

LU Factorization

Geometric Algorithms
Lecture 12

Practice Problem

$$\begin{bmatrix} 1 & 2 \\ 3 & 7 \end{bmatrix}$$

Determine the inverse of the above matrix in every way that we've discussed

Answer

$$A = \begin{bmatrix} 1 & 2 \\ 3 & 7 \end{bmatrix}$$

$$\frac{1}{ad-bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1}$$

$$\frac{1}{7-6} \begin{bmatrix} 7 & -2 \\ -3 & 1 \end{bmatrix} = \begin{bmatrix} 7 & -2 \\ -3 & 1 \end{bmatrix}$$

$$A \vec{x} = \vec{e}_1$$

$$\begin{bmatrix} 1 & 2 & 1 \\ 3 & 7 & 0 \end{bmatrix} \sim \begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & -3 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & 7 \\ 0 & 1 & -3 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 \\ 3 & 7 \end{bmatrix} \vec{x} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$A \vec{x} = \vec{e}_2$$

$$\begin{bmatrix} 1 & 2 & 0 \\ 3 & 7 & 1 \end{bmatrix} \sim \begin{bmatrix} 1 & 2 & 0 \\ 0 & 1 & 1 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & -2 \\ 0 & 1 & 1 \end{bmatrix}$$

Answer

$$\begin{bmatrix} 1 & 2 \\ 3 & 7 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 & 1 & 0 \\ 3 & 7 & 0 & 1 \end{bmatrix} \sim \begin{bmatrix} 1 & 2 & 1 & 0 \\ 0 & 1 & -3 & 1 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & 7 & -2 \\ 0 & 1 & -3 & 1 \end{bmatrix}$$

$$A \vec{x} = \begin{bmatrix} 3 \\ 10 \end{bmatrix}$$

$$\vec{x} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 & 3 \\ 3 & 7 & 10 \end{bmatrix} \sim \begin{bmatrix} 1 & 2 & 3 \\ 0 & 1 & 1 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix}$$

$$A^{-1} \begin{bmatrix} 3 \\ 10 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} 7 & -2 \\ -3 & 1 \end{bmatrix} \begin{bmatrix} 3 \\ 10 \end{bmatrix} =$$

$$\begin{bmatrix} 7(3) - 2(10) \\ -9 + 10 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Objectives

- » Motivate **matrix factorization** in general, and the LU factorization in specific
- » Recall elementary row operations and connect them to matrices
- » Look at the **LU factorization**, how to find it, and how to use it

LU Factorization

Matrix Factorization

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A **factorization** of a matrix A is an equation which expresses A as a product of one or more matrices, e.g.,

$$A = BC$$

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So far, we've been given two factors and asked to find their product

Factorization is the harder direction

Reasons to Factorize

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Writing A as the product of multiple matrices can

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» make computing with A faster

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- » expose important information about A

Reasons to Factorize

Writing A as the product of multiple matrices can

» make computing with A faster LU Decomposition

» make working with A easier

» expose important information about A

The Problem

Question. For an matrix A , solve the equations

$$A\mathbf{x} = \mathbf{b}_1 \quad , \quad A\mathbf{x} = \mathbf{b}_2 \quad \dots \quad A\mathbf{x} = \mathbf{b}_{k-1} \quad , \quad A\mathbf{x} = \mathbf{b}_k$$

In other words: we want to solve several matrix equations over the same matrix

The Problem

Question. For a matrix A , solve (for X) in the equation

$$AX = B$$

where X and B are matrices of appropriate dimension

This is (essentially) the same question

The Problem

Question. Solve $AX = B$

If A is *invertible*, then we have a solution:

Find A^{-1} and then $X = A^{-1}B$

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Question. Solve $AX = B$

If A is *invertible*, then we have a solution:

Find A^{-1} and then $X = A^{-1}B$

What if A^{-1} is not invertible?

Even if it is, can we do it faster?

LU Factorization at a High Level

Given a $m \times n$ matrix A , we are going to factorize A as

$$A = \underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ * & 1 & 0 & 0 \\ * & * & 1 & 0 \\ * & * & * & 1 \end{bmatrix}}_L \underbrace{\begin{bmatrix} \blacksquare & * & * & * & * \\ 0 & \blacksquare & * & * & * \\ 0 & 0 & 0 & \blacksquare & * \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}}_{\substack{\text{echelon form of } A \\ U}}$$

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echelon form of A

Note. This applies to non-square matrices

What are "L" and "U"?

L stands for "lower" as in *lower triangular*

U stands for "upper" as in *upper triangular*

$$A = \begin{bmatrix} 1 & 0 & 0 & 0 \\ * & 1 & 0 & 0 \\ * & * & 1 & 0 \\ * & * & * & 1 \end{bmatrix} \begin{bmatrix} \blacksquare & * & * & * \\ 0 & \blacksquare & * & * \\ 0 & 0 & \blacksquare & * \\ 0 & 0 & 0 & \blacksquare \end{bmatrix}$$

L U

The Fundamental Question

$$A = LU$$

echelon form of A

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We know how to build U , that's just the forward phase of Gaussian elimination

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How do we build L ?

The Fundamental Question

$$A = LU$$

echelon form of A

We know how to build U , that's just the forward phase of Gaussian elimination

How do we build L ?

The idea. L "implements" the row operations of the forward phase

Elementary Matrices

Recall: Elementary Row Operations

scaling	multiply a row by a number
interchange	switch two rows
replacement	add a scaled equation to another

The First Key Observation

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Elementary row operations are **linear transformations**
(viewed as transformation on columns)

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(viewed as transformation on columns)

Example: Scale row 2 by 5

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \xrightarrow{R_2 \leftarrow 5R_2} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 5a_{21} & 5a_{22} & 5a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

Example: Scaling

Restricted to one column, we see this is the above linear transformation

$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} \mapsto \begin{bmatrix} v_1 \\ 5v_2 \\ v_3 \end{bmatrix}$$

Example: Scaling

$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} \mapsto \begin{bmatrix} v_1 \\ 5v_2 \\ v_3 \end{bmatrix}$$

Let's build the matrix which implements it:

$$\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \mapsto \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \mapsto \begin{bmatrix} 0 \\ 5 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \mapsto \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 5 & 5 & 5 \\ 1 & 1 & 1 \end{bmatrix}$$

Another Example: Scaling + Replacement

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \longrightarrow \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ (a_{31} - 2a_{11}) & (a_{32} - 2a_{12}) & (a_{33} - 2a_{13}) \end{bmatrix}$$

$$R_3 \leftarrow (R_3 - 2R_1)$$

Another Example: Scaling + Replacement

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \mapsto \begin{bmatrix} x_1 \\ x_2 \\ x_3 - 2x_1 \end{bmatrix} \quad \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \mapsto \begin{bmatrix} 1 \\ 0 \\ -2 \end{bmatrix} \quad \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \mapsto \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

$$R_3 \leftarrow (R_3 - 2R_1)$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -2 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \mapsto \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ -1 & -1 & -1 \end{bmatrix}$$

Elementary row operations are
linear, so they are implemented
by matrices

General Elementary Scaling Matrix

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & k & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

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$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & k & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

If we want to perform $R_3 \leftarrow kR_3$ then we need the identity matrix but with the entry $A_{33} = k$.

General Elementary Scaling Matrix

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If we want to perform $R_3 \leftarrow kR_3$ then we need the identity matrix but with the entry $A_{33} = k$.

If we want to perform $R_i \leftarrow kR_i$ then we need the identity matrix but with the entry $A_{ii} = k$.

General Replacement Matrix

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ k & 0 & 0 & 1 \end{bmatrix}$$

General Replacement Matrix

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ k & 0 & 0 & 1 \end{bmatrix}$$

If we want to perform $R_4 \leftarrow R_4 + kR_1$, then we need the identity matrix but with the entry $A_{41} = k$.

General Replacement Matrix

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ k & 0 & 0 & 1 \end{bmatrix}$$

If we want to perform $R_4 \leftarrow R_4 + kR_1$, then we need the identity matrix but with the entry $A_{41} = k$.

If we want to perform $R_i \leftarrow R_i + kR_j$, then we need the identity matrix but with the entry $A_{ij} = k$.

General Swap Matrix

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

If we want to swap R_2 and R_3 , then we need the identity matrix, but with R_2 and R_3 swapped.

Elementary Matrices

Definition. An **elementary matrix** is a matrix obtained by applying a single row operation to the identity matrix I

Example.

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \xrightarrow{R_2 \leftrightarrow R_3} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

How To: Finding Elementary Matrices

Question. Find the matrix implementing the elementary row operation op

Solution. Apply op to the identity matrix of the appropriate size

$$R_2 \leftarrow R_2 + 3R_1$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \longrightarrow \begin{bmatrix} 1 & 0 & 0 & 0 \\ 3 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Products of Elementary Matrices

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Taking stock:

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- » Remember that Matrix multiplication is transformation composition (i.e., do one then the other)

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Taking stock:

- » Elementary matrices implement elementary row operations
- » Remember that Matrix multiplication is transformation composition (i.e., do one then the other)

So we can implement any sequence of row operations as a product of elementary matrices

How to: Matrices implementing Row Operations

Question. Find the matrix implementing a sequence of row operations op_1, op_2, \dots

Solution. Apply the row operations in sequence to the identity matrix of the appropriate size

Question

Find the matrix implementing the following sequence of elementary row operations on a $3 \times n$ matrix.

$$R_2 \leftarrow 3R_2$$

$$R_1 \leftarrow R_1 + R_2$$

$$R_2 \leftrightarrow R_3$$

Then multiply it with the all-ones 3×3 matrix.

Answer

$$R_2 \leftarrow 3R_2$$

$$R_1 \leftarrow R_1 + R_2$$

$$R_2 \leftrightarrow R_3$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 1 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 3 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\rightarrow \begin{bmatrix} 1 & 3 & 0 \\ 0 & 0 & 1 \\ 0 & 3 & 0 \end{bmatrix}$$

check:

$$\begin{bmatrix} 1 & 3 & 0 \\ 0 & 0 & 1 \\ 0 & 3 & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 4 & 4 & 4 \\ 1 & 1 & 1 \\ 3 & 3 & 3 \end{bmatrix}$$

Second Key Observation

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This also means the product of elementary matrices is invertible

$$(E_1 E_2 E_3 E_4)^{-1} = E_4^{-1} E_3^{-1} E_2^{-1} E_1^{-1}$$

!! the order reverses !!

Question (Conceptual)

Describe the inverse transformation for each elementary row operation

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Question (Conceptual)

Describe the inverse transformation for each elementary row operation

The inverse of scaling by k is scaling by $1/k$

The inverse of $R_i \leftarrow R_i + kR_j$ is $R_i \leftarrow R_i - kR_j$

The inverse of swapping is swapping again

Recall: Elementary Row Operations

scaling	multiply a row by a number
interchange	switch two rows
replacement	add a scaled equation to another

Recall: Elementary Row Operations

We only need these two for the forward phase

interchange

switch two rows

replacement

add a scaled equation to another

Recall: Elementary Row Operations

We'll assume we only need this

replacement add a scaled equation to another

Reminder: LU Factorization at a High Level

Given a $m \times n$ matrix A , we are going to factorize A as

$$A = \begin{matrix} & \begin{matrix} \text{Echelon form of } A \end{matrix} \\ \begin{bmatrix} 1 & 0 & 0 & 0 \\ * & 1 & 0 & 0 \\ * & * & 1 & 0 \\ * & * & * & 1 \end{bmatrix} & \begin{bmatrix} \blacksquare & * & * & * & * \\ 0 & \blacksquare & * & * & * \\ 0 & 0 & 0 & \blacksquare & * \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \\ L & U \end{matrix}$$

Gaussian Elimination and Elementary Matrices

$$A \sim A_1 \sim A_2 \sim \dots \sim A_k$$

Consider a sequence of elementary row operations from A to an echelon form

Each step can be represent as a **product with an elementary matrix**

Gaussian Elimination and Elementary Matrices

$$A \sim E_1 A \sim E_2 E_1 A \sim \dots \sim E_k E_{k-1} \dots E_2 E_1 A$$

Gaussian Elimination and Elementary Matrices

$$A \sim E_1 A \sim E_2 E_1 A \sim \dots \sim E_k E_{k-1} \dots E_2 E_1 A$$

This exactly tells us that if B is the final echelon form we get then

$$B = (E_k E_{k-1} \dots E_2 E_1) A = EA$$

where E implements a sequence of row operations. So:

Gaussian Elimination and Elementary Matrices

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This exactly tells us that if B is the final echelon form we get then

$$B = \overset{\text{Invertible}}{(E_k E_{k-1} \dots E_2 E_1)} A = EA$$

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Gaussian Elimination and Elementary Matrices

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Invertible

$$B = (E_k E_{k-1} \dots E_2 E_1) A = EA$$

where E implements a sequence of row operations. So:

$$A = E^{-1} B = (E_1^{-1} E_2^{-1} \dots E_{k-1}^{-1} E_k^{-1}) B$$

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```
1  FUNCTION LU_Factorization(A):
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```
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2      L ← identity matrix
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LU Factorization Algorithm

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1  FUNCTION LU_Factorization( $A$ ):  
2       $L \leftarrow$  identity matrix  
3       $U \leftarrow A$ 
```

LU Factorization Algorithm

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1  FUNCTION LU_Factorization(A):  
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3      U ← A  
4      convert U to an echelon form by GE forward step # without swaps
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6          E ← the matrix implementing OP
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5      FOR each row operation OP in the prev step:  
6          E ← the matrix implementing OP  
7          L ← L @ E-1      # note the multiplication on the right  
8      RETURN (L, U)      we'll see how to do this more efficiently
```

The forward part of Gaussian
elimination is matrix
factorization

The "L" Part

$$E = E_k E_{k-1} \dots E_2 E_1$$

This a product of elementary matrices

So $L = E^{-1} = E_1^{-1} E_2^{-1} \dots E_{k-1}^{-1} E_k^{-1}$ **!! the order reverses !!**

We won't prove this, but it's worth thinking about: **why is this lower triangular?**

And can we build this in a more efficient way?

demo

How To: LU Factorization by hand

Question. Find a LU Factorization for the matrix A (assuming no swaps)

Solution.

- » Start with L as the identity matrix
- » Find U by the forward part of GE
- » For each operation $R_i \leftarrow R_i + kR_j$, set L_{ij} to $-k$

Practice Problem

$$\begin{bmatrix} 1 & 2 \\ 3 & 7 \end{bmatrix}$$

Determine an LU factorization of the above matrix using this procedure

Answer

$$\begin{bmatrix} 1 & 2 \\ 3 & 7 \end{bmatrix}$$

Determine an LU factorization of the above matrix using this procedure

Analyzing LU Factorization

Analyzing Linear Algebra Algorithms

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We will not use $O(\cdot)$ notation!

Analyzing Linear Algebra Algorithms

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For numerics, we care about number of **F**loating-oint
Operations (FLOPs):

- >> addition
- >> subtraction
- >> multiplication
- >> division
- >> square root

Analyzing Linear Algebra Algorithms

We will not use $O(\cdot)$ notation!

For numerics, we care about number of **F**loating-oint
Operations (FLOPs):

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$2n$ vs. n is very different
when $n \sim 10^{20}$

Dominant Terms

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That said, we don't care about *exact* bounds

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A function $f(n)$ is ***asymptotically equivalent*** to $g(n)$ if

$$\lim_{i \rightarrow \infty} \frac{f(i)}{g(i)} = 1$$

Dominant Terms

That said, we don't care about *exact* bounds

A function $f(n)$ is ***asymptotically equivalent*** to $g(n)$ if

$$\lim_{i \rightarrow \infty} \frac{f(i)}{g(i)} = 1$$

For polynomials, they are equivalent to their dominant term

Dominant Terms

the dominant term of a polynomial is the monomial with the highest degree

$$\lim_{i \rightarrow \infty} \frac{3x^3 + 100000x^2}{3x^3} = 1$$

$3x^3$ dominates the function even though the coefficient for x^2 is so large

How To: Solving systems with the LU

Question. Solve the equation $A\mathbf{x} = \mathbf{b}$ given that $A = LU$ is a LU factorization.

Solution. First solve $L\mathbf{x} = \mathbf{b}$ to get a solution \mathbf{c} , then solve $U\mathbf{x} = \mathbf{c}$ to get a solution \mathbf{d} .

Verify:

How To: Solving systems with the LU

Question. Solve the equation $A\mathbf{x} = \mathbf{b}$ given that $A = LU$ is a LU factorization.

Solution. First solve $L\mathbf{x} = \mathbf{b}$ to get a solution \mathbf{c} , then solve $U\mathbf{x} = \mathbf{c}$ to get a solution \mathbf{d} .

Why is this better than just solving $A\mathbf{x} = \mathbf{b}$?

FLOPs for Solving General Systems

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The following FLOP estimates are based on $n \times n$ matrices

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GE Backward: $\sim 2n^2$ FLOPS

Matrix Inversion: $\sim 2n^3$ FLOPS

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Matrix Inversion: $\sim 2n^3$ FLOPS

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Solving by matrix inversion: $\sim 2n^3$ FLOPS

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The following FLOP estimates are based on $n \times n$ matrices

Gaussian Elimination: $\sim \frac{2n^3}{3}$ FLOPS

GE Forward: $\sim \frac{2n^3}{3}$ FLOPS

GE Backward: $\sim 2n^2$ FLOPS

Matrix Inversion: $\sim 2n^3$ FLOPS

Matrix-Vector Multiplication: $\sim 2n^2$ FLOPS

Solving by matrix inversion: $\sim 2n^3$ FLOPS

Solving by Gaussian elimination: $\sim \frac{2n^3}{3}$ FLOPS

FLOPS for solving LU systems

LU Factorization: $\sim \frac{2n^3}{3}$ FLOPS

Solving $L\mathbf{x} = \mathbf{b}$: $\sim 2n^2$ FLOPS (by "forward" elimination)

Solving $U\mathbf{x} = \mathbf{c}$: $\sim 2n^2$ FLOPS (already in echelon form)

Solving by LU Factorization: $\sim \frac{2n^3}{3}$ FLOPS

If you solve several matrix equations for the same matrix, LU factorization is faster than matrix inversion on the first equation, and the same (asymptotically) in later equations (and it works for rectangular matrices).

Other Considerations: Density

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If A doesn't have too many entries (A is **sparse**), then it's likely that L and U won't either.

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If A doesn't have too many entries (A is **sparse**), then it's likely that L and U won't either.

But A^{-1} may have *many* entries (A^{-1} is **dense**)

Other Considerations: Density

If A doesn't have too many entries (A is **sparse**), then it's likely that L and U won't either.

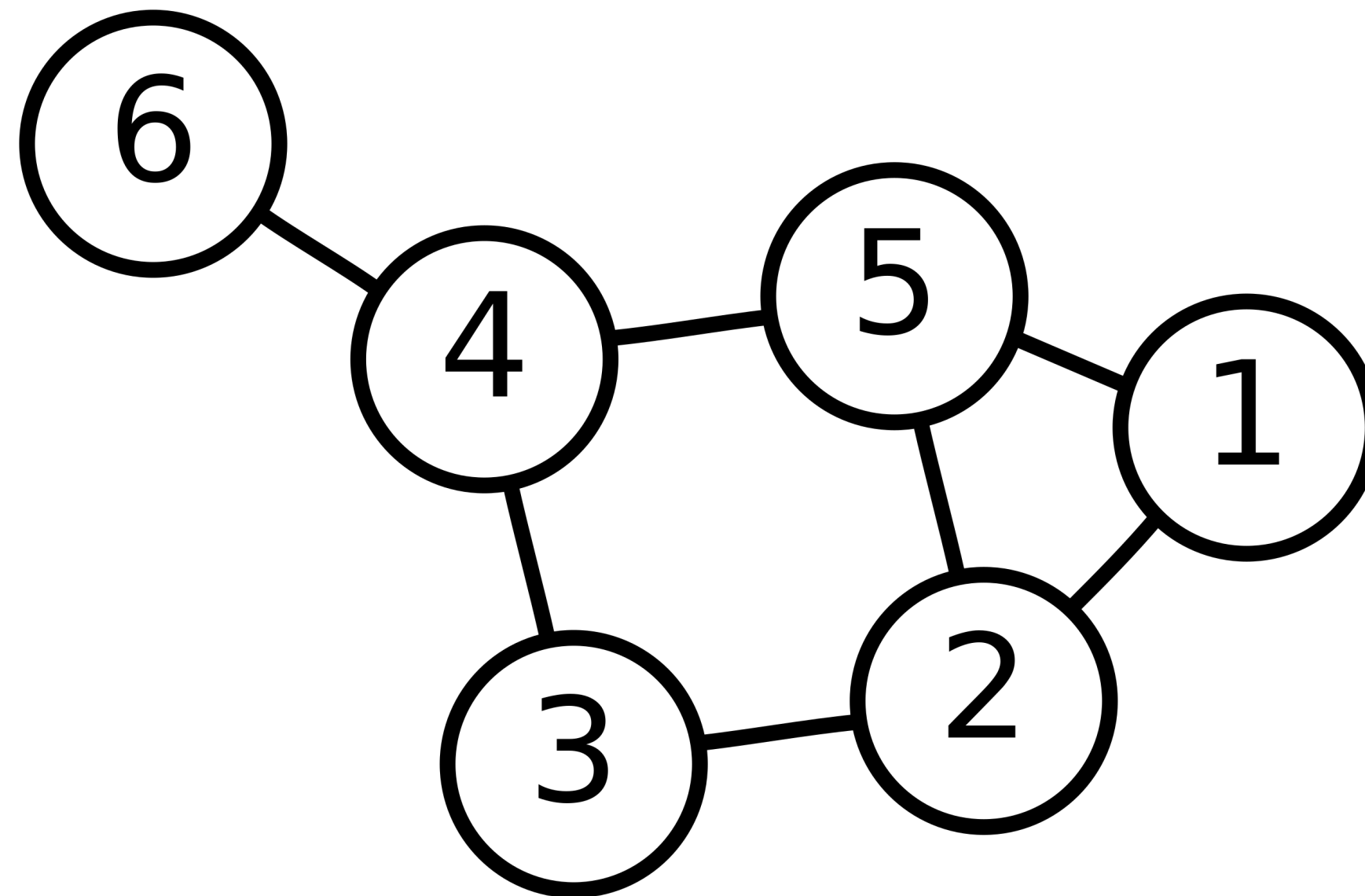
But A^{-1} may have *many* entries (A^{-1} is **dense**)

Sparse matrices are faster to compute with and better with respect to storage.

Algebraic Graph Theory

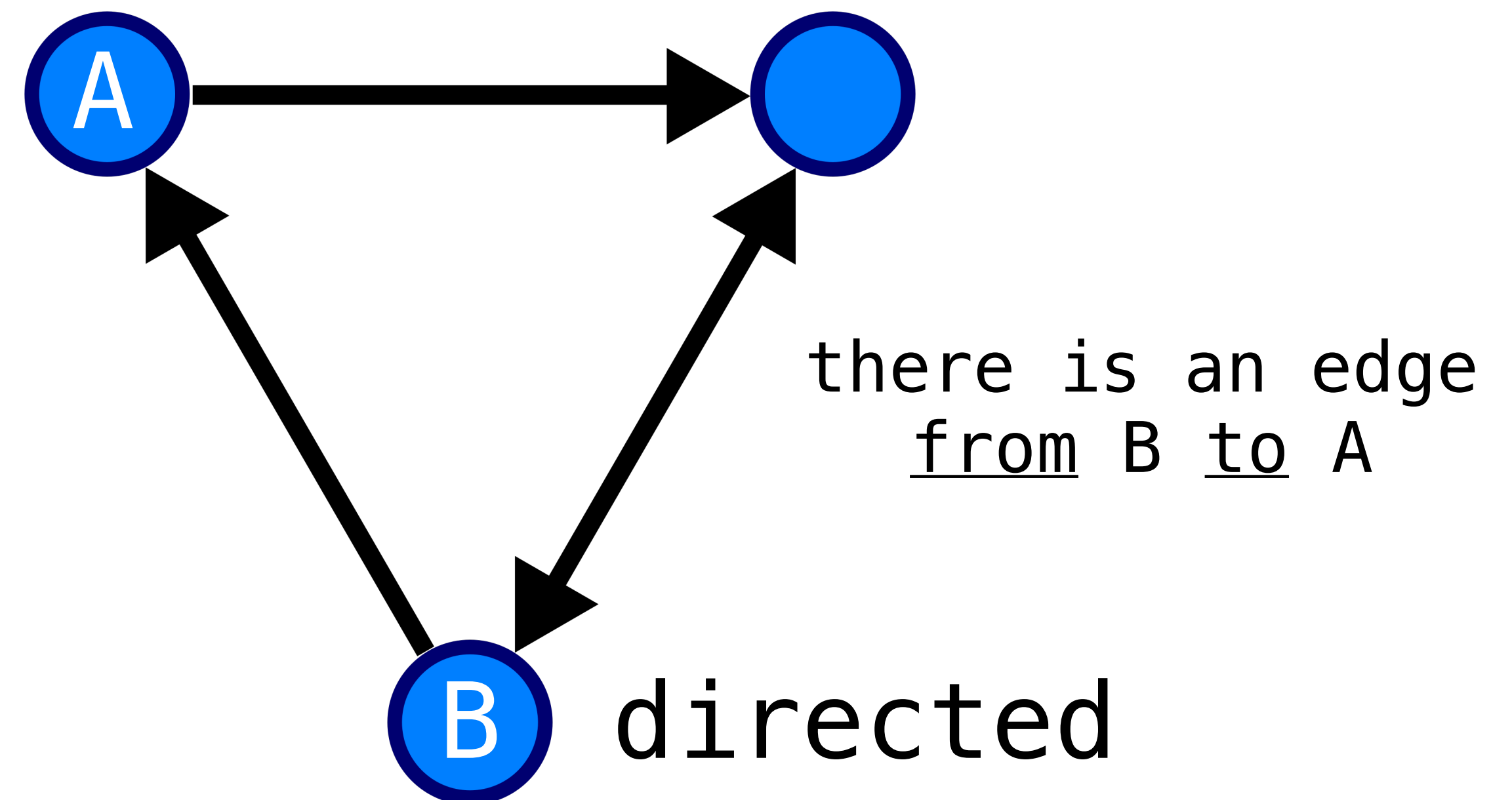
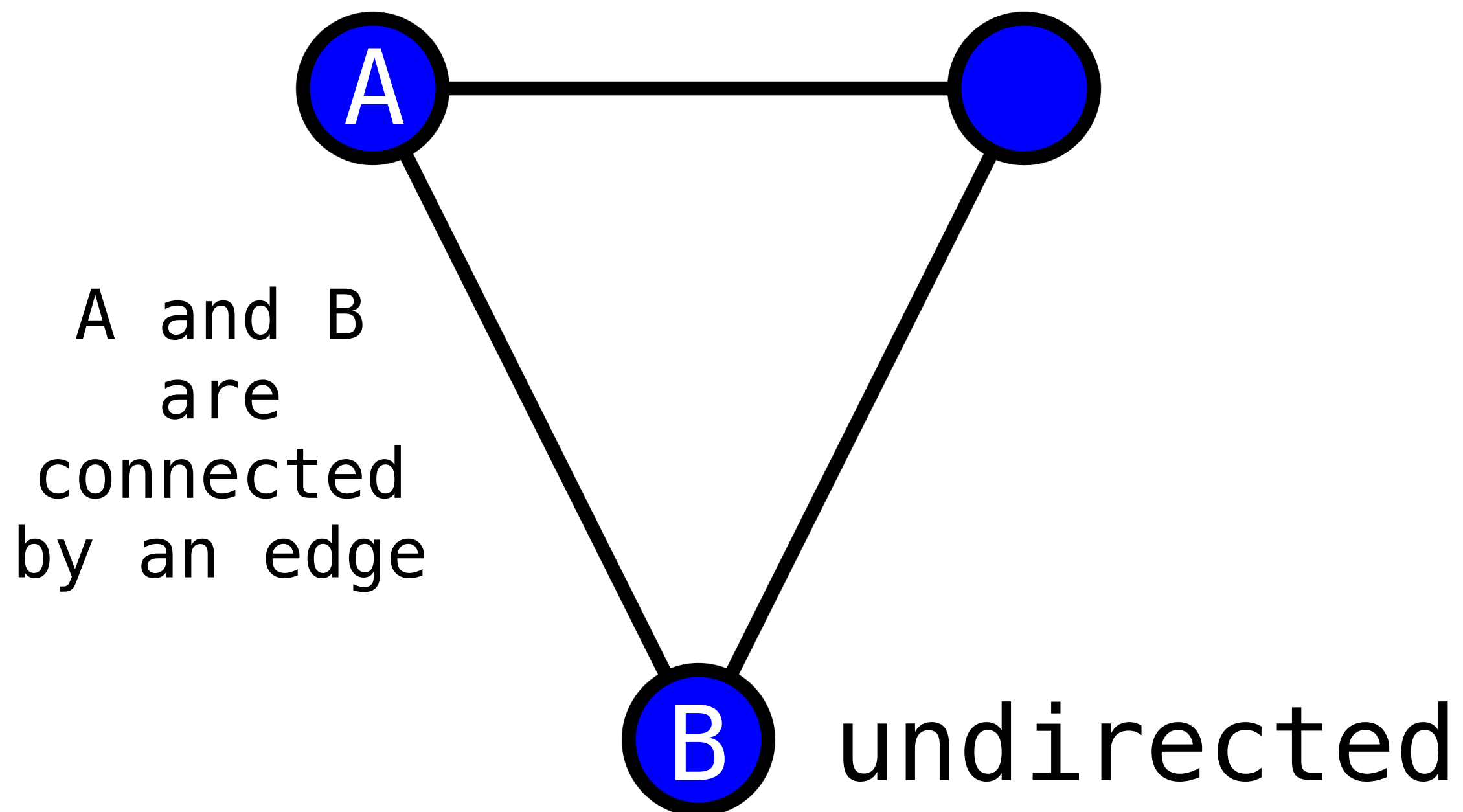
Graphs

Definition (Informal). A graph is a collection of nodes with edges between them.



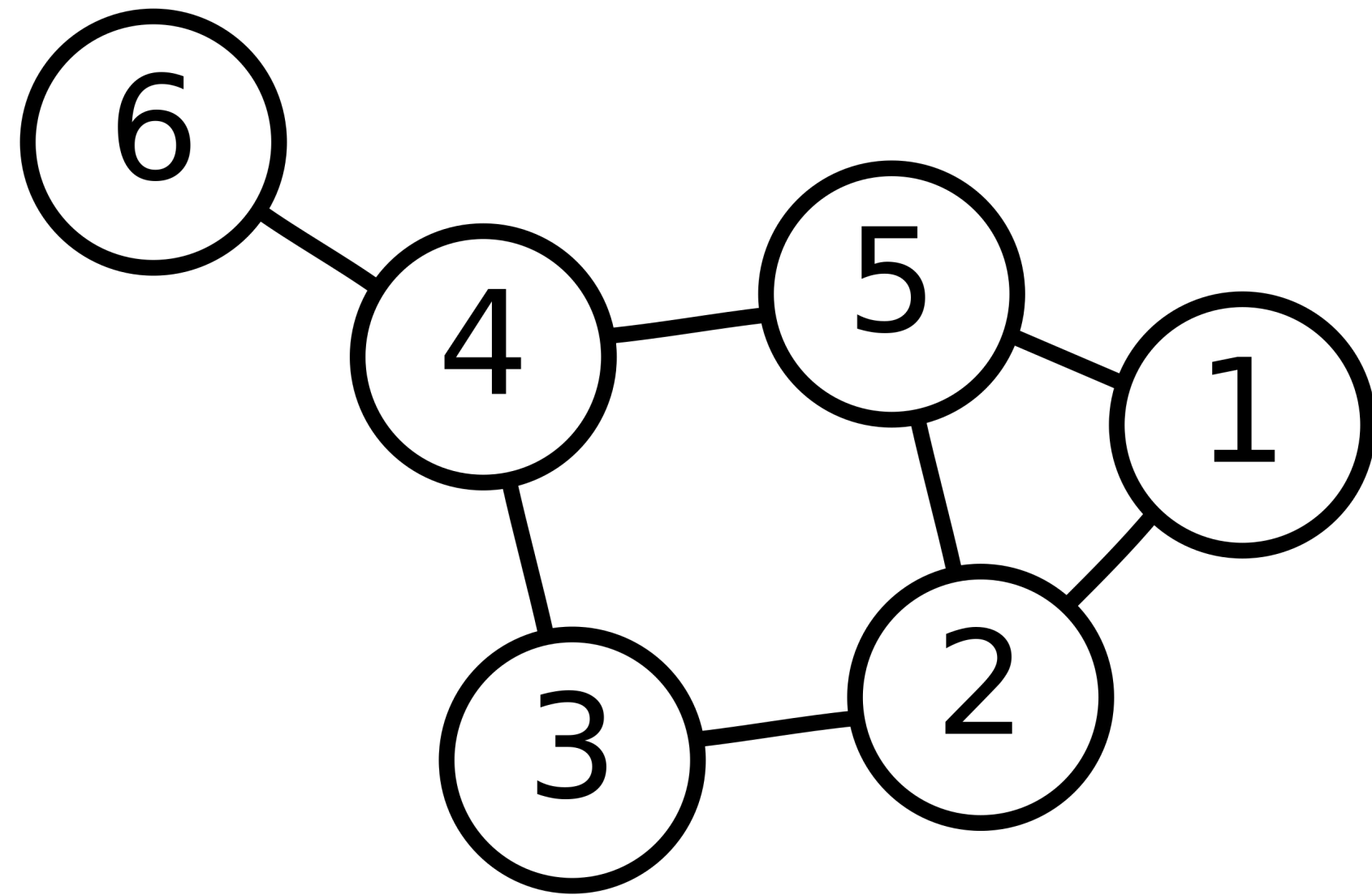
Directed vs. Undirected Graphs

A graph is **directed** if its edges have a direction.

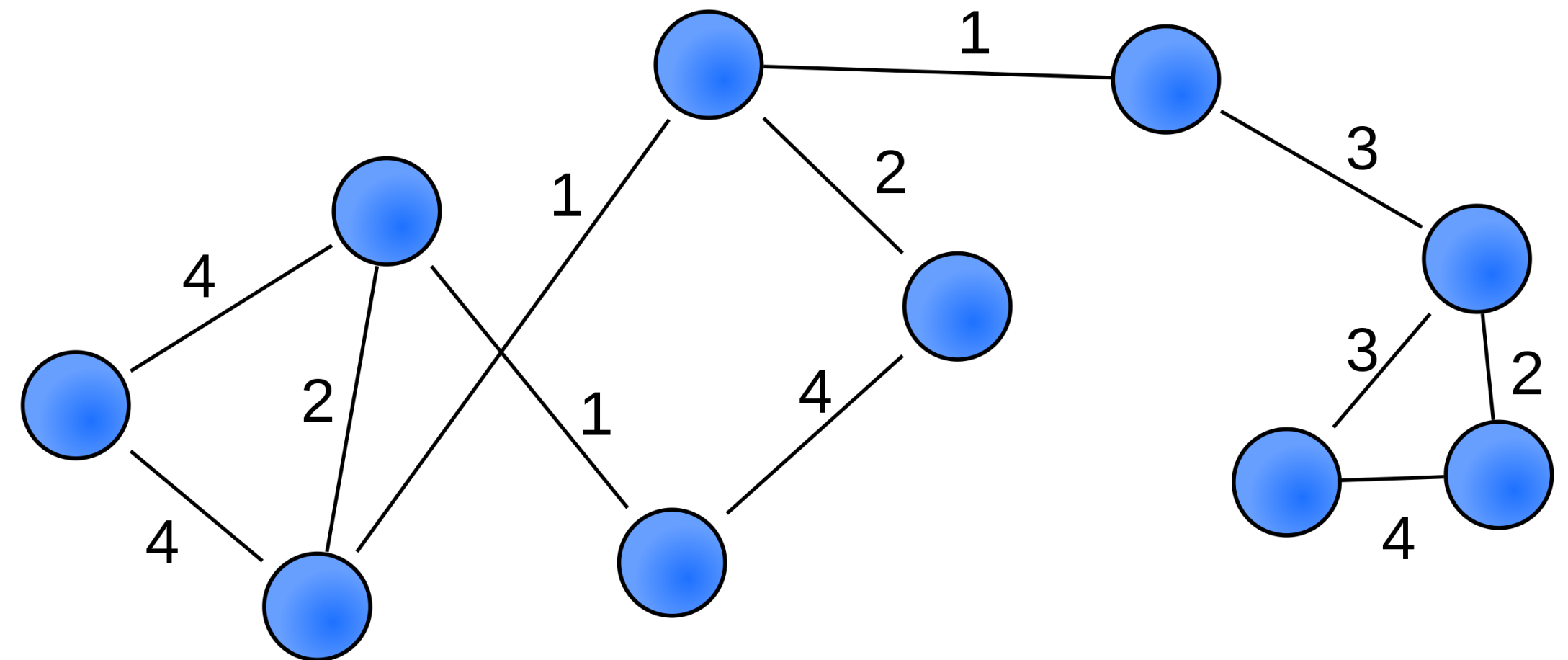


Weighted vs Unweighted graphs

A graph is **weighted** if its edges have associated values.



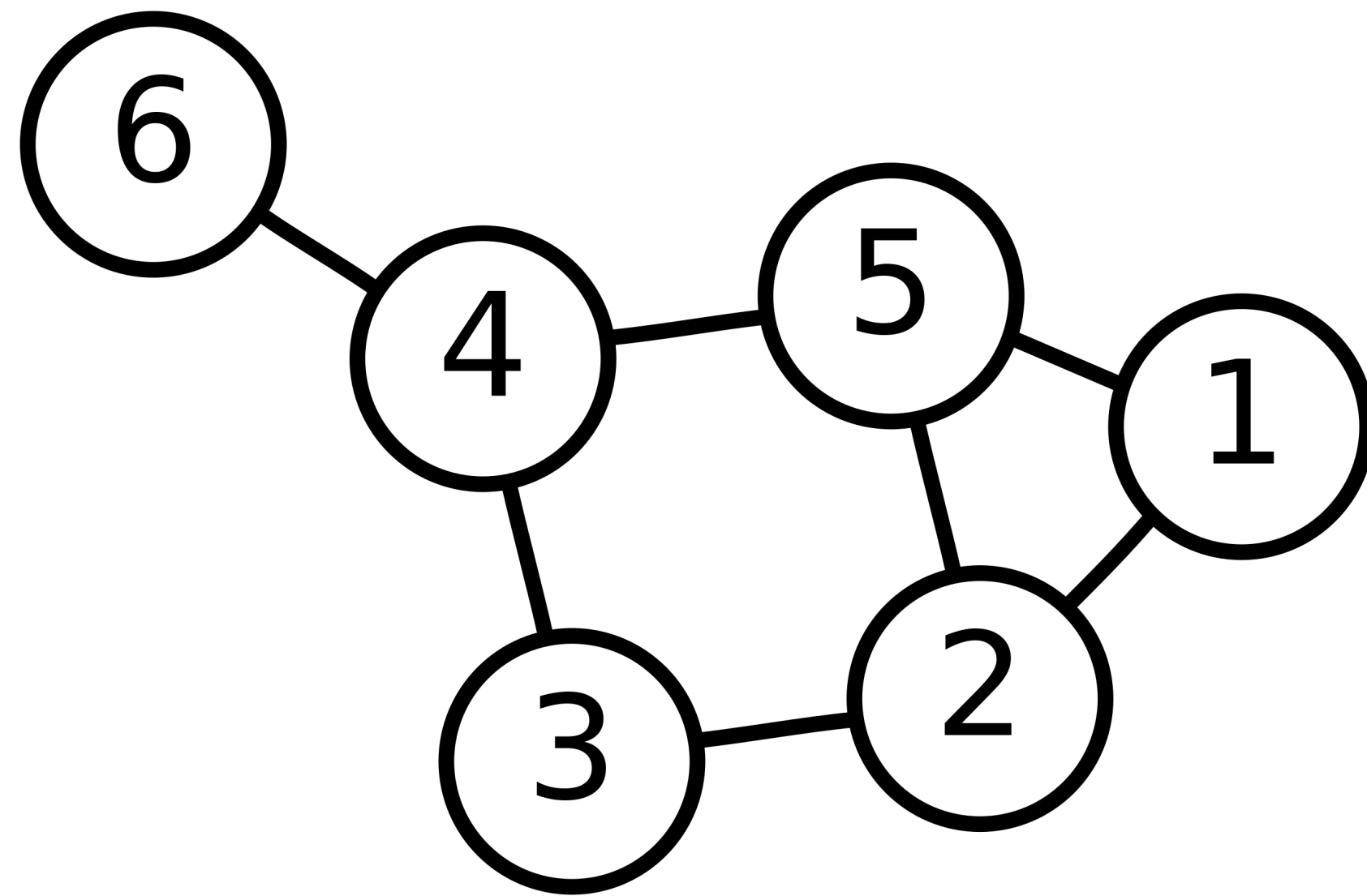
unweighted



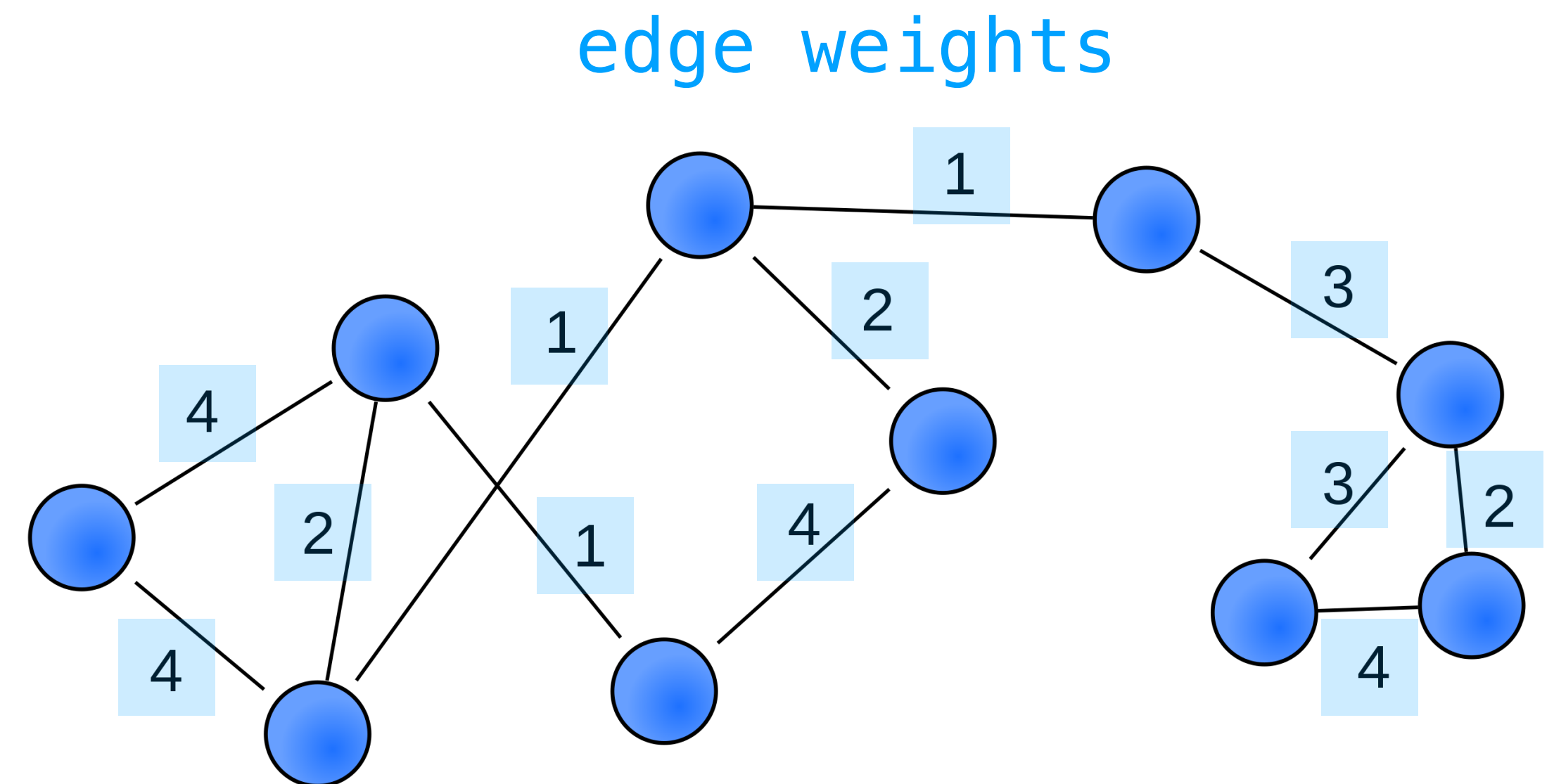
weighted

Weighted vs Unweighted graphs

A graph is **weighted** if its edges have associated values.



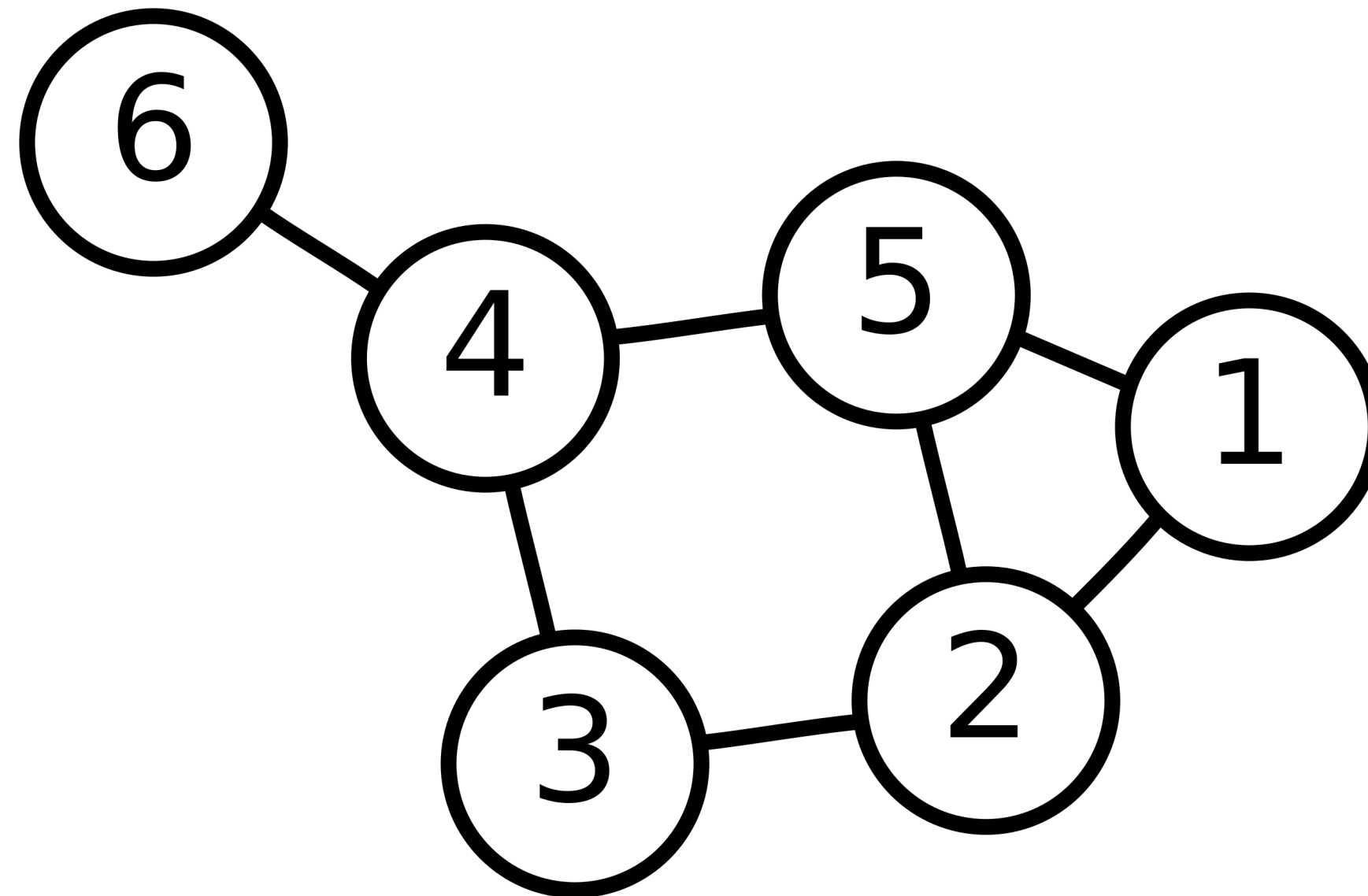
unweighted



weighted

Simple Graphs

A graph is **simple** if it is undirected, has no self loops, and no multi-edges.



Four Kinds of Graphs

directed

undirected

weighted

nodes are traffic lights
edges are streets
weights are number of lanes

nodes are musicians
edges are collaborations
weights are number of collaborations

unweighted

nodes are instagram users
edges are follows

nodes are bodies of land
edges are pedestrian bridges

Four Kinds of Graphs

directed

undirected

weighted

nodes are traffic lights
edges are streets
weights are number of lanes

nodes are musicians
edges are collaborations
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nodes are instagram users
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nodes are bodies of land
edges are pedestrian bridges

Today

Four Kinds of Graphs

directed

undirected

weighted

nodes are traffic lights
edges are streets
weights are number of lanes

Markov Chains

nodes are musicians
edges are collaborations
weights are number of collaborations

unweighted

nodes are instagram users
edges are follows

nodes are bodies of land
edges are pedestrian bridges

Today

Fundamental Question

Fundamental Question

How do we represent a graph
formally in a computer?

Fundamental Question

How do we represent a graph formally in a computer?

There are a couple ways, but one way is to use matrices.

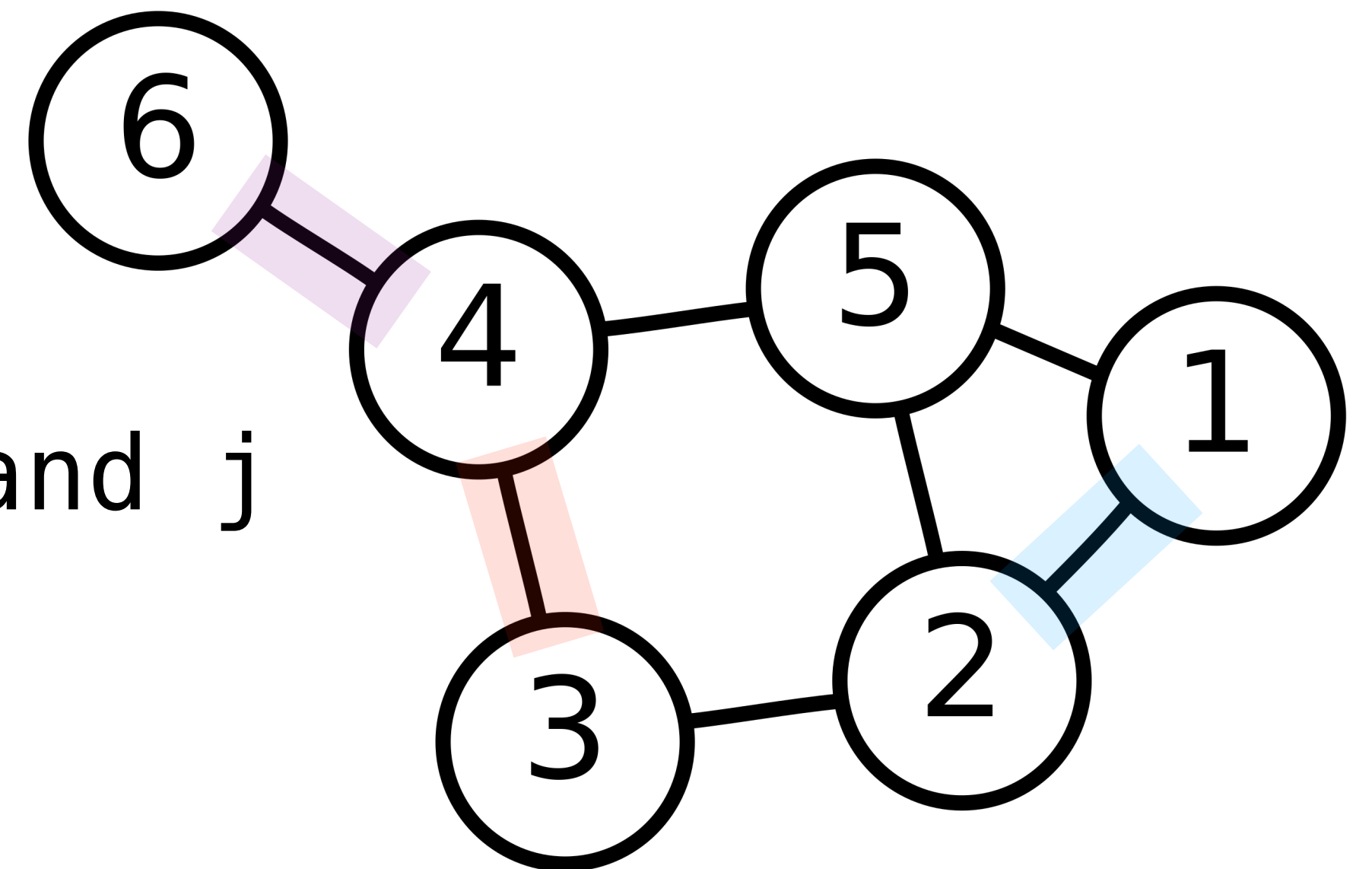
Adjacency Matrices

Let G be an simple graph with its nodes labeled by numbers 1 through n .

We can create the **adjacency matrix** A for G as follows.

$$A_{ij} = \begin{cases} 1 & \text{there is an edge between } i \text{ and } j \\ 0 & \text{otherwise} \end{cases}$$

$$\begin{matrix} & & A_{12} & & A_{34} & & A_{46} \\ A_{21} & \begin{bmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix} \end{matrix}$$



Symmetric Matrices

Definition. A $n \times n$ matrix is **symmetric** if

$$A^T = A$$

Example.

$$\begin{bmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}$$

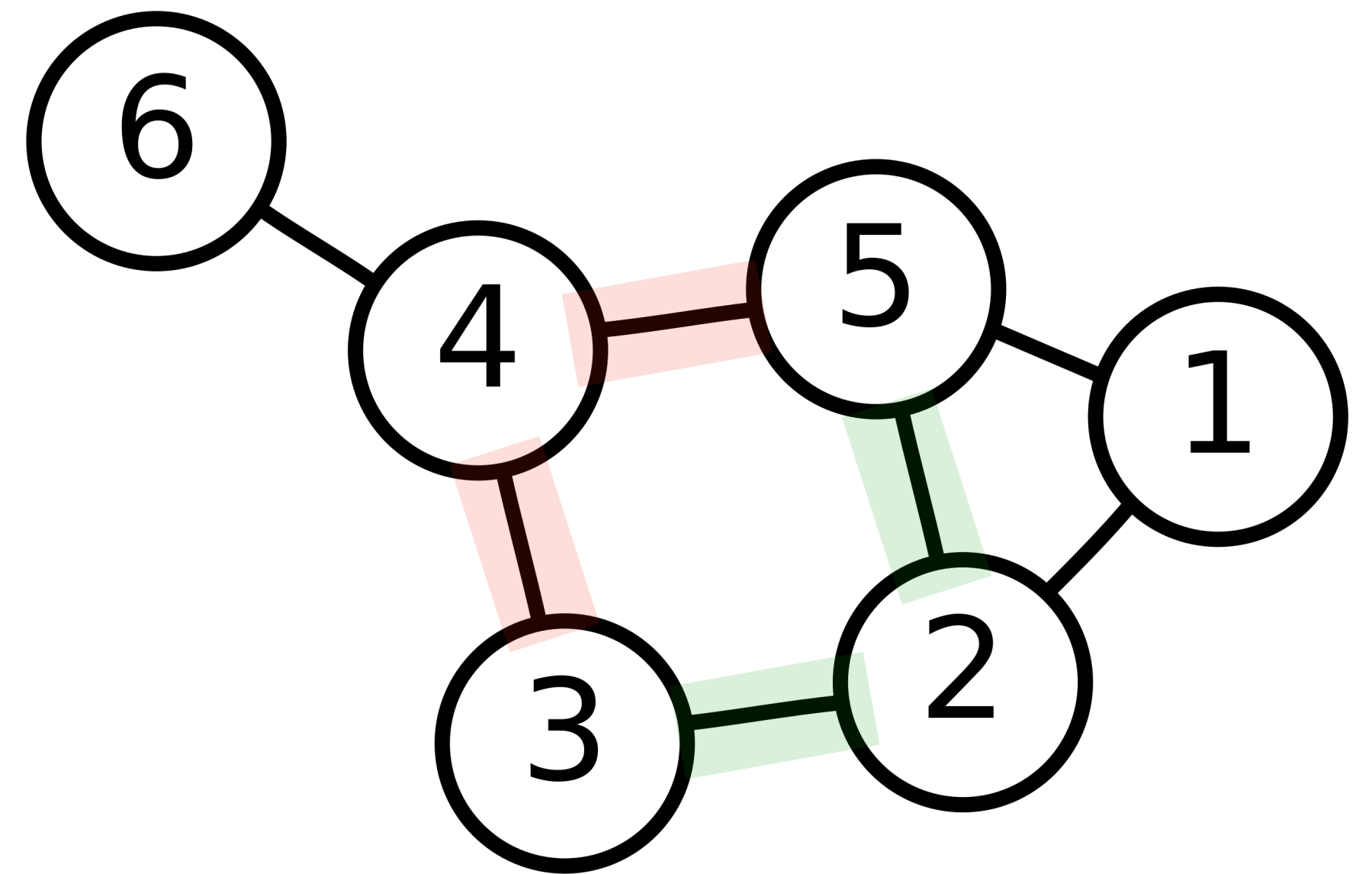
Once we have an adjacency matrix,
we can do linear algebra on
graphs.

Example: Squared Adjacency Matrices

Given an adjacency matrix A , can we interpret anything meaningful from A^2 ?

Example: Squared Adjacency Matrices

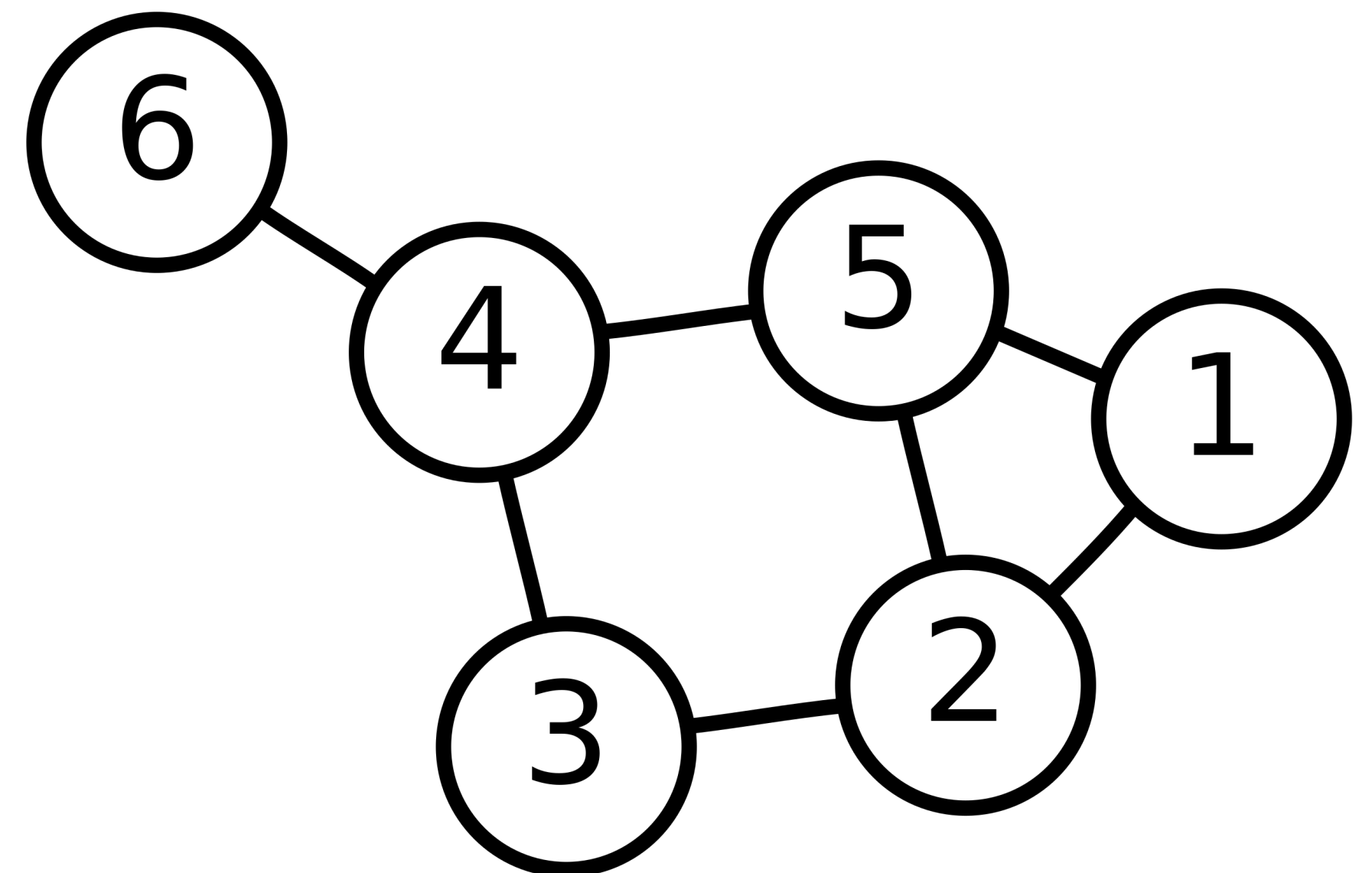
$$\begin{bmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}
 \begin{bmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}$$



$$(A^2)_{53} = 1(0) + 1(1) + 0(0) + 1(1) + 0(0) + 0(0) = 2$$

Example: Squared Adjacency Matrices

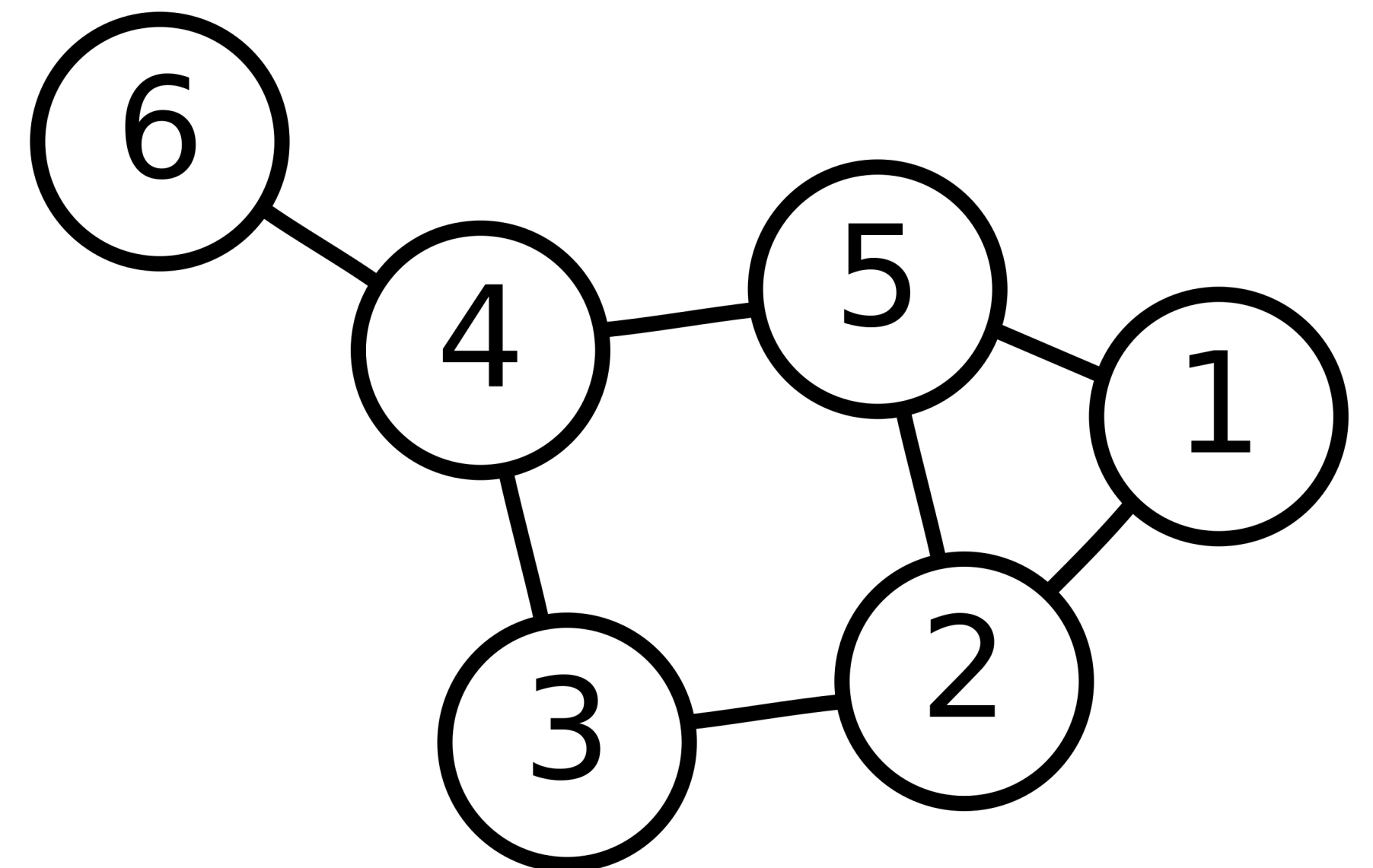
$$(A^2)_{ij} = A_{i1}A_{1j} + A_{i2}A_{2j} + \dots + A_{in}A_{nj}$$



Example: Squared Adjacency Matrices

$$(A^2)_{ij} = A_{i1}A_{1j} + A_{i2}A_{2j} + \dots + A_{in}A_{nj}$$

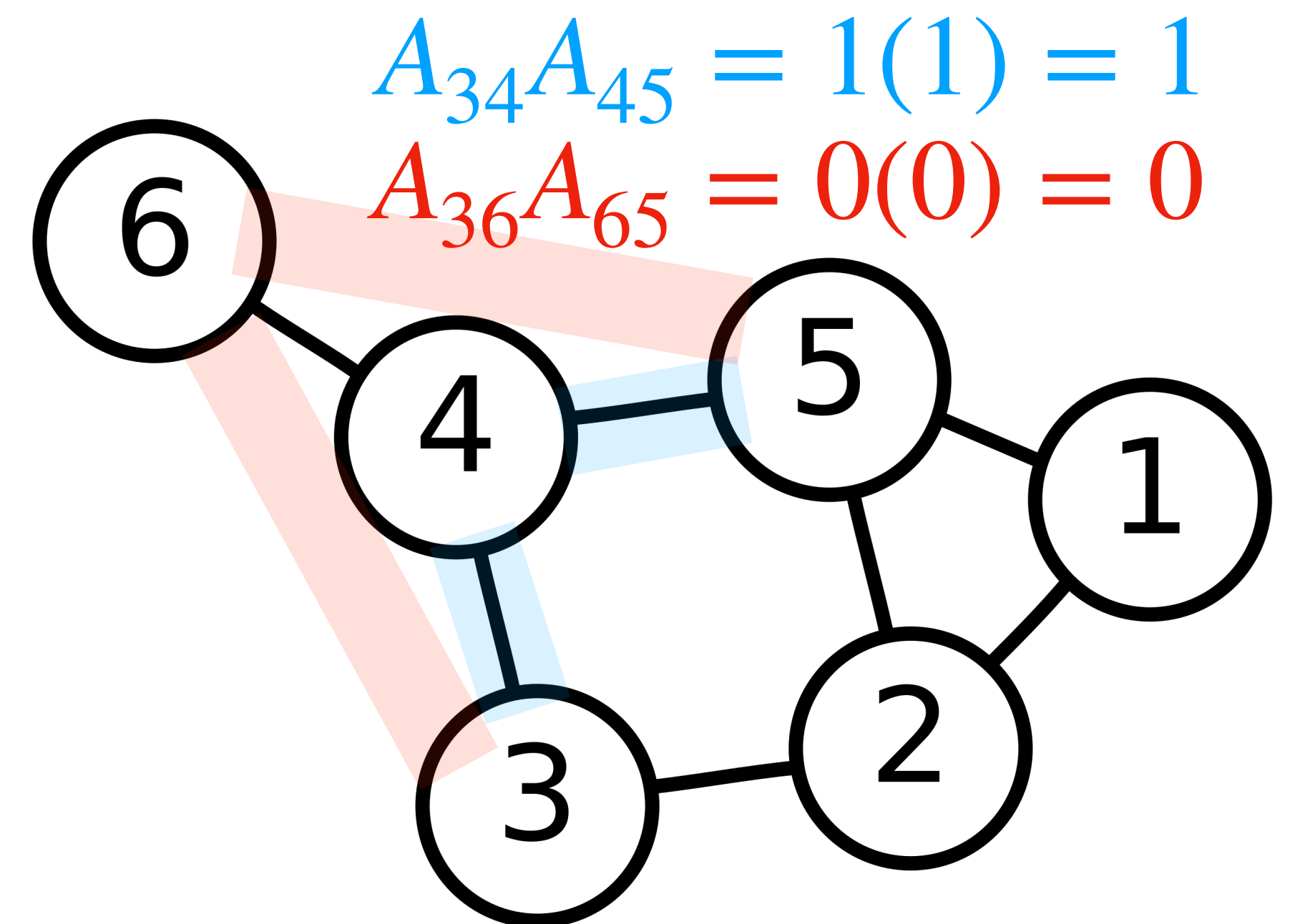
$$A_{ik}A_{kj} = \begin{cases} 1 & \text{there are edges } i \text{ to } k \text{ and } k \text{ to } j \\ 0 & \text{otherwise} \end{cases}$$



Example: Squared Adjacency Matrices

$$(A^2)_{ij} = A_{i1}A_{1j} + A_{i2}A_{2j} + \dots + A_{in}A_{nj}$$

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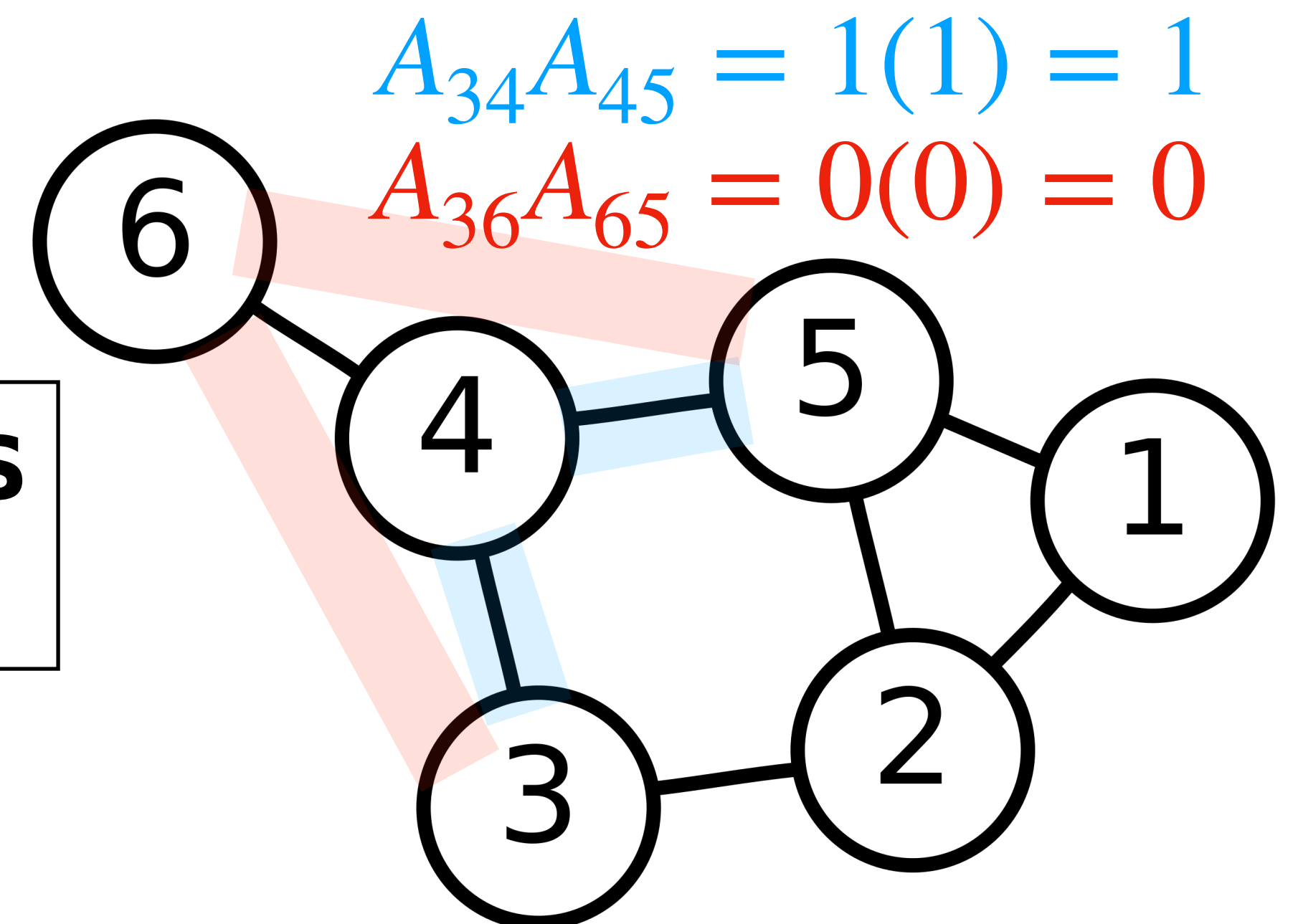


Example: Squared Adjacency Matrices

$$(A^2)_{ij} = A_{i1}A_{1j} + A_{i2}A_{2j} + \dots + A_{in}A_{nj}$$

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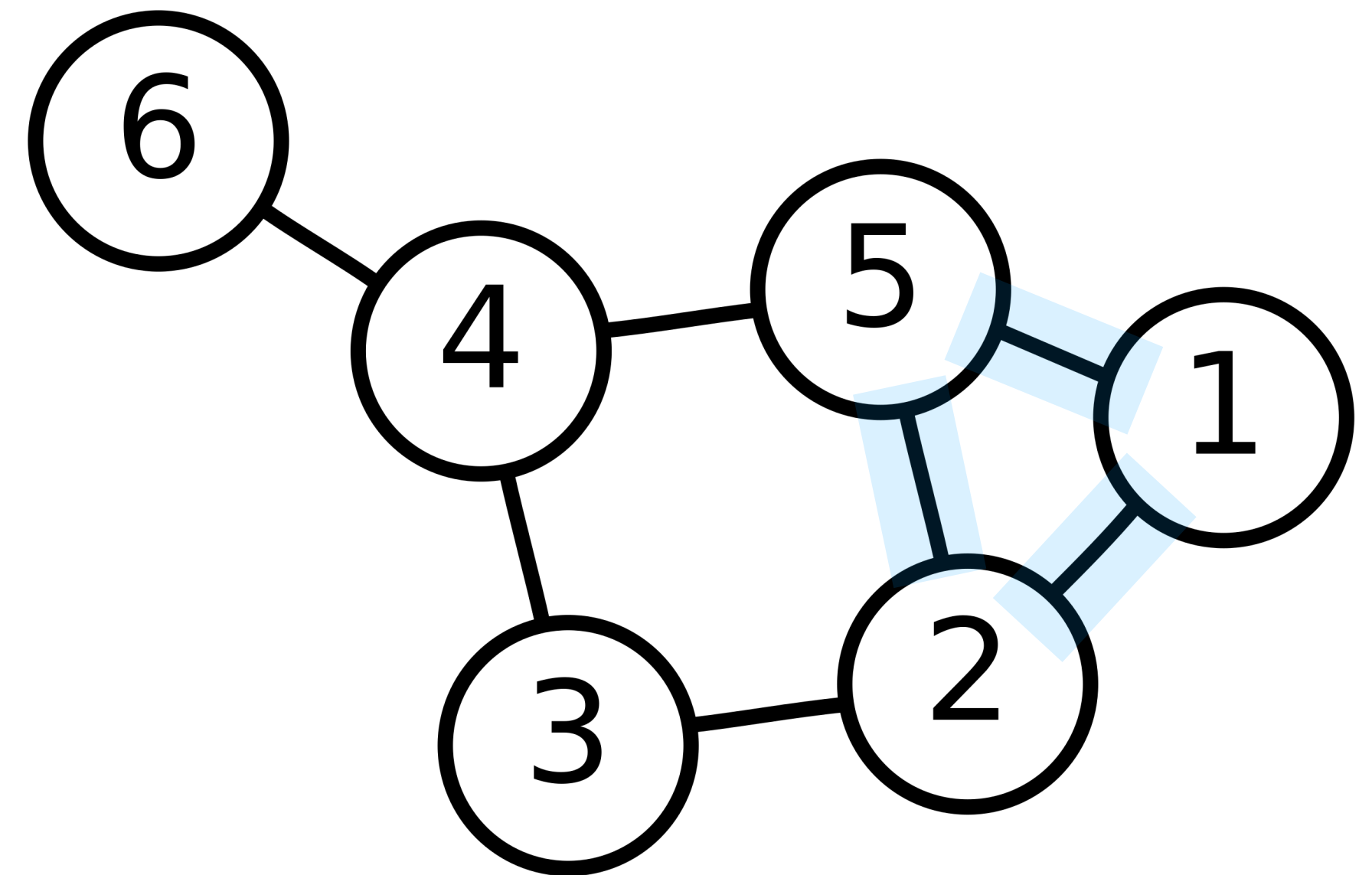
$$(A^2)_{ij} = \text{number of 2-step paths from } i \text{ to } j$$



Application: Triangle Counting

A **triangle** in an undirected graph is a set of three distinct nodes with edges between every pair of nodes.

Triangles in a social network represent mutual friends and tight cohesion (among other things)



Application: Triangle Counting (Naive)

```
FUNCTION tri_count_naive(A):
```

```
    count = 0
```

```
    for i from 1 to n:
```

```
        for j from i + 1 to n:
```

```
            for k from j + 1 to n:
```

```
                if  $A_{ij} = 1$  and  $A_{jk} = 1$  and  $A_{ki} = 1$ : # an edge between each pair
```

```
                    count += 1:
```

```
RETURN count
```

Application: Triangle Counting

Theorem. For an adjacency matrix A , the number of triangle containing the edge (i,j) is

$$(A^2)_{ij} * A_{ij}$$

Verify:

Application: Triangle Counting

FUNCTION tri_count(A):

 compute A^2

 count \leftarrow sum of $(A^2)_{ij} * A_{ij}$ for all distinct i and j

RETURN count / 6 # why divided by 6?

Application: Triangle Counting

FUNCTION tri_count(A):

in NumPy '*' is entry-wise multiplication

also called the HADAMARD PRODUCT

count \leftarrow sum of the entries of $A^2 * A$

RETURN count / 6

Application: Triangle Counting

```
FUNCTION tri_count(A):
```

```
    # in NumPy '*' is entry-wise multiplication
```

```
    #      also called the HADAMARD PRODUCT
```

```
    # and 'np.sum' sums the entry of a matrix
```

```
RETURN np.sum( (A @ A) * A ) / 6
```

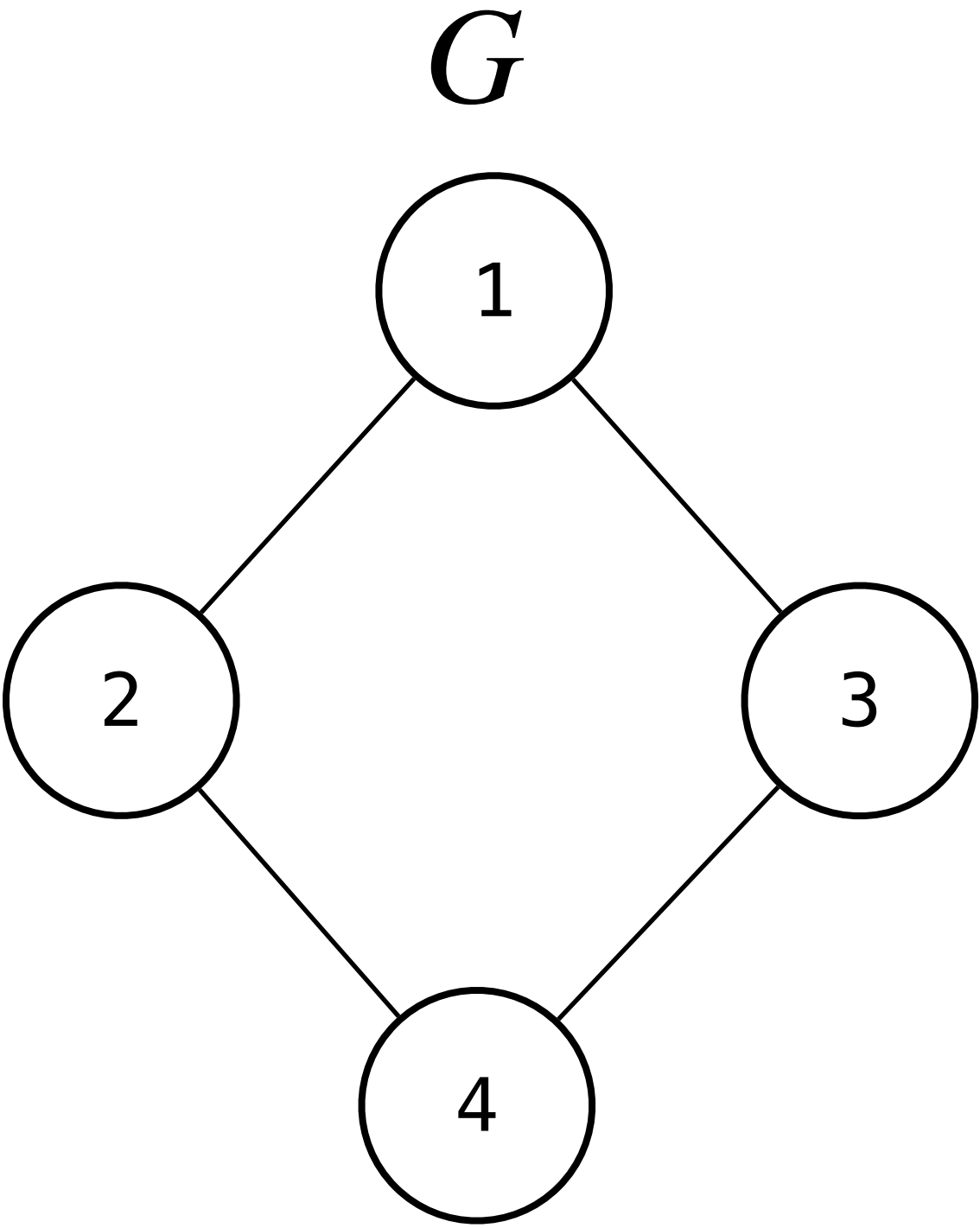
demo

Another Application: Reachability

Question: If A^2 gives us information about length 2 paths, then what about A^k ?

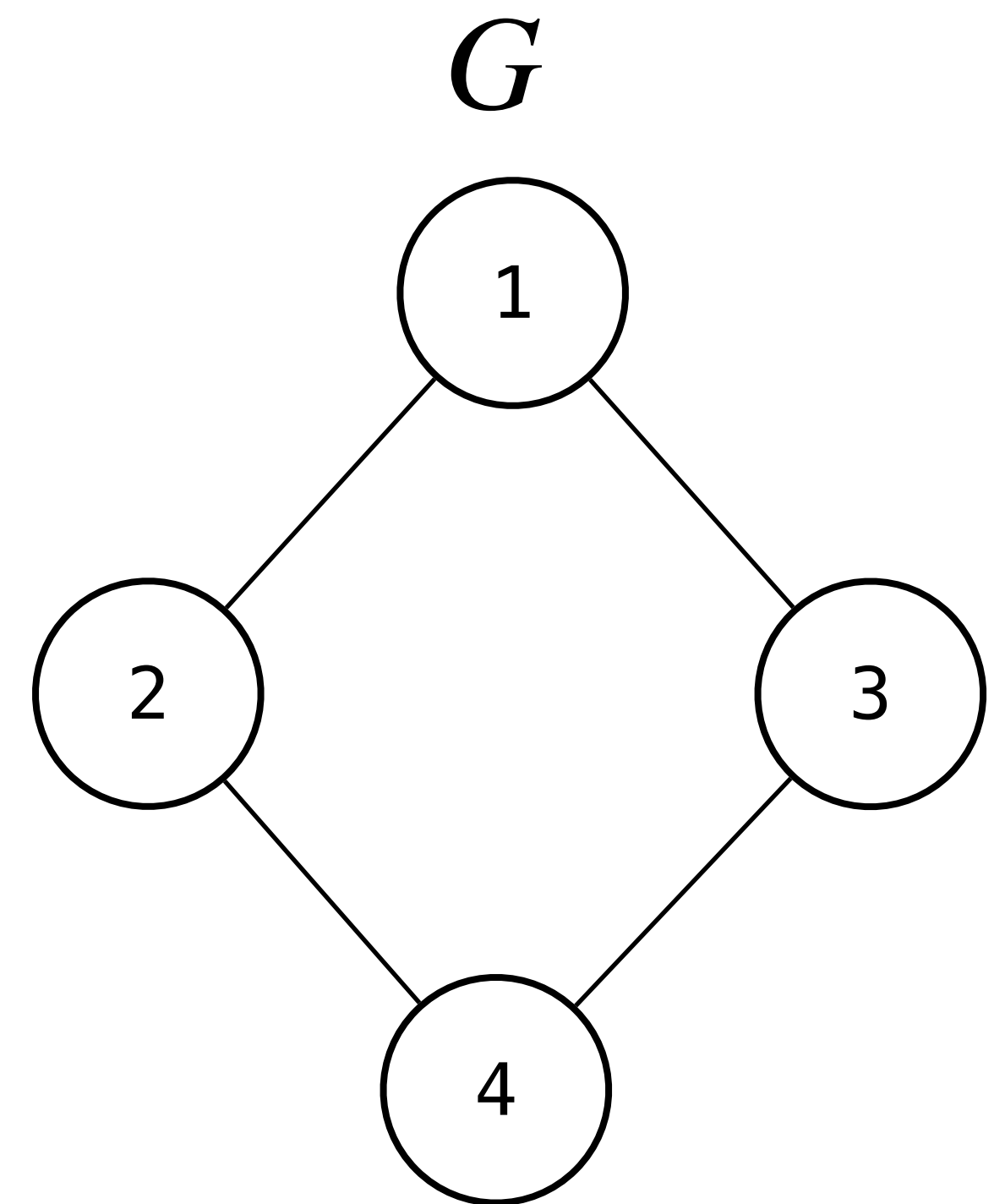
A^k gives us information about k -length paths.

Example



Example

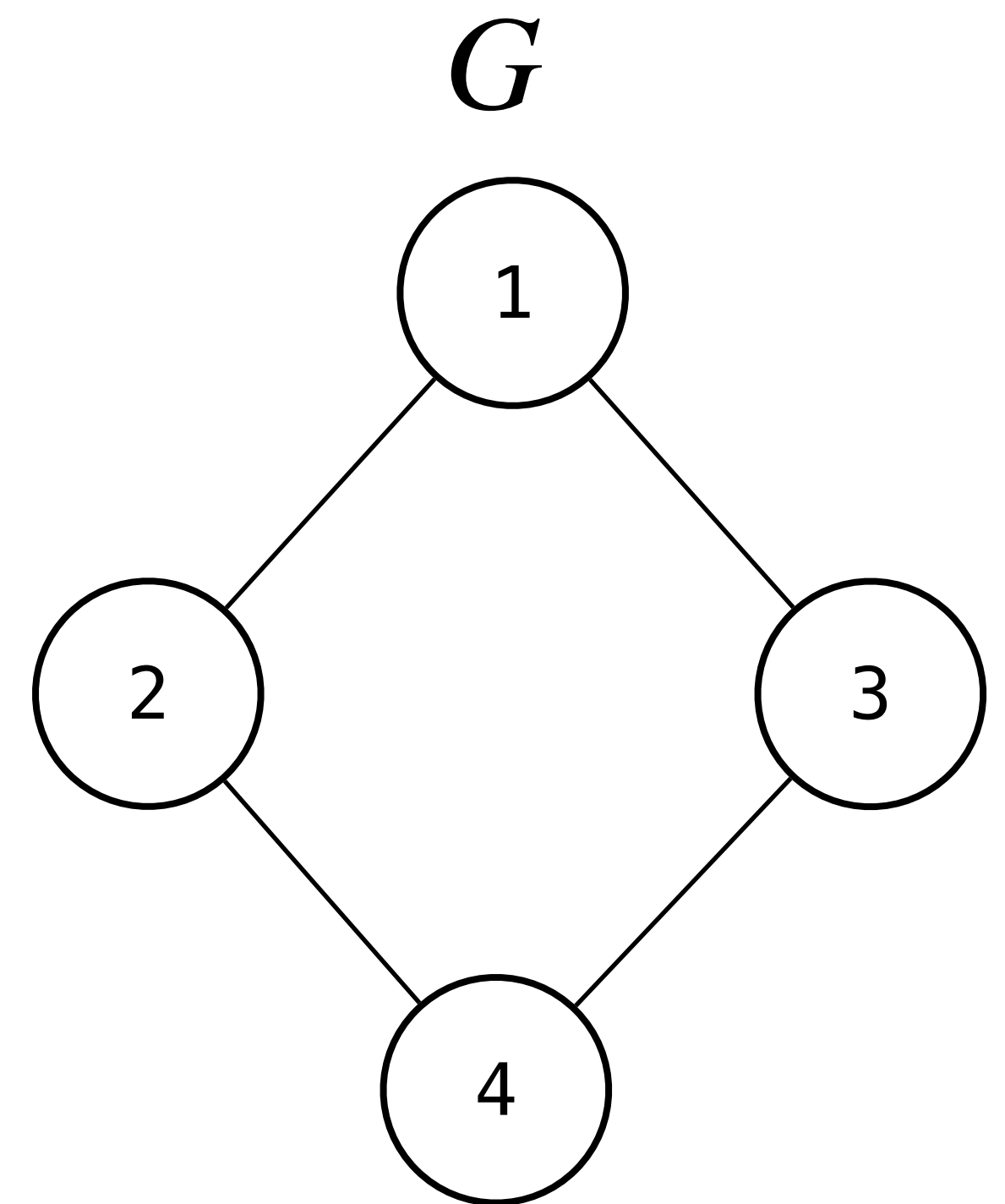
$$\begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} = \text{adjacency matrix for } G$$



Example

$$\begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} = \text{adjacency matrix for } G$$

$$\begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}^2 = \begin{bmatrix} 2 & 0 & 0 & 2 \\ 0 & 2 & 2 & 0 \\ 0 & 2 & 2 & 0 \\ 2 & 0 & 0 & 2 \end{bmatrix}$$

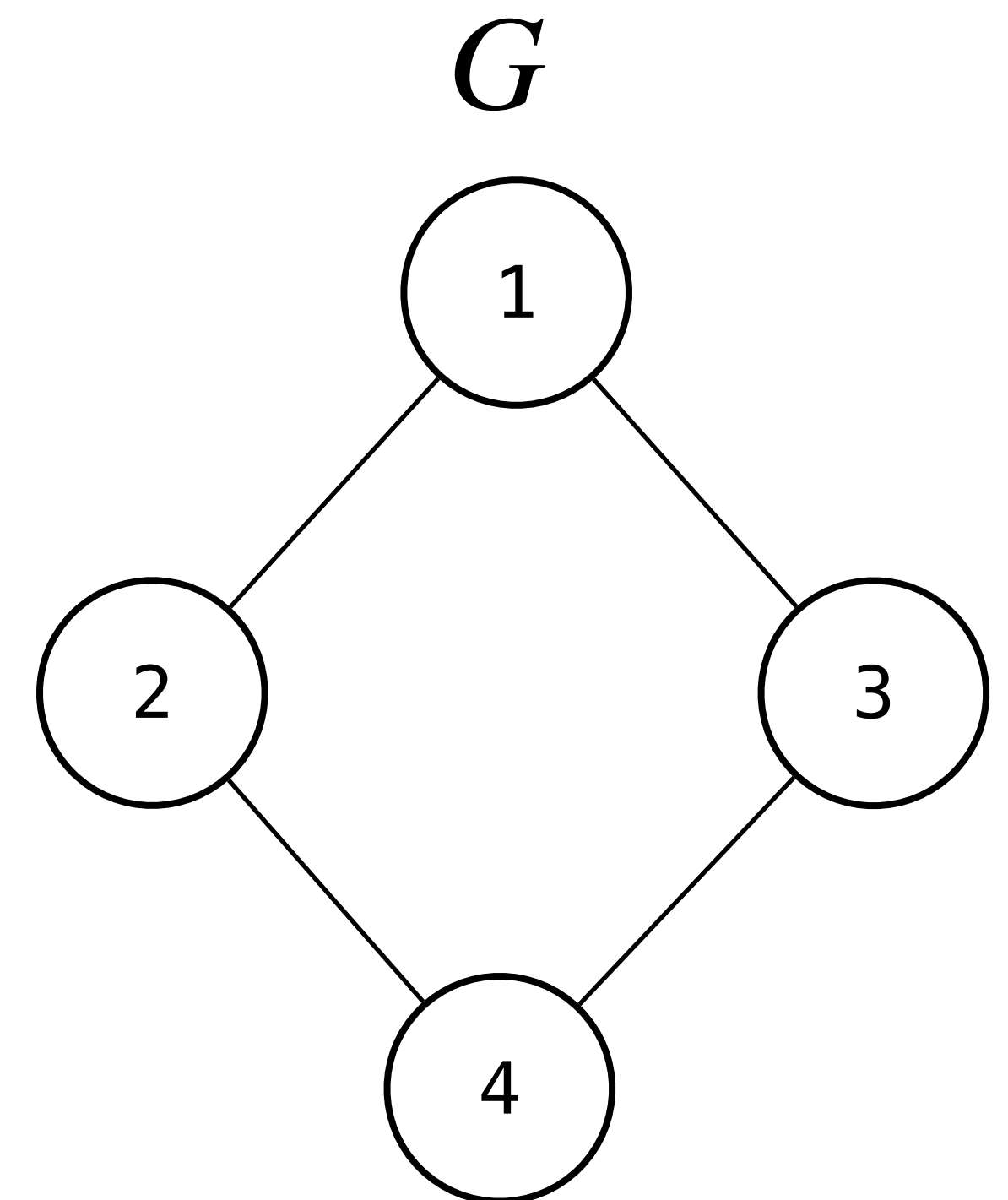


Example

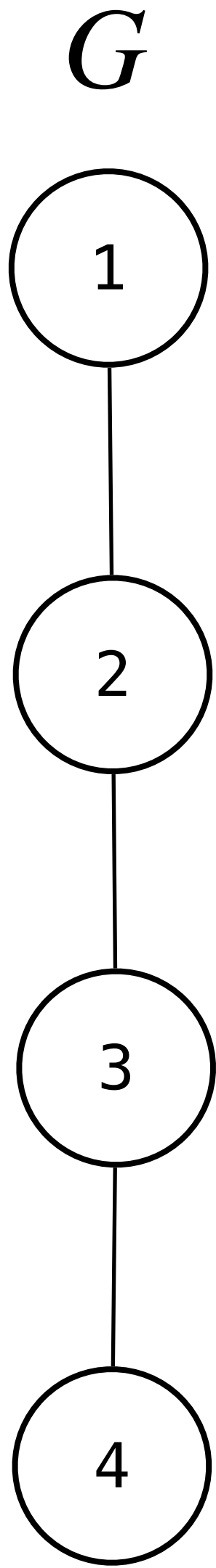
$$\begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} = \text{adjacency matrix for } G$$

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$$\begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}^3 = \begin{bmatrix} 2 & 0 & 0 & 2 \\ 0 & 2 & 2 & 0 \\ 0 & 2 & 2 & 0 \\ 2 & 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 4 & 4 & 0 \\ 4 & 0 & 0 & 4 \\ 4 & 0 & 0 & 4 \\ 0 & 4 & 4 & 0 \end{bmatrix}$$

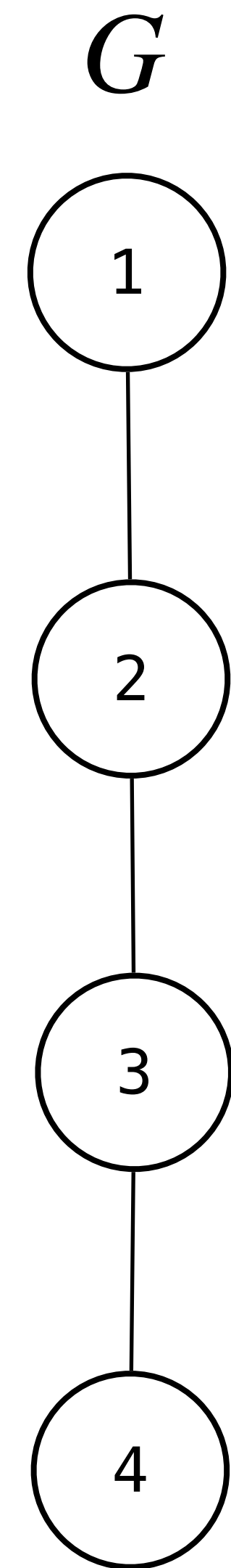


Example



Example

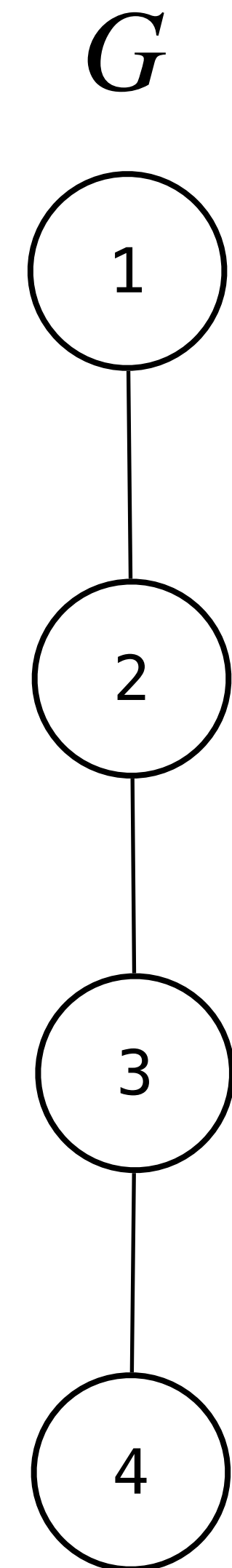
$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \text{adjacency matrix for } G$$



Example

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \text{adjacency matrix for } G$$

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}^2 = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 2 & 0 & 1 \\ 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}$$

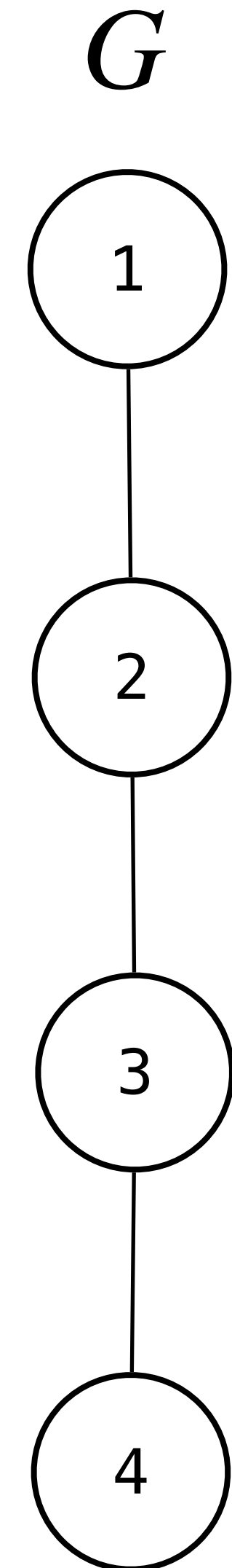


Example

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \text{adjacency matrix for } G$$

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}^2 = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 2 & 0 & 1 \\ 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}^3 = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 2 & 0 & 1 \\ 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 2 & 0 & 1 \\ 2 & 0 & 3 & 0 \\ 0 & 3 & 0 & 2 \\ 1 & 0 & 2 & 0 \end{bmatrix}$$

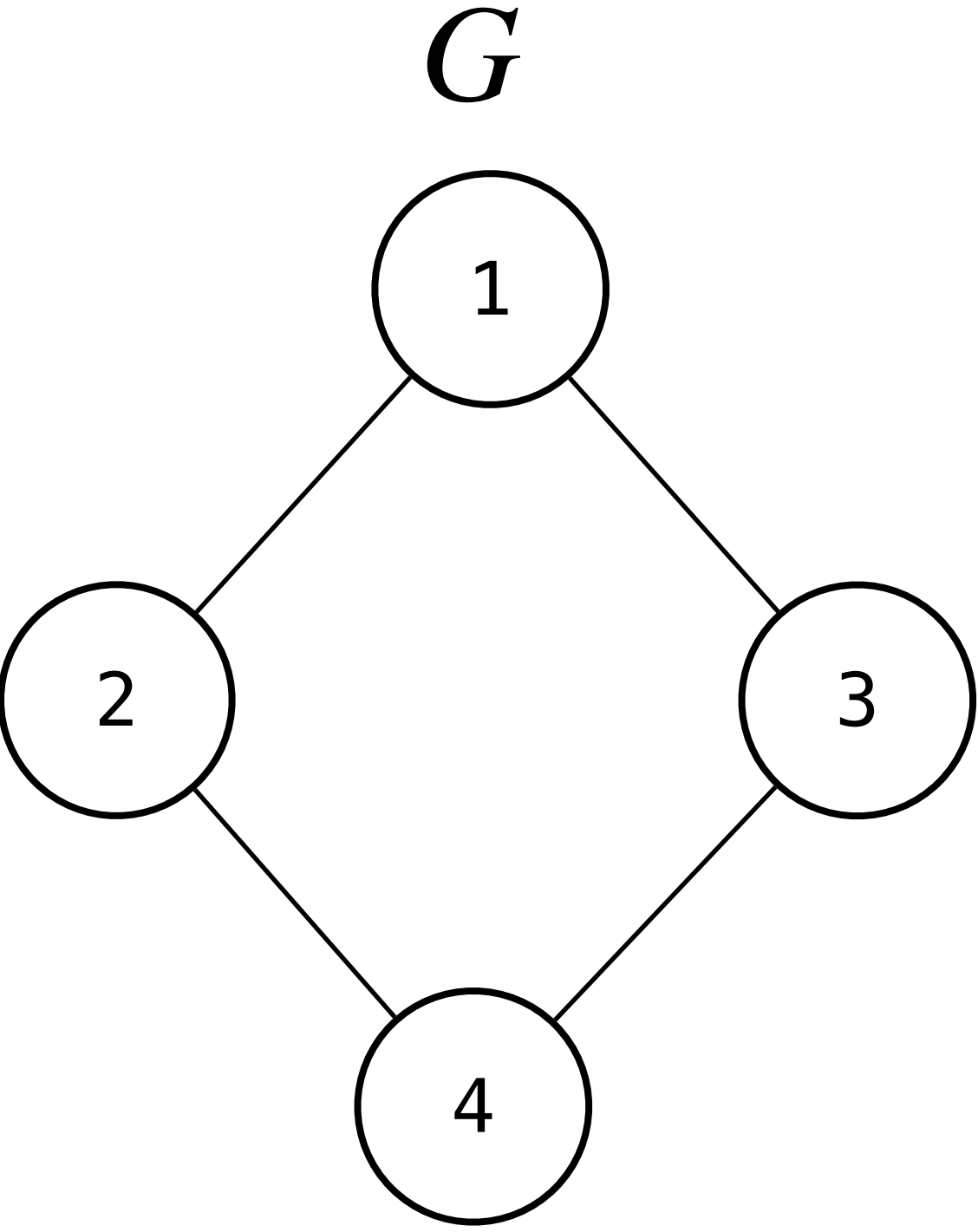


Another Application: Reachability

Theorem: Let G be a simple graph.

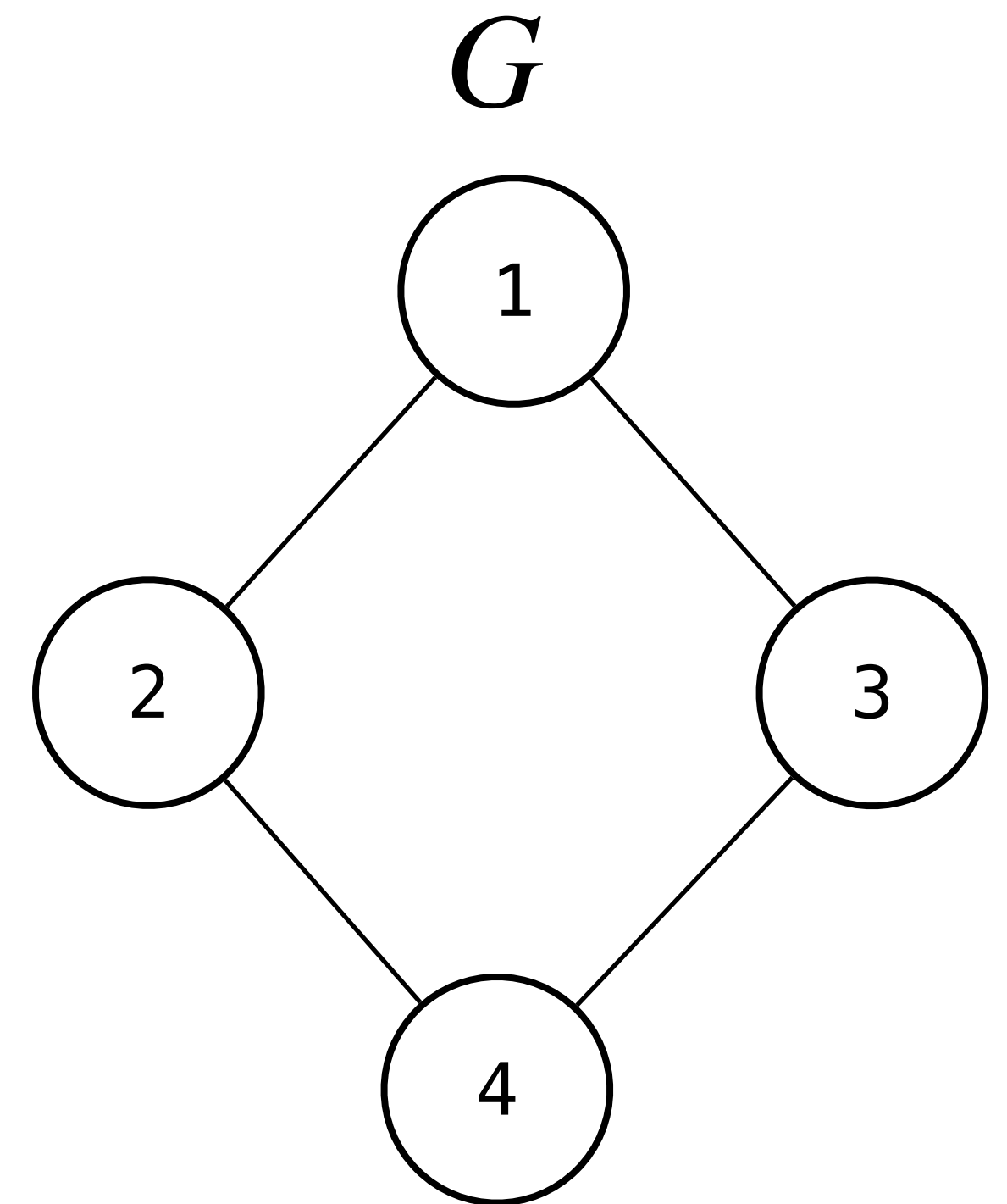
- $(A_G^k)_{ij}$ is the number of paths of length **exactly** k from v_i to v_j .
- $((A_G + I)^k)_{ij}$ is nonzero if and only if there is a path of length at **at most** k from v_i to v_j .

Example



Example

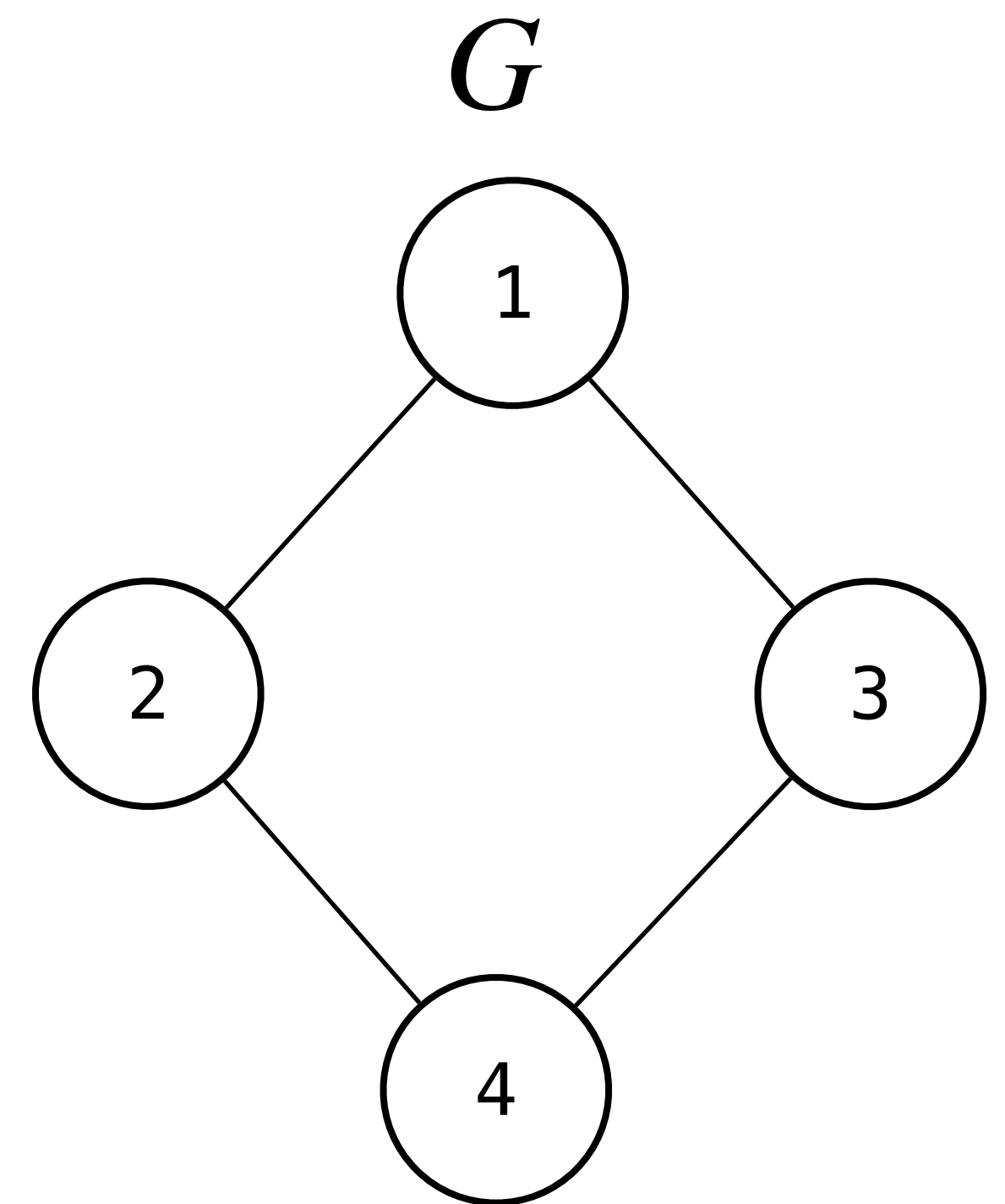
$$\begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{bmatrix} = (\text{adjacency matrix for } G) + I$$



Example

$$\begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{bmatrix} = (\text{adjacency matrix for } G) + I$$

$$\begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{bmatrix}^2 = \begin{bmatrix} 3 & 2 & 2 & 2 \\ 2 & 3 & 2 & 2 \\ 2 & 2 & 3 & 2 \\ 2 & 2 & 2 & 3 \end{bmatrix}$$

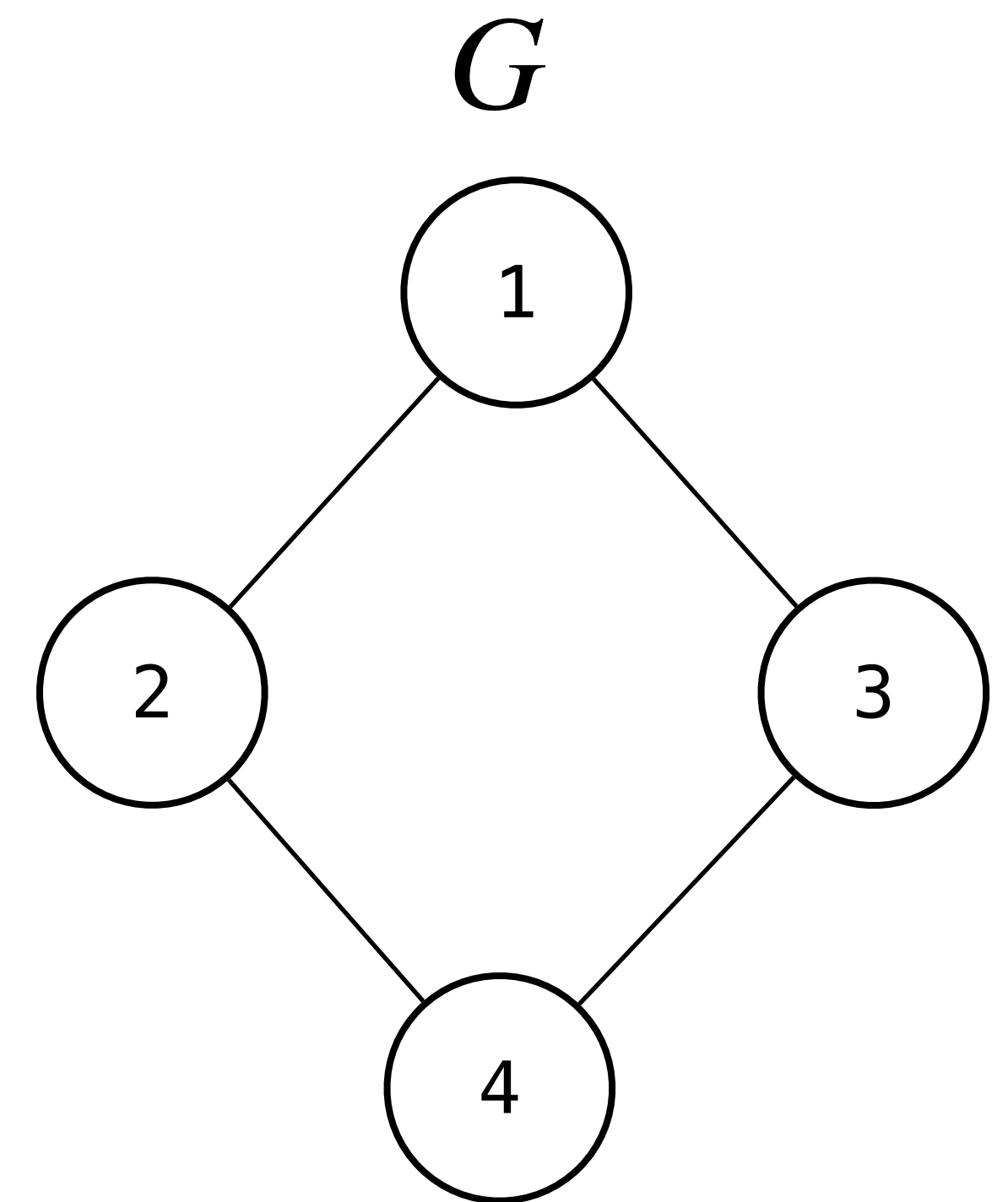


Example

$$\begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{bmatrix} = (\text{adjacency matrix for } G) + I$$

$$\begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{bmatrix}^2 = \begin{bmatrix} 3 & 2 & 2 & 2 \\ 2 & 3 & 2 & 2 \\ 2 & 2 & 3 & 2 \\ 2 & 2 & 2 & 3 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}^3 = \begin{bmatrix} 3 & 2 & 2 & 2 \\ 2 & 3 & 2 & 2 \\ 2 & 2 & 3 & 2 \\ 2 & 2 & 2 & 3 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 6 & 6 & 6 & 7 \\ 6 & 6 & 7 & 6 \\ 6 & 7 & 6 & 6 \\ 7 & 6 & 6 & 6 \end{bmatrix}$$



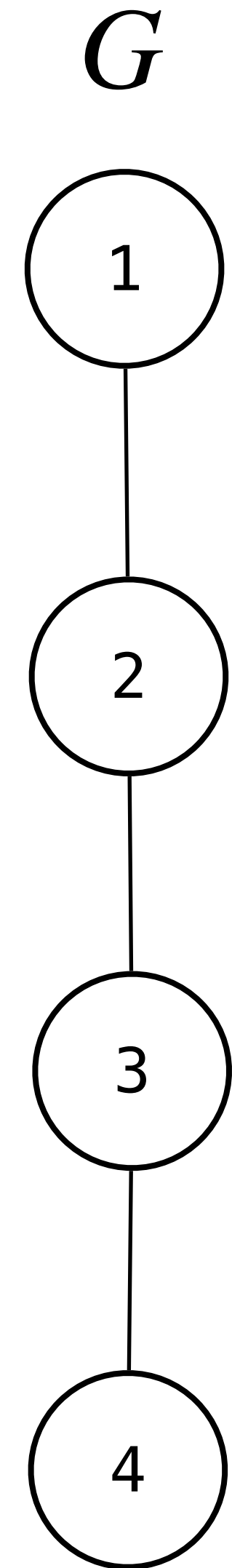
How To: Reachability

Question: Given a simple graph G determine how many nodes v_i can reach in at least k steps.

Answer: Find $(A_G + I)^k$ and count the number of nonzero elements in column i .

Question

Determine the $(A_G + I)^2$ and $(A_G + I)^3$ and interpret the results.



Summary

Matrix inverses allow us to easily solve many matrixes equations over the same A

LU Factorizations allows us to do the same, but more generally more efficiently

Adjacency matrices are linear algebraic representations of graphs