Clustering and Mixture Models

Machine Learning
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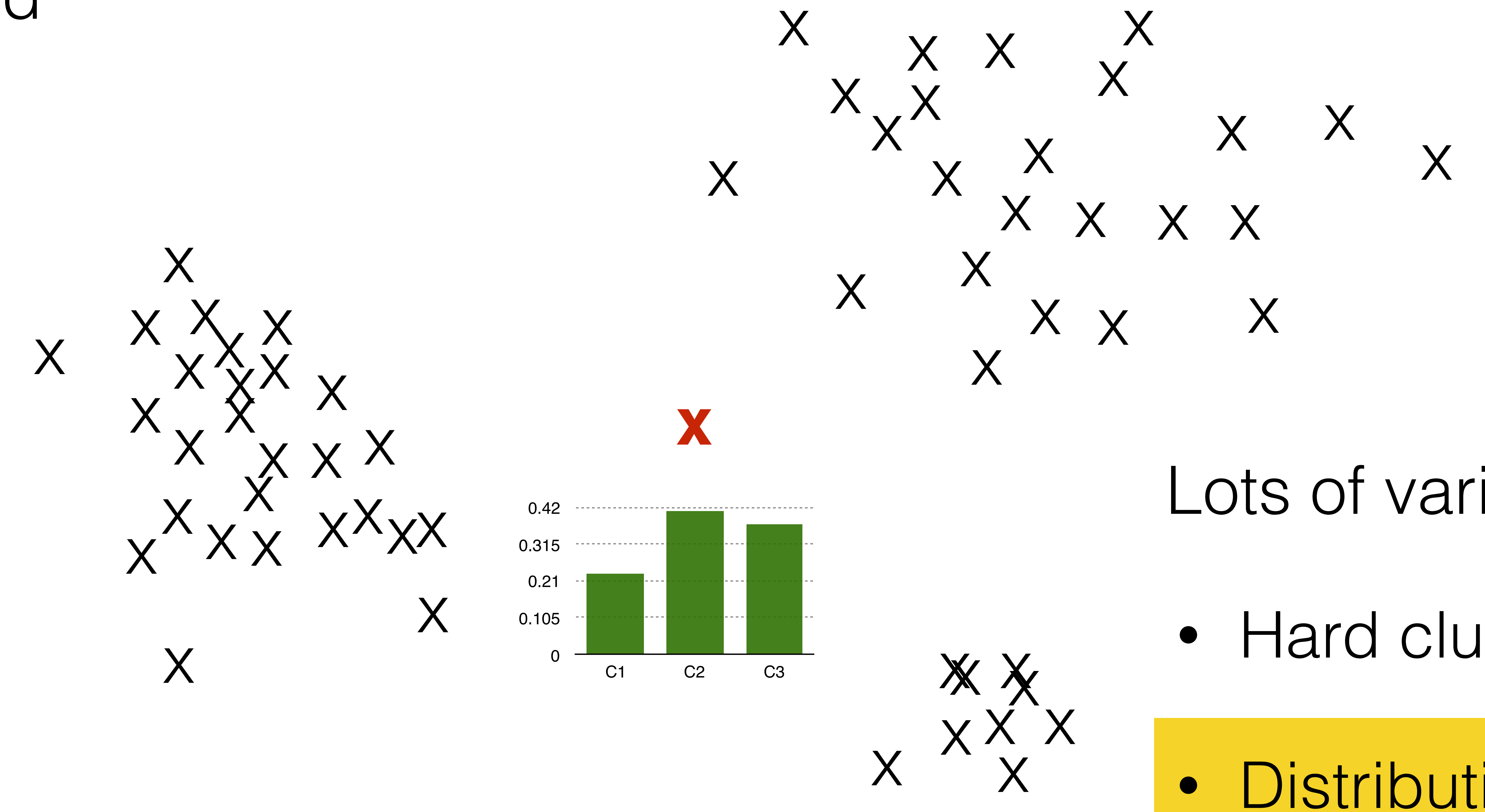
Outline

- Clustering intuition
- Mixture models
- Mixture of Gaussians
- Expectation maximization
- Variational expectation maximization

Clustering

unsupervised



Lots of variants:

- Hard cluster assignment
- Distribution-based
- Hierarchical, etc.

Mixture Models

$$X = \{x_1, \dots, x_n\}$$

$$P(X) = \prod_{i=1}^{n} \sum_{c_i=1}^{K} p(c_i) p(x_i | c_i)$$

probability of $\mathbf{x_i}$ if **i** is in cluster $\mathbf{c_i}$

probability that example **i** is in cluster $\mathbf{c_i}$

generative process:

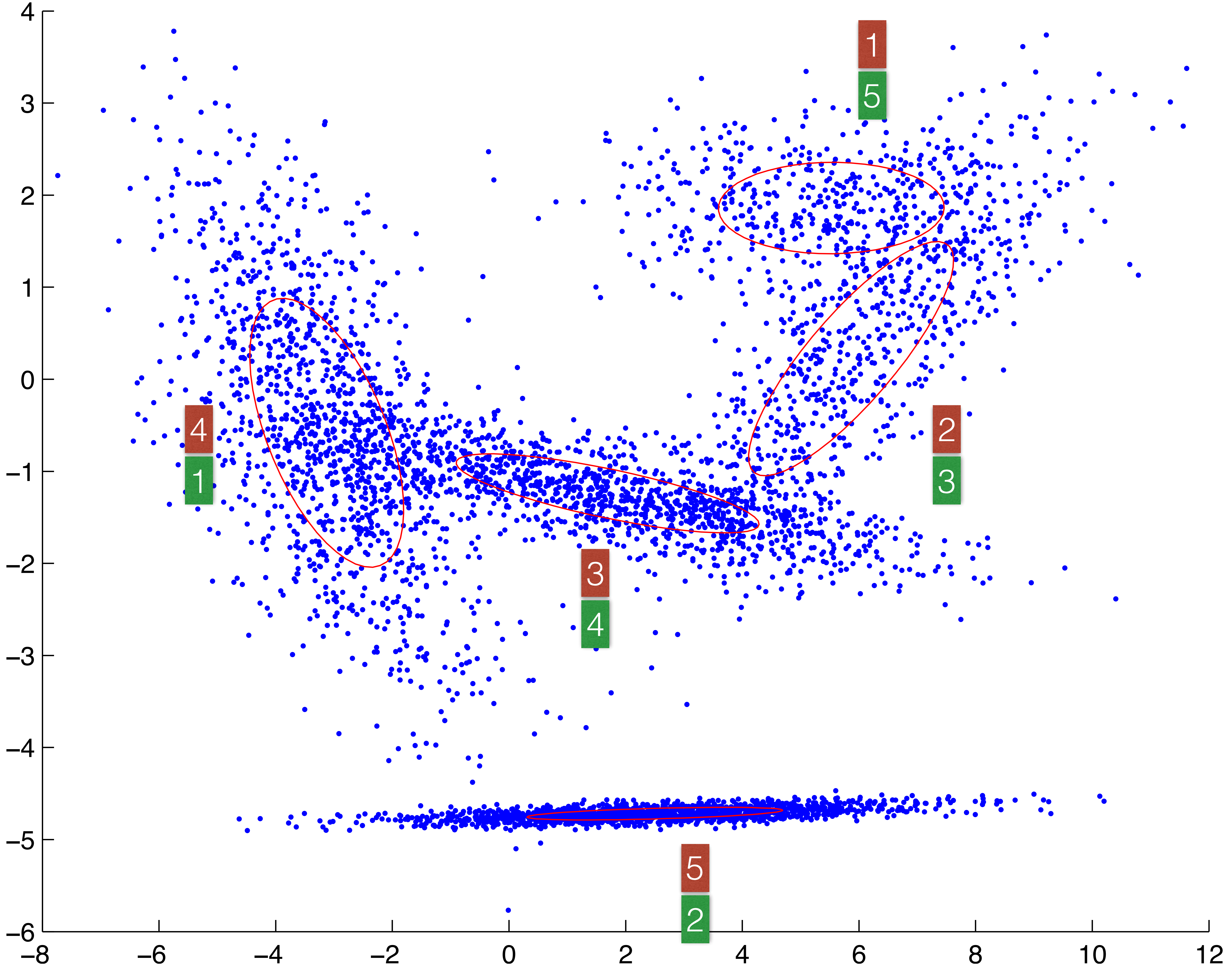
1. Sample cluster
2. Sample data example from cluster distribution

Gaussian Mixture Model

$$P(x) = \sum_{c=1}^{K} p(c) \frac{1}{\sqrt{2\pi|\Sigma_c|}} \exp\left(-\frac{1}{2}(x-\mu_c)^\top \Sigma_c^{-1}(x-\mu_c)\right)$$

multinomial cluster membership

multivariate Gaussian data $\mathcal{N}(x|\mu_c, \Sigma_c)$



“clouds” can overlap

no identity for clusters

Expectation Maximization Recipe

Input: $x_i \qquad i \in \{1, \ldots, n\}$

GMM parameters:

$$p(c) \quad \mu_c \quad \Sigma_c \qquad c \in \{1, \ldots, K\}$$

Latent variables:

$$z_i \in \{1, \ldots, K\}$$

Latent variable probabilities: $p(z_i)$

$$\sum_{c=1}^{K} p(c) = \sum_{c=1}^{K} p(z_i = c) = 1$$

E-step: fit latent variable probabilities

$$p(z_i = c) \leftarrow \frac{p(c)\mathcal{N}(x_i | \mu_c, \Sigma_c)}{\sum_{c'=1}^{K} p(c')\mathcal{N}(x_i | \mu_{c'}, \Sigma_{c'})}$$

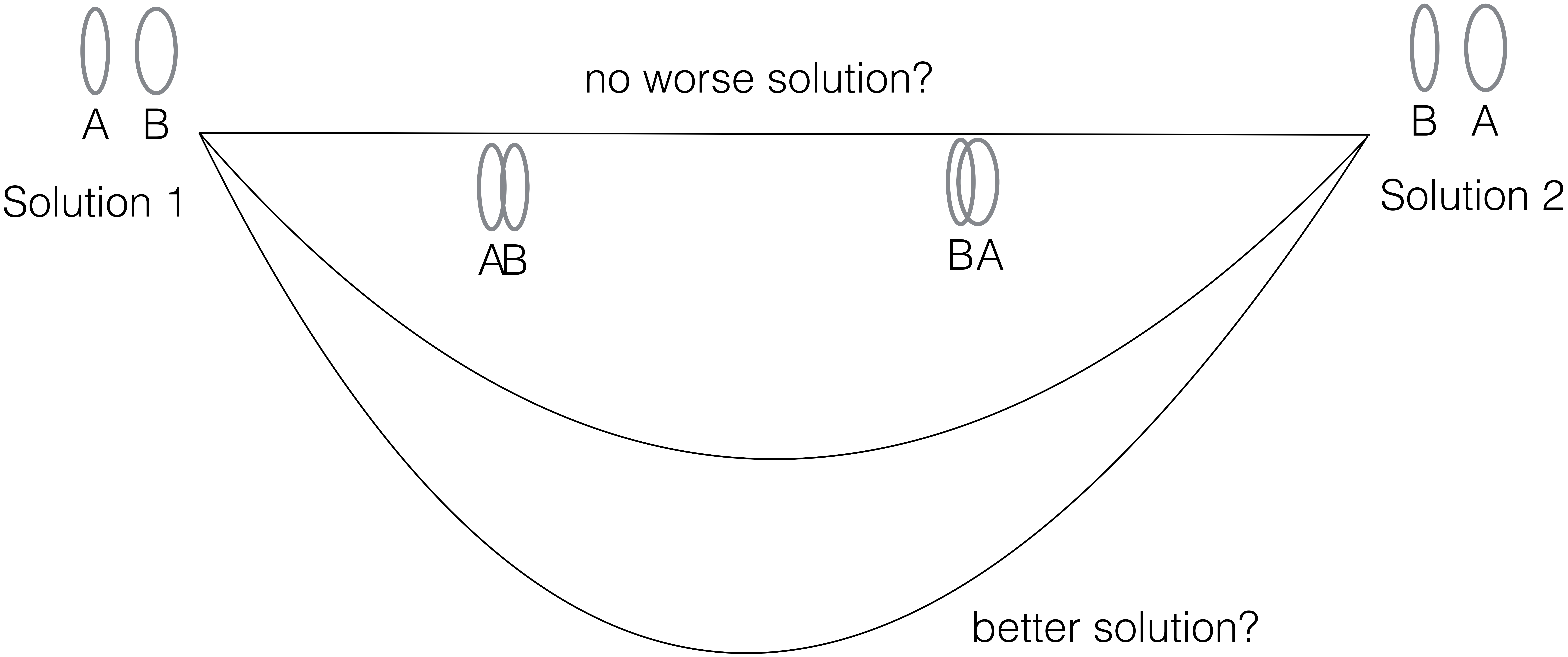
M-step: fit GMM parameters using expected likelihood

$$p(c) \leftarrow \frac{1}{n} \sum_{i=1}^{n} p(z_i = c)$$

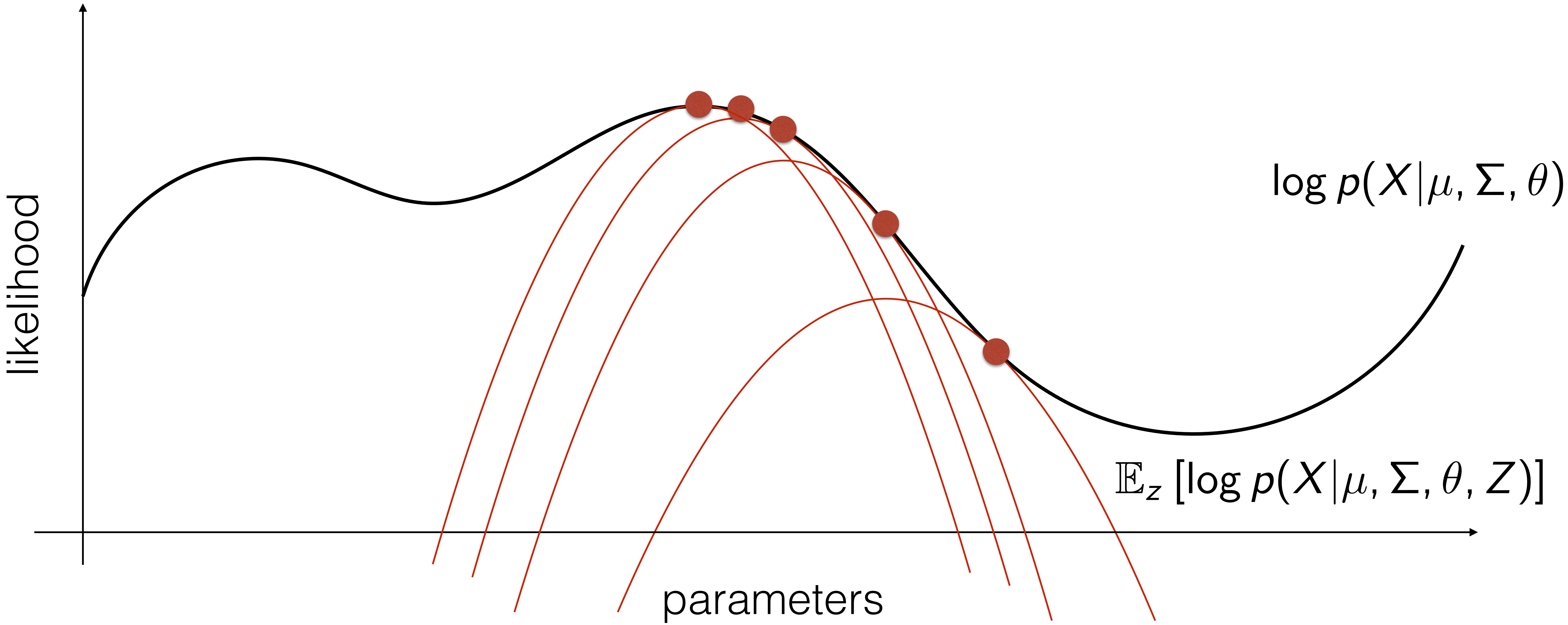
$$\mu_c \leftarrow \frac{\sum_{i=1}^{n} p(z_i = c) x_i}{\sum_{i=1}^{n} p(z_i = c)}$$

$$\Sigma_c \leftarrow \frac{\sum_{i=1}^{n} p(z_i = c)(x_i - \mu_c)(x_i - \mu_c)^\top}{\sum_{i=1}^{n} p(z_i = c)}$$

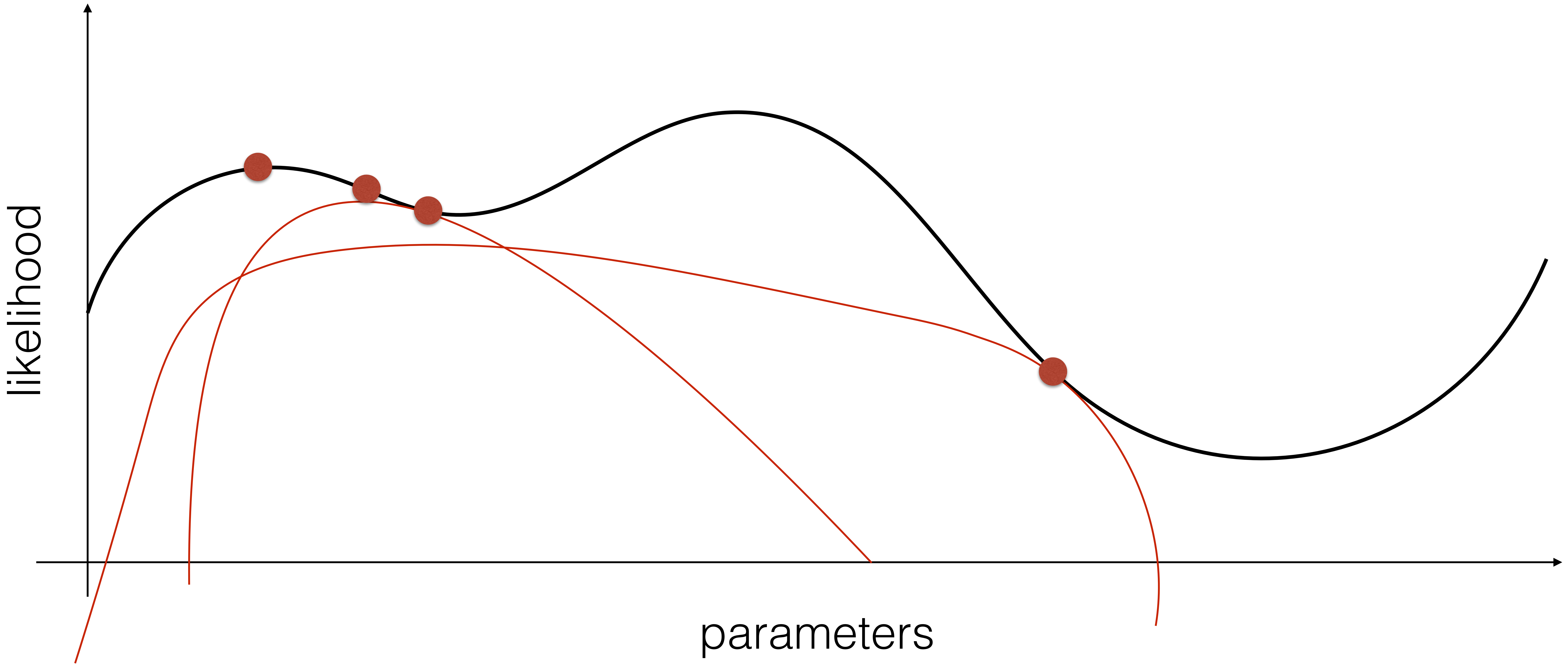
Non-Convexity of GMM NLL



EM as Maximizing Lower Bound



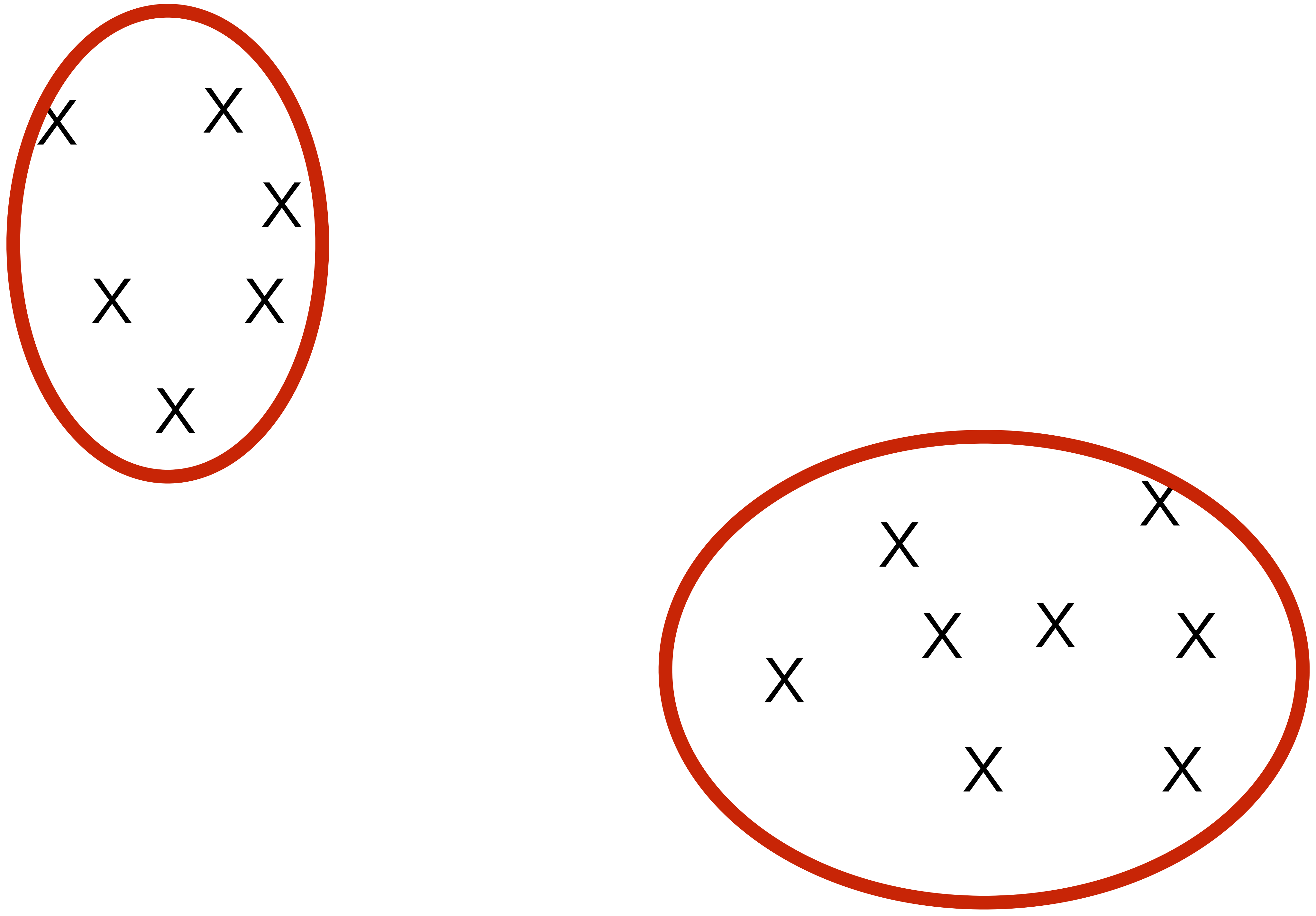
EM as Maximizing Lower Bound



Initialization

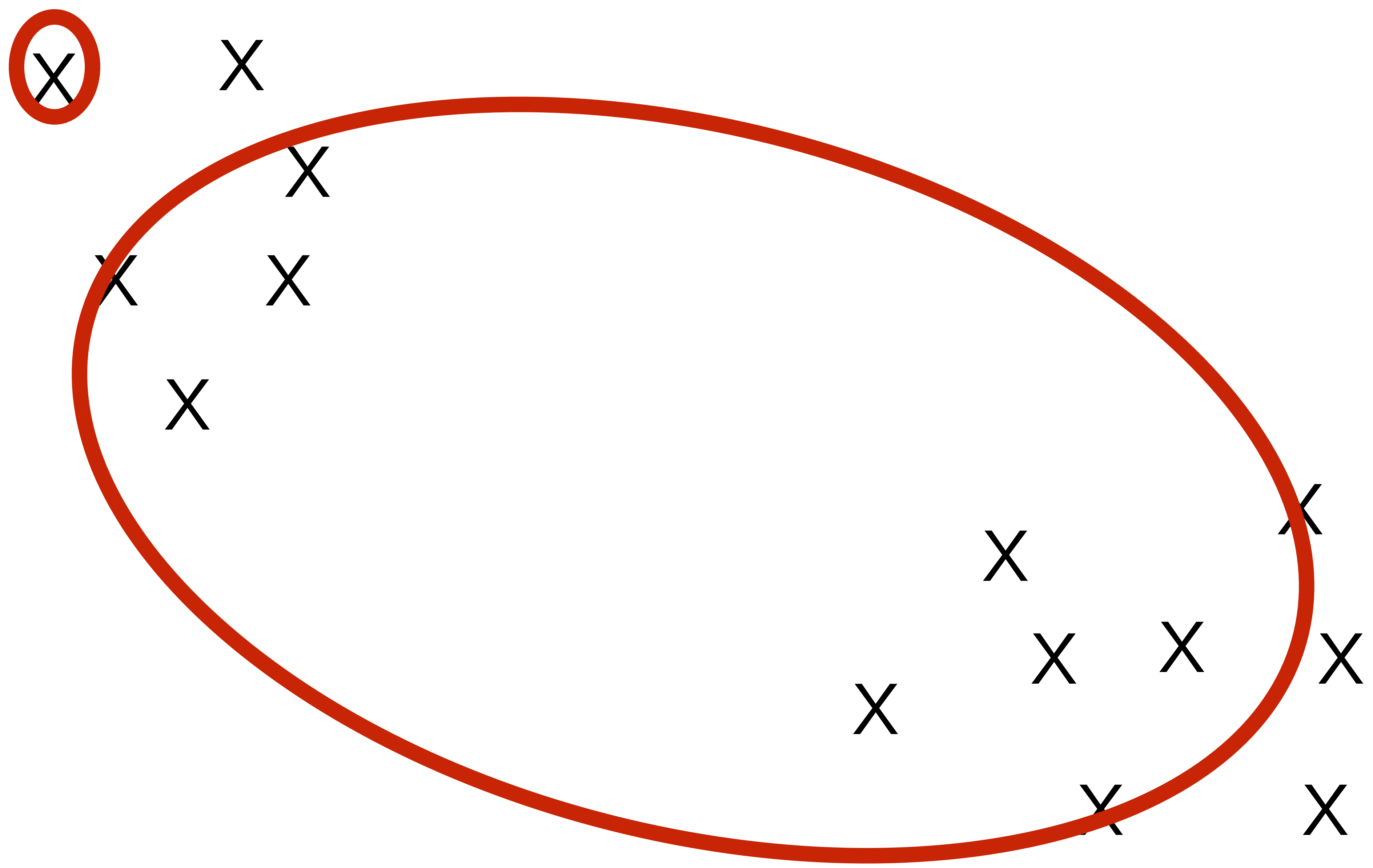
- Some heuristics:
  - Completely random
  - Fit a single Gaussian to all data; randomly perturb K copies
  - Randomly initialize cluster memberships. Start with M-step

EM Likelihood Landscape



Global maximum?

$\Sigma_c \to [0]$ $\quad$ $L \to \infty$



$$\sum_{i=1}^{n} \log \sum_{c=1}^{K} p(c) \frac{1}{\sqrt{2\pi|\Sigma_c|}} \exp\left(-\frac{1}{2}(x_i - \mu_c)^\top \Sigma_c^{-1}(x_i - \mu_c)\right)$$

$$\int_{-\infty}^{\infty} p(x)dx = 1$$

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Fixes

- Good initialization
- Constrain covariance to have some bandwidth on each dimension

Summary of EM for GMMs

- Gaussian mixture models: fit data with weighted combination of Gaussians
- Non-convex likelihood
  - Estimate probability of each point being in each Gaussian
  - Use probabilities to maximize expected likelihood
  - Iterate until local minimum

Variational Derivation of EM

Marginal Likelihood

$$p(X|\theta)$$
$$= \int_Z p(X, Z|\theta) dZ$$
$$\sum_Z p(X, Z|\theta)$$

e.g., $X = \{x_1, \dots, x_n\}$

$$\theta = \{\mu_1, \dots, \mu_K, \Sigma_1, \dots, \Sigma_K, \dots p(c)\}$$

$Z = \{z_1, \dots, z_n\}$ (cluster memberships)

$$p(X, Z|\theta) = \prod_{i=1}^{n} p(z_i) \mathcal{N}(x_i|\mu_{z_i}, \Sigma_{z_i})$$

$$\log p(X|\theta) = \log \sum_Z p(X, Z|\theta)$$

log marginal likelihood

$$\underset{\theta}{\operatorname{argmax}} \ \log \sum_Z p(X, Z|\theta)$$

learning objective

Jensen's Inequality

For any convex function φ,

$$\varphi(\mathbb{E}[X]) \leq \mathbb{E}[\varphi(X)]$$

For any concave function ϕ,

$$\phi(\mathbb{E}[X]) \geq \mathbb{E}[\phi(X)]$$

$$\log(\mathbb{E}[X]) \geq \mathbb{E}[\log X]$$

Variational Bound

$$\log(\mathbb{E}[X]) \geq \mathbb{E}[\log X]$$

$$\sum_Z q(Z) = 1$$

$$\begin{aligned}
\log \sum_Z p(X, Z|\theta) &= \log \sum_Z \frac{q(Z)}{q(Z)} p(X, Z|\theta) \\
&= \log \sum_Z q(Z) \frac{p(X, Z|\theta)}{q(Z)} \\
&\geq \sum_Z q(Z) \log \frac{p(X, Z|\theta)}{q(Z)} \\
&= \sum_Z q(Z) \log p(X, Z|\theta) - \sum_Z q(Z) \log q(Z)
\end{aligned}$$

Variational Bound

expectation entropy

$$\log \sum_Z p(X, Z|\theta) \geq \sum_Z q(Z) \log p(X, Z|\theta) - \sum_Z q(Z) \log q(Z)$$

We can pick any ***q*** distribution and the bound holds

$$\operatorname*{argmax}_{\theta, q \in Q} \sum_Z q(Z) \log p(X, Z|\theta) - \sum_Z q(Z) \log q(Z)$$

$$q(Z) = \prod_{i=1}^{n} q(z_i) \qquad \sum_{z_i} q(z_i) = 1$$

Fully Factorized Variational Family

$$\operatorname*{argmax}_{\theta, q \in Q} \sum_{Z} q(Z) \log p(X, Z|\theta) - \sum_{Z} q(Z) \log q(Z)$$

$$q(Z) = \prod_{i=1}^{n} q(z_i) \qquad \sum_{z_i} q(z_i) = 1$$

$$\operatorname*{argmax}_{\theta, q \in Q} \sum_{i=1}^{n} \sum_{z_i} q(z_i) \log p(x_i, z_i|\theta) - q(z_i) \log q(z_i)$$

Point Distributions

$$\underset{\theta, q \in Q}{\operatorname{argmax}} \sum_{Z} q(Z) \log p(X, Z|\theta) - \sum_{Z} q(Z) \log q(Z)$$

$$q(Z) = \prod_{i=1}^{n} q(z_i) \qquad q(z_i) = \begin{cases} 1 & \text{if } z_i = \hat{z}_i \\ 0 & \text{otherwise} \end{cases}$$

$$\underset{\theta, q \in Q}{\operatorname{argmax}} \sum_{i=1}^{n} \sum_{z_i} q(z_i) \log p(x_i, z_i|\theta) - q(z_i) \log q(z_i)$$

$$\underset{\theta, q \in Q, \hat{Z}}{\operatorname{argmax}} \sum_{i=1}^{n} \log p(x_i, \hat{z}_i|\theta)$$

point distributions are often easier to compute, but less robust

Point Distributions for GMMs

$$\underset{\theta, q \in Q, \hat{Z}}{\operatorname{argmax}} \sum_{i=1}^{n} \log p(x_i, \hat{z}_i | \theta)$$

$$\sum_{i=1}^{n} \log \mathcal{N}(x_i | \mu_{\hat{z}_i}, \Sigma_{\hat{z}_i})$$

$$\hat{z}_i \leftarrow \underset{z}{\operatorname{argmax}} \; \log \mathcal{N}(x_i | \mu_z, \Sigma_z)$$

$$\mu_z \leftarrow \frac{\sum_{i; \hat{z}_i = z} x_i}{\sum_{i; \hat{z}_i = z} 1} \qquad \Sigma_z \leftarrow \frac{\sum_{i; \hat{z}_i = z} (x_i - \mu_i)(x_i - \mu_i)^\top}{\sum_{i; \hat{z}_i = z} 1}$$

K-means

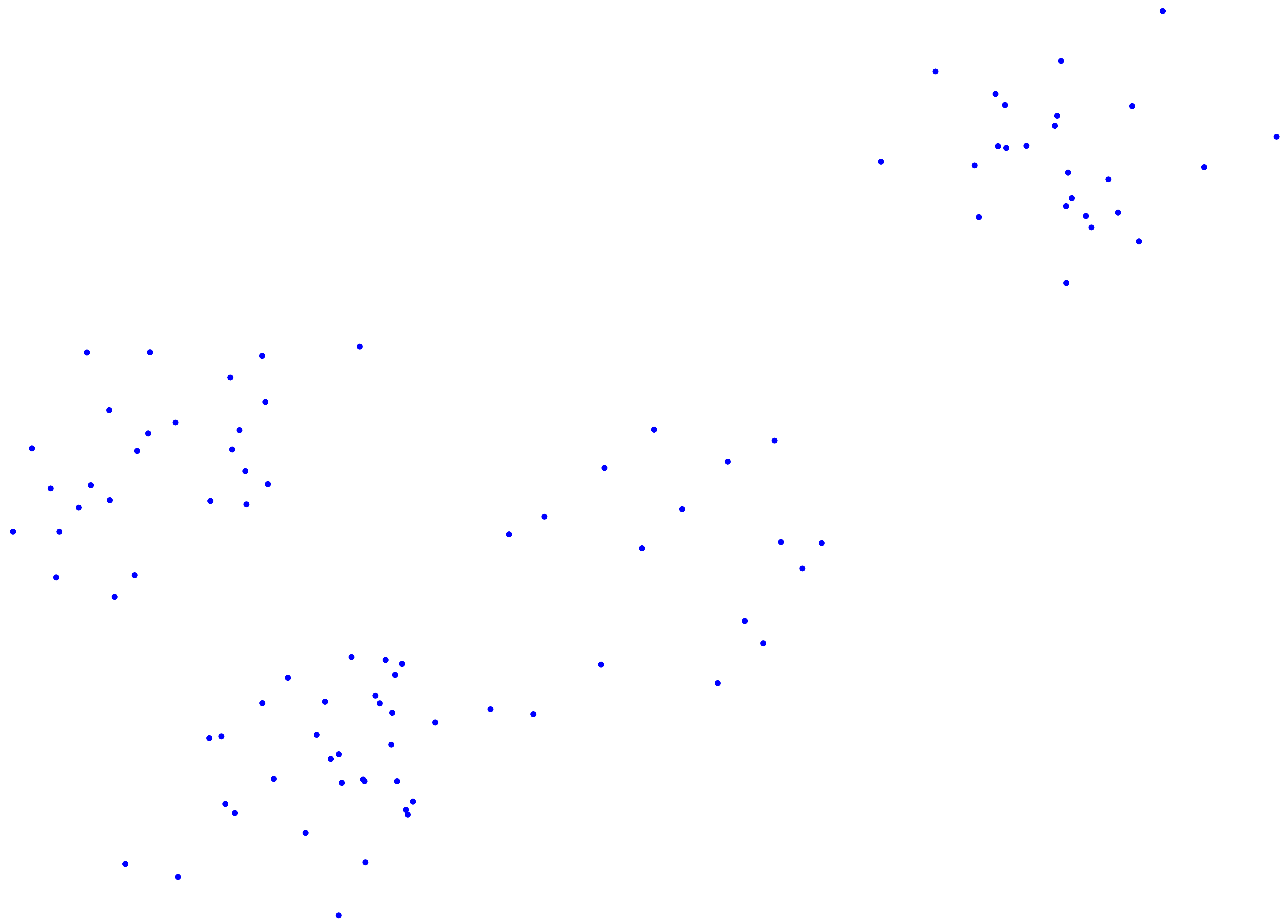
$$\hat{z}_i \leftarrow \underset{z}{\operatorname{argmin}} \, ||x_i - \mu_z||$$

assign points to closest mean

$$\mu_z \leftarrow \frac{\sum_{i; \hat{z}_i = z} x_i}{\sum_{i; \hat{z}_i = z} 1}$$

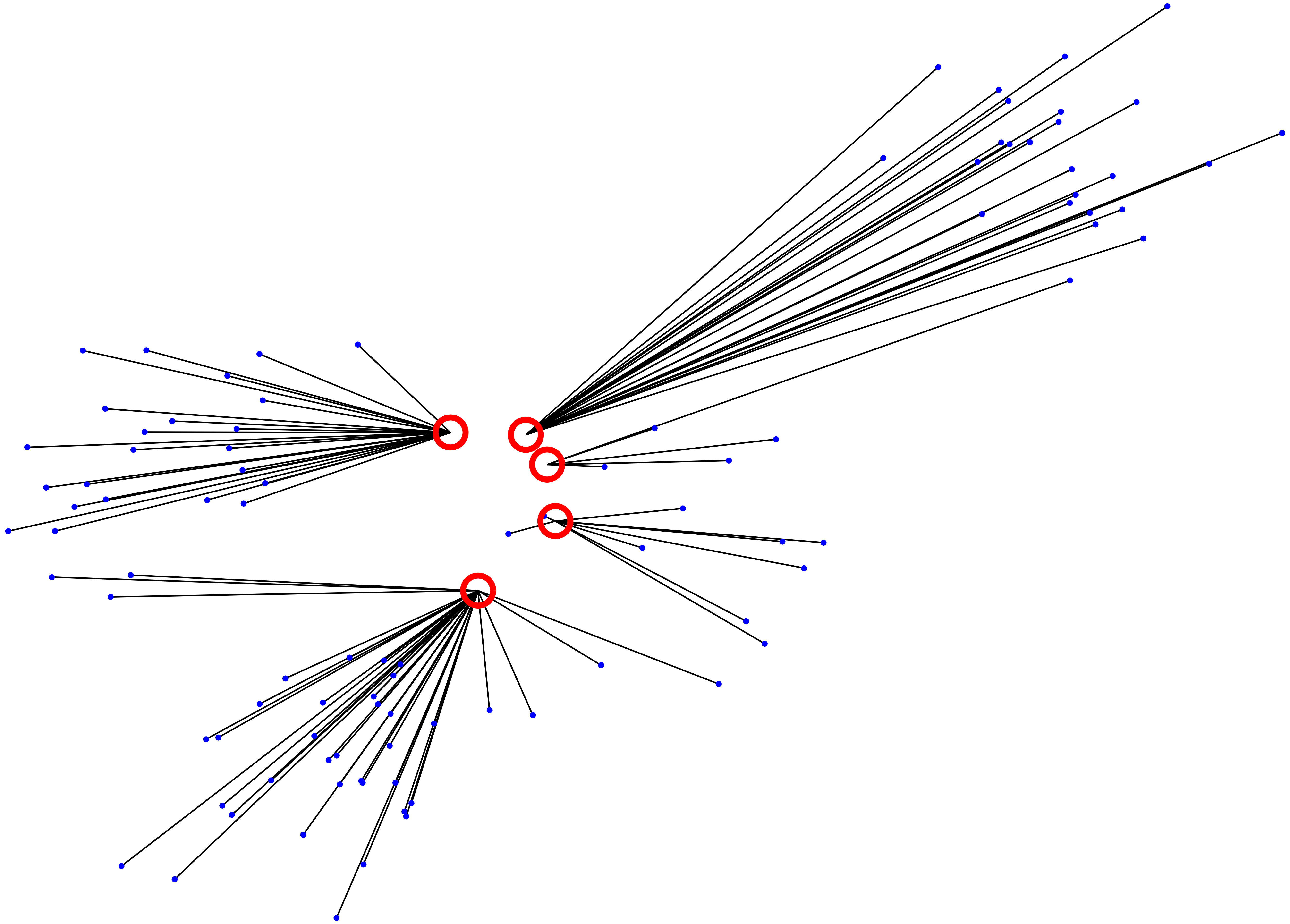
set means to average of points in cluster

Example



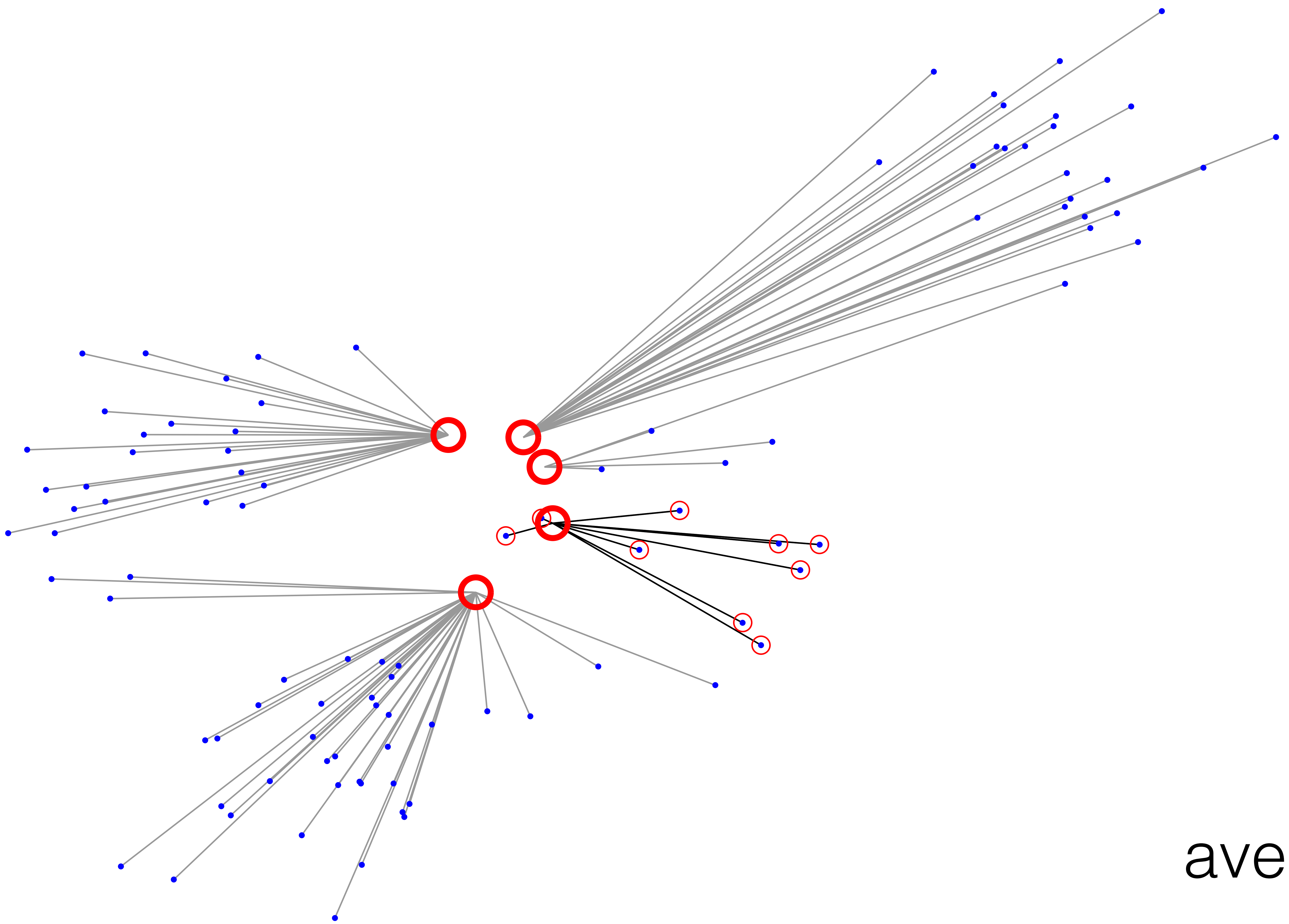
input data

Example



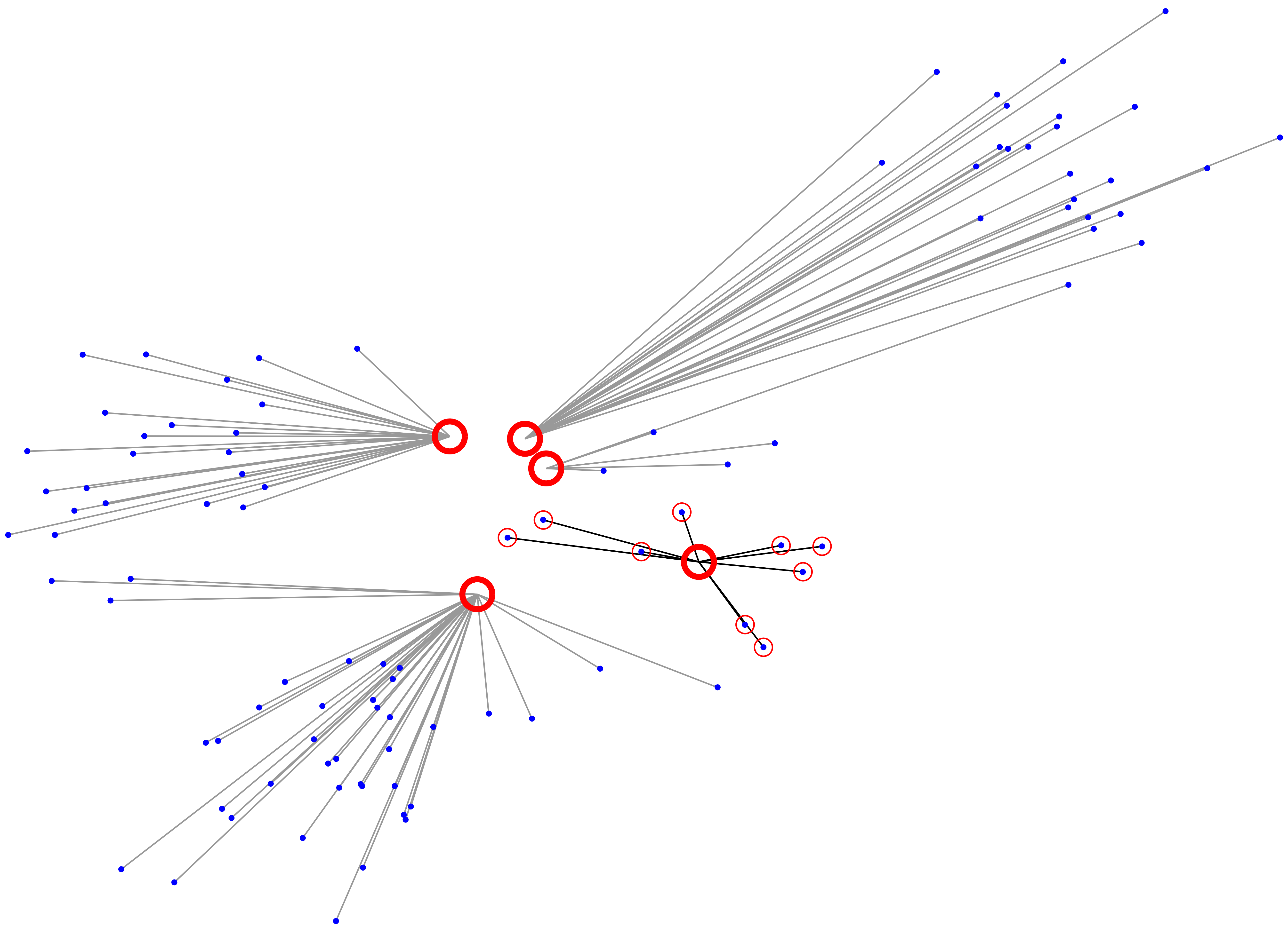
assign points to
initialized means

Example



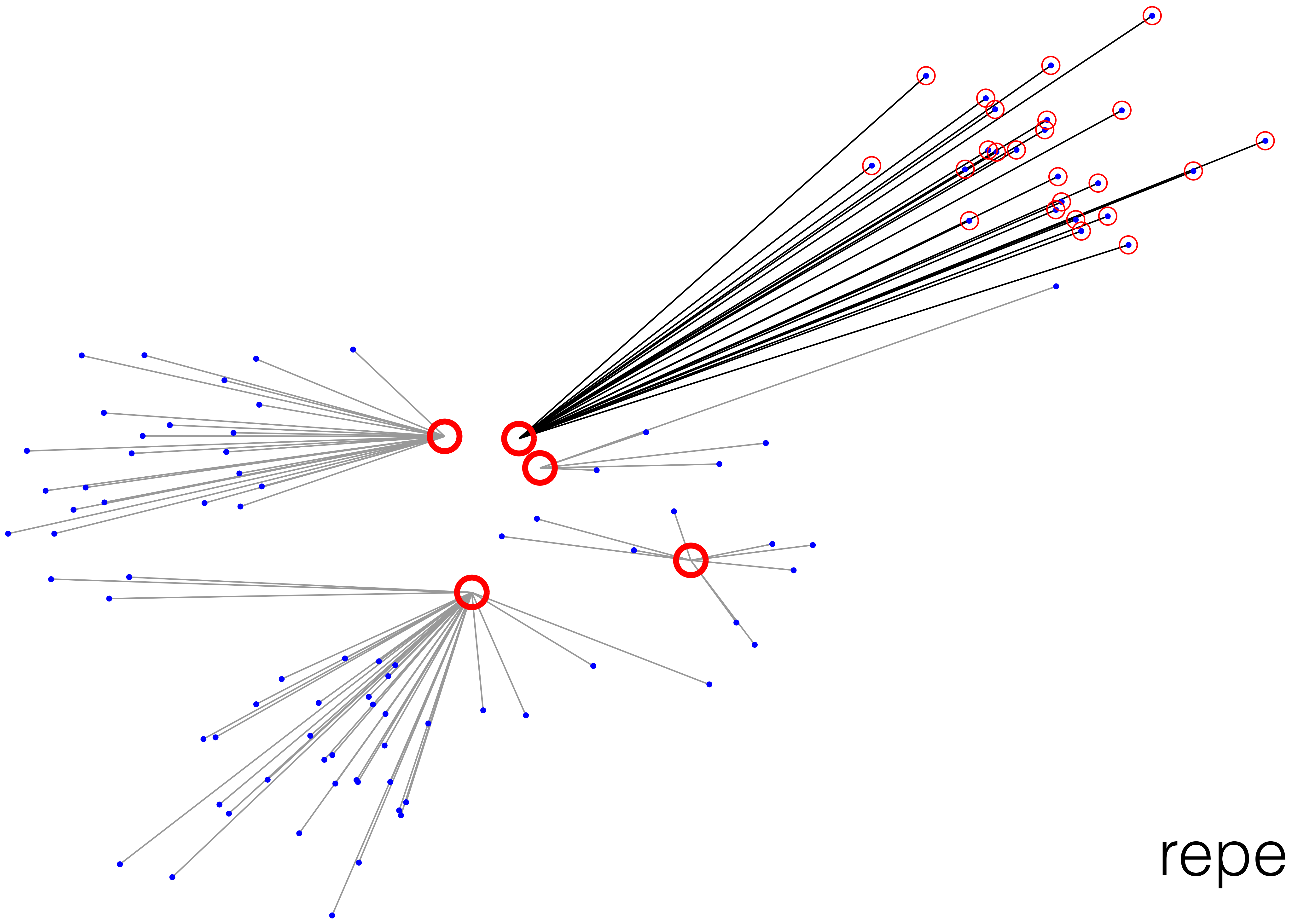
average each cluster

Example



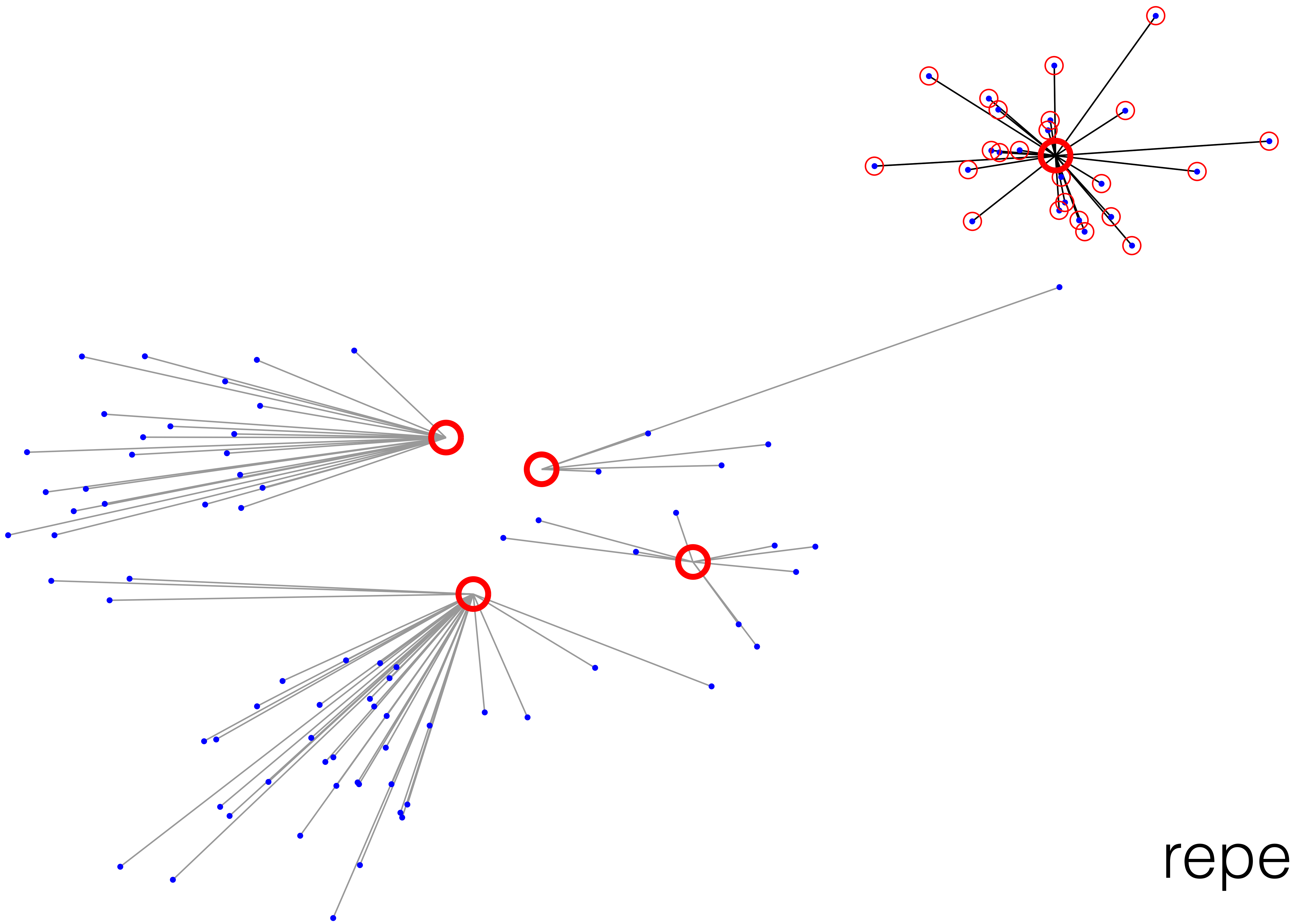
update mean

Example



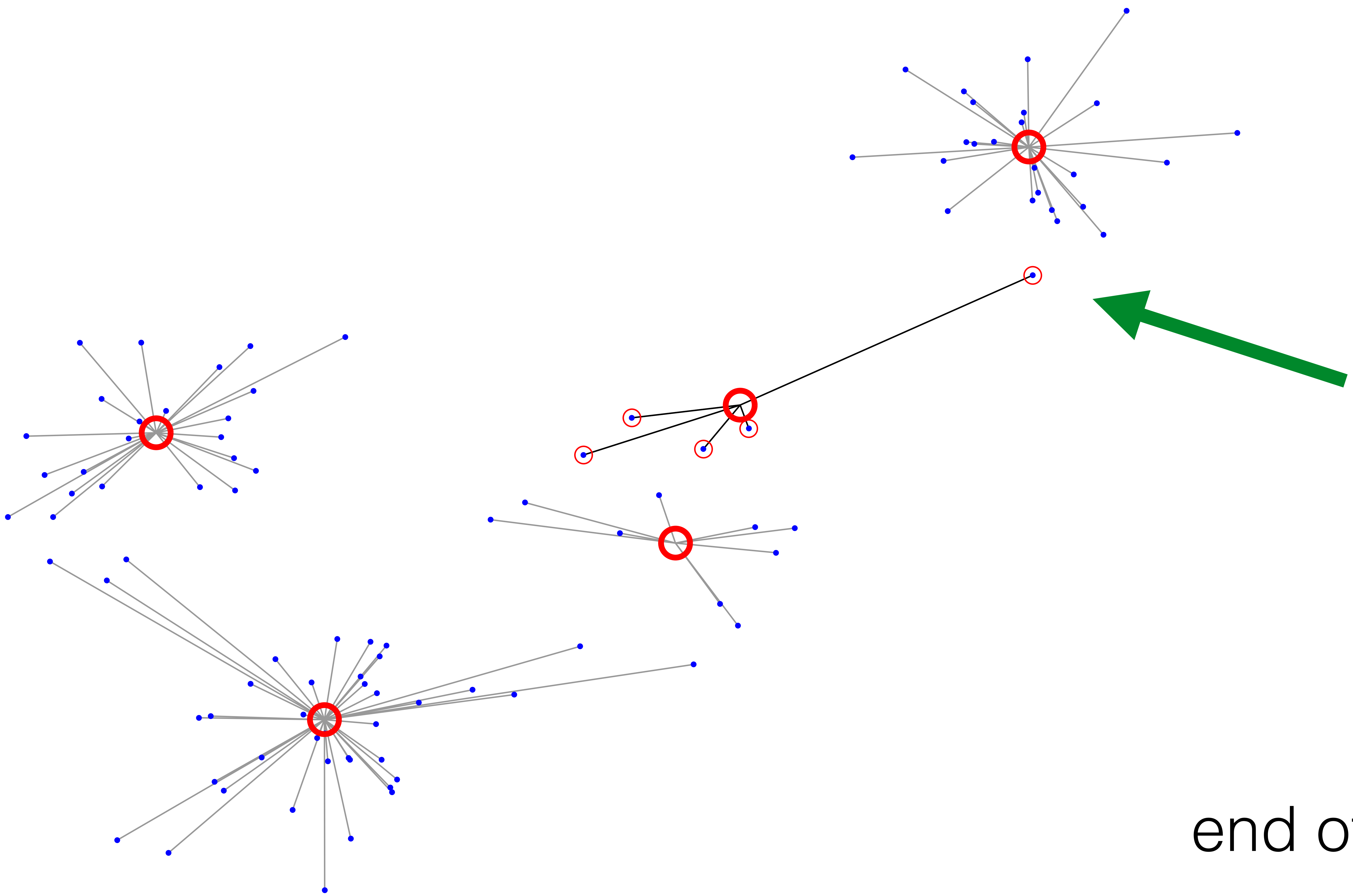
repeat for all clusters

Example



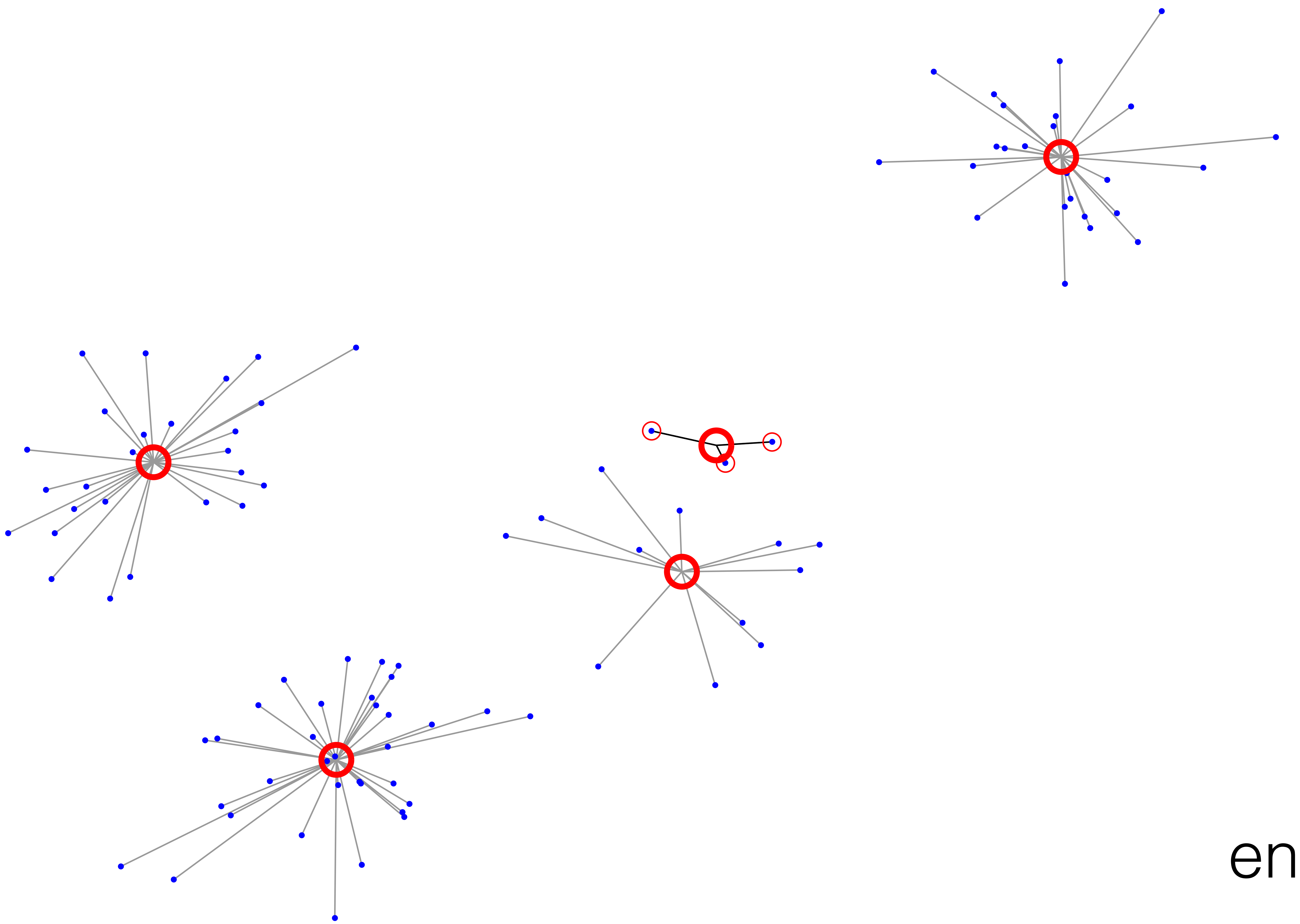
repeat for all clusters

Example



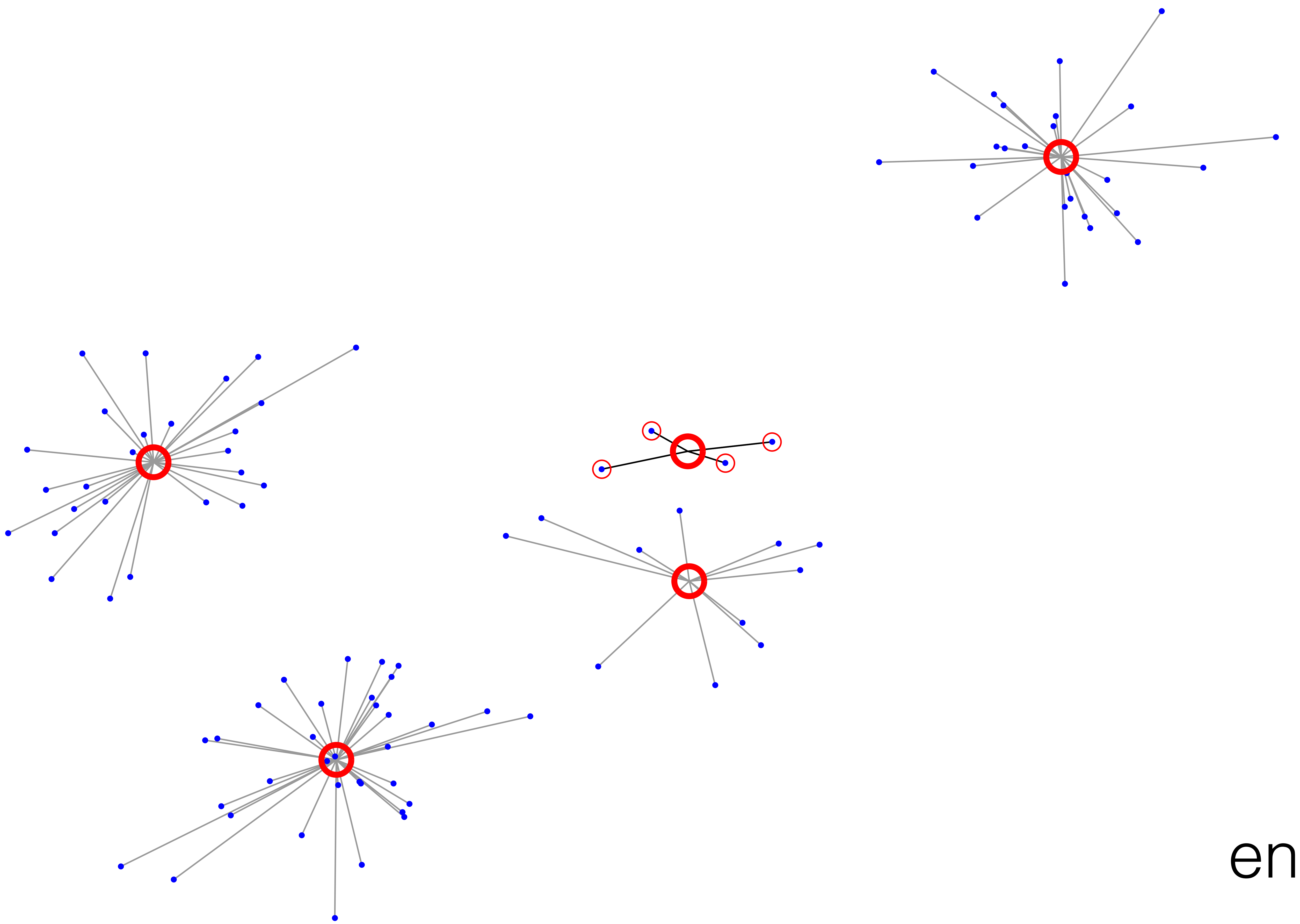
end of iteration 1

Example



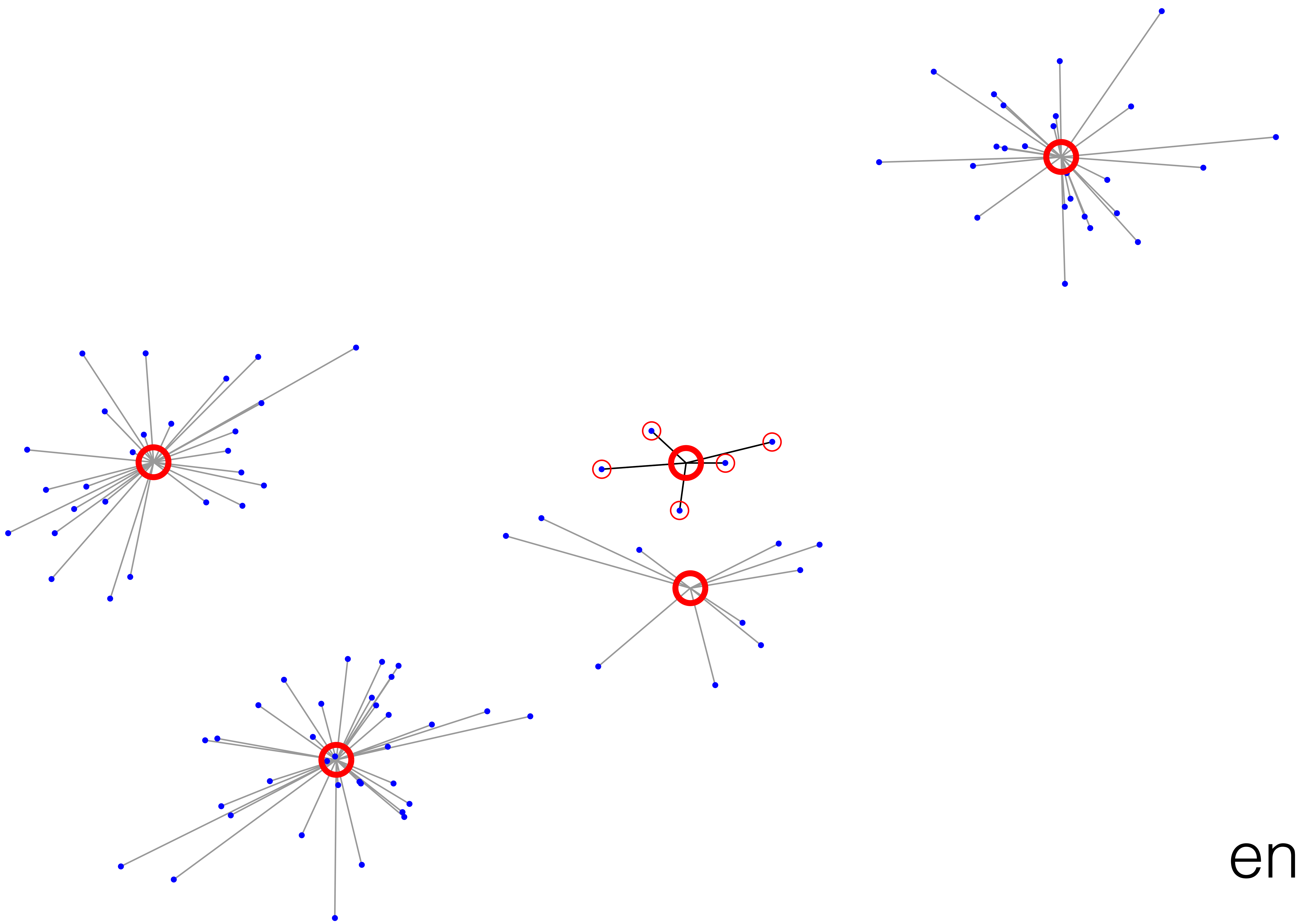
end of iteration 2

Example



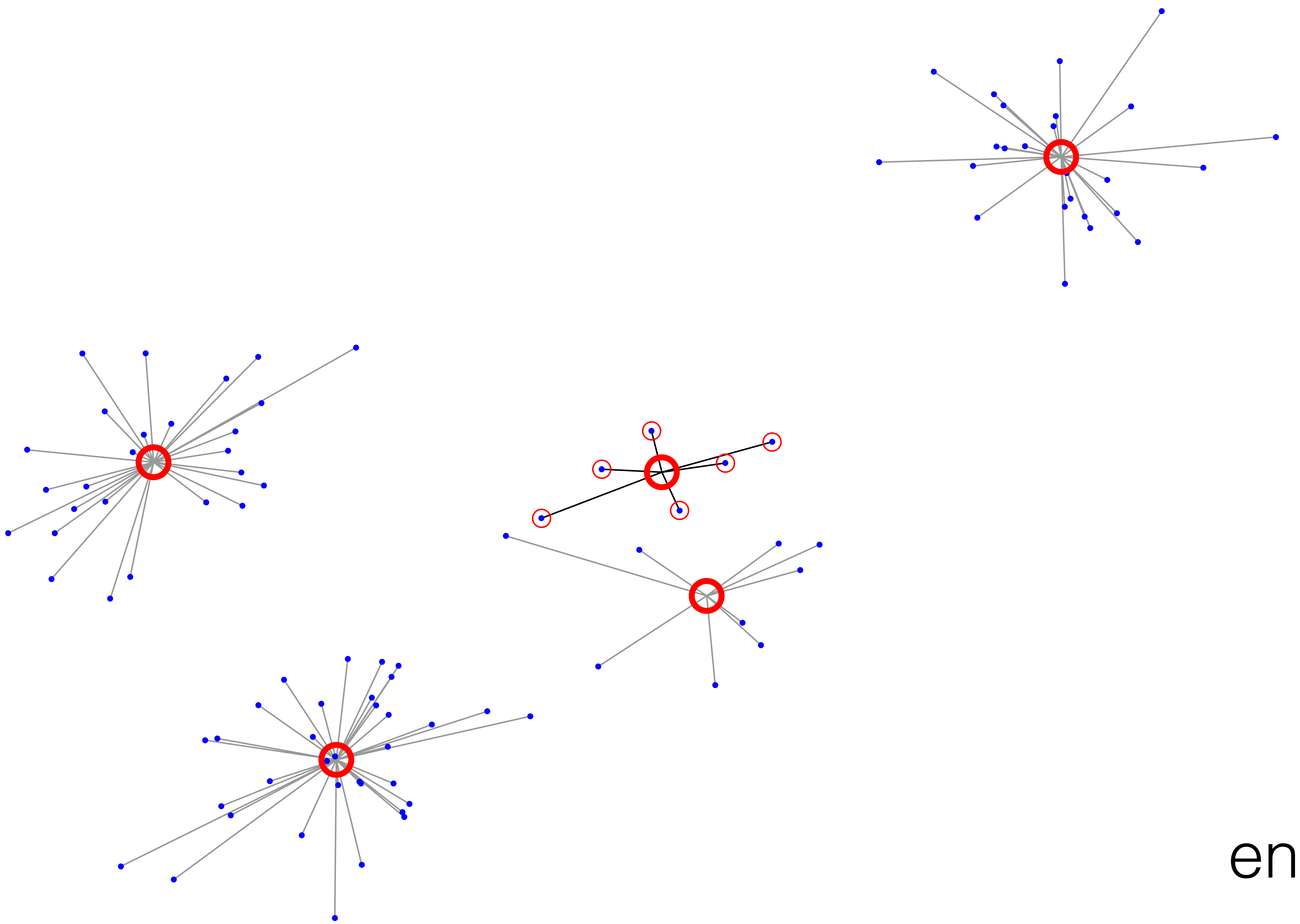
end of iteration 3

Example



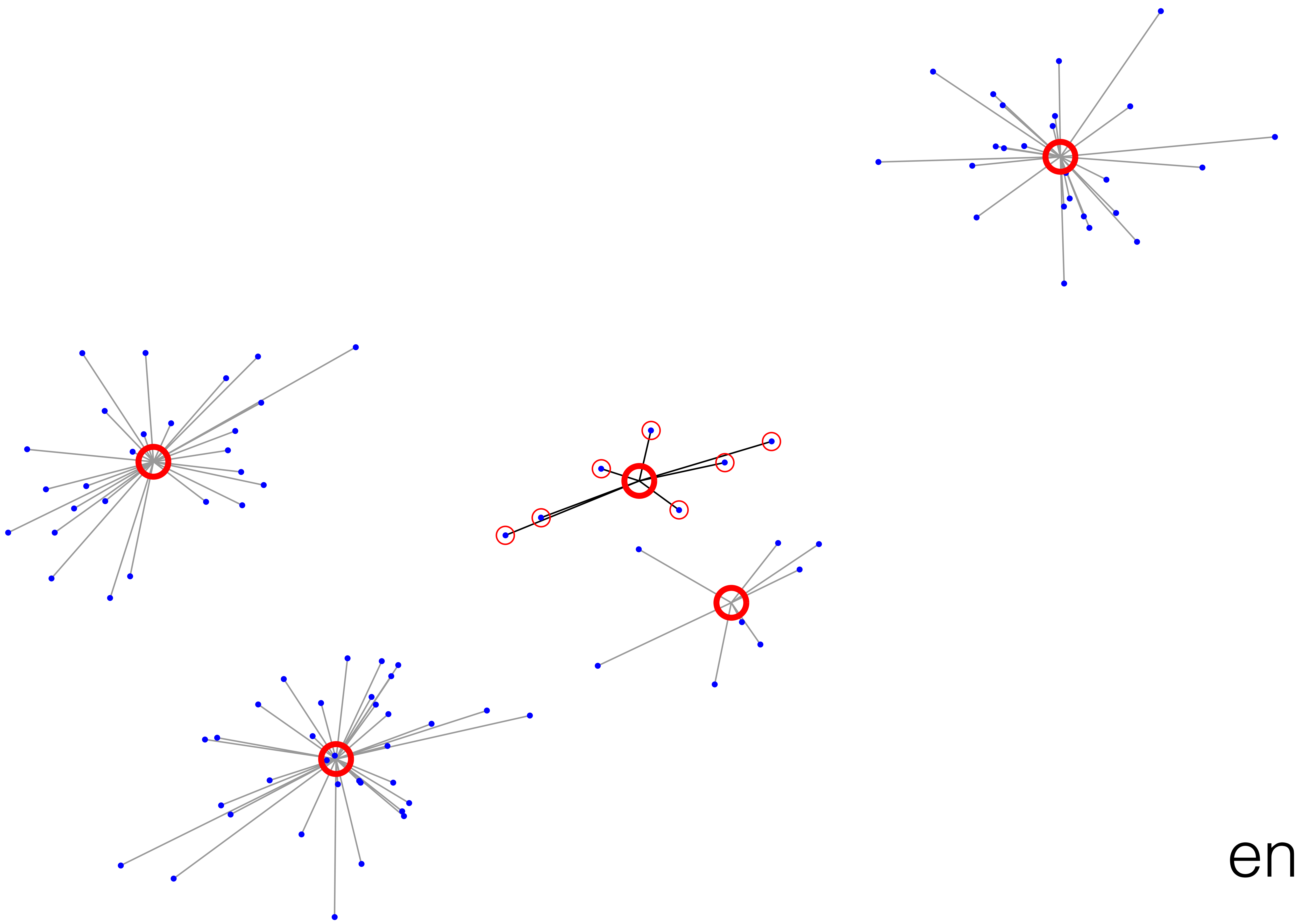
end of iteration 4

Example



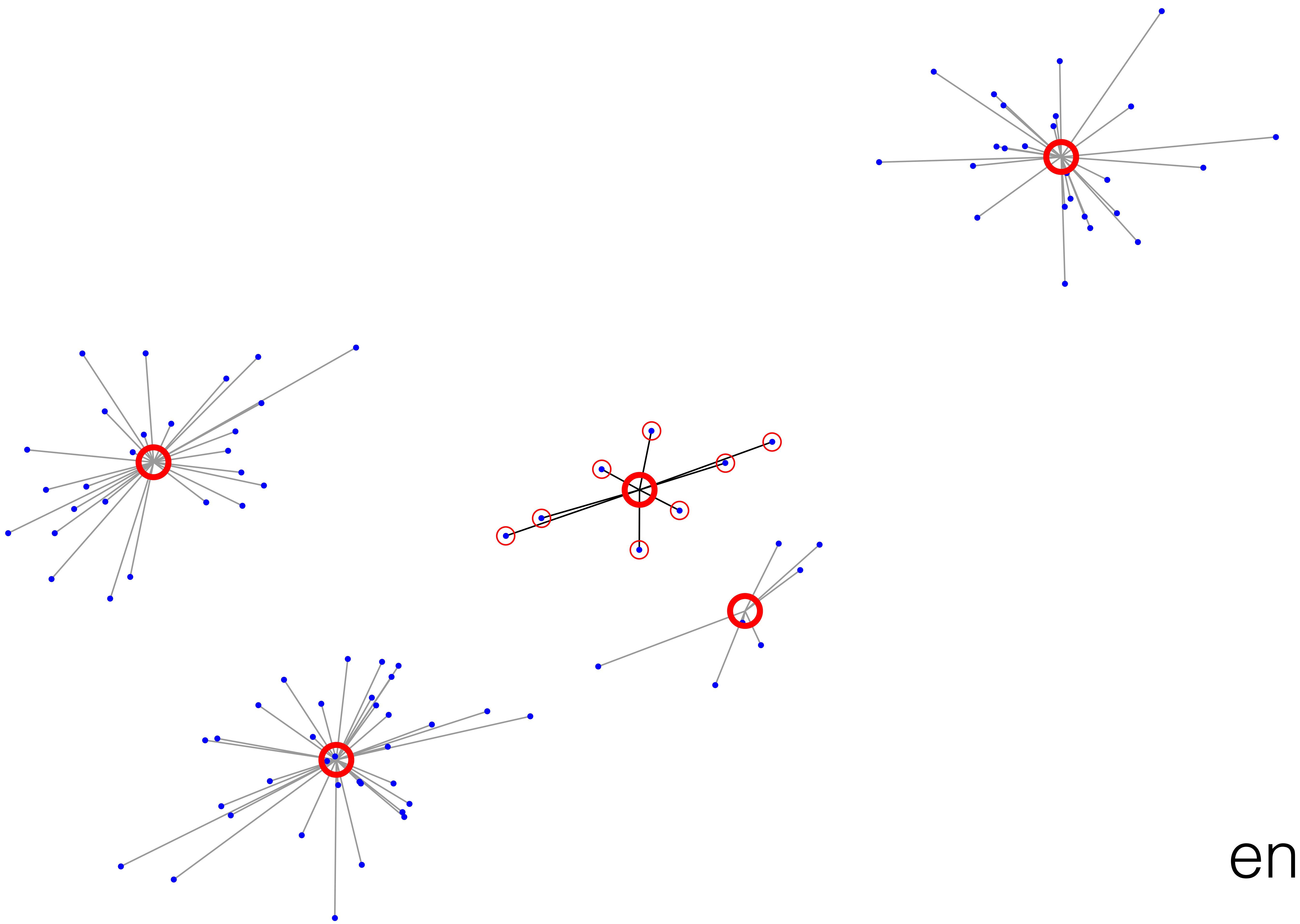
end of iteration 5

Example



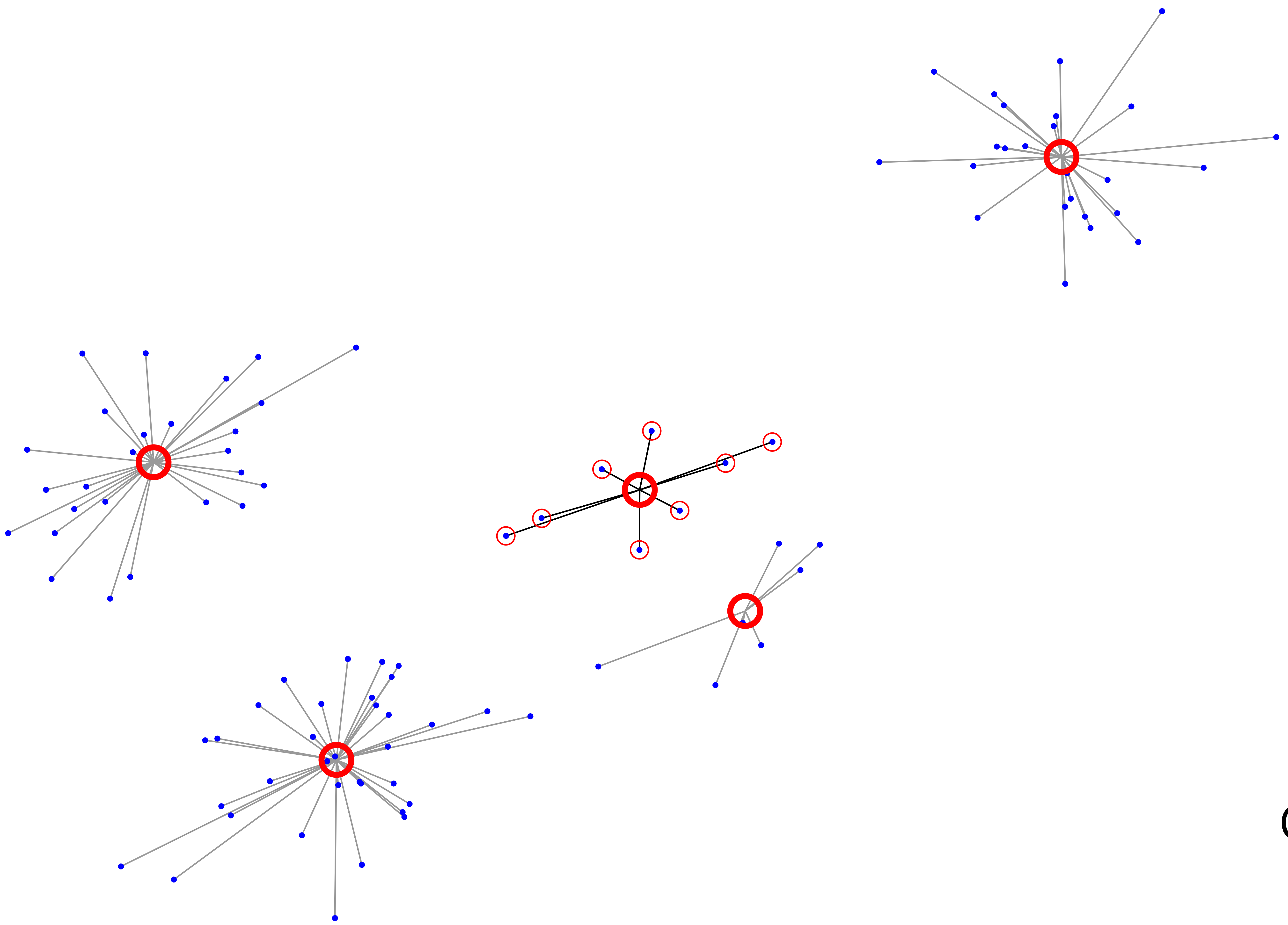
end of iteration 6

Example



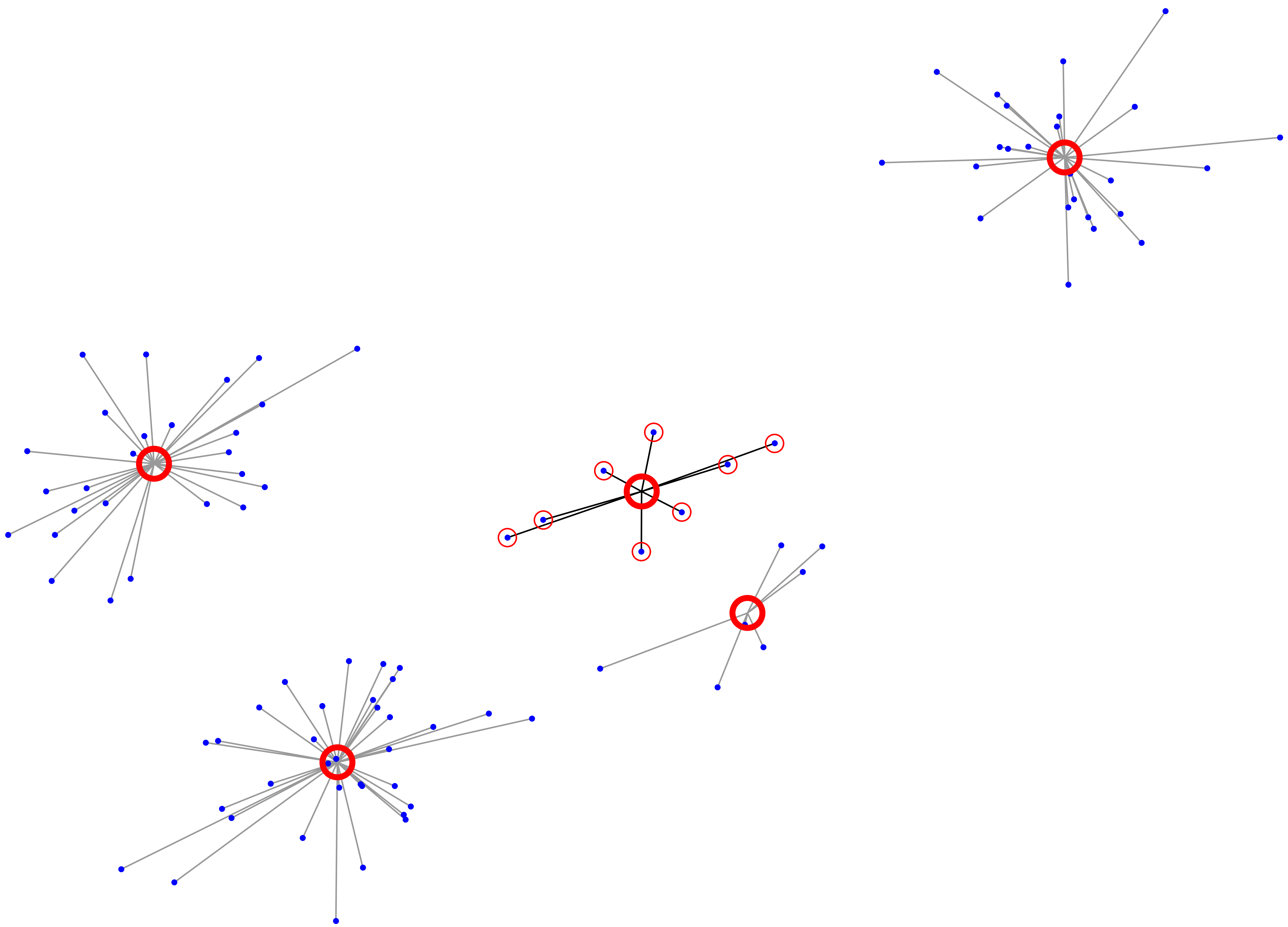
end of iteration 7

Example



converged at
iteration 8

Example



Summary of Variational EM

- Used Jensen's inequality to derive lower bound on log marginal likelihood

- Bound uses variational distribution **q**. We get to choose what family of **q** distributions to consider

- Using fully-factorized multinomial distributions for **q** gets EM

- Fully-factorized point distributions gets "hard"-EM, and using fixed, spherical covariance gets K-means