important pages
  - This is an iterative algorithm that converges to a fixed-point
  - For this exercise, the graph will consist of directed edges, to simulate the unidirectional nature of hyperlinks



## Exercise 14: PageRank iterative algorithm

- Given an  $N \times N$  adjacency matrix  $\mathbf{A}$  and a damping factor  $\alpha$ , compute the vector  $\mathbf{r}$  of page ranks of each vertex
- Initially, all entries of  $\mathbf{r}$  have value  $1/N$
- At each iteration:
  - distribute the rank of a vertex among its neighbors (linked pages)
  - compute the new rank of a vertex as the sum of the contributions of all vertices that point to it (and a damping factor component)
  - if the old ranks and new ranks are close, end the computation
- If  $\mathbf{r}[i]$  is the rank of vertex  $i$ , and  $\mathbf{d}[i]$  is the number of edges originating from vertex  $i$  (out-degree of vertex  $i$ ), then at each iteration we compute a new rank for each vertex  $j$  as:

$$\mathbf{r}[j] = \frac{1 - \alpha}{N} + \sum_{i \in \mathbf{A}(:, j)} \mathbf{r}[i] \cdot \frac{\alpha}{\mathbf{d}[i]}$$

where  $\mathbf{A}(:, j)$  are those vertices that have outgoing edges to vertex  $j$

# What you will create

```
import pygraphblas as grb

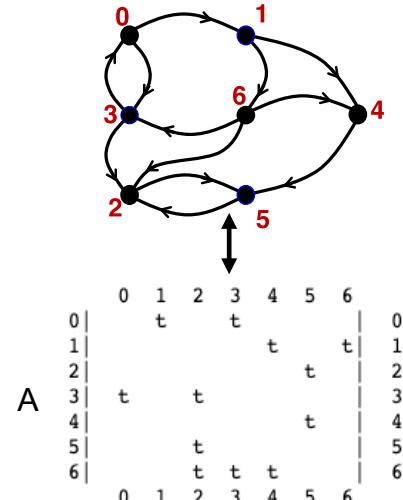
rowID = [0,0,1,1,2,3,3,4,5,6,6,6]
colID = [1,3,4,6,5,0,2,5,2,2,3,4]
vals  = [True]*len(rowID)
A = grb.Matrix.from_lists(rowID, colID, vals)

r = pagerank(A)
print(r)
```

A

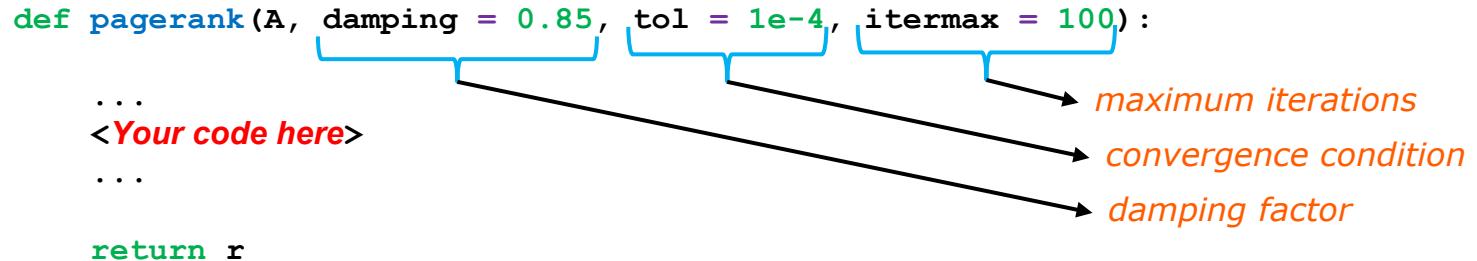
	0	1	2	3	4	5	6		0	1	2	3	4	5	6	
0		t		t					0		0	0.0429				0
1					t		t		1		1	0.0397				1
2						t			2		2	0.387				2
3	t		t						3	→	3	0.0505				3
4					t				4		4	0.0491				4
5			t						5		5	0.392				5
6				t	t	t			6		6	0.0383				6
	0	1	2	3	4	5	6		0	1	2	3	4	5	6	

r



# The pagerank function

```
def pagerank(A, damping = 0.85, tol = 1e-4, itermax = 100):  
    ...  
<Your code here>  
    ...  
    return r
```



The diagram illustrates the parameters of the `pagerank` function with annotations:

- A blue bracket underlines the first three parameters: `damping`, `tol`, and `itermax`.
- Three black arrows point from these underlined parameters to their respective descriptions:
  - An arrow points from `damping` to the text *damping factor*.
  - An arrow points from `tol` to the text *convergence condition*.
  - An arrow points from `itermax` to the text *maximum iterations*.

# Preparing for the iterations

- Number of vertices in graph:

```
n = A.nrows
```

- A vector of initial page ranks:

```
r = grb.Vector.sparse(grb.FP32, n)
r[:] = 1.0 / n
```

- Computing the vector of out-degrees:

A								d	0	1	2
0	1	2	3	4	5	6		0	1	2	
0	t	t				0	A.reduce_vector(out=d,	0  2			
1			t	t	t  1		mon=grb.types.FP32.PLUS_MONOID)	1  2			
2				t	2			2  1			
3	t	t			3	→		3  2			
4				t	4			4  1			
5		t			5			5  1			
6		t	t	t	6			6  3			
	0	1	2	3	4	5	6				

# Inside the iterations

- If we define a working vector  $\mathbf{w}$  such that

$$\mathbf{w}[i] = \mathbf{r}[i] \cdot \frac{\alpha}{\mathbf{d}[i]}$$

and reset

$$\mathbf{r}[i] = \frac{1 - \alpha}{N}$$

then we can update the page rank with a vector-matrix product

$$\mathbf{r} = \mathbf{r} + \mathbf{w} \oplus \cdot \otimes \mathbf{A}$$

<b>A</b>							
<b>w</b>	0	1	2	3	4	5	6
0   $\mathbf{w}[0]$	0	$t$	$t$				0
1   $\mathbf{w}[1]$	1			$t$	$t$		1
2   $\mathbf{w}[2]$	2				$t$		2
3   $\mathbf{w}[3]$	$\oplus \cdot \otimes$	3	$t$	$t$			3
4   $\mathbf{w}[4]$		4			$t$		4
5   $\mathbf{w}[5]$		5		$t$			5
6   $\mathbf{w}[6]$		6	$t$	$t$	$t$		6
	0	1	2	3	4	5	6

→

0   $\mathbf{w}[3]$	0						
1   $\mathbf{w}[0]$	1						
2   $\mathbf{w}[3] + \mathbf{w}[5] + \mathbf{w}[6]$	2						
3   $\mathbf{w}[0] + \mathbf{w}[6]$	3						
4   $\mathbf{w}[1] + \mathbf{w}[6]$	4						
5   $\mathbf{w}[2] + \mathbf{w}[4]$	5						
6   $\mathbf{w}[1]$	6						

# Tips for inside the loop body

- Save the current value of the **r** vector so that you can compare later: `t[:] = r[:]` note – the colons are important to make a copy as opposed to just copying handles
- Use element-wise operation to compute the vector **w** (hint: you may want to pre-compute  $\alpha/d[i]$ )
- Use vector-matrix multiplication to compute  $w \oplus . \otimes A$  and accumulate with the reset value of vector **r**
- Compute the absolute differences of all new (**r**) and old (**t**) values of the page rank of each vertex (hint: use element-wise operation and `apply`)
- Use `reduce_float` to compute the sum of all absolute differences and compare with the convergence condition `tol` (but limit the maximum number of iterations to `itermax`)

## vxm VS mxv

Name	Math	pygraphblas examples ( <code>import pygraphblas as grb</code> )
mxv	$r \odot = A \oplus . \otimes w$	<code>mxv(self, other, cast=None, out=None, semiring=None, mask=None, accum=None, desc=None)</code>
vxm	$r^T \odot = w^T \oplus . \otimes A$	<code>vxm(self, other, cast=None, out=None, semiring=None, mask=None, accum=None, desc=None)</code>

```
w.vxm(A, out=r, accum=grb.FP32.PLUS,  
semiring=grb.FP32.PLUS_TIMES)
```

## vxm VS mxv

Name	Math	pygraphblas examples ( <code>import pygraphblas as grb</code> )
mxv	$r \odot = A \oplus \cdot \otimes w$	<code>mxv(self, other, cast=None, out=None, semiring=None, mask=None, accum=None, desc=None)</code>
vxm	$r^T \odot = w^T \oplus \cdot \otimes A$	<code>vxm(self, other, cast=None, out=None, semiring=None, mask=None, accum=None, desc=None)</code>

input  
vector



```
w.vxm(A, out=r, accum=grb.FP32.PLUS,  
      semiring=grb.FP32.PLUS_TIMES)
```

## vxm VS mxv

Name	Math	pygraphblas examples ( <code>import pygraphblas as grb</code> )
mxv	$r \odot = A \oplus \cdot \otimes w$	<code>mxv(self, other, cast=None, out=None, semiring=None, mask=None, accum=None, desc=None)</code>
vxm	$r^T \odot = w^T \oplus \cdot \otimes A$	<code>vxm(self, other, cast=None, out=None, semiring=None, mask=None, accum=None, desc=None)</code>

input vector      input matrix

```
w.vxm(A, out=r, accum=grb.FP32.PLUS,  
semiring=grb.FP32.PLUS_TIMES)
```

## vxm VS mxv

Name	Math	pygraphblas examples ( <code>import pygraphblas as grb</code> )
mxv	$r \odot = A \oplus \cdot \otimes w$	<code>mxv(self, other, cast=None, out=None, semiring=None, mask=None, accum=None, desc=None)</code>
vxm	$r^T \odot = w^T \oplus \cdot \otimes A$	<code>vxm(self, other, cast=None, out=None, semiring=None, mask=None, accum=None, desc=None)</code>

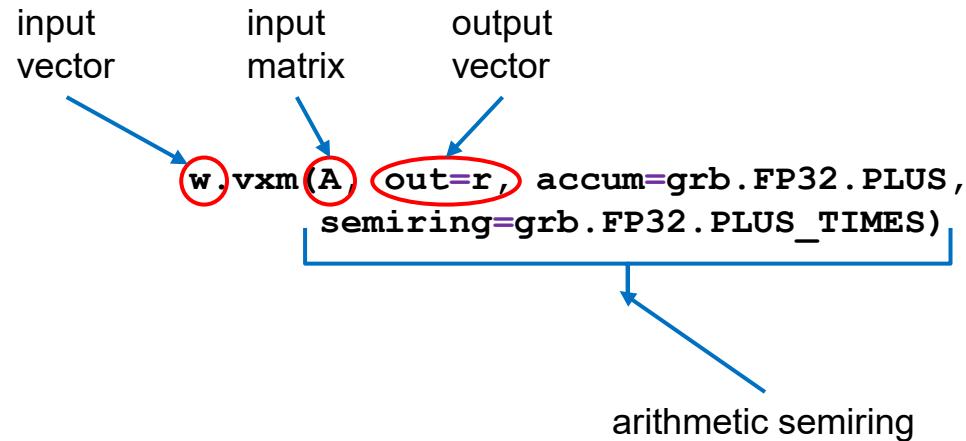
input vector      input matrix      output vector

The diagram shows three labels above a code snippet: "input vector", "input matrix", and "output vector". Three blue arrows point from these labels to the corresponding arguments in the code below. The first arrow points to "w", the second to "A", and the third to "out=r".

```
w.vxm(A, out=r, accum=grb.FP32.PLUS,  
semiring=grb.FP32.PLUS_TIMES)
```

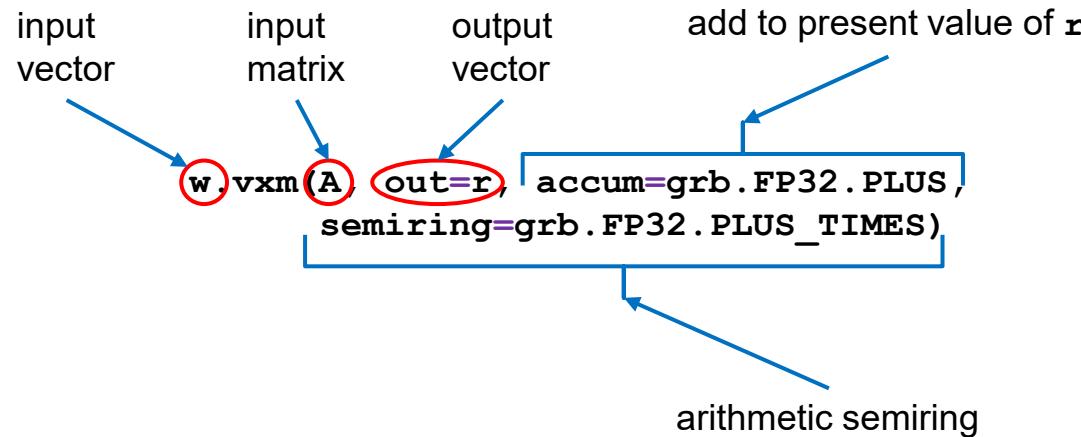
## vxm VS mxv

Name	Math	pygraphblas examples ( <code>import pygraphblas as grb</code> )
mxv	$r \odot = A \oplus \cdot \otimes w$	<code>mxv(self, other, cast=None, out=None, semiring=None, mask=None, accum=None, desc=None)</code>
vxm	$r^T \odot = w^T \oplus \cdot \otimes A$	<code>vxm(self, other, cast=None, out=None, semiring=None, mask=None, accum=None, desc=None)</code>



## vxm VS mxv

Name	Math	pygraphblas examples ( <code>import pygraphblas as grb</code> )
mxv	$r \odot = A \oplus . \otimes w$	<code>mxv(self, other, cast=None, out=None, semiring=None, mask=None, accum=None, desc=None)</code>
vxm	$r^T \odot = w^T \oplus . \otimes A$	<code>vxm(self, other, cast=None, out=None, semiring=None, mask=None, accum=None, desc=None)</code>



# apply operation

Name	Math	pygraphblas examples ( <code>import pygraphblas as grb</code> )
apply (vector)	$u \odot= f(v)$	<code>apply(self, op, out=None, mask=None, accum=None, desc=None)</code>
apply (matrix)	$C \odot= f(A)$	<code>apply(self, op, out=None, mask=None, accum=None, desc=None)</code>

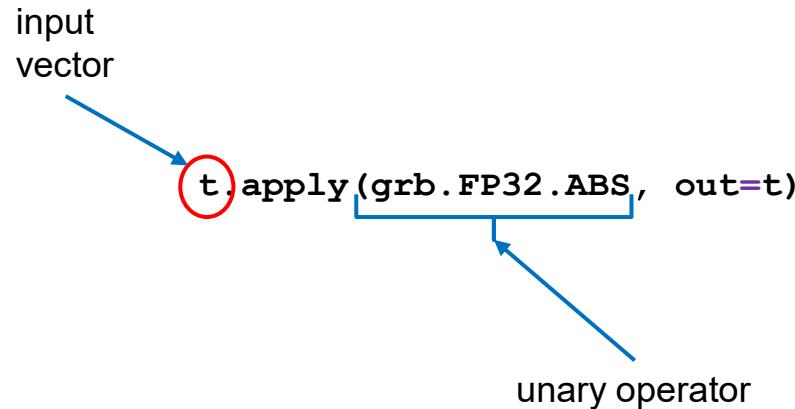
input  
vector



```
t.apply(grb.FP32.ABS, out=t)
```

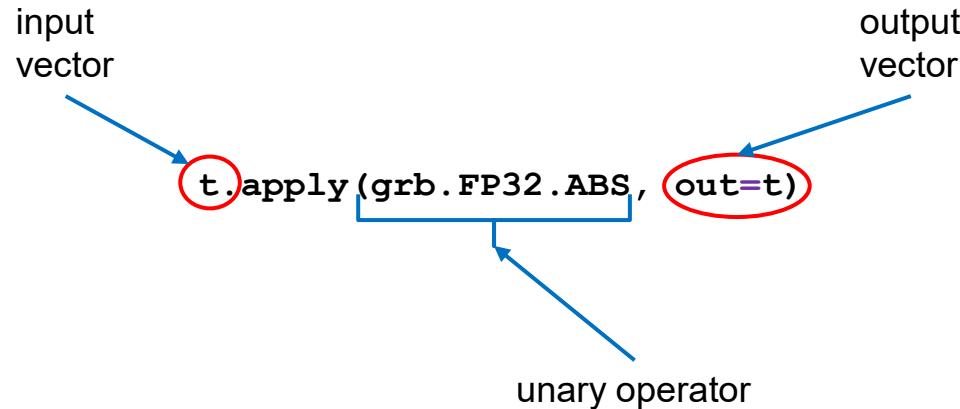
# apply operation

Name	Math	pygraphblas examples ( <code>import pygraphblas as grb</code> )
apply (vector)	$u \odot= f(v)$	<code>apply(self, op, out=None, mask=None, accum=None, desc=None)</code>
apply (matrix)	$C \odot= f(A)$	<code>apply(self, op, out=None, mask=None, accum=None, desc=None)</code>



# apply operation

Name	Math	pygraphblas examples ( <code>import pygraphblas as grb</code> )
apply (vector)	$u \odot= f(v)$	<code>apply(self, op, out=None, mask=None, accum=None, desc=None)</code>
apply (matrix)	$C \odot= f(A)$	<code>apply(self, op, out=None, mask=None, accum=None, desc=None)</code>



# Exercise 14: Solution

```
def pagerank(A, damping = 0.85, tol = 1e-4, itermax = 100):
    n = A.nrows
    t = grb.Vector.dense(grb.FP32, n)
    r = grb.Vector.dense(grb.FP32, n, fill = 1.0/n) # r[:] = 1.0/n
    d = grb.Vector.dense(grb.FP32, n, fill=damping) # d[:] = damping
    A.reduce_vector(out=d, accum=grb.FP32.DIV,
                    mon=grb.FP32.PLUS_MONOID)

    for i in range(itermax):
        t[:] = r[:]
        w = t * d
        r[:] = (1 - damping) / n
        w.vxm(A, out=r, accum=grb.FP32.PLUS,
               semiring=grb.FP32.PLUS_TIMES)

        # test for convergence
        t = t - r
        t.apply(grb.FP32.ABS, out=t)
        rdiff = t.reduce_float(grb.FP32.PLUS_MONOID)
        if rdiff <= tol:
            break

    return r
```

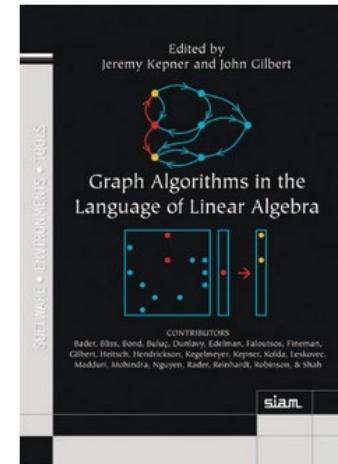
# The GraphBLAS Operations of PageRank

Operation Name	Mathematical Notation
mxm	$C \langle M, r \rangle = C \odot A \oplus . \otimes B$
mxv	$w \langle m, r \rangle = w \odot A \oplus . \otimes u$
vxm	$w^T \langle m^T, r \rangle = w^T \odot u^T \oplus . \otimes A$
eWiseMult	$C \langle M, r \rangle = C \odot A \otimes B$
	$w \langle m, r \rangle = w \odot u \otimes v$
eWiseAdd	$C \langle M, r \rangle = C \odot A \oplus B$
	$w \langle m, r \rangle = w \odot u \oplus v$
extract	$C \langle M, r \rangle = C \odot A(i, j)$
	$w \langle m, r \rangle = w \odot u(i)$
assign	$C \langle M, r \rangle(i, j) = C(i, j) \odot A$
	$w \langle m, r \rangle(i) = w(i) \odot u$
reduce (row)	$w \langle m, r \rangle = w \odot [\oplus_j A(:, j)]$
reduce (scalar)	$s = s \odot [\oplus_{i,j} A(i, j)]$
	$s = s \odot [\oplus_i u(i)]$
apply	$C \langle M, r \rangle = C \odot f_u(A)$
	$w \langle m, r \rangle = w \odot f_u(u)$
apply(indexop)	$C \langle M, r \rangle = C \odot f_i(A, \text{ind}(A), s)$
	$w \langle m, r \rangle = w \odot f_i(u, \text{ind}(u), s)$
select	$C \langle M, r \rangle = C \odot A \langle f_i(A, \text{ind}(A), s) \rangle$
	$w \langle m, r \rangle = w \odot u \langle f_i(u, \text{ind}(u), s) \rangle$
transpose	$C \langle M, r \rangle = C \odot A^T$
kronecker	$C \langle M, r \rangle = C \odot A \otimes B$

We've expanded our repertoire of GraphBLAS operations

# Conclusion and next steps

- The GraphBLAS define a standard API for “Graph Algorithms in the Language of Linear Algebra”.
  - <https://github.com/GraphBLAS/LAGraph>
- A wide range of algorithms are variations of the basic breadth first traversal for a graph.
- To reach GraphBLAS mastery
  - Attend the Graph Architectures Programming and Learning (GrAPL) workshop at IPDPS
  - Attend GraphBLAS BoFs at HPEC and Supercomputing
  - Explore the challenge problems included with this tutorial
  - Work through the algorithms in the Graph book →



# Appendices

- 
- MxM: the low-level details of the GraphBLAS operations
  - Common patterns for algorithmic reasoning
  - Challenge Problems:
    - Some key algorithms with the GraphBLAS
  - Reference materials

# GraphBLAS: details of operations

- When you read the GraphBLAS C API specification, the operations are described in a manner that may seem obtuse.
- The definitions, however, are presented in this way for good reasons:
  - to cover the full range of variations exposed by the various arguments and to express the operation without ever specifying the undefined elements (i.e. the “zeros” of the semiring).
  - To avoid any reference to the non-stored elements of the sparse matrix. In sparse arrays, the undefined elements are usually assumed to be the “zero of the semiring”. By defining the operations without any reference to those “un-stored values”, we can freely change the semirings between operations without having to update the un-stored elements.

**GrB\_mxm()**

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

Matrix Multiplication ... the way we learned it in school

$$\mathbf{C}(i, j) = \bigoplus_{k=1}^l \mathbf{A}(i, k) \otimes \mathbf{B}(k, j)$$

$$\mathbf{A} : \mathbb{S}^{m \times l}$$

$$\mathbf{B} : \mathbb{S}^{l \times n}$$

$$\mathbf{C} : \mathbb{S}^{m \times n}$$

---

Matrix Multiplication ... set notation to ignore un-stored elements

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

With set notation, it's easier to define the operations over a matrix as  
the semi-ring changes

# GrB\_mxM(): Function Signature

```
GrB_Info GrB_mxM(GrB_Matrix           *C,
                  const GrB_Matrix      Mask,
                  const GrB_BinaryOp    accum,
                  const GrB_Semiring    op,
                  const GrB_Matrix       A,
                  const GrB_Matrix       B,
                  const GrB_Descriptor  desc);
```

**C** (INOUT) An existing GraphBLAS matrix. On input, the matrix provides values that may be accumulated with the result of the matrix product. On output, the matrix holds the results of this operation.

**Mask** (IN) A “write” mask that controls which results from this operation are stored into the output matrix C (optional). If no mask is desired, GrB\_NULL is specified. The Mask dimensions must match those of the matrix C and the domain of the Mask matrix must be of type bool or any “built-in” GraphBLAS type.

**accum** (IN) A binary operator used for accumulating entries into existing C entries. For assignment rather than accumulation, GrB\_NULL is specified.

**op** (IN) Semiring used in the matrix-matrix multiply:  $\text{op} = \langle D_1, D_2, D_3, \oplus, \otimes, 0 \rangle$ .

**A** (IN) The GraphBLAS matrix holding the values for the left-hand matrix in the multiplication.

**B** (IN) The GraphBLAS matrix holding the values for the right-hand matrix in the multiplication.

**desc** (IN) Operation descriptor (optional). If a *default* descriptor is desired, GrB\_NULL should be used. Valid fields are as follows:

Argument	Field	Value	Description
C	GrB_OUTP	GrB_REPLACE	Output matrix C is cleared (all elements removed) before result is stored in it.
Mask	GrB_MASK	GrB_SCMP	Use the structural complement of Mask.
A	GrB_INP0	GrB_TRAN	Use transpose of A for operation.
B	GrB_INP1	GrB_TRAN	Use transpose of B for operation.

# GrB\_mxM(): Function Signature

```
GrB_Info GrB_mxM(GrB_Matrix           *C,  
                  const GrB_Matrix      Mask,  
                  const GrB_BinaryOp    accum,  
                  const GrB_Semiring    op,  
                  const GrB_Matrix       A,  
                  const GrB_Matrix       B,  
                  const GrB_Descriptor desc);
```

GrB\_Info return values:

GrB_SUCCESS	Blocking mode: Operations completed successfully. Nonblocking mode: consistency tests passed on dimensions and domains for input arguments
GrB_PANIC	Unknown Internal error
GrB_OUTOFMEM	Not enough memory for the operation
GrB_DIMENSION_MISMATCH	Matrix dimensions are incompatible.
GrB_DOMAIN_MISMATCH	Domains of matrices are incompatible with the domains of the accumulator, semiring, or mask.

# Standard function behavior

- Consider the following code:

```
GrB_Descriptor_new(&desc) ;  
GrB_Descriptor_set(desc, GrB_OUTP, GrB_REPLACE) ;  
GrB_Descriptor_set(desc, GrB_INP0, GrB_TRANS) ;  
GrB_mxm(&C, M, Int32Add, Int32AddMul, A, B, desc) ;
```

int32AddMul semiring  
int32Add accumulation

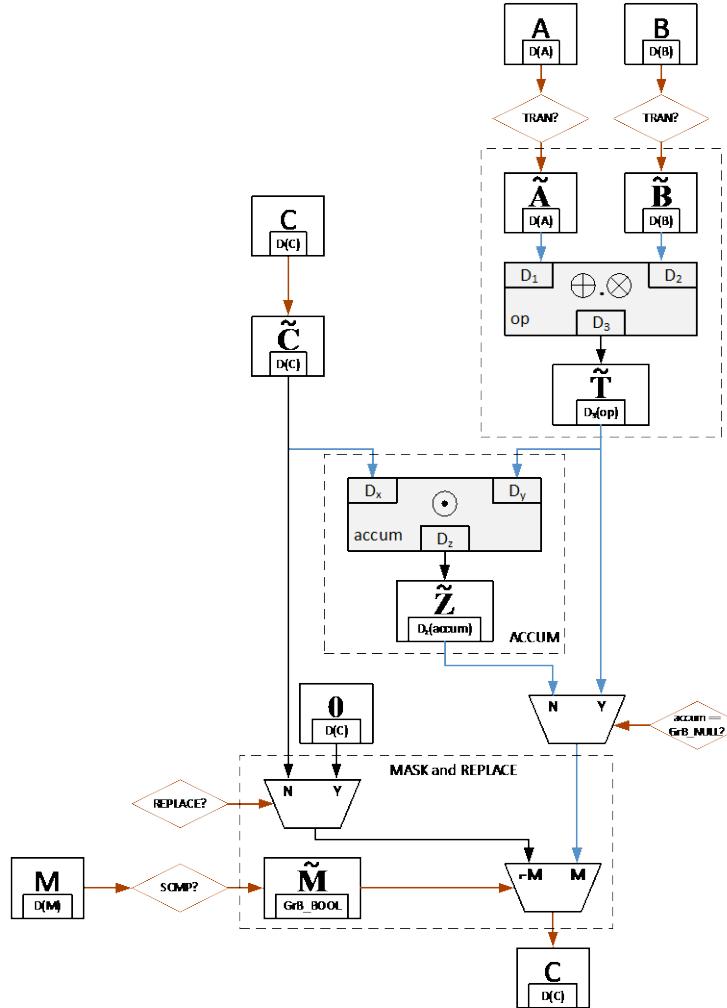
Form input operands and mask based on descriptor	C, B, M, A $\leftarrow A^T$
Test the domains and sizes for consistency.	int32, dims match
Carry out the indicated operation	$T \leftarrow A *_{\cdot} + B$ , $Z \leftarrow C + T$
Apply the write-mask to select output values	$Z \leftarrow Z \cap M$
Replace mode: delete elements in output object and replace with output values	$C \leftarrow Z$
Merge mode: Assign output value (i,j) to element (i,j) of output object, but leave other elements of the output object alone.	

# MXM flowchart

To understand what happens inside a graphBLAS operation, consider matrix multiply.

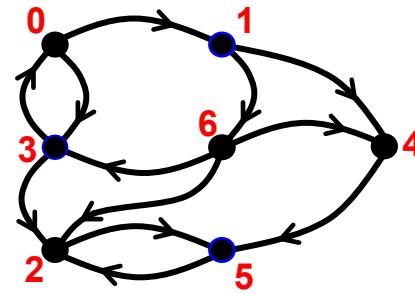
All the operations follow this basic format

```
GrB_Info GrB_mxm(  
    GrB_Matrix          C,  
    const GrB_Matrix     M,  
    const GrB_BinaryOp   accum,  
    const GrB_Semiring   op,  
    const GrB_Matrix     A,  
    const GrB_Matrix     B,  
    const GrB_Descriptor desc);
```



# Exercise: Matrix Matrix Multiplication

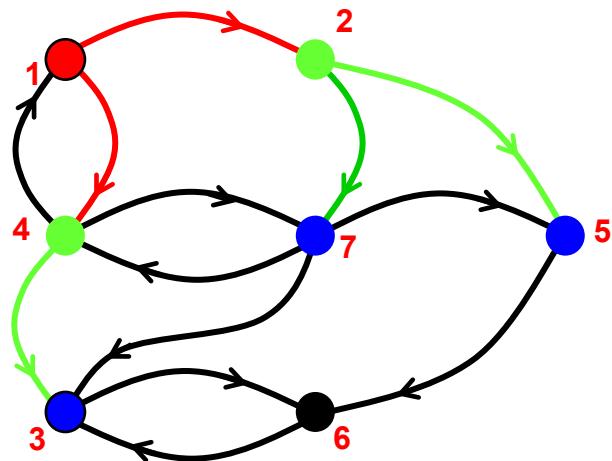
- Multiply the adjacency matrix from our “logo graph” by itself.
- Print resulting matrix and interpret the result
- Hint: Do the multiply again and compare results.  
Do you see the pattern?



# Appendices

- MxM: the low-level details of the GraphBLAS operations
- • Common patterns for algorithmic reasoning
- Challenge Problems:
  - Some key algorithms with the GraphBLAS
- Reference materials

# SpMSpV: Sparse-Matrix/Sparse-Vector Multiplication



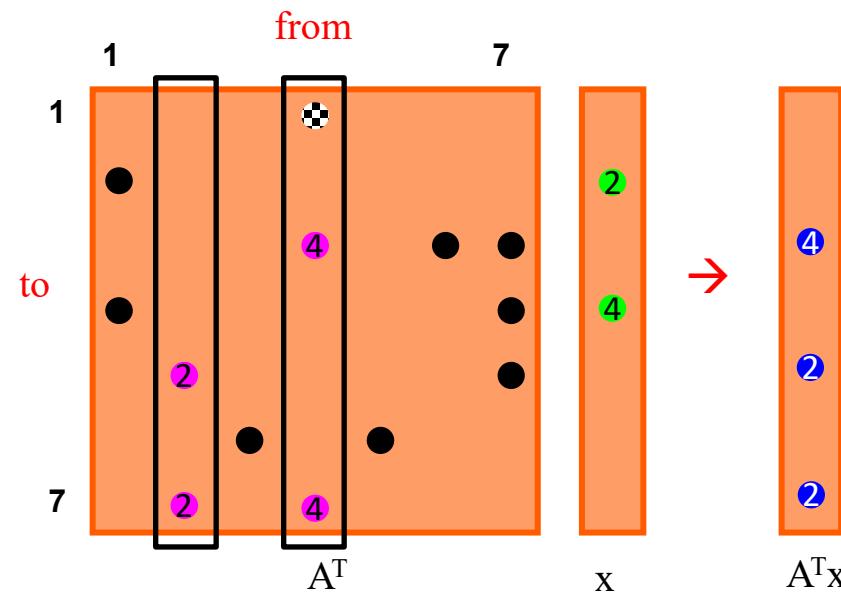
parents (p):

0  
1  
4  
1  
2  
2

**SpMSpV: single-source graph traversal**  
Used in BFS, CC, matching, ordering, etc.

$y = A \cdot mxv(x, \text{mask}=p, \text{desc}=\text{descriptor.T0})$

A: sparse adjacency matrix  
x: sparse input vector (previous frontier)  
p: mask (already discovered vertices)



# SpMSpM: Sparse-Matrix/Sparse-Matrix Multiplication

**SpGEMM: multi-source graph traversal**

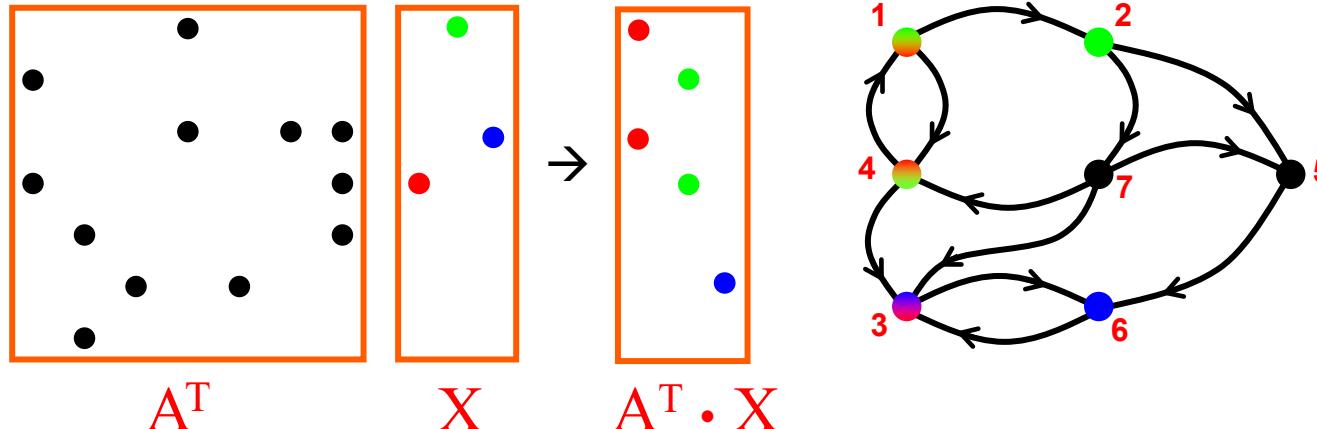
Ex: multi-source BFS, betweenness centrality, triangle counting\*, Markov clustering\*

`Y=A.mxm(X, mask=P, desc=descriptor.T0)`

A: sparse adjacency matrix

X: sparse input matrix (previous frontier), n-by-b where b is the #sources

P: mask (already discovered vertices), multi-vector version of p from previous slide



\*: shown in later slides

# SpMM: Sparse-Matrix/dense-Matrix Multiplication

SpMM: feature aggregation from neighbors

Used in Graph neural networks, graph embedding, etc.

$W = A \text{.mxm}(H, \text{desc=descriptor.T0})$

A: sparse adjacency matrix, n-by-n

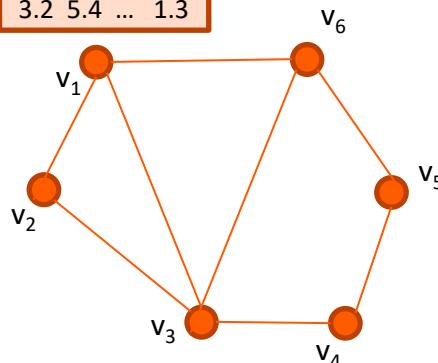
H: input dense matrix, n-by-f where  $f \ll n$  is the feature dimension

W: output dense matrix, new features

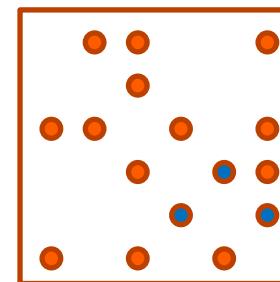
We call this  
dense matrix,  
H, a “tall  
skinny”  
Matrix

$O(f)$  feature vector

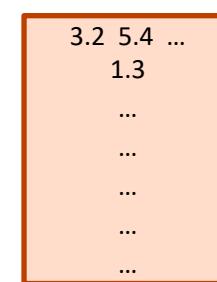
3.2 5.4 ... 1.3



$W =$



$A^T$

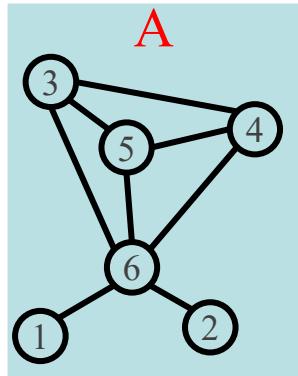


$H$

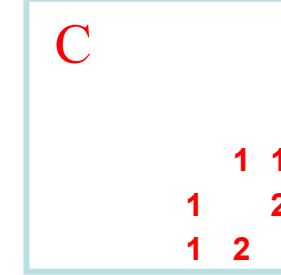
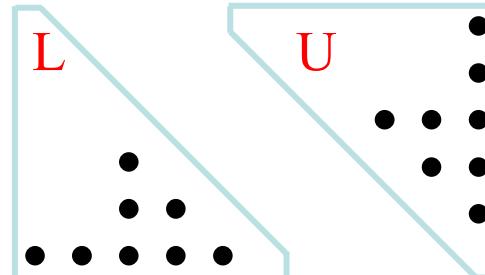
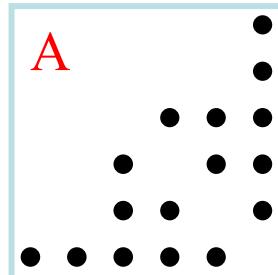
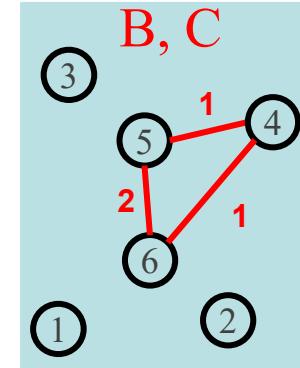
# SpMSpM Example: Triangle Counting

Triangle counting is also multi-source(in fact, all sources) traversal.  
It just stops after one traversal iteration only, discovering all wedges

$$B = L \cdot mxm(U)$$



$A = L + U$  (hi->lo + lo->hi)  
 $L \times U = B$  (wedge, low hinge)  
 $A \wedge B = C$  (closed wedge)  
 $\text{sum}(C)/2 = 4 \text{ triangles}$



# SpMSpM Example: Triangle Counting

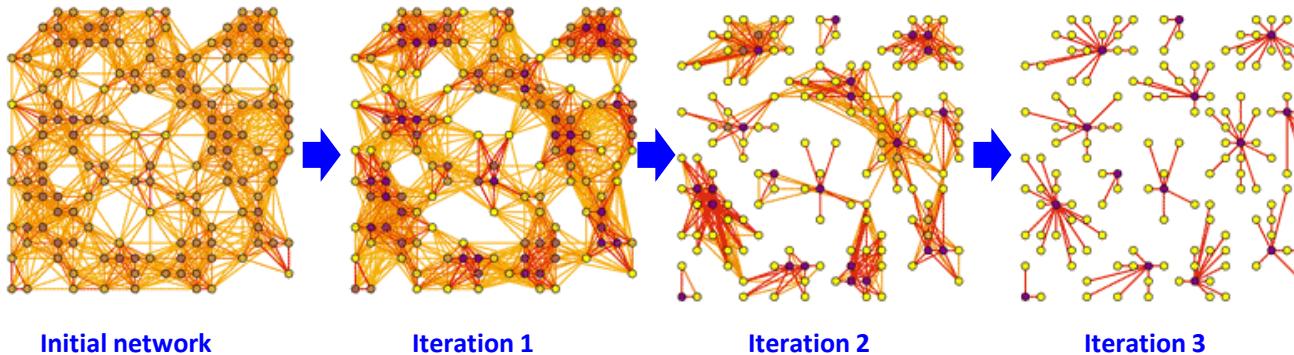
Markov clustering is also multi-source (in fact, all sources) traversal.

It alternates between SpGEMM and element-wise or column-wise pruning

```
C=A.mxm(A, desc=descriptor.TOT1)
```

A: sparse normalized adjacency matrix

C: denser (but still sparse) pre-pruned matrix for next iteration



At each iteration:

**Step 1 (Expansion):** Squaring the matrix while pruning (a) small entries, (b) denser columns

**Naïve implementation:** sparse matrix-matrix product (SpGEMM), followed by column-wise top-K selection and column-wise pruning

**Step 2 (Inflation) :** taking powers entry-wise

# Appendices

- MxM: the low-level details of the GraphBLAS operations
- Common patterns for algorithmic reasoning
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# Challenge problems

- Triangle counting
- Direction optimizing Breadth first search
- Betweenness Centrality

# Notation

operation/method	description	notation
<code>mxm</code>	matrix-matrix multiplication	$C(M) \odot= A \oplus_{\cdot} \otimes B$
<code>vxm</code>	vector-matrix multiplication	$w^T \langle m^T \rangle \odot= u^T \oplus_{\cdot} \otimes A$
<code>mxv</code>	matrix-vector multiplication	$w \langle m \rangle \odot= A \oplus_{\cdot} \otimes u$
<code>eWiseAdd</code>	element-wise addition using operator $\text{op}$ on elements in the set union of structures of $A/B$ and $u/v$	$C(M) \odot= A \text{ op}_{\cup} B$ $w \langle m \rangle \odot= u \text{ op}_{\cup} v$
<code>eWiseMult</code>	element-wise multiplication using operator $\text{op}$ on elements in the set intersection of structures of $A/B$ and $u/v$	$C(M) \odot= A \text{ op}_{\cap} B$ $w \langle m \rangle \odot= u \text{ op}_{\cap} v$
<code>extract</code>	extract submatrix from matrix $A$ using indices $i$ and indices $j$ extract the $j$ th column vector from matrix $A$ extract subvector from $u$ using indices $i$	$C(M) \odot= A(i,j)$ $w \langle m \rangle \odot= A(:,j)$ $w \langle m \rangle \odot= u(i)$
<code>assign</code>	assign matrix to submatrix with mask for $C$ assign scalar to submatrix with mask for $C$ assign vector to subvector with mask for $w$ assign scalar to subvector with mask for $w$	$C(M) \langle i,j \rangle \odot= A$ $C(M) \langle i,j \rangle \odot= s$ $w \langle m \rangle \langle i \rangle \odot= u$ $w \langle m \rangle \langle i \rangle \odot= s$
<code>subassign</code> (GxB)	assign matrix to submatrix with submask for $C(i,j)$ assign scalar to submatrix with submask for $C(i,j)$ assign vector to subvector with submask for $w(i)$ assign scalar to subvector with submask for $w(i)$	$C(i,j)(M) \odot= A$ $C(i,j)(M) \odot= s$ $w(i)\langle m \rangle \odot= u$ $w(i)\langle m \rangle \odot= s$
<code>apply</code>	apply unary operator $f$ with optional thunk $k$	$C(M) \odot= f(A, k)$ $w \langle m \rangle \odot= f(u, k)$
<code>select</code>	apply select operator $f$ with optional thunk $k$	$C(M) \odot= f(A, k)$ $\dots$
<code>reduce</code>	row-wise reduce matrix to column vector reduce matrix to scalar reduce vector to scalar	$w \langle m \rangle \odot= [\oplus_j A(:,j)]$ $s \odot= [\oplus_{i,j} A(i,j)]$ $s \odot= [\oplus_i u(i)]$
<code>transpose</code>	transpose	$C(M) \odot= A^T$
<code>dup</code>	duplicate matrix duplicate vector	$C \leftrightarrow A$ $w \leftrightarrow u$
<code>build</code>	matrix from tuples vector from tuples	$C \leftrightarrow \{i,j,x\}$ $w \leftrightarrow \{i,x\}$
<code>extractTuples</code>	extract index arrays $(i,j)$ and value arrays $(x)$	$\{i,j,x\} \leftrightarrow A$ $\{i,x\} \leftrightarrow u$
<code>extractElement</code>	extract element to scalar	$s = A(i,j)$ $s = u(i)$
<code>setElement</code>	set element	$C(i,j) = s$ $w(i) = s$

# Triangle Counting

---

**Algorithm 6:** Triangle counting.

---

**Data:**  $\mathbf{A} \in \mathbb{B}^{n \times n}$

**Result:**  $t \in \text{UINT64}$

1 **Function** *TriangleCount*

2     sample the *mean* and *median* degree of  $\mathbf{A}$

3     **if** *mean* >  $4 \times \text{median}$  **then**

4          $\mathbf{p}$  = permutation to sort degree, ascending order

5          $\mathbf{A} = \mathbf{A}(\mathbf{p}, \mathbf{p})$

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

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

8          $\mathbf{C}\langle s(\mathbf{L}) \rangle = \mathbf{L} \text{ plus.pair } \mathbf{U}^T$

9          $t = [+_{ij} \mathbf{C}(i, j)]$

# Breadth First Search

---

**Algorithm 2:** Direction-Optimizing Parent BFS.

---

**Input:**  $\mathbf{A}, \mathbf{A}^T, startVertex$

1 **Function** *DirectionOptimizingBFS*

2    $q(startVertex) = 0$

3   **for**  $level = 1$  **to**  $nrows(\mathbf{A}) - 1$  **do**

4     **if** *Push*( $\mathbf{A}, q$ ) **then**

5        $q^T \langle \neg s(p^T), r \rangle = q^T \text{ any. secondi } \mathbf{A}$

6       **else**

7        $q \langle \neg s(p), r \rangle = \mathbf{A}^T \text{ any. secondi } q$

8        $p(s(q)) = q$

9       **if** *nvals*( $q$ ) = 0 **then**

10        **return**

---

# Betweenness Centrality

Algorithm 3: Betweenness centrality.

```
1 Function BrandesBC
2   // P(k, j) = # paths from kth source to node j
3   // F: # paths in the current frontier
4   let:  $\mathbf{P} \in \mathbb{Q}_{64}^{ns \times n}$ 
5   let:  $\mathbf{F} \in \mathbb{Q}_{64}^{ns \times n}$ 
6    $\mathbf{P}(1 : k, s) = 1$ 
7   // First frontier:
8    $\mathbf{F}(\neg s(\mathbf{P})) = \mathbf{P}$  plus.first  $\mathbf{A}$ 
9   // BFS phase:
10  for  $d = 0$  to nrows( $\mathbf{A}$ ) do
11    let:  $\mathbf{S}[d] \in \mathbb{B}^{ns \times n}$ 
12     $\mathbf{S}[d](s(\mathbf{F})) = 1$  // S[d] = pattern of F
13     $\mathbf{P} += \mathbf{F}$ 
14     $\mathbf{F}(\neg s(\mathbf{P}), r) = \mathbf{F}$  plus.first  $\mathbf{A}$ 
15    if nvals( $\mathbf{F}$ ) = 0 then
16      break
17
18  // Backtrack phase:
19  let:  $\mathbf{B} \in \mathbb{Q}_{64}^{ns \times n}$ 
20   $\mathbf{B}(:) = 1.0$ 
21  let:  $\mathbf{W} \in \mathbb{Q}_{64}^{ns \times n}$ 
22  for  $i = d - 1$  downto 0 do
23     $\mathbf{W}(s(\mathbf{S}[i]), r) = \mathbf{B} \text{ div}_\cap \mathbf{P}$ 
24     $\mathbf{W}(s(\mathbf{S}[i - 1]), r) = \mathbf{W}$  plus.first  $\mathbf{A}^\top$ 
25     $\mathbf{B} += \mathbf{W} \times_\cap \mathbf{P}$ 
26
27  // centrality(j) =  $\sum_i (\mathbf{B}(i, j) - 1)$ 
28   $\mathbf{centrality}(:) = -ns$ 
29   $\mathbf{centrality} += [+_i \mathbf{B}(i, :)])$ 
```

# Appendices

- MxM: the low-level details of the GraphBLAS operations
- Common patterns for algorithmic reasoning
- Challenge Problems:
  - Some key algorithms with the GraphBLAS
- • Reference materials

# Full set of GraphBLAS opaque objects

Table 2.1: GraphBLAS opaque objects and their types.

GrB_Object types	Description
GrB_Type	User-defined scalar type.
GrB_UnaryOp	Unary operator, built-in or associated with a single-argument C function.
GrB_BinaryOp	Binary operator, built-in or associated with a two-argument C function.
GrB_Monoid	Monoid algebraic structure.
GrB_Semiring	A GraphBLAS semiring algebraic structure.
GrB_Matrix	Two-dimensional collection of elements; typically sparse.
GrB_Vector	One-dimensional collection of elements.
GrB_Descriptor	Descriptor object, used to modify behavior of methods.

# Error codes returned by GraphBLAS methods

## API Errors

Error code	Description
GrB_UNINITIALIZED_OBJECT	A GraphBLAS object is passed to a method before new was called on it.
GrB_NULL_POINTER	A NULL is passed for a pointer parameter.
GrB_INVALID_VALUE	Miscellaneous incorrect values.
GrB_INVALID_INDEX	Indices passed are larger than dimensions of the matrix or vector being accessed.
GrB_DOMAIN_MISMATCH	A mismatch between domains of collections and operations when user-defined domains are in use.
GrB_DIMENSION_MISMATCH	Operations on matrices and vectors with incompatible dimensions.
GrB_OUTPUT_NOT_EMPTY	An attempt was made to build a matrix or vector using an output object that already contains valid tuples (elements).
GrB_NO_VALUE	A location in a matrix or vector is being accessed that has no stored value at the specified location.

# Error codes returned by GraphBLAS methods

## Execution Errors

Error code	Description
GrB_OUT_OF_MEMORY	Not enough memory for operations.
GrB_INSUFFICIENT_SPACE	The array provided is not large enough to hold output.
GrB_INVALID_OBJECT	One of the opaque GraphBLAS objects (input or output) is in an invalid state caused by a previous execution error.
GrB_INDEX_OUT_OF_BOUNDS	Reference to a vector or matrix element that is outside the defined dimensions of the object.
GrB_PANIC	Unknown internal error.

# GraphBLAS predefined operators

- A subset of operators from Table 2.3 of the GraphBLAS specification

Identifier	Domains	Description	
GrB_LOR	bool x bool $\rightarrow$ bool	$f(x,y) = x \vee y$	Logical OR
GrB_LAND	bool x bool $\rightarrow$ bool	$f(x,y) = x \wedge y$	Logical AND
GrB_EQ_T	$T \times T \rightarrow$ bool	$f(x,y) = (x==y)$	Equal
GrB_MIN_T	$T \times T \rightarrow T$	$f(x,y) = (x < y) ? x : y$	minimum
GrB_MAX_T	$T \times T \rightarrow T$	$f(x,y) = (x > y) ? x : y$	maximum
GrB_PLUS_T	$T \times T \rightarrow T$	$f(x,y) = x + y$	addition
GrB_TIMES_T	$T \times T \rightarrow T$	$f(x,y) = x * y$	multiplication
GrB_FIRST_T	$T \times T \rightarrow T$	$f(x,y) = x$	First argument
GrB_SECOND_T	$T \times T \rightarrow T$	$f(x,y) = y$	Second argument

Where  $T$  is a suffix indicating type and includes **FP32**, **FP64**, **INT32**, **UINT32**, **BOOL**

Note: **GrB\_FIRST** and **GrB\_SECOND** are not commutative operators

This is a subset of the defined types and operators. See table 2.3 for the full list.

# GraphBLAS Operations (a subset from the Math Spec\*)

Name	Math	pygraphblas examples ( <code>import pygraphblas as grb</code> )
mxm	$C \odot= A \oplus\otimes B$	<code>mxm(self, other, cast=None, out=None, semiring=None, mask=None, accum=None, desc=None)</code>
mxv	$w \odot= A \oplus\otimes v$	<code>mxv(self, other, cast=None, out=None, semiring=None, mask=None, accum=None, desc=None)</code>
vxm	$w^T \odot= v^T \oplus\otimes A$	<code>vxm(self, other, cast=None, out=None, semiring=None, mask=None, accum=None, desc=None)</code>
eWiseMult	$C \odot= A \otimes B$	<code>emult(self, other, mult_op=None, cast=None, out=None, mask=None, accum=None, desc=None)</code>
	$w \odot= u \otimes v$	<code>emult(self, other, mult_op=None, cast=None, out=None, mask=None, accum=None, desc=None)</code>
eWiseAdd	$C \odot= A \oplus B$	<code>eadd(self, other, add_op=None, cast=None, out=None, mask=None, accum=None, desc=None)</code>
	$w \odot= u \oplus v$	<code>eadd(self, other, add_op=None, cast=None, out=None, mask=None, accum=None, desc=None)</code>
reduce	$w \odot= \bigoplus_j A(:,j)$	<code>reduce_vector(self, mon=None, out=None, mask=None, accum=None, desc=None)</code>

\* Mathematical foundations of the GraphBLAS, Kepner et. al. HPEC'2016

# GraphBLAS Operations (a subset from the Math Spec\*)

Name	Math	pygraphblas examples ( <code>import pygraphblas as grb</code> )
mxm	$C \odot= A \oplus_{\cdot} \otimes B$	<code>A.mxm(B, out=C, accum=grb.INT64.PLUS)</code>  <code>with Accum=grb.INT64.PLUS:</code> <code>C = A@B</code>
mxv	$w \odot= A \oplus_{\cdot} \otimes v$	<code>with grb.INT64.PLUS_TIMES:</code> <code>w = A@v</code>
vxm	$w^T \odot= v^T \oplus_{\cdot} \otimes A$	<code>w = v.vxm(A, mask=None, accum=grb.FP32.PLUS)</code>
eWiseMult	$C \odot= A \otimes B$  $w \odot= u \otimes v$	<code>A.emult(B, out=C, accum=grb.INT32.PLUS)</code>  <code>w=u*v</code>
eWiseAdd	$C \odot= A \oplus B$  $w \odot= u \oplus v$	<code>C = A+B</code>  <code>w=y.eadd(v, add_op=grb.FP64.DIV)</code>
reduce	$w \odot= \bigoplus_j A(:,j)$	<code>A.reduce_vector(out=w, accum=grb.FP32.PLUS)</code>

\* Mathematical foundations of the GraphBLAS, Kepner et. al. HPEC'2016