

# Lecture 16

## ***Graph Data Structures***

Fall 2025

Prof. Khoa Luu  
[khoaluu@uark.edu](mailto:khoaluu@uark.edu)

# Major Topics In This Course

1. Introduction
2. Reviews (Link List, OOP, Binary Tree, BT Search)
3. Self-balancing Binary Search Tree (AVL, Multiway Search, Red-Black)
4. Splay Tree
5. Balanced Search Tree Review
6. Heap Methods
7. Hashing Methods
8. Graph Data Structures
10. Graph CNN
11. Data Structures in Deep Learning
12. Final Project Presentations

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# Outline

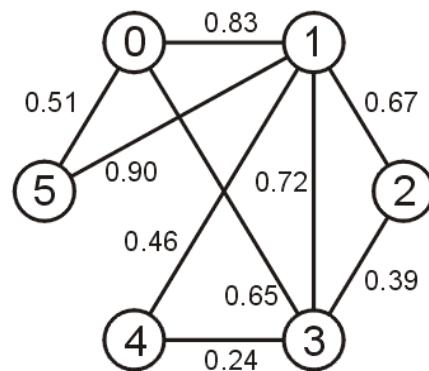
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- In this topic, we will cover the representation of graphs on a computer
- We will examine:
  - an adjacency matrix representation
  - smaller representations and pointer arithmetic
  - sparse matrices and linked lists

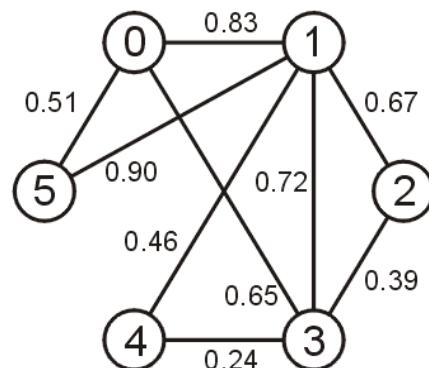
# Background

- You are required to store a graph with a given number of vertices numbered 0 through  $n - 1$



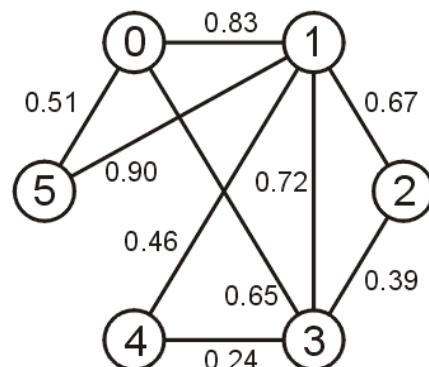
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- You are required to store a graph with a given number of vertices numbered 0 through  $n - 1$
- Initially, there are no edges between these  $n$  vertices



# Background

- You are required to store a graph with a given number of vertices numbered 0 through  $n - 1$
- Initially, there are no edges between these  $n$  vertices
- The **insert** command adds edges to the graph while the number vertices remains unchanged



# Background

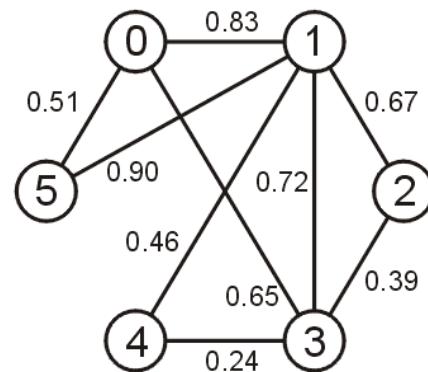
- In this lecture, we will look at techniques for storing the edges of a graph

# Background

- In this lecture, we will look at techniques for storing the edges of a graph
- This lecture will focus on weighted graphs, however, for unweighted graphs, one can easily use `bool` in place of `double`

# Background

- To demonstrate these techniques, we will look at storing the edges of the following graph:



# Adjacency Matrix

A graph of  $n$  vertices may have up to ? edges

# Adjacency Matrix

A graph of  $n$  vertices may have up to

$$\binom{n}{2} = \frac{n(n-1)}{2} = \mathbf{O}(n^2)$$

edges

The first straight-forward implementation is an adjacency matrix

# Adjacency Matrix

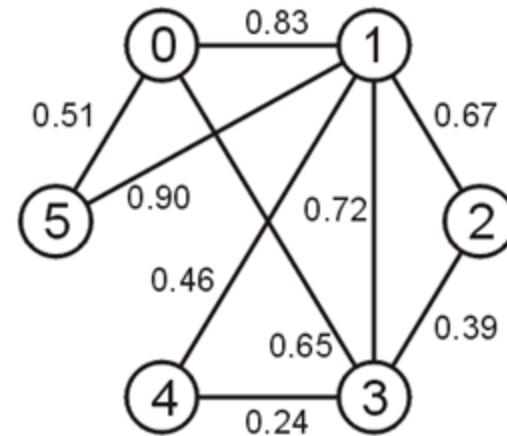
Define an  $n \times n$  matrix  $\mathbf{A} = (a_{ij})$  and if the vertices  $v_i$  and  $v_j$  are connected with weight  $w$ , then set  $a_{ij} = w$  and  $a_{ji} = w$

# Adjacency Matrix

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That is, the matrix is symmetric, e.g.,

	0	1	2	3	4	5
0		0.83		0.65		0.51
1	0.83		0.67	0.72	0.46	0.90
2		0.67		0.39		
3	0.65	0.72	0.39		0.24	
4		0.46		0.24		
5	0.51	0.90				



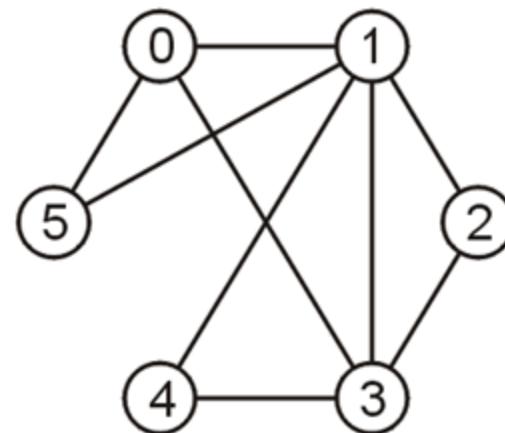
# Adjacency Matrix

An unweighted graph may be saved as an array of Boolean values

- vertices  $v_i$  and  $v_j$  are connected then set

$$a_{ij} = a_{ji} = \text{true}$$

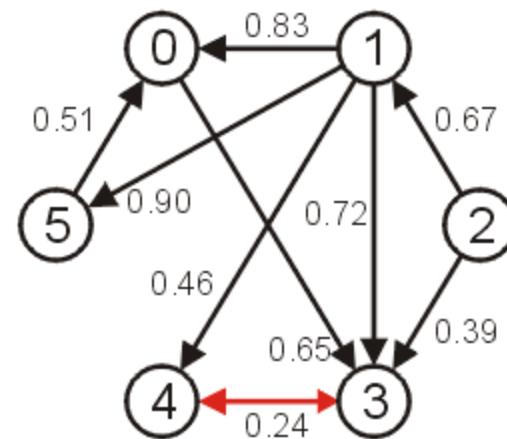
	0	1	2	3	4	5
0	T		F	T	F	T
1	T		T	T	T	T
2	F	T		T	F	F
3	T	T	T		T	F
4	F	T	F	T		F
5	T	T	F	F	F	



# Adjacency Matrix

If the graph was directed, then the matrix would not necessarily be symmetric

	0	1	2	3	4	5
0				0.65		
1	0.83			0.72	0.46	0.90
2		0.67		0.39		
3					0.24	
4				0.24		
5	0.51					



# Adjacency Matrix

First we must allocate memory for a **two-dimensional array**

C++ does not have native support for anything more than one-dimensional arrays, thus how do we store a two-dimensional array?

# Adjacency Matrix

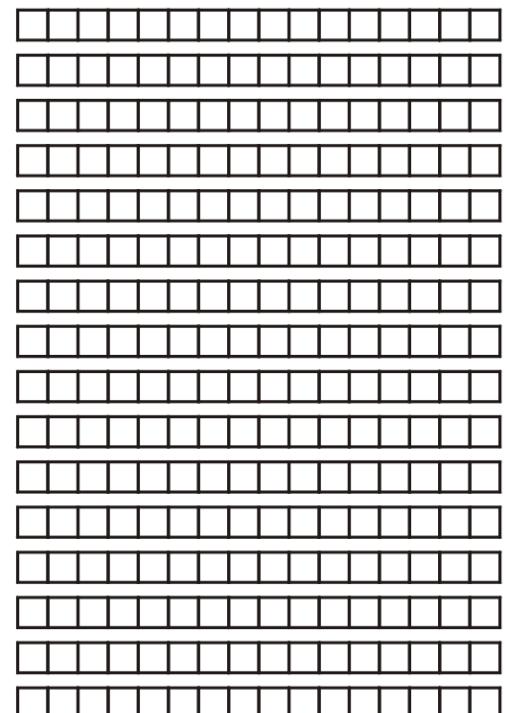
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C++ does not have native support for anything more than one-dimensional arrays, thus how do we store a two-dimensional array?

- as an array of arrays

# Adjacency Matrix

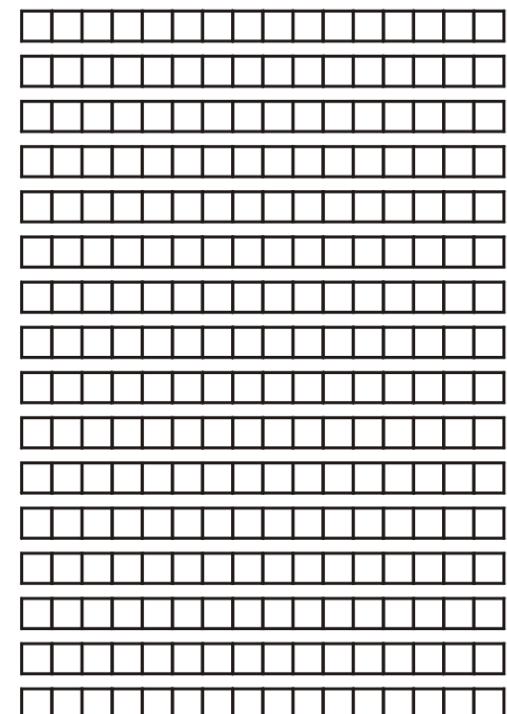
Suppose we require a  $16 \times 16$  matrix of double-precision floating-point numbers



# Adjacency Matrix

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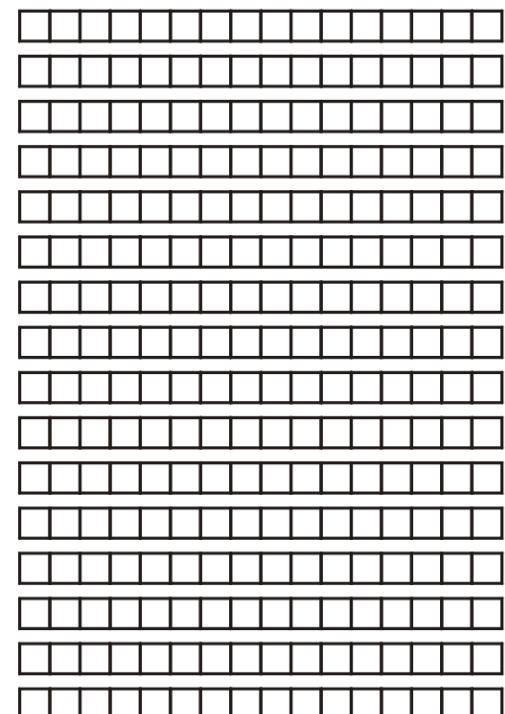
Each row of the matrix can be represented by ?



# Adjacency Matrix

Suppose we require a  $16 \times 16$  matrix of double-precision floating-point numbers

Each row of the matrix can be represented by an array

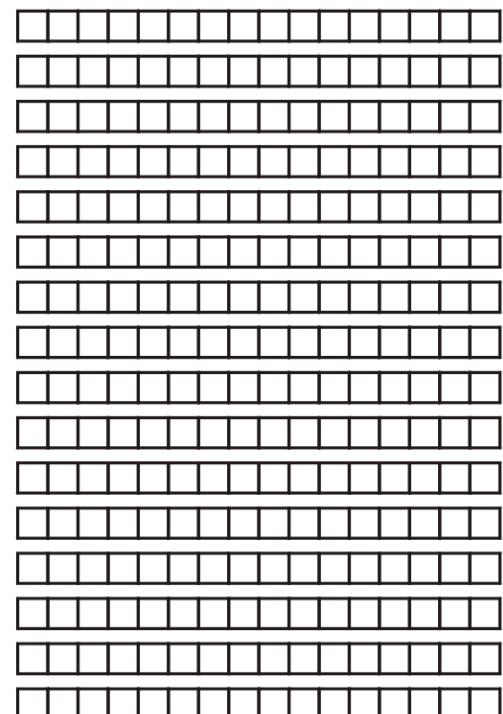


# Adjacency Matrix

Suppose we require a  $16 \times 16$  matrix of double-precision floating-point numbers

Each row of the matrix can be represented by an array

The address of the first entry must be stored in ?



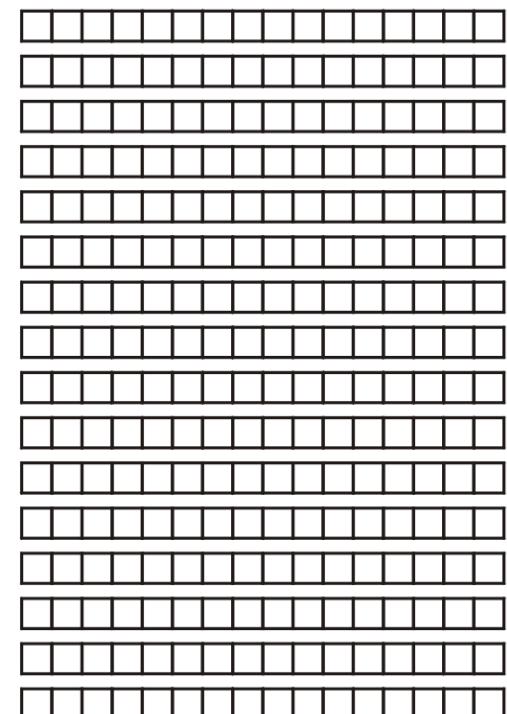
# Adjacency Matrix

Suppose we require a  $16 \times 16$  matrix of double-precision floating-point numbers

Each row of the matrix can be represented by an array

The address of the first entry must be stored in **a pointer to a double**:

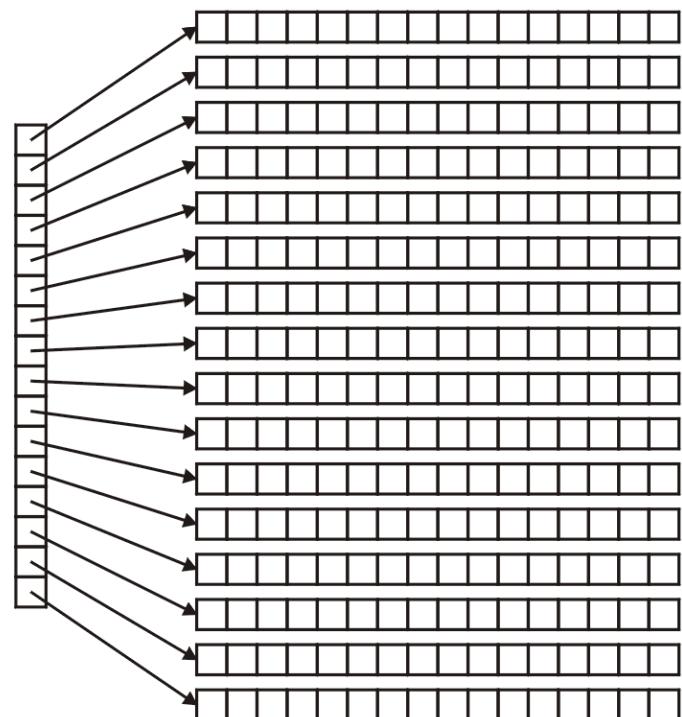
```
double *
```



# Adjacency Matrix

However, because we must store 16 of these pointers-to-doubles, it makes sense that we store these in an array

What is the declaration  
of this array?

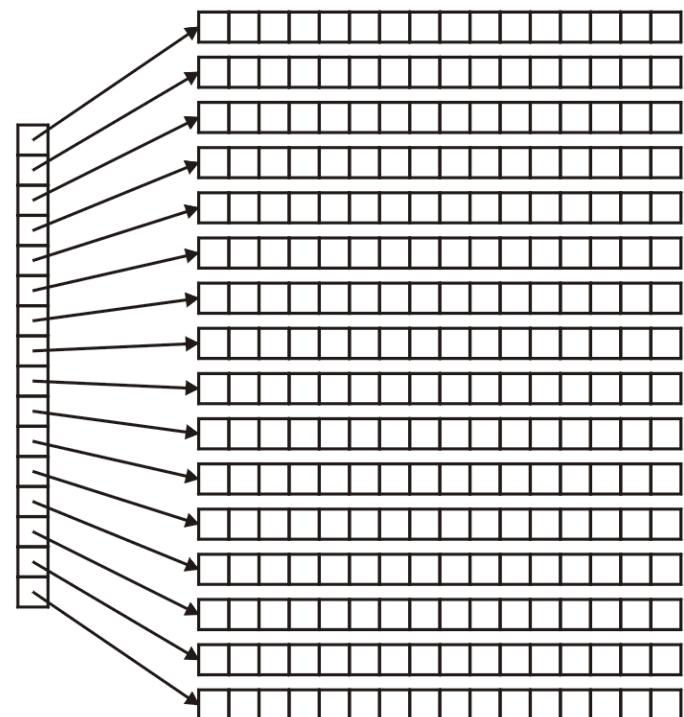


# Adjacency Matrix

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Well, we must store a  
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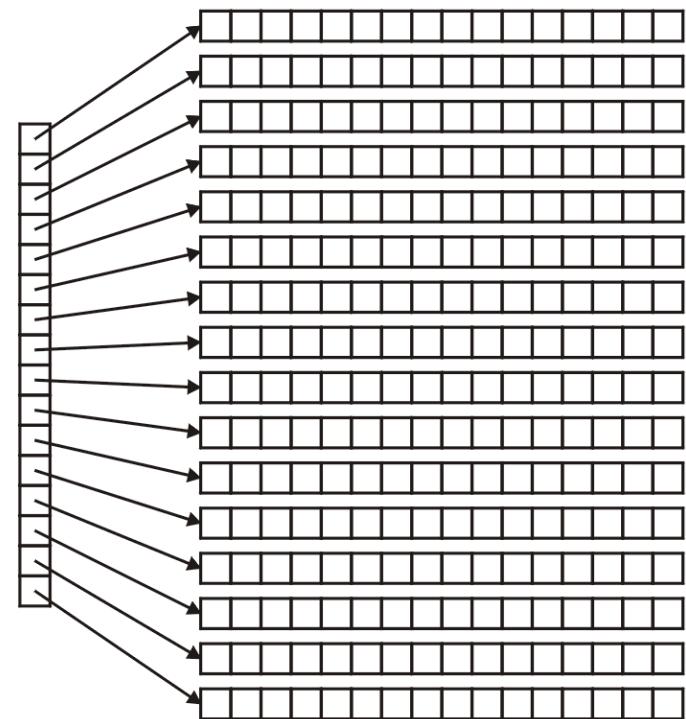
# Adjacency Matrix

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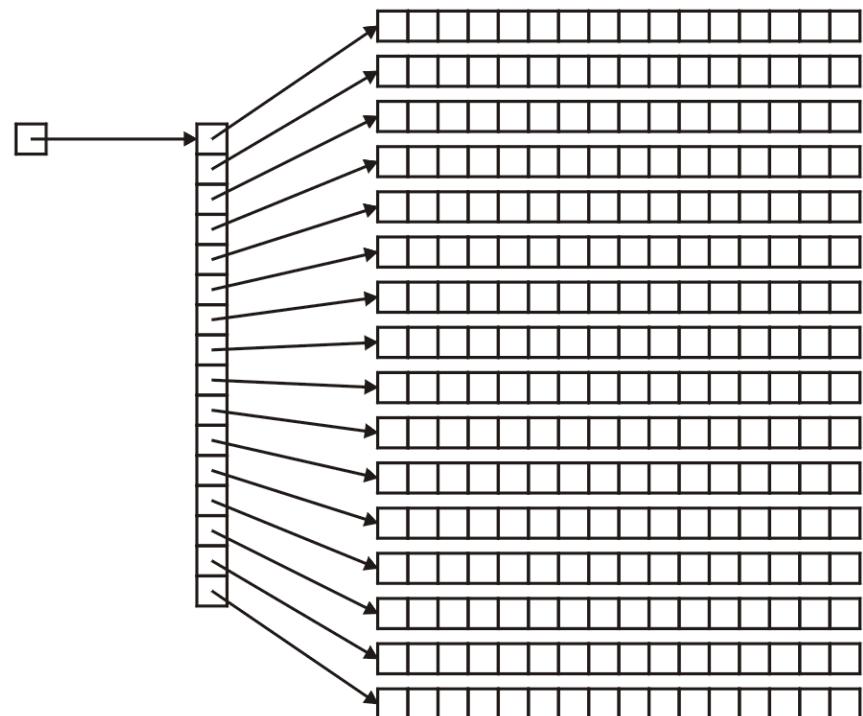
That is: `double **`



# Adjacency Matrix

Thus, the address of the first array must be declared to be:

```
double **matrix;
```

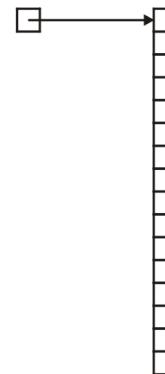


# Adjacency Matrix

The next question is memory allocation

First, we must allocate the memory for the array of pointers to doubles:

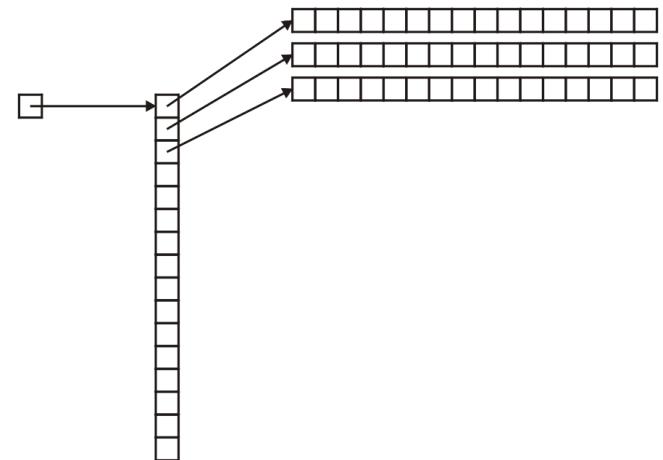
```
matrix = new double * [16];
```



# Adjacency Matrix

Next, to each entry of this matrix, we must assign the memory allocated for an array of doubles

```
for ( int i = 0; i < 16; ++i ) {  
    matrix[i] = new double[16];  
}
```



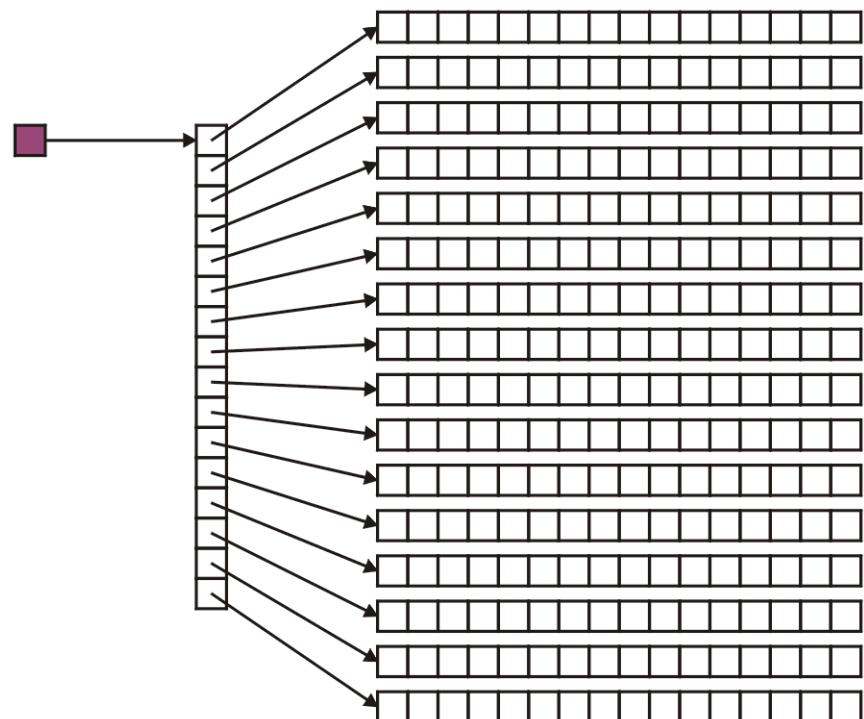
# Adjacency Matrix

Accessing a matrix is done through a double index, e.g.,  
`matrix[3][4]`

You can interpret this as `(matrix[3])[4]`

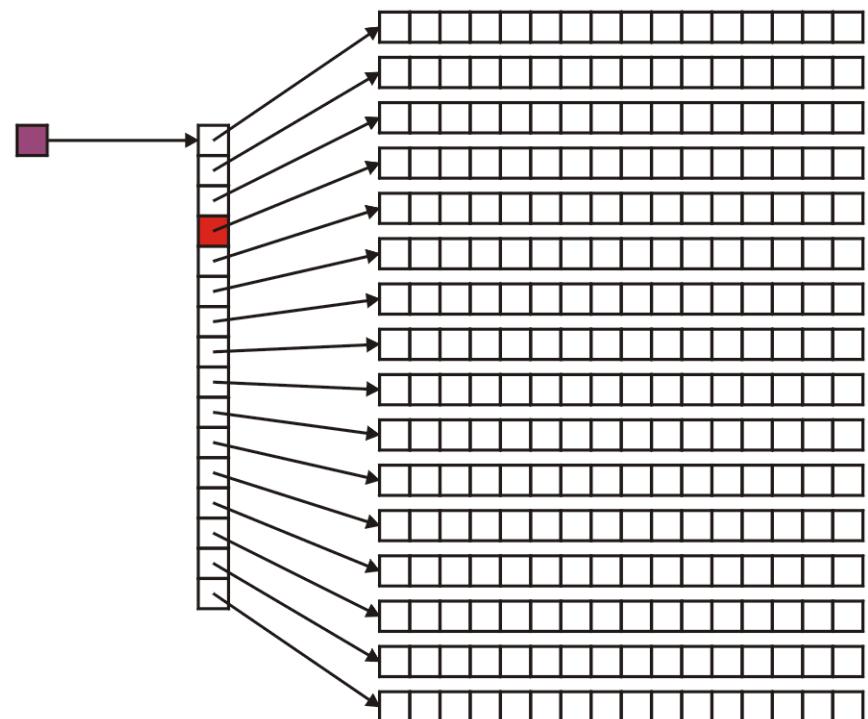
# Adjacency Matrix

Recall that in `matrix[3][4]`, the variable `matrix` is a pointer-to-a-pointer-to-a-double:



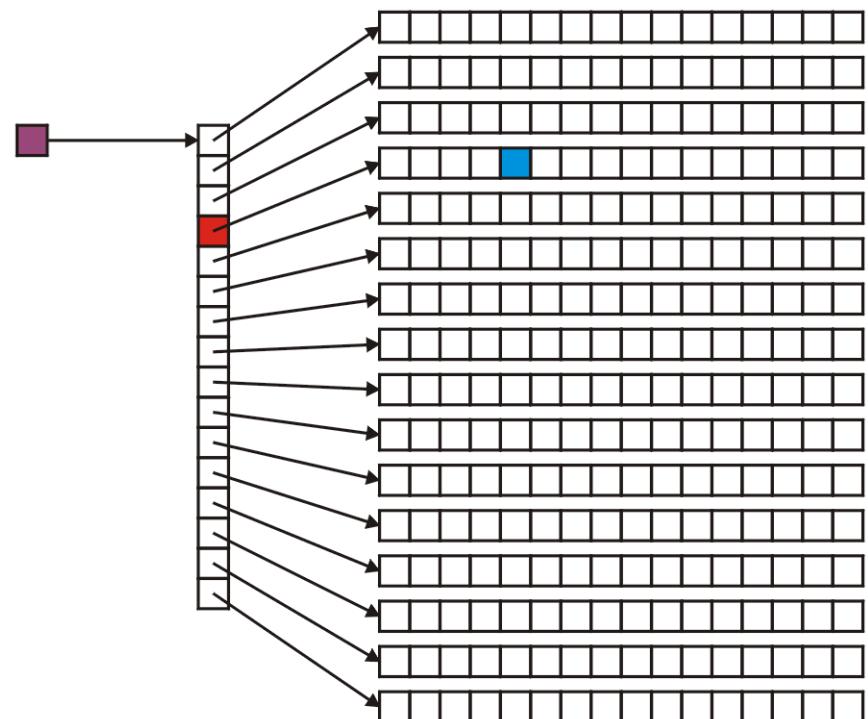
# Adjacency Matrix

Therefore, **matrix[3]** is a pointer-to-a-double:



# Adjacency Matrix

And consequently, `matrix[3][4]` is a double:



# C++ Notation Warning

Do not use `matrix[3, 4]` because:

- in C++, the comma operator evaluates the operands in order from left-to-right
- the *value* is the last one

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Do not use `matrix[3, 4]` because:

- in C++, the comma operator evaluates the operands in order from left-to-right
- the *value* is the last one

Therefore, `matrix[3, 4]` is equivalent to calling `matrix[4]`

Try it:

```
int i = (3, 4);  
cout << i << endl;
```

# C++ Notation Warning

Many things will compile if you try to use this notation:

```
matrix = new double[N, N];
```

will allocate an array of  $N$  doubles, just like:

```
matrix = new double[N];
```

However, this is likely not to do what you really expect...

# Adjacency Matrix

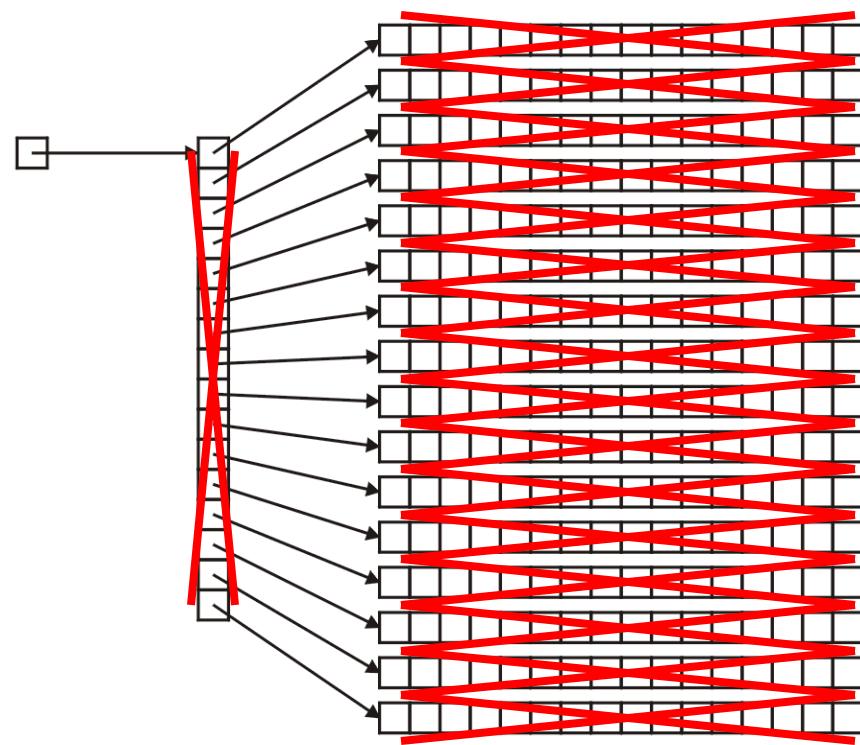
Now, once you've used the matrix, you must also delete it...

# Adjacency Matrix

Recall that for each call to `new[ ]`, you must have a corresponding call to `delete[ ]`

Therefore, we must use  
a for-loop to delete the  
arrays

- implementation up to you



# Default Values

Question: what do we do about vertices which are not connected?

- the value 0
- a negative number, e.g.,  $-1$
- positive infinity:  $\infty$

The last is the most logical, in that it makes sense that two vertices which are not connected have an infinite distance between them

# Default Values

To use infinity, you may declare a constant static member variable INF:

```
#include <limits>

class Weighted_graph {
    private:
        static const double INF;
        // ...
        // ...
};

const double Weighted_graph::INF =
    std::numeric_limits<double>::infinity();
```

# Default Values

In this case, you can initialize your array as follows:

```
for ( int i = 0; i < N; ++i ) {  
    for ( int j = 0; j < N; ++j ) {  
        matrix[i][j] = INF;  
    }  
  
    matrix[i][i] = 0;  
}
```

It makes intuitive sense that the distance from a node to itself is 0

# Default Values

If we are representing an unweighted graph, use Boolean values:

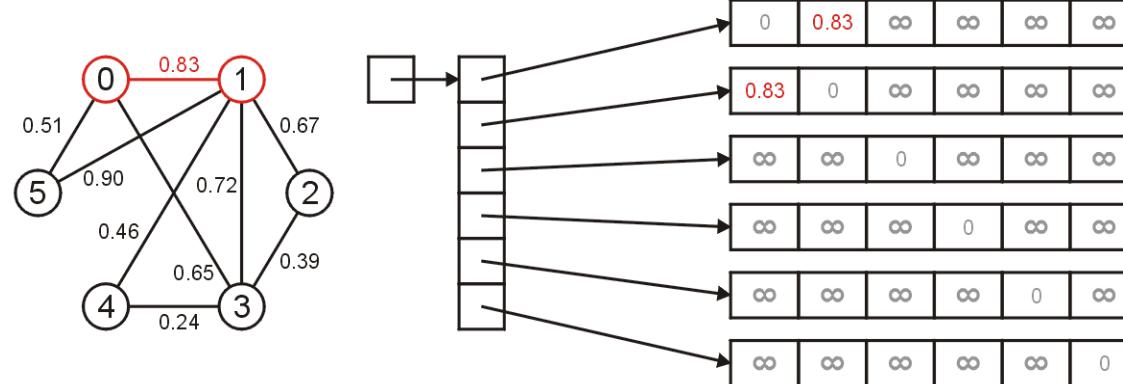
```
for ( int i = 0; i < N; ++i ) {  
    for ( int j = 0; j < N; ++j ) {  
        matrix[i][j] = false;  
    }  
  
    matrix[i][i] = true;  
}
```

It makes intuitive sense that a vertex is connected to itself



# Adjacency Matrix

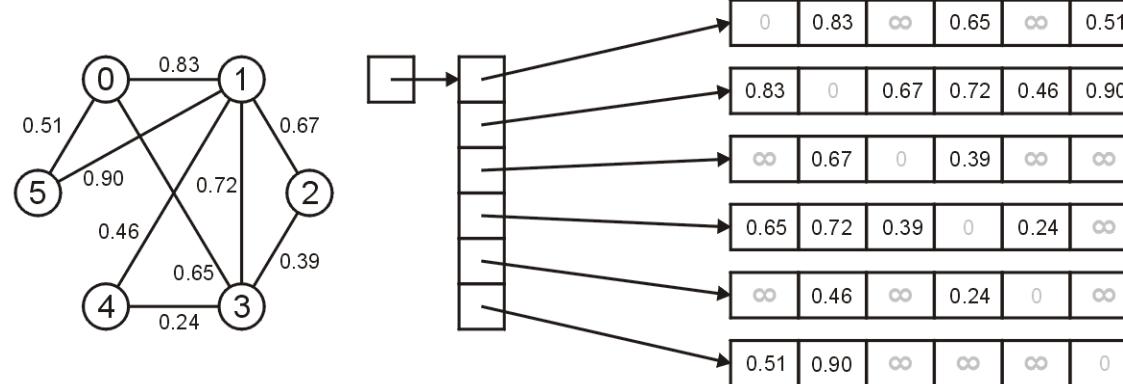
To insert the edge between 0 and 1 with weight 0.83, we set  
`matrix[0][1] = matrix[1][0] = 0.83;`



# Adjacency Matrix

The final result is shown as follows

Note, however, that these six arrays could be anywhere in memory...



# Adjacency Matrix

We have now looked at how we can store an adjacency graph in C++

Next, we will look at:

- Two improvements for the array-of-arrays implementations, including:
  - allocating the memory for the matrix in a single contiguous block of code, and
  - a lower-triangular representation; and
- A sparse linked-list implementation

# Adjacency Matrix Improvement

To begin, we will look at the first improvement:

- allocating all of the memory of the arrays in a single array with  $n^2$  entries

# Adjacency Matrix Improvement

For those of you who would like to reduce the number of calls to `new`, consider the following idea:

- allocate an array of 16 pointers to doubles
- allocate an array of  $16^2 = 256$  doubles

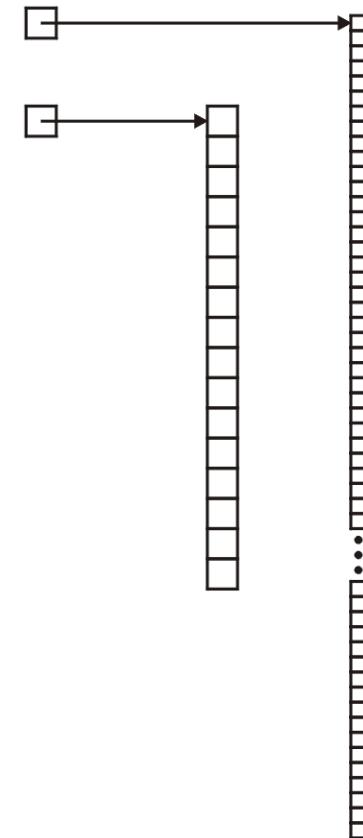
Then, assign to the 16 pointers in the first array the addresses of entries

0, 16, 32, 48, 64, ..., 240

# Adjacency Matrix Improvement

First, we allocate memory:

```
matrix = new double * [16];  
double * tmp = new double[256];
```



# Adjacency Matrix Improvement

Next, we allocate the addresses:

```
matrix = new double * [16];
double * tmp = new double[256];

for ( int i = 0; i < 16; ++i ) {
    matrix[i] = &( tmp[16*i] );
}
```

This assigns:

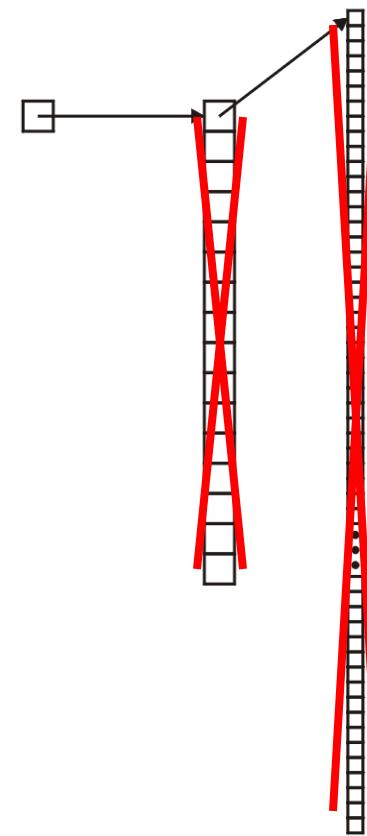
```
matrix[ 0 ] = &( tmp[ 0 ] );
matrix[ 1 ] = &( tmp[ 16 ] );
matrix[ 2 ] = &( tmp[ 32 ] );
.
.
.
matrix[15] = &( tmp[240] );
```



# Adjacency Matrix Improvement

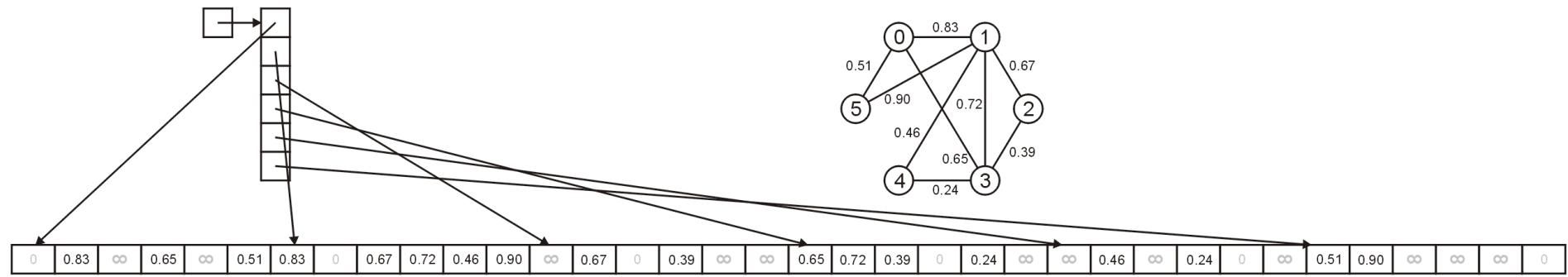
Deleting this array is easier:

```
delete [] matrix[0];  
delete [] matrix;
```



# Adjacency Matrix Improvement

Our sample graph would be represented as follows:



# Lower-triangular adjacency matrix

Next we will look at another improvement which can be used for undirected graphs

We will store only half of the entries

- To do this, we must also learn about pointer arithmetic

# Lower-triangular adjacency matrix

Note also that we are not storing a directed graph: therefore, we really need only store half of the matrix

Thus, instead of 256 entries, we really only require 120 entries

A 10x10 grid containing the following non-zero entries:

- (1, 1) = 0
- (2, 2) = 0
- (3, 3) = 0
- (4, 4) = 0
- (5, 5) = 0
- (6, 6) = 0
- (7, 7) = 0
- (8, 8) = 0
- (9, 9) = 0

# Lower-triangular adjacency matrix

The memory allocation for this would be straight-forward, too:

```
matrix = new double * [16];
matrix[0] = 0;
matrix[1] = new double[120];

for( int i = 2; i < 16; ++i ) {
    matrix[i] = matrix[i - 1] + i - 1;
}
```

# Lower-triangular adjacency matrix

- What we are using here is pointer arithmetic:
  - in C/C++, you can add values to a pointer
  - the question is, what does it mean to set:

```
ptr = ptr + 1;
```

or

```
ptr = ptr + 2;
```

# Lower-triangular adjacency matrix

- Suppose we have a pointer-to-a-double:

```
double * ptr = new double( 3.14 );
```

where:

- the pointer has a value of **0x53A1D780**, and
- the representation of 3.14 is **0x40091Eb851EB851F**

53A1D780	53A1D781	53A1D782	53A1D783	53A1D784	53A1D785	53A1D786	53A1D787	53A1D788
40	09	1E	B8	51	EB	85	1F	??

# Lower-triangular adjacency matrix

- If we just added one to the address, then this would give us the value **0x53A1D781**, but this contains no useful information...

53A1D780	53A1D781	53A1D782	53A1D783	53A1D784	53A1D785	53A1D786	53A1D787	53A1D788
40	09	1E	B8	51	EB	85	1F	??



# Lower-triangular adjacency matrix

- The only logical interpretation of `ptr + 1` is to go to the *next* location a different double could exist, *i.e.*, `0x53A1D788`

53A1D780	53A1D781	53A1D782	53A1D783	53A1D784	53A1D785	53A1D786	53A1D787	53A1D788	
40	09	1E	B8	51	EB	85	1F	??	

# Lower-triangular adjacency matrix

Therefore, if we define:

```
double * array = new double[4];
```

then the following are all equivalent:

<b>array[0]</b>	<b>*array</b>
<b>array[1]</b>	<b>* (array + 1)</b>
<b>array[2]</b>	<b>* (array + 2)</b>
<b>array[3]</b>	<b>* (array + 3)</b>

# Lower-triangular adjacency matrix

- Thus, the following code simply adds appropriate amounts to the pointer:

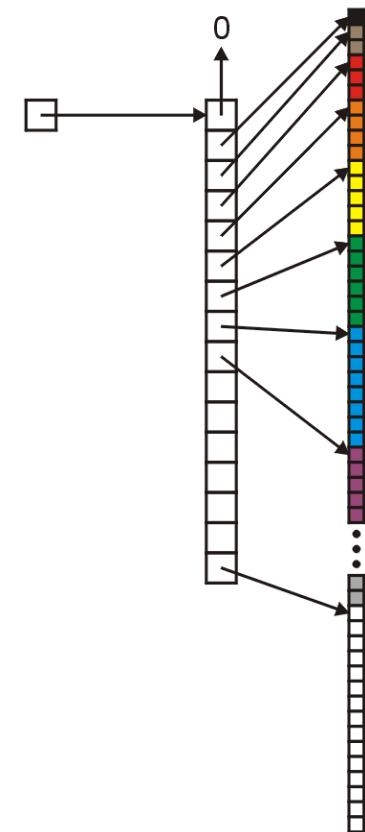
```
matrix = new double *[N];
matrix[0] = nullptr;
matrix[1] = new double[N*(N - 1)/2];

for( int i = 2; i < N; ++i ) {
    matrix[i] = matrix[i - 1] + i - 1;
}
```

# Lower-triangular adjacency matrix

Visually, we have, for  $N = 16$ , the following:

```
matrix[0] = nullptr;  
matrix[1] = &( tmp[0] );  
matrix[2] = &( tmp[1] );  
matrix[3] = &( tmp[3] );  
matrix[4] = &( tmp[6] );  
matrix[5] = &( tmp[10] );  
matrix[6] = &( tmp[15] );  
matrix[7] = &( tmp[21] );  
matrix[7] = &( tmp[28] );  
.  
.  
.  
matrix[15] = &( tmp[105] );
```



# Lower-triangular adjacency matrix

The only thing that we would have to do is ensure that we always put the larger number first:

```
void insert( int i, int j, double w ) {
    if ( j < i ) {
        matrix[i][j] = w;
    } else {
        matrix[j][i] = w;
    }
}
```

# Lower-triangular adjacency matrix

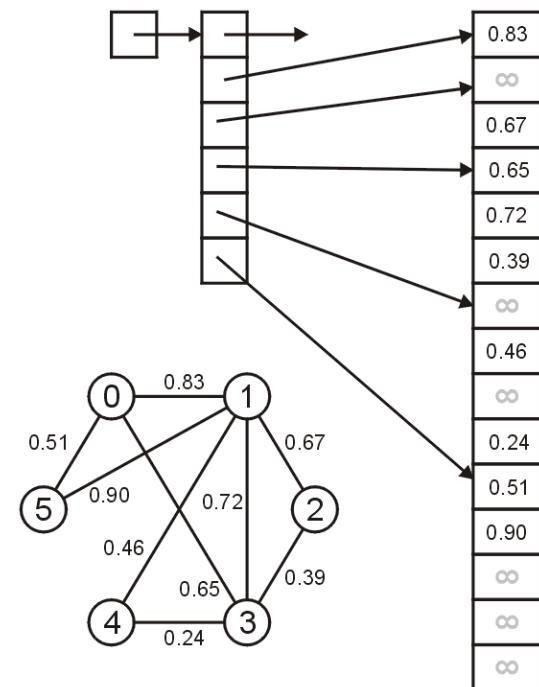
- A slightly less efficient way of writing this would be:

```
void insert( int i, int j, double w ) {  
    matrix[max(i,j)][min(i,j)] = w;  
}
```

- The benefits (from the point-of-view of clarity) are much more significant...

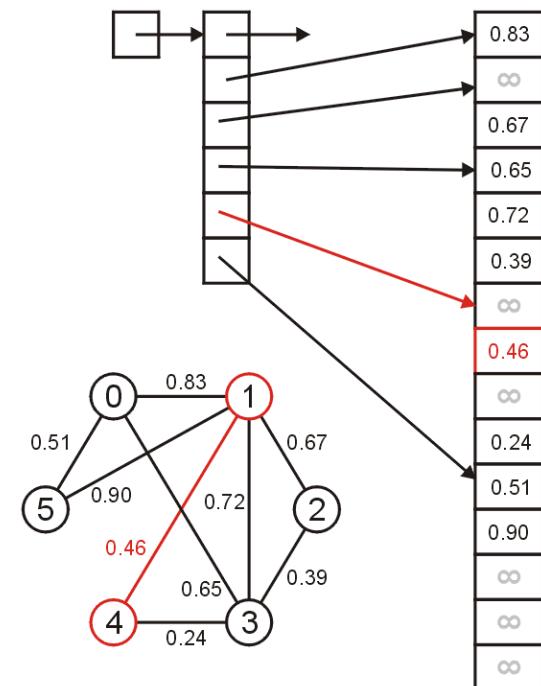
# Lower-triangular adjacency matrix

- Our example graph is stored using this representation as shown here
- Notice that we do not store any 0's, nor do we store any duplicate entries
- The second array has only 15 entries, versus 36



# Lower-triangular adjacency matrix

- To determine the weight of the edge connecting vertices 1 and 4, we must look up the entry  
**matrix[4][1]**



# Sparse Matrices

- Finally we will consider the problem with sparse matrices and we will look at one implementation using linked lists

# Sparse Matrices

- The memory required for creating an  $n \times n$  matrix using an array-of-arrays is:

$$4 \text{ bytes} + 4n \text{ bytes} + 8n^2 \text{ bytes} = \Theta(n^2) \text{ bytes}$$

# Sparse Matrices

- The memory required for creating an  $n \times n$  matrix using an array-of-arrays is:  
$$4 \text{ bytes} + 4n \text{ bytes} + 8n^2 \text{ bytes} = \Theta(n^2) \text{ bytes}$$
- This could potentially waste a significant amount of memory:
  - consider all intersections in US as vertices and streets as edges
  - how could we estimate the number of intersections in US?

# Sparse Matrices

- Matrices where less than 5% of the entries are not the default value (either infinity or 0, or perhaps some other default value) are said to be *sparse*

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# Sparse Matrices

- Matrices where less than 5% of the entries are not the default value (either infinity or 0, or perhaps some other default value) are said to be *sparse*
- Matrices where most entries (25% or more) are not the default value are said to be *dense*
- Clearly, these are not hard limits

# Sparse Matrices

- Assume that each intersection connects, on average, four other intersections
- Therefore, less than 0.0005% of the entries of the matrix are used to store connections
  - the rest are storing the value *infinity*

# Sparse Matrices

- We will look at a very efficient sparse-matrix implementation with the last topic
- Here, we will consider a simpler implementation:
  - use an array of linked lists to store edges
- Note, however, that each node in a linked list must store two items of information:
  - the connecting vertex and the weight

# Sparse Matrices

- One possible solution:
  - modify the **SingleNode** data structure to store both an integer and a double:

```
class SingleNode {  
    private:  
        int adacent_vertex;  
        double edge_weight;  
        SingleNode * next_node;  
  
    public:  
        SingleNode( int, double SingleNode = 0 );  
        double weight() const;  
        int vertex() const;  
        SingleNode * next() const;  
};
```
  - exceptionally inefficient

# Sparse Matrices

A better solution is to create a new class which stores a vertex-edge pair

```
class Pair {  
    private:  
        double edge_weight;  
        int adacent_vertex;  
    public:  
        Pair( int, double );  
        double weight() const;  
        int vertex() const;  
};
```

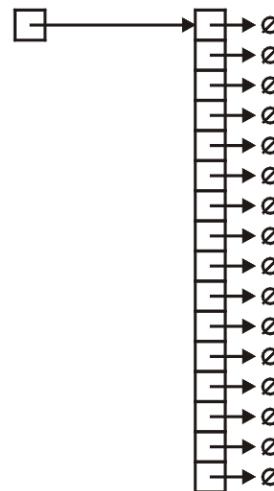
Now create an array of linked-lists storing these pairs

# Sparse Matrices

Thus, we define and create the array:

```
SingleList<Pair> * array;
```

```
array = new SingleList<Pair>[16];
```



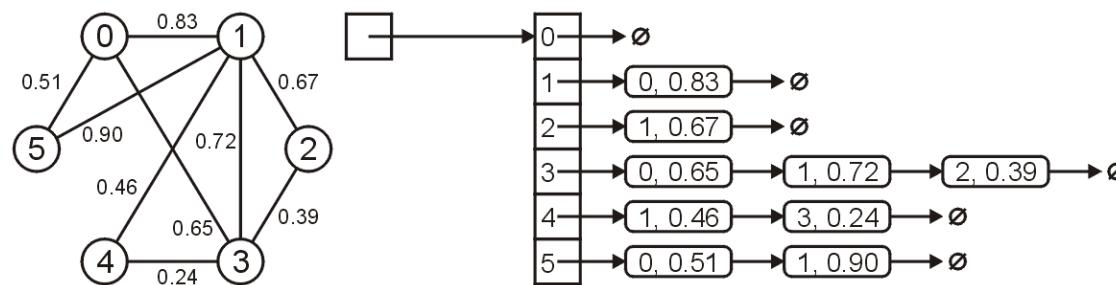
# Sparse Matrices

As before, to reduce redundancy, we would only insert the entry into the entry corresponding with the larger vertex

```
void insert( int i, int j, double w ) {  
    if ( i < j ) {  
        array[j].push_front( Pair(i, w) );  
    } else {  
        array[i].push_front( Pair(j, w) );  
    }  
}
```

# Sparse Matrices

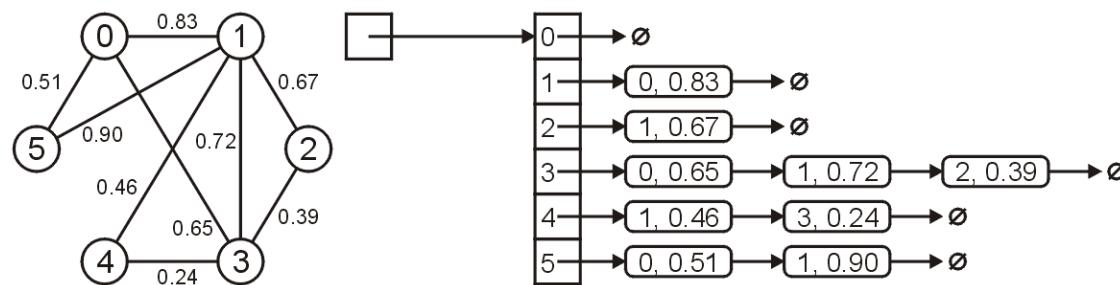
For example, the graph shown below would be stored as



# Sparse Matrices

Later, we will see an even more efficient implementation

- The old an new Yale sparse matrix formats



# Summary

- In this lecture, we have looked at a number of graph representations
- C++ lacks a *matrix* data structure
  - must use array of arrays
- The possible factors affecting your choice of data structure are:
  - weighted or unweighted graphs
  - directed or undirected graphs
  - dense or sparse graphs