Mixture Models & EM

Lecture outline

- Brief review
  - what k-means CANNOT do
- How to model each cluster?
  - e.g., spherical Gaussians (brief review)
- Mixture Models
  - motivation, formulation
  - estimation, the EM algorithm
  - selecting the number of mixture components

Recall: K-means

- K-means clustering
  - initialize K different means
  - assign each data point to the closest cluster mean
  - re-estimate cluster means based on the points assigned to them
  - iterate until convergence

What K-means cannot do?

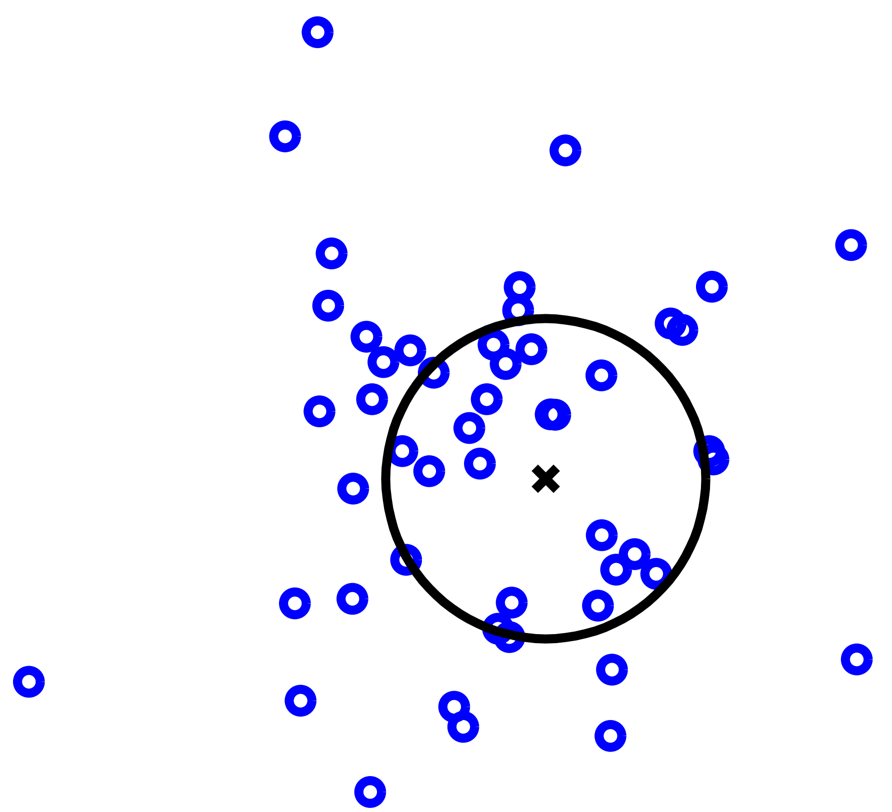
- It cannot handle overlapping clusters
- It cannot represent clusters with different “spreads”
- It cannot properly deal with clusters that have different numbers of points

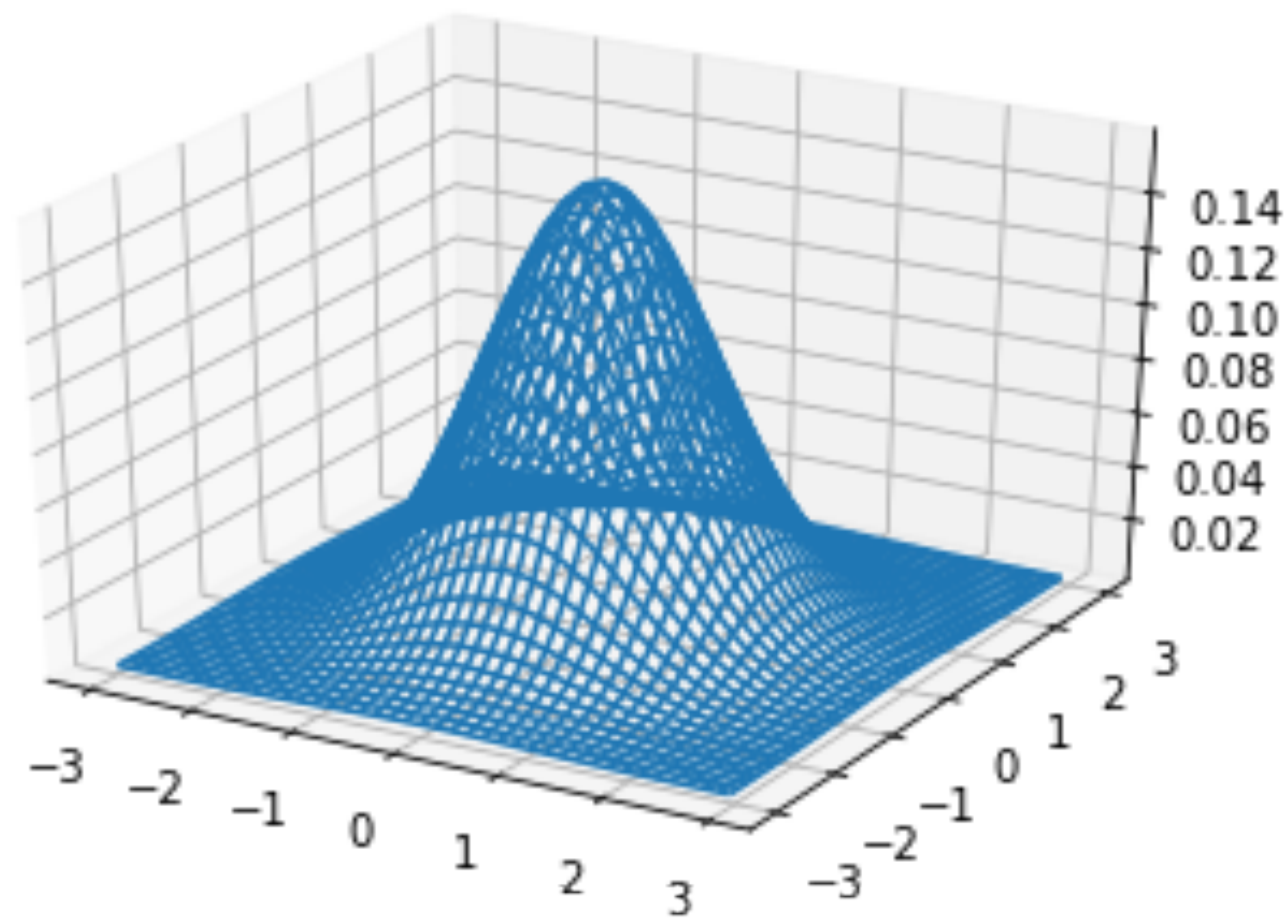
Recall: spherical Gaussian

- The pdf of a spherical Gaussian

$$N(x; \mu, \sigma^2 I) = \frac{1}{(2\pi\sigma^2)^{d/2}} \exp\left(-\frac{1}{2\sigma^2} \|x - \mu\|^2 \right)$$

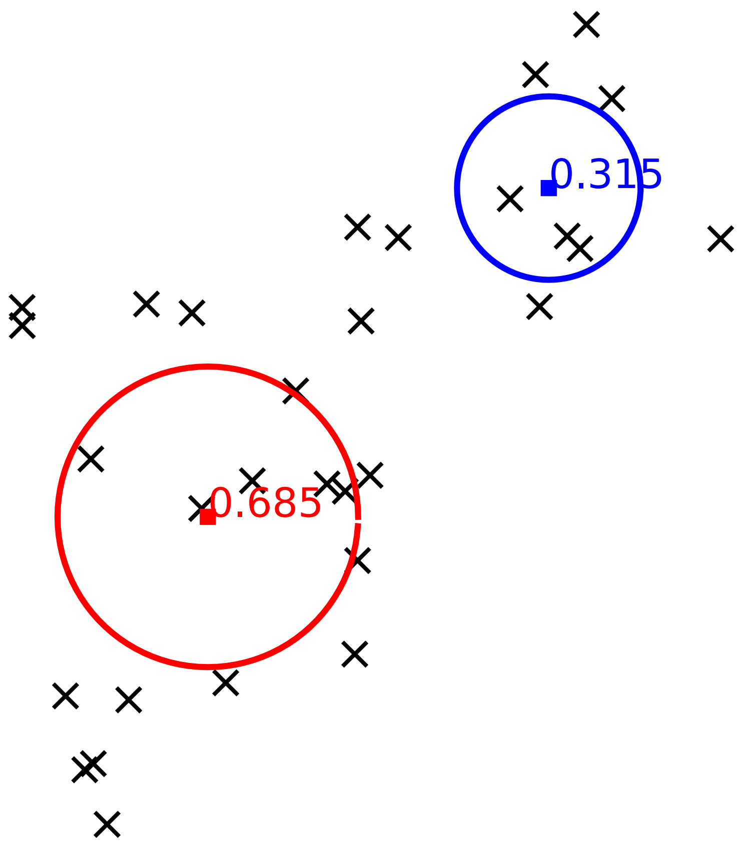
- Graphical representation (when dim d = 2) in terms of mean and stdv





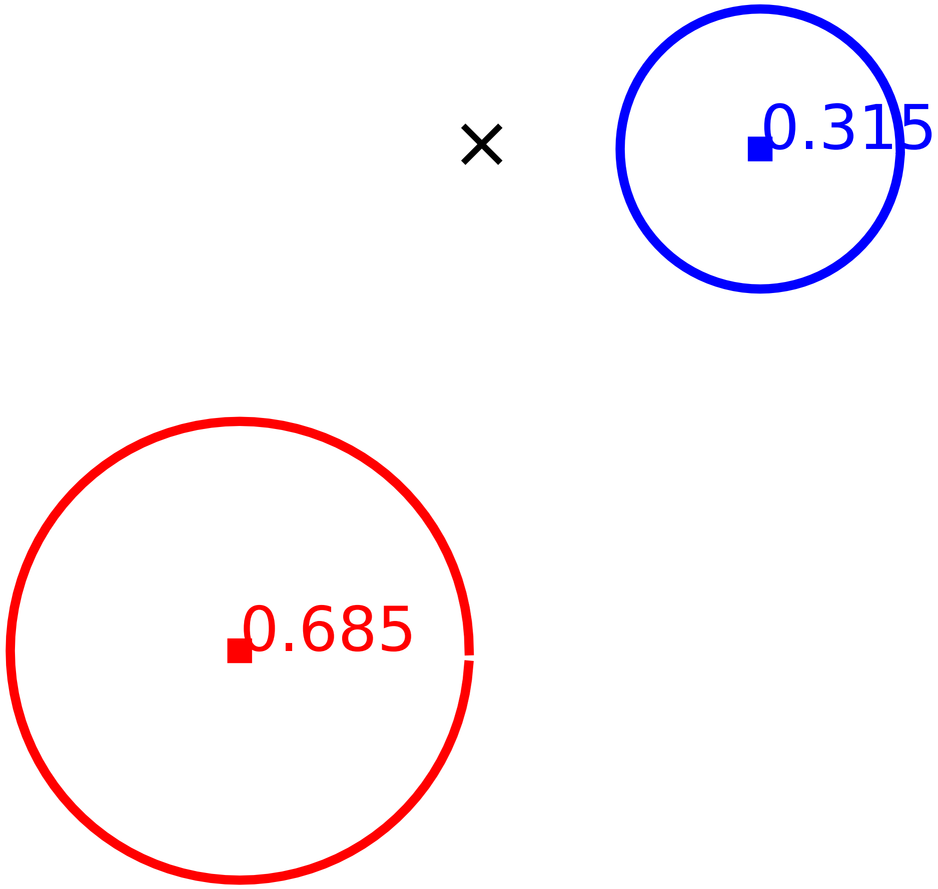
Mixture model: overview

- We use a spherical Gaussian to model each cluster
- These cluster models can have different means, variances (spreads), as well as "sizes"
- A mixture model combines these "components" into an overall probability model $P(x;\theta)$



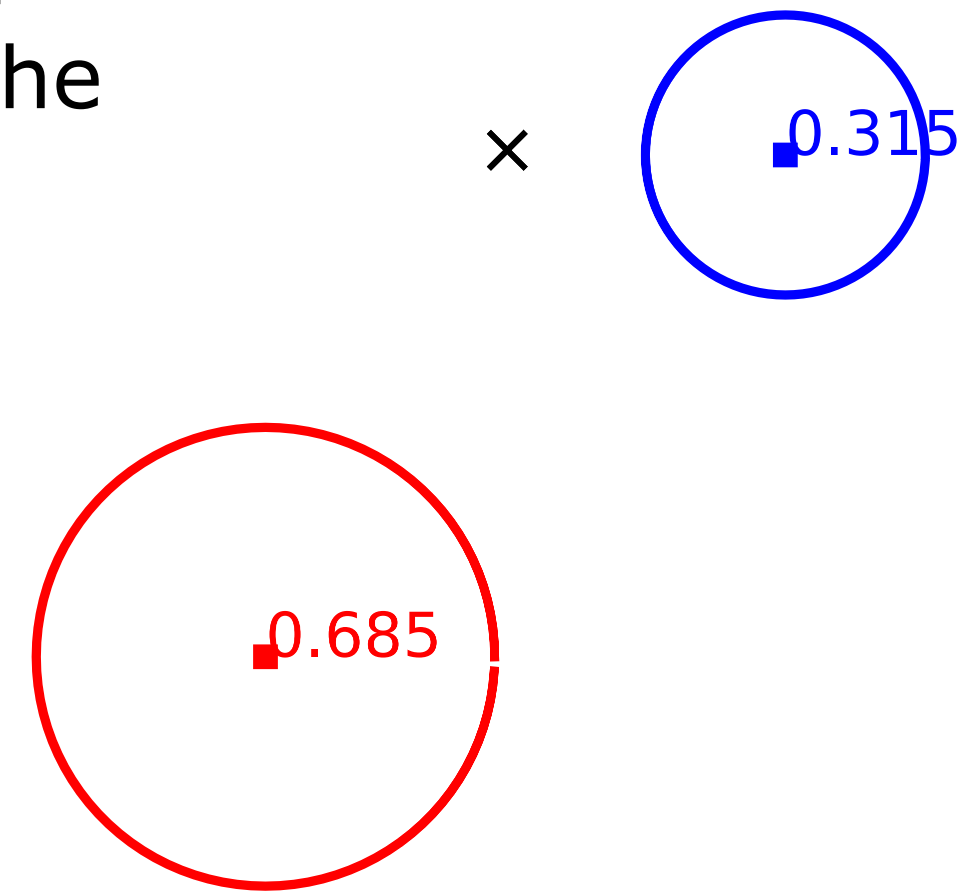
Mixture model: data generation

- We consider alternative ways that each data point x could have been created



Mixture model: data generation

- We consider alternative ways that each data point x could have been created:
  - select a cluster
  - select x from the cluster model



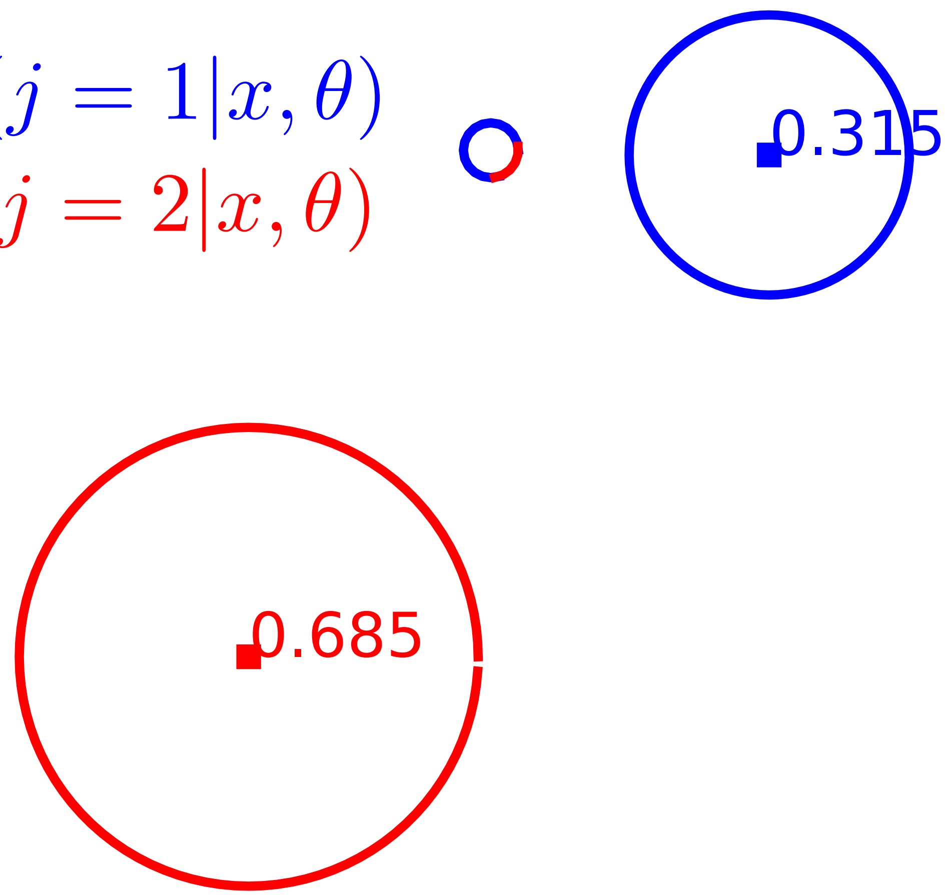
$$P(x;\theta) = p_1 N(x;\mu^{(1)},\sigma_1^2 I) + p_2 N(x;\mu^{(2)},\sigma_2^2 I)$$

Mixture model: posterior

- We can also infer (after the fact) which cluster likely generated each point by evaluating the posterior probability

$P(j = 1|x, \theta)$

$P(j = 2|x, \theta)$



$$P(j = 1|x, \theta) = \frac{p_1 N(x; \mu^{(1)}, \sigma_1^2 I)}{p_1 N(x; \mu^{(1)}, \sigma_1^2 I) + p_2 N(x; \mu^{(2)}, \sigma_2^2 I)}$$

Mixture models: estimation

- The goal is to find the parameters of the mixture model that maximize the log-likelihood that the data points came from the mixture distribution

$$l(D;\theta) = \sum_{i=1}^{n} \log P(x^{(i)};\theta)$$

$$= \sum_{i=1}^{n} \log \left[\sum_{j=1}^{K} p_j N(x^{(i)}; \mu^{(j)}, \sigma_j^2 I) \right]$$

- The difficulty lies in the fact that the Gaussian cluster models cannot be estimated independently (since we don't know which data points they should generate)

The EM algorithm: overview

- The EM algorithm solves the problem by iteratively re-assigning points to clusters (softly) and re-estimating the corresponding cluster models (cf. K-means)

- **Initialize** mixture

- **E-step** (complete the data)
  - evaluate the posterior probability that each data point came from a particular cluster

- **M-step** (maximize expected log-likelihood)
  - use the posterior probabilities (now fixed) as cluster specific weights on data points to separately re-estimate each cluster model

The EM algorithm (iterative)

- **Initialize:**
  - e.g. means as randomly selected points, all variances set to overall variance, uniform mixing proportions
- **E-step:** calculate posterior assignments

$$p(j|i) = \frac{p_j N(x^{(i)}; \mu^{(j)}, \sigma_j^2 I)}{P(x^{(i)}|\theta)}, \quad j = 1, \ldots, K, \quad i = 1, \ldots, n$$

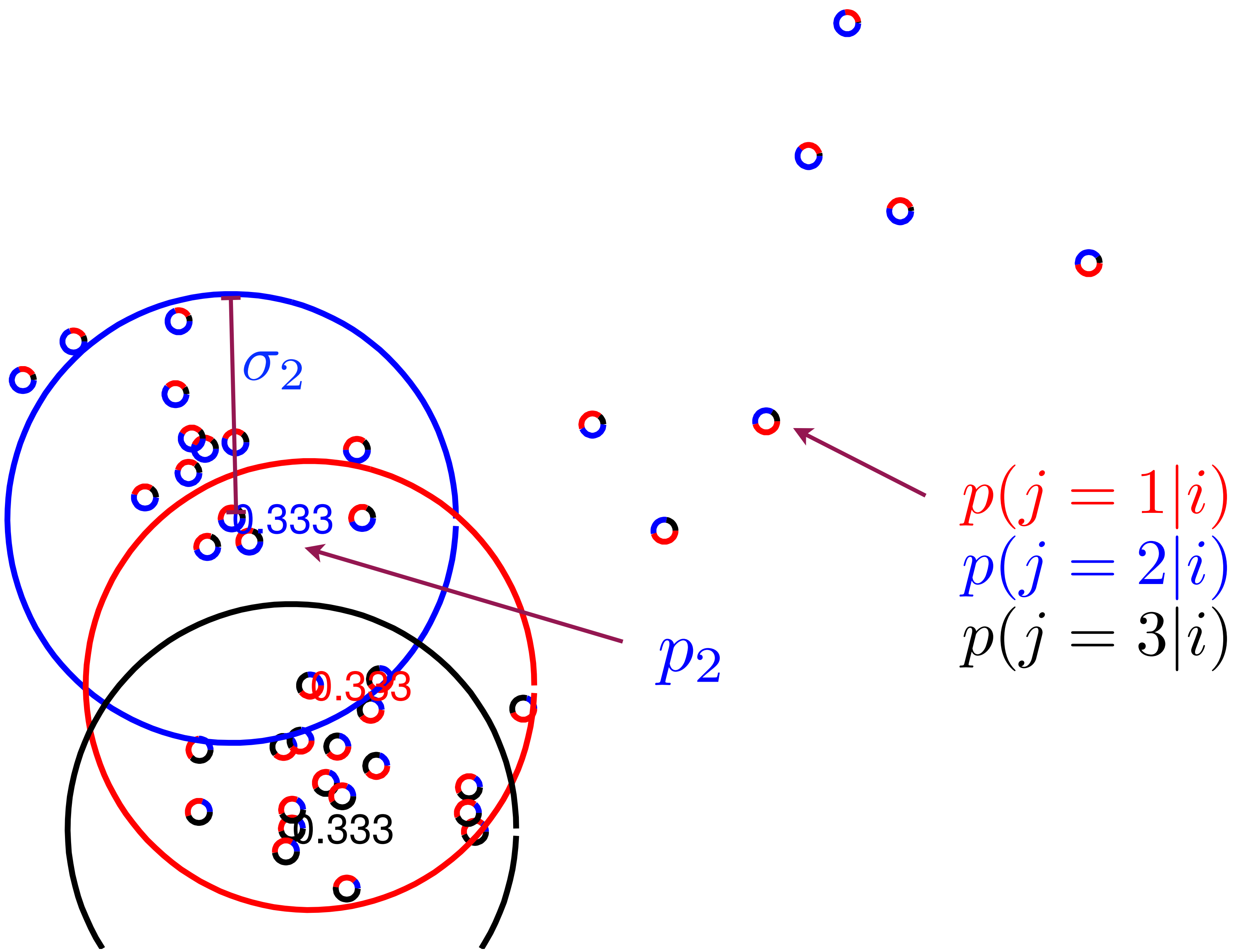
- **M-step:** maximize

$$\tilde{l}(D; \theta) = \sum_{j=1}^{K} \sum_{i=1}^{n} p(j|i) \log \left[\frac{p_j N(x^{(i)}; \mu^{(j)}, \sigma_j^2 I)}{p(j|i)} \right]$$

with respect to mixture parameters while keeping $p(j|i)$ fixed

Mixture of Gaussians example

- initial 3-component mixture



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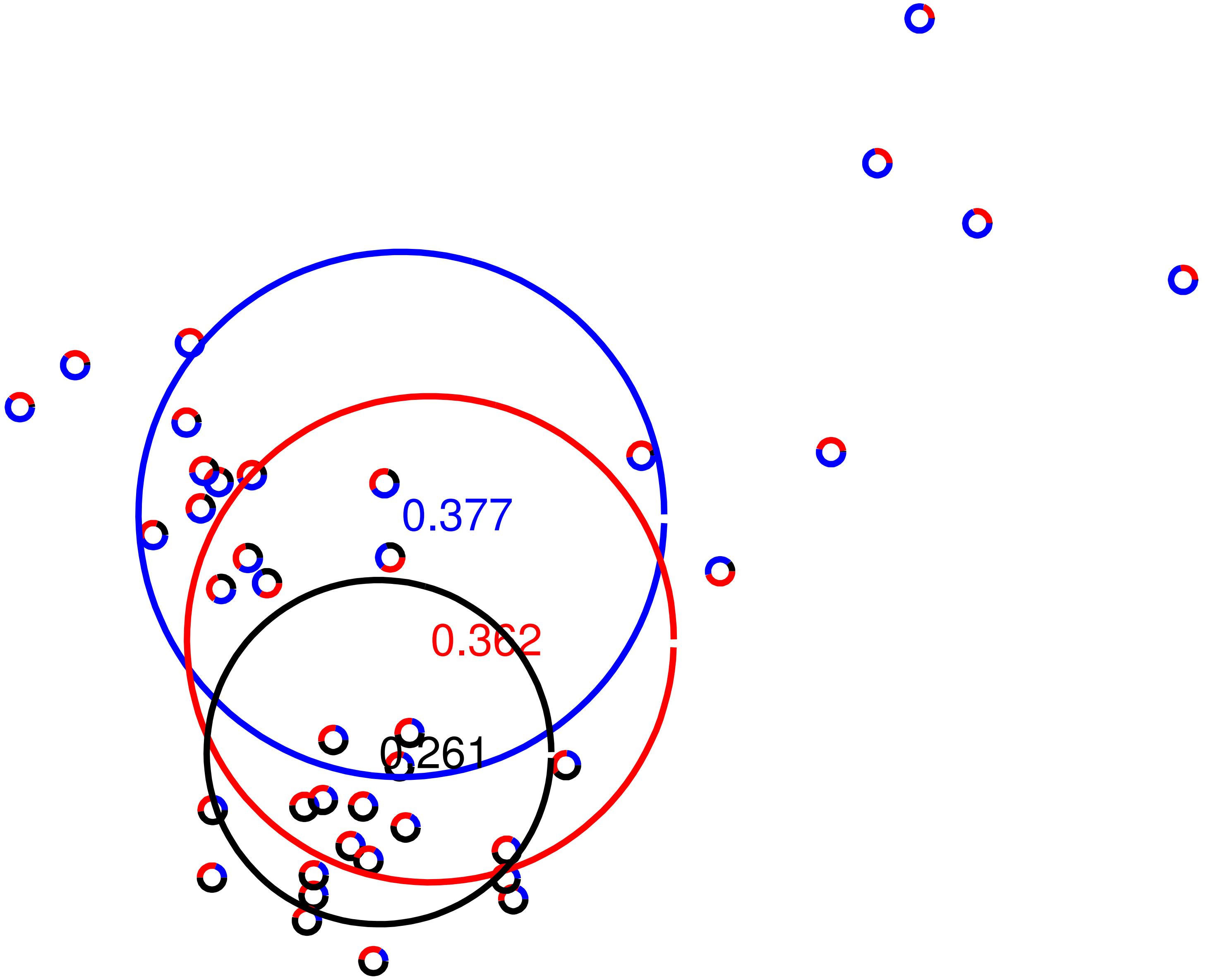

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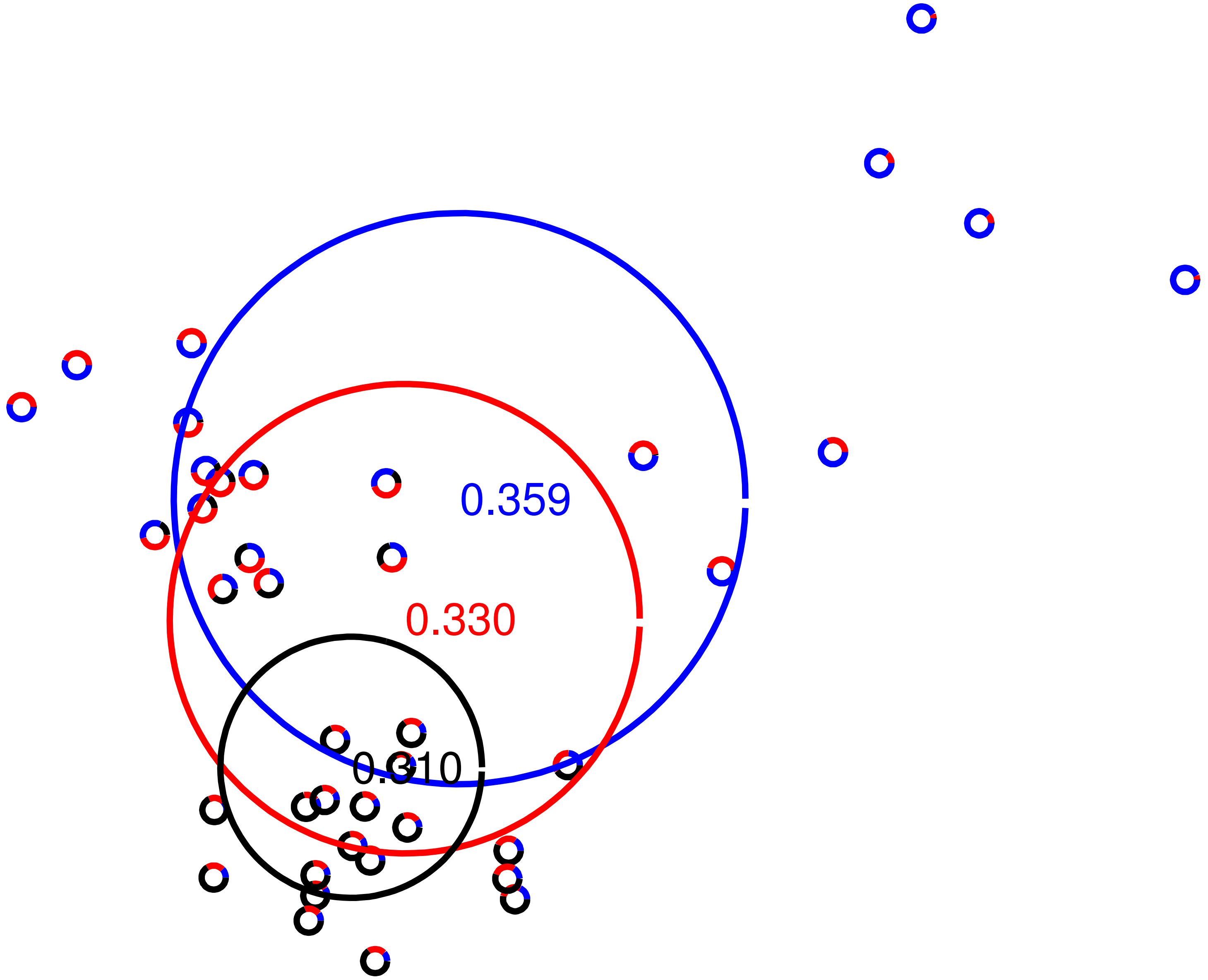

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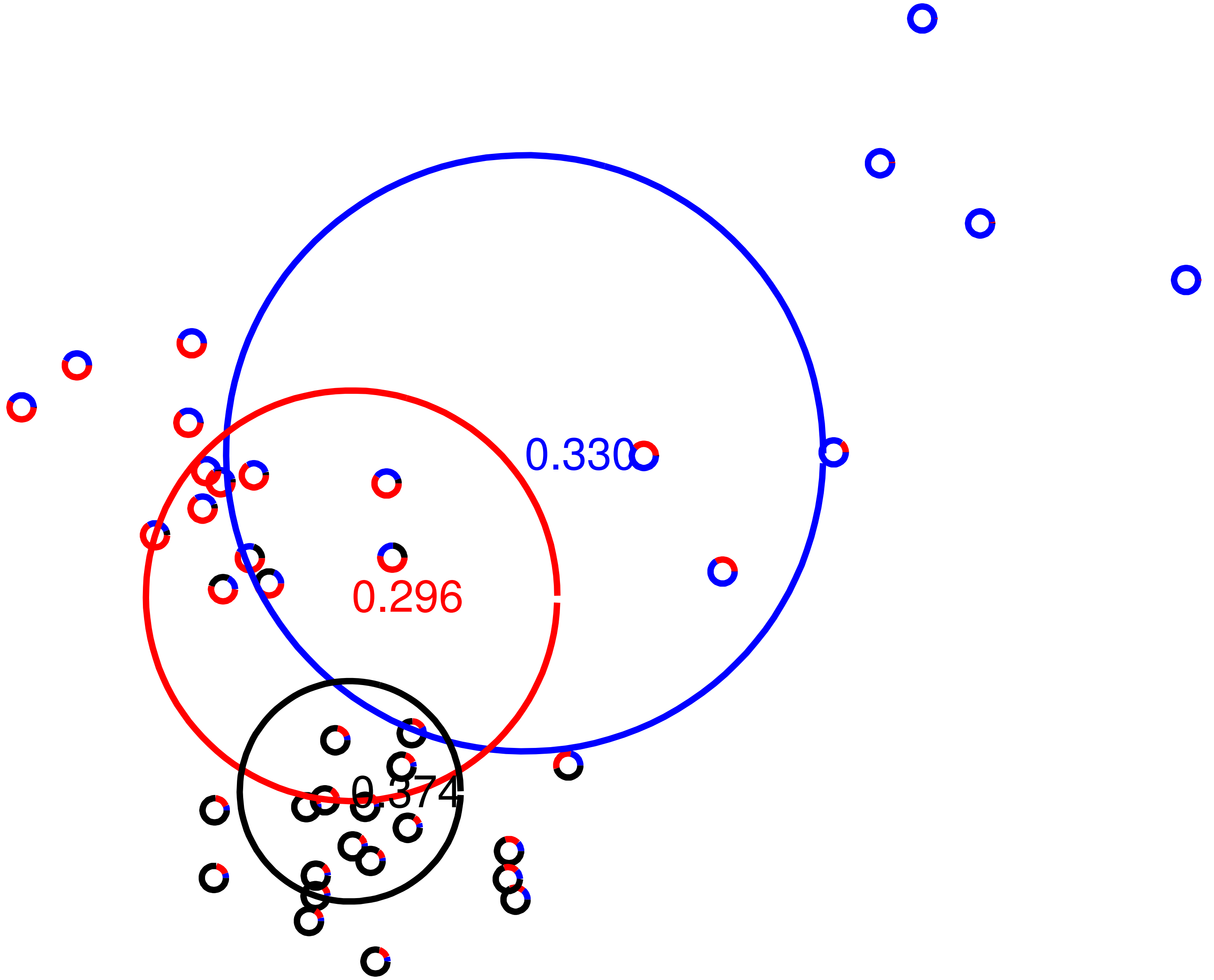

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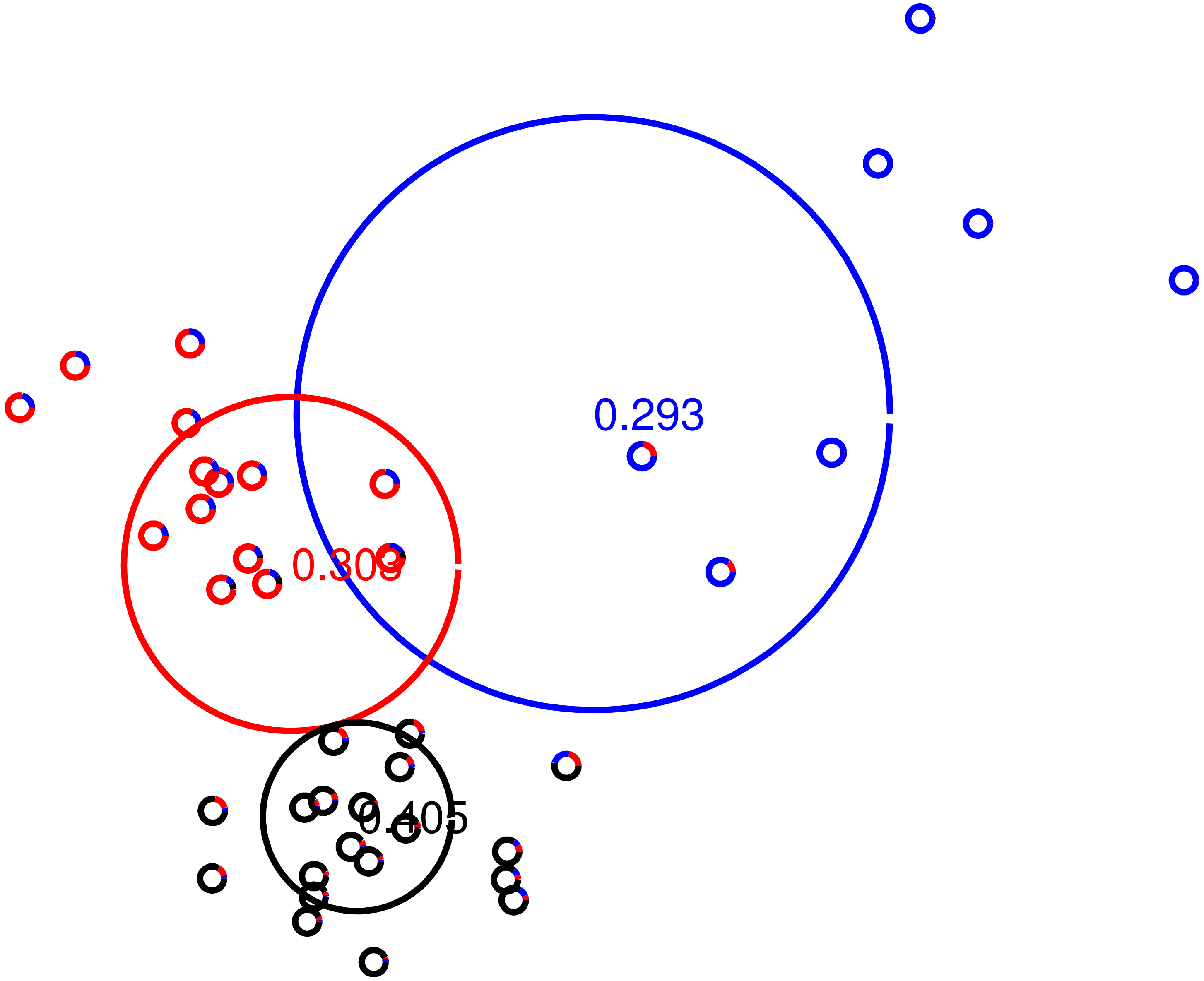

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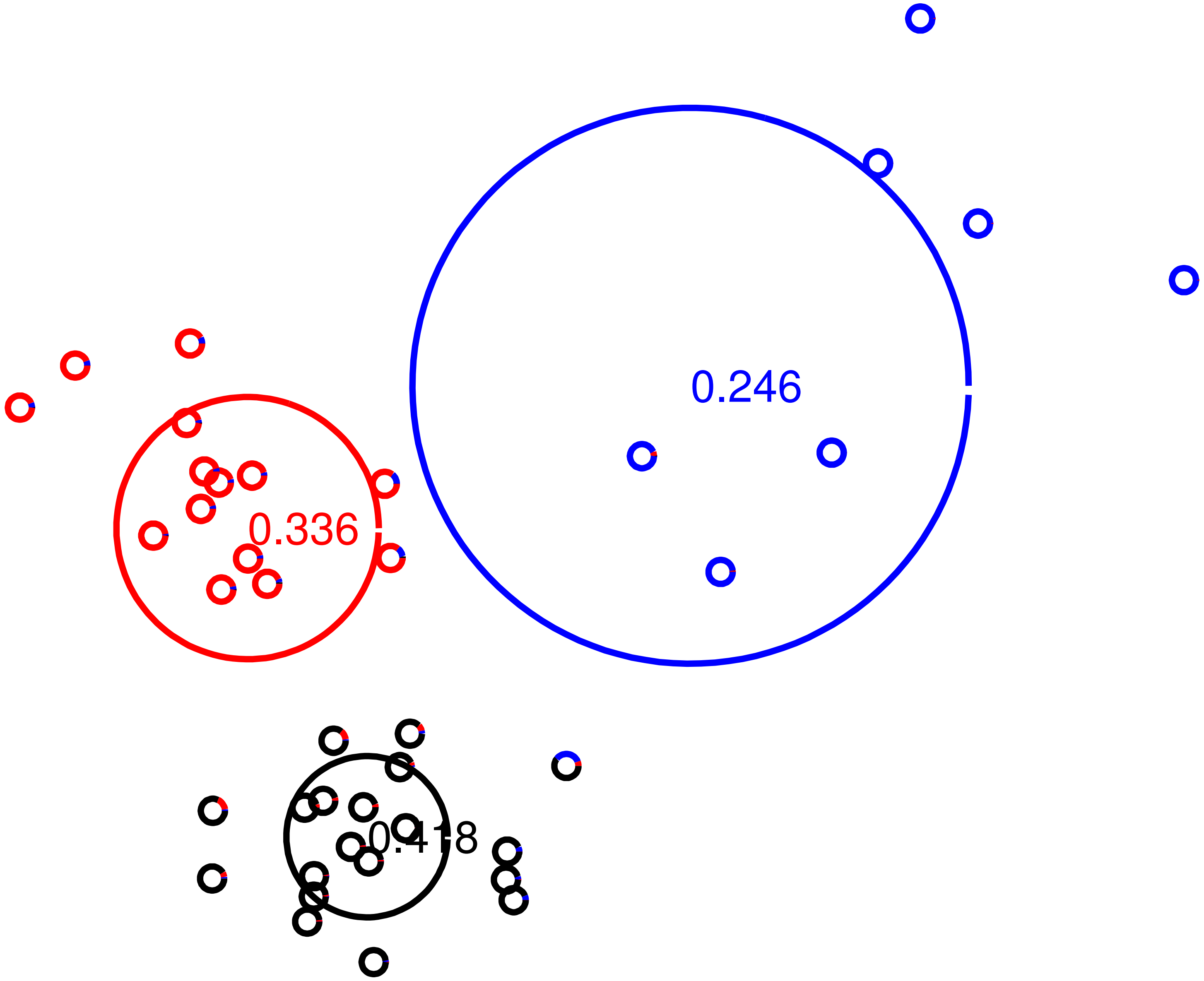

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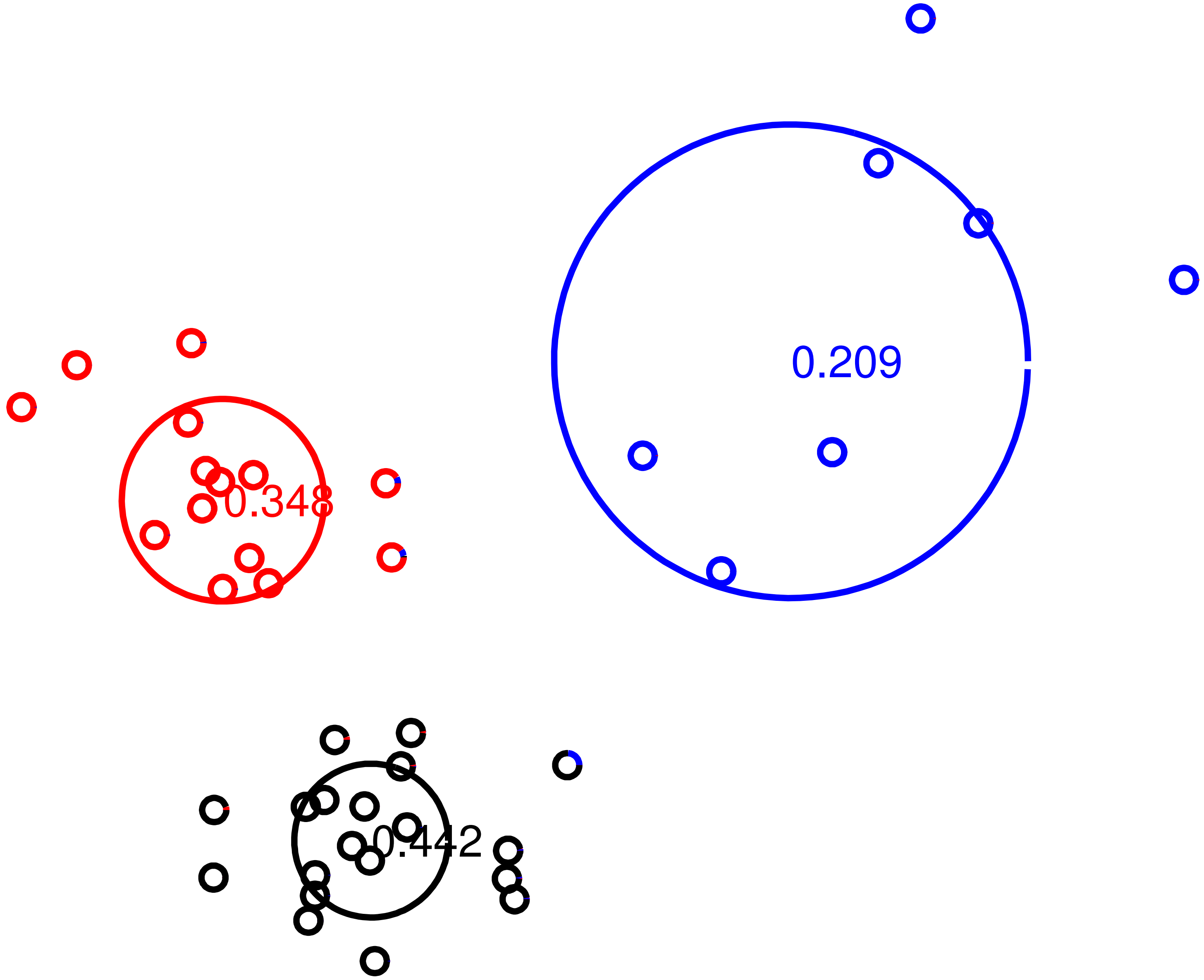

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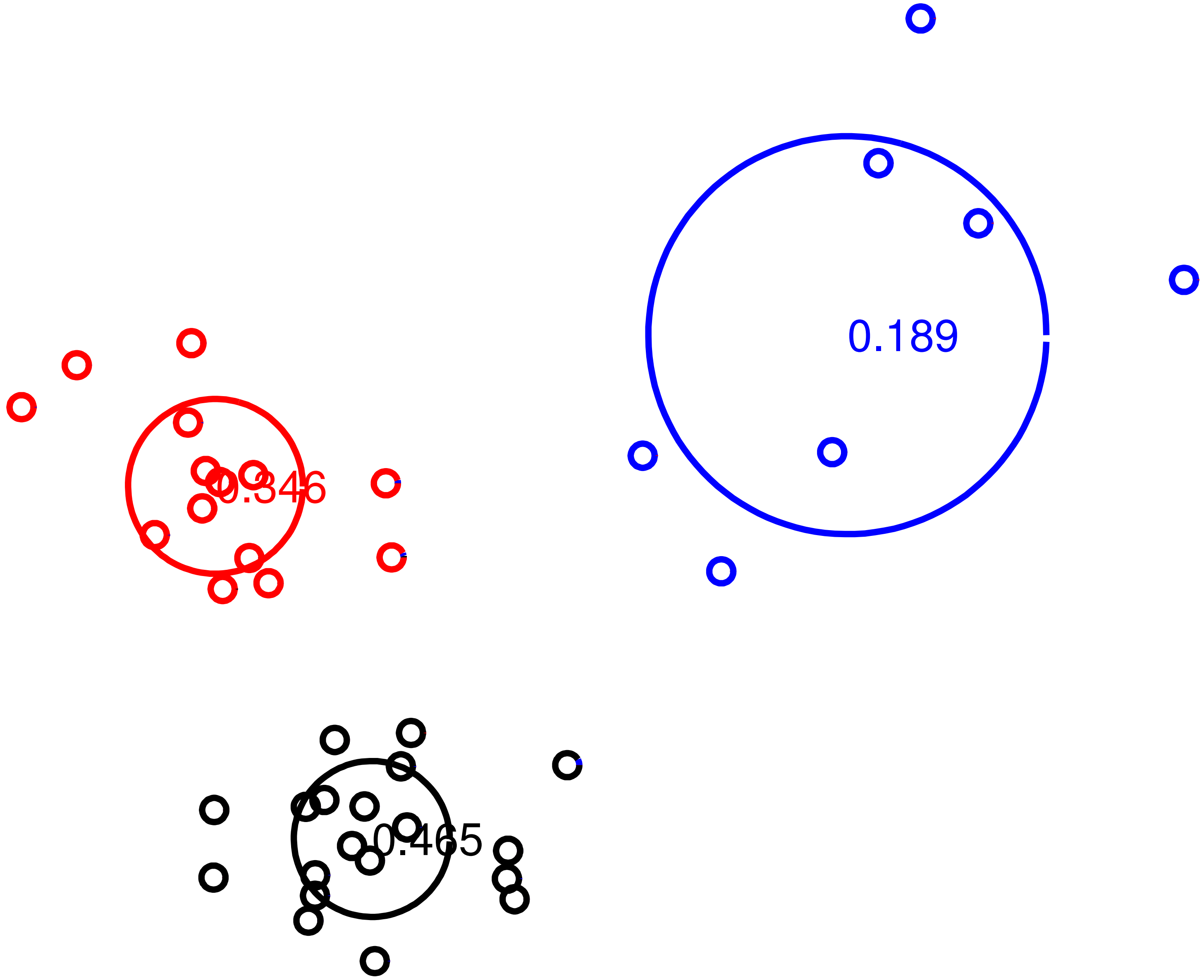

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Mixture of Gaussians example

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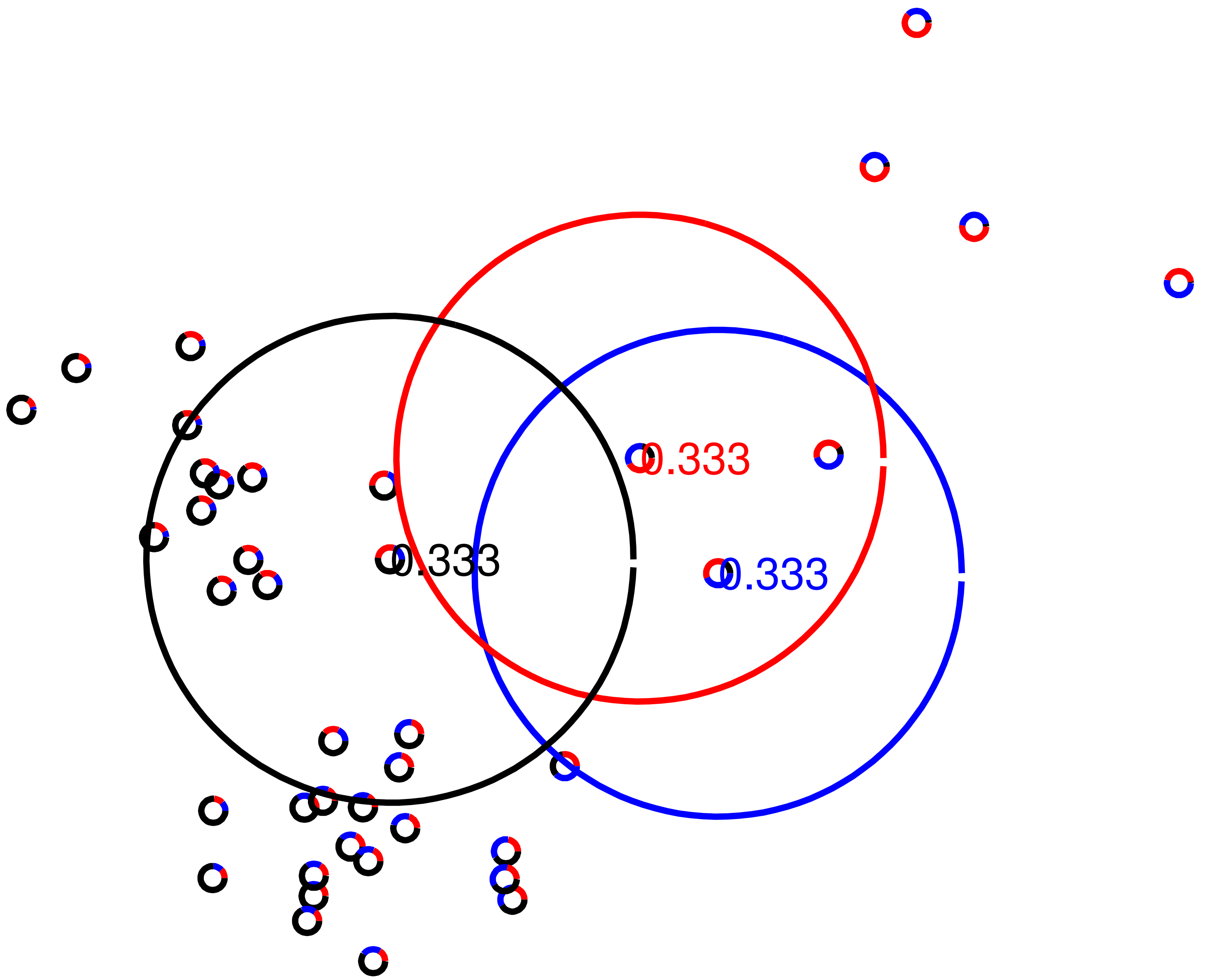

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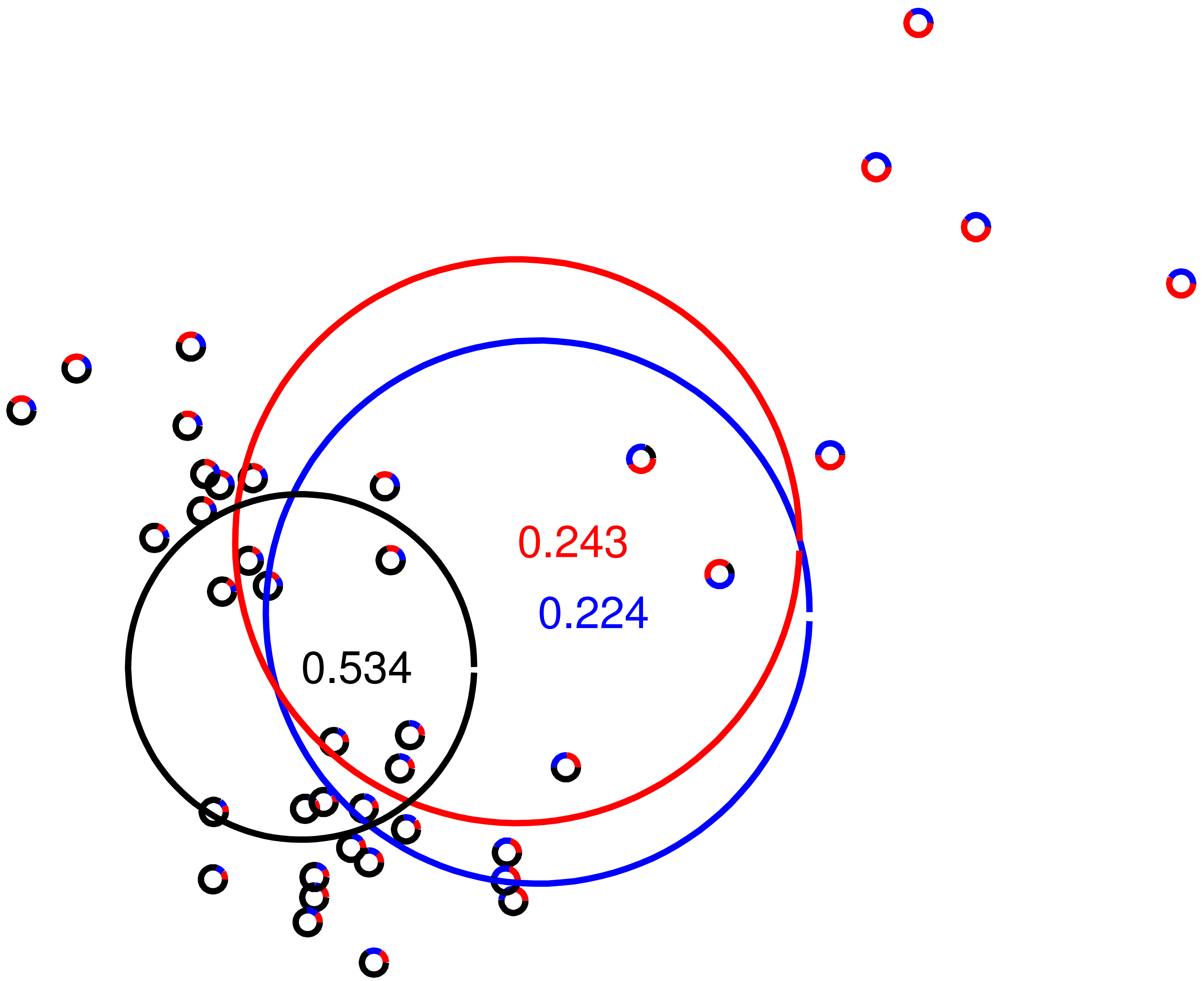

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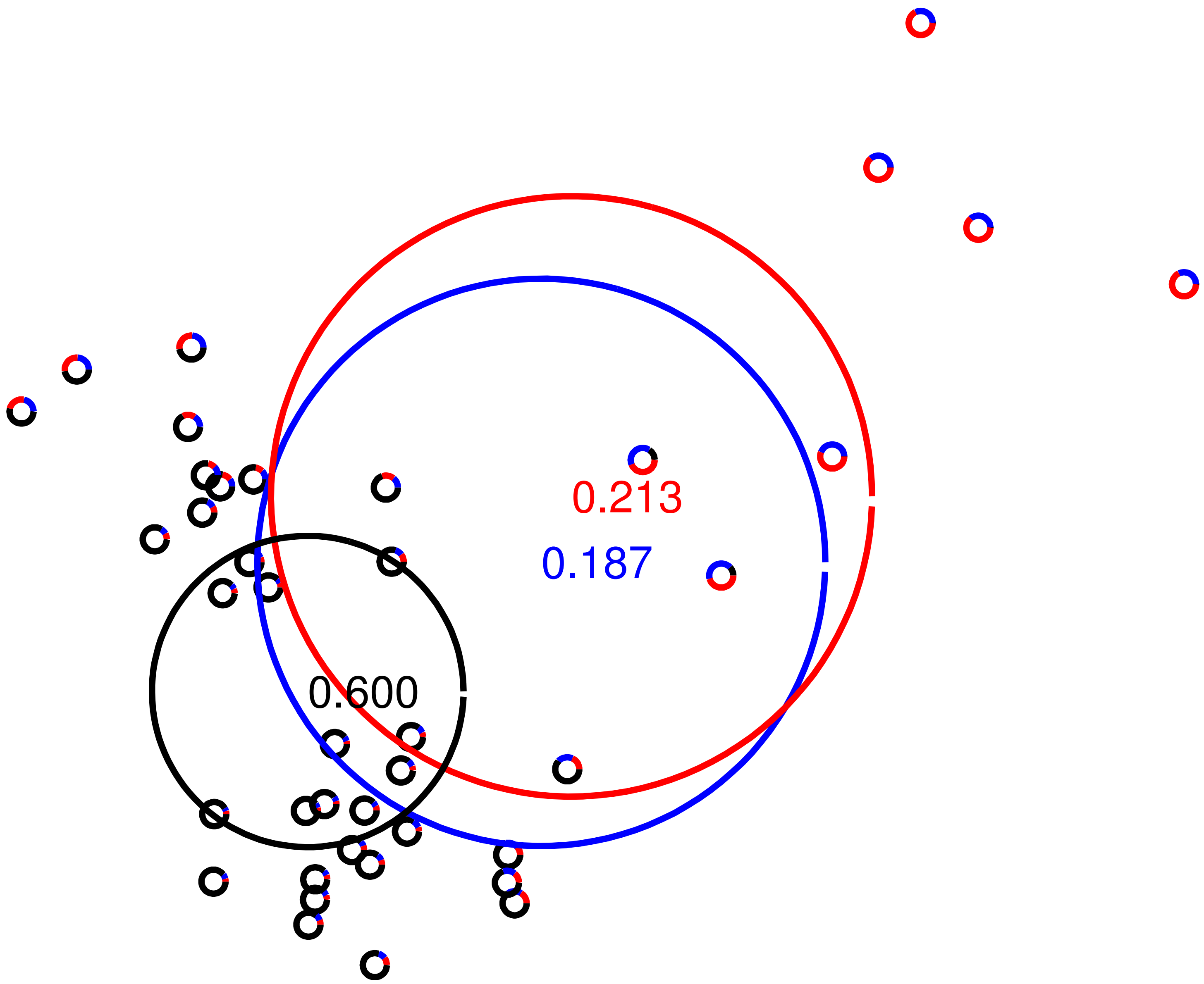

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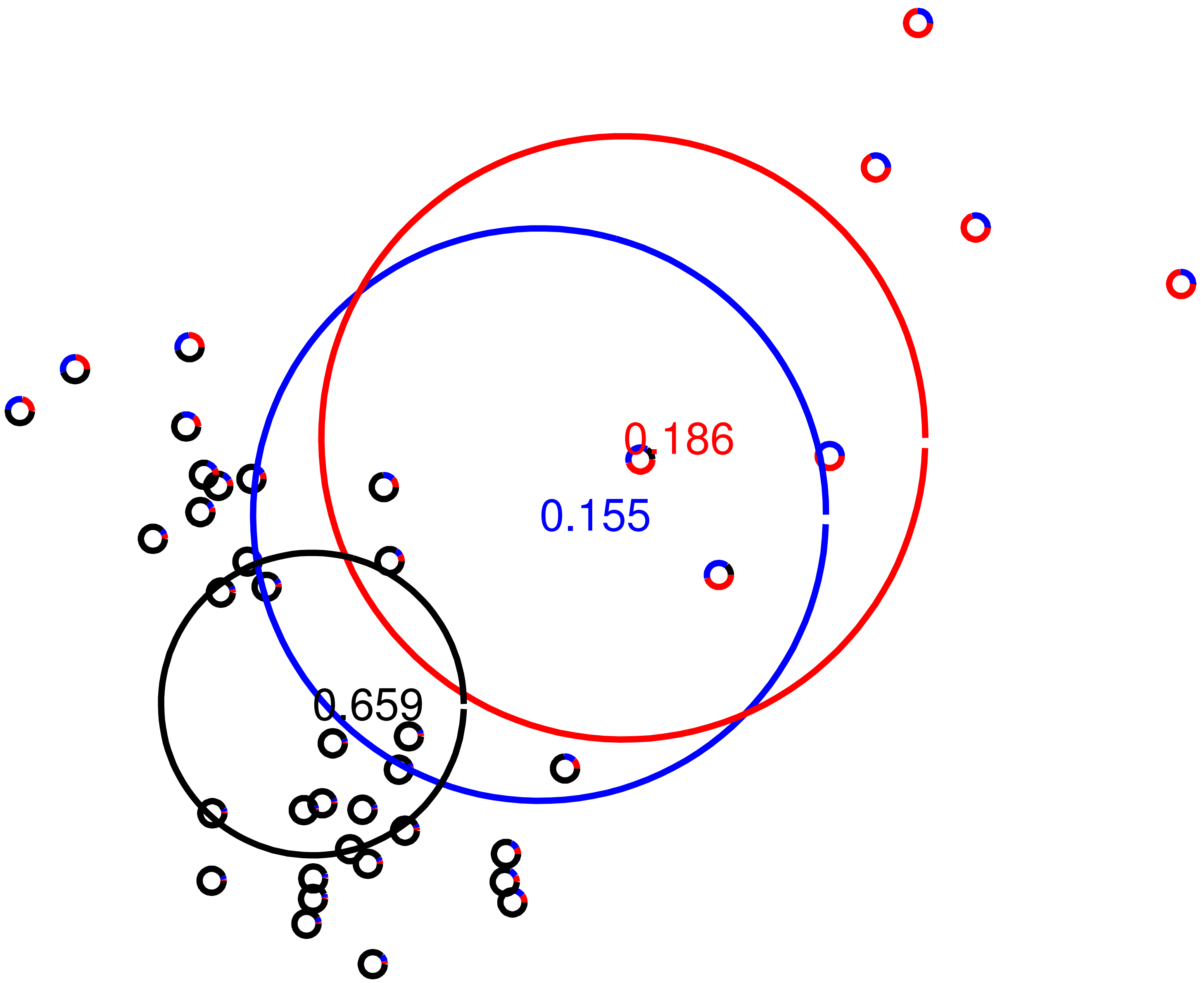

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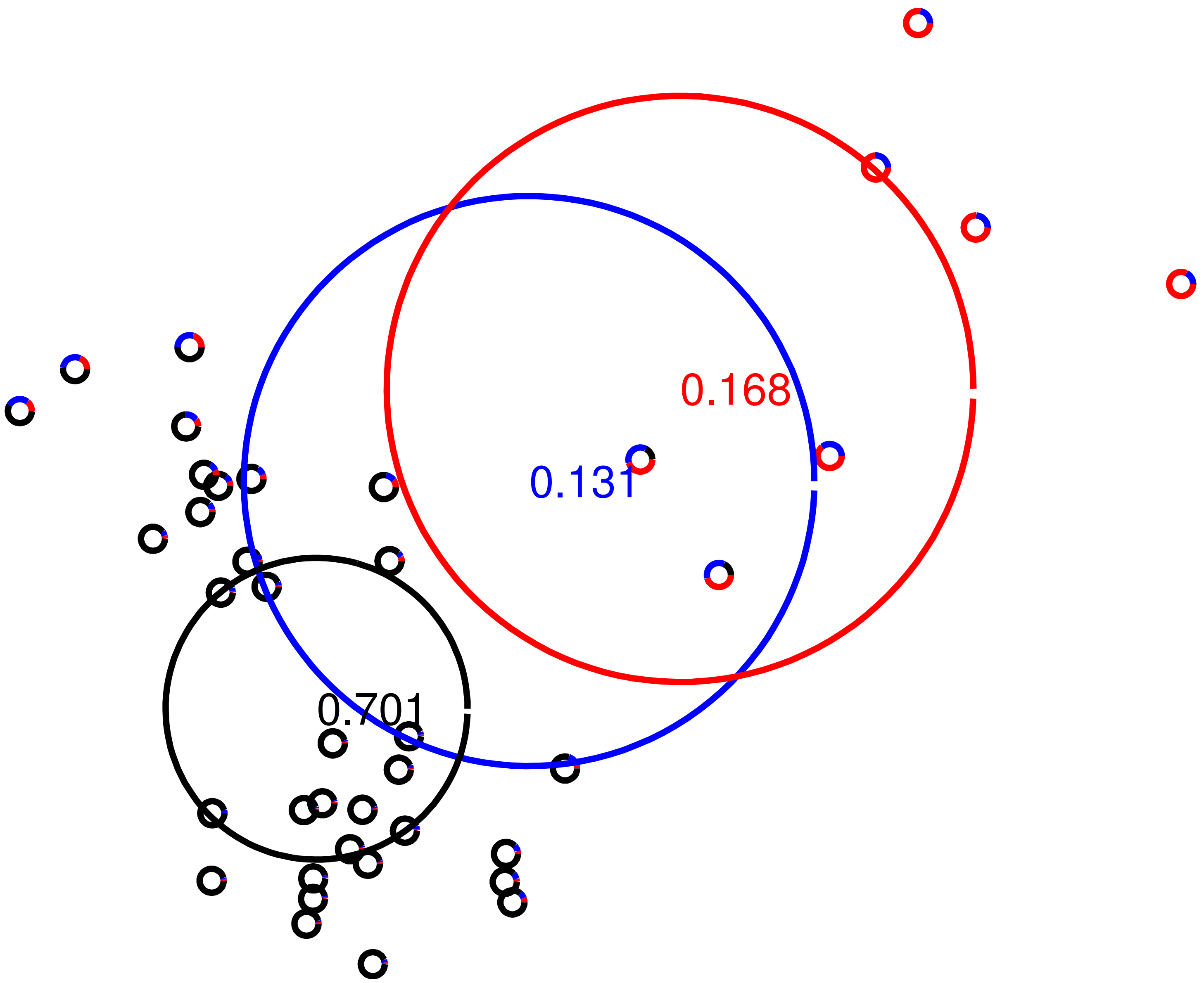

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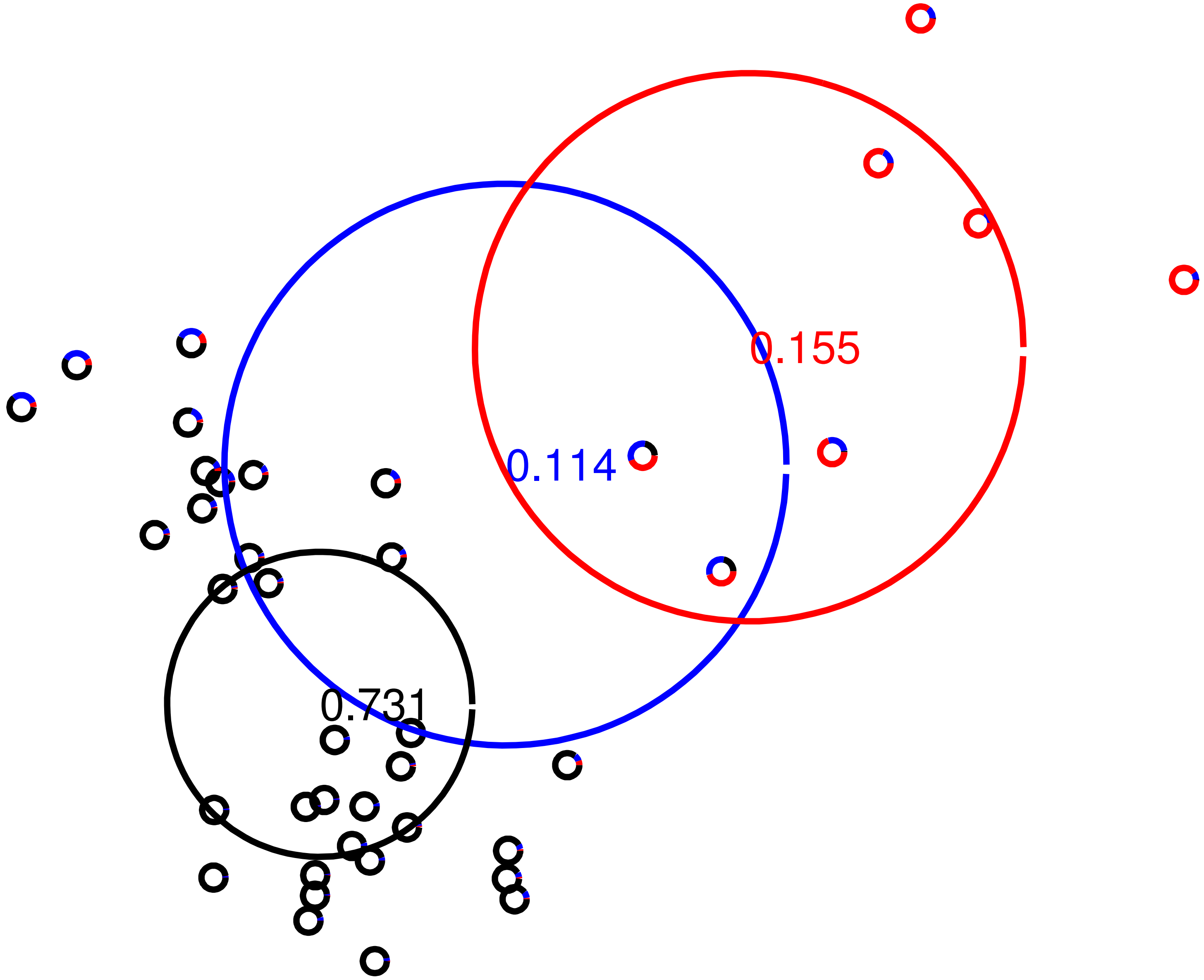

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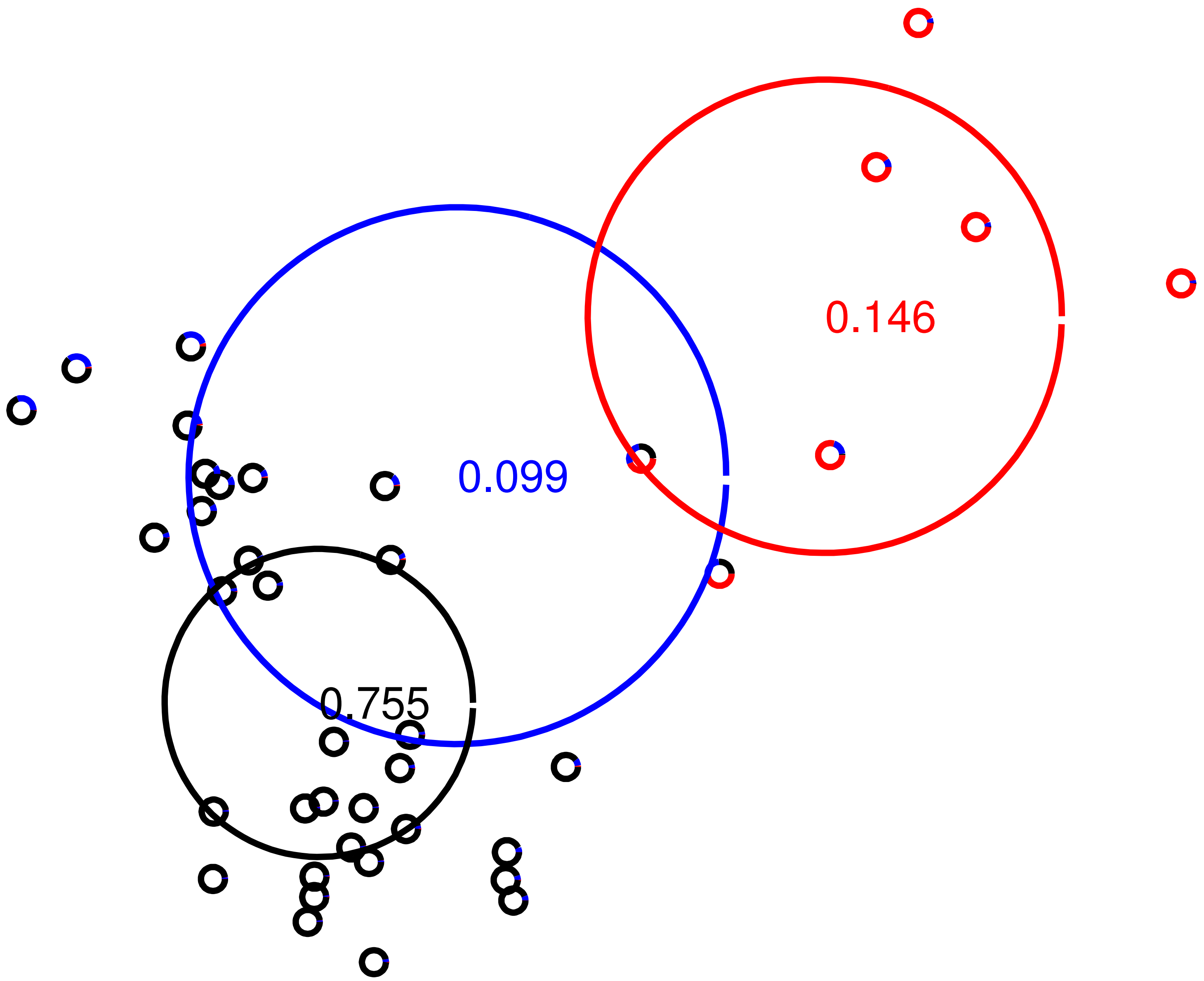

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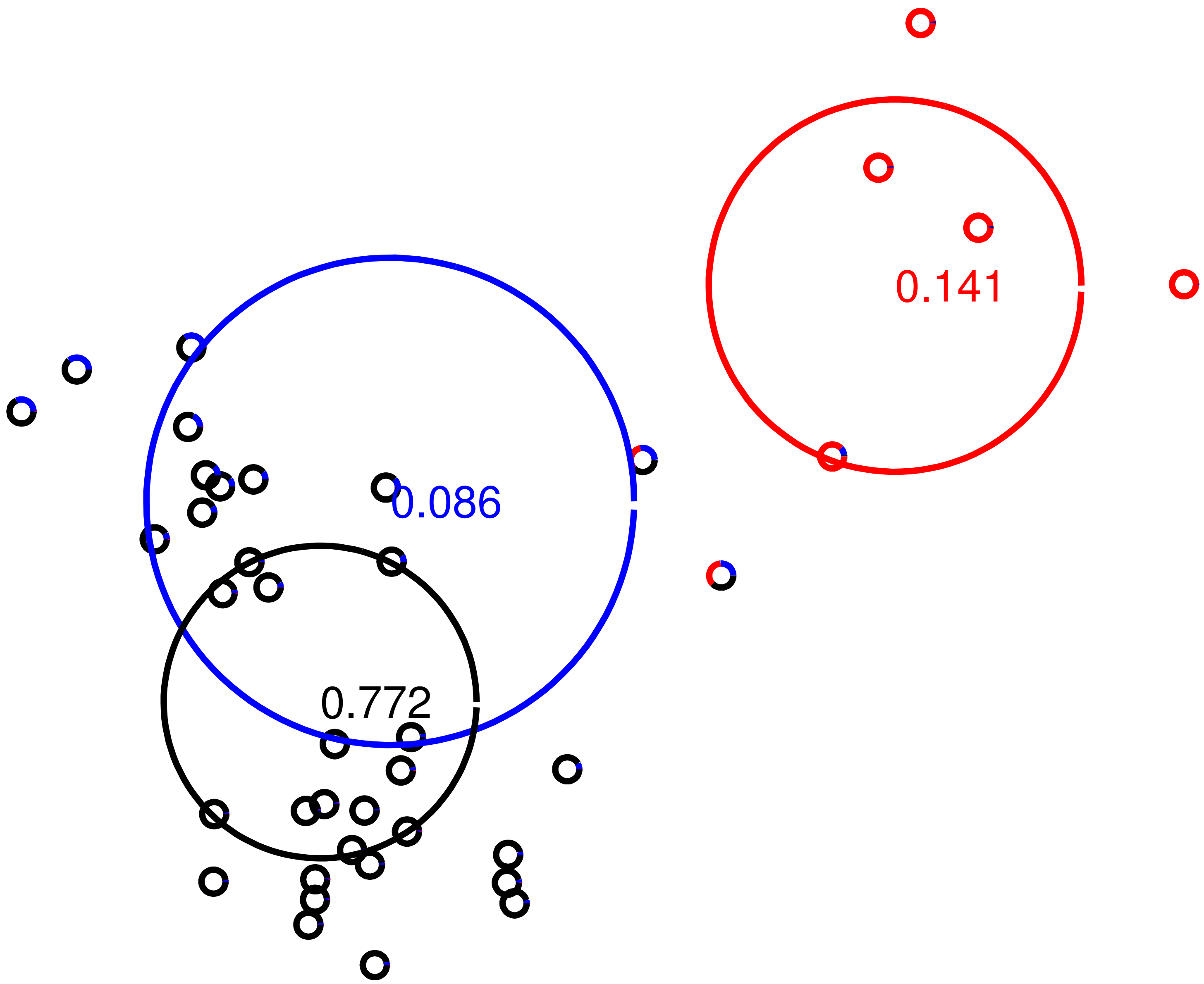

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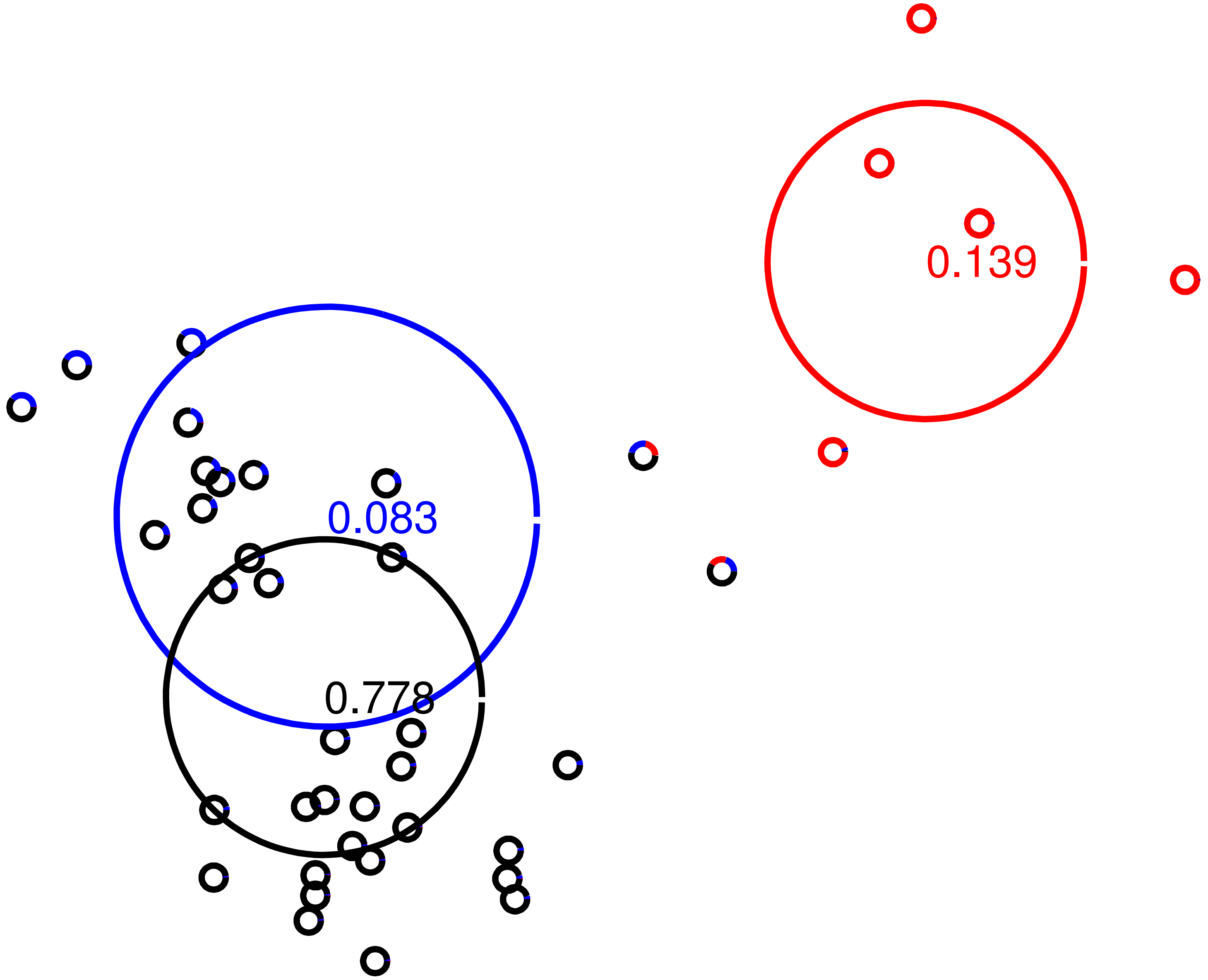

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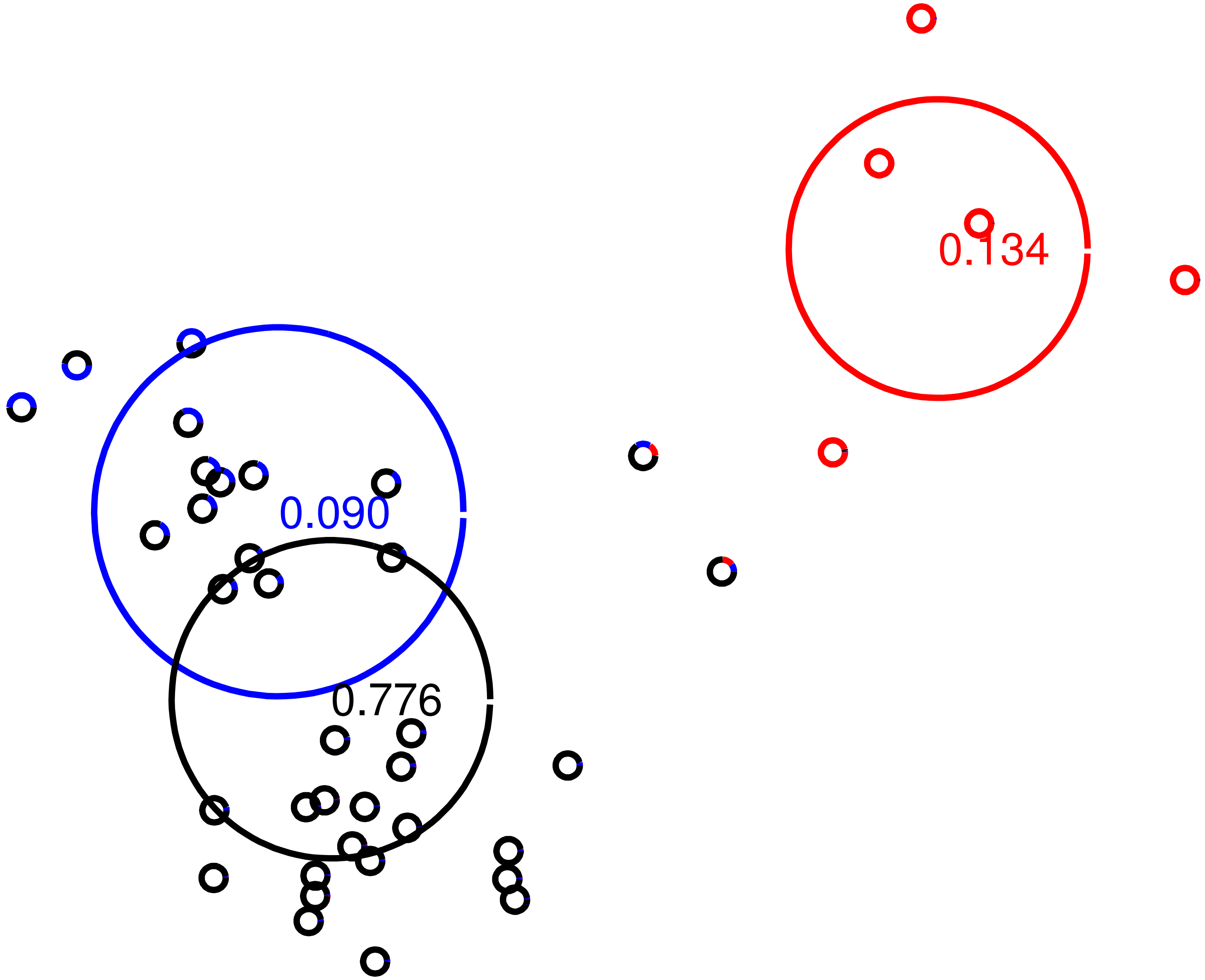

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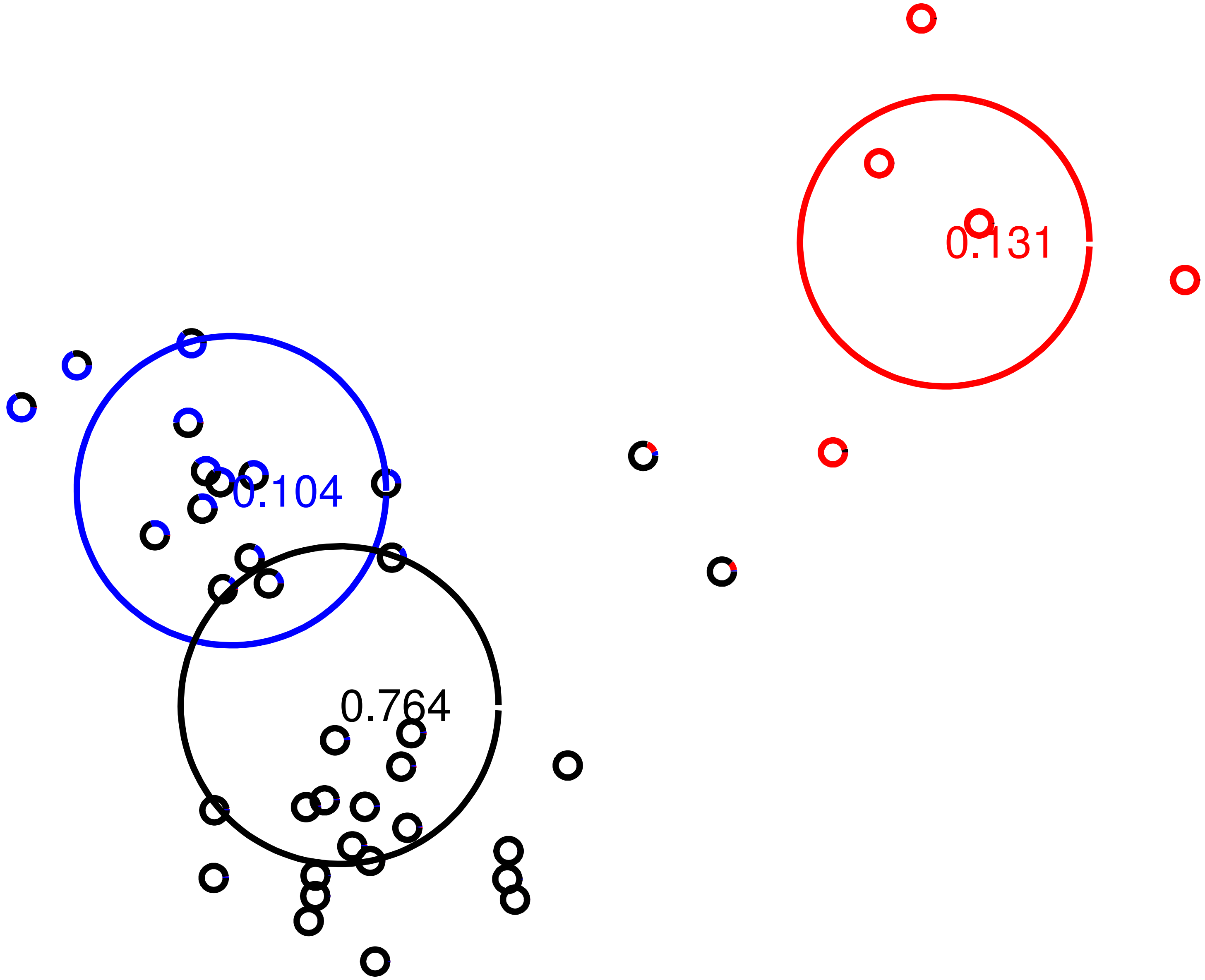

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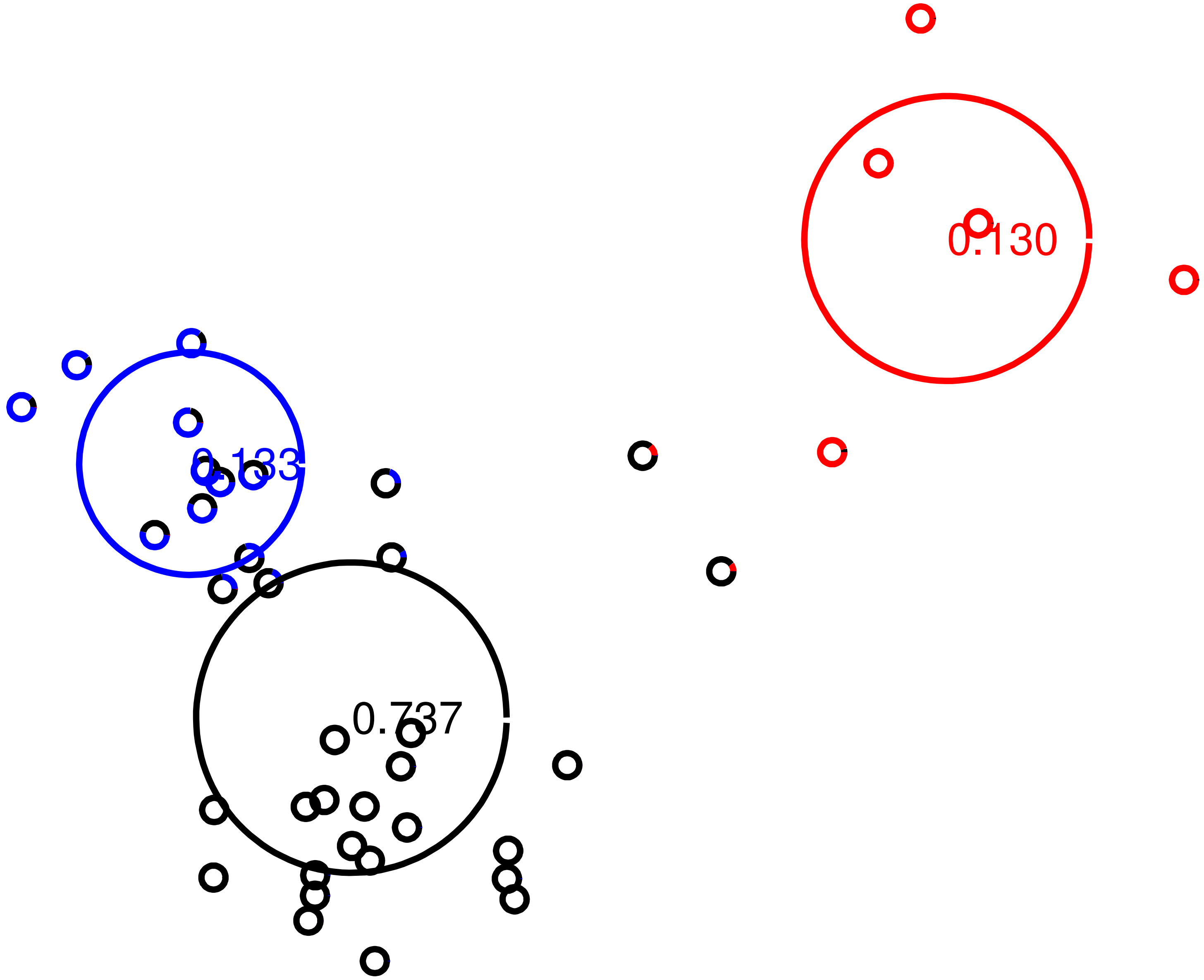

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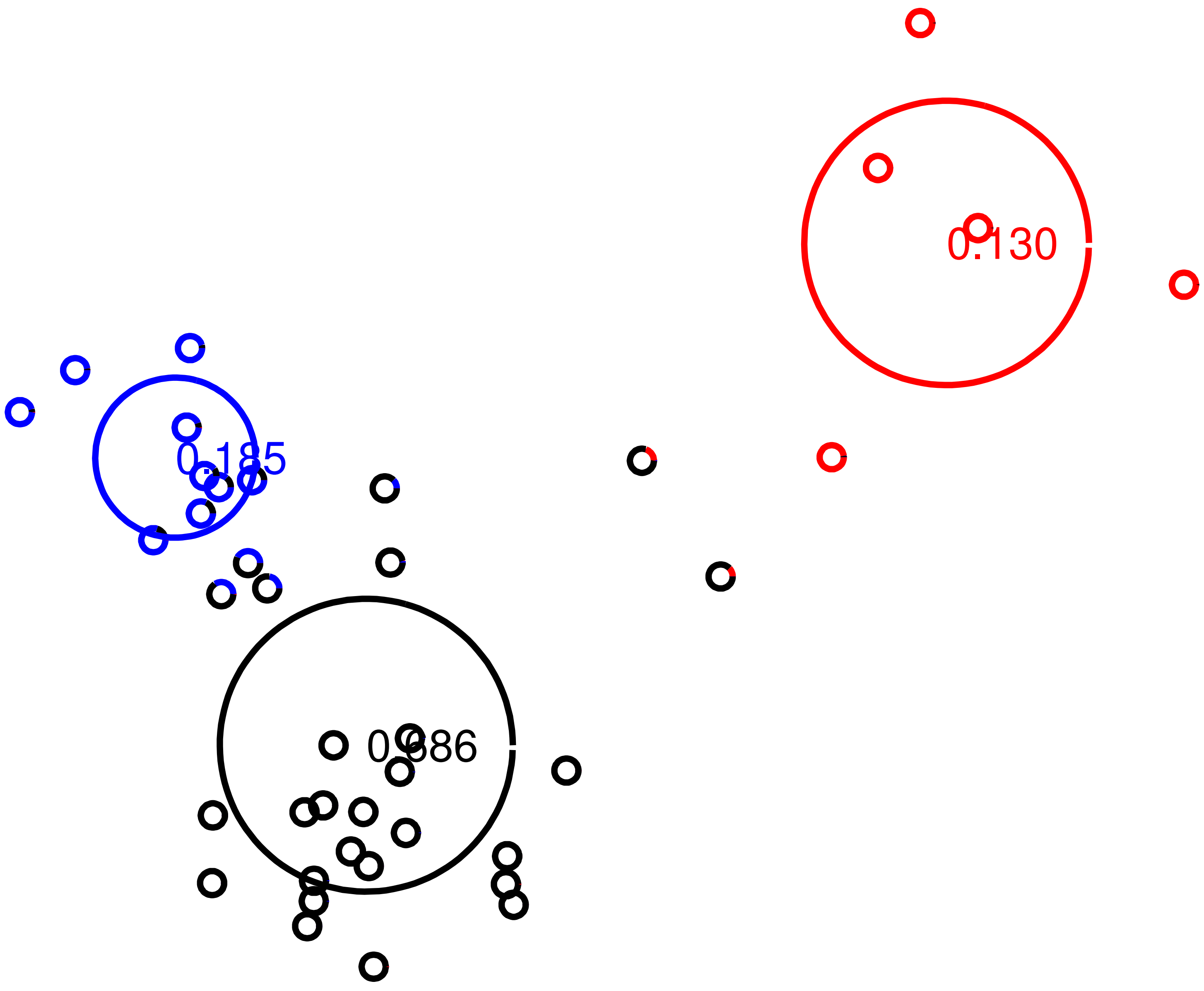
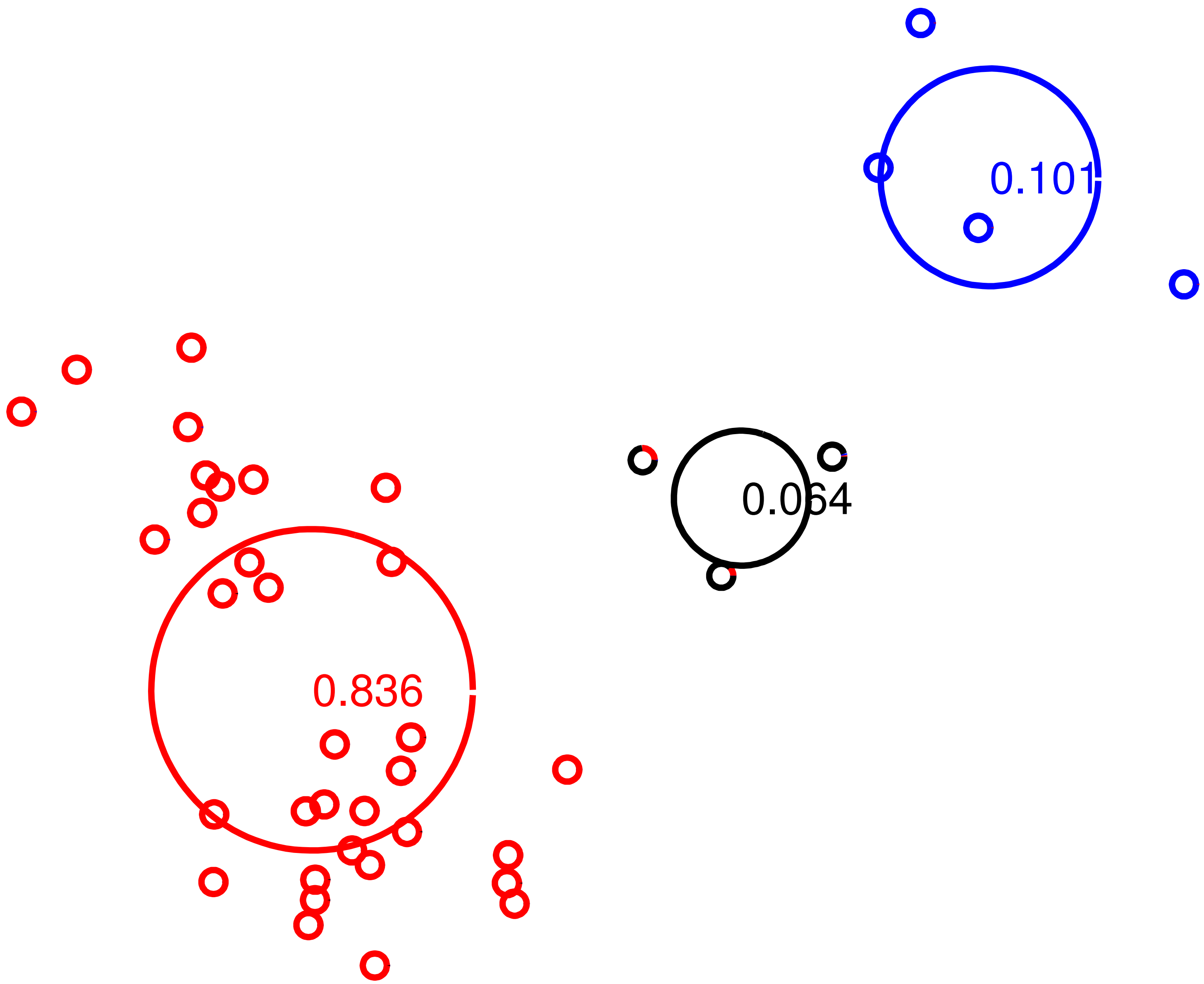
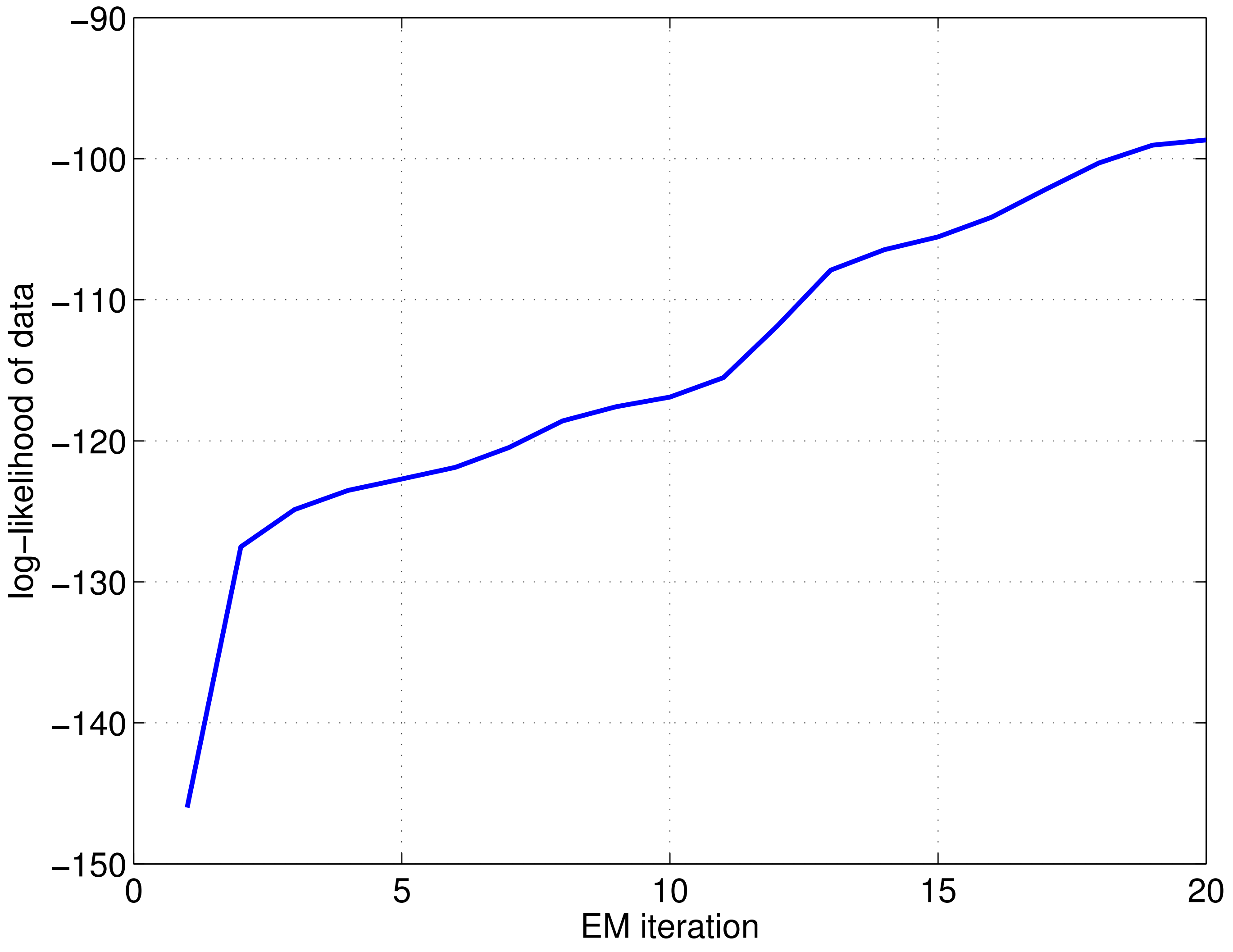


Doesn’t always work… well



The EM algorithm

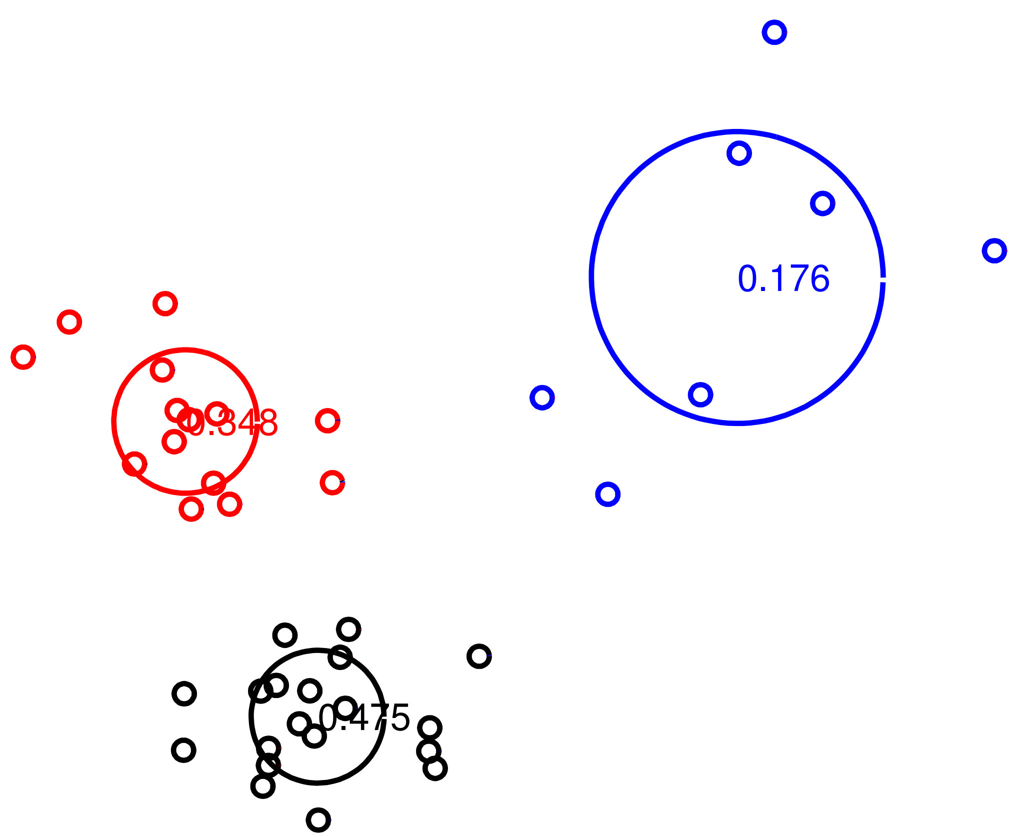


- The EM-algorithm monotonically increases the log-likelihood of the training data (cf. K-means)

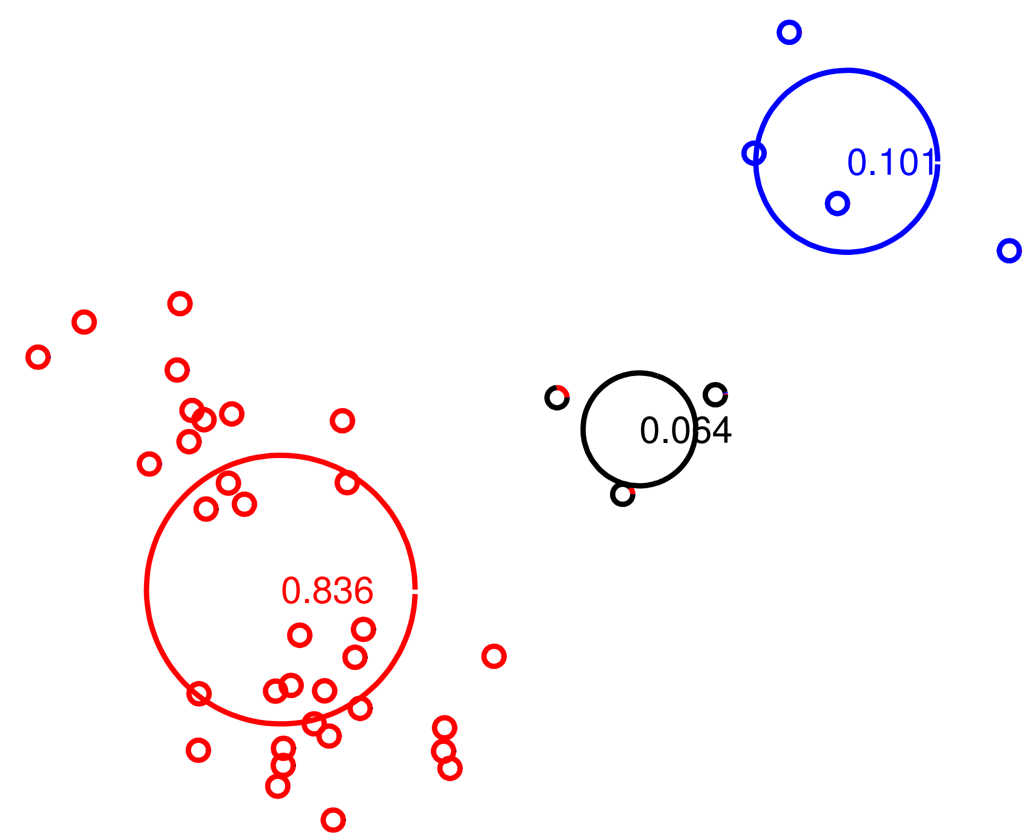
$$l(D;\theta) < l(D;\theta') < l(D;\theta'') < \dots$$

Locally optimal solutions

- The EM-algorithm is guaranteed to find a locally optimal solution by monotonically increasing the log-likelihood (the estimation problem with respect to θ is typically not convex)
- Whether the algorithm converges to the globally optimal solution depends on the initialization



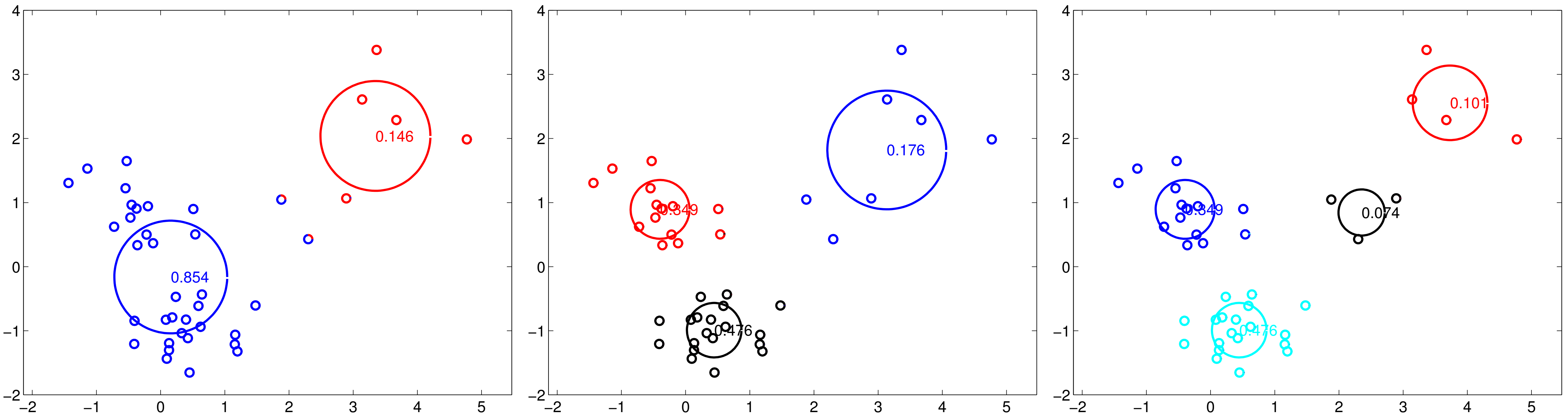
$$l(D;\hat{\theta}) = -98.64$$



$$l(D;\hat{\theta}) = -114.82$$

Model selection

- We can run the EM-algorithm with different numbers of components. Need to specify a criterion for selecting among the different models.



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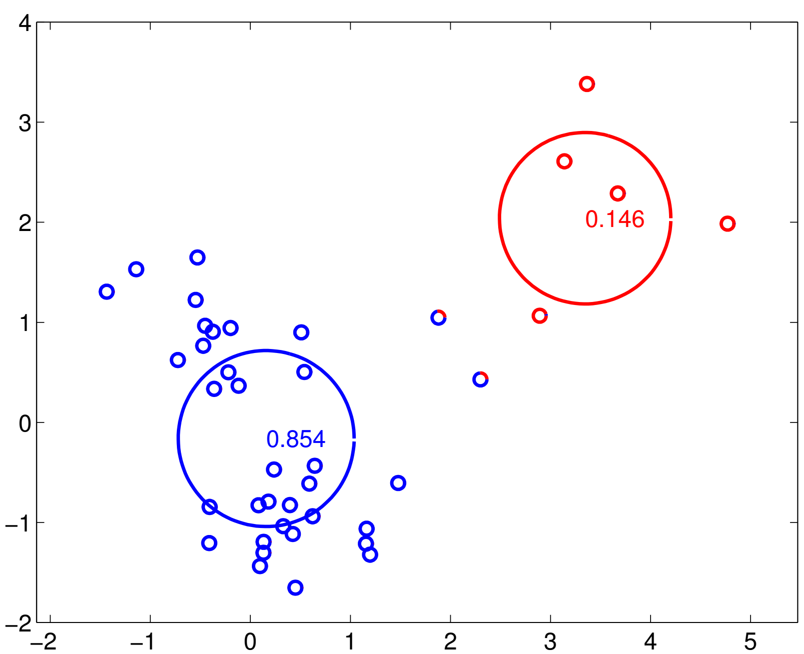
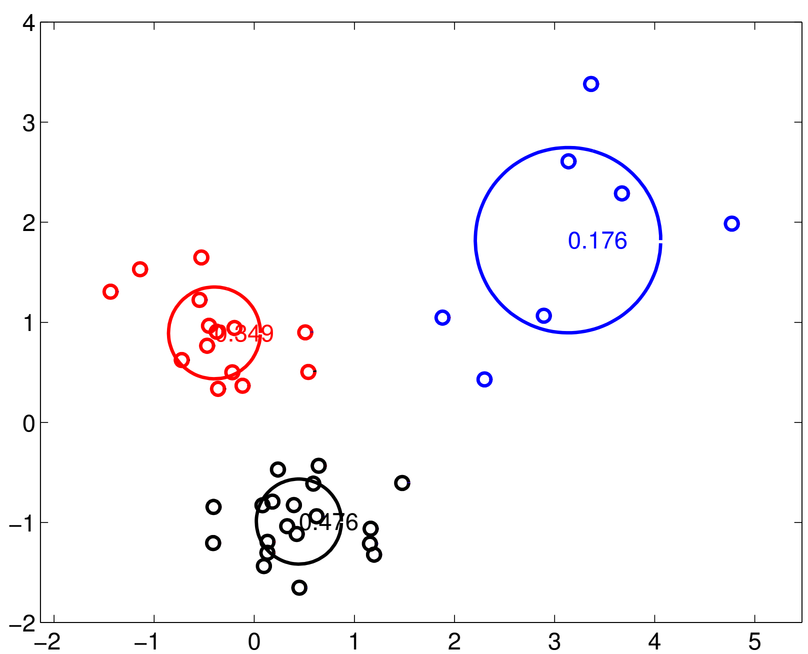


$$l(D; \hat{\theta}) = -118.25$$



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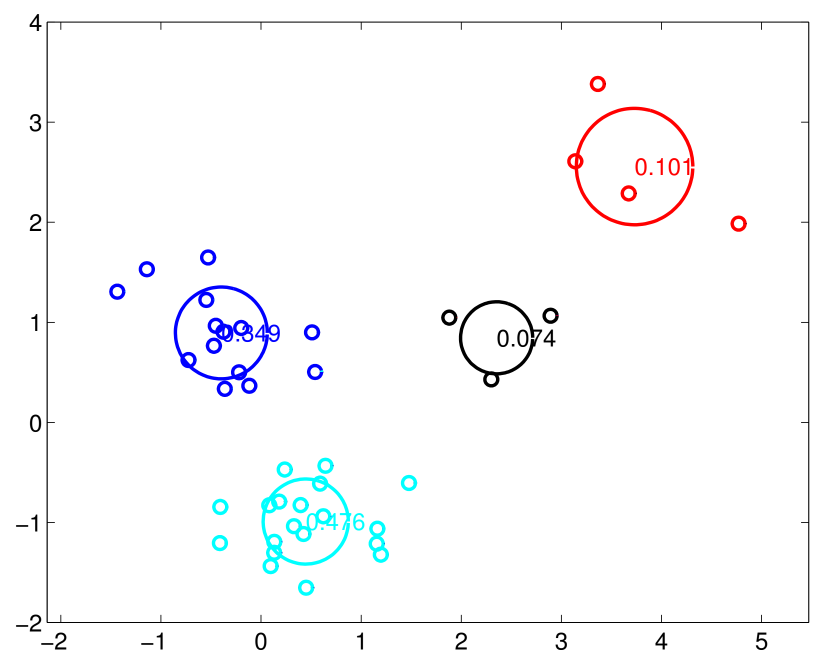

$$l(D; \hat{\theta}) = -94.11$$

Model selection

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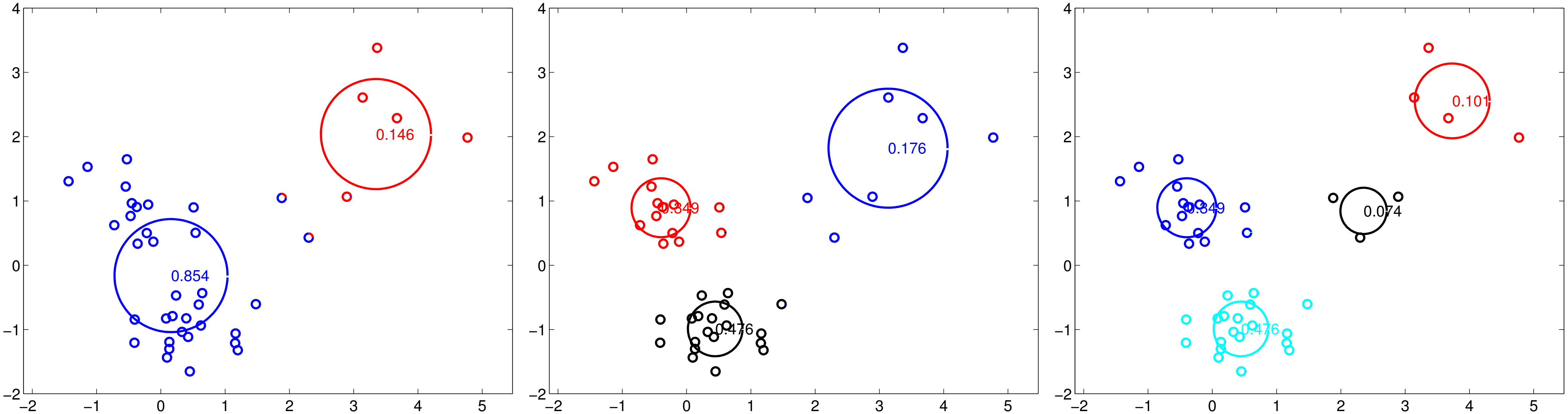

$l(D;\hat{\theta}) = -118.25$ $\quad l(D;\hat{\theta}) = -98.64$ $\quad l(D;\hat{\theta}) = -94.11$

- Basing the selecting on the value of log-likelihood would invariably lead to the largest number of components

Key things to know

- K-means failures
- Mixture model as a latent variable generative model
- Evaluating posterior probabilities
- Mixture estimation
  - ML criterion
  - complete data case
  - EM algorithm
- Why ML cannot be used to select the number of mixture components