Machine Learning for Data Science (CS4786)
Lecture 11

Spectral Embedding + Clustering

Thought Experiment

- For each user i we specify embedding (location) y_i
- How do we find good locations $y_1, \ldots, y_n$?
- What are good properties?

Key Principle

- Points are centered at 0
- Keep your Friends close
(sum of distances between linked nodes should be small)
- Variance or spread amongst the nodes should be large

Key Principle

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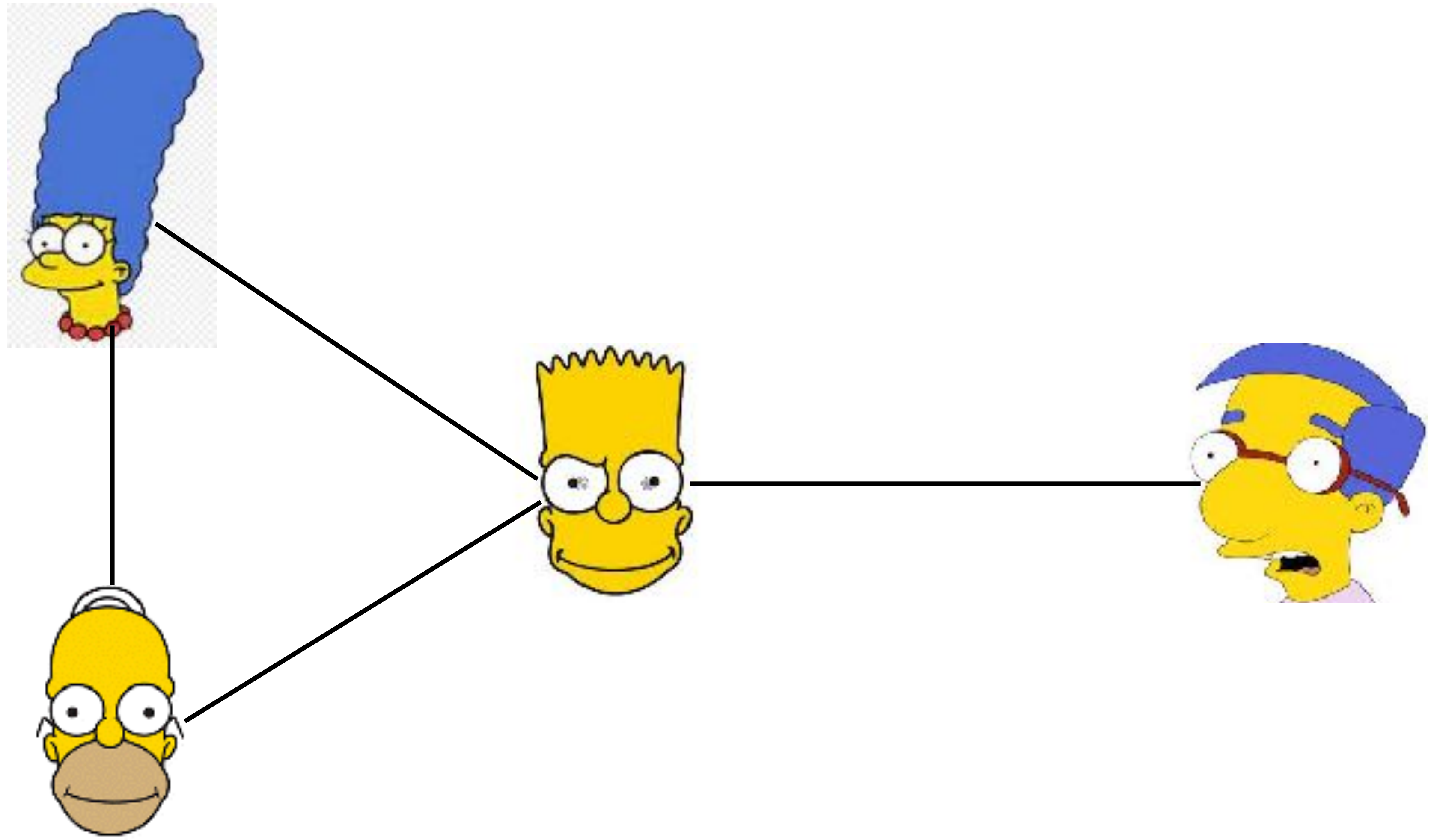
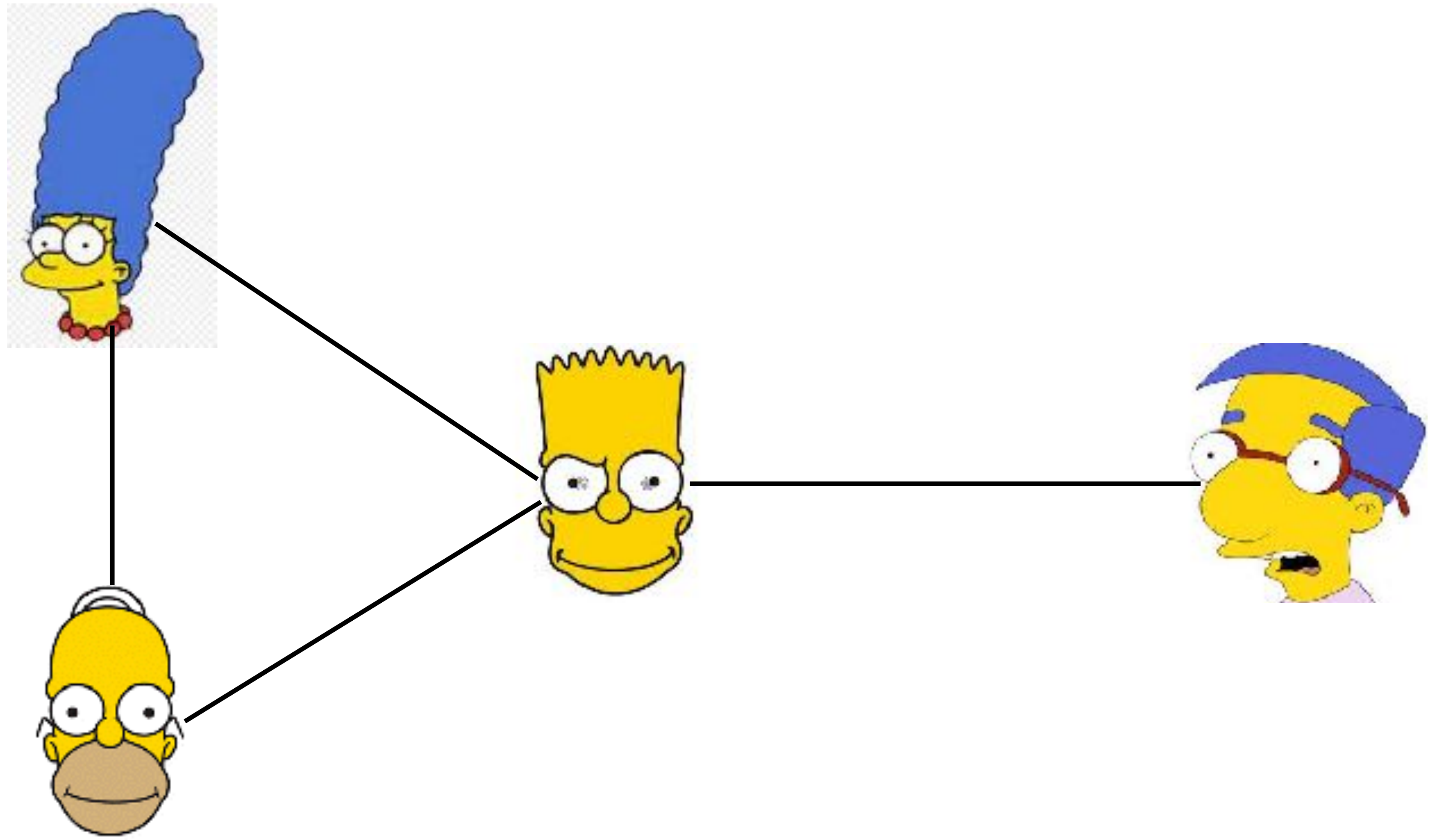
REPRESENTING THE GRAPH



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

Representing the Graph



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

The Laplacian Matrix

$$L = \cancel{D} - A$$

	2	0	0	0
	0	2	0	0
	0	0	3	0
	0	0	0	1

$-$

	0	1	1	0
	1	0	1	0
	1	1	0	1
	0	0	1	0

Key Principle

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- **Variance or spread should be large** $\text{Maximize} \; \frac{1}{n}\|y\|_2^2$

$$\text{Minimize} \; \frac{y^\top L y}{\|y\|_2^2} \quad \text{s.t.} \; y \perp \mathbf{1}$$

$$\text{Minimize} \; y^\top L y \quad \text{s.t.} \; \|y\|_2^2 = 1 \quad y \perp \mathbf{1}$$

KEY PRINCIPLE

- Points are centered at 0 $y^\top \mathbf{1} = 0$
- Keep your Friends close $\text{minimize} \quad y^\top L y$
- Variance or spread should be large $\text{Maximize } \frac{1}{n}\|y\|_2^2$

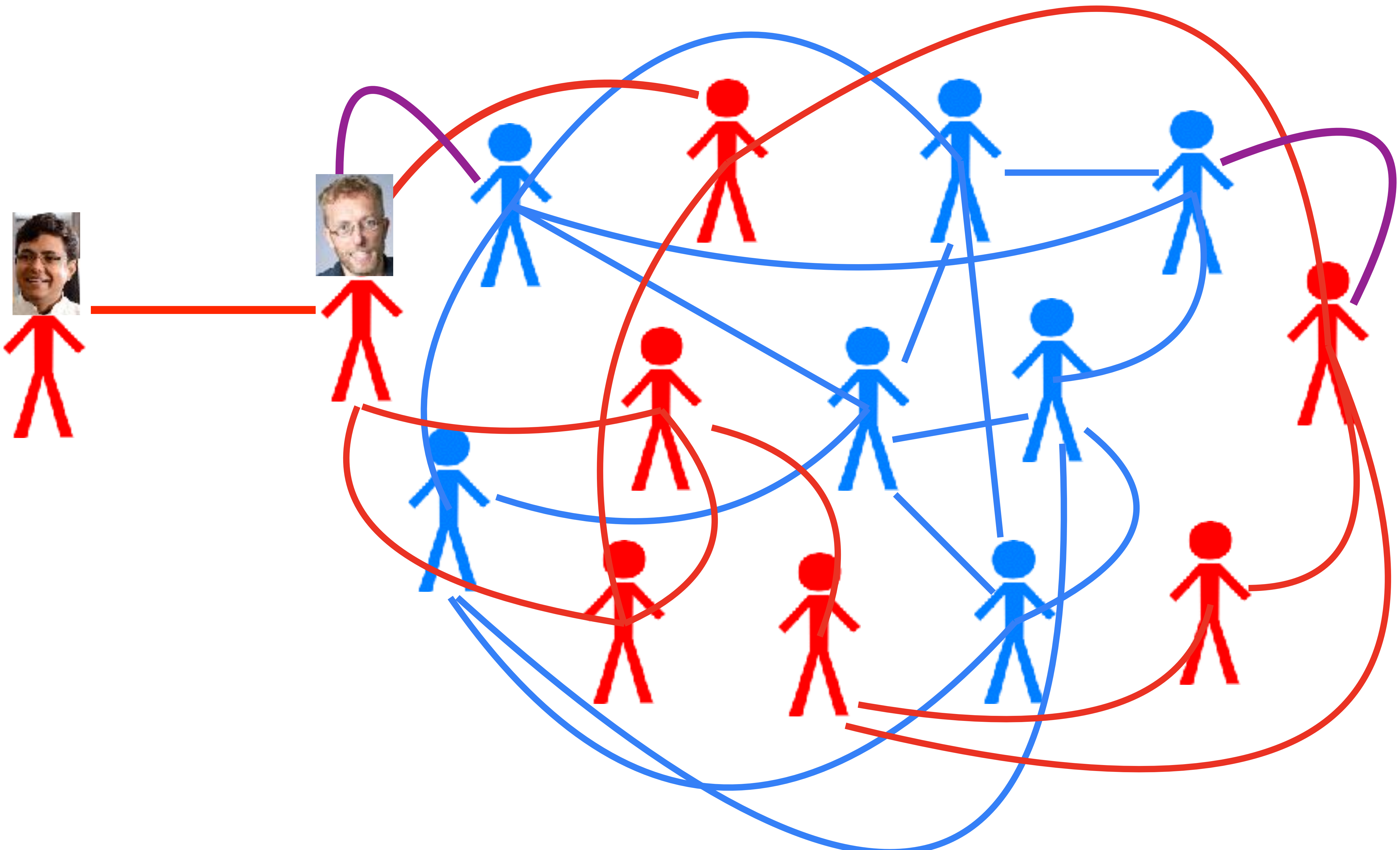
$$\text{Minimize } y^\top L y \quad \text{s.t. } \|y\|_2^2 = 1 \quad y \perp \mathbf{1}$$

$$y = \text{ Second smallest eigenvector of } L$$

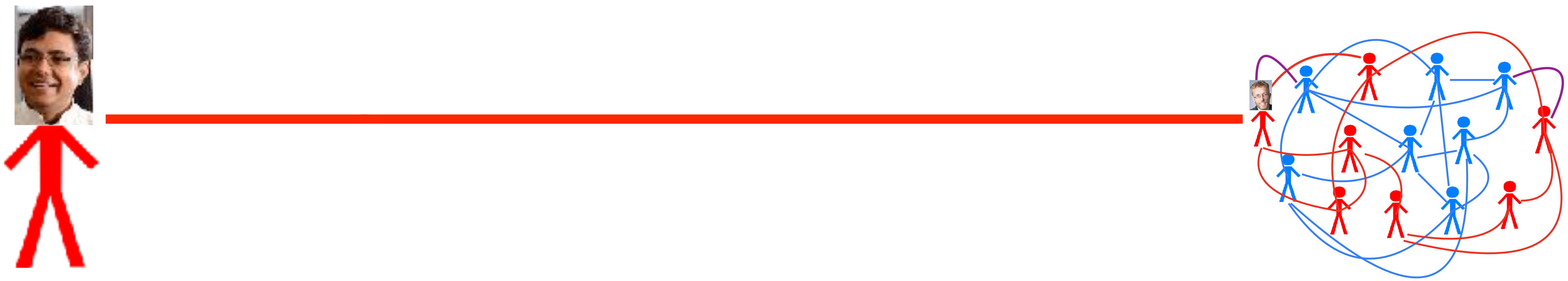
Spectral Clustering Algorithm (Unnormalized)

1. Given matrix A calculate diagonal matrix D s.t. $D_{i,i} = \sum_{j=1}^{n} A_{i,j}$
2. Calculate the Laplacian matrix $L = D - A$
3. Find eigen vectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$ of L (ascending order of eigenvalues)
4. Pick the K eigenvectors with smallest eigenvalues to get $\mathbf{y}_1, \ldots, \mathbf{y}_n \in \mathbb{R}^K$
5. Use K-means clustering algorithm on $\mathbf{y}_1, \ldots, \mathbf{y}_n$

Trouble Makers



TROUBLE MAKERS



- Variance is high
- Almost all connected nodes have same (small value)

What was the problem?

- Pushing few nodes far away from the rest increased variance
- But these nodes were ones with one or few links
- We want nodes with fewer links to account for lesser of the variance

Normalized Spectral Embedding

- Nodes linked to each other are close to each other
- Variance or spread should be large
  - But variance under what distribution?
  - Higher degree nodes are more important!
  - Lets try a distribution where probability of picking node is proportional to its degree
    - so pushing loners away does not account for much variance
    - There is more incentive to push the famous people outwards

Normalized Spectral Embedding

$$\text{Define distribution with } p_i = \frac{D_{i,i}}{\sum_{j=1}^{n} D_{j,j}} = \frac{D_{i,i}}{|E|}$$

- Keep your Friends close $\quad \text{minimize} \quad y^\top L y$
- Points are centered at 0 $\quad \sum_{i=1}^{n} p_i y_i = 0 \qquad \sum_{i=1}^{n} D_{i,i} y_i = 0$
- Variance or spread should be large

$$\text{Maximize} \sum_{i=1}^{n} p_i y_i^2 = \frac{1}{|E|} \sum_{i=1}^{n} D_{i,i} y_i^2 = \frac{1}{|E|} y^\top D y$$

Normalized Spectral Embedding

- Keep your Friends close $\quad \text{minimize} \quad y^\top L y$
- Points are centered at 0 $\quad \sum_{i=1}^{n} D_{i,i} y_i = 0$
- Variance or spread should be large $\quad \text{Maximize} \quad y^\top D y$

$$\text{Minimize} \quad \frac{y^\top L y}{y^\top D y} \quad \text{s.t.} \quad \sum_{i=1}^{n} D_{i,i} y_i = 0$$

$$\text{Define } u = D^{1/2} y \text{ so that } \frac{y^\top L y}{y^\top D y} = \frac{u^\top D^{-1/2} L D^{-1/2} u}{\|u\|^2}$$

$$\text{and } \sum_{i=1}^{n} D_{i,i} y_i = \sum_{i=1}^{n} D_{i,i}^{1/2} u_i = 0 \Rightarrow \text{diag}(D^{1/2}) \perp u$$

Normalized Spectral Embedding

- Keep your Friends close $\text{minimize} \quad y^\top L y$
- Points are centered at 0 $\sum_{i=1}^{n} D_{i,i} y_i = 0$
- Variance or spread should be large $\text{Maximize} \quad y^\top D y$

$$\text{Minimize } u^\top D^{-1/2} L D^{-1/2} u \qquad \text{s.t. } \|u\| = 1 \ \& \ u \perp \mathrm{diag}(D^{1/2})$$

$$\text{Solution: Second smallest eigen vector of } D^{-1/2} L D^{-1/2}$$

Normalized Spectral Embedding

- More generally if probability of a node i is proportional to some p_i then solution to normalized spectral clustering is
  - Second smallest eigen vector of $P^{-1/2} L P^{-1/2}$ where $P = \mathrm{diag}(p)$
  - For K dimensional representation, we can take 2nd to K+1'th smallest eigenvectors say $u_2, \ldots, u_{K+1}$
- $Y = P^{-1/2} U$

Clustering

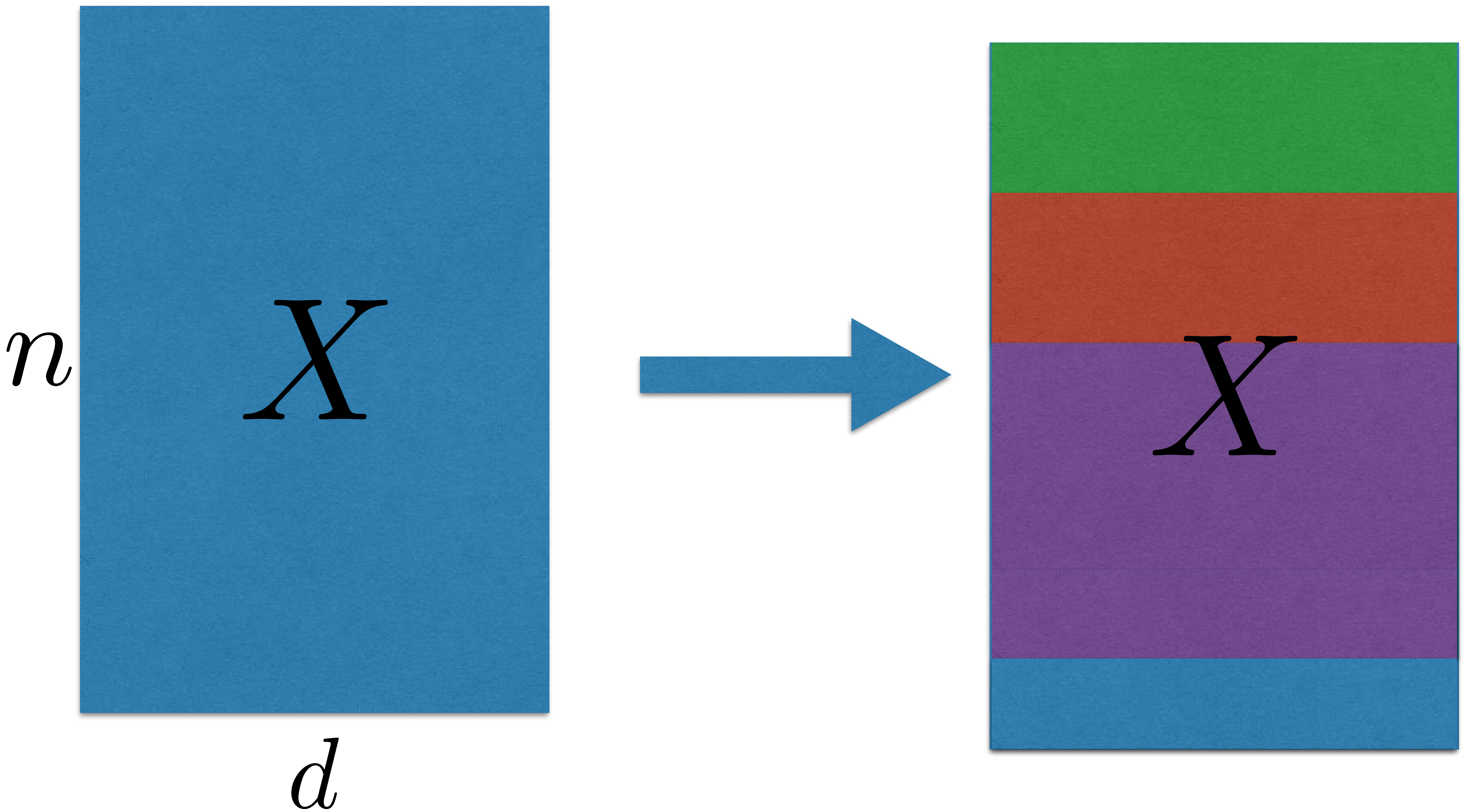
CLUSTERING

- Grouping sets of data points s.t.
  - points in same group are similar
  - points in different groups are dissimilar
- A form of unsupervised classification where there are no predefined labels

Clustering

- Partition data into K disjoint groups
- Compression or Quantization
  - Compress n points into K representatives/groups
- Visualization or Understanding
  - Taxonomy: Animals Vs plants Vs Microbes, Science Vs Math Vs Social Sciences
  - Segmentation: different types of customers, students etc. Find natural groupings in data
- What this does not include: items belonging to more than one type

Clustering



Clustering

- Grouping sets of data points s.t.
  - points in same group are similar
  - points in different groups are dissimilar
- A form of unsupervised classification where there are no predefined labels

Some Notations

- Kary clustering is a partition of $\mathbf{x}_1, \ldots, \mathbf{x}_n$ into K groups
- For now assume the magical K is given to use
- Clustering given by $C_1, \ldots, C_K$, the partition of data points.
- Given a clustering, we shall use $c(\mathbf{x}_t)$ to denote the cluster identity of point $\mathbf{x}_t$ according to the clustering.
- Let n_j denote $|C_j|$, clearly $\sum_{j=1}^{K} n_j = n$.

How do we formalize a good clustering objective?

How do we formalize?

Say dissimilarity$(\mathbf{x}_t, \mathbf{x}_s)$ measures dissimilarity between $\mathbf{x}_t$ & $\mathbf{x}_s$

Given two clustering $\{C_1, \ldots, C_K\}$ (or c) and $\{C'_1, \ldots, C'_K\}$ (or c')

How do we decide which is better?

- points in same cluster are not dissimilar
- points in different clusters are dissimilar

Clustering Criterion

- Minimize total within-cluster dissimilarity

$$M_1 = \sum_{j=1}^{K} \sum_{s,t \in C_j} \text{dissimilarity}(x_t, x_s)$$

- Maximize between-cluster dissimilarity

$$M_2 = \sum_{\mathbf{x}_s, \mathbf{x}_t : c(\mathbf{x}_s) \neq c(\mathbf{x}_t)} \text{dissimilarity}(x_t, x_s)$$

- Maximize smallest between-cluster dissimilarity

$$M_3 = \min_{\mathbf{x}_s, \mathbf{x}_t : c(\mathbf{x}_s) \neq c(\mathbf{x}_t)} \text{dissimilarity}(x_t, x_s)$$

- Minimize largest within-cluster dissimilarity

$$M_4 = \max_{j \in [K]} \max_{s,t \in C_j} \text{dissimilarity}(x_t, x_s)$$