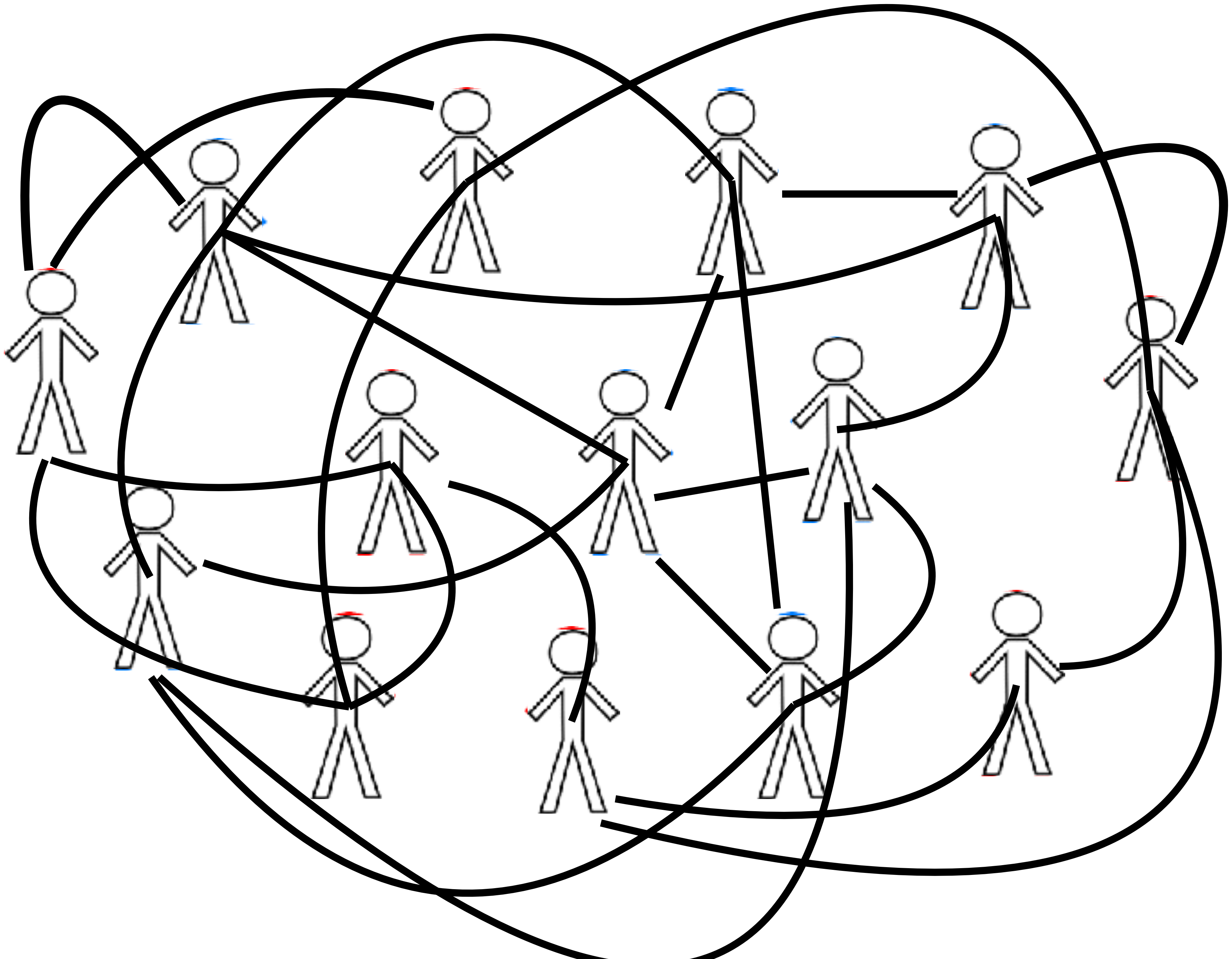
Machine Learning for Data Science (CS4786)
Lecture 13

Spectral Embedding

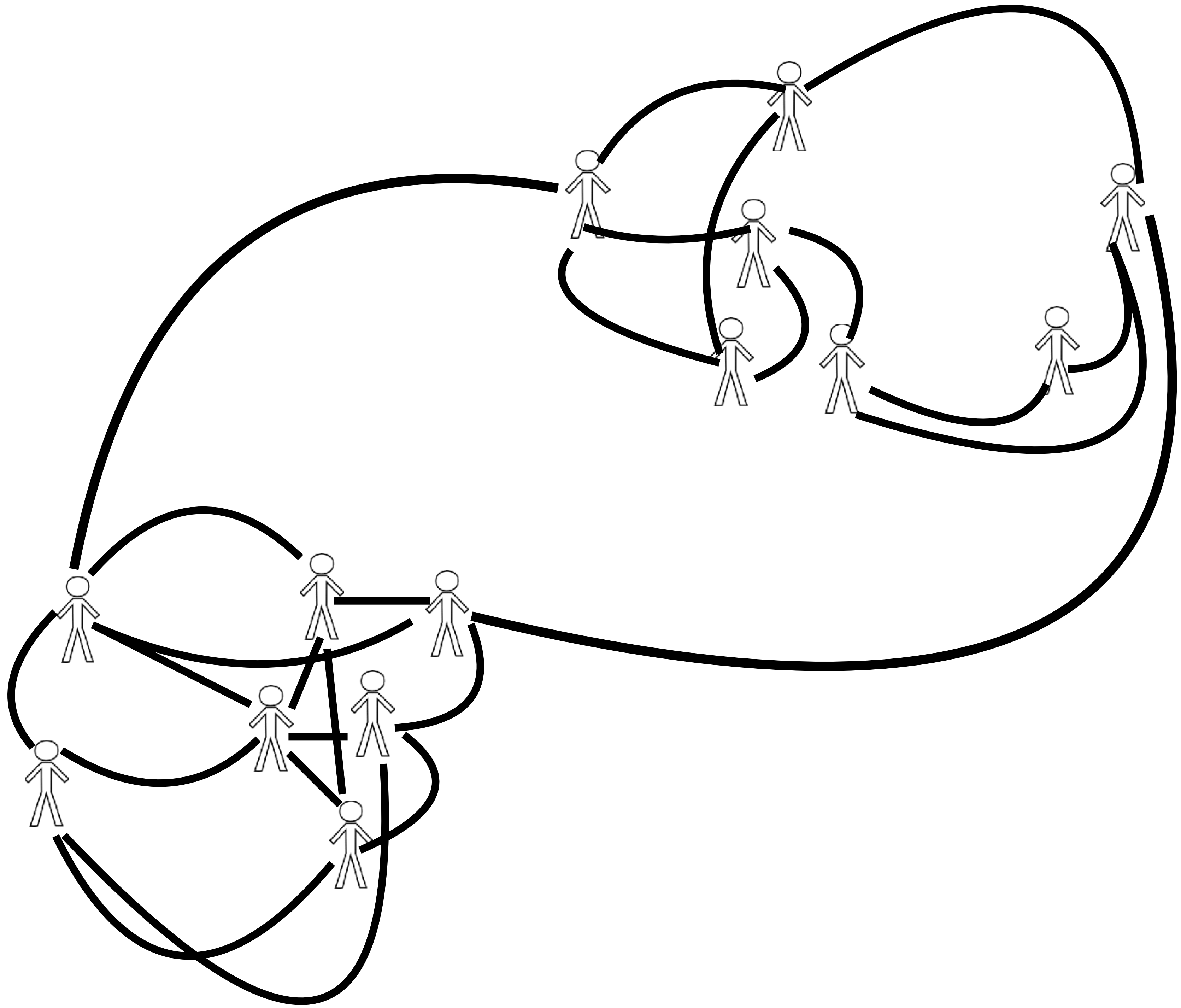
Spectral Embedding

Motivating Example



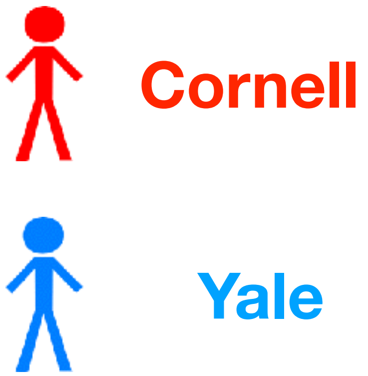
What can you say from this network?

Motivating Example



How about now?

Motivating Example



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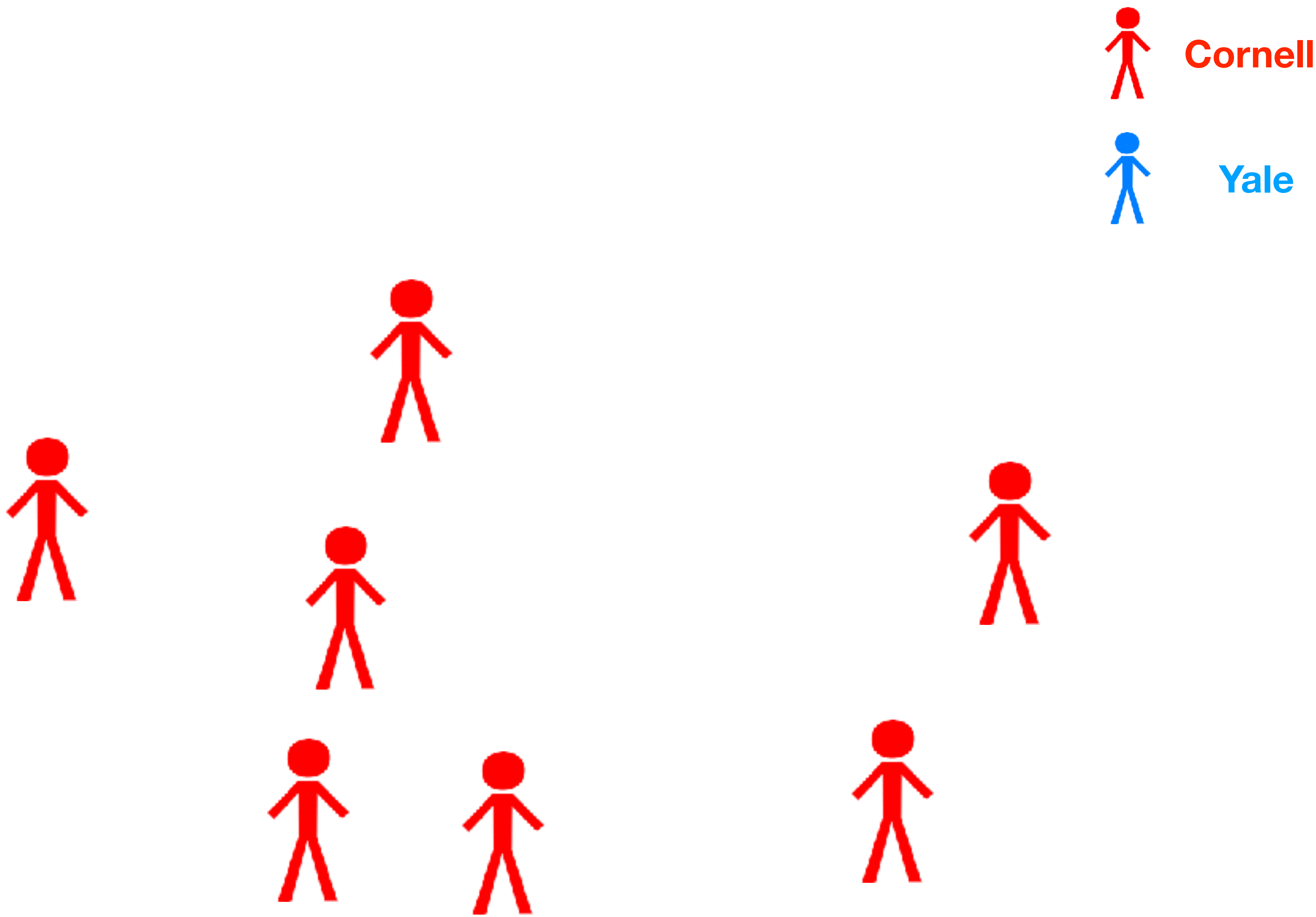

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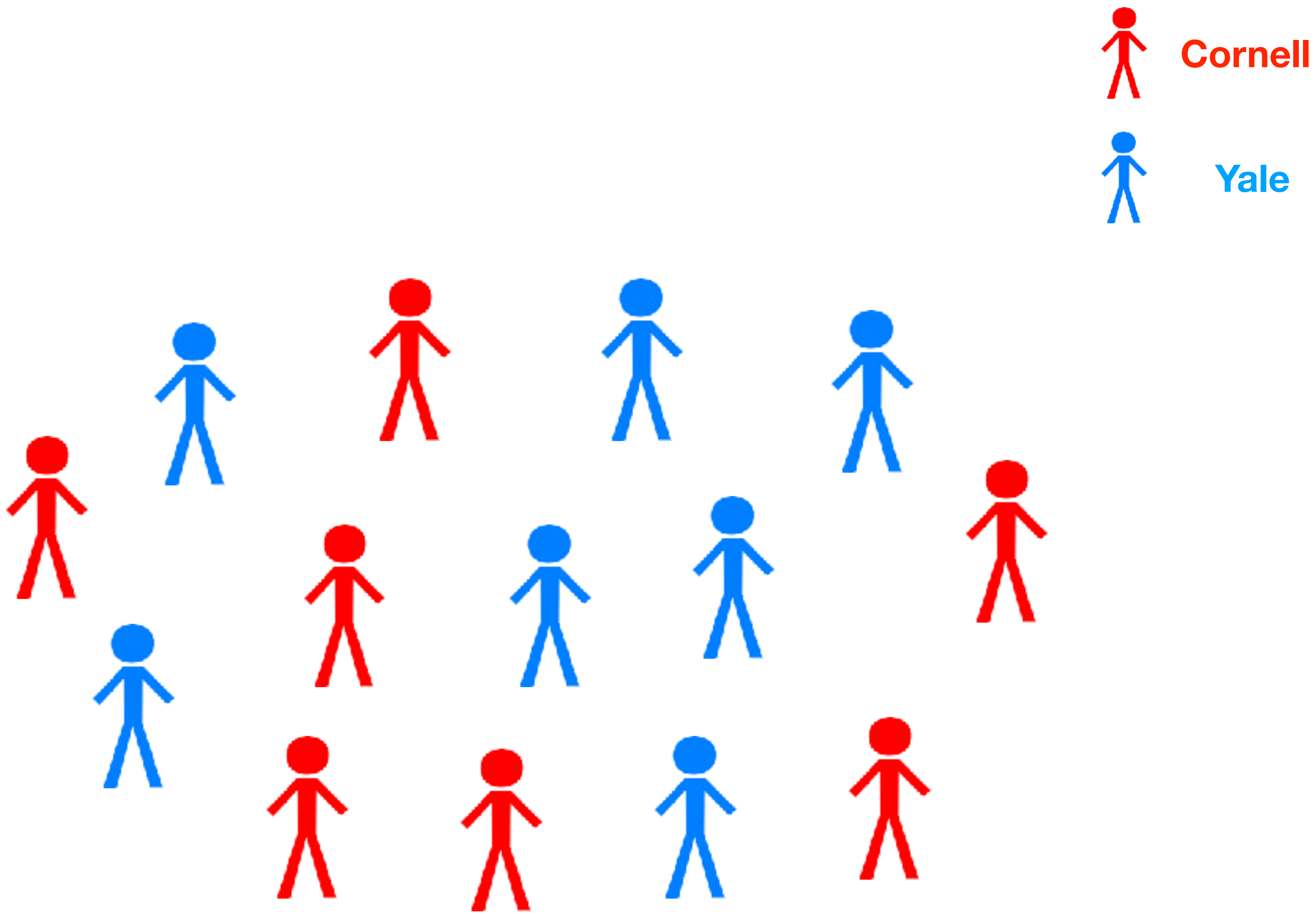

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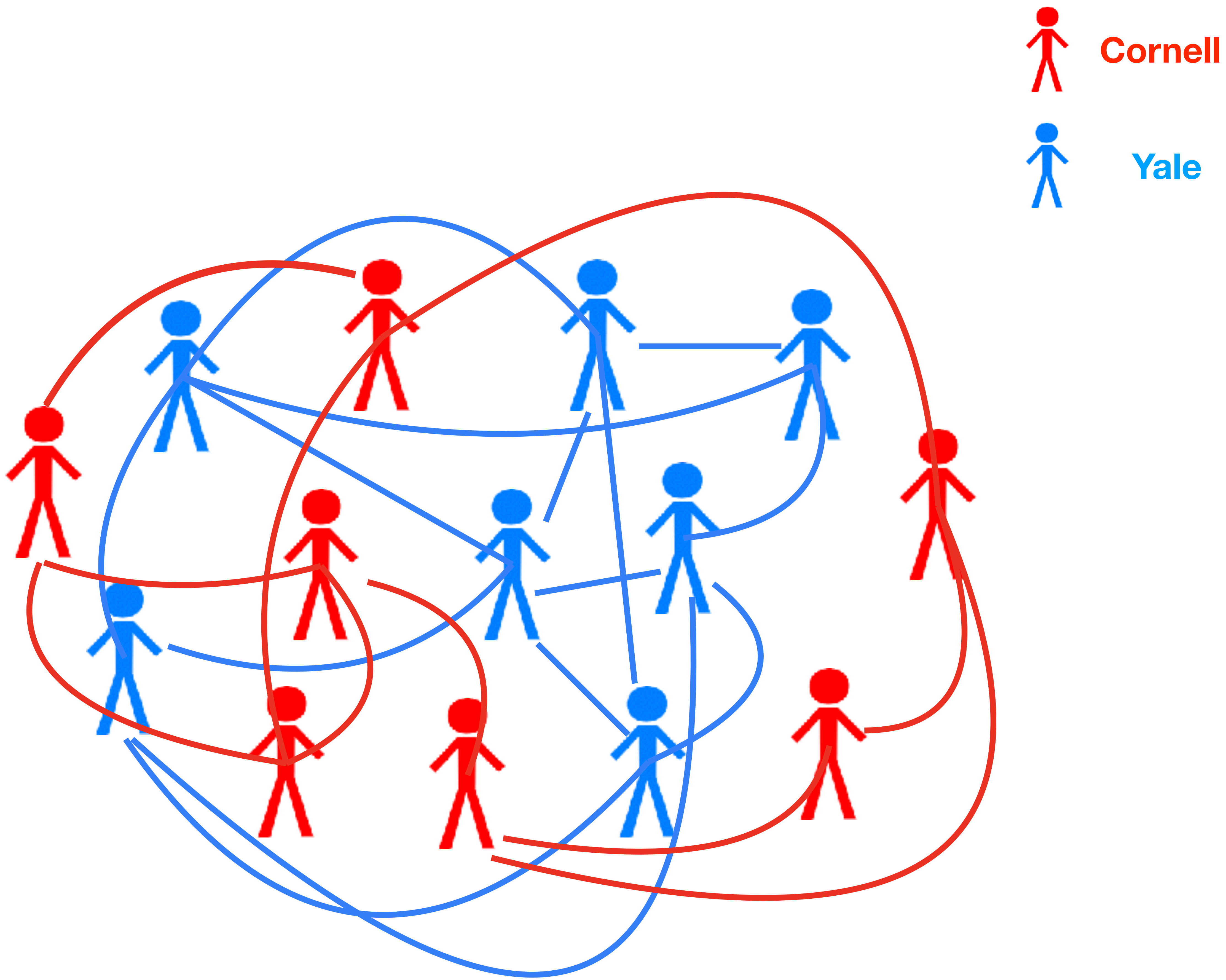
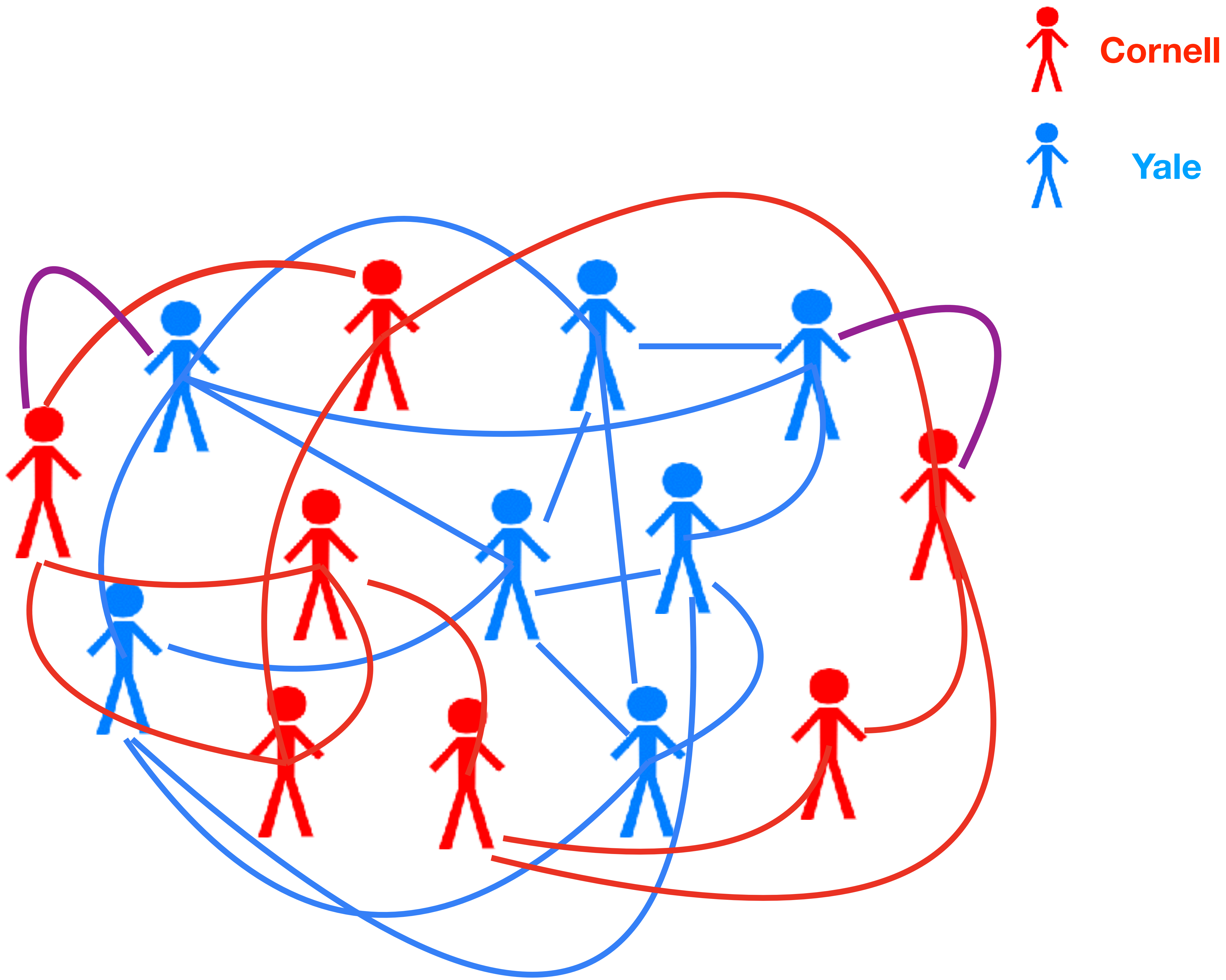


MOTIVATING EXAMPLE



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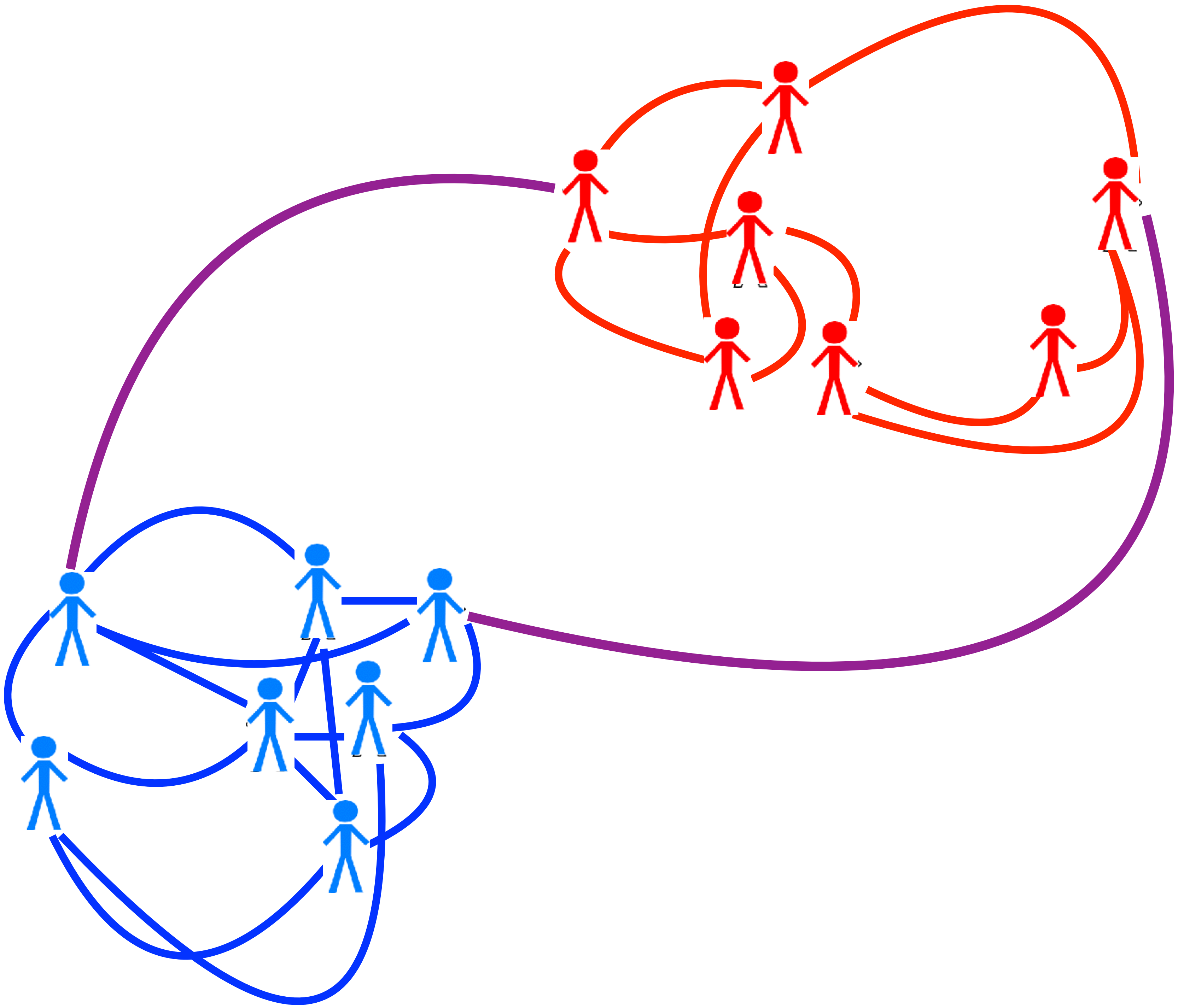

Graph Embedding

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- GOAL: Place vertices (users) of the graph in appropriate locations (in a K dimensional space)

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- 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

Key Principle

How do we do this?

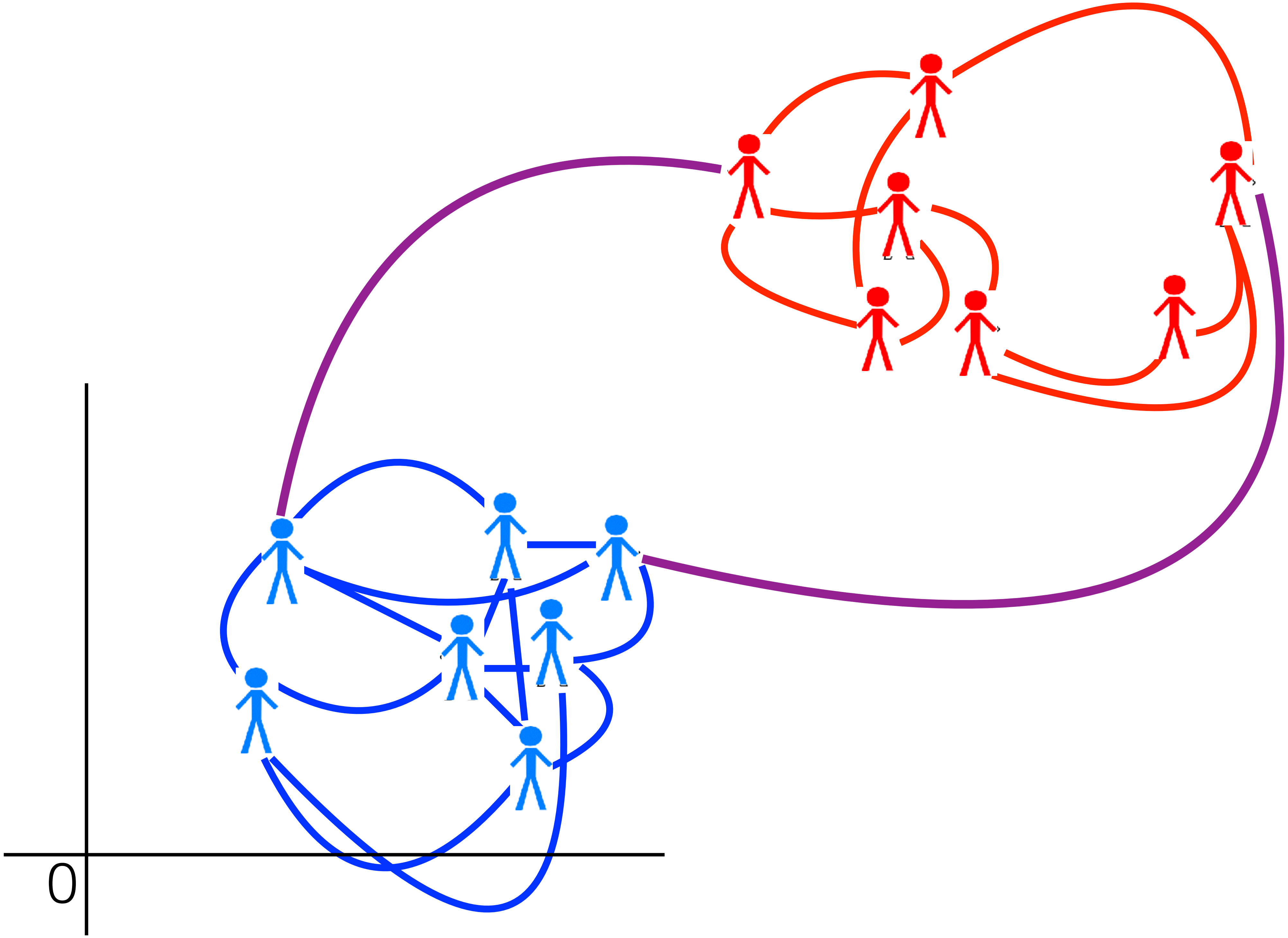
How do we do this?

- 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



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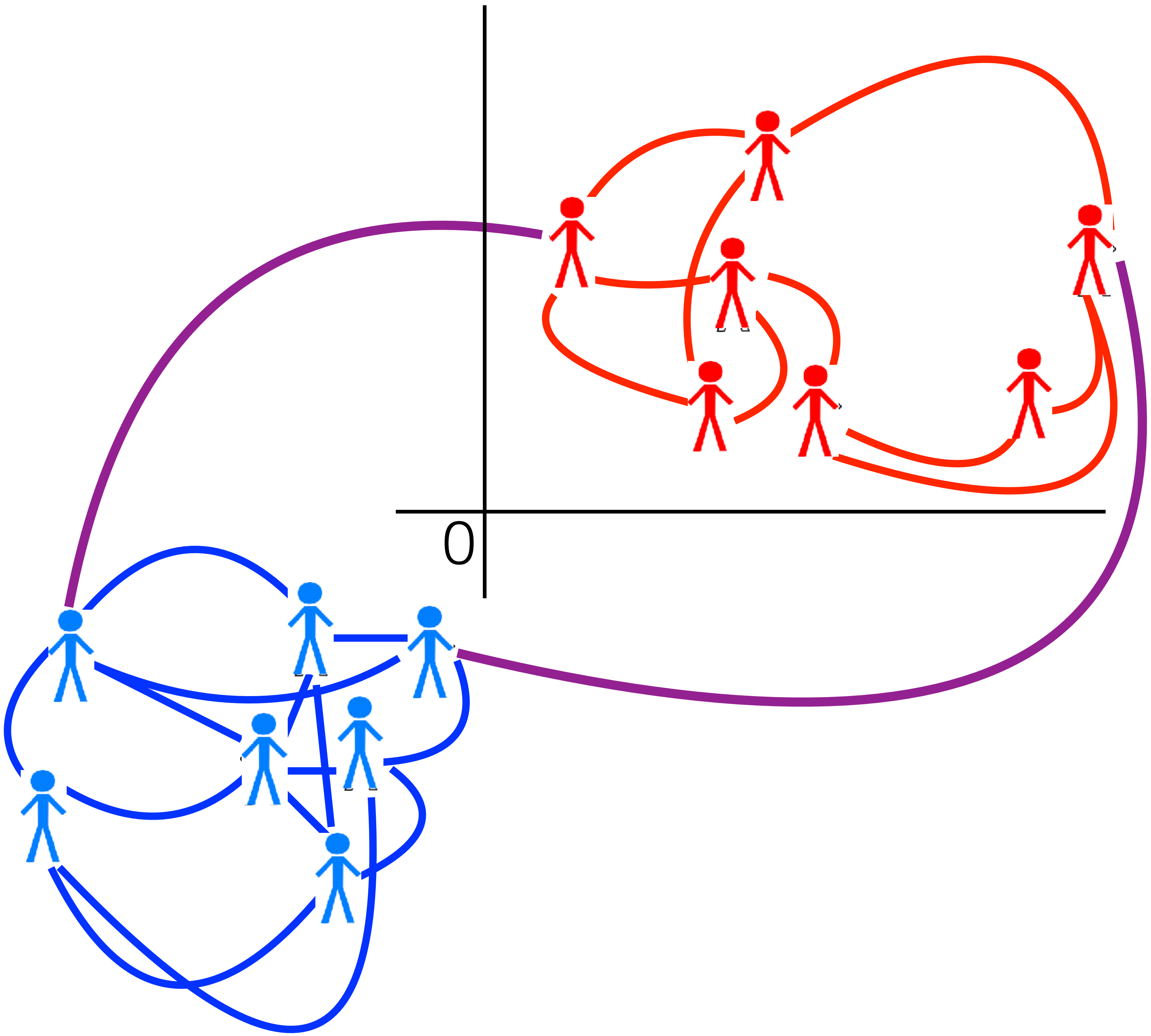

Key Principle

- **Points are centered at 0**

Key Principle

Key Principle

Make total distance between friends small:

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

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

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Spread around the points!

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Spread around the points!

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

Key Principle

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

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Spectral Embedding

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

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$$\Updownarrow$$

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

KEY PRINCIPLE

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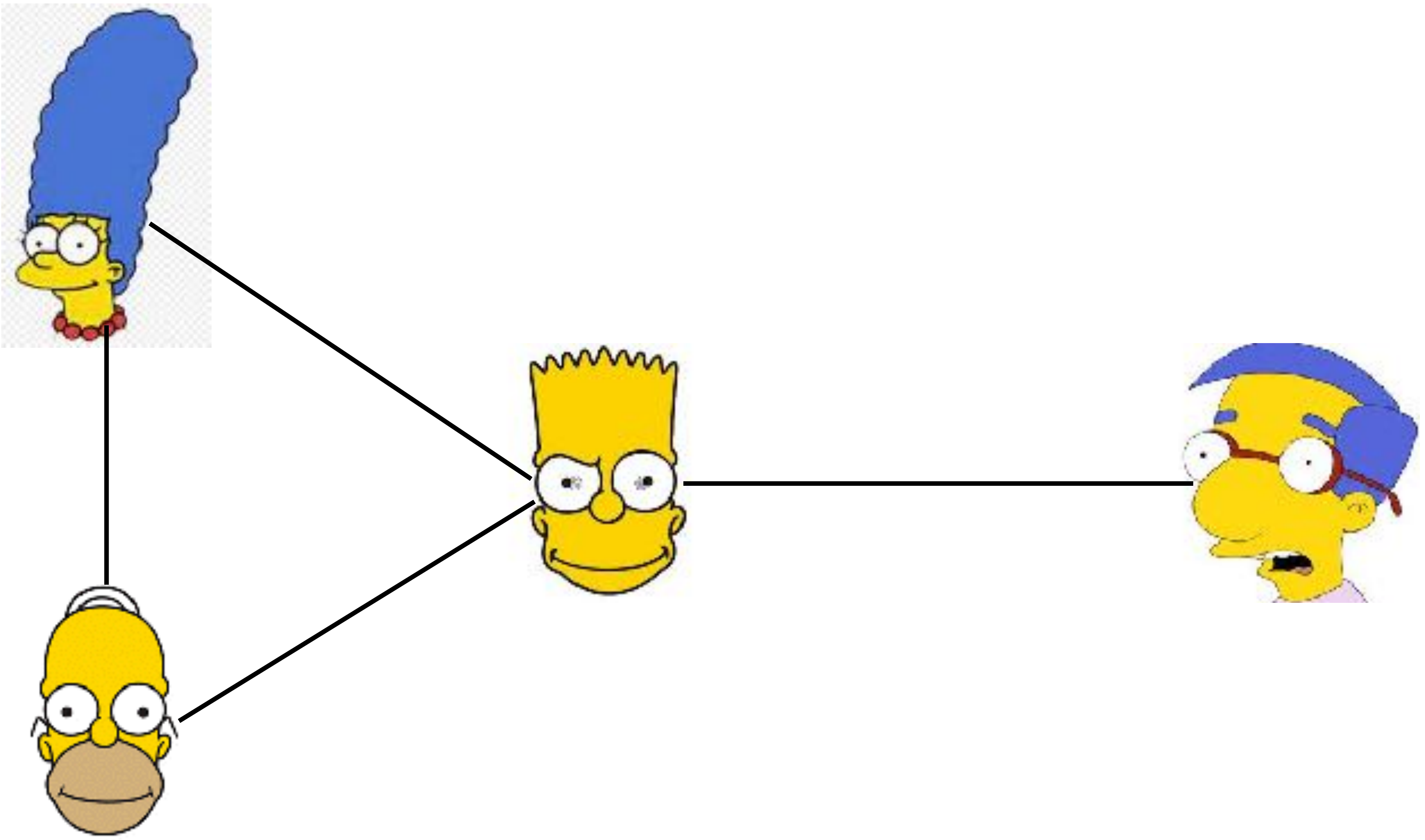
Representing the Graph



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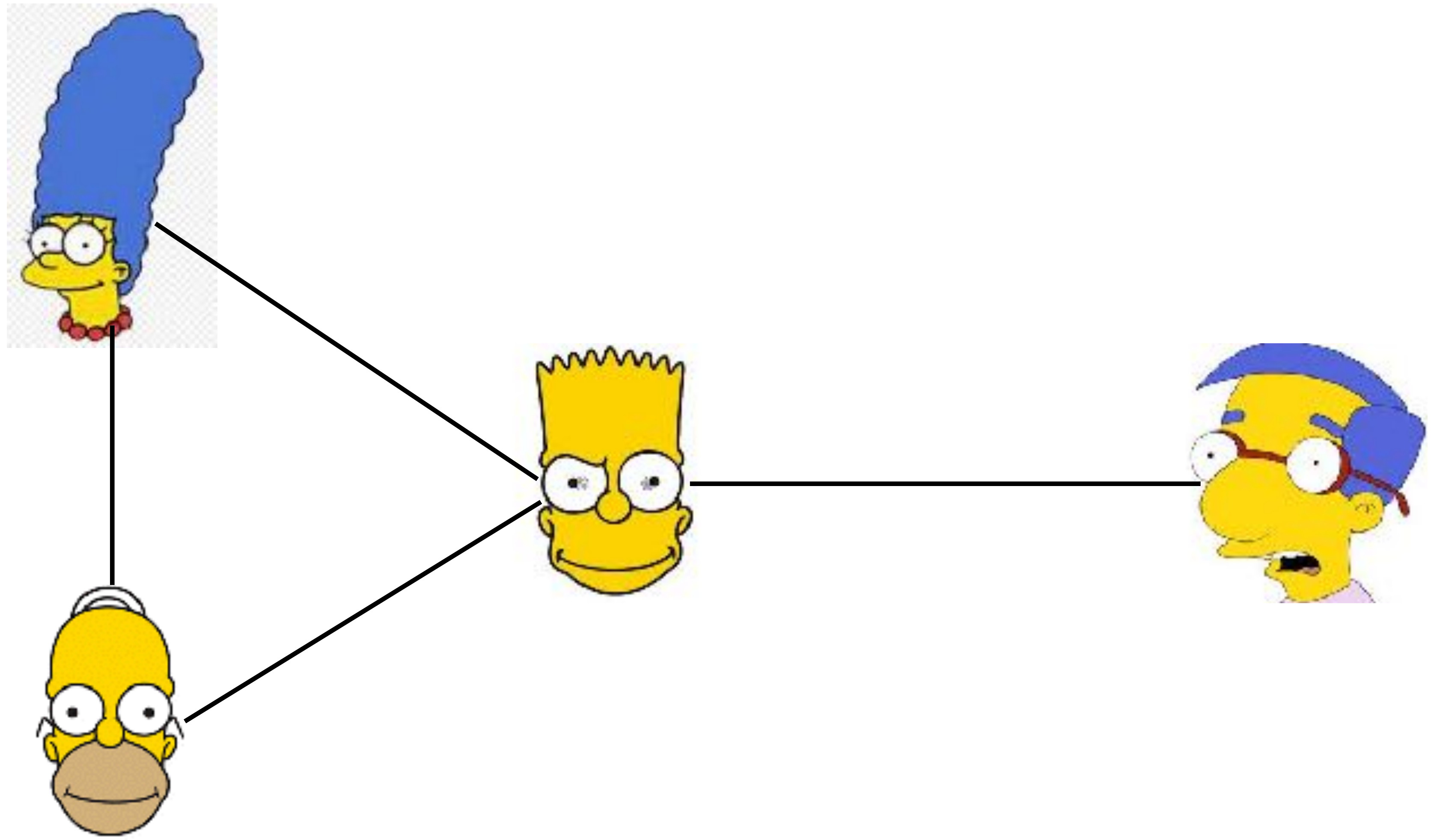

A =

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

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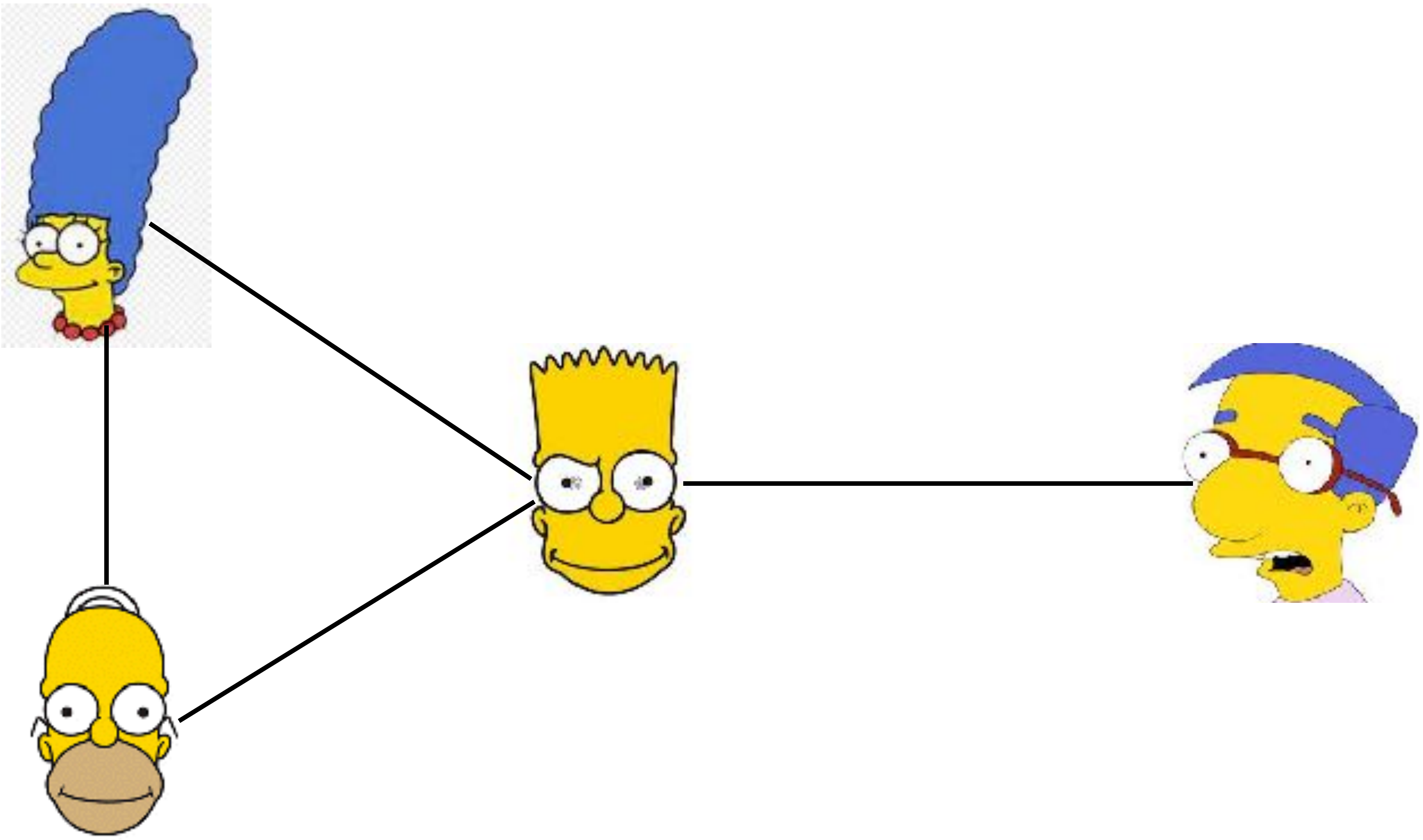

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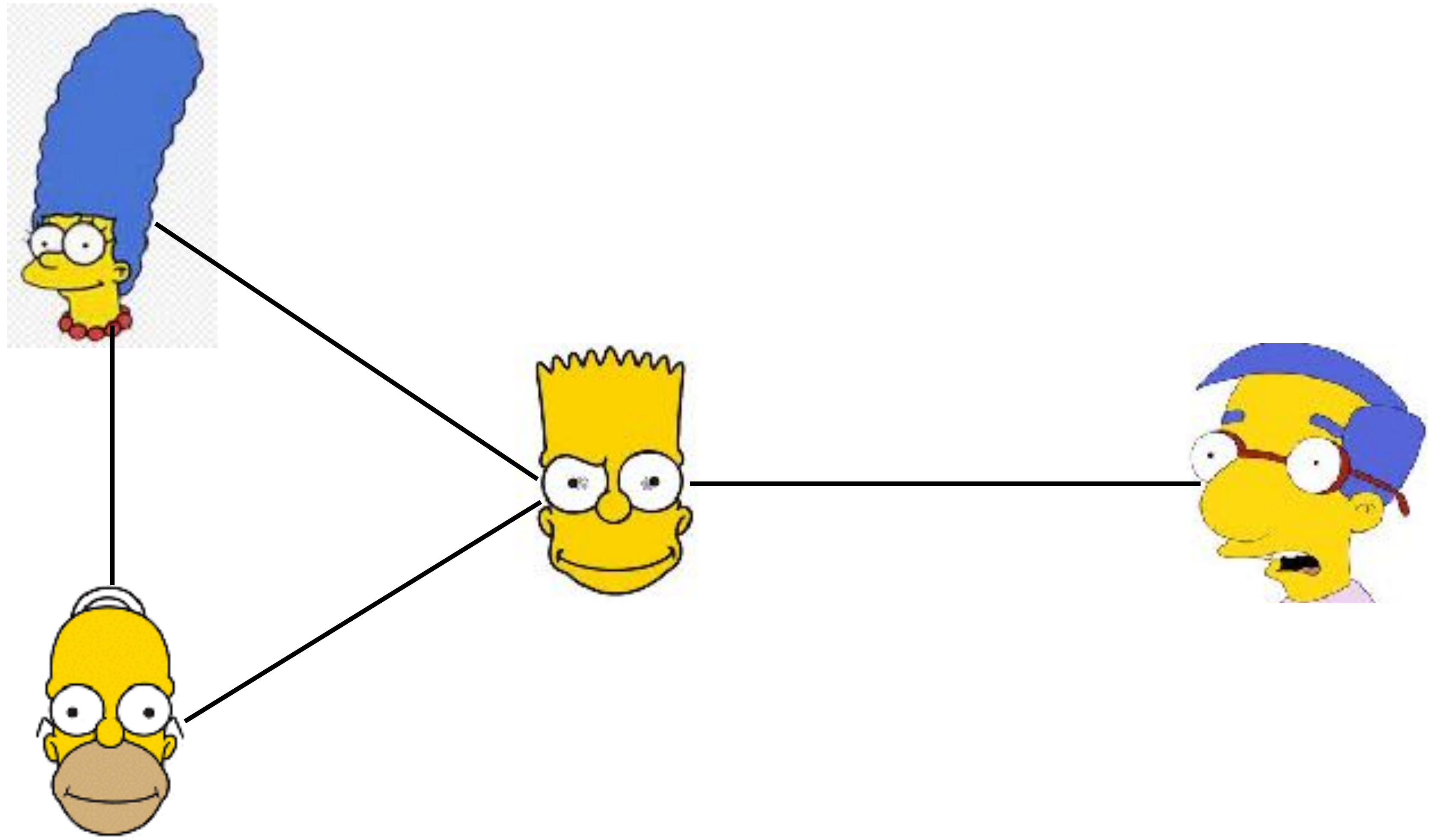

D =

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

Why the Laplacian?

$$\text{Obj}(y_1, \ldots, y_n) = \sum_{(i,j) \in \text{ Friends}} (y_i - y_j)^2$$

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Why the Laplacian?

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\text{Obj}(y_1, \ldots, y_n) &= \sum_{(i,j) \in \text{ Friends}} (y_i - y_j)^2 \\
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&= \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)
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&= \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_iy_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_iy_j\right)
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&= \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)
\end{aligned}
$$

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&= \sum_{i=1}^{n} D_{i,i}\; y_i^2 - \sum_{i=1}^{n}\sum_{j=1}^{n} A_{i,j}y_iy_j \\
&= \left(y^\top Dy - y^\top Ay\right) \\
&= y^\top (D-A)y = y^\top Ly
\end{aligned}
$$

The Laplacian Matrix

$$L = D - A$$

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$$L = D - A$$

	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

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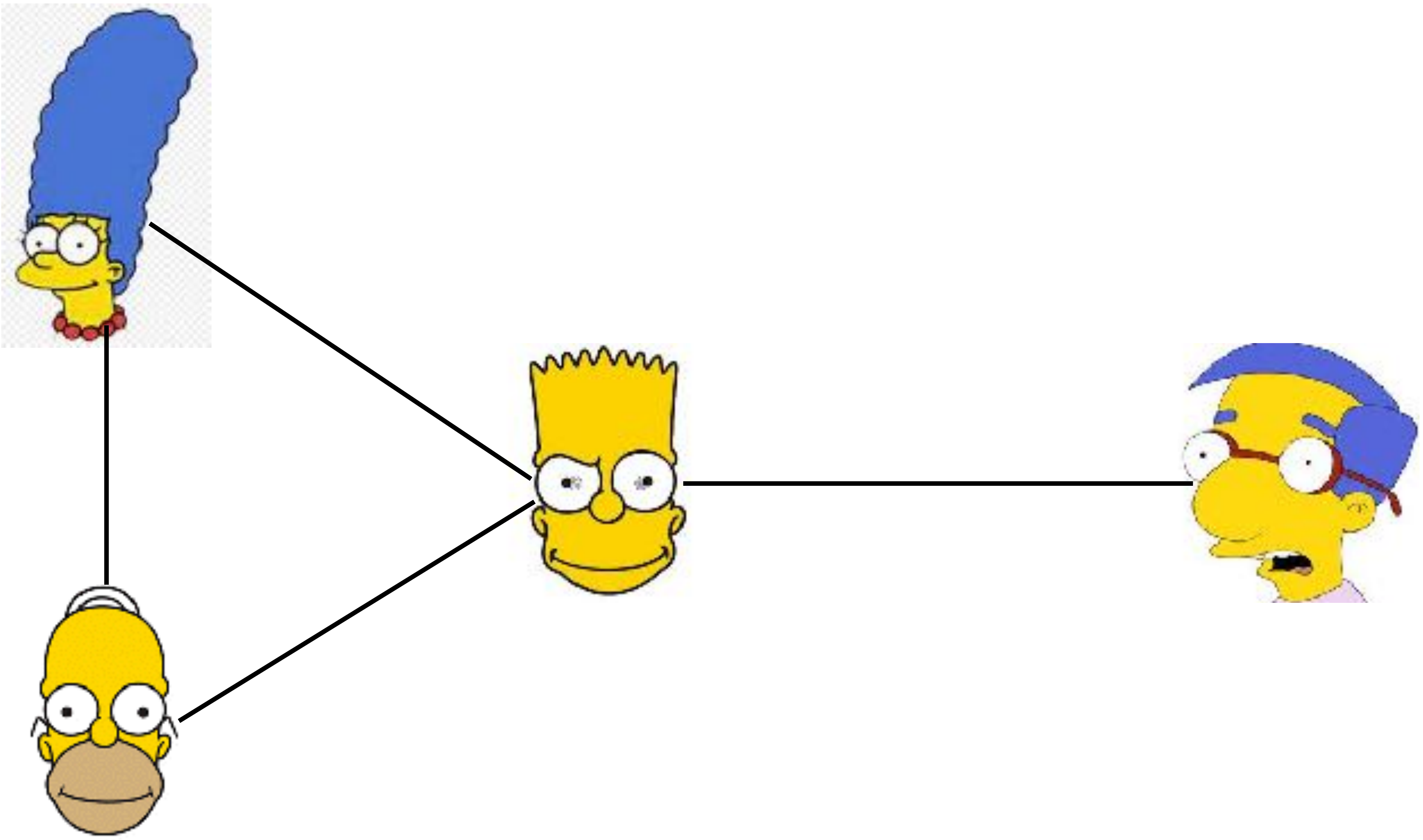
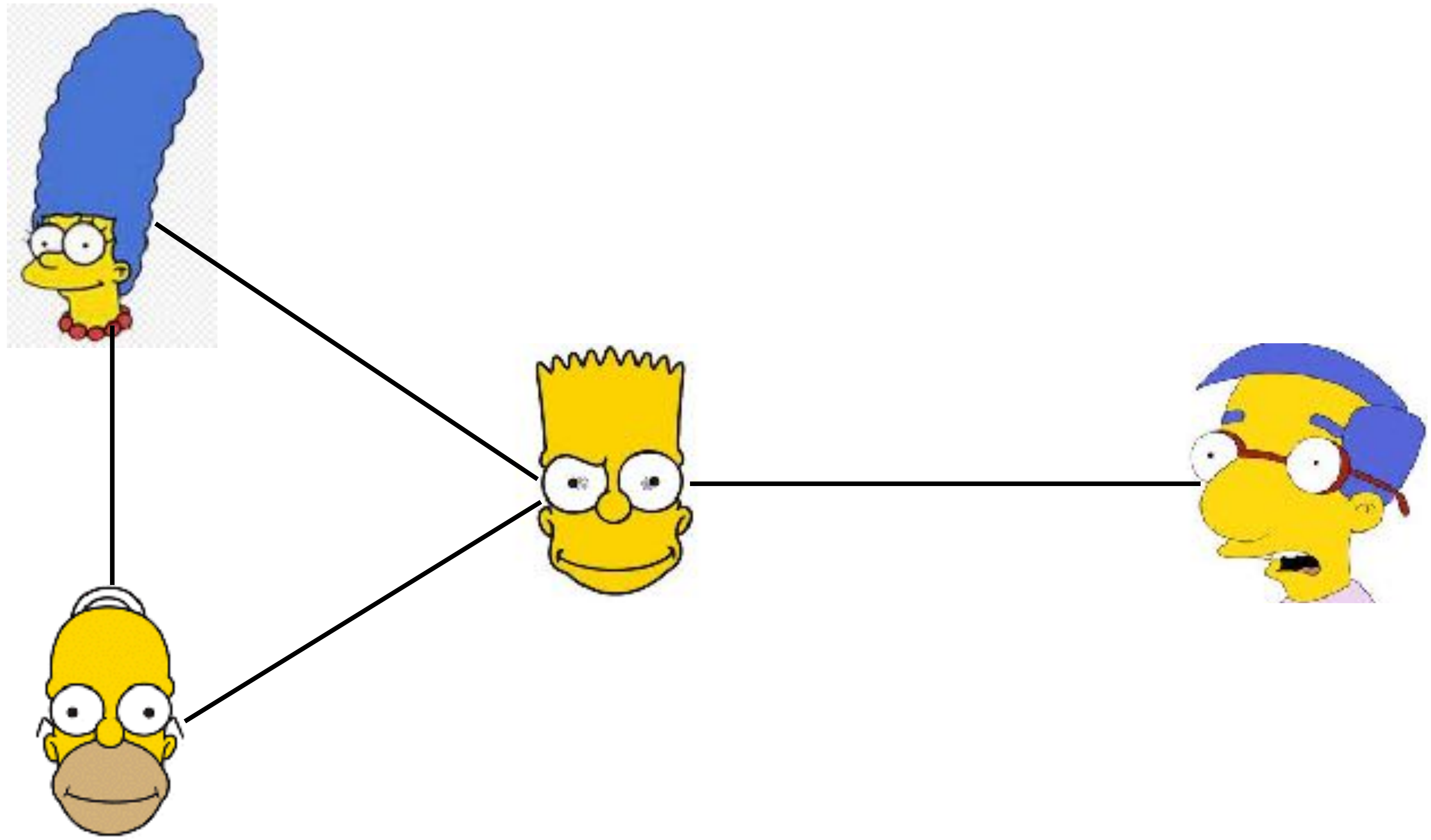


REPRESENTING THE GRAPH



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**
- Variance or spread should be large

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Maximize Variance

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Maximize Variance

$$\text{Var}(y_1, \ldots, y_n) = \frac{1}{n}\sum_{t=1}^{n}(y_t - \text{mean}(y))^2$$

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Maximize Variance

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

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

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

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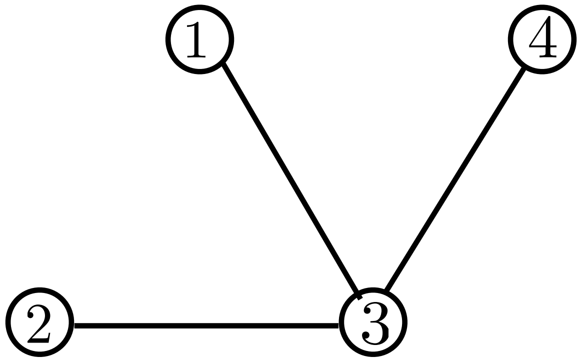
Examples



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

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

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

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- For $K > 1$ dimensional embedding

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- First dimension is the second smallest eigenvector

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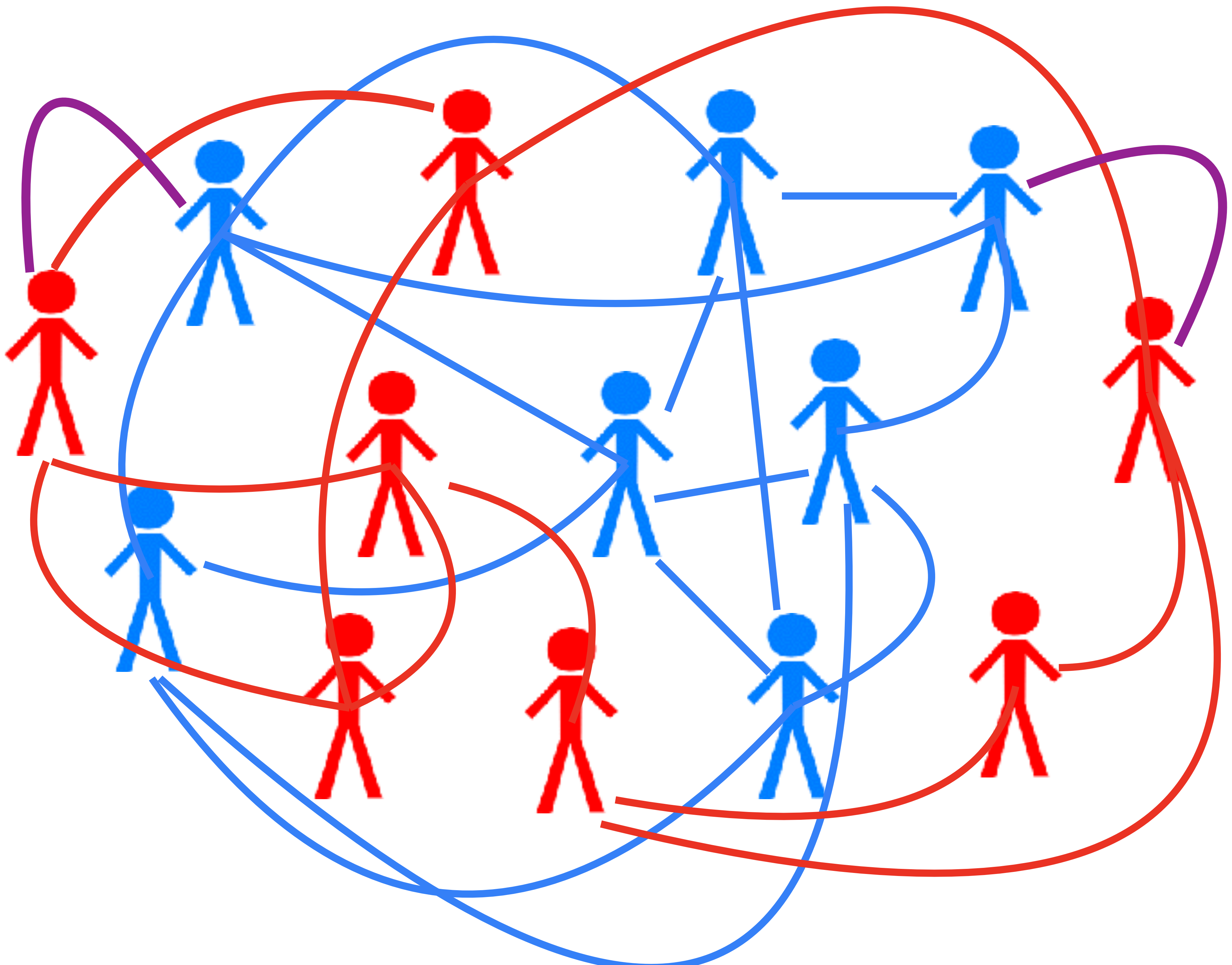
Spectral Embedding

- 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



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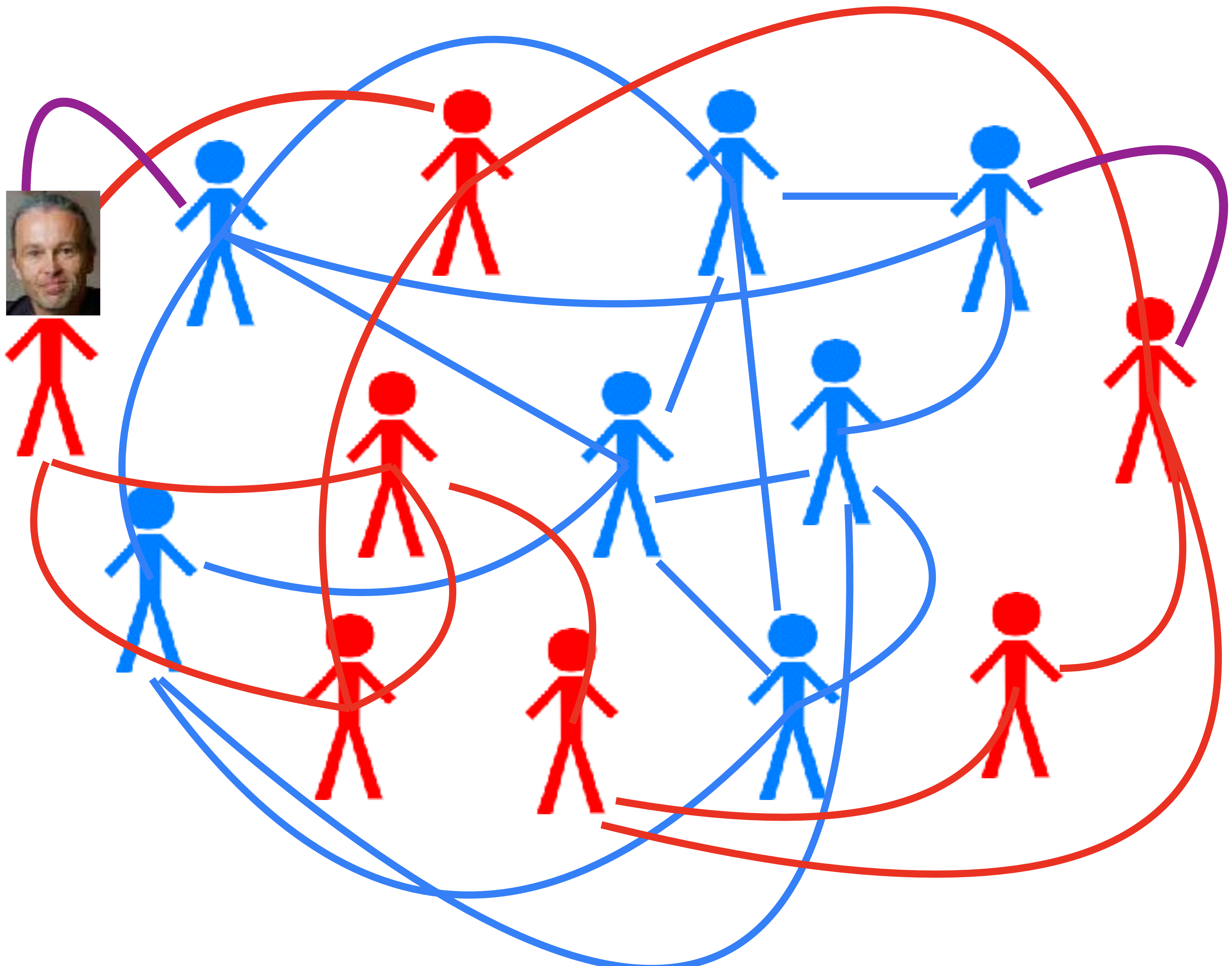

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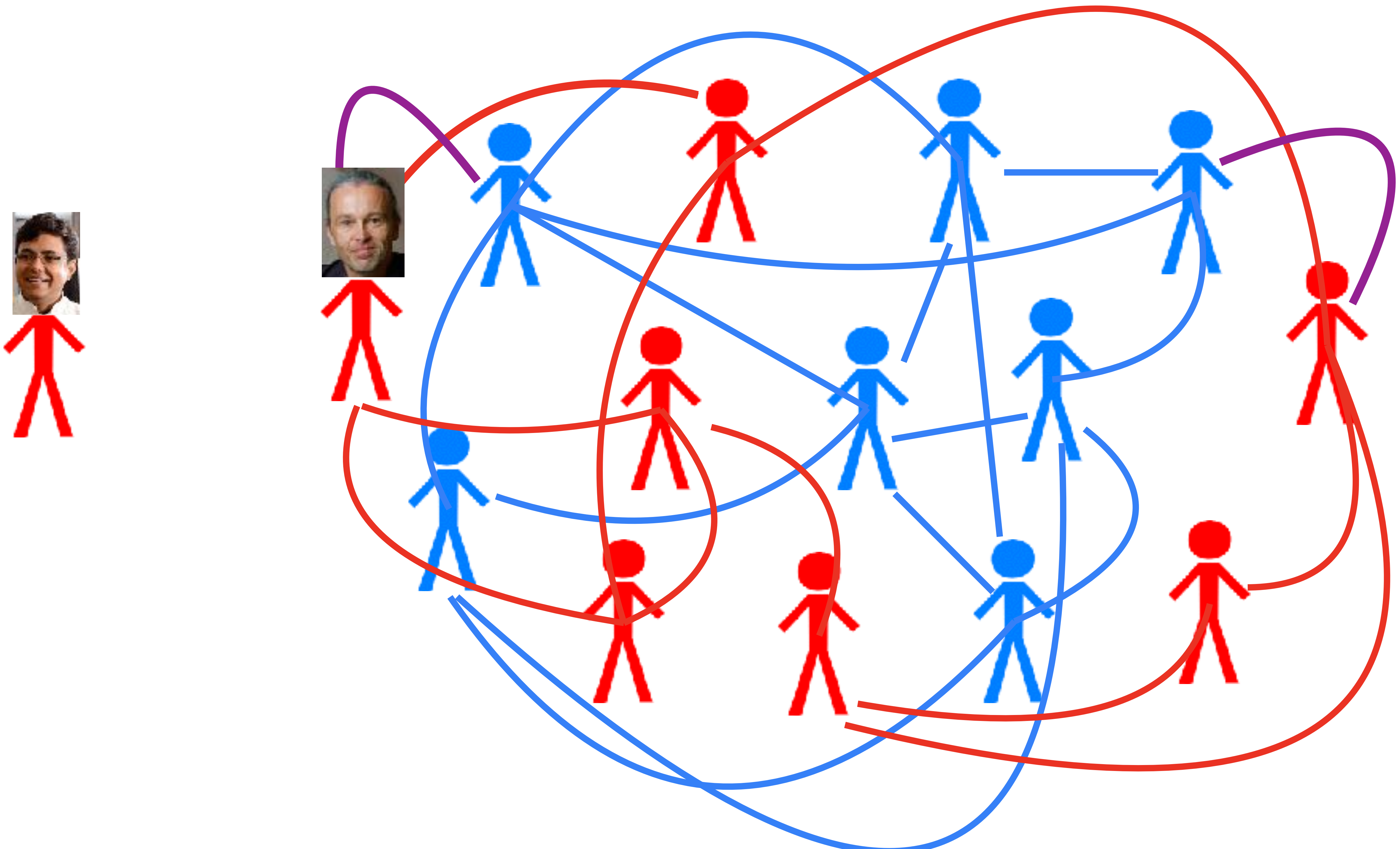

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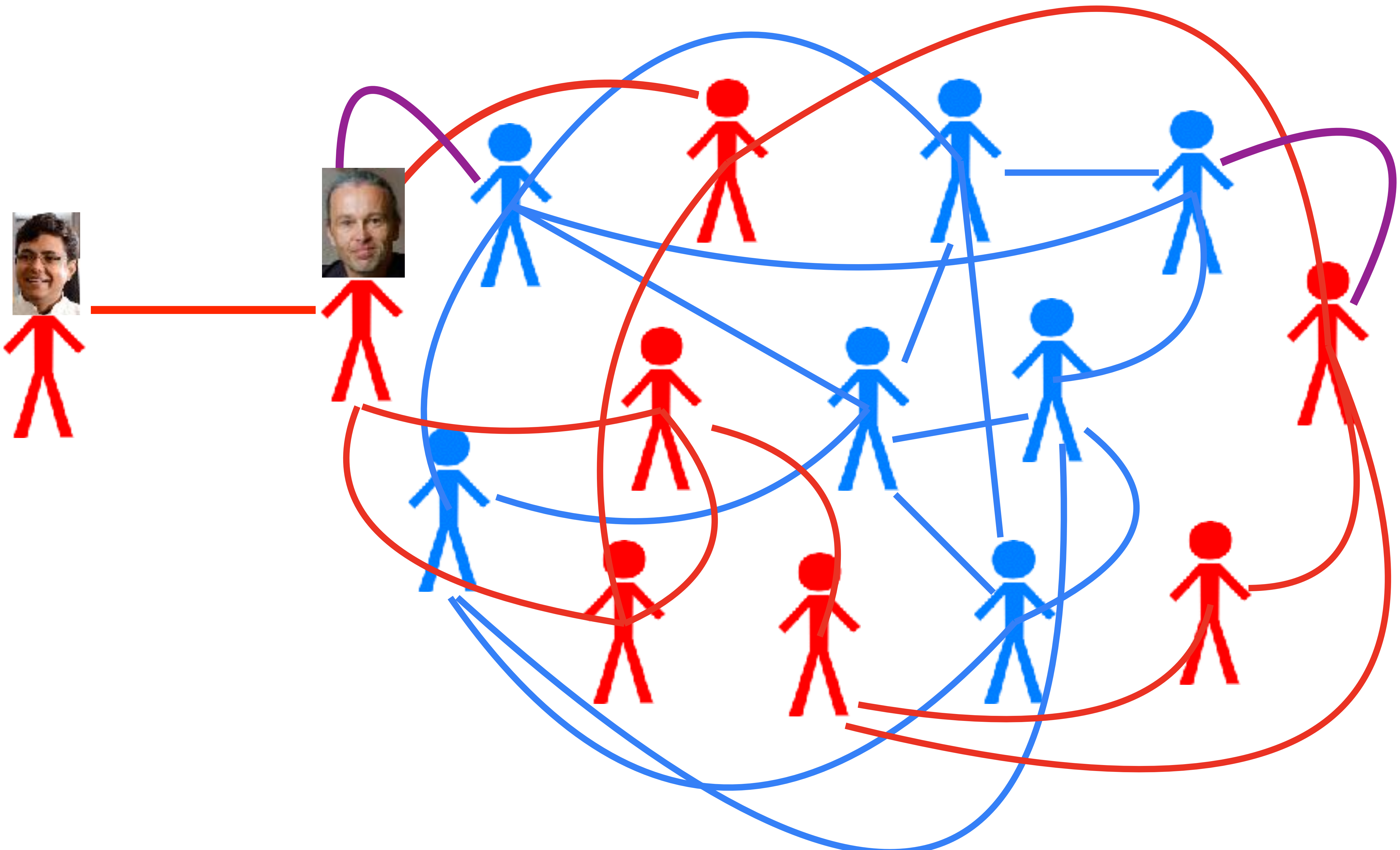

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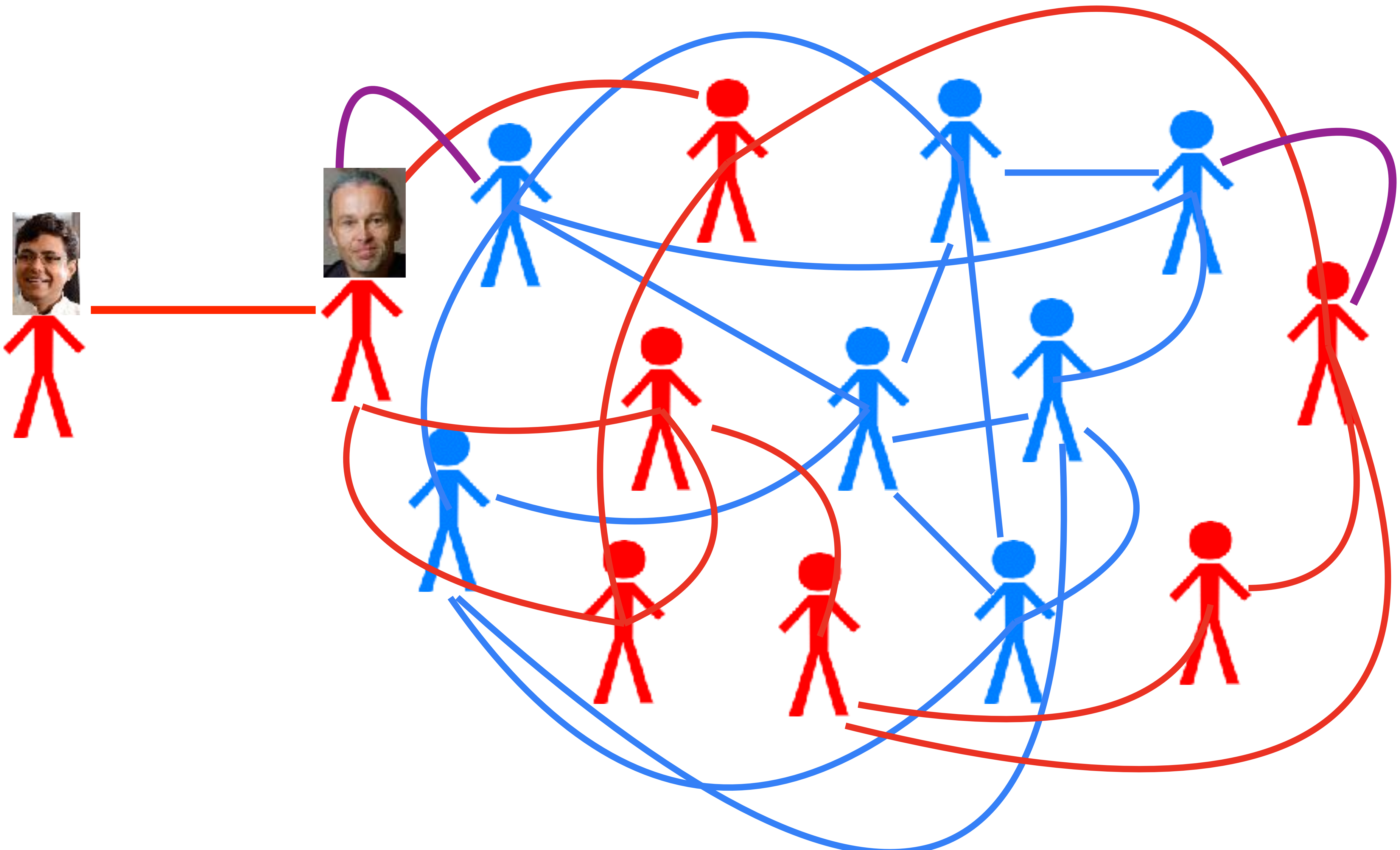

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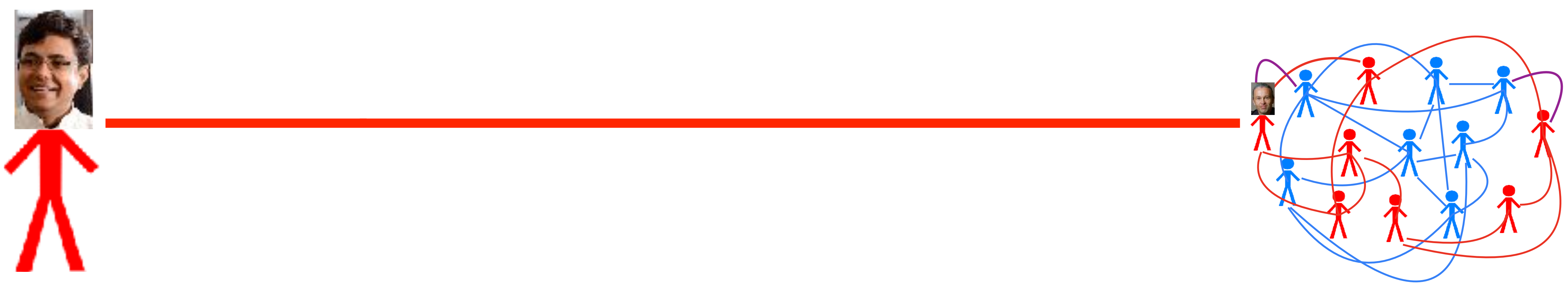

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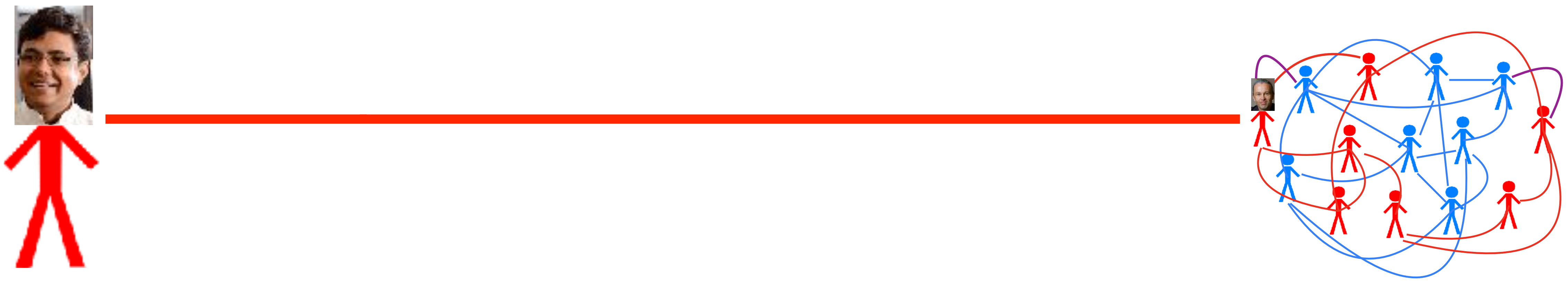
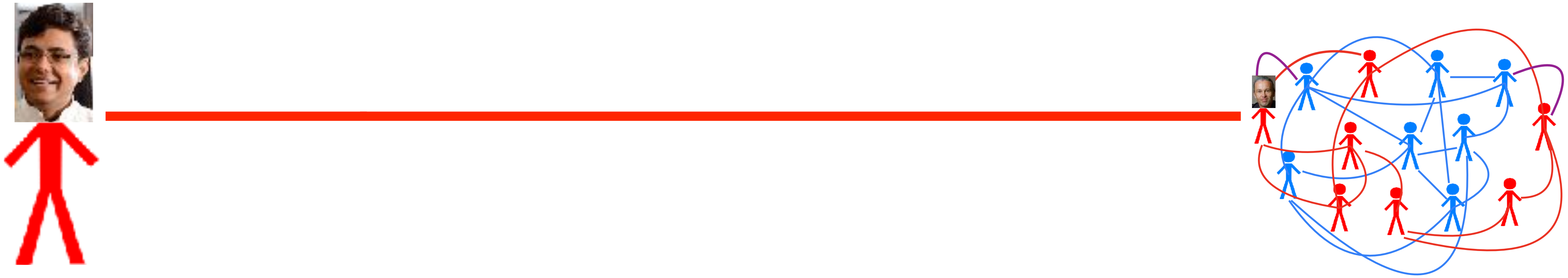


- Variance is high

Trouble Makers



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

Demo

What was the problem?

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- Pushing few nodes far away from the rest increased variance

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- But these nodes were ones with one or few links

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- 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

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  - Higher degree nodes are more important!

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

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

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

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

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- Variance or spread should be large $\text{Maximize} \quad y^\top D y$

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

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

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 $u_2, \ldots, u_{K+1}$
- $Y = P^{-1/2} U$

Demo