• CSCI 8314 • Spring 2019 •

SPARSE MATRIX COMPUTATIONS

Class time : Mo & We 09:45 – 11:00am

Room : Akerman 227

Instructor : Yousef Saad

URL : www-users.cselabs.umn.edu/classes/Spring-2019/csci8314/

About this class: Objectives

Set 1 An introduction to sparse matrices and sparse matrix computations.

- Sparse matrices;
- Sparse matrix direct methods ;
- Graph theory viewpoint; graph theory methods;

Set 2 Iterative methods and eigenvalue problems

- Iterative methods for linear systems
- Algorithms for sparse eigenvalue problems and the SVD
- Possibly: nonlinear equations

Set 3 Applications of sparse matrix techniques

- Applications of graphs; Graph Laplaceans; Networks ...;
- Standard Applications (PDEs, ..)
- Applications in machine learning
- Data-related applications
- Other instances of sparse matrix techniques

Logistics:

- We will use Canvas only to post grades
- Main class web-site is :

`www-users.cselabs.umn.edu/classes/Spring-2019/csci8314/`

- There you will find :

- Lecture notes
- Schedule of assignments/ tests
- Announcements for class,
- On occasion: Exercises [do before indicated class]
- .. and more

About lecture notes:

➤ Lecture notes (like this first set) will be posted on the class web-site – usually before the lecture. [if I am late do not hesitate to send me e-mail]

➤ Note: format used in lectures may be formatted differently – but same contents.

➤ Review them to get some understanding if possible before class.

➤ Read the relevant section (s) in the texts or references provided

➤ Lecture note sets are grouped by topics (sections in the textbook) rather than by lecture.

➤ In the notes the symbol ✍ indicates suggested easy exercises or questions – often [not always] done in class.

Occasional in-class practice exercises

- Posted in advance – see HWs web-page
- Do them before class. No need to turn in anything.

Matlab

- We will often use matlab for testing algorithms.
- Other documents will be posted in the matlab web-site.
- Most important:
- .. I post the matlab diaries used for the demos (if any).

CSCI 8314: SPARSE MATRIX COMPUTATIONS

GENERAL INTRODUCTION

- **General introduction - a little history**
- **Motivation**
- **Resources**
- **What will this course cover**

What this course is about

➤ Solving linear systems and (to a lesser extent) eigenvalue problems with matrices that are sparse.

➤ Sparse matrices : matrices with mostly zero entries [details later]

➤ Many applications of sparse matrices...

➤ ... and we are seing more with new applications everywhere

A brief history

Sparse matrices have been identified as important early on – origins of terminology is quite old. Gauss defined the first method for such systems in 1823. Varga used explicitly the term 'sparse' in his 1962 book on iterative methods.

`https://www-users.cs.umn.edu/~saad/PDF/icerm2018.pdf`

➤ Special techniques used for sparse problems coming from Partial Differential Equations

➤ One has to wait until to the 1960s to see the birth of the general technology available today

➤ Graphs introduced as tools for sparse Gaussian elimination in 1961 [Seymour Parter]

- Early work on reordering for banded systems, envelope methods
- Various reordering techniques for general sparse matrices introduced.
- Minimal degree ordering [Markowitz - 1957] ...
- ... later used in Harwell MA28 code [Duff] - released in 1977.
- Tinney-Walker Minimal degree ordering for power systems [1967]
- Nested Dissection [A. George, 1973]
- SPARSPAK [commercial code, Univ. Waterloo]
- Elimination trees, symbolic factorization, ...

History: development of iterative methods

- 1950s up to 1970s : focus on “relaxation” methods

- Development of 'modern' iterative methods took off in the mid-70s. but...

- ... The main ingredients were in place earlier [late 40s, early 50s: Lanczos; Arnoldi ; Hestenes (a local!) and Stiefel; ....]

- The next big advance was the push of ‘preconditioning’: in effect a way of combining iterative and (approximate) direct methods – [Meijerink and Van der Vorst, 1977]

History: eigenvalue problems

➤ Another parallel branch was followed in sparse techniques for large eigenvalue problems.

➤ A big problem in 1950s and 1960s : flutter of airplane wings.. This leads to a large (sparse) eigenvalue problem

➤ Overlap between methods for linear systems and eigenvalue problems [Lanczos, Arnoldi]

Resources

[See the "links" page in the course web-site]

- Matrix market

```
http://math.nist.gov/MatrixMarket/
```

- SuiteSparse site (Formerly : Florida collection)

```
http://faculty.cse.tamu.edu/davis/suitesparse.html
```

- SPARSKIT, etc.

```
http://www.cs.umn.edu/~saad/software
```

Resources – continued

Books: on sparse direct methods.

- Book by Tim Davis [SIAM, 2006] see syllabus for info
- Best reference [old, out-of print, but still the best]:

• Alan George and Joseph W-H Liu, Computer Solution of Large Sparse Positive Definite Systems, Prentice-Hall, 1981. Englewood Cliffs, NJ.

- Of interest mostly for references:

• I. S. Duff and A. M. Erisman and J. K. Reid, Direct Methods for Sparse Matrices, Clarendon press, Oxford, 1986.

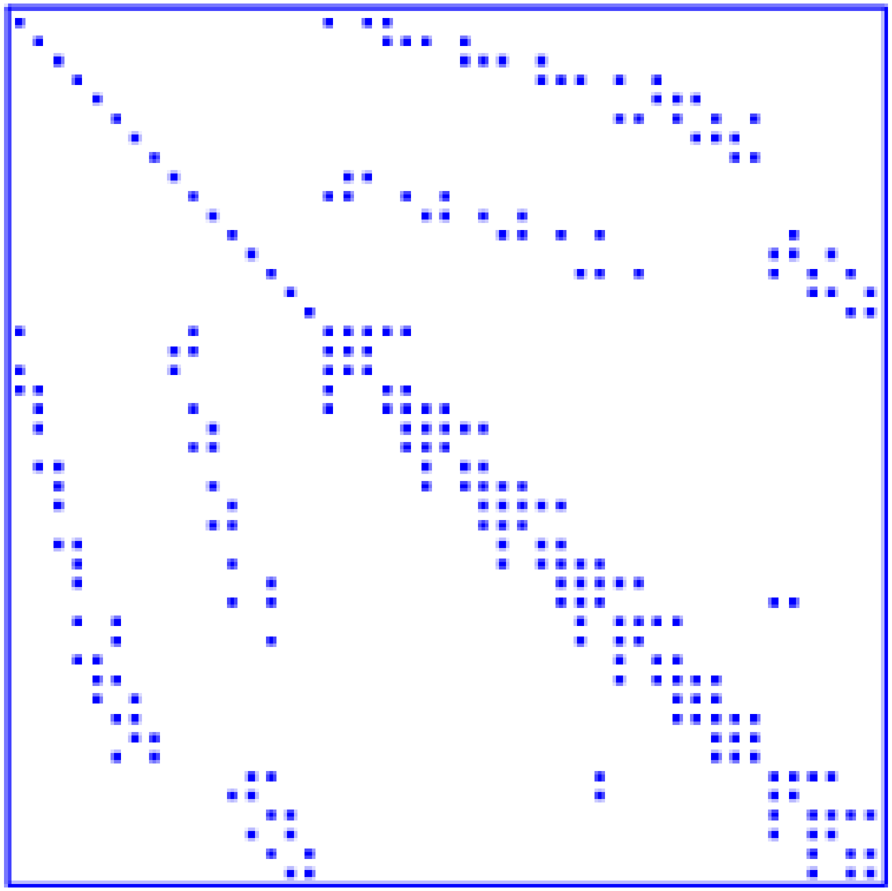
Overall plan for the class

- We will begin by sparse matrices in general, their origin, storage, manipulation, etc..
- Graph theory viewpoint
- We will then spend some time on sparse direct methods
- .. back to graphs: Graph Laplaceans and applications; Networks; ...
- .. and then on eigenvalue problems and
- ... iterative methods for linear systems
- ... Plan is still in progress.

SPARSE MATRICES

- See Chap. 3 of text
- See the "links" page on the class web-site
- See also the various sparse matrix sites.
- Introduction to sparse matrices
- Sparse matrices in matlab –

What are sparse matrices?



Pattern of a small sparse matrix

- Vague definition: matrix with few nonzero entries
- For all practical purposes: an $m \times n$ matrix is sparse if it has $O(\min(m, n))$ nonzero entries.
- This means roughly a constant number of nonzero entries per row and column -
- This definition excludes a large class of matrices that have $O(\log(n))$ nonzero entries per row.
- Other definitions use a slow growth of nonzero entries with respect to n or m.

‘‘..matrices that allow special techniques to take advantage of the large number of zero elements.” (J. Wilkinson)

A few applications which lead to sparse matrices:

Structural Engineering, Computational Fluid Dynamics, Reservoir simulation, Electrical Networks, optimization, Google Page rank, information retrieval (LSI), circuit similation, device simulation, ...

Goal of Sparse Matrix Techniques

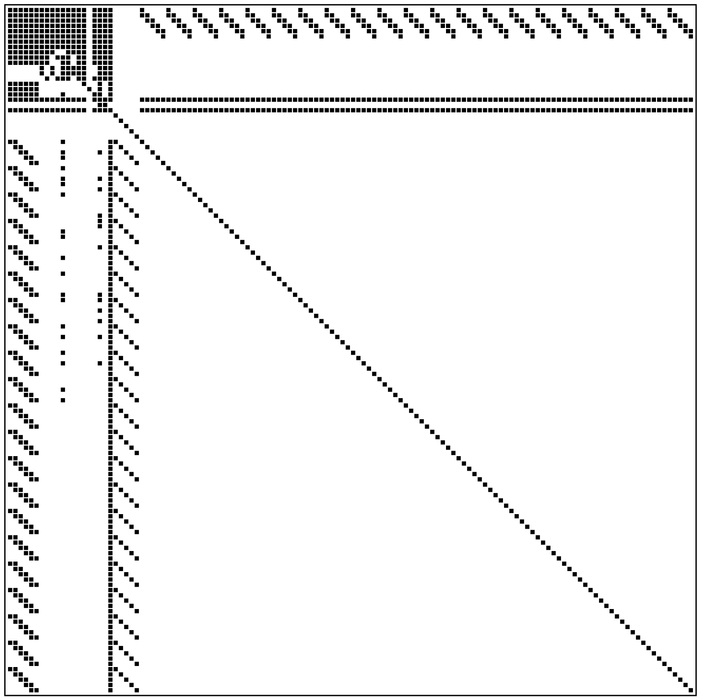
➤ To perform standard matrix computations economically i.e., without storing the zeros of the matrix.

Example: To add two square dense matrices of size n requires $O(n^2)$ operations. To add two sparse matrices A and B requires $O(nnz(A) + nnz(B))$ where $nnz(X)$ = number of nonzero elements of a matrix X.

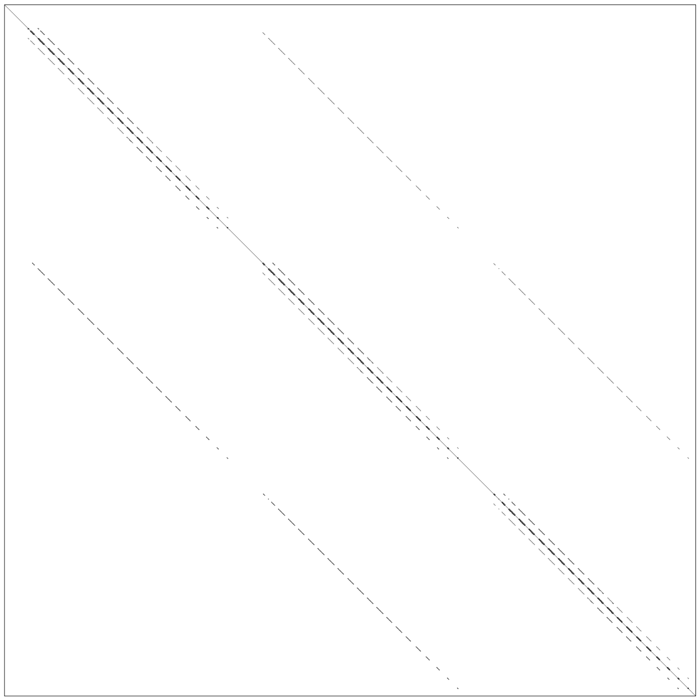
➤ For typical Finite Element /Finite difference matrices, number of nonzero elements is $O(n)$.

Remark: A^{-1} is usually dense, but L and U in the LU factorization may be reasonably sparse (if a good technique is used)

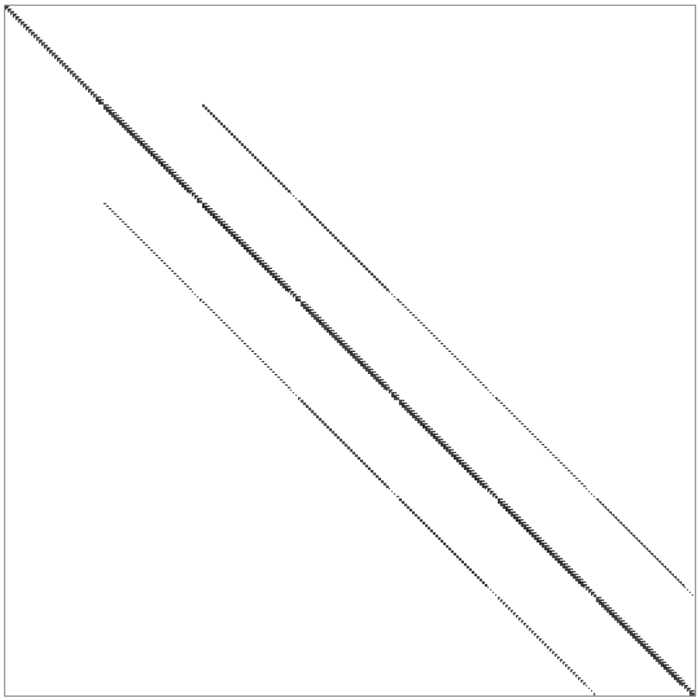
Nonzero patterns of a few sparse matrices



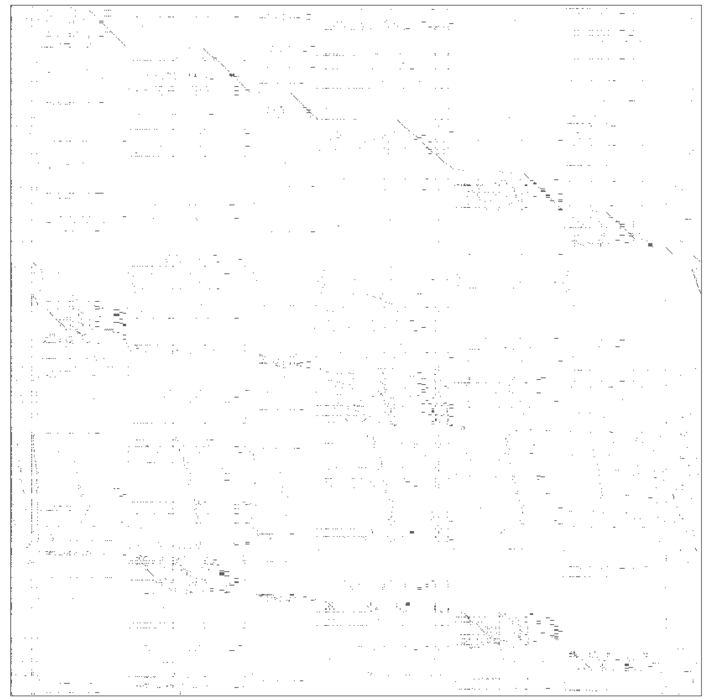
ARC130: Unsymmetric matrix from laser problem. a.r.curtis, oct 1974



SHERMAN5: fully implicit black oil simulator 16 by 23 by 3 grid, 3 unk



PORES3: Unsymmetric MATRIX FROM PORES



BP_1000: UNSYMMETRIC BASIS FROM LP PROBLEM BP

Types of sparse matrices

➤ Two types of matrices: **structured** (e.g. Sherman5) and **unstructured** (e.g. BP_1000)

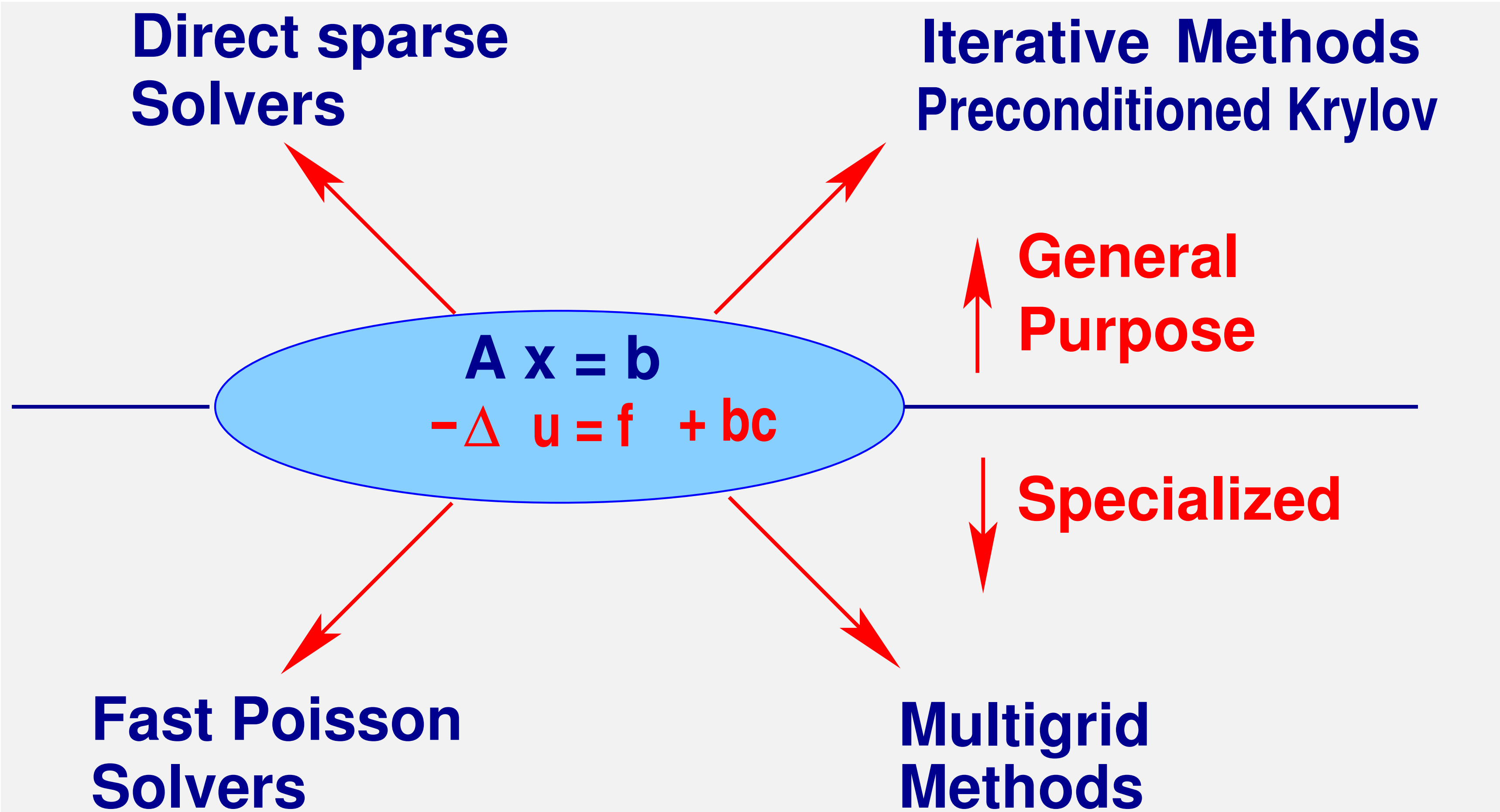
➤ The matrices PORES3 and SHERMAN5 are from Oil Reservoir Simulation. Often: 3 unknowns per mesh point (Oil , Water saturations, Pressure). Structured matrices.

➤ 40 years ago reservoir simulators used rectangular grids.

➤ Modern simulators: Finer, more complex physics ➤ harder and larger systems. Also: unstructured matrices

➤ A naive but representative challenge problem: $\mathbf{100 \times 100 \times 100}$ grid + about 10 unknowns per grid point ➤ $\boldsymbol{N \approx 10^7}$, and $\boldsymbol{nnz \approx 7 \times 10^8}$.

Solving sparse linear systems: existing methods



Two types of methods for general systems:

➤ Direct methods : based on sparse Gaussian eimination, sparse Cholesky,..

➤ Iterative methods: compute a sequence of iterates which converge to the solution - preconditioned Krylov methods..

Remark: These two classes of methods have always been in competition.

➤ 40 years ago solving a system with $n = 10,000$ was a challenge

➤ Now you can solve this in a fraction of a second on a laptop.

➤ Sparse direct methods made huge gains in efficiency. As a result they are very competitive for 2-D problems.

➤ 3-D problems lead to more challenging systems [inherent to the underlying graph]

Difficulty:

- No robust 'black-box' iterative solvers.
- At issue: Robustness in conflict with efficiency.

➤ Iterative methods are starting to use some of the tools of direct solvers to gain 'robustness'

Consensus:

1. Direct solvers are often preferred for two-dimensional problems (robust and not too expensive).

2. Direct methods loose ground to iterative techniques for three-dimensional problems, and problems with a large degree of freedom per grid point,

Sparse matrices in matlab

- Matlab supports sparse matrices to some extent.
- Can define sparse objects by conversion

```
A = sparse(X) ;  X = full(A)
```

- Can show pattern

```
spy(X)
```

- Define the analogues of `ones`, `eye`:

```
speye(n,m),   spones(pattern)
```

➤ A few reorderings functions provided.. [will be studied in detail later]

```
symrcm, symamd, colamd, colperm
```

➤ Random sparse matrix generator:

`sprand(S)` or `sprand(m,n, density)`

(also textttsprandn(...))

➤ Diagonal extractor-generator utility:

```
spdiags(A) , spdiags(B,d,m,n)
```

➤ Other important functions:

```
spalloc(..)  , find(..)
```

Graph Representations of Sparse Matrices

- Graph theory is a fundamental tool in sparse matrix techniques.

DEFINITION. A graph G is defined as a pair of sets $G = (V, E)$ with $E \subset V \times V$. So G represents a binary relation. The graph is undirected if the binary relation is reflexive. It is directed otherwise. V is the vertex set and E is the edge set.

Example: Given the numbers 5, 3, 9, 15, 16, show the two graphs representing the relations

R1: Either $x < y$ or y divides x.

R2: x and y are congruent modulo 3. [mod(x,3) $=$ mod(y,3)]

➤ Adjacency Graph $G = (V, E)$ of an $n \times n$ matrix A :

- Vertices $V = \{1, 2, ..., n\}$.
- Edges $E = \{(i, j) | a_{ij} \neq 0\}$.

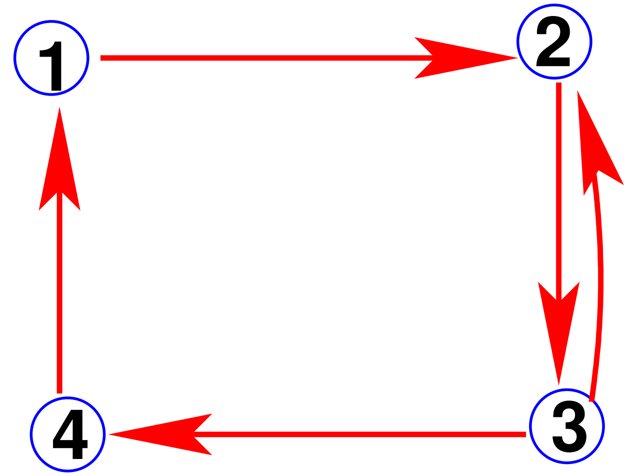
➤ Often self-loops (i, i) are not represented [because they are always there]

➤ Graph is undirected if the matrix has a symmetric structure:

$$a_{ij} \neq 0 \quad \text{iff} \quad a_{ji} \neq 0.$$

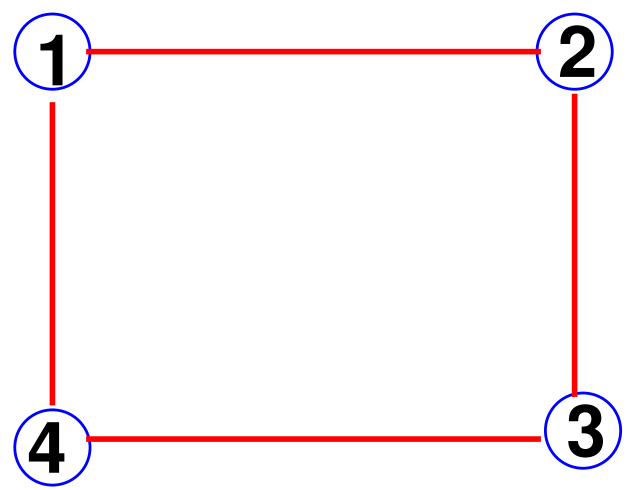
Example: (directed graph)

$$\begin{bmatrix} & \star & & \\ & & \star & \\ & \star & & \star \\ \star & & & \end{bmatrix}$$



Example: (undirected graph)

$$\begin{bmatrix} & \star & & \star \\ \star & & \star & \\ & \star & & \star \\ \star & & \star & \end{bmatrix}$$



✍ Adjacency graph of:

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

✍ Graph of a tridiagonal matrix? Of a dense matrix?

✍ Recall what a star graph is. Show a matrix whose graph is a star graph. Consider two situations: Case when center node is labeled first and case when it is labeled last.

- Note: Matlab now has a *graph* function.
- `G = graph(A)` creates adjacency graph from A
- G is a matlab class/
- `G.Nodes` will show the vertices of G
- `G.Edges` will show its edges.
- `plot(G)` will show a representation of the graph

✍ Do the following:

- Load the matrix 'Bmat.mat' located in the class web-site (see 'matlab' folder)
- Visualize pattern (`spy(B)`) + find: Number of nonzero elements, size, ...
- Generate graph - without self-edges:

```
G = graph(B,'OmitSelfLoops'
```

- Plot the graph –
- $1M question: Any idea on how this plot is generated?