# Graph Convolutional Networks (GCN)

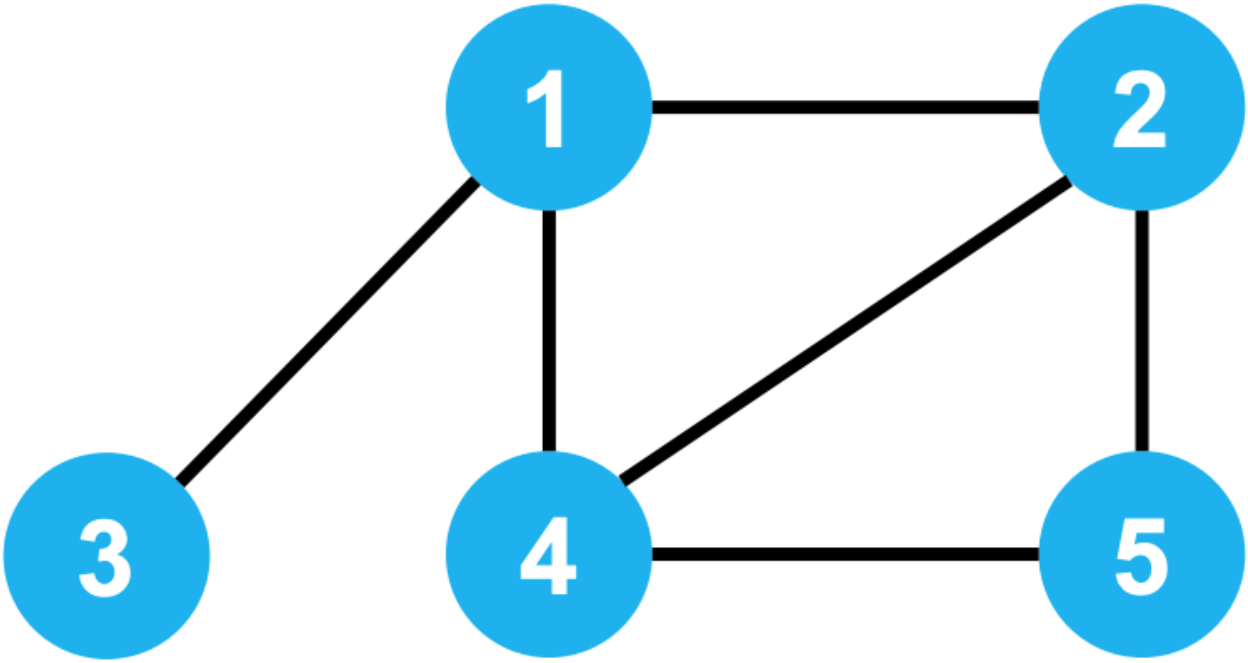
- Semi-Supervised Classification with Graph Convolutional Networks

## 1. Introduction to Graph

### Graph Basics

A Graph is defined as $G = (V, E)$

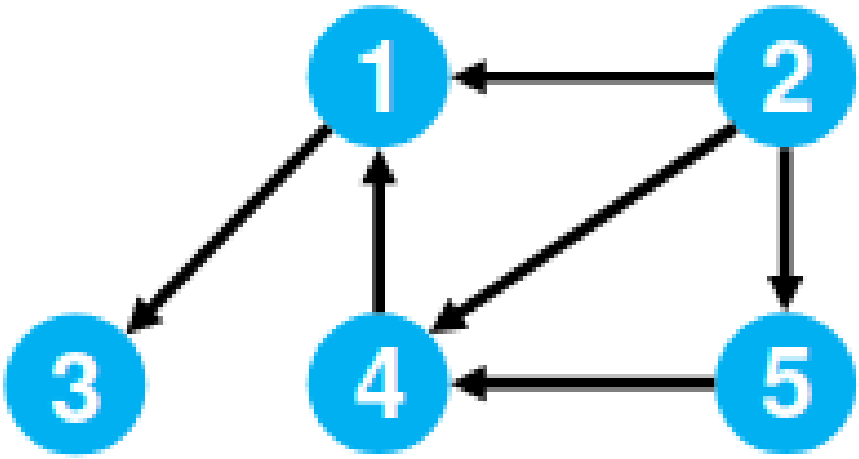
- V: a finite, nonempty set of vertices
- E: a set of edges / pairs of vertices




```
V = {1,2,3,4,5}
E = {(1,2),(1,3),(1,4),(2,4),(2,5),(4,5)}
```

**Graph type**

- Undirected: edge (u,v) = edge (v,u)
- Directed: edge (u,v) goes from vertex u to vertex v; $(u, v) \neq (v, u)$
- Weighted: edges associate with weights




```
V = {1,2,3,4,5}
E = {(2,1),(1,3),(4,1),(2,4),(2,5),(5,4)}
```

**Terminate**

- Adjacent

  If there is an edge (u,v), then u and v are adjacent.

- Incident

  If there id an edge (u,v), the edge (u,v) is incident from u and is incident to v.

- Degree:

  The degree of a vertex u is the number of edges incident on u.

  - in-degree of u: edges (x,u) in a directed graph.
  - out-degree of u: edges (u,x) in a directed graph.
  - Degree = in-degree + out-degree
  - Isolated vertex: degree = 0

- Connected:

  - Two vertices are connected if there is a path between them.
  - A connected graph has a path from every vertex to every other.

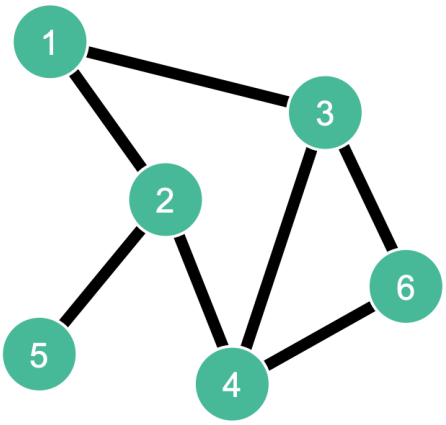
## Graph Representations

How to represent a graph in computer programs?

**Adjacency Matrix**

Adjacency matrix = $N \times N$ matrix A with $A[i][j] = 1$ if (i,j) is an edge.

$$A_{ij} := \begin{cases} 1 & \text{if (i,j)} \in E \\ 0 & \text{otherwise} \end{cases}$$




| | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| 1 | | 1 | 1 | | | |
| 2 | 1 | | | 1 | 1 | |
| 3 | 1 | | | 1 | | 1 |
| 4 | | 1 | 1 | | | 1 |
| 5 | | 1 | | | | |
| 6 | | | 1 | 1 | | |

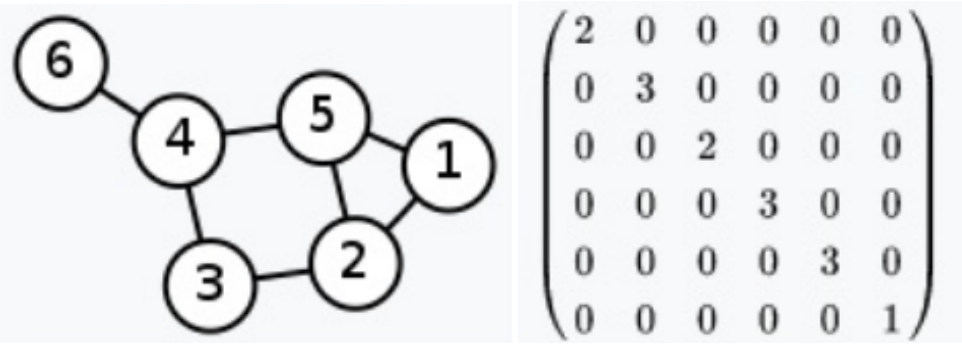
- For undirected graphs, A is symmertric, $A = A^T$
- If weighted, store weights instead of bits in $A$

**Degree Matrix**

Degree matrix is a `diagonal matrix` wich contains information about the degree of each vertex.

Given a graph $G = (V, E)$ with $|V| = n$, the `degree matrix` D for G is a $N \times N$ diagonal matrix defined as:

$$D_{ij} := \begin{cases} deg(v_i) & \text{if i = j} \\ 0 & \text{otherwise} \end{cases}$$




$$\begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

## 2. Spectral Graph Theory

In mathmatics, `spectral graph theory` is the study of the properties of a graph in relationship to the `characteristic polynomial`, `eigenvalues`, and `eigenvectors` of matrices associated with the graph, such as its adjacency matrix or `Laplacian matrix`.

### Laplacian matrix

Given a simple graph G with n vertices, its Laplacian matrix L is defined as :

$$L = D - A$$

where D is the degree matrix and A is the adjacency matrix of the graph.

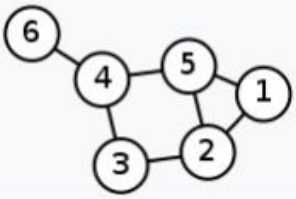
$$L_{ij} := \begin{cases} deg(v_i) & \text{if } i = j \\ -1 & \text{if } i \neq j \text{ and } v_i \text{is adjaceney to } v_j \\ 0 & \text{otherwise} \end{cases}$$

where $deg(v_i)$ is the degree of the vertex $i$.

**Properties**

- L is symmetric matrix.
- L is positive-semidefinite matrix.

**Example**

| Labeled graph | Degree matrix | Adjacency matrix | Laplacian matrix |
|---|---|---|---|
|  | $\begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 2 & -1 & 0 & 0 & -1 & 0 \\ -1 & 3 & -1 & 0 & -1 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & -1 & 0 & -1 & 3 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}$ |

**Other Laplacian matrix**

- Random walk normallized Laplacian matrix

$$L^{rw} = D^{-1}L = I - D^{-1}A$$

- Symmetric normalized Laplacian matrix

$$L^{\text{sym}} = D^{-1/2}LD^{-1/2} = I - D^{-1/2}AD^{-1/2}$$

**Orthogonal diagonalization**

Because L is a real-symmetric matrix, it can be diagonalized by an orthogonal matrix.

$$L = U\Lambda U^T$$

where

- U is a eigenvector of L, and is orthgonoally matrix: $UU^T = I, U^{-1} = U^T$.
- $\Lambda$ is a diagonal matrix that consists of the eigenvalue of L.

$$L = U \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix} U^{-1} \qquad L = U \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix} U^{T}$$

## 3. Laplace operator

The `Laplace operator` or `Laplacian` is a `differential operator` given by the `divergence` of the `gradient` of a function on `Euclidean space`.

It defined as `the divergence (∇·) of the gradient (∇f)`.

The Laplacian of f is defined by:

$$\Delta f = \nabla^2 f = \nabla \cdot \nabla f$$

where

$$\nabla = \left( \frac{\partial}{\partial_{x_1}}, \cdots, \frac{\partial}{\partial_{x_n}} \right)$$

So

$$\Delta f = \sum_{i=1}^{n} \frac{\partial^2 f}{\partial x_i^2}$$

Heat Conduction Model on Graph

Heat conduction (or `thermal conduction`) is the movement of heat from one object to another one that has different temperatures when they are touching each other.

```
Heat flows from the hotter object to the colder one.
```

**Heat Conduction Model on One-dimension**


For node $i$, it's only connected with node $i-1$ and node $i+1$, and the temperatures will be changed by these two nodes (receive from node $i+1$, transfer to node $i-1$).

If the current temperature of node $i$ is $\phi_i$,

$$\frac{d\phi_i}{dt} = k(\phi_{i+1} - \phi_i) + k(\phi_i - \phi_{i-1})$$

$$\frac{d\phi_i}{dt} - k[(\phi_{i+1} - \phi_i) - (\phi_i - \phi_{i-1})] = 0$$

$$\frac{\partial \phi}{\partial t} - k\frac{\partial^2 \phi}{\partial x^2} = 0$$

$$\frac{\partial \phi}{\partial t} - k\frac{\partial^2 \phi}{\partial x^2} = 0$$

$$\frac{\partial \phi}{\partial t} - k\Delta\phi = 0$$

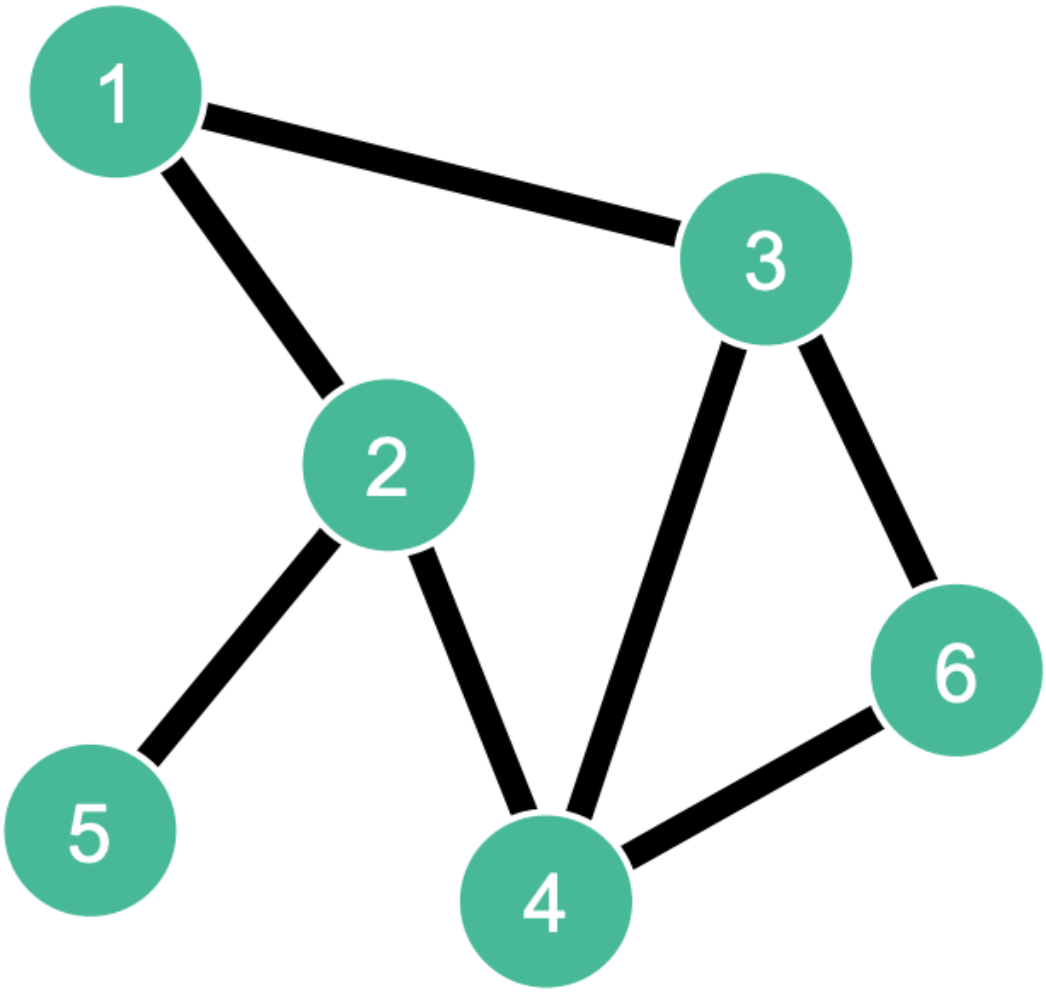
=>

1. 在歐式空間中，某溫度升高的速度正比於該點周圍的溫度分佈，用Laplace operator衡量
2. Laplace operator是二階導數對高維空間的推廣

**Heat Conduction Model on Graph**

現在讓我們將熱傳播模型推廣到Graph上

如下圖中所示，點1只和點2跟點3發生熱交換，點5的熱量要通過點2間接傳過來，而沒有直接熱交換。




根據一維熱傳播模型，這Graph上溫度隨時間的變化可以寫成以下：

$$\frac{d\phi_i}{dt} = -k \sum_j A_{ij}(\phi_i - \phi_j)$$

where A is adjacency matrix

=>

$$\frac{d\phi_i}{dt} = -k \sum_j A_{ij}(\phi_i - \phi_j) \qquad = -k[\phi_i \sum_j A_{ij} - \sum_j A_{ij}\phi_j] \ = -k[deg(i)\phi_i - \sum_j A_{ij}\phi_j]$$

=>

$$ \begin{bmatrix} \frac{d\phi_1}{dt} \ \frac{d\phi_2}{dt} \ \cdots \ \frac{d\phi_n}{dt} \ \end{bmatrix} = -k \begin{bmatrix} deg(1) \times \phi_1 \ deg(2) \times \phi_2 \ \cdots \ deg(n) \times \phi_n \ \end{bmatrix}$$

- kA

$$\begin{bmatrix} \phi_1 \ \phi_2 \ \cdots \ \phi_n \ \end{bmatrix}$$

define $\phi = [\phi_1, \phi_2, \cdots, \phi_n]^T$ , then

$$\frac{d\phi}{dt} = -kD\phi + kA\phi \qquad = -k(D - A)\phi$$

=>

$$\frac{d\phi}{dt} + kL\phi = 0$$

=>

$$L = D - A$$

**推廣到GCN**

假設在圖中各個節點流動的東西不是熱量，而是特徵(Feature)，而是訊息(Message)，那問題就自然被推廣到了GCN。

所以GCN就是在一張Graph Network中特徵(Feature)和訊息(Message)中的流動傳播。

## 4. Convolution and Forurier Transfornm

- Convolution

  The convolution of $f$ and $g$ is written $f * g$,

$$(f * g)(t) = \int_{-\infty}^{\infty} f(\tau)g(t-\tau)d\tau$$

- Fourier Transform

$$Ff(w) = \int_{-\infty}^{\infty} f(x)e^{-iwx}dx$$

- Inverse Fourier transform

$$F^{-1}f(x) = \int_{-\infty}^{\infty} f(w)e^{iwx}dx$$

推導

$$h(z) = \int_{-\infty}^{\infty} f(x)g(z-x)dx$$

$$Ff * g(z) = Fh(z) \qquad = \int_{-\infty}^{\infty} h(z)e^{-iwz}dz \ = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x)g(z-x)e^{-iwz}dxdz \qquad = \int_{-\infty}^{\infty} f(x)(\int_{-\infty}^{\infty} g(z-x)e^{-iwz}dz)dx$$

Let $y = z - x$, $dy = dz$

$$Ff * g = \int_{-\infty}^{\infty} f(x)(\int_{-\infty}^{\infty} g(y)e^{-iw(y+x)}dy)dx \qquad = \int_{-\infty}^{\infty} f(x)e^{-iwx}dx \int_{-\infty}^{\infty} g(y)e^{-iwy}dy \ = Ff \cdot Fg$$

$$f * g = F^{-1}Ff \cdot Fg$$

## 5. Graph Fourier

- Traditional Fourier

$$F(W) = \hat{f}(w) = \int_{-\infty}^{\infty} f(x)e^{-iwx}dx$$

- Graph Fourier

$$F(\lambda_i) = \hat{f}(\lambda_i) = \sum_{k=1}^{N} f(k)u_i^*(k)$$

$$\begin{pmatrix} \hat{f}(\lambda_1) \\ \hat{f}(\lambda_2) \\ \vdots \\ \hat{f}(\lambda_N) \end{pmatrix} = \begin{pmatrix} u_1(1) & u_1(2) & \dots & u_1(N) \\ u_2(1) & u_2(2) & \dots & u_2(N) \\ \vdots & \vdots & \ddots & \vdots \\ u_N(1) & u_N(2) & \dots & u_N(N) \end{pmatrix} \begin{pmatrix} f(1) \\ f(2) \\ \vdots \\ f(N) \end{pmatrix}$$

=> $\hat{f} = U^T f$

- Traditional Inverse Fourier

$$F^{-1}[F(w)] = f(x) = \int_{-\infty}^{\infty} F(w) e^{iwx} dx$$

- Graph Inverse Fourier

$$f(i) = \sum_{k=1}^{N} \hat{f}(\lambda_i) u_k(i)$$

=> $f = U\hat{f}$

## 6. Graph Convolution

- Traditional Convolution

$$f * h = F^{-1} Ff \cdot Fh$$

- Graph convolution

$$(f * h)_G = U((U^T f) \odot (U^T h))$$

where $\odot$ is the element-wised product (as known as `Hadamard product`).

Let $\hat{h}(\lambda_i) = \sum_{k=1}^{N} h(k) u_i^*(k)$, then:

$$(f * h)_G = U \begin{pmatrix} \hat{h}(\lambda_1) & & \\ & \ddots & \\ & & \hat{h}(\lambda_n) \end{pmatrix} U^T f$$