Machine Learning for Data Science (CS4786)
Lecture 10

t-SNE and Spectral Embedding

Stochastic Neighborhood Embedding

- Use a probabilistic notion of which points are neighbors.

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- Goal: Find $\mathbf{y}_1, \ldots, \mathbf{y}_n$ with stochastic neighborhood distribution Q such that "P and Q are similar"

  i.e. minimize:

$$\mathrm{KL}(P \| Q) = \sum_{s,t} P_{s,t} \log\left(\frac{P_{s,t}}{Q_{s,t}}\right) = \sum_{s,t} P_{s,t} \log\left(P_{s,t}\right) - \sum_{s,t} P_{s,t} \log\left(Q_{s,t}\right)$$

Choice for Q

- Just like we defined P, we can define Q for a given $\mathbf{y}_1, \ldots, \mathbf{y}_n$ by

$$q_{t \to s} = \frac{\exp(-\frac{\|\mathbf{y}_s - \mathbf{y}_t\|^2}{2\sigma^2})}{\sum_{u \neq t} \exp(-\frac{\|\mathbf{y}_u - \mathbf{y}_t\|^2}{2\sigma^2})}$$

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  - For d dimensional gaussians, most points are found at distance $\sqrt{d}$ from mean!
  - If we use gaussians in both high and low dimensional space, all the points are squished in to a small space
  - Too many points crowd the center!

Demo

Method II: t-SNE

- Instead for Q we use, student t distribution which is heavy tailed:

$$q_{t \to s} = \frac{\left(1 + \|\mathbf{y}_s - \mathbf{y}_t\|^2\right)^{-1}}{\sum_{u \neq t} \left(1 + \|\mathbf{y}_u - \mathbf{y}_t\|^2\right)^{-1}}$$

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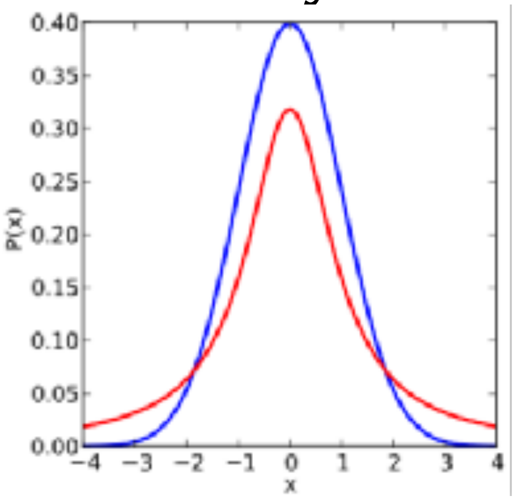

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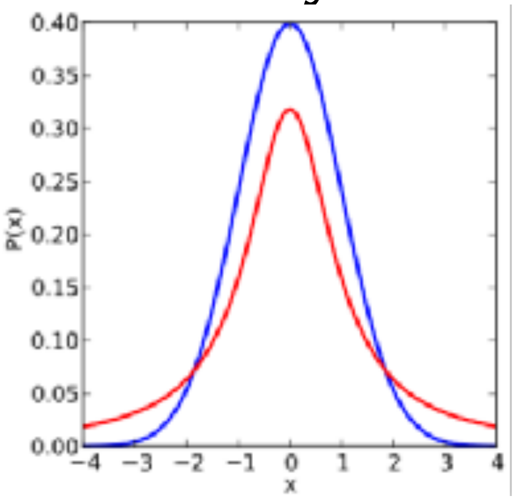

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- It can be verified that

$$\nabla_{\mathbf{y}_t} \mathrm{KL}(P\|Q) = 4 \sum_{s=1}^{n} (P_{s,t} - Q_{s,t})(\mathbf{y}_t - \mathbf{y}_s)\left(1 + \|\mathbf{y}_s - \mathbf{y}_t\|^2\right)^{-1}$$

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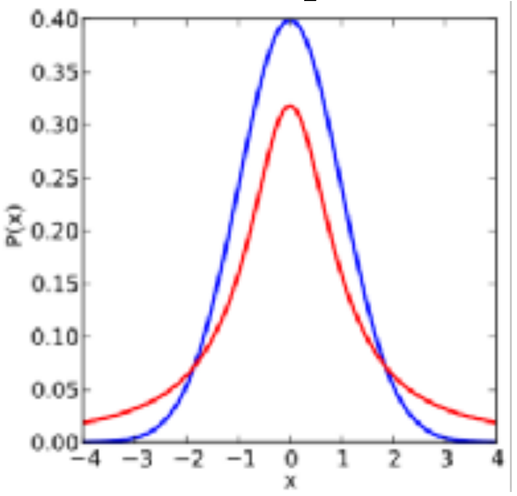

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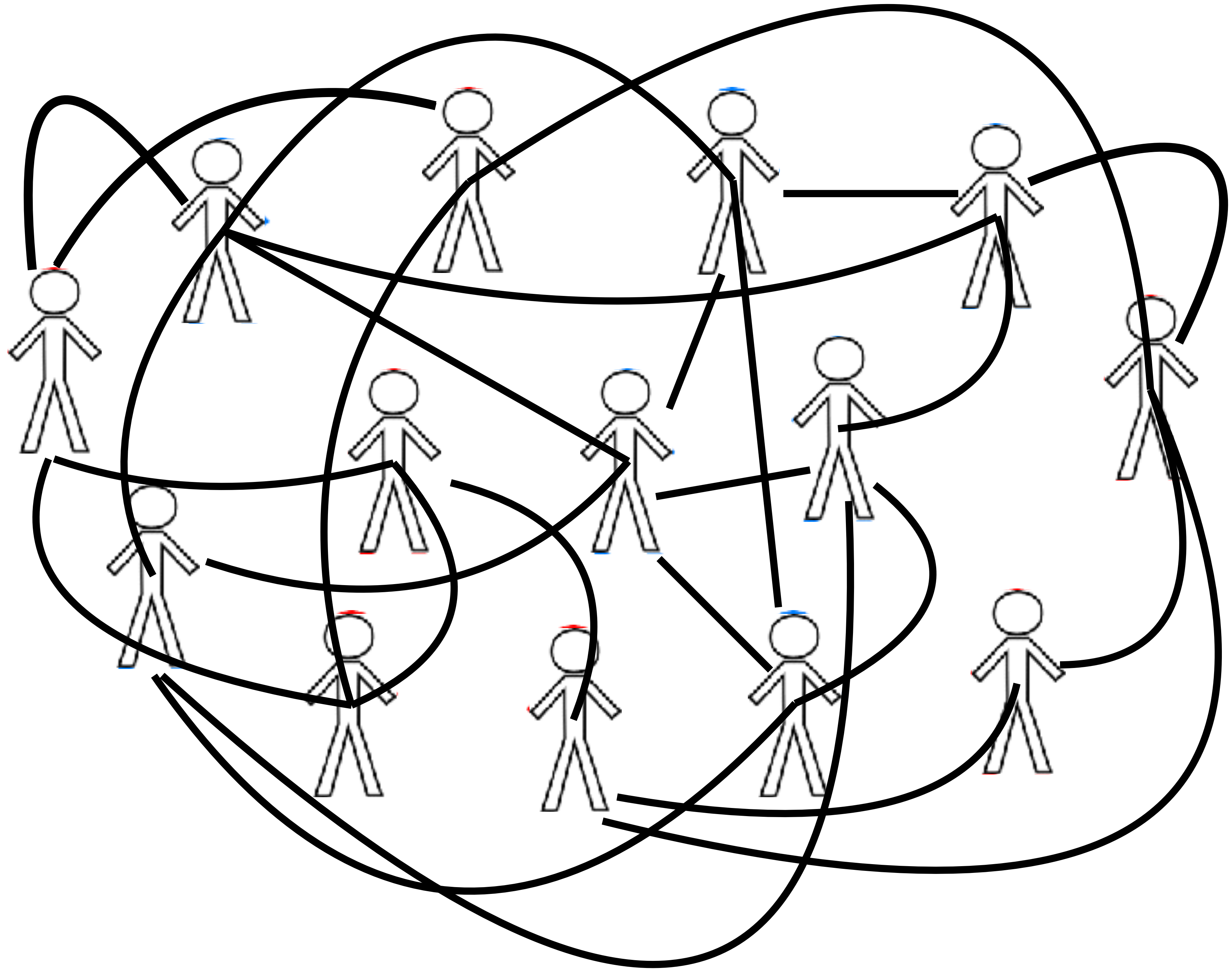
- Algorithm: Find $\mathbf{y}_1, \ldots, \mathbf{y}_n$ by performing gradient descent

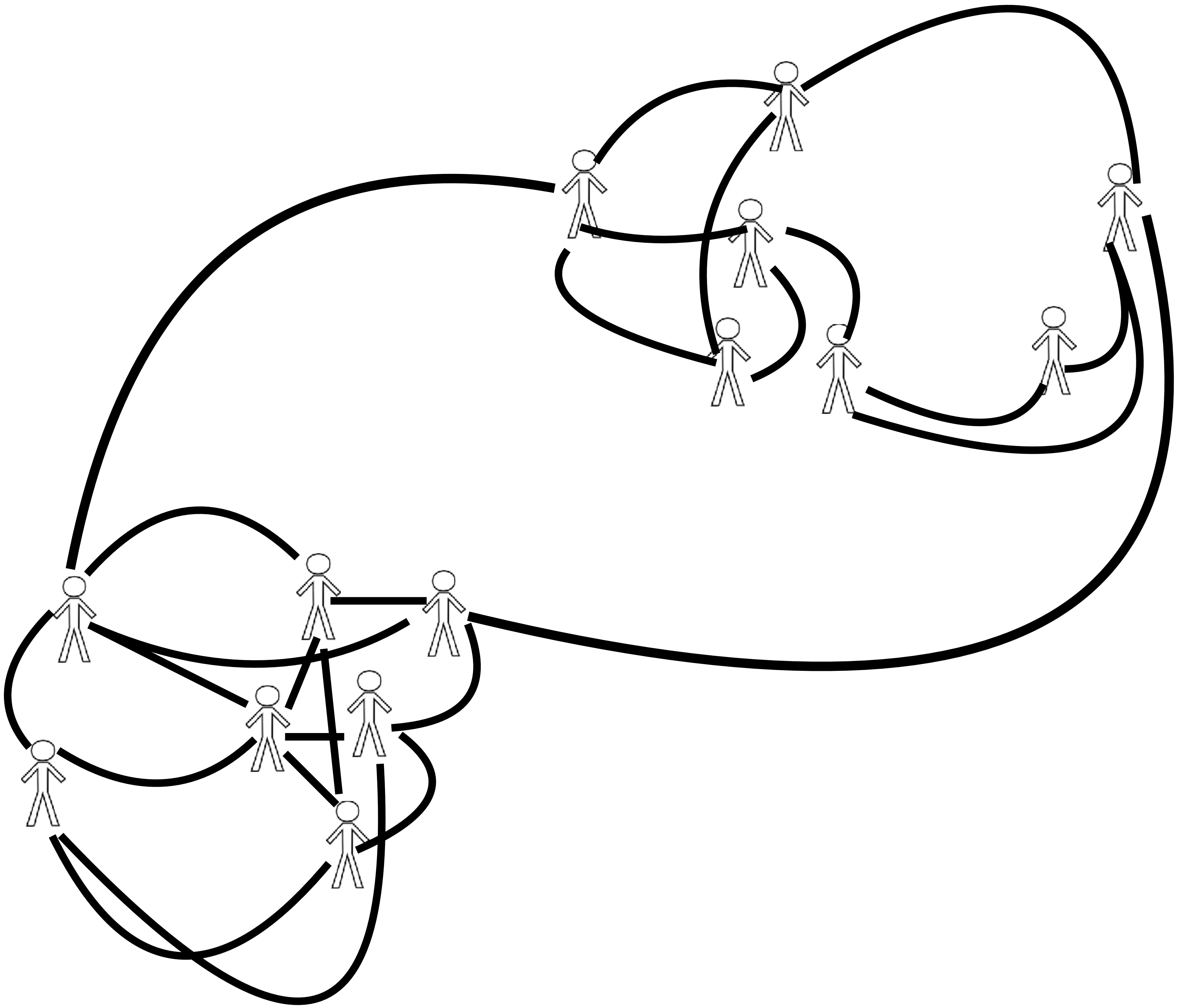
Demo

Motivating Example



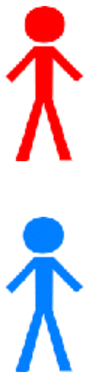
What can you say from this network?

Motivating Example



How about now?

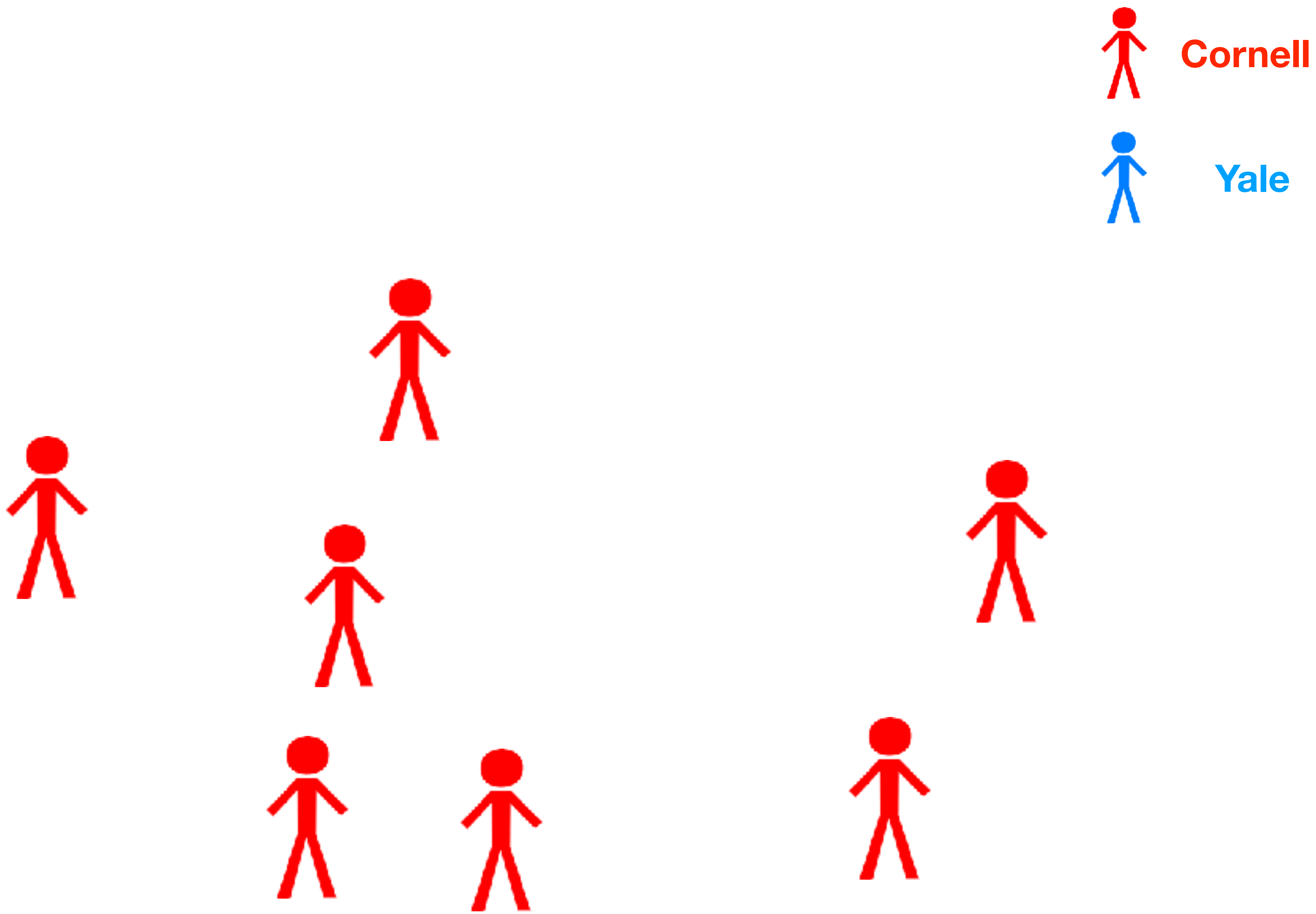
Motivating Example



Cornell

Yale

Motivating Example



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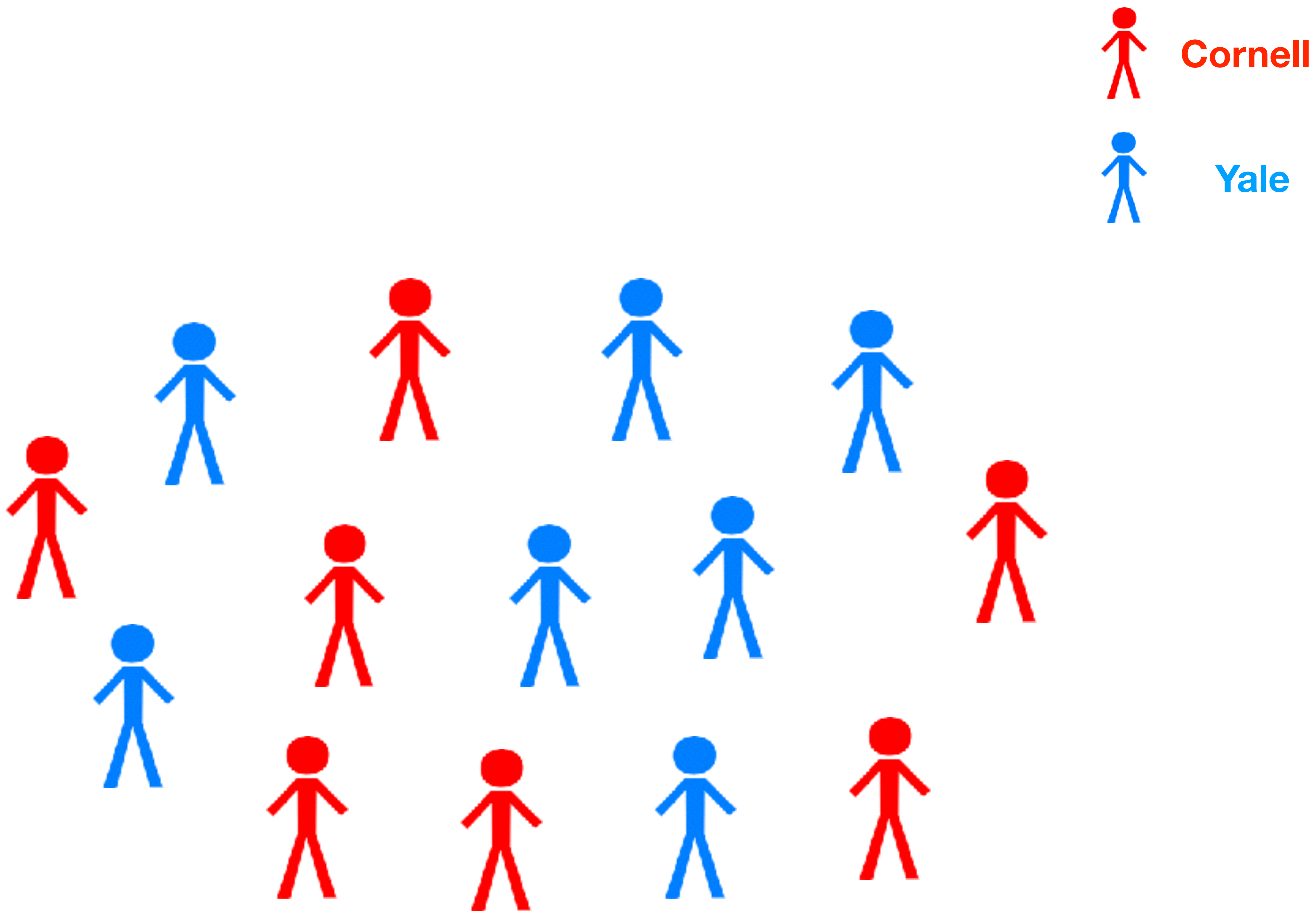

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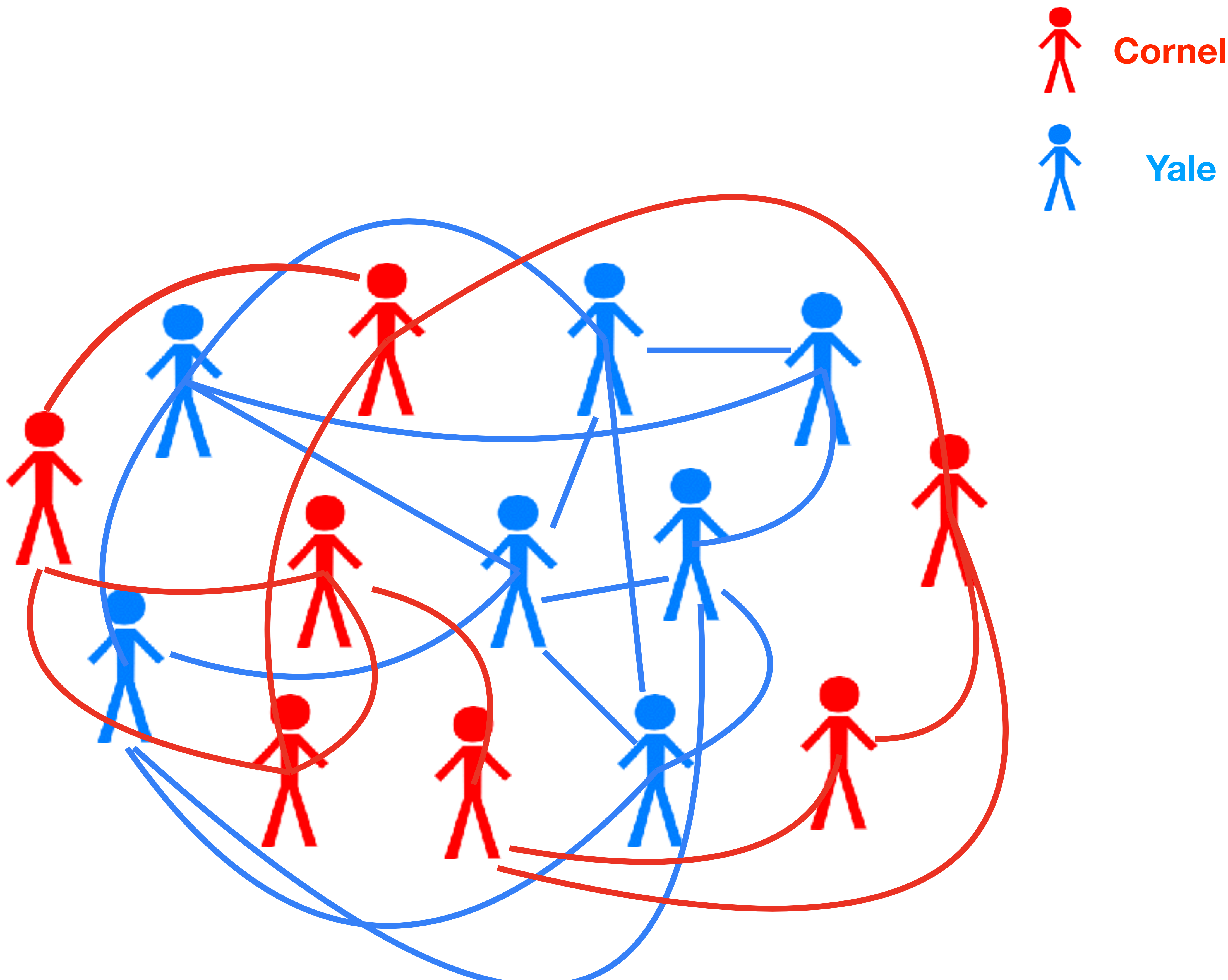

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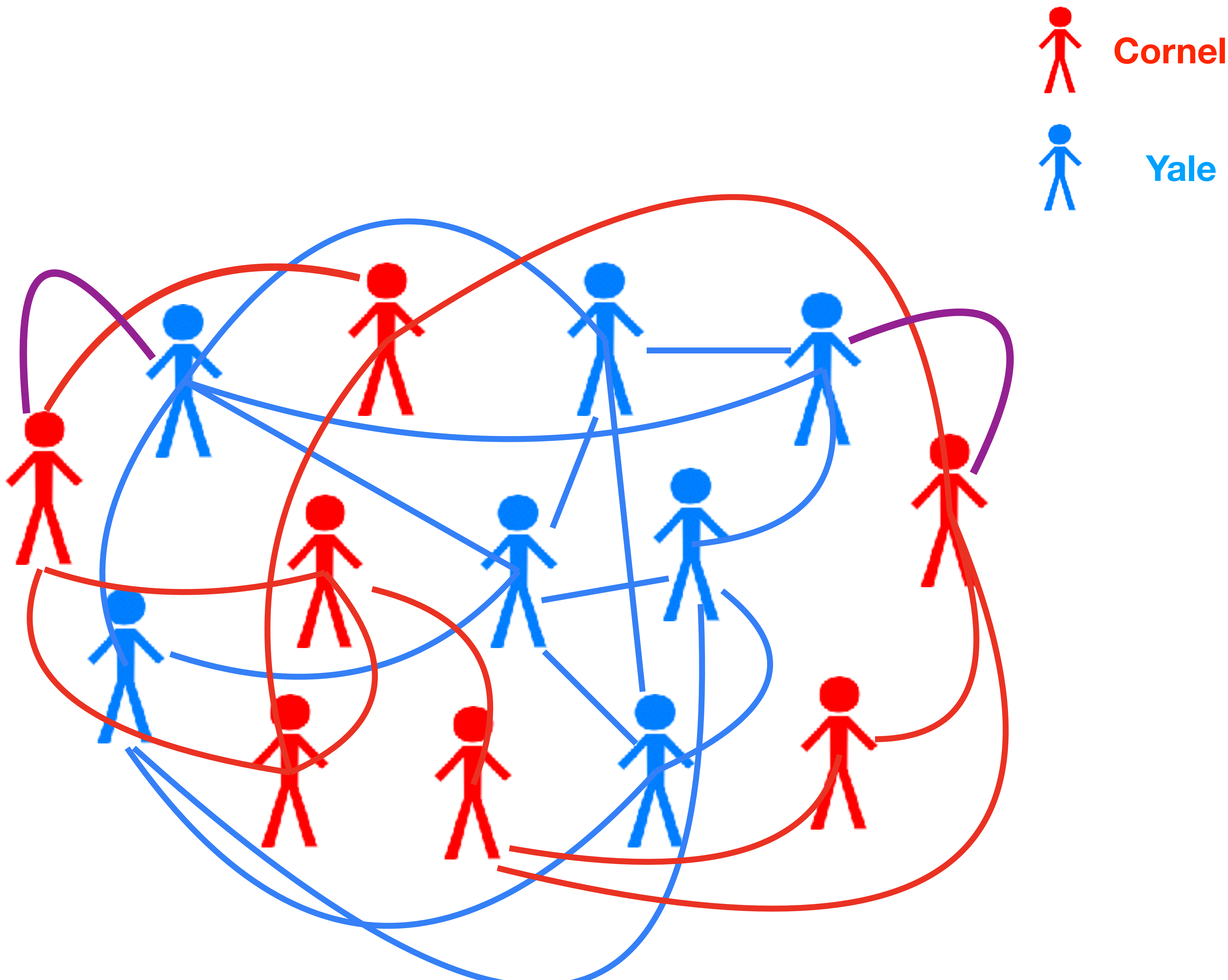

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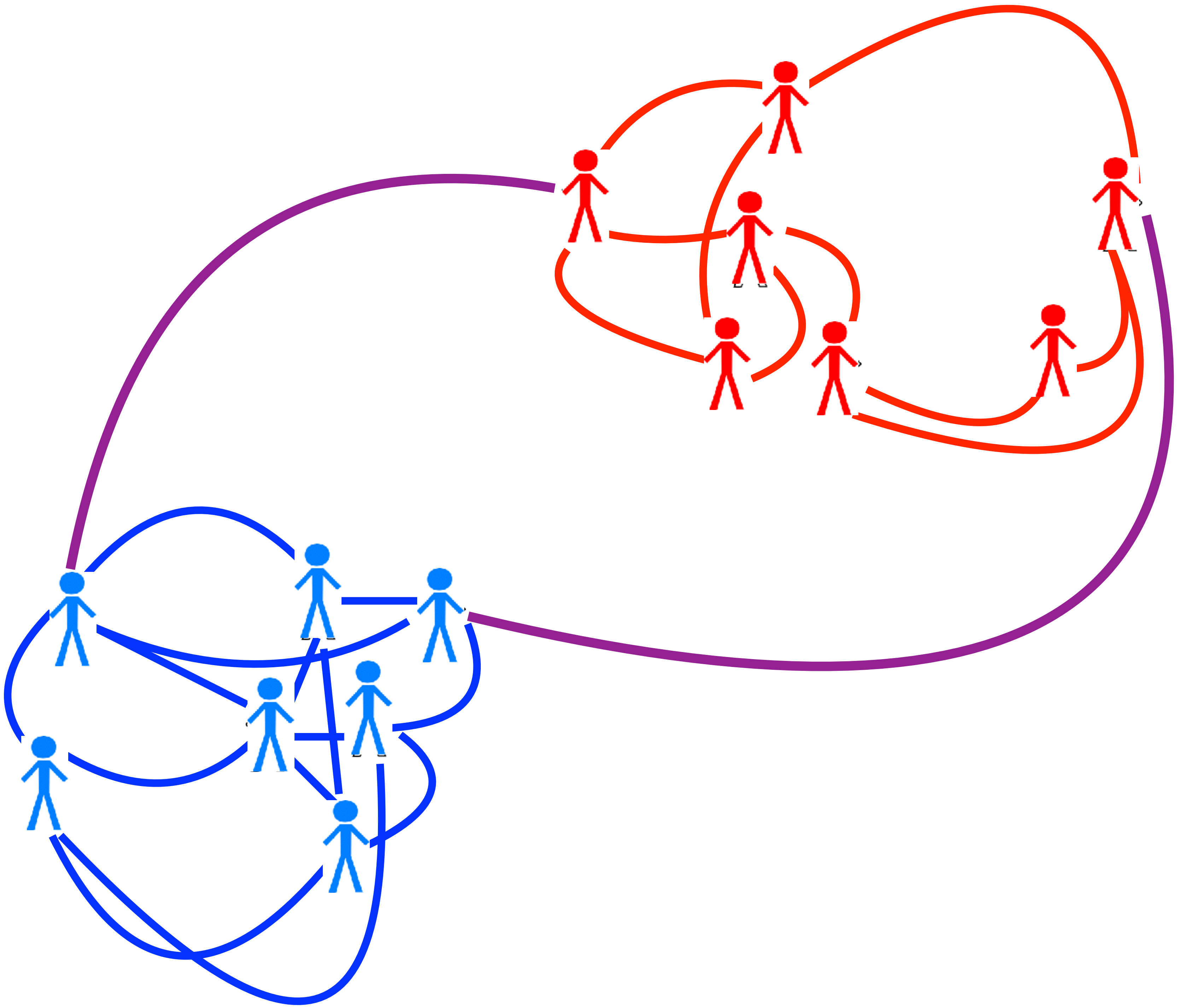

Graph Embedding

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

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- 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?

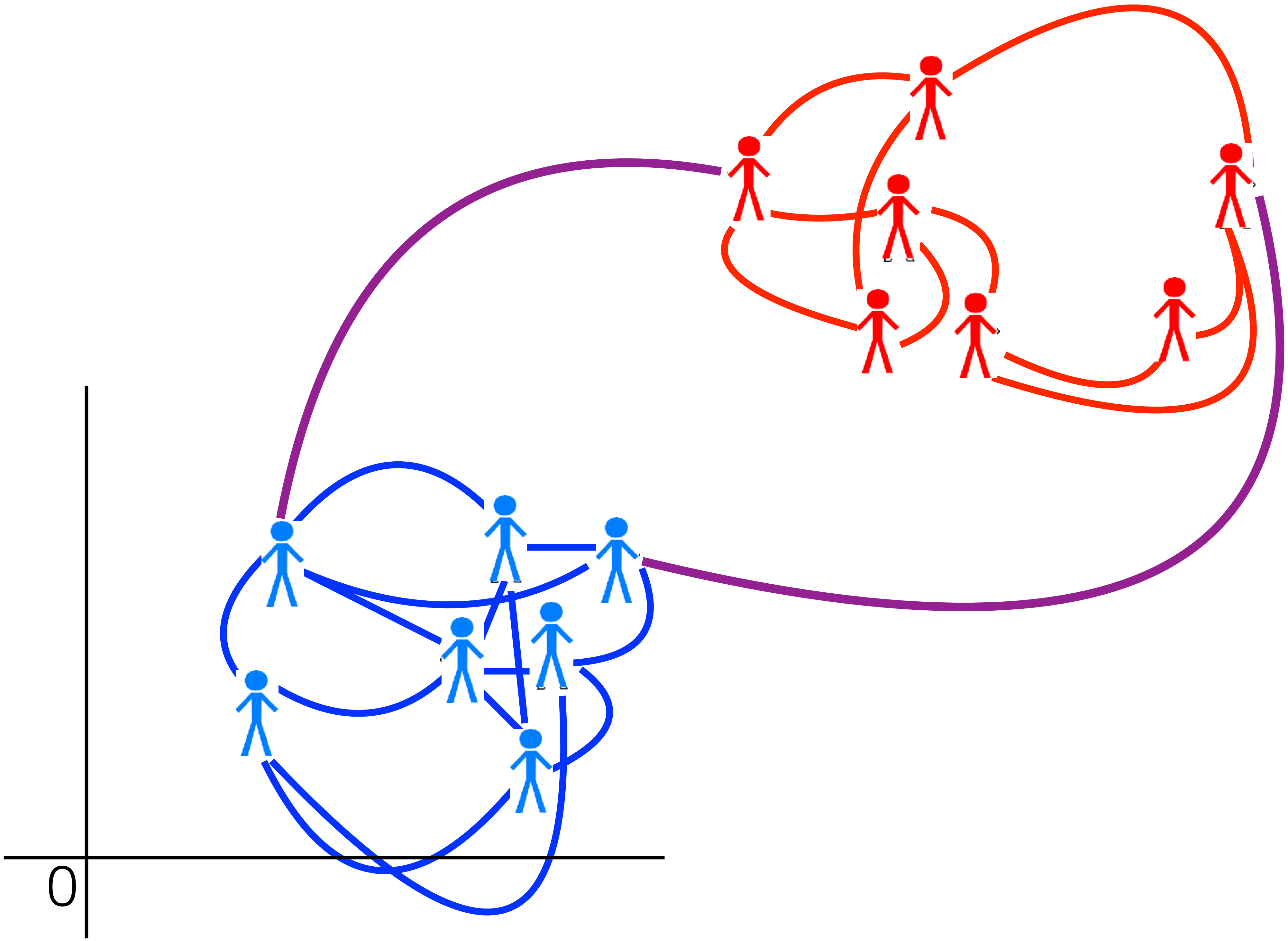
How do we do this?

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

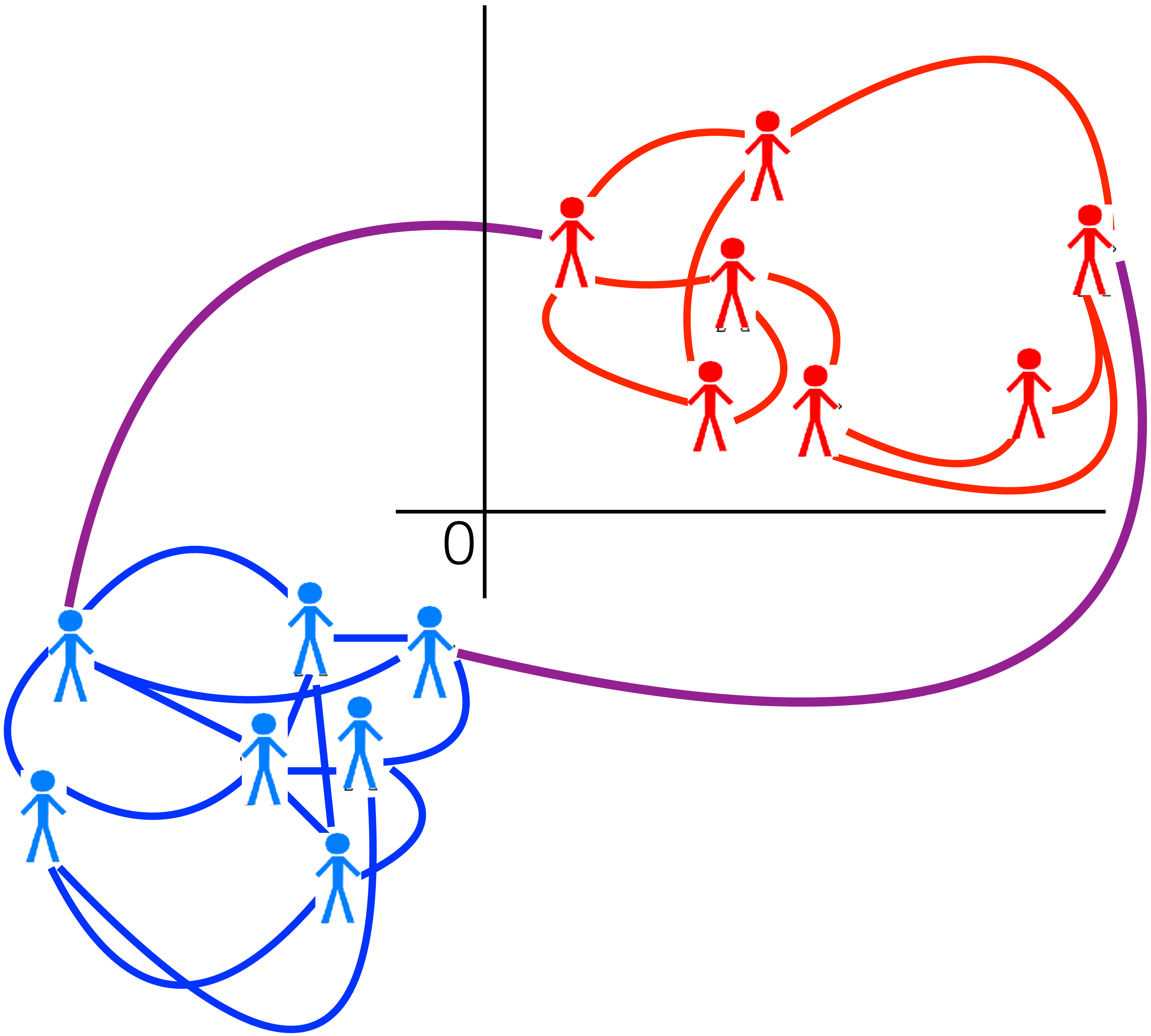
Thought Experiment

- 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



Centering locations



Key Principle

- **Points are centered at 0**

Key Principle

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)

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

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Make $\text{Var}(y_1, \ldots, y_n)$ 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

- Points are centered at 0 $y^\top \mathbf{1} = 0$
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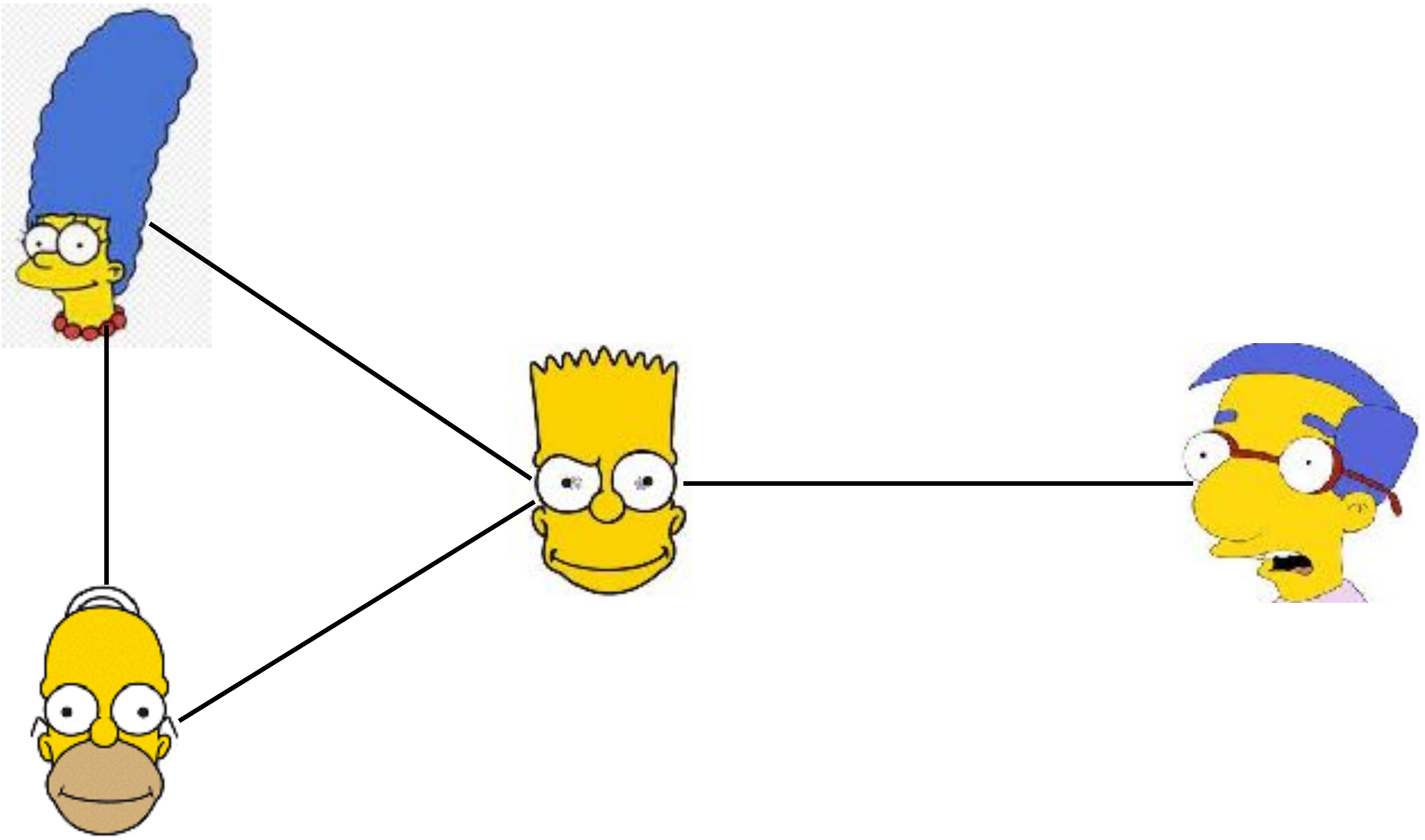
Representing the Graph



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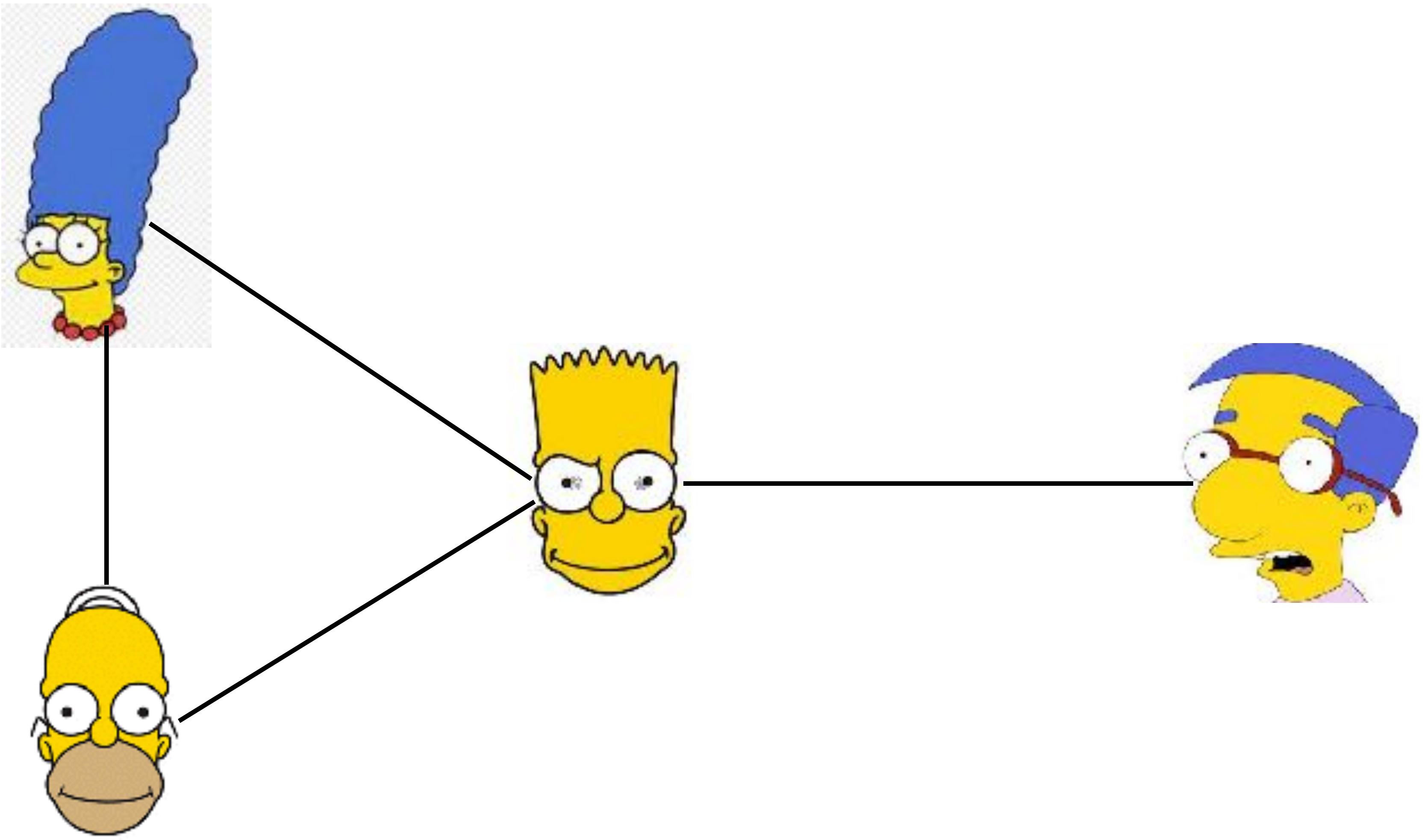

A =

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

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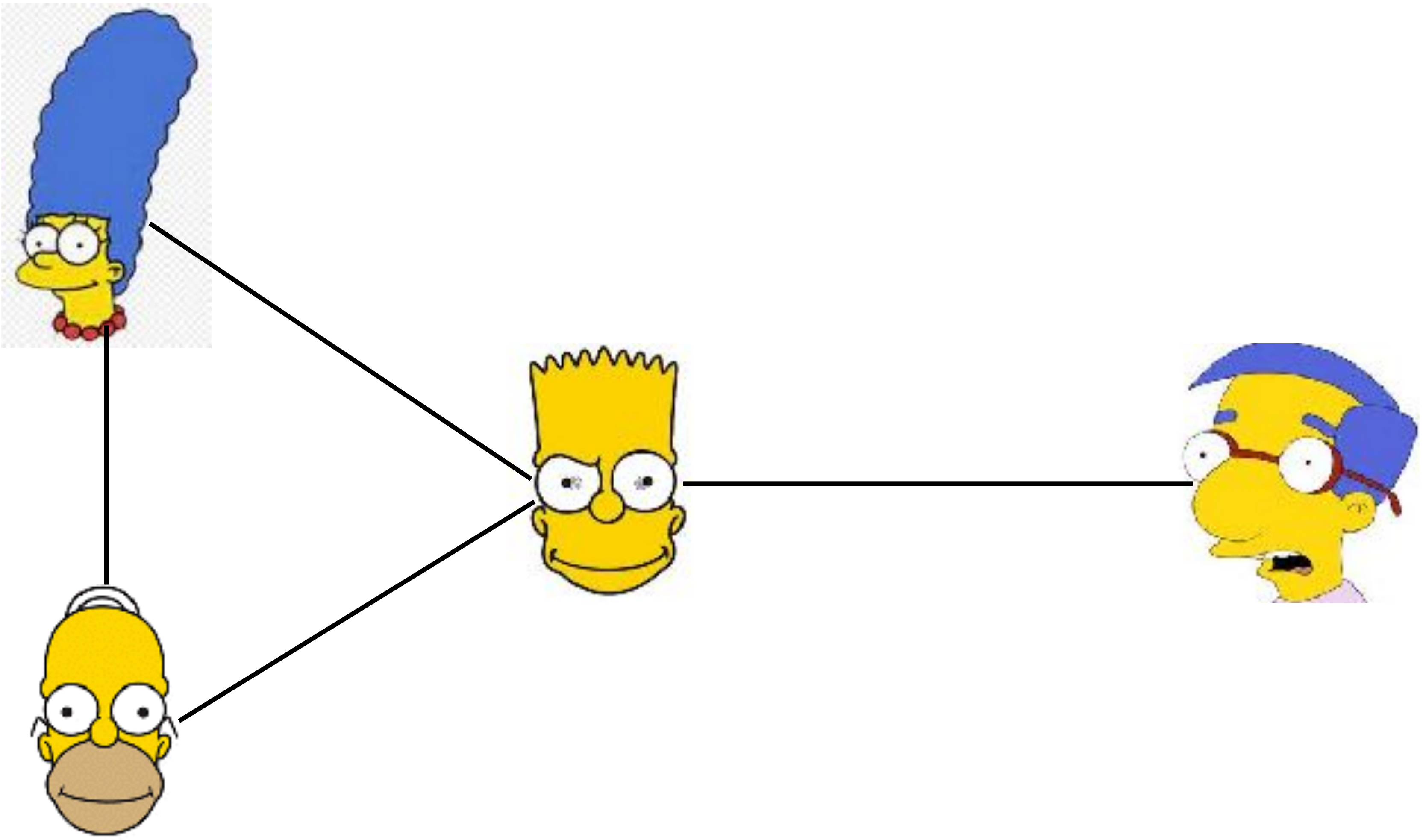

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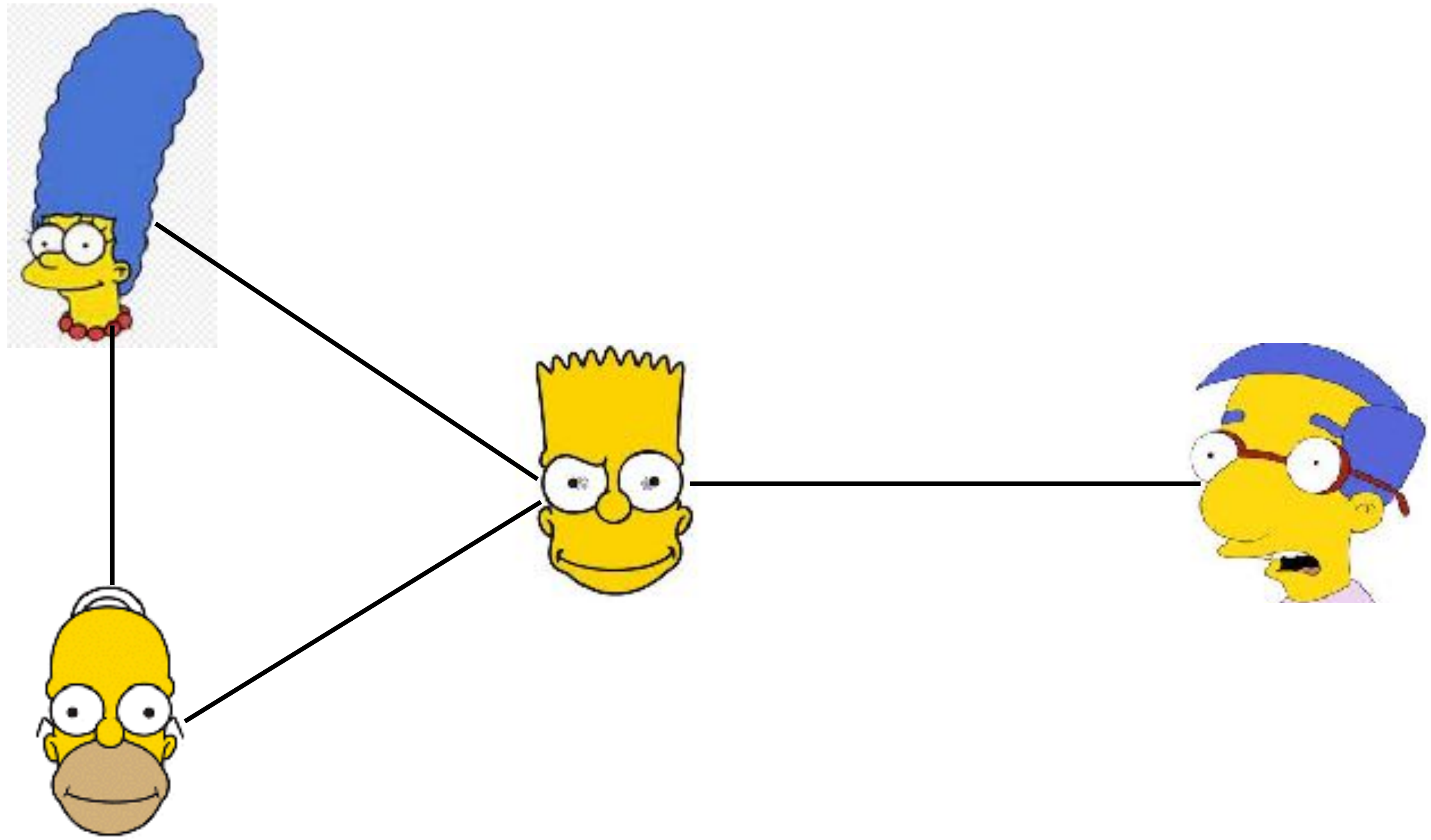

D =

	2	0	0	0
	0	2	0	0
	0	0	3	0
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Why the Laplacian?

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

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$$= \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{i,j} (y_i - y_j)^2$$

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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)
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&= \left(y^\top D y - y^\top A y \right) \\
&= y^\top (D - A) y = y^\top L y
\end{aligned}
$$

The Laplacian Matrix

$$L = D - A$$

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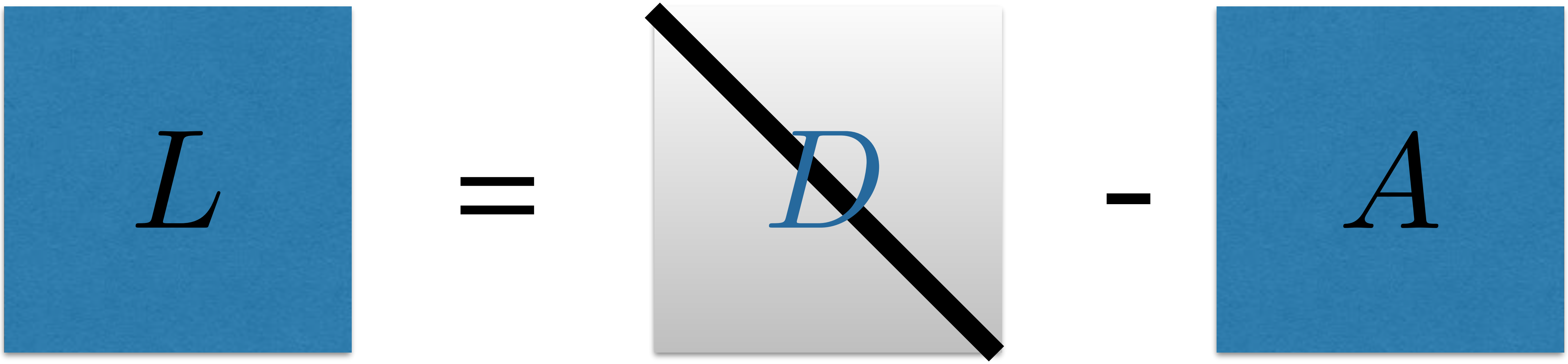

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–

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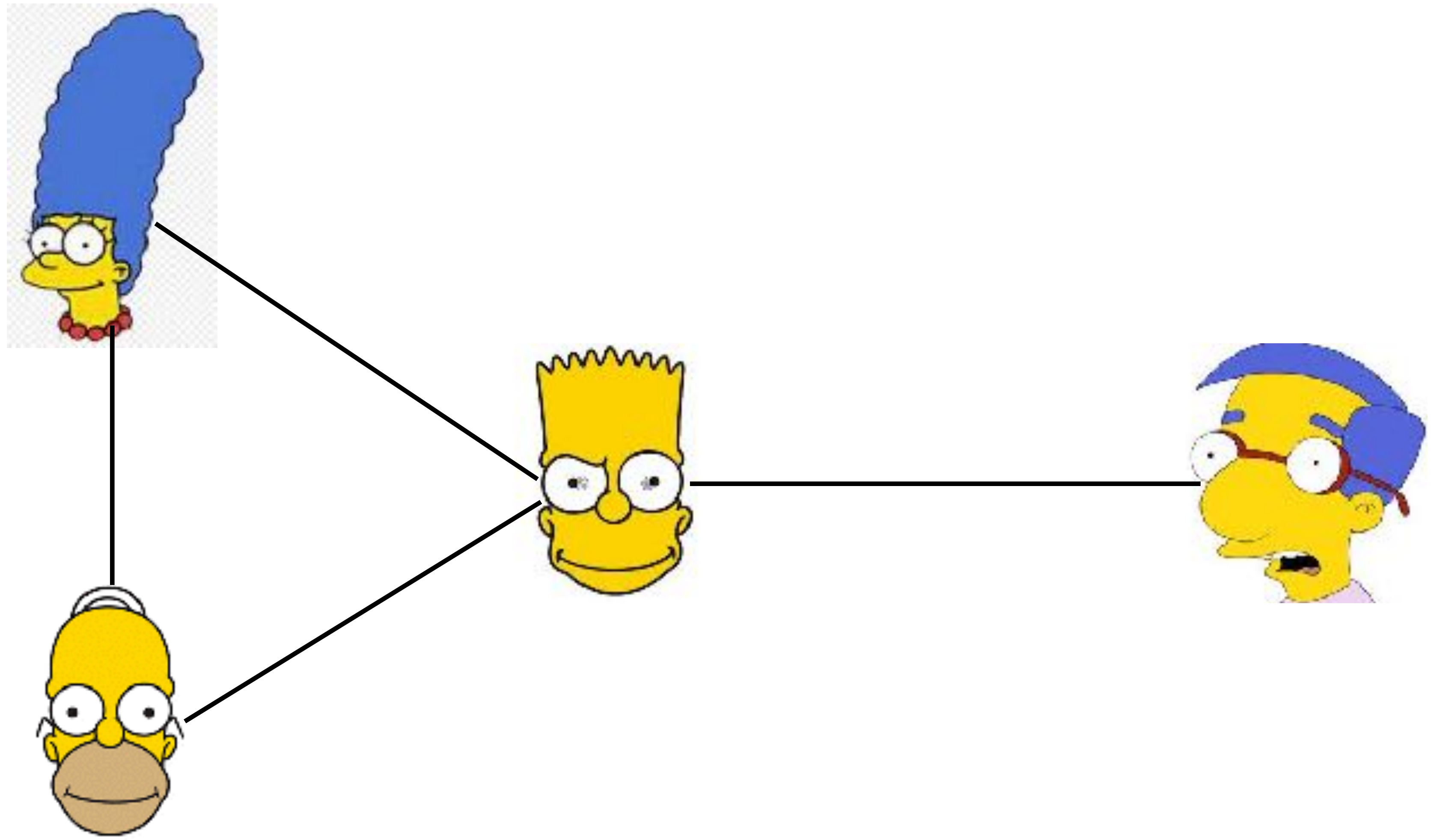

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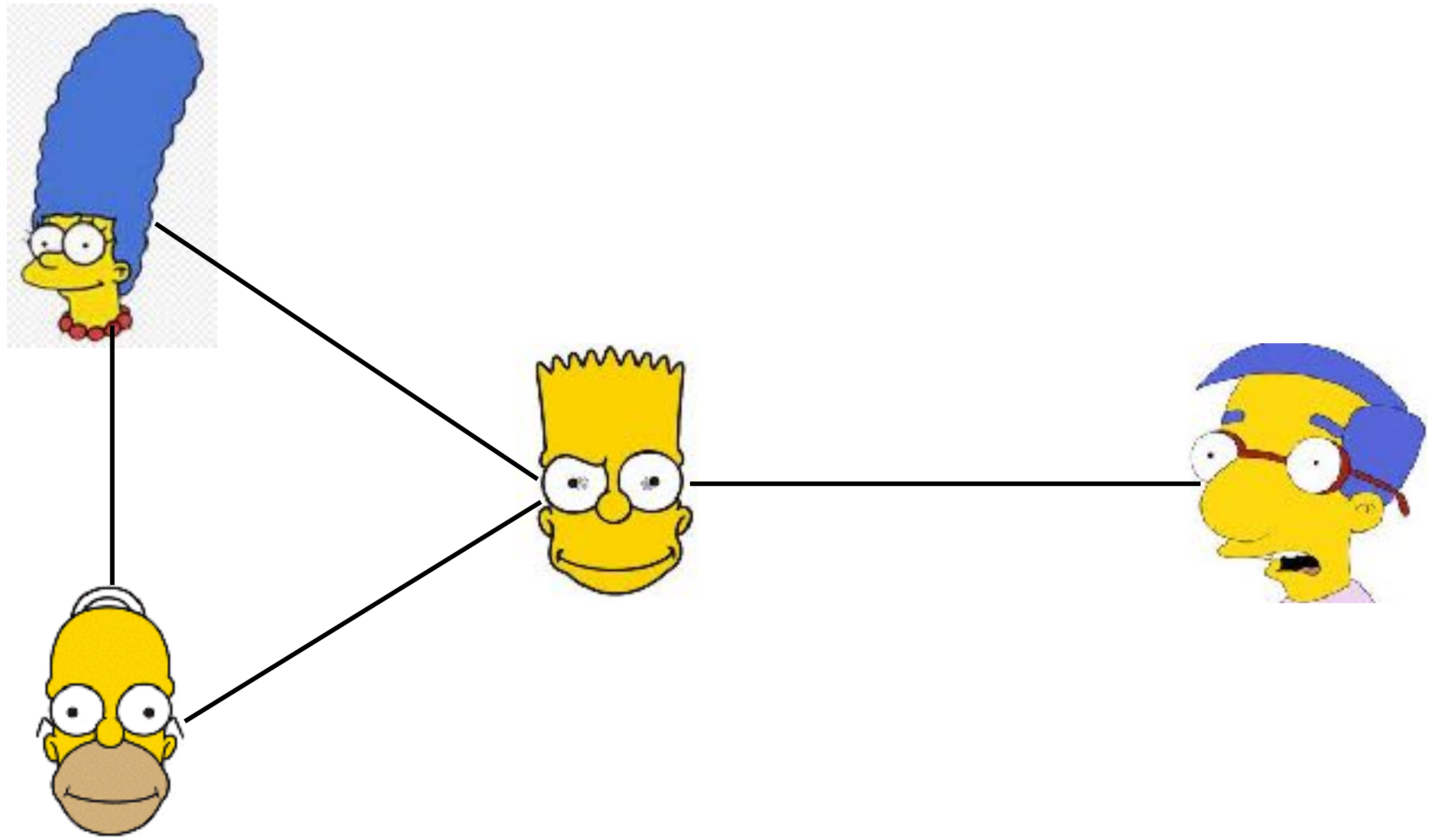

L =

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

Key Principle

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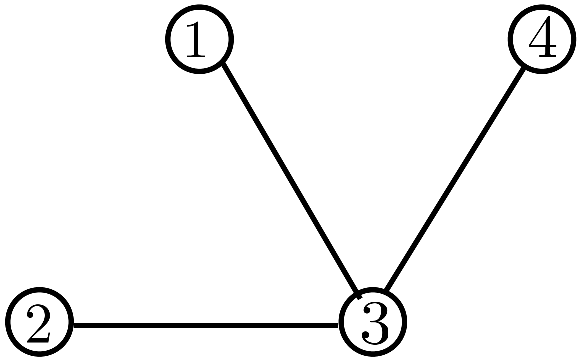
Examples



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

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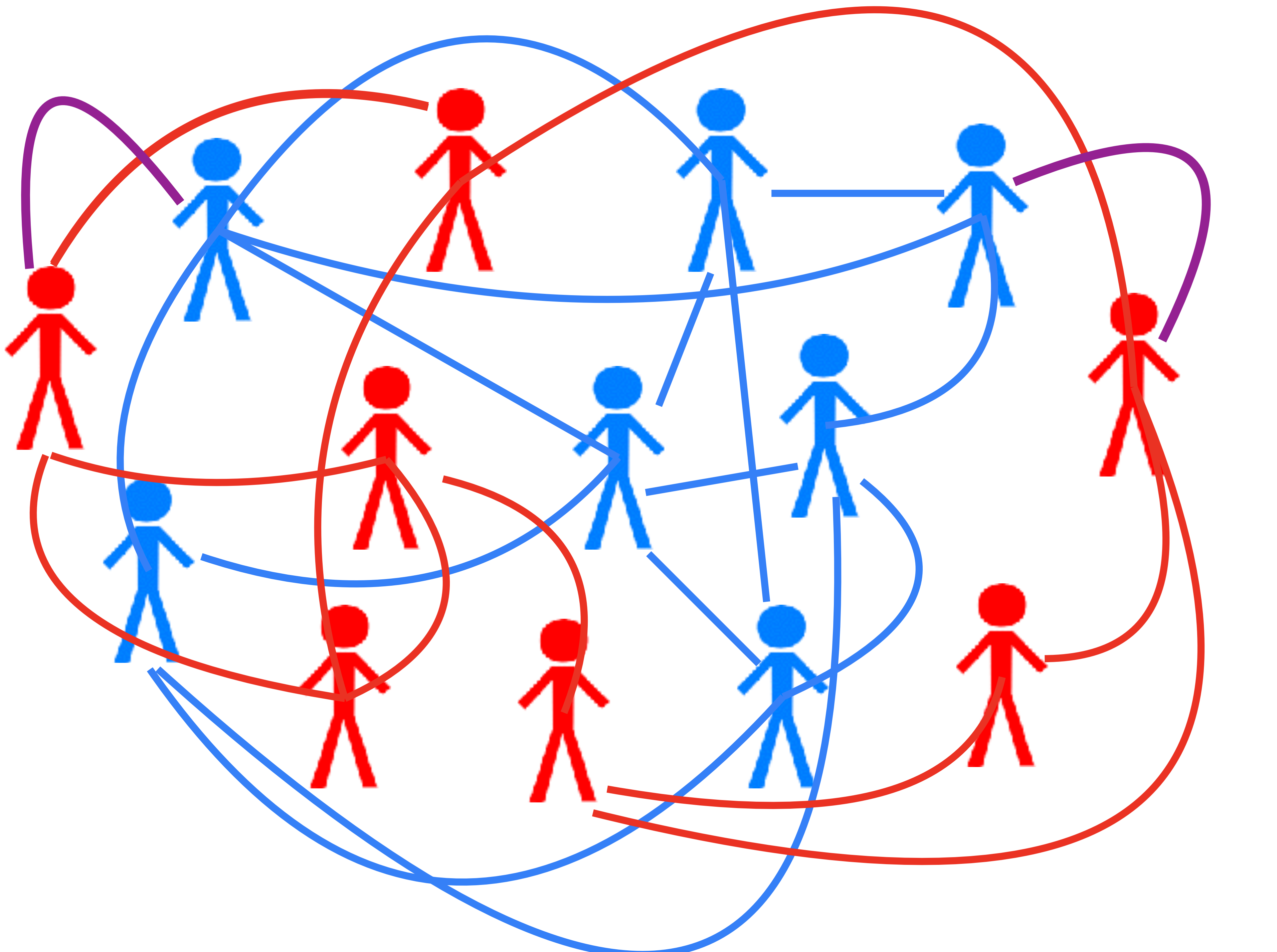
- (Unnormalized) Spectral clustering: compute $2 : K + 1$ smallest eigen vectors
- Set Y_i to be the i'th row

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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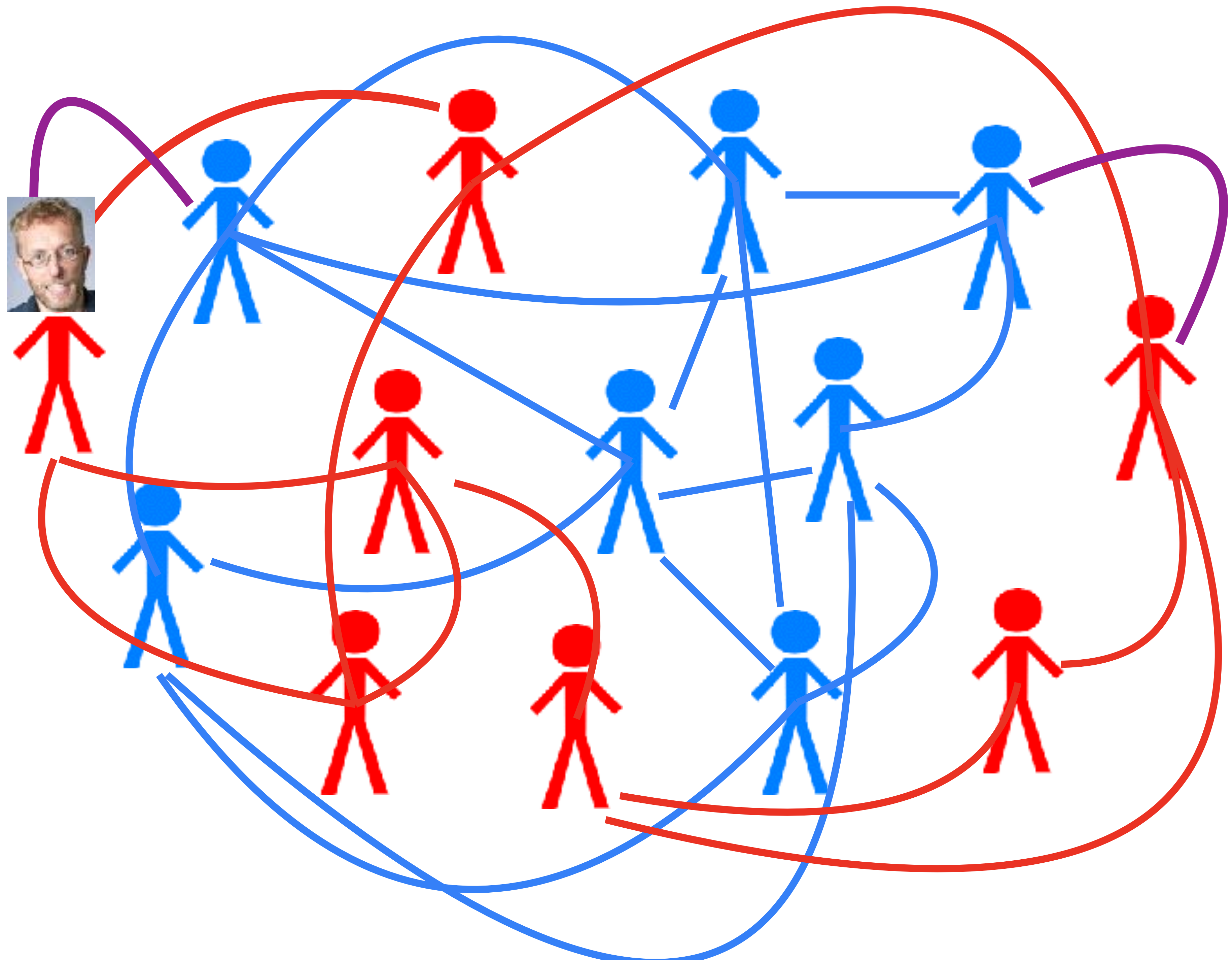

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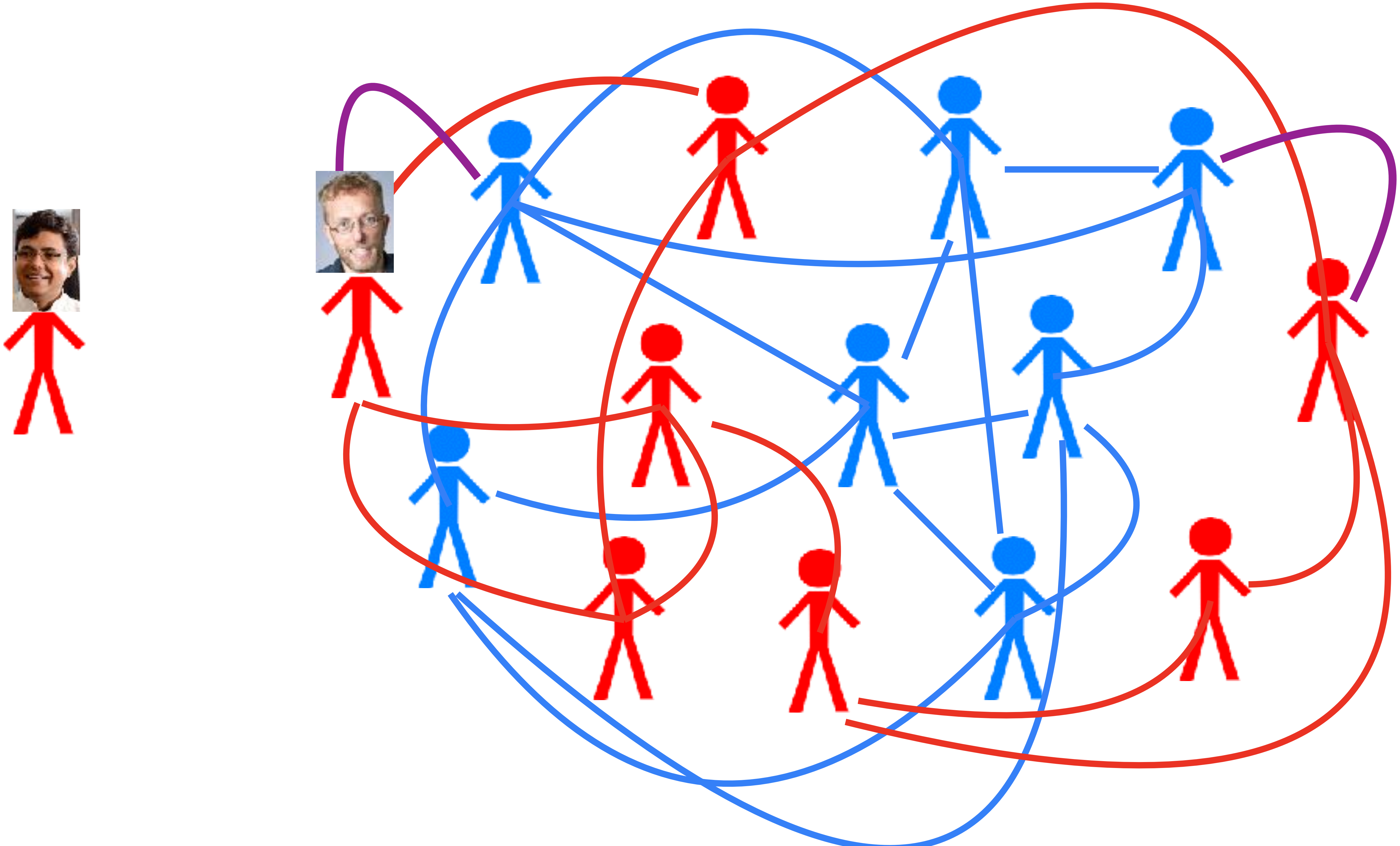

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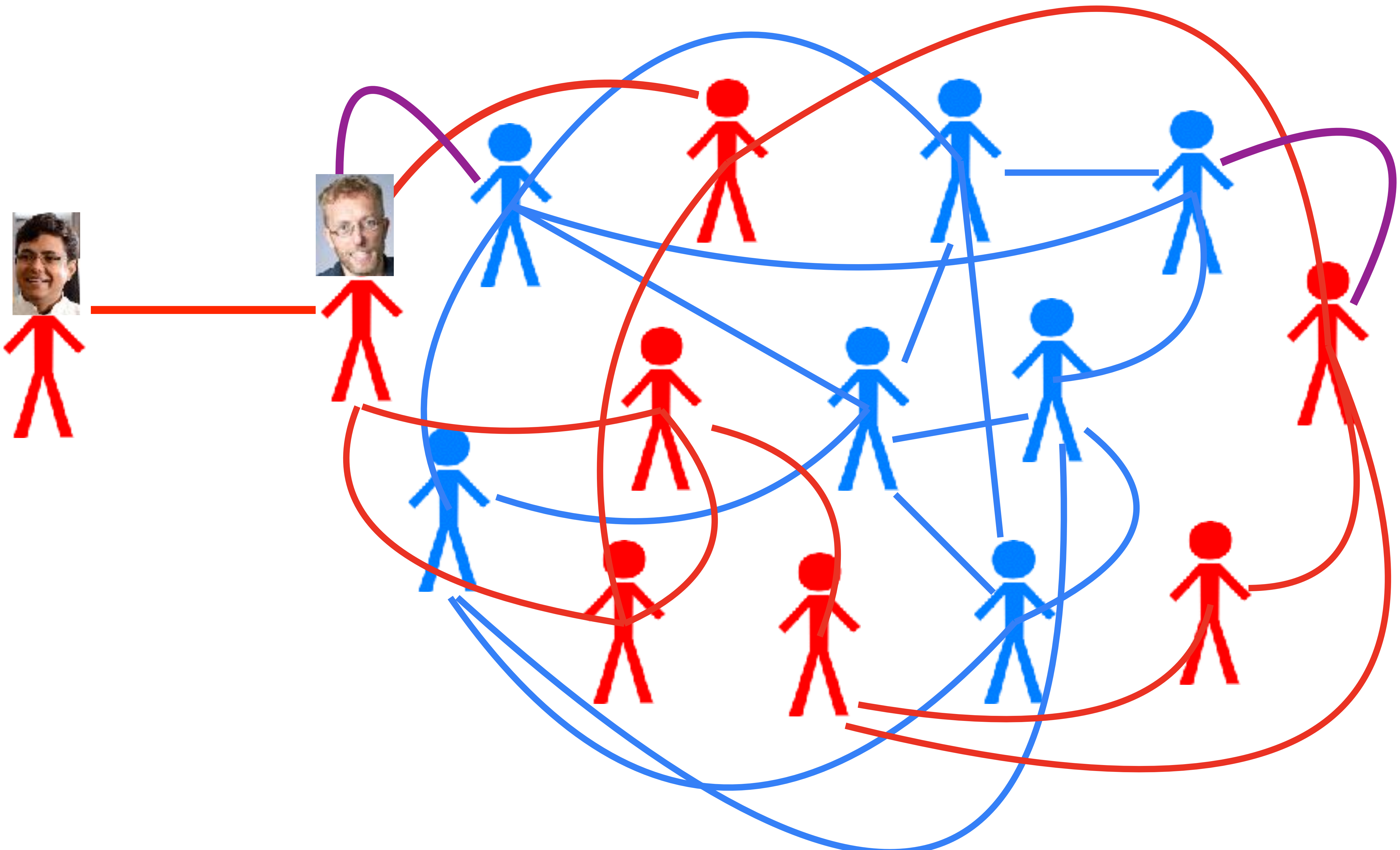

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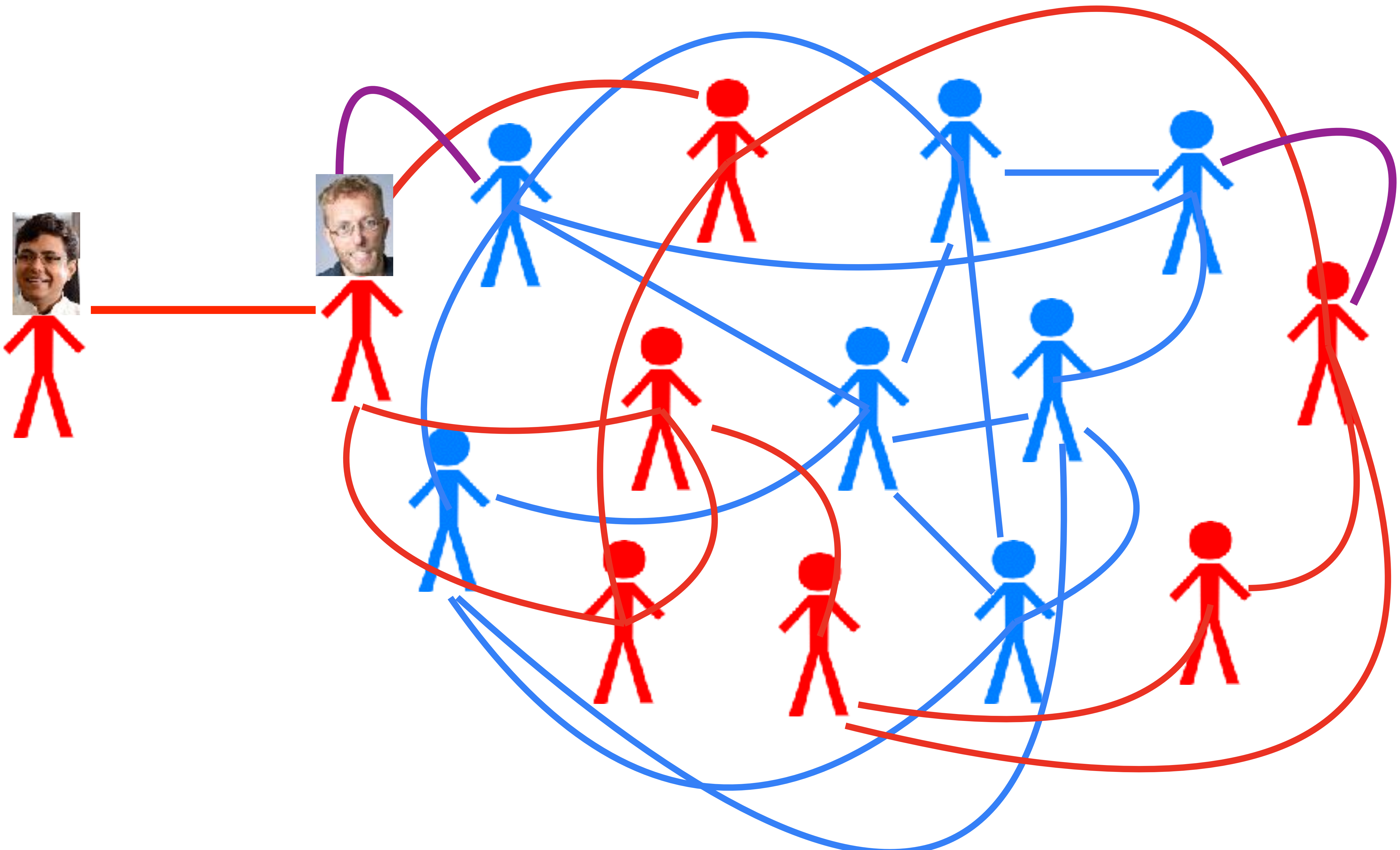

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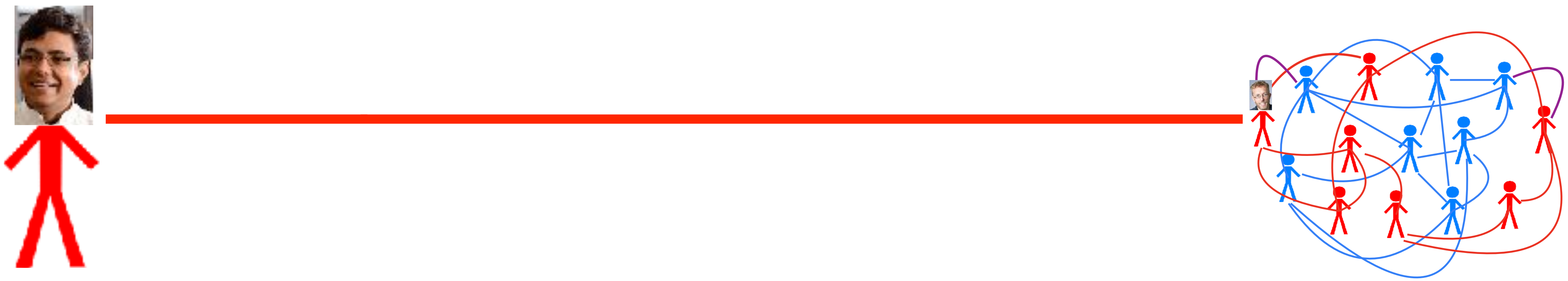

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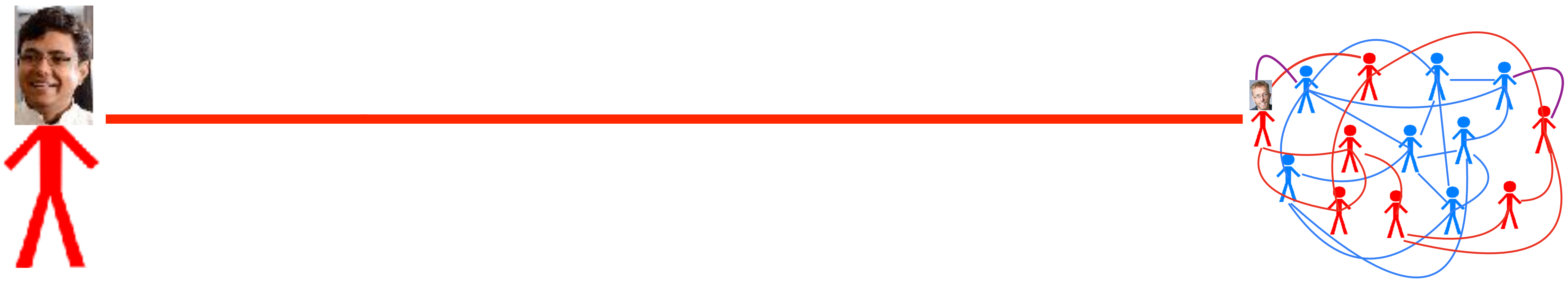

- Variance is high

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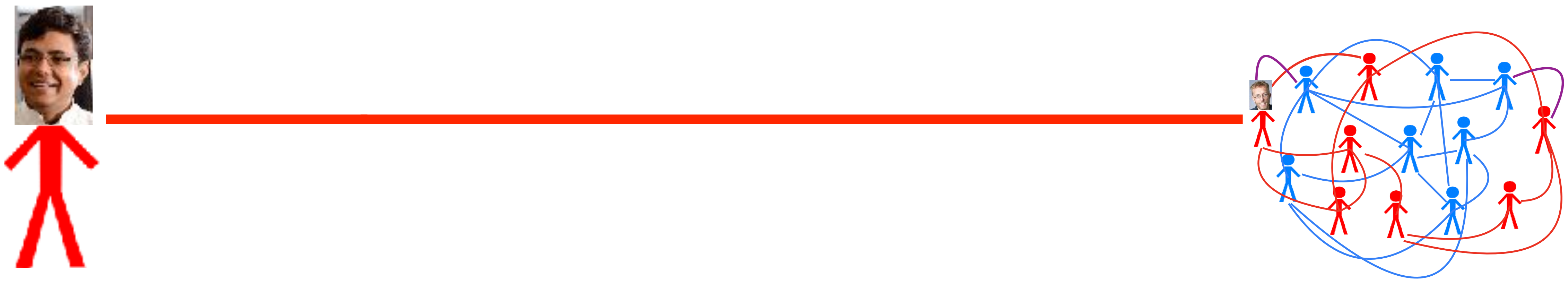

- Variance is high
- Almost all connected nodes have same (small value)

Demo

Normalized Spectral Embedding

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- Nodes linked to each other are close to each other

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  - But variance under what distribution?
  - Higher degree nodes are more important!
  - Lets try distribution given by p_i \propto D_{i,i}