Spectral Clustering

Recall:

- Weighted graph – (G, w) $|V| = n$.
- Incidence matrix – M.
- Laplacian matrix $(n \times n)$: $L = M^T M$.

$$L_{ij} = \begin{cases} \overset{= \sum_{k \neq i} w(v_i, v_k)}{\deg(v_i)} & i = j \\ -w(v_i, v_j) & i \neq j \end{cases}$$

- $L \cdot \underline{\underline{1}} = \underline{0}$ ($\underline{1}$ = eignevector with eig. value $\lambda = 0$)

all ones

Binary Clustering:

Denote: $\underbrace{\overset{0 \, =}{\lambda_1} \leq \lambda_2 \leq \cdots \leq \lambda_n}_{\text{all eig. values of } L}$

Find $\underline{u}^{(2)}$ = eig. vector for λ_2.

Then:

$u_i^{(k)} > 0 \Rightarrow v_i$ cluster 0

$u_i^{(k)} < 0 \Rightarrow v_i$ cluster 1

Questions:

(1) Why does it work?

(2) What happes when we have more than two clusters?

THE LAPLACIAN MATRIX

$$(G, w) \to M \to L = M^T M.$$

ALTERNATIVE DEFINITION:

- W = weight matrix $(n \times n)$

$$W_{i,j} = w(v_i, v_j)$$

- $d_i = \deg(v_i) = \sum_{j \neq i} W_{i,j}$

$$D = \operatorname{diag}(d_1, \_\_, d_n) = \begin{pmatrix} d_1 & & & 0 \\ & d_2 & & \\ & & \ddots & \\ 0 & & & d_n \end{pmatrix}$$

- Then: $L = D - W$

L = real values + symmetric $\Rightarrow$ diagonalisable.

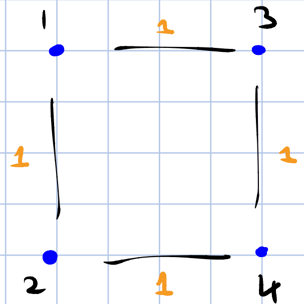
+ positive semi-definite (PSD) $\downarrow$ all eig-vals are ≥ 0

Eigenvalues:

$$\underset{\substack{\| \\ 0}}{\lambda_1} \leq \lambda_2 \leq \lambda_3 \leq \cdots \leq \lambda_n$$

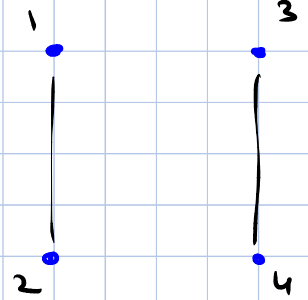
Q: What is $\operatorname{Ker}(L)$? $(L \cdot \underline{v} = \underline{0})$

(we know $\underline{1} \in \operatorname{Ker}(L)$).

Ex. $G_1 =$ 

$$\to L_1 = \begin{array}{c} \begin{array}{cccc} & (1,2) & (1,3) & (1,4) \\ & \downarrow & \downarrow & \downarrow \end{array} \\ \begin{pmatrix} 2 & -1 & -1 & 0 \\ -1 & 2 & 0 & -1 \\ -1 & 0 & 2 & -1 \\ 0 & -1 & -1 & 2 \end{pmatrix} \end{array}$$

$\operatorname{Ker}(L_1) = \operatorname{Span}(\underline{1})$

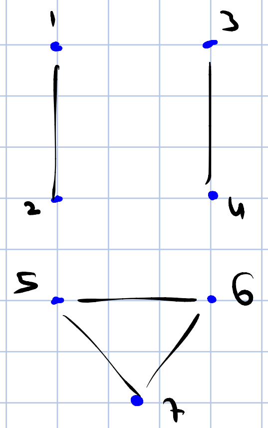
$G_2 =$  $\rightarrow \quad L_2 = \begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix}$

$L_2 \cdot \overbrace{\begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}}^{v_1} = \underline{0} \qquad L_2 \cdot \overbrace{\begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}}^{v_2} = \underline{0}$

$\hookrightarrow \quad L_2 \cdot (\alpha v_1 + \beta v_2) = \underline{0}$

$\Downarrow$

$\mathrm{Ker}(L_2) = \mathrm{Span}(v_1, v_2)$

$G_3 =$  $\rightarrow \quad L_3 = \begin{pmatrix} \begin{matrix} 1 & -1 \\ -1 & 1 \end{matrix} & & 0 \\ & \begin{matrix} 1 & -1 \\ -1 & 1 \end{matrix} & \\ 0 & & \begin{matrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{matrix} \end{pmatrix}$

$v_1 = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad v_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad v_3 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \\ 1 \end{pmatrix}$

$L_3 \cdot v_1 = L_3 \cdot v_2 = L_3 \cdot v_3 = \underline{0}$

$\mathrm{Ker}(L_3) = \mathrm{Span}(v_1, v_2, v_3)$

<u>Conclusion:</u>

$\dim(\mathrm{Ker}(L)) = \#$ connected components in G.

THEOREM:

(G, W) – weighted graph

$C_1, C_2, \dots, C_k \subset V \rightarrow$ the connected components of G.

(C_i is connected, and no edges between C_i and any other C_j)

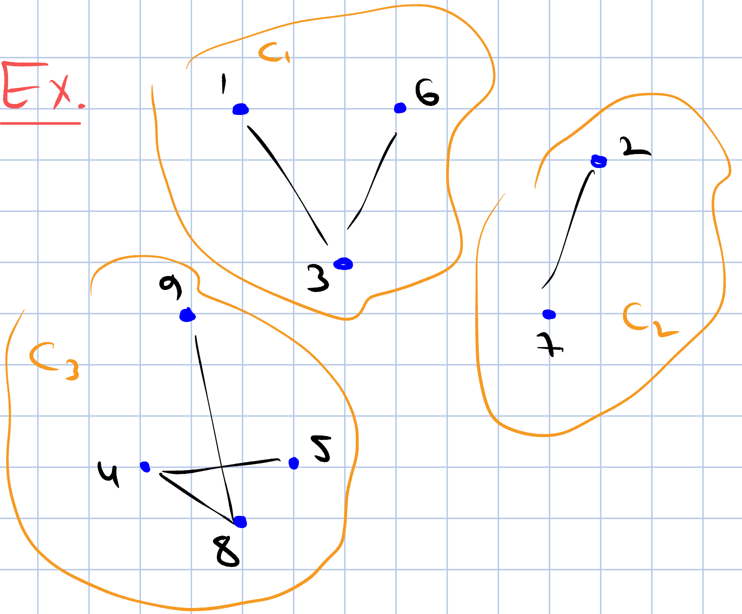
Define: $u^{(1)}, u^{(2)}, \dots, u^{(k)} \in \mathbb{R}^n$

$$u^{(j)}_i = \begin{cases} 1 & v_i \in C_j \\ 0 & \text{otherwise.} \end{cases}$$

Then: $\operatorname{Ker}(L) = \operatorname{Span}(u^{(1)}, \dots, u^{(k)})$

$(\dim \operatorname{Ker}(L) = k)$

Ex.



$$(u^{(1)}, u^{(2)}, u^{(3)}) = \begin{array}{cc} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix} & \begin{array}{l} \leftarrow v_1 \\ \leftarrow v_2 \\ \leftarrow v_3 \\ \vdots \\ \\ \\ \\ \\ \leftarrow v_9 \end{array} \end{array} \quad \#$$

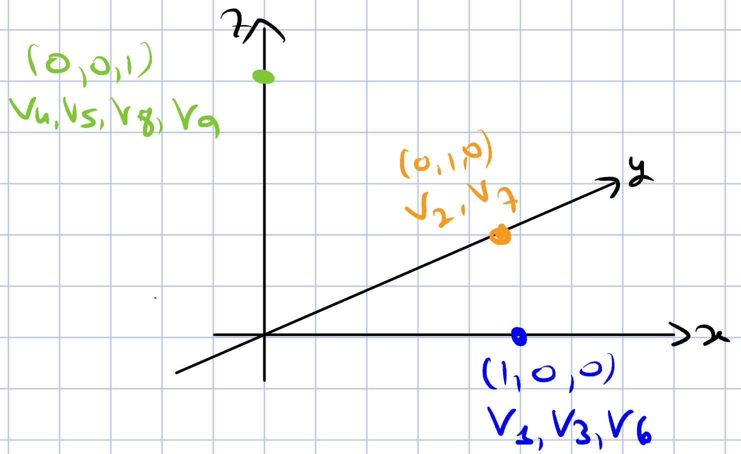
Define: $P : V \rightarrow \mathbb{R}^3$

$P(v_i) = R_i = i\text{-th row of } \#$

$P(V_1) = P(V_3) = P(V_6) = (1,0,0)$

$P(V_2) = P(V_7) = (0,1,0)$

$P(V_4) = P(V_5) = P(V_8) = P(V_9) = (0,0,1)$



→ apply a clustering algorithm (k-means)

↓

find the components / clusters of G.

Q1:

$Ker(L) = Span(u^{(1)}, \_\_, u^{(k)})$

what if we chose a different basis?

A1:

$U = (u^{(1)}, u^{(2)}, u^{(3)})$

$A \in \mathbb{R}^{3\times3}$ - invertible

New basis: $\tilde{U} = U \cdot A$.

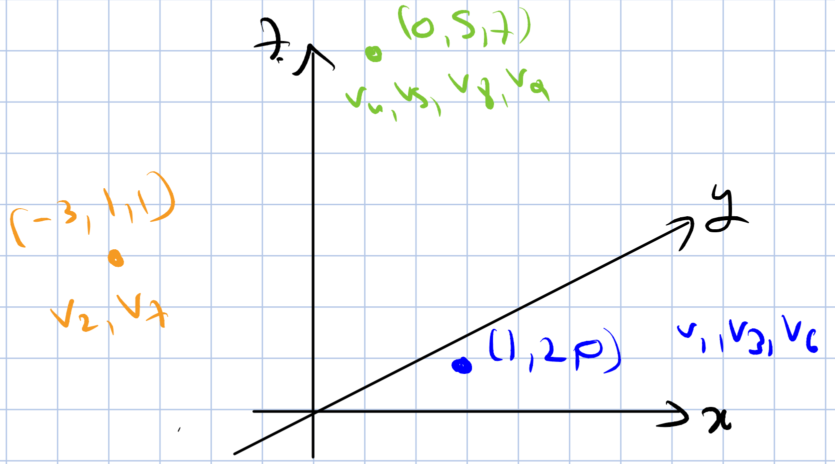
example: $A = \begin{pmatrix} 1 & 2 & 0 \\ -3 & 1 & 1 \\ 0 & 5 & 7 \end{pmatrix}$

$$U = (u^{(1)}, u^{(2)}, u^{(3)}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix}$$

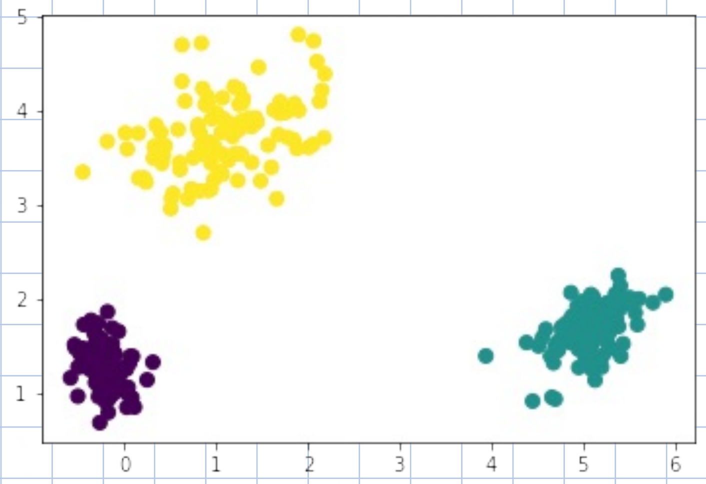
$$A = \begin{pmatrix} 1 & 2 & 0 \\ -3 & 1 & 1 \\ 0 & 5 & 7 \end{pmatrix}$$

$$\tilde{U} = U \cdot A = \begin{pmatrix} 1 & 2 & 0 \\ -3 & 1 & 1 \\ 1 & 2 & 0 \\ 0 & 5 & 7 \\ 0 & 5 & 7 \\ 1 & 2 & 0 \\ -3 & 1 & 1 \\ 0 & 5 & 7 \\ 0 & 5 & 7 \end{pmatrix}$$

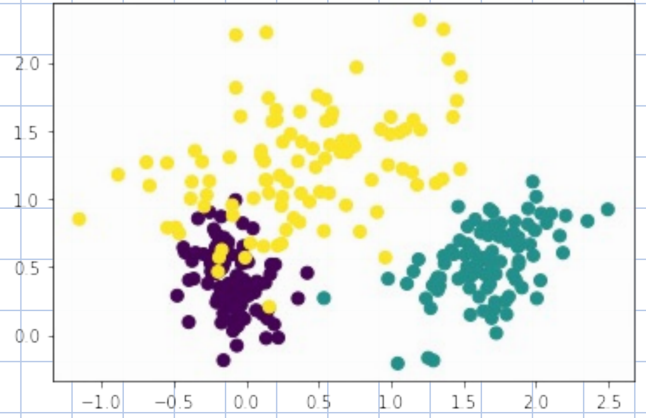
Apply Đ the same way:



Q2: This method works well when clusters are well-separated



What happens if this isn't the case?



→ graph will be connected

$\ker(L) = Sp(\mathbb{1})$

A2:

Assume G is connected.

$$\underset{\substack{\| \\ 0}}{\lambda_1} < \lambda_2 \leq \lambda_3 \leq \cdots \leq \lambda_n$$

(G disconnected $\Rightarrow \lambda_1 = \lambda_2 = \cdots = \lambda_k = 0$
k = num. components)

Before (G disconnected):

$$\lambda_1 = \lambda_2 = \cdots = \lambda_k = 0$$

P = projection on eigen-space of $\lambda_1, \_\_, \lambda_k$ (all 0)

Now: (G connected $\lambda_2 > 0$)

$u^{(j)}$ = eigen-vector for λ_j

no information $\overset{\mathbb{1}}{\shortparallel}$

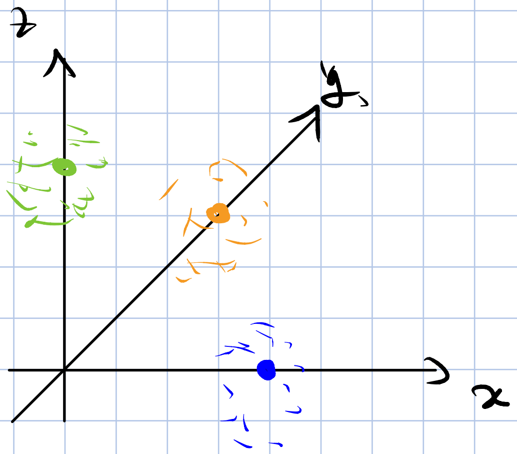
$$U = (\cancel{u^{(1)}}, u^{(2)}, \_\_, u^{(k)})$$

$$\begin{pmatrix} 1 & 7 & 2 & -1 \\ 1 & 7 & 6 & 7 \\ 1 & -3 & 2 & 17 \\ 1 & & & \\ \vdots & & \vdots & \\ 1 & & & \end{pmatrix}$$

Define: $P : V \to \mathbb{R}^{k-1}$

$P(v_i) = R_i$ = i-th row of U

Expected result:



If we have "nice enough" clusters vertices in the same cluster will lie next to each other.

↓

Run clustering algorithm (k-means)

ALGORITHM (SPECTRAL CLUSTERING)

Input: $W \in \mathbb{R}^{n \times n}$ - weights.
$k = \#$ clusters.

- Construct: $L = D - W$
- Find $\cancel{u^{(1)}}, u^{(2)}, \_\_\_, u^{(k)} \in \mathbb{R}^n$ - eigen-vecs. corresponding to $\cancel{\lambda_1}, \lambda_2, \_\_, \lambda_k$ (lowest)
- Construct: $U = \left(\underset{\downarrow}{u^{(2)}}, \underset{\downarrow}{\top}, \underset{\downarrow}{u^{(k)}} \right)$
- Map: $V_i \to R_i$ (i-th row) $\in \mathbb{R}^{k-1}$
- Run any clustering algorithm on $R(V_1), \_\_, R(V_n)$
$\quad \overset{\shortparallel}{R_1}, \_\_, R_n \subseteq \mathbb{R}^{k-1}$

Ex. $\underline{k=2}$

$$\text{Find } \underset{\overset{\shortparallel}{0}}{\lambda_1}, \lambda_2 \Rightarrow \underset{\overset{\shortparallel}{\underline{1}}}{u^{(1)}}, u^{(2)} \rightarrow \left.\begin{pmatrix} \cancel{u^{(1)}} & u^{(2)} \\ \downarrow & \downarrow \end{pmatrix}\right\} n$$

→ cluster the data using $u^{(2)}$ only.

$$V_i \longrightarrow u_i^{(2)}$$

$\underline{1}$ – eig. vec for $\lambda_1 = 0$

$u^{(2)}$ – eig vec for $\lambda_2 > 0$

$$\Downarrow$$

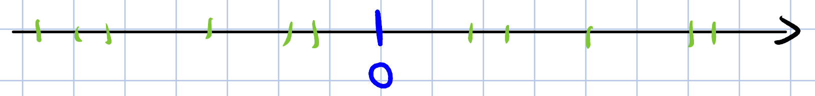
$$\underline{1} \perp u^{(2)}$$

$$\Downarrow$$

$$0 = \langle \underline{1}, u^{(2)} \rangle = \sum_{i=1}^{n} u_i^{(2)}$$

$$\Downarrow$$

$$\frac{1}{n}\sum_{i=1}^{n} u_i^{(2)} = 0$$



center of values is at 0.

⇒ naive clustering:

$$\begin{cases} 1 & u_i^{(2)} > 0 \\ 0 & u_i^{(2)} < 0 \end{cases}$$

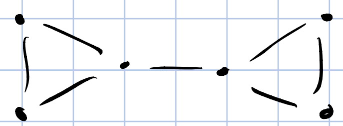
⊗ this is not necessarily the best solution, but it's good & simple

Concluding Remarks

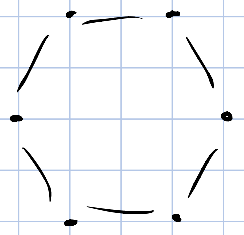
- Adding new points – need to run everything all over again.
  (as opposed to k-means, GMM)
- k – num. of clusters – chosen in advance.
- Weakness – may fail for clusters with varying densities.
- G is connected iff $\lambda_2 > 0$
  measures "how well" the graph is connected

Ex.

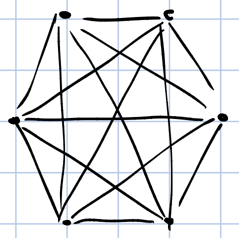
$\lambda_2 = 0.26$



$\lambda_2 = 0.43$



$\lambda_2 = 1$



$\lambda_2 = 6.$