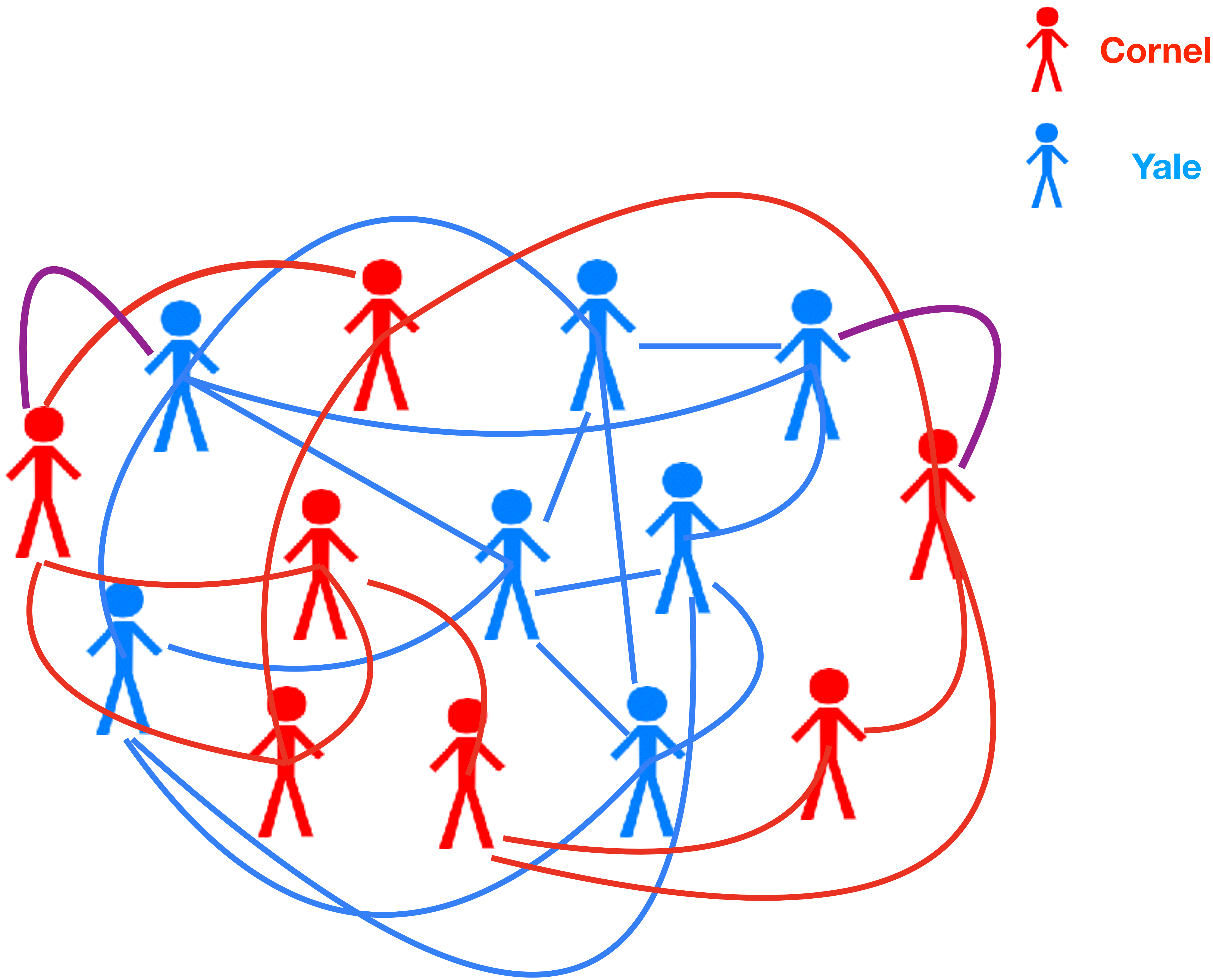
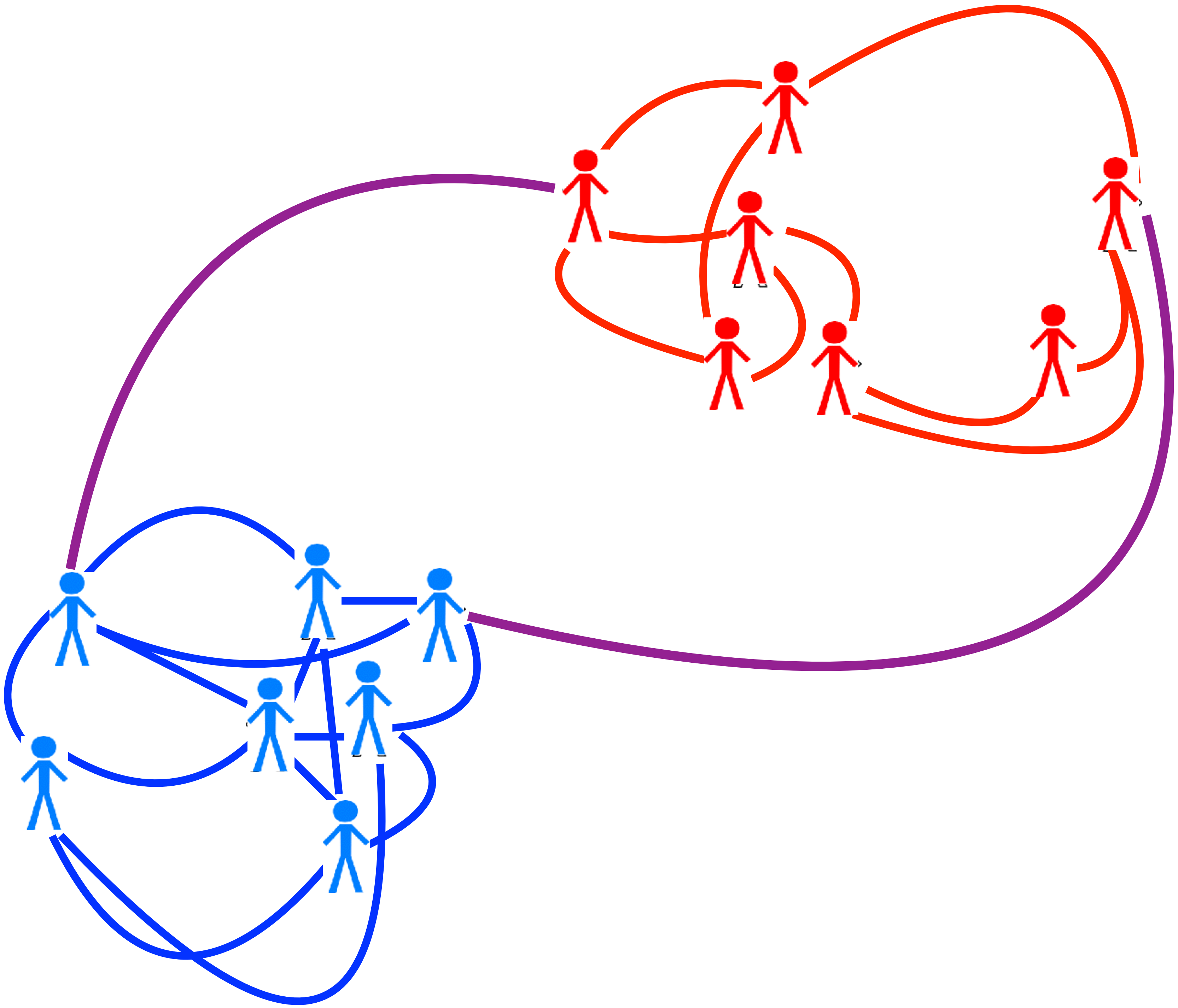
Machine Learning for Data Science (CS4786)
Lecture 10

Spectral Embedding

Motivating Example



Motivating Example



Graph Embedding

- GOAL: Place vertices (users) of the graph in appropriate locations (in a K dimensional space)
- Distances between vertices (users) should be representative of some desired properties of the graph
  - Eg. Cornell folks are together, all Yale folks are together

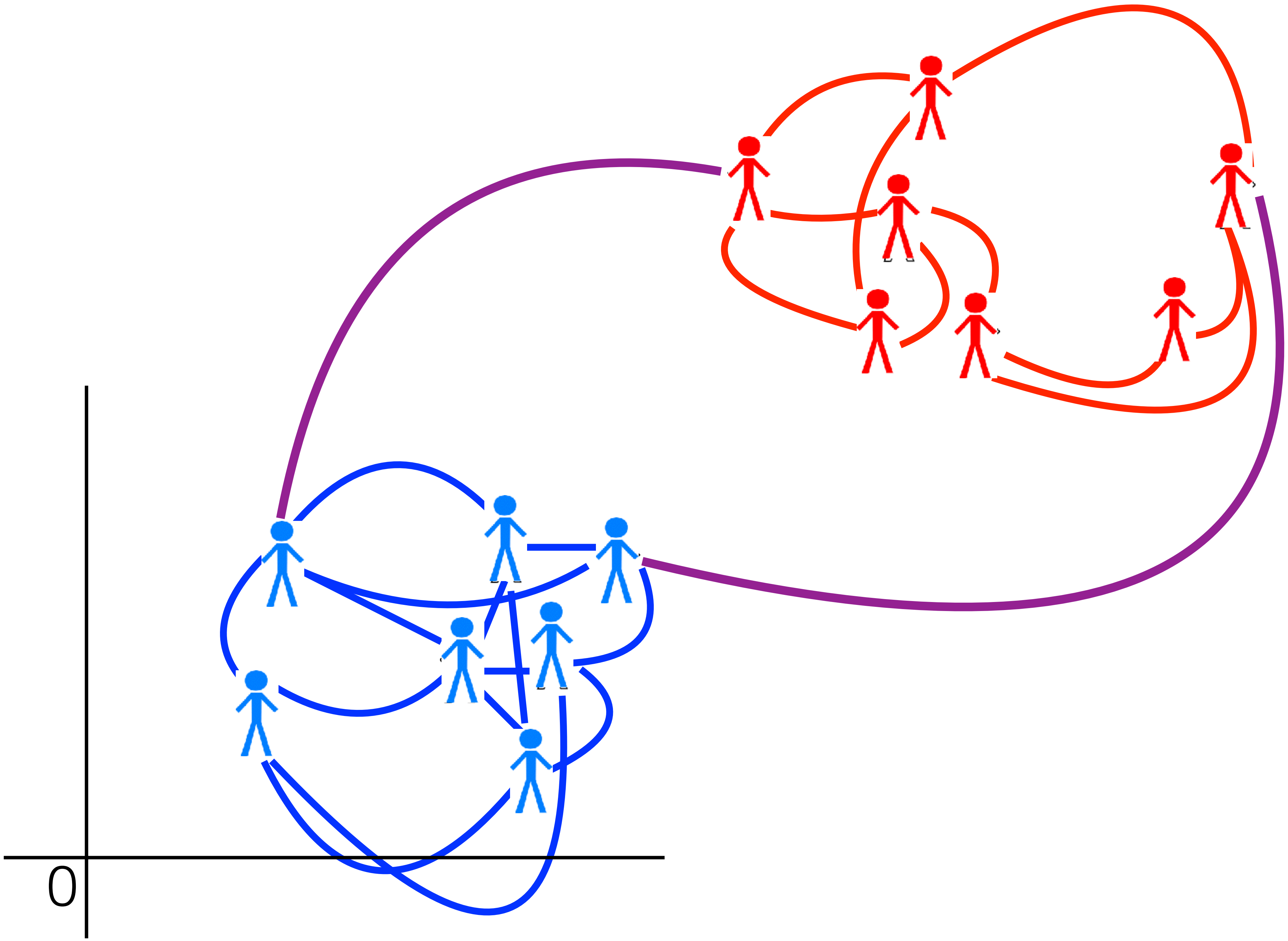
How do we do this?

- If I gave you a proposed location how would you evaluate it for instance?
- What are the desirable properties?

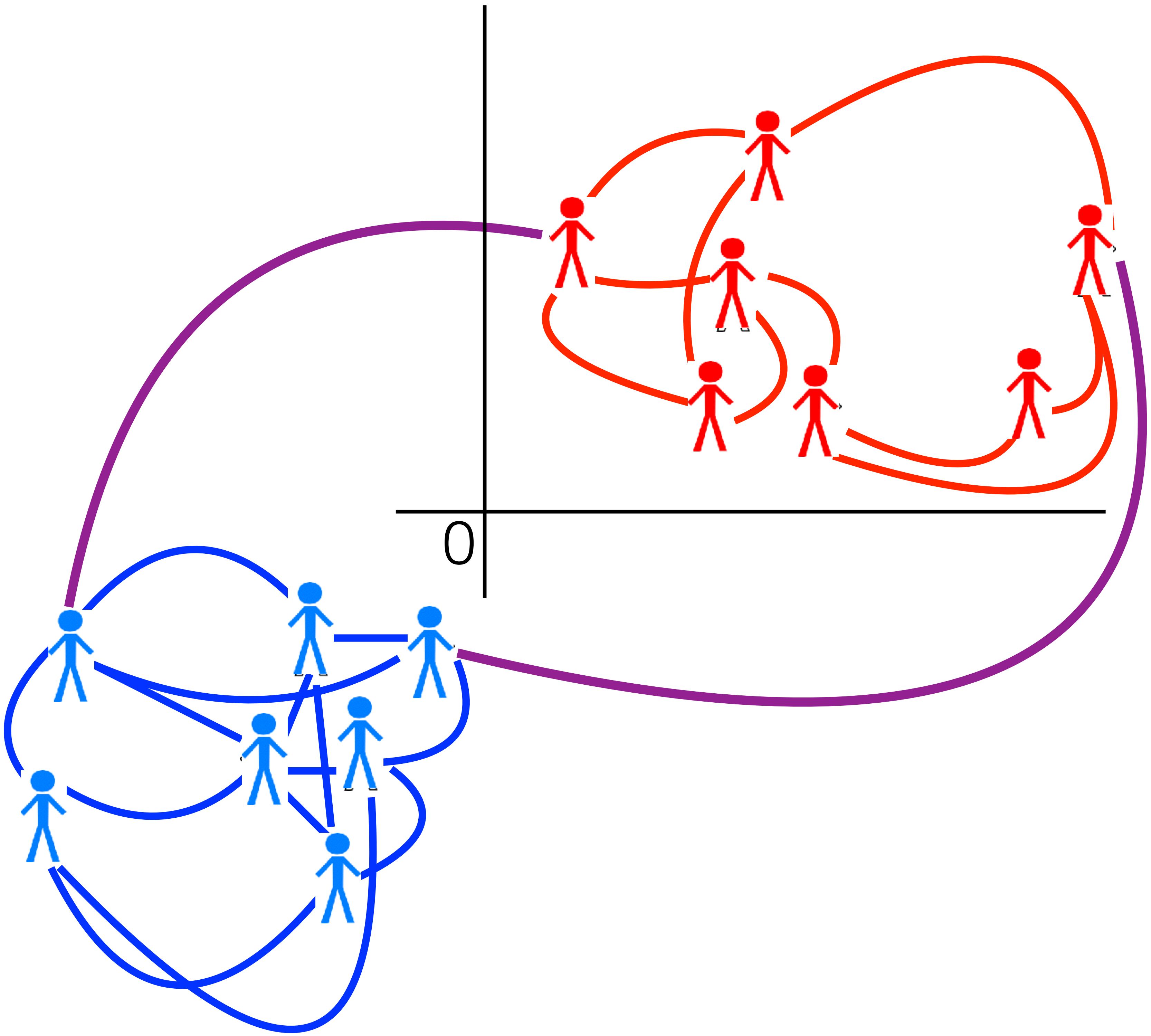
Thought Experiment

- 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?

Centering locations



Centering locations



KEY PRINCIPLE

- **Points are centered at 0**

Key Principle

Make total distance between friends small:

$$\mathrm{Obj}(y_1, \ldots, y_n) = \sum_{(i,j) \in E} \mathrm{dist}^2(y_i, y_j)$$

KEY PRINCIPLE

- Points are centered at 0
- **Keep your Friends close**
  (sum of distances between linked nodes should be small)

Key Principle

If all $y's$ are at same location then friends are all close

Spread around the points!

Make $\mathrm{Var}(y_1, \ldots, y_n)$ large.

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**

Spectral Embedding

- Lets start with one dimensional projection
- Single number y_i for each node i
- Lets review the three desired properties

Key Principle

- **Points are centered at 0**
- Keep your Friends close
- Variance or spread amongst the nodes should be large

$$\frac{1}{n}\sum_{t=1}^{n} y_t = 0$$

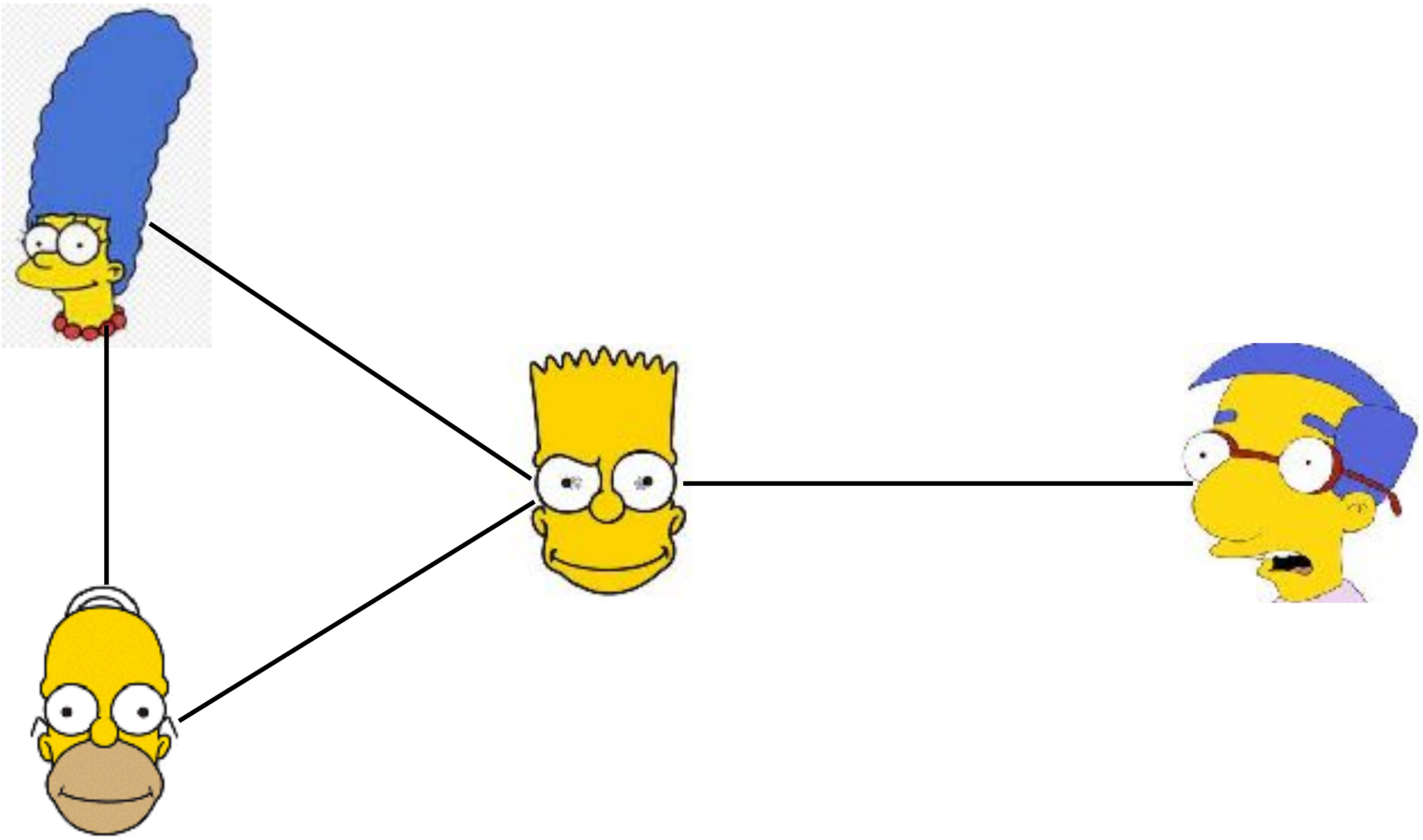
$$\Updownarrow$$

$$y^\top \mathbf{1} = 0$$

KEY PRINCIPLE

- Points are centered at 0 $y^\top \mathbf{1} = 0$
- **Keep your Friends close**
- Variance or spread should be large

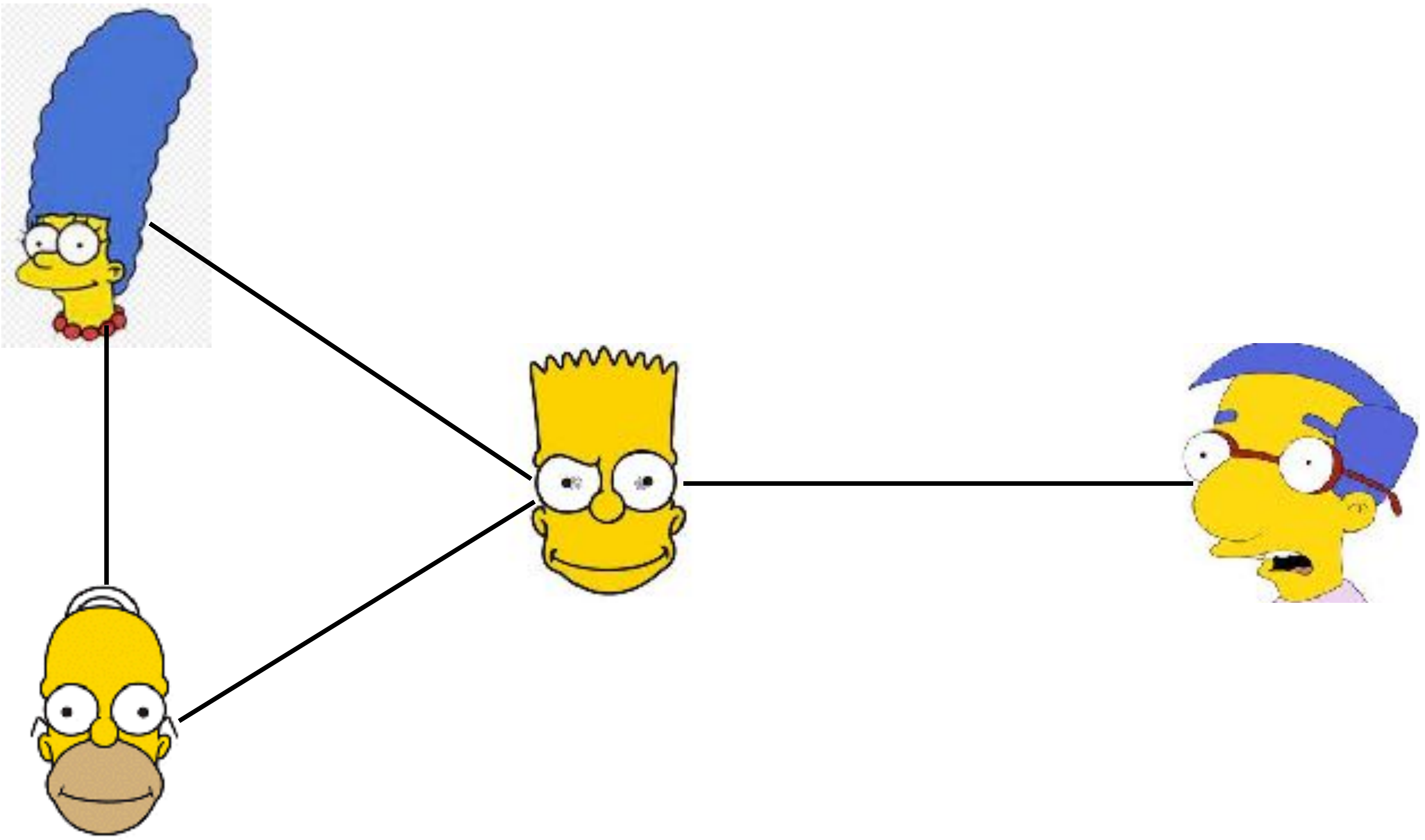
Representing the Graph



A =

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

Representing the Graph



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

Why the Laplacian?

$$
\begin{aligned}
\mathrm{Obj}(y_1, \dots, y_n) &= \sum_{(i,j) \in \text{ Friends}} (y_i - y_j)^2 \\
&= \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{i,j} (y_i - y_j)^2 \\
&= \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{i,j} \left(y_i^2 + y_j^2 - 2 y_i y_j\right) \\
&= \frac{1}{2} \left(\sum_{i=1}^{n} \left(\sum_{j=1}^{n} A_{i,j} \right) y_i^2 + \sum_{j=1}^{n} \left(\sum_{i=1}^{n} A_{i,j} \right) y_j^2 - 2 \sum_{i=1}^{n} \sum_{j=1}^{n} A_{i,j} y_i y_j \right) \\
&= \frac{1}{2} \left(\sum_{i=1}^{n} D_{i,i} y_i^2 + \sum_{j=1}^{n} D_{j,j} y_j^2 - 2 \sum_{i=1}^{n} \sum_{j=1}^{n} A_{i,j} y_i y_j \right) \\
&= \sum_{i=1}^{n} D_{i,i} \; y_i^2 - \sum_{i=1}^{n} \sum_{j=1}^{n} A_{i,j} y_i y_j \\
&= \left(y^\top D y - y^\top A y \right) \\
&= y^\top (D - A) y = y^\top L y
\end{aligned}
$$

The Laplacian Matrix

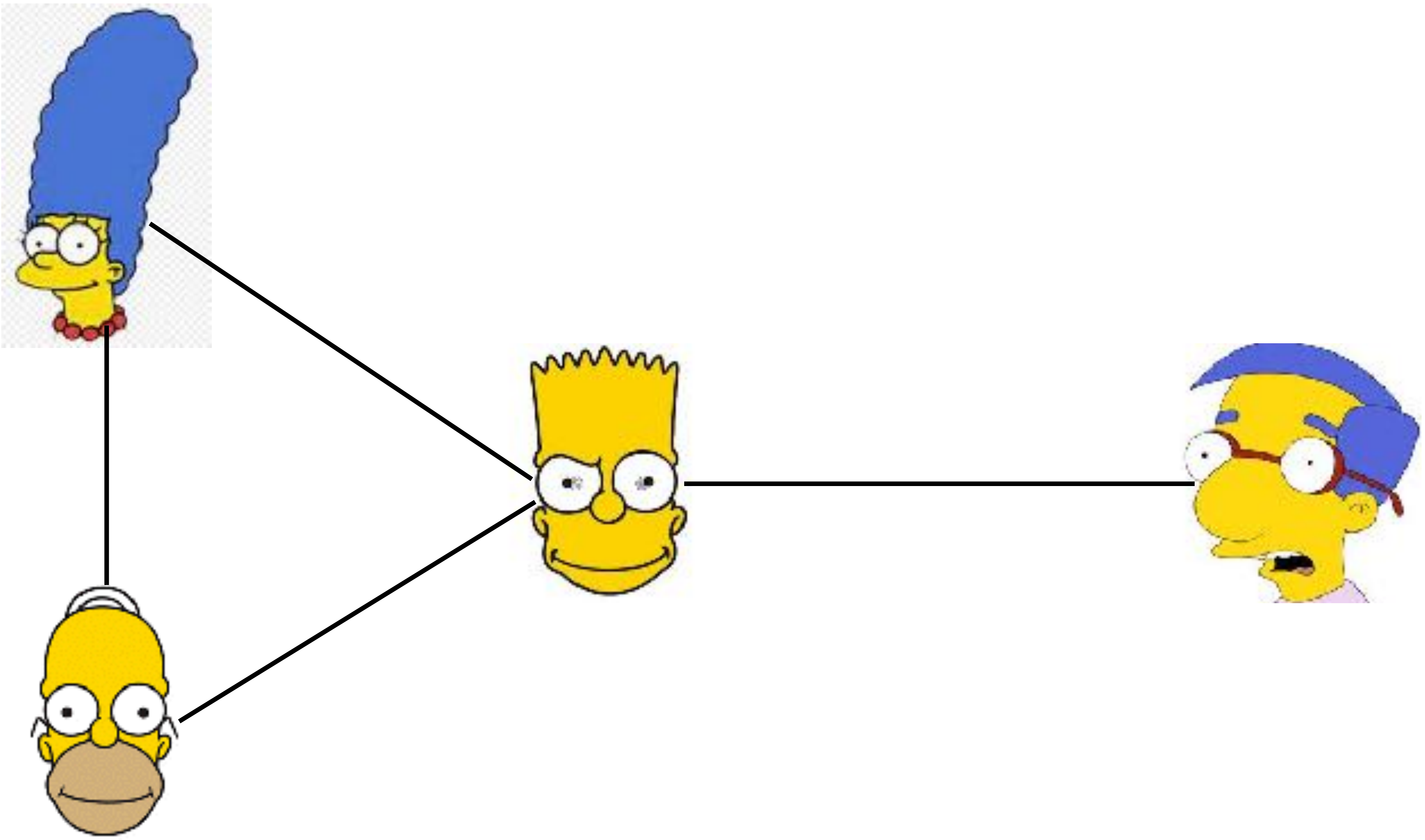
$$L = \cancel{D} - A$$

				
	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

Representing the Graph



L =

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

KEY PRINCIPLE

- Points are centered at 0 $y^\top \mathbf{1} = 0$
- **Keep your Friends close** $\text{minimize} \;\; y^\top L y$
- Variance or spread should be large

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Maximize Variance

$$\begin{aligned}\mathrm{Var}(y_1, \ldots, y_n) &= \frac{1}{n}\sum_{t=1}^{n}(y_t - \mathrm{mean}(y))^2 \\ &= \frac{1}{n}\sum_{t=1}^{n} y_t^2 = \frac{1}{n}\|y\|_2^2\end{aligned}$$

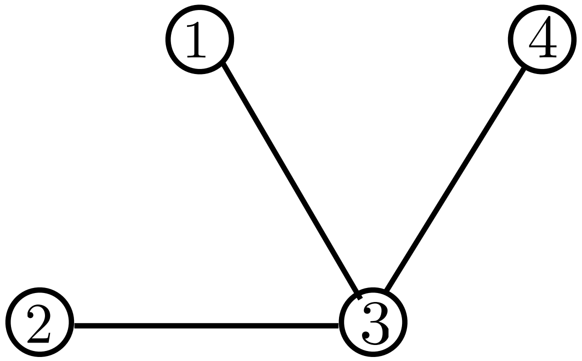
Key Principle

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

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

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

EXAMPLES



- Fact: For a connected graph, exactly one, the smallest of eigenvalues is 0, corresponding eigenvector is $(1, 1, \ldots, 1)^\top / \sqrt{n}$

KEY PRINCIPLE

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

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

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

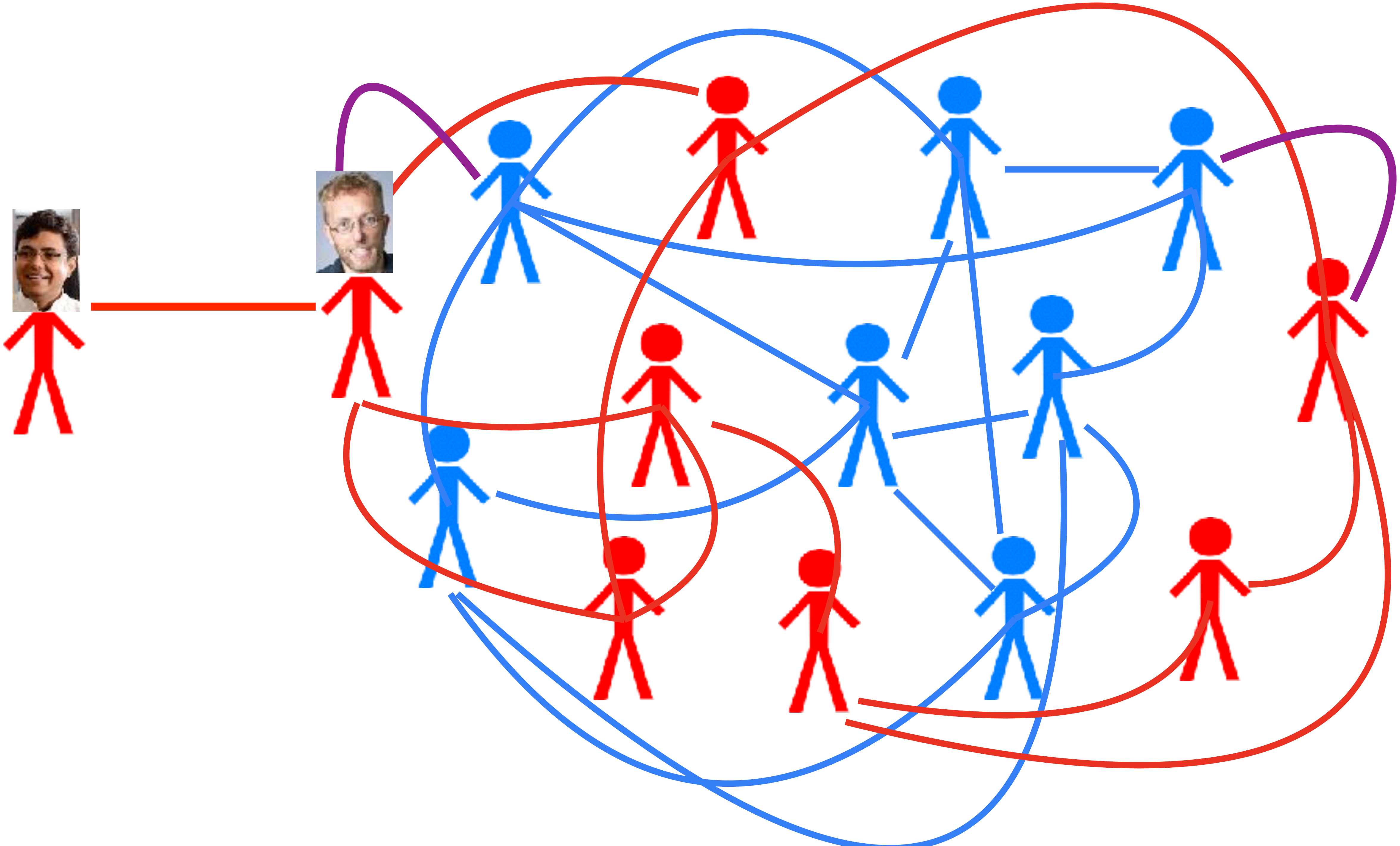
Spectral Embedding

- For $K > 1$ dimensional embedding
- First dimension is the second smallest eigenvector
- Second dimension is the third smallest eigenvector and so on ...
- (Unnormalized) Spectral clustering: compute $2 : K + 1$ smallest eigen vectors
- Set Y_i to be the i'th row

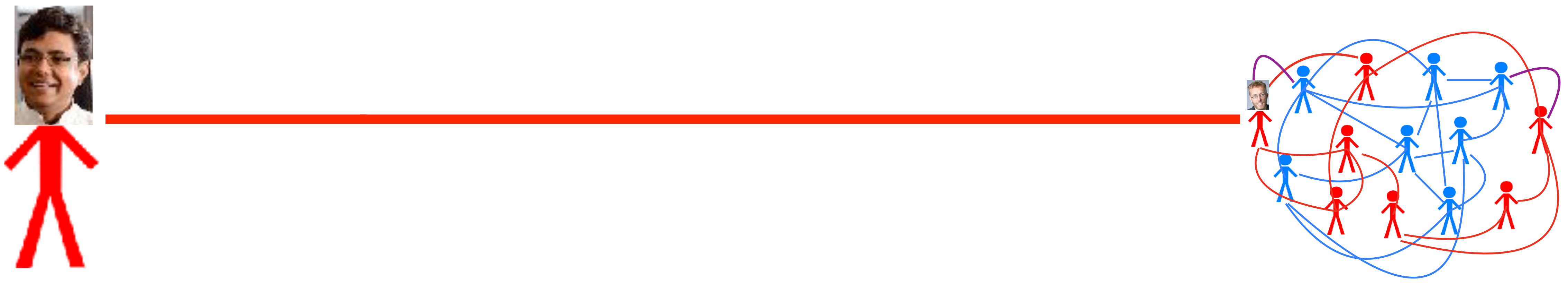
Spectral Clustering Algorithm (Unnormalized)

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)

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 distribution given by p_i \propto D_{i,i}