Structural Zeros in GraphBLAS

(*Working document for discussion with the* GraphBLAS *team at large*)

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1 Introduction

When vectors and matrices are used to represent adjacency matrices, sets of vertices, sets of edges, and properties of those edges and vertices, the elements of those vectors and matrices have to represent two different concepts. First, they have to represent the presence or absence of an edge or vertex. Second, they have to represent values associated with those vertices and edges, such as weight or capacity.

Sparse matrices and vectors lead themselves to this dual representation role. A missing edge or vertex is denoted by the absence of the corresponding element in the sparse representation of the matrix or vector. We call those element *structural zeros*. When an element is present and its value is zero, we call it a *zero value*.

We believe it is important to distinguish between structural zeros and zero values. In particular, when performing operations on semirings, structural zeros *always* act as the addition identity and multiplication annihilator. The zero value behavior depends on the actual addition and multiplication operators for that semiring. (That is, the semiring zero may not be the standard zero (0) value. For example, in an *arctic semiring*, the zero is $-\infty$.)

This document presents a formulation for the GraphBLAS operations that focuses on the structural zeros of vectors and matrices. In particular, it ensures that structural zeros always behave as the addition identity and multiplication annihilator. Furthermore, it defines a precise semantics even when the data values and operators do not constitute a semiring. (For example, in the case of floating-point numbers or user-defined operators.) It is really meant to be a working document and to serve as a discussion point only. In its current state, the document only defines some functions of the GraphBLAS, although we believe the formulation can be extended to all proposed operations.

2 Basic concepts

Let Ω be an integer ≥ 1. An *index* is an integer in the range $[0, \Omega)$.

Let D be a set of unique values. An element of D is called a *scalar*.

A vector $\mathbf{v} = \{(i, \mathbf{v}(i))\}$ is a set of tuples $(i, \mathbf{v}(i))$ where $0 \leq i < \Omega$ and $\mathbf{v}(i) \in D$. A particular value of i can only appear at most once in $\mathbf{v}$. We also define the set $\mathbf{i}(\mathbf{v}) = \{i \mid (i, \mathbf{v}(i)) \in \mathbf{v}\}$.

A matrix $\mathbf{A} = \{(i, j, \mathbf{A}(i, j))\}$ is a set of tuples $(i, j, \mathbf{A}(i, j))$ where $0 \leq i < \Omega$, $0 \leq j < \Omega$, and $\mathbf{A}(i, j) \in D$. A particular pair of values i, j can only appear at most once in $\mathbf{A}$. We also define the sets $\mathbf{i}(\mathbf{A}) = \{i \mid \exists (i, j, \mathbf{A}(i, j)) \in \mathbf{A}\}$ and $\mathbf{j}(\mathbf{A}) = \{j \mid \exists (i, j, \mathbf{A}(i, j)) \in \mathbf{A}\}$. (These are the sets of nonempty rows and columns of $\mathbf{A}$, respectively.)

If $\mathbf{A}$ is a matrix, then $\mathbf{A}(:, j) = \{(i, \mathbf{A}(i, j)) \mid (i, j, \mathbf{A}(i, j)) \in \mathbf{A}\}$ is a vector called the j-th *column* of $\mathbf{A}$. Correspondingly, if $\mathbf{A}$ is a matrix, then $\mathbf{A}(i, :) = \{(j, \mathbf{A}(i, j)) \mid (i, j, \mathbf{A}(i, j)) \in \mathbf{A}\}$ is a vector called the i-th *row* of $\mathbf{A}$. We will use rows and columns when defining operations on matrices.

3 Operations

We here define just a subset of the proposed GraphBLAS operations. It is our goal to extend this approach to all operations but we believe this subset illustrates the principles of the approach. Also, although we only show variants with mask (and negated mask) for one operation (**vxm**), we plan to add such variants to most (if not all) operations.

$\mathbf{w} = \mathbf{ewiseadd}(\mathbf{u}, \oplus, \mathbf{v})$

Let $\mathbf{u}$ and $\mathbf{v}$ be vectors. Then, $\mathbf{w}$ is a vector defined as follows:

$$\begin{aligned} \mathbf{i}(\mathbf{w}) &= \mathbf{i}(\mathbf{u}) \cup \mathbf{i}(\mathbf{v}) && (1) \\ \mathbf{w}(i) &= \mathbf{u}(i) \oplus \mathbf{v}(i), \forall i \in (\mathbf{i}(\mathbf{u}) \cap \mathbf{i}(\mathbf{v})) && (2) \\ \mathbf{w}(i) &= \mathbf{u}(i), \forall i \in (\mathbf{i}(\mathbf{w}) - \mathbf{i}(\mathbf{v})) && (3) \\ \mathbf{w}(i) &= \mathbf{v}(i), \forall i \in (\mathbf{i}(\mathbf{w}) - \mathbf{i}(\mathbf{u})) && (4) \end{aligned}$$

$\mathbf{w} = \mathbf{ewiseadd}(\mathbf{u}, \oplus, a)$

Let $\mathbf{u}$ be a vector and a be a scalar. Then, $\mathbf{w}$ is a vector defined as follows:

$$\begin{aligned} \mathbf{i}(\mathbf{w}) &= \mathbf{i}(\mathbf{u}) && (5) \\ \mathbf{w}(i) &= \mathbf{u}(i) \oplus a, \forall i \in \mathbf{i}(\mathbf{w}) && (6) \end{aligned}$$

$\mathbf{w} = \mathbf{ewiseadd}(a, \oplus, \mathbf{u})$

Let $\mathbf{u}$ be a vector and a be a scalar. Then, $\mathbf{w}$ is a vector defined as follows:

$$\begin{aligned} \mathbf{i}(\mathbf{w}) &= \mathbf{i}(\mathbf{u}) && (7) \\ \mathbf{w}(i) &= a \oplus \mathbf{u}(i), \forall i \in \mathbf{i}(\mathbf{w}) && (8) \end{aligned}$$

$\mathbf{w} = \mathbf{ewisemult}(\mathbf{u}, \otimes, \mathbf{v})$

Let $\mathbf{u}$ and $\mathbf{v}$ be vectors. Then, $\mathbf{w}$ is a vector defined as follows:

$$\begin{aligned} \mathbf{i}(\mathbf{w}) &= \mathbf{i}(\mathbf{u}) \cap \mathbf{i}(\mathbf{v}) && (9) \\ \mathbf{w}(i) &= \mathbf{u}(i) \otimes \mathbf{v}(i), \forall i \in \mathbf{i}(\mathbf{w}) && (10) \end{aligned}$$

$\mathbf{w} = \mathbf{ewisemult}(\mathbf{u}, \otimes, a)$

Let $\mathbf{u}$ be a vector and a be a scalar. Then, $\mathbf{w}$ is a vector defined as follows:

$$\begin{aligned} \mathbf{i}(\mathbf{w}) &= \mathbf{i}(\mathbf{u}) && (11) \\ \mathbf{w}(i) &= \mathbf{u}(i) \otimes a, \forall i \in \mathbf{i}(\mathbf{w}) && (12) \end{aligned}$$

$\mathbf{w} = \mathbf{ewisemult}(a, \otimes, \mathbf{u})$

Let $\mathbf{u}$ be a vector and a be a scalar. Then, $\mathbf{w}$ is a vector defined as follows:

$$\begin{aligned} \mathbf{i}(\mathbf{w}) &= \mathbf{i}(\mathbf{u}) && (13) \\ \mathbf{w}(i) &= a \otimes \mathbf{u}(i), \forall i \in \mathbf{i}(\mathbf{w}) && (14) \end{aligned}$$

$\mathbf{c} = \mathbf{vxm}(\mathbf{a}, \oplus, \otimes, \mathbf{B})$

Let $\mathbf{a}$ be a vector and let $\mathbf{B}$ be a matrix. Then $\mathbf{c}$ is a vector defined as follows:

$$\begin{aligned} \mathbf{c} &= \emptyset && (15) \\ \mathbf{for}(i \in \mathbf{i}(\mathbf{a}))\ \mathbf{c} &= \mathbf{ewiseadd}(\mathbf{c}, \oplus, \mathbf{ewisemult}(\mathbf{a}(i), \otimes, \mathbf{B}(i,:))) && (16) \end{aligned}$$

$\mathbf{c} = \mathbf{vxm}(\mathbf{a}, \oplus, \otimes, \mathbf{B}, \mathbf{m})$

Let $\mathbf{a}$ and $\mathbf{m}$ be vectors and let $\mathbf{B}$ be a matrix. Then $\mathbf{c}$ is a vector defined as follows:

$$\begin{aligned} \mathbf{c} &= \emptyset && (17) \\ \mathbf{for}(i \in \mathbf{i}(\mathbf{a}) \mid i \in \mathbf{i}(\mathbf{m}))\ \mathbf{c} &= \mathbf{ewiseadd}(\mathbf{c}, \oplus, \mathbf{ewisemult}(\mathbf{a}(i), \otimes, \mathbf{B}(i,:))) && (18) \end{aligned}$$

$\mathbf{c} = \mathbf{vxm}(\mathbf{a}, \oplus, \otimes, \mathbf{B}, \overline{\mathbf{m}})$

Let $\mathbf{a}$ and $\mathbf{m}$ be vectors and let $\mathbf{B}$ be a matrix. Then $\mathbf{c}$ is a vector defined as follows:

$$\begin{aligned} \mathbf{c} &= \emptyset && (19) \\ \mathbf{for}(i \in \mathbf{i}(\mathbf{a}) \mid i \notin \mathbf{i}(\mathbf{m}))\ \mathbf{c} &= \mathbf{ewiseadd}(\mathbf{c}, \oplus, \mathbf{ewisemult}(\mathbf{a}(i), \otimes, \mathbf{B}(i,:))) && (20) \end{aligned}$$

$\mathbf{C} = \mathbf{mxm}(\mathbf{A}, \oplus, \otimes, \mathbf{B})$

Let $\mathbf{A}$ and $\mathbf{B}$ be matrices. Then $\mathbf{C}$ is a matrix defined as follows:

$$\begin{aligned} \mathbf{C} &= \emptyset & (21) \\ \mathbf{for}(i \in \mathbf{i}(\mathbf{A}))\ \mathbf{C} &= \mathbf{C} \cup \{(i, j, \mathbf{v}(j)) \mid (j, \mathbf{v}(j)) \in \mathbf{vxm}(\mathbf{A}(i, :), \oplus, \otimes, \mathbf{B})\} & (22) \end{aligned}$$

$\mathbf{C} = \mathbf{mxm}(\mathbf{A}, \oplus, \otimes, \mathbf{B}, \mathbf{m})$

Let $\mathbf{A}$ and $\mathbf{B}$ be matrices, and let $\mathbf{m}$ be a vector. Then $\mathbf{C}$ is a matrix defined as follows:

$$\begin{aligned} \mathbf{C} &= \emptyset & (23) \\ \mathbf{for}(i \in \mathbf{i}(\mathbf{A}) \mid i \in \mathbf{i}(\mathbf{m}))\ \mathbf{C} &= \mathbf{C} \cup \{(i, j, \mathbf{v}(j)) \mid (j, \mathbf{v}(j)) \in \mathbf{vxm}(\mathbf{A}(i, :), \oplus, \otimes, \mathbf{B})\} & (24) \end{aligned}$$

4 Observations

Some (or all) of observations below are probably obvious or repetitive, but we believe they should be stated for clarity and completeness.

1. Vectors and matrices have no explicit size or shape. Implicitly, their are constrained in size and shape by the valid range of indices $[0, \Omega)$.

2. Those *potential* elements of a vector or matrix that are not defined are called *structural zeros*. The above specifications of operations on vectors and matrices never reference a structural zero.

3. In contrast, a vector $\mathbf{v}$ or a matrix $\mathbf{A}$ can have elements $\mathbf{v}(i)$ and $\mathbf{A}(i, j)$, respectively such that $\mathbf{v}(i) = 0$ and $\mathbf{A}(i, j) = 0$. These elements are called *zero values* and are operated on when performing an operation on the vector and/or matrix.

4. Structural zeros *always* behave as additive identities and multiplicative annihilators, irrespective of the choice of domain D and operators $(\oplus, \otimes)$. The same cannot be said of zero values.

5. When $(D, \oplus, \otimes, 0)$ is a semiring (*i.e.*, the zero value is the semiring zero) then the result of the GraphBLAS operations, as defined above, are exactly the same as if operating in dense matrices and vectors with the structural zeros replaced by zero values.

6. When $(D, \oplus, \otimes, z)$ is a semiring (z is the semiring zero) then the result of the GraphBLAS operations, as defined above, are exactly the same as if operating in dense matrices and vectors with the structural zeros replaced by z.

7. The two observations above imply that the specifications presented in this document for GraphBLAS operations do not preclude any storage and/or computation optimization for the *common cases*. We call common cases those that we know (inside GraphBLAS) the

semiring we are operating on. (This includes knowing the semantics of the operations and the semiring zero.) Furthermore, the specification still produces deterministic results when we cannot tell what we are operating on, or even if it is a semiring at all.

8. If D is the set of IEEE floating-point numbers (single- or double-precision), then a structural zero does not propagate NaNs, whereas a zero value does. (Whether NaNs should be propagated or not is a separate discussion.)

A Alternative formulation

We now present a formulation in which vectors and matrices have well defined sizes and shapes. That is, the space of potential non-structural zeros is more restricted than $[0, \Omega)$.

A vector $\mathbf{v} = \langle N, \{(i, \mathbf{v}(i))\}\rangle$ is defined by a size $N > 0$ and a set of tuples $(i, \mathbf{v}(i))$ where $0 \leq i < N$ and $\mathbf{v}(i) \in D$. A particular value of i can only appear at most once in $\mathbf{v}$. We define $n(\mathbf{v}) = N$ and $L(\mathbf{v}) = \{(i, \mathbf{v}(i))\}$. We also define the set $\mathbf{i}(\mathbf{v}) = \{i \mid (i, \mathbf{v}(i)) \in \mathbf{v}\}$.

A matrix $\mathbf{A} = \langle N, M, \{(i, j, \mathbf{A}(i, j))\}\rangle$ is defined by its number of rows $N > 0$, its number of columns $M > 0$ and a set of tuples $(i, j, \mathbf{A}(i, j))$ where $0 \leq i < N$, $0 \leq j < M$, and $\mathbf{A}(i, j) \in D$. A particular pair of values i, j can only appear at most once in $\mathbf{A}$. We define $n(\mathbf{A}) = N$, $m(\mathbf{A}) = M$ and $L(\mathbf{A}) = \{(i, j, \mathbf{A}(i, j))\}$. We also define the sets $\mathbf{i}(\mathbf{A}) = \{i \mid \exists(i, j, \mathbf{A}(i, j)) \in \mathbf{A}\}$ and $\mathbf{j}(\mathbf{A}) = \{j \mid \exists(i, j, \mathbf{A}(i, j)) \in \mathbf{A}\}$. (These are the sets of nonempty rows and columns of $\mathbf{A}$, respectively.)

If $\mathbf{A}$ is a matrix and $0 \leq j < N$, then $\mathbf{A}(:, j) = \langle N, \{(i, \mathbf{A}(i, j)) \mid (0 \leq j < M) \wedge ((i, j, \mathbf{A}(i, j)) \in \mathbf{A})\}\rangle$ is a vector called the j-th *column* of $\mathbf{A}$. Correspondingly, if $\mathbf{A}$ is a matrix and $0 \leq i < M$, then $\mathbf{A}(i, :) = \langle M, \{(j, \mathbf{A}(i, j)) \mid (0 \leq i < N) \wedge ((i, j, \mathbf{A}(i, j)) \in \mathbf{A})\}\rangle$ is a vector called the i-th *row* of $\mathbf{A}$. We will use rows and columns when defining operations on matrices.

The various operations can be defined as follows:

$\mathbf{w} = \mathbf{ewiseadd}(\mathbf{u}, \oplus, \mathbf{v})$

Let $\mathbf{u}$ and $\mathbf{v}$ be vectors. Then, $\mathbf{w}$ is a vector defined as follows:

if $n(\mathbf{u}) \neq n(\mathbf{v})$ **then**

$$\mathbf{w} = \mathbf{nil} \tag{25}$$

else

$$\begin{aligned} n(\mathbf{w}) &= n(\mathbf{u}) && (26)\\ \mathbf{i}(\mathbf{w}) &= \mathbf{i}(\mathbf{u}) \cup \mathbf{i}(\mathbf{v}) && (27)\\ \mathbf{w}(i) &= \mathbf{u}(i) \oplus \mathbf{v}(i), \forall i \in (\mathbf{i}(\mathbf{u}) \cap \mathbf{i}(\mathbf{v})) && (28)\\ \mathbf{w}(i) &= \mathbf{u}(i), \forall i \in (\mathbf{i}(\mathbf{w}) - \mathbf{i}(\mathbf{v})) && (29)\\ \mathbf{w}(i) &= \mathbf{v}(i), \forall i \in (\mathbf{i}(\mathbf{w}) - \mathbf{i}(\mathbf{u})) && (30) \end{aligned}$$

endif

$\mathbf{w} = \mathbf{ewiseadd}(\mathbf{u}, \oplus, a)$

Let $\mathbf{u}$ be a vector and a be a scalar. Then, $\mathbf{w}$ is a vector defined as follows:

$$\begin{aligned} n(\mathbf{w}) &= n(\mathbf{u}) && (31) \\ \mathbf{i}(\mathbf{w}) &= \mathbf{i}(\mathbf{u}) && (32) \\ \mathbf{w}(i) &= \mathbf{u}(i) \oplus a, \forall i \in \mathbf{i}(\mathbf{w}) && (33) \end{aligned}$$

$\mathbf{c} = \mathbf{vxm}(\mathbf{a}, \oplus, \otimes, \mathbf{B})$

Let $\mathbf{a}$ be a vector and let $\mathbf{B}$ be a matrix. Then $\mathbf{c}$ is a vector defined as follows:

if $n(\mathbf{a}) \neq n(\mathbf{B})$ **then**

$$\mathbf{c} = \mathbf{nil} \tag{34}$$

else

$$\begin{aligned} n(\mathbf{c}) &= n(\mathbf{a}) && (35) \\ L(\mathbf{c}) &= \emptyset && (36) \\ \mathbf{for}(i \in \mathbf{i}(\mathbf{a}))\ \mathbf{c} &= \mathbf{ewiseadd}(\mathbf{c}, \oplus, \mathbf{ewisemult}(\mathbf{a}(i), \otimes, \mathbf{B}(i,:))) && (37) \end{aligned}$$

endif

$\mathbf{C} = \mathbf{mxm}(\mathbf{A}, \oplus, \otimes, \mathbf{B})$

Let $\mathbf{A}$ and $\mathbf{B}$ be matrices. Then $\mathbf{C}$ is a matrix defined as follows:

if $m(\mathbf{A}) \neq n(\mathbf{B})$ **then**

$$\mathbf{C} = \mathbf{nil} \tag{38}$$

else

$$\begin{aligned} n(\mathbf{C}) &= n(\mathbf{A}) && (39) \\ m(\mathbf{C}) &= m(\mathbf{B}) && (40) \\ L(\mathbf{C}) &= \emptyset && (41) \\ \mathbf{for}(i \in \mathbf{i}(\mathbf{A}))\ L(\mathbf{C}) &= L(\mathbf{C}) \cup \{(i, j, \mathbf{v}(j)) \mid (j, \mathbf{v}(j)) \in \mathbf{vxm}(\mathbf{A}(i,:), \oplus, \otimes, \mathbf{B})\} && (42) \end{aligned}$$

endif