香港科技大學
THE HONG KONG
UNIVERSITY OF SCIENCE
AND TECHNOLOGY

COMP 5212
Machine Learning
Lecture 11

Unsupervised Learning: Clustering, Expectation Maximization

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Oct 15, 2024

Midterm Exam

- Oct 24, in-class (130pm-250pm, locations TBA)

Review: How to Choose Prior

- Inject prior human knowledge to regularize the estimate
  - Could learn better if data is limited

- Posterior easy to compute
  - Conjugate prior

Conjugate Prior

If $P(\theta)$ is conjugate prior for $P(D|\theta)$, then Posterior has same form as prior

Posterior = Likelihood x Prior

$$P(\theta|D) = P(D|\theta) \times P(\theta)$$

P(theta)	P(D|theta)	P(theta|D)
Gaussian	Gaussian	Gaussian
Beta	Bernoulli	Beta
Dirichlet	Multinomial	Dirichlet

Review: MLE vs. MAP

Maximum Likelihood estimation (MLE)

Choose value that maximizes the probability of observed data

$$\widehat{\theta}_{MLE} = \arg\max_{\theta} P(D|\theta)$$

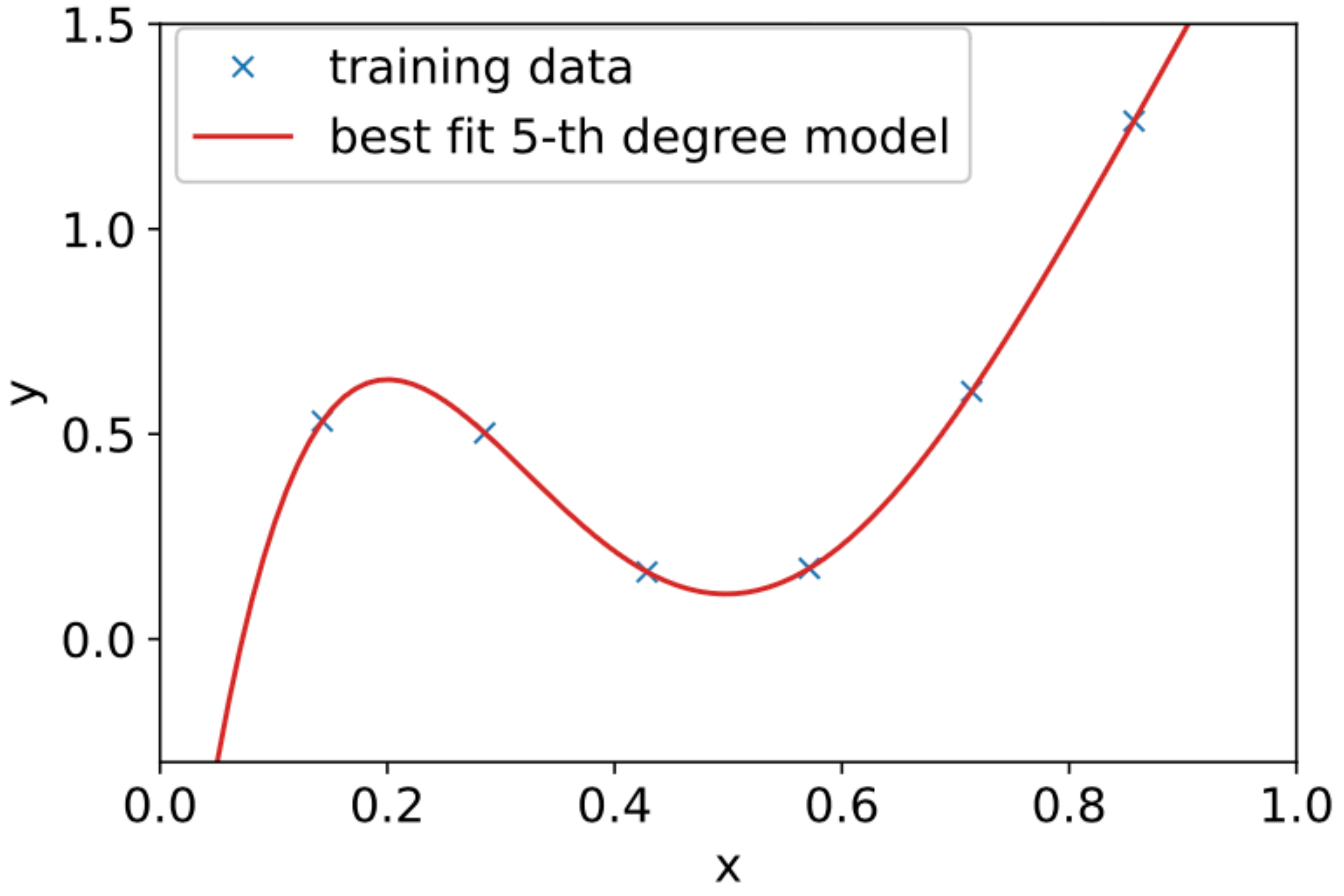
Maximum *a posteriori* (MAP) estimation

Choose value that is most probable given observed data and prior belief

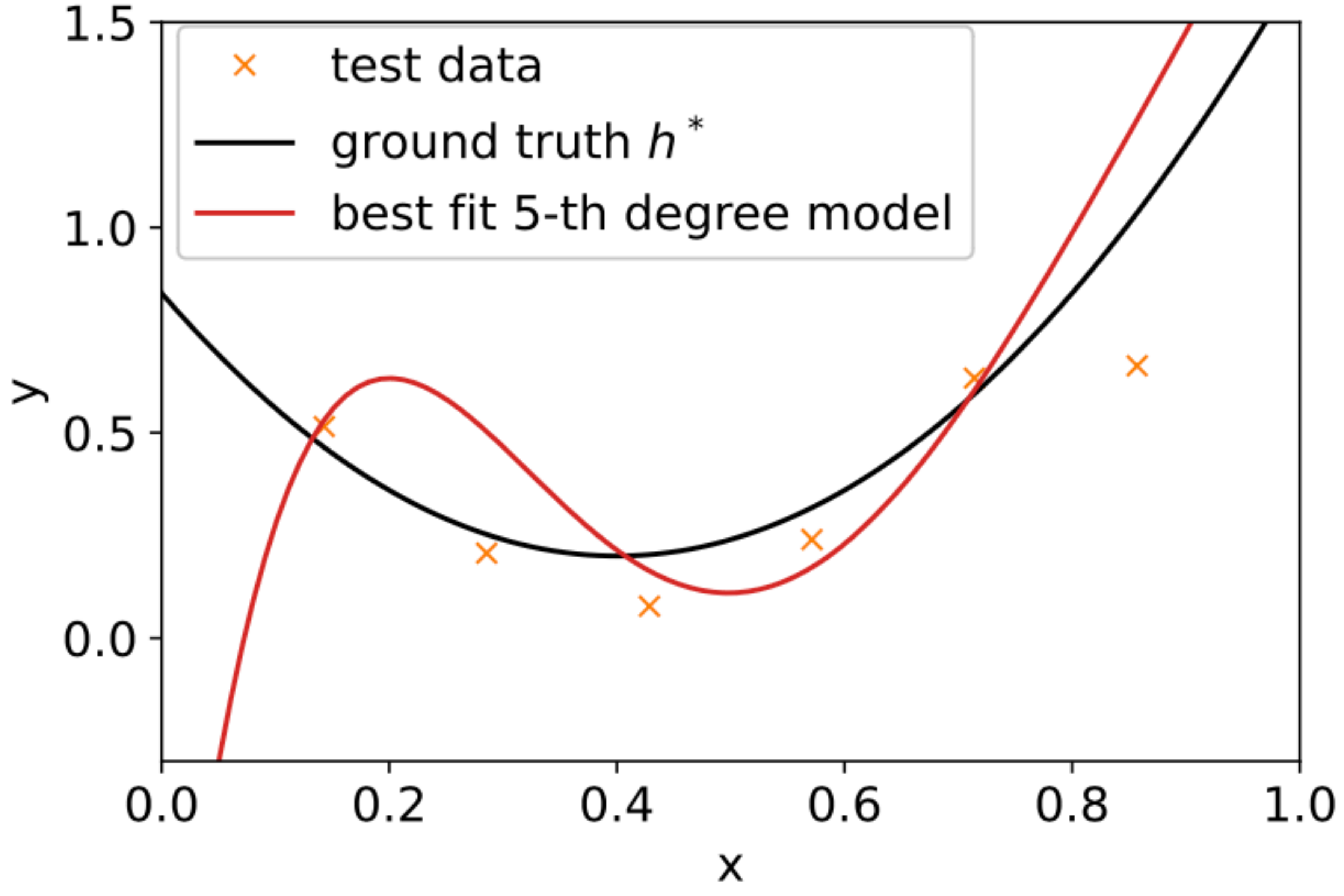
$$\begin{aligned} \widehat{\theta}_{MAP} &= \arg\max_{\theta} P(\theta|D) \\ &= \arg\max_{\theta} P(D|\theta)P(\theta) \end{aligned}$$

When are they the same?

Recap: Generalization



Zero training error



Large test error

How Do We Know Generalization in Practice

- We don't have test data, cannot compute test error

Hold-out or Cross-validation

Hold-out method

Hold – out procedure:

n data points available $D \equiv \{X_i, Y_i\}_{i=1}^{n}$

Use the validation dataset to mimic the test case

1) Split into two sets (randomly and preserving label proportion):

Training dataset $D_T = \{X_i, Y_i\}_{i=1}^{m}$

Validation/Hold-out dataset $D_V = \{X_i, Y_i\}_{i=m+1}^{n}$

2) Train classifier on D_T. Report error on validation dataset D_V.
Overfitting if validation error is much larger than training error

Validation Error

In case of gradient descent, we can observe whether the validation error increases

Drawback of Hold-Out Method

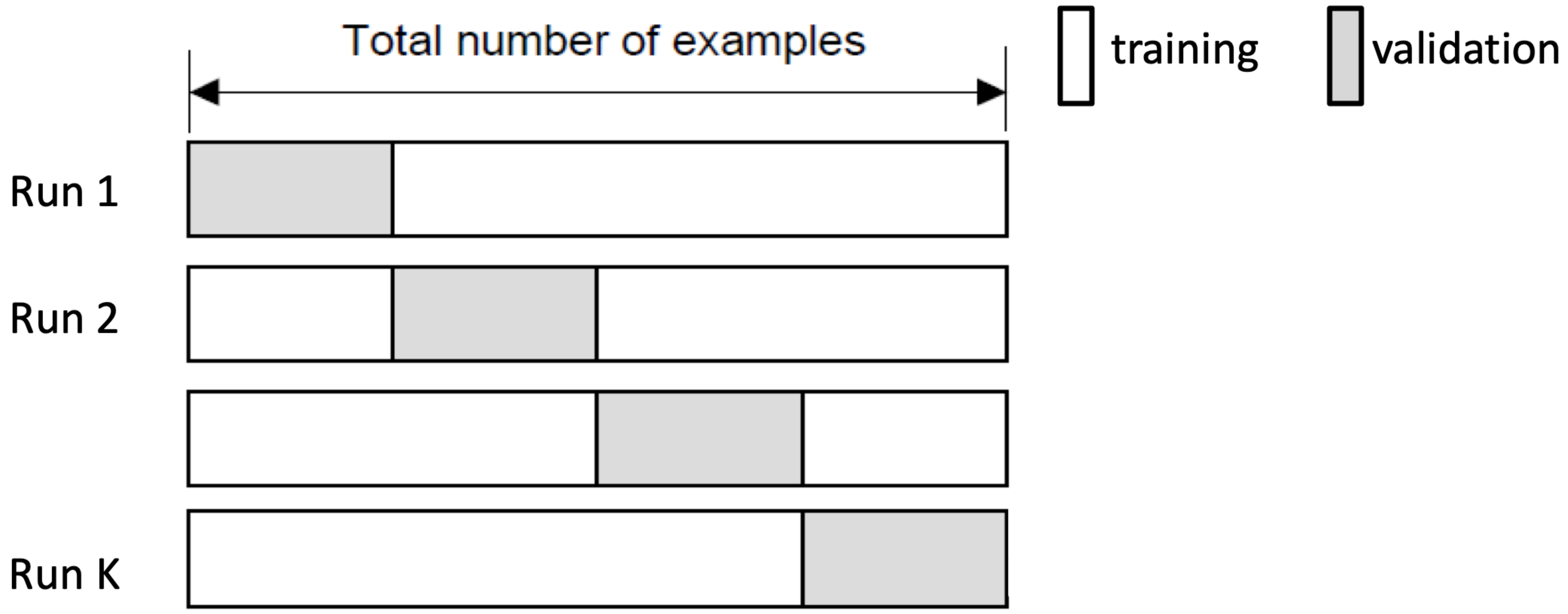
- Validation error may be misleading if we get an “unfortunate” split

Validation is essentially mimicking the test

Cross-Validation

K-fold cross-validation

Create K-fold partition of the dataset.
Do K runs: train using K-1 partitions and calculate validation error on remaining partition (rotating validation partition on each run).
Report average validation error



Drawback of Cross-Validation

- Cannot be used to select a specific model, more often used to select method design, hyperparameters, etc.

- Expensive

Hold-out is more commonly used nowadays, and the validation dataset is provided in advance

Hold-Out Method

Validation is essentially mimicking the test, always try to pick validation data that may align with test data, unnecessarily to hold out training data for validation

Train, Validation, Test

Validation dataset is another set of pairs $\{(\hat{x}^{(1)}, \hat{y}^{(1)}), \cdots, (\hat{x}^{(m)}, \hat{y}^{(m)})\}$

Does not overlap with training dataset

Test dataset is another set of pairs $\{(\tilde{x}^{(1)}, \tilde{y}^{(1)}), \cdots, (\tilde{x}^{(L)}, \tilde{y}^{(L)})\}$

Does not overlap with training and validation dataset

Completely unseen before deployment

Realistic setting

Validation is Very Important

- Track underfitting/overfitting (in case of iterative training)
- Decide when to stop training
- Select hyperparameters

Hyperparameter tuning

When you tune hyperparameters harder, it is more likely the validation error would mismatch the test error, because you are overfitting on the validation

Hyperparameter tuning is a form of training

Good ML Practice

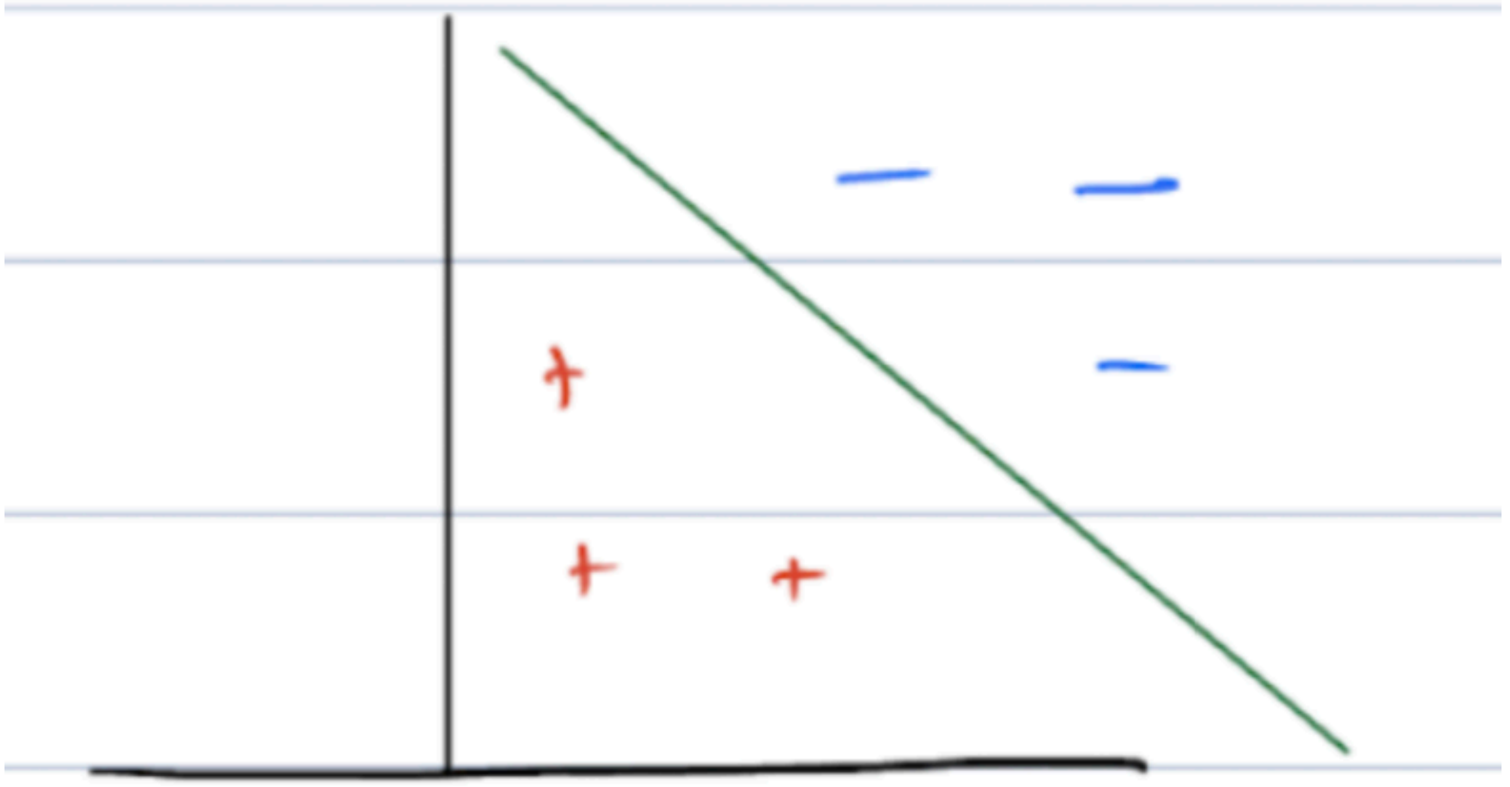
- Do not look at or evaluate on the test dataset

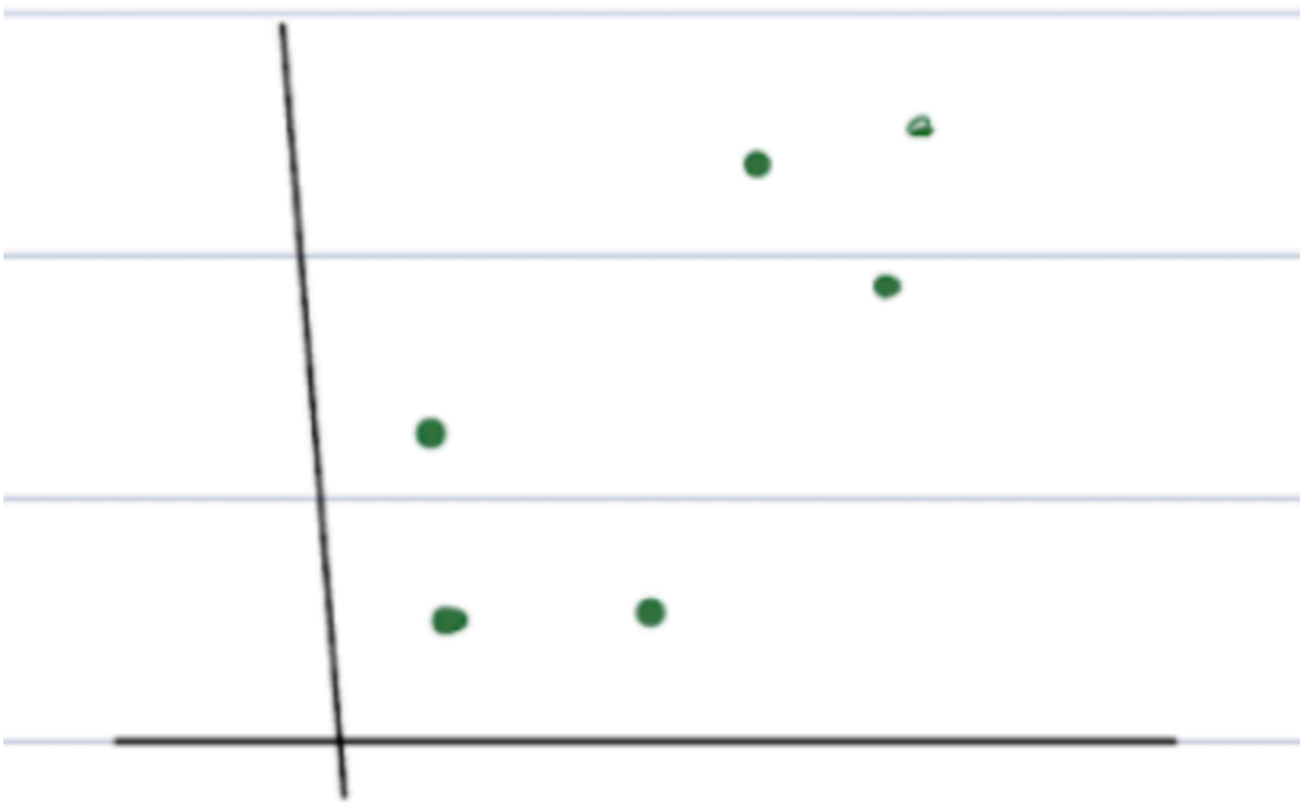
  Many people are implicitly using test dataset as validation

- Always track the training and validation metrics/errors/losses

Unsupervised Learning

No labels, only x is given





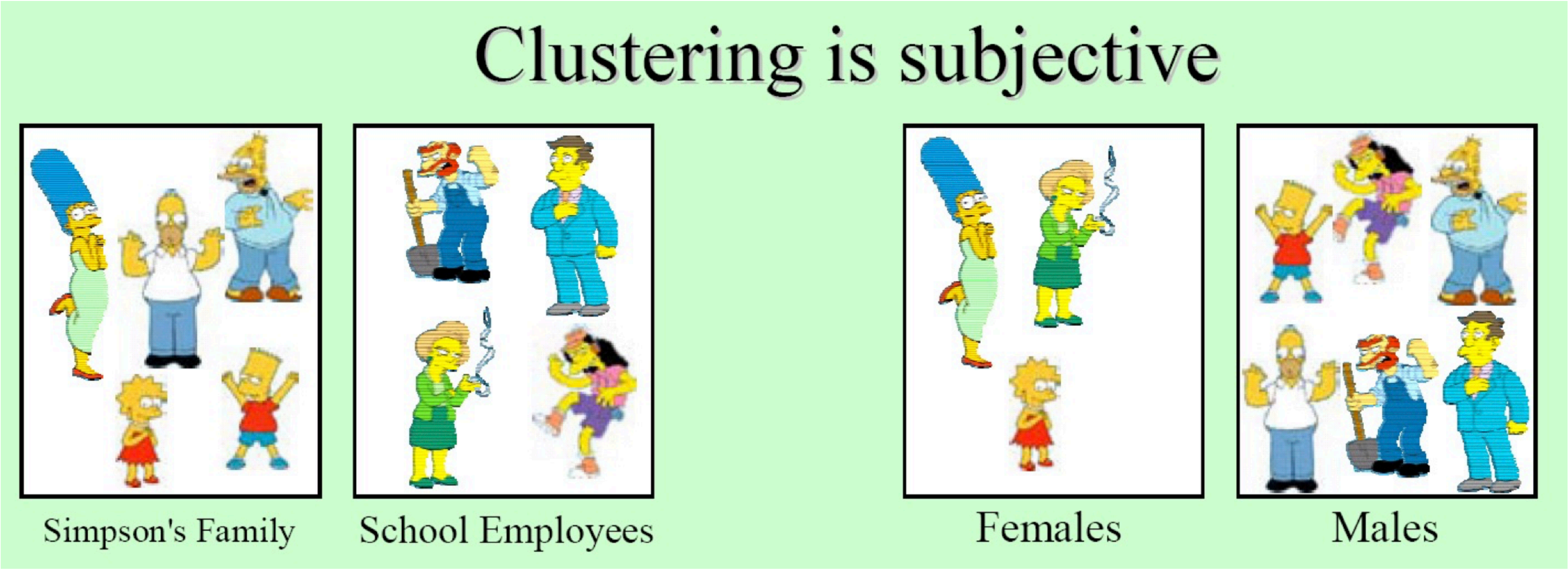
Unsupervised learning is typically “harder” than supervised learning

What is Clustering

Clustering: the process of grouping a set of objects into classes of similar objects

- high intra-class similarity
- low inter-class similarity
- It is the most common form of unsupervised learning

Similarity is subjective



Distance Metrics

$x = (x_1, x_2, \ldots, x_p)$
$y = (y_1, y_2, \ldots, y_p)$

Euclidean distance

$$d(x, y) = \sqrt[2]{\sum_{i=1}^{p} |x_i - y_i|^2}$$

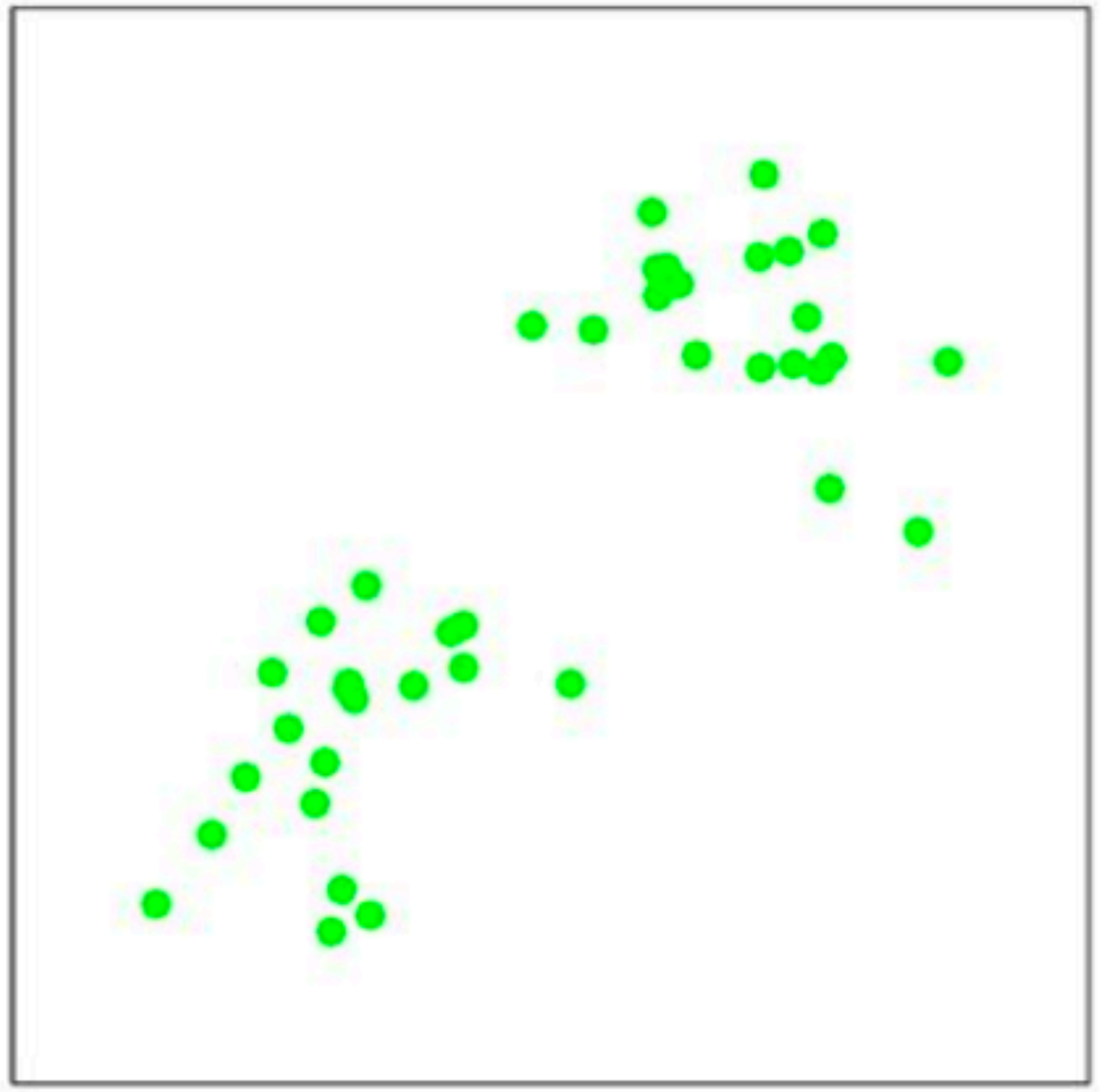
Manhattan distance

$$d(x, y) = \sum_{i=1}^{p} |x_i - y_i|$$

Sup-distance

$$d(x, y) = \max_{1 \le i \le p} |x_i - y_i|$$

K-Means Clustering



K-Means

Algorithm

Input – Desired number of clusters, *k*

Initialize – the *k* cluster centers (randomly if necessary)

Iterate –

1. Assign points to the nearest cluster centers

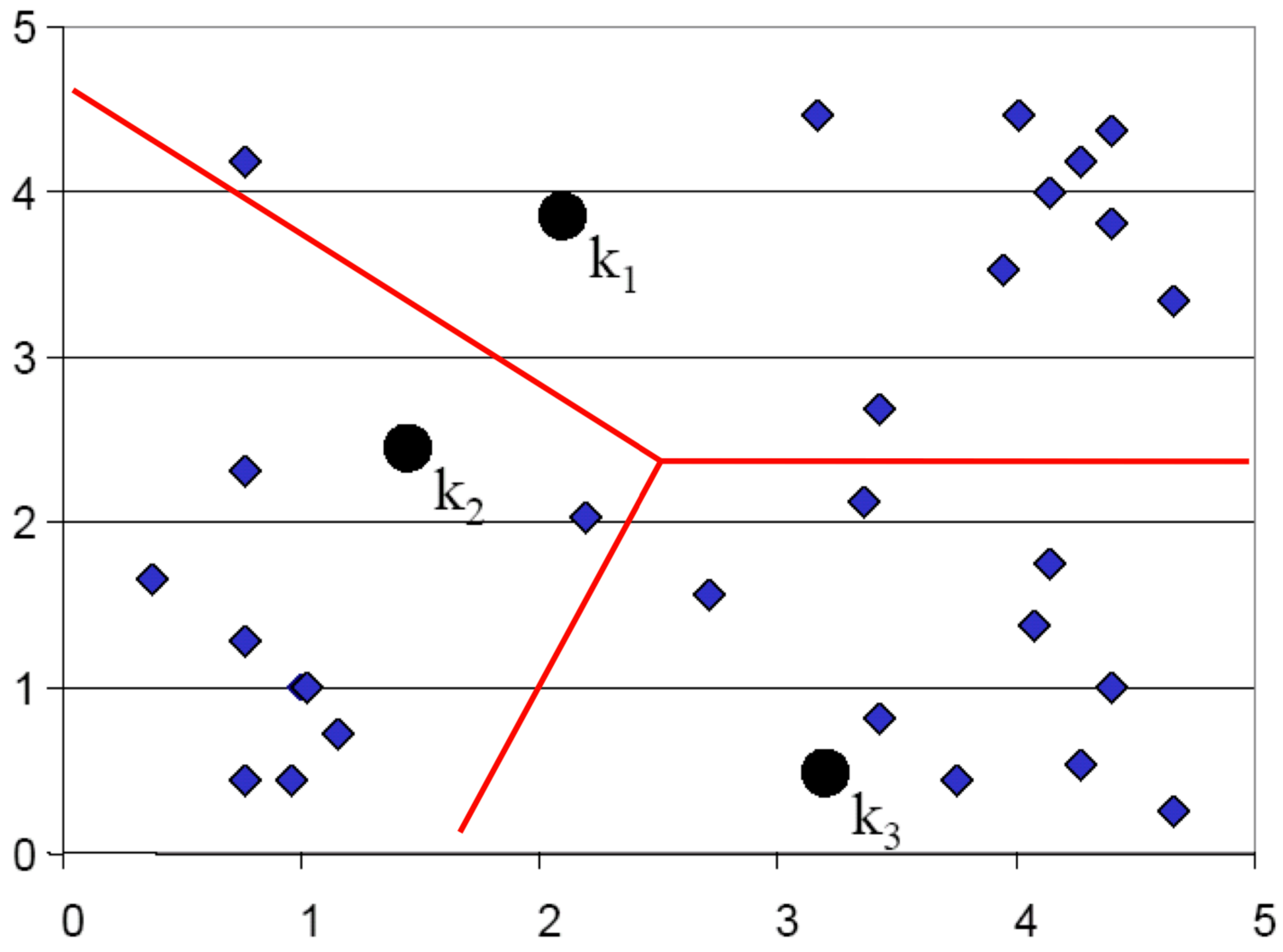
2. Re-estimate the *k* cluster centers (aka the centroid or mean), by assuming the memberships found above are correct.

$$\vec{\mu}_k = \frac{1}{\mathcal{C}_k} \sum_{i \in \mathcal{C}_k} \vec{x}_i$$

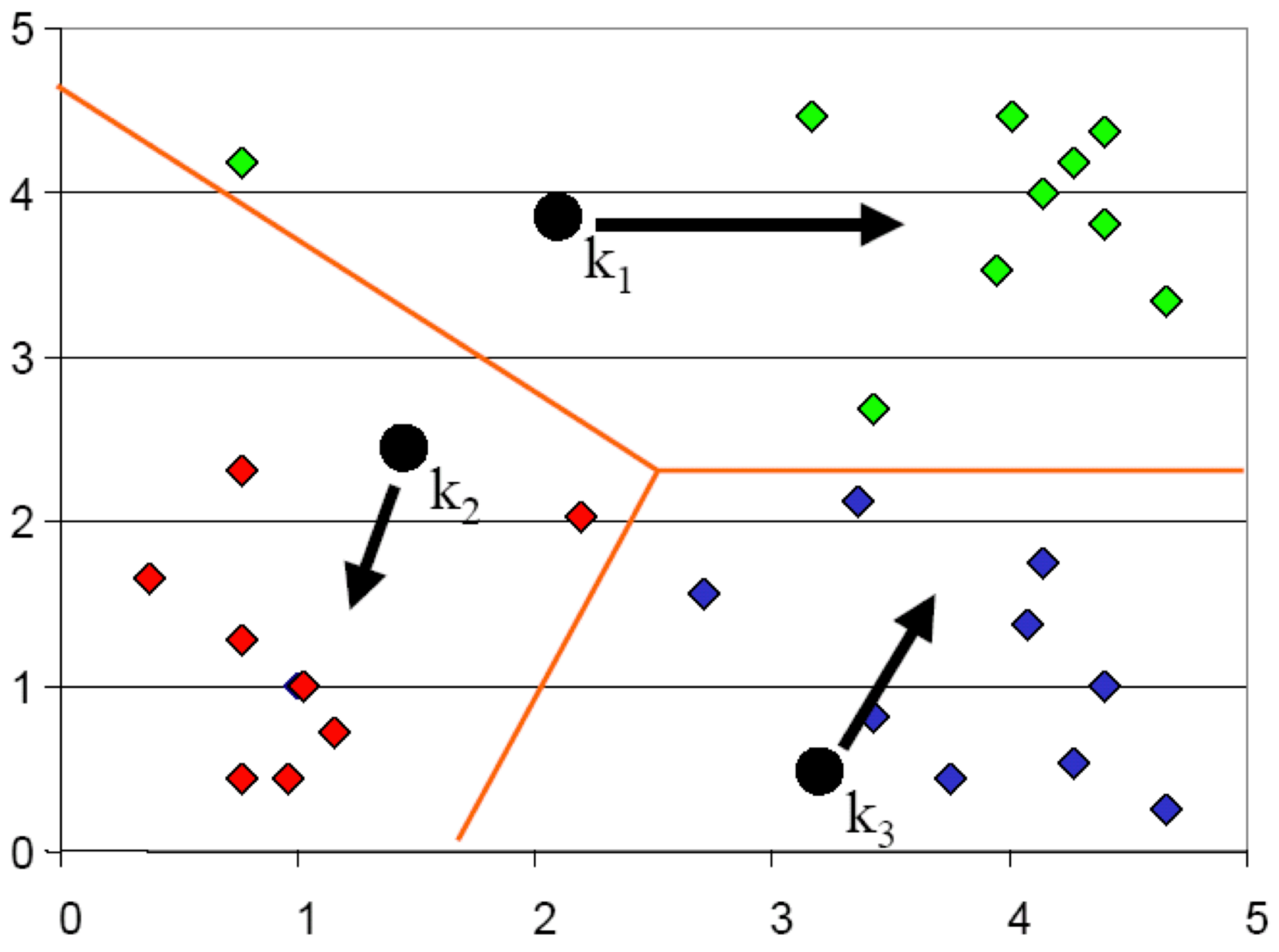
Termination –

If none of the objects changed membership in the last iteration, exit.
Otherwise go to 1.

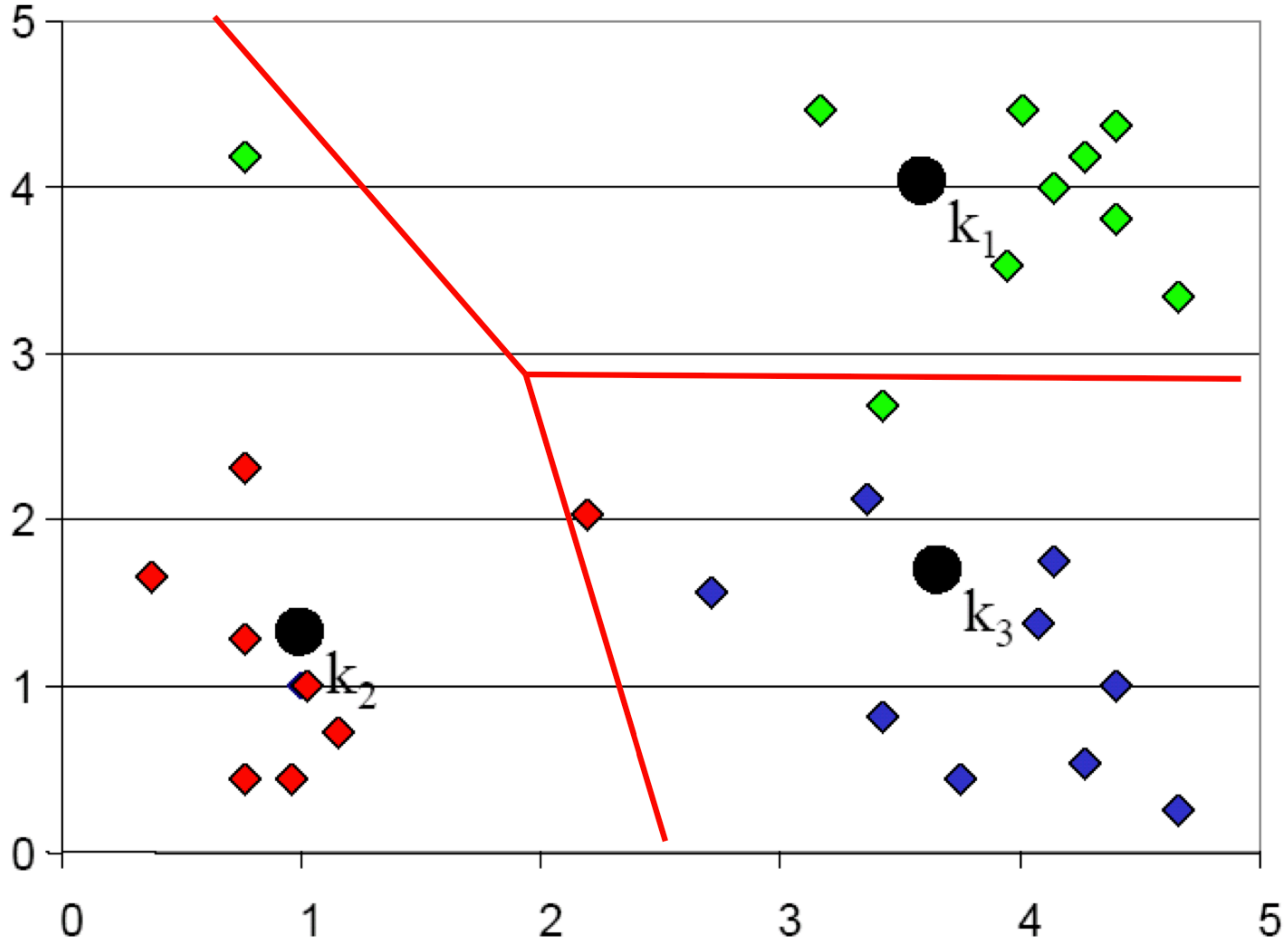
K-Means: Step 1



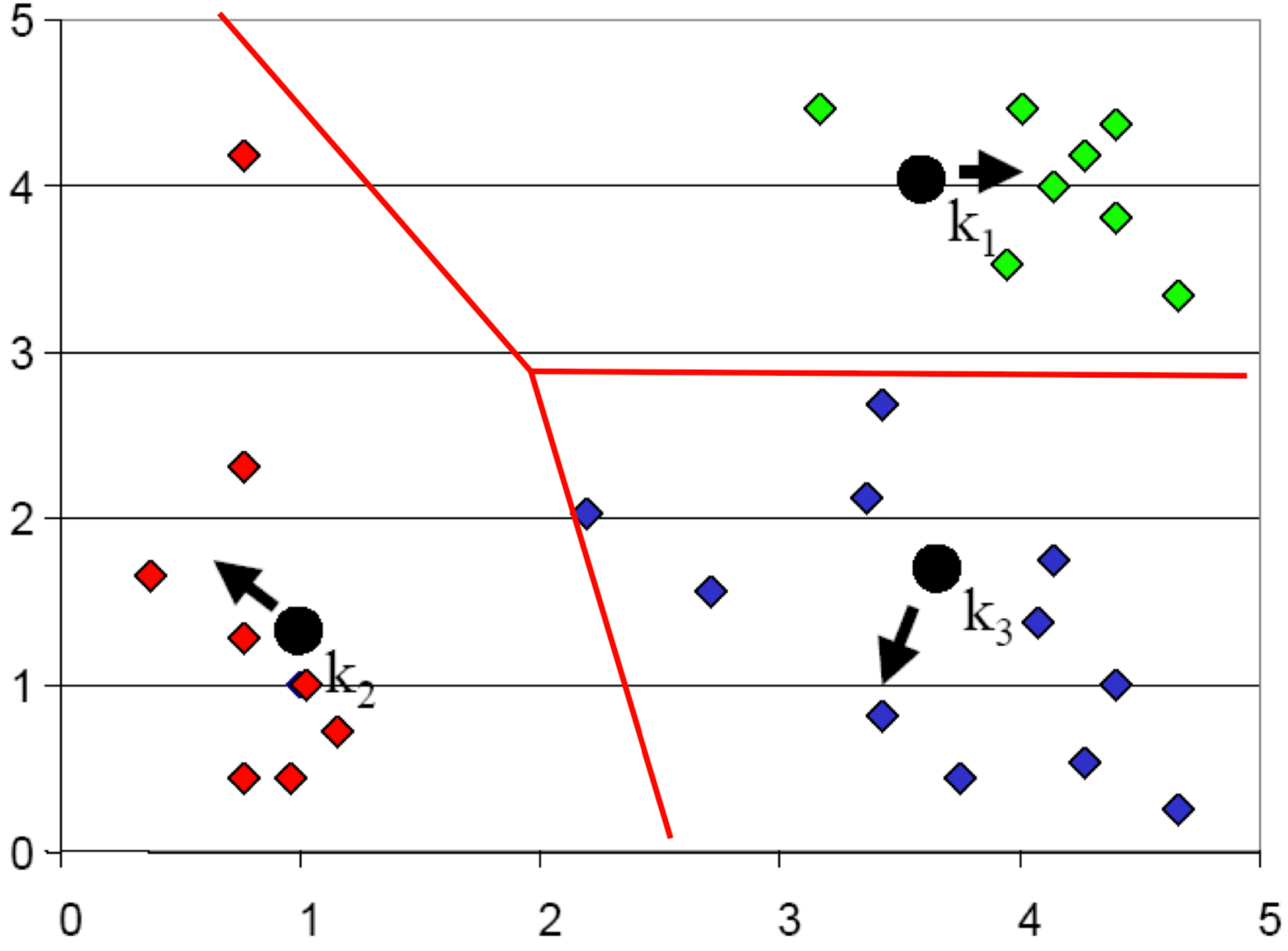
K-Means: Step 2



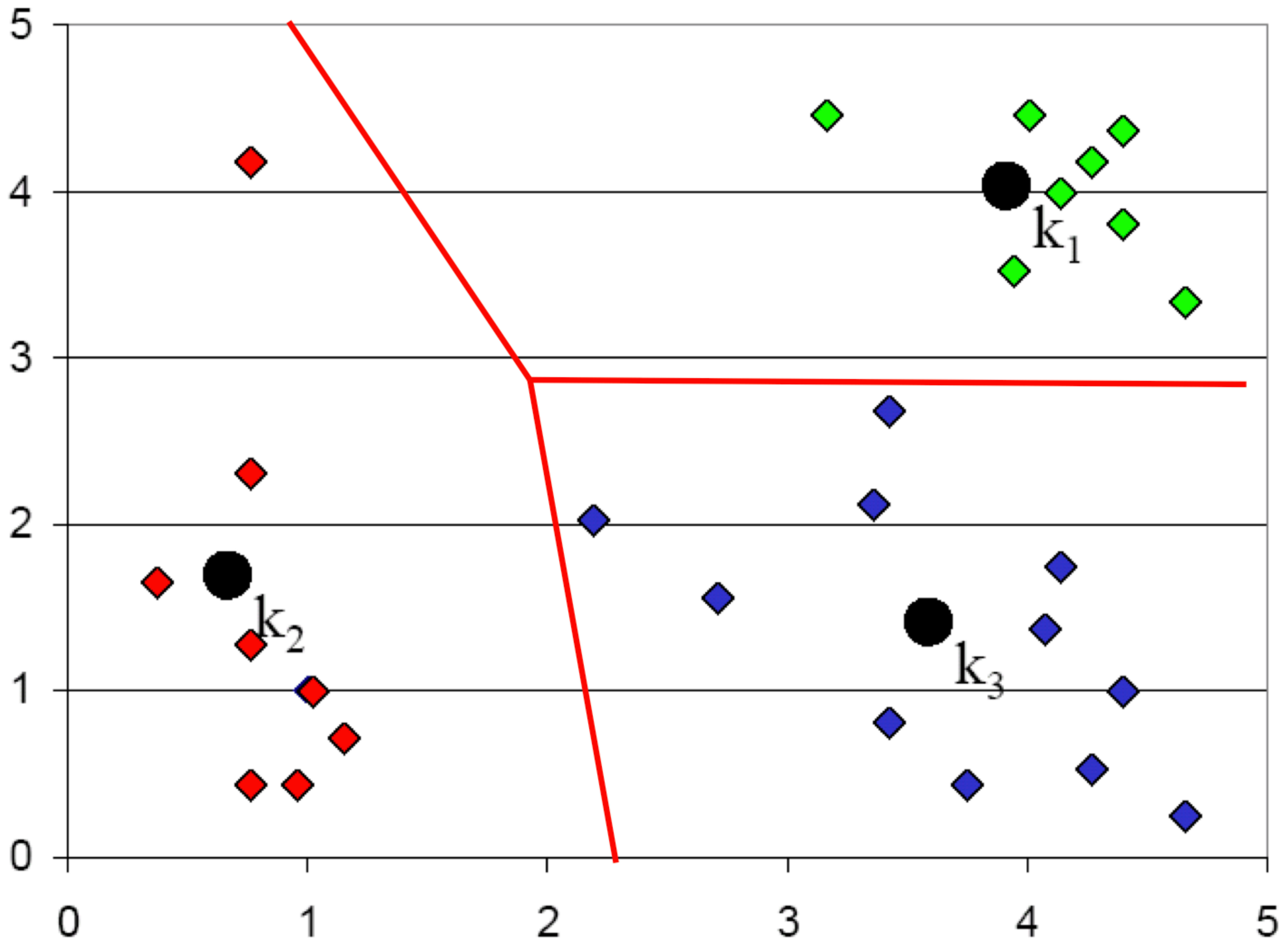
K-Means: Step 3



K-Means: Step 4



K-Means: Step 5



Objective of K-Means

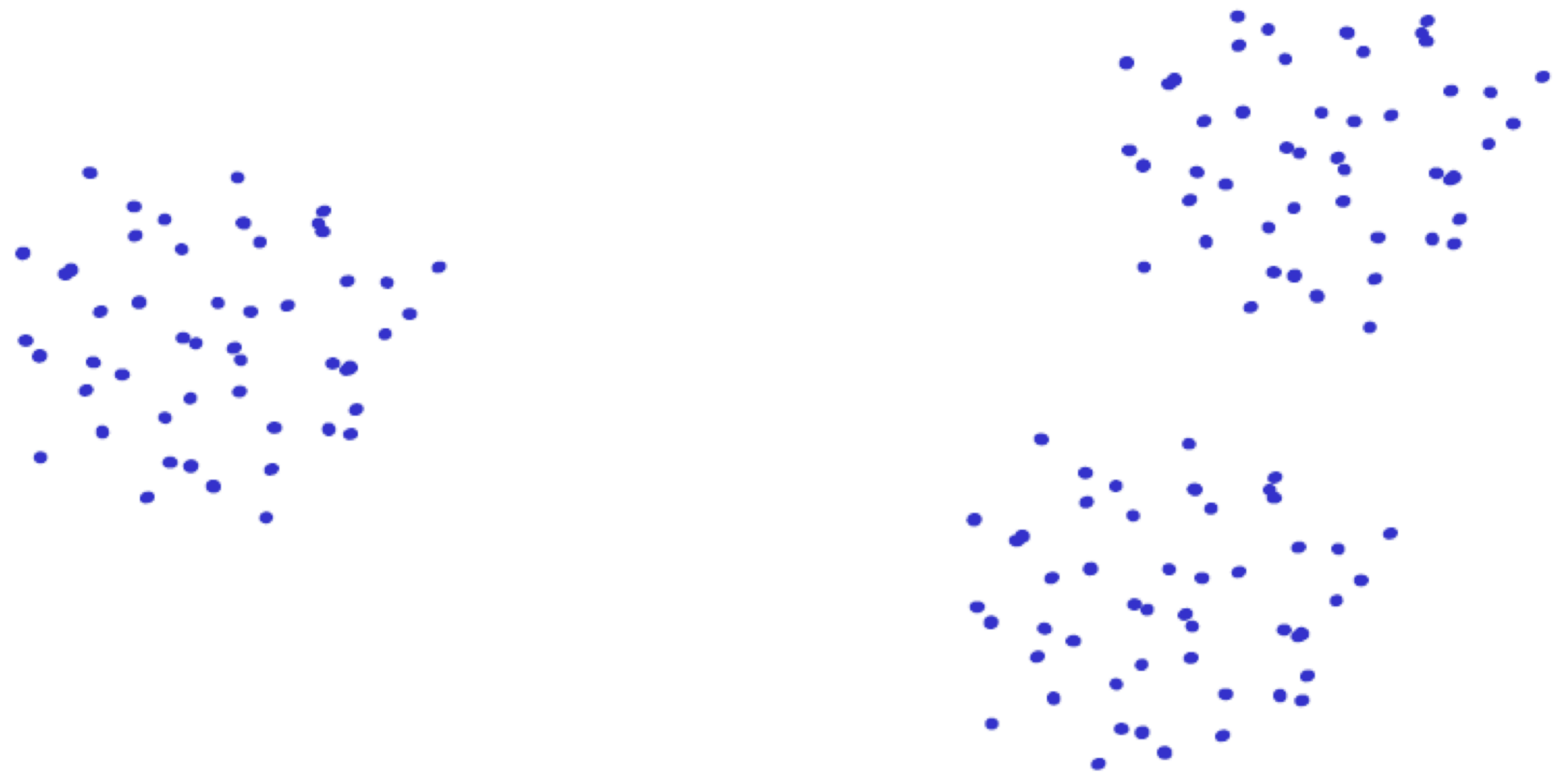
$$J(C, \mu) = \sum_{i=1}^{n} \|x^{(i)} - \mu^{C^{(i)}}\|^2$$ decreases momonotonically.

Proof?

K-means does not find a global minimus in this objective (it is NP-Hard)

Initialization of Centers

Results are sensitive to the initialization



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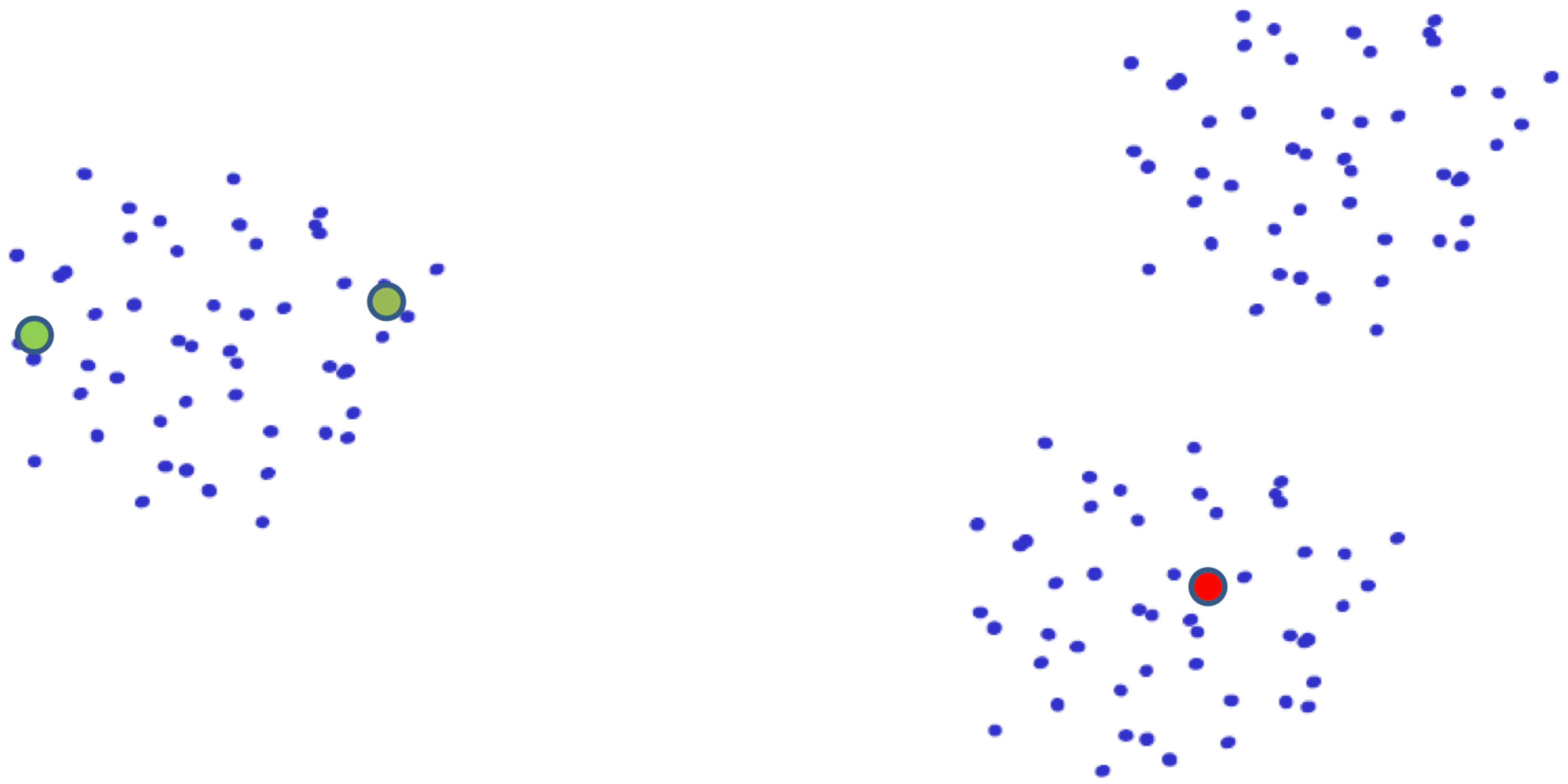

Initialization of Centers

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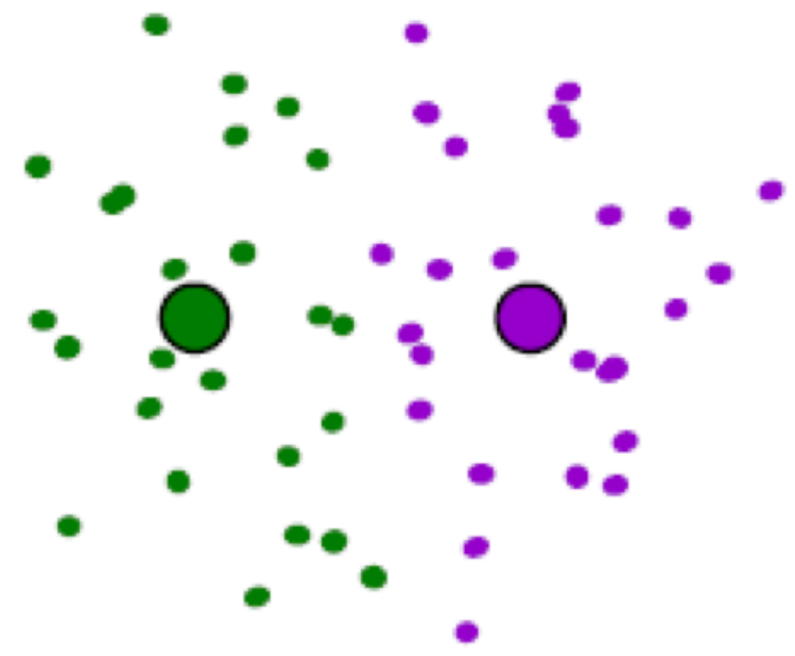
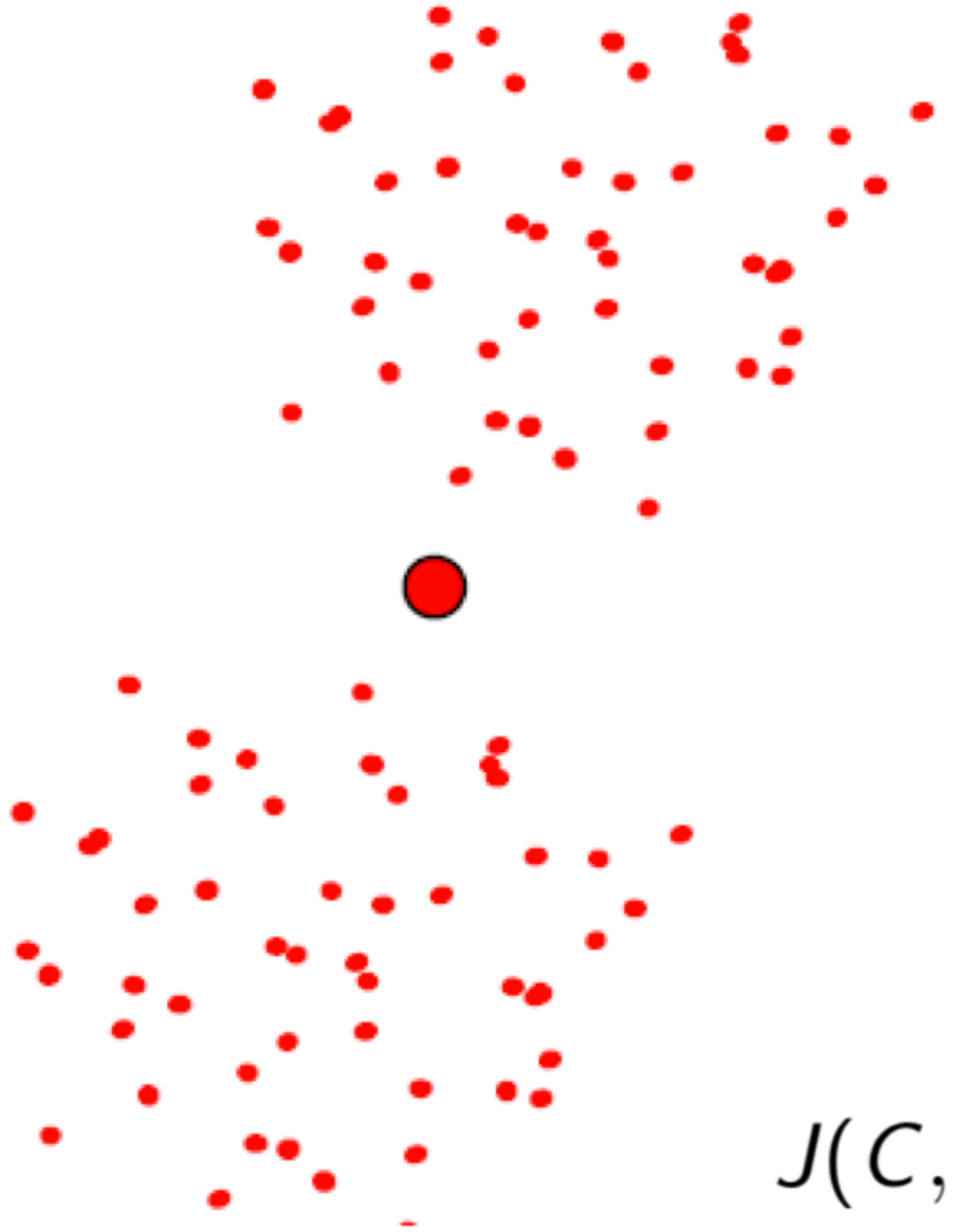




$$J(C, \mu) = \sum_{i=1}^{n} \|x^{(i)} - \mu^{C^{(i)}}\|^2$$

1. Try out multiple starting points and compare the objective
2. K-means++ algorithm improves the initialization

Model Selection of K-Means (or Unsupervised Learning in General)

Try out multiple starting points and compare the objective

$$J(C, \mu) = \sum_{i=1}^{n} \|x^{(i)} - \mu^{C^{(i)}}\|^2$$

This is unsupervised metric

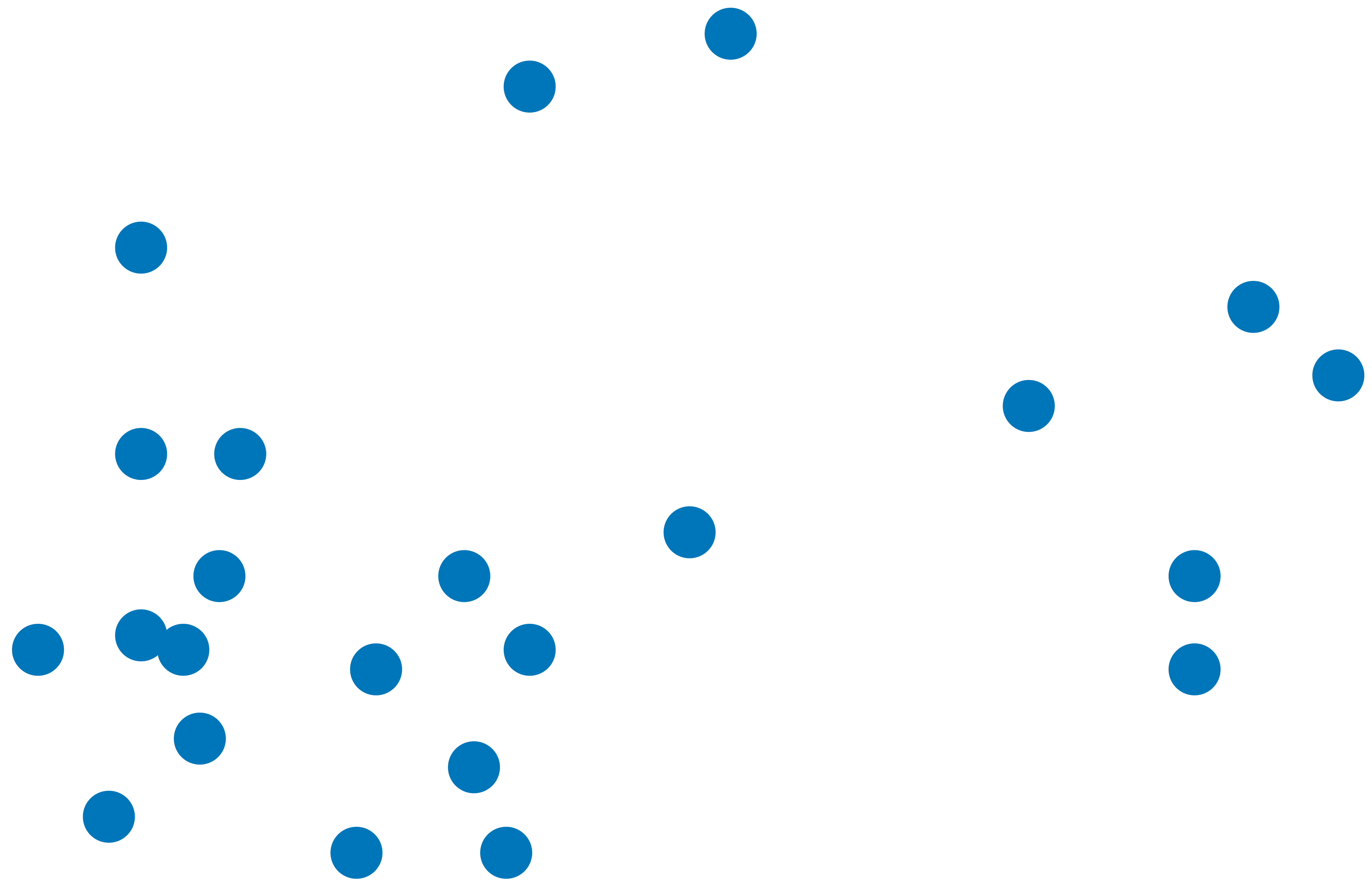
Sometimes people use supervised metrics for validation, which is not strictly unsupervised learning

1. Compute the metric on training set or test set?
2. For unsupervised learning, what is the difference of train and test?
3. Is it reasonable to assume the test input (x) is given?
4. If now I give you some data examples, ask you to cluster them. Are these data training or test?

Expectation Maximization (EM)

EM for Gaussian Mixture Model

Given a training set $\{x^{(1)}, \ldots x^{(n)}\}$ No Labels



We have discussed the supervised case in Gaussian Discriminative Model

Modeling data distribution is a fundamental goal in ML, not necessarily for classification

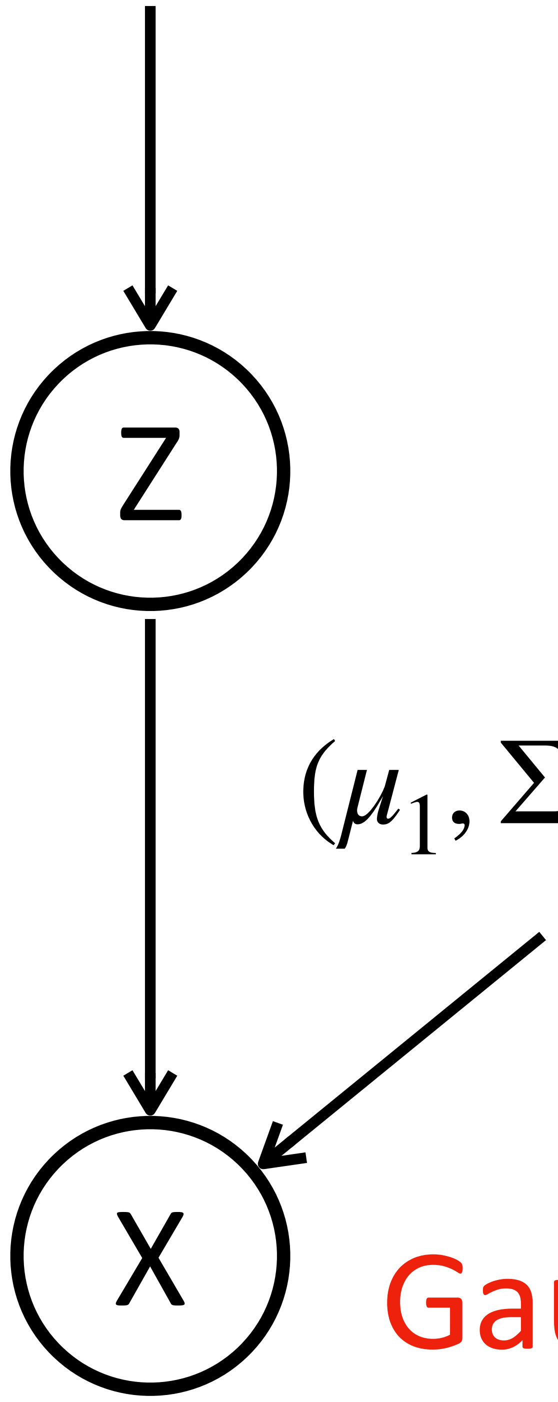
The Generative Model

p(z): multinomial , k classes(e.g. uniform)

K is a hyperparameter based on our assumption

We assume the generative process as:

Label



Data

$(\mu_1, \Sigma_1), (\mu_2, \Sigma_2), \ldots (\mu_k, \Sigma_k)$

1. For each data point, sample its label z_i from p(z)

2. Sample $x_i \sim N(\mu_{z_i}, \Sigma_{z_i})$

Gaussian Mixture Model (GMM)

Same as Gaussian Discriminative Analysis, but Z is observed in GDA

Recap: How did we do in GDA?

Binary classification: $y \in \{0,1\}, x \in R^d$

Assumption

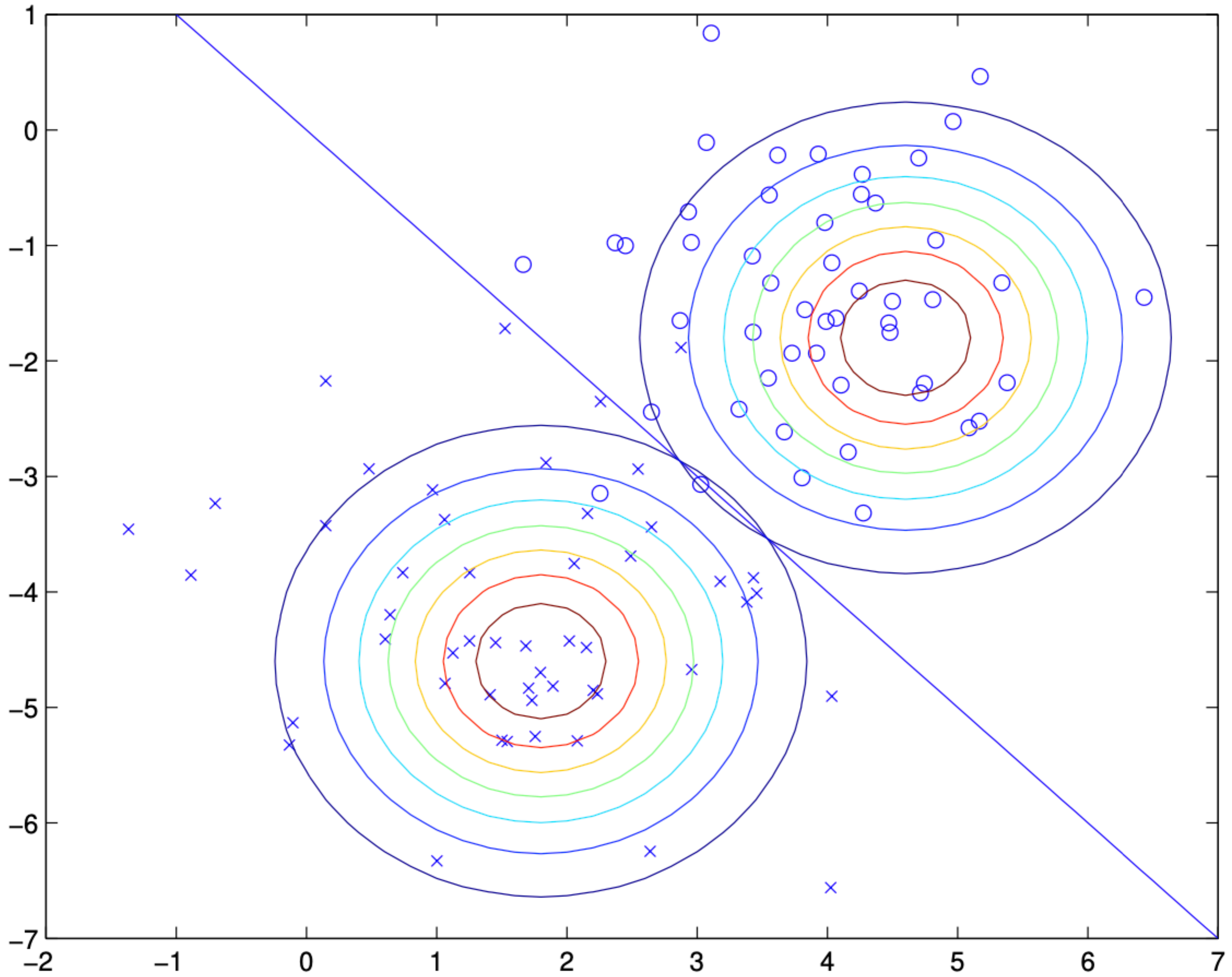
$$
\begin{aligned}
y &\sim \text{Bernoulli}(\phi) \\
x|y=0 &\sim \mathcal{N}(\mu_0, \Sigma) \\
x|y=1 &\sim \mathcal{N}(\mu_1, \Sigma)
\end{aligned}
$$

$$
\begin{aligned}
p(y) &= \phi^y (1-\phi)^{1-y} \\
p(x|y=0) &= \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_0)^T \Sigma^{-1} (x-\mu_0)\right) \\
p(x|y=1) &= \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_1)^T \Sigma^{-1} (x-\mu_1)\right)
\end{aligned}
$$

Recap: How did we do in GDA?

$$\begin{aligned}\ell(\phi, \mu_0, \mu_1, \Sigma) &= \log \prod_{i=1}^{n} p(x^{(i)}, y^{(i)}; \phi, \mu_0, \mu_1, \Sigma) \\ &= \log \prod_{i=1}^{n} p(x^{(i)} | y^{(i)}; \mu_0, \mu_1, \Sigma) p(y^{(i)}; \phi).\end{aligned}$$

$$\begin{aligned}\phi &= \frac{1}{n} \sum_{i=1}^{n} 1\{y^{(i)} = 1\} \\ \mu_0 &= \frac{\sum_{i=1}^{n} 1\{y^{(i)} = 0\} x^{(i)}}{\sum_{i=1}^{n} 1\{y^{(i)} = 0\}} \\ \mu_1 &= \frac{\sum_{i=1}^{n} 1\{y^{(i)} = 1\} x^{(i)}}{\sum_{i=1}^{n} 1\{y^{(i)} = 1\}} \\ \Sigma &= \frac{1}{n} \sum_{i=1}^{n} (x^{(i)} - \mu_{y^{(i)}})(x^{(i)} - \mu_{y^{(i)}})^T\end{aligned}$$



The Generative Model

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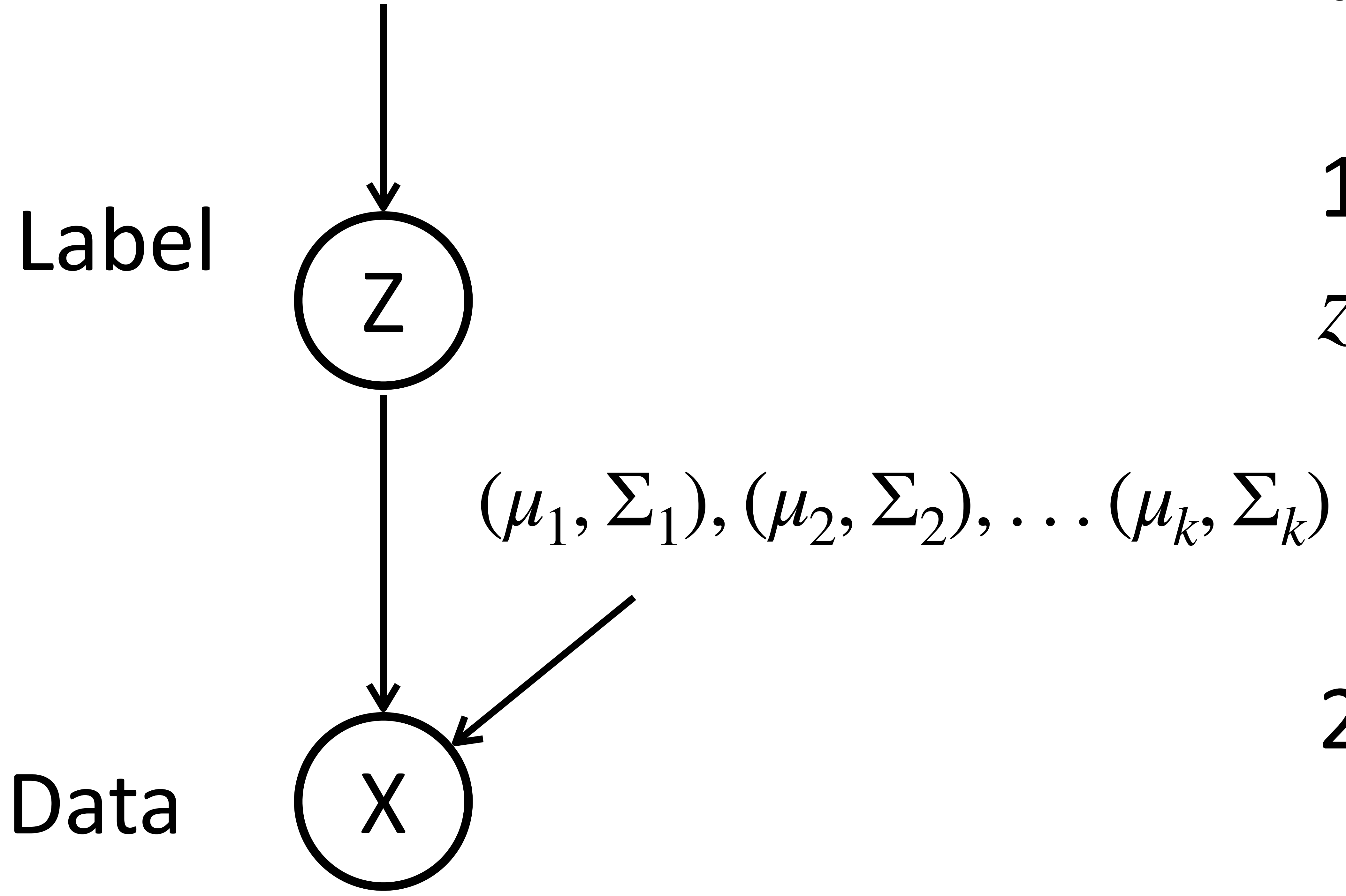

We assume the generative process as:

1. For each data point, sample its label z_i from p(z)

2. Sample $x_i \sim N(\mu_{z_i}, \Sigma_{z_i})$

Same as Gaussian Discriminative Analysis, but Z is observed in GDA

Maximum Likelihood Estimation for GMM

Modeling data distribution is a fundamental goal in ML

Supervised:

$\text{argmax}_{\phi,\mu,\Sigma} \log p(x, z)$

Unsupervised:

$\boxed{\text{argmax}_{\phi,\mu,\Sigma} \log p(x)}$

How to compute this?

$\Downarrow$

Prediction:

$$p(z \mid x) \propto p(z)p(x \mid z)$$

Maximum Likelihood Estimation for GMM

$$\begin{aligned}\ell(\phi, \mu, \Sigma) &= \sum_{i=1}^{n} \log p(x^{(i)}; \phi, \mu, \Sigma) \\ &= \sum_{i=1}^{n} \log \sum_{z^{(i)}=1}^{k} p(x^{(i)}|z^{(i)}; \mu, \Sigma) p(z^{(i)}; \phi).\end{aligned}$$

1. Intractable (no closed-form for the solution)
2. Expensive when k is large (if you want to do gradient descent)

Things are easy when we know z..

In case we know z

$$\ell(\phi, \mu, \Sigma) = \sum_{i=1}^{n} \log p(x^{(i)}|z^{(i)}; \mu, \Sigma) + \log p(z^{(i)}; \phi).$$

$$\begin{aligned}
\phi_j &= \frac{1}{n}\sum_{i=1}^{n} 1\{z^{(i)} = j\}, \\
\mu_j &= \frac{\sum_{i=1}^{n} 1\{z^{(i)} = j\} x^{(i)}}{\sum_{i=1}^{n} 1\{z^{(i)} = j\}}, \\
\Sigma_j &= \frac{\sum_{i=1}^{n} 1\{z^{(i)} = j\} (x^{(i)} - \mu_j)(x^{(i)} - \mu_j)^T}{\sum_{i=1}^{n} 1\{z^{(i)} = j\}}.
\end{aligned}$$

Expectation maximization is to infer the latent variables first (z here), and maximize the likelihood given the inferred z

Expectation Maximization for GMM

Repeat until convergence:

{

No parameter change in E-step

(E-step) For each i, j, set

$$w_j^{(i)} := p(z^{(i)} = j | x^{(i)}; \phi, \mu, \Sigma)$$

Compute the posterior distribution, given current parameters

(M-step) Update the parameters:

$$\begin{aligned} \phi_j &:= \frac{1}{n} \sum_{i=1}^{n} w_j^{(i)}, \\ \mu_j &:= \frac{\sum_{i=1}^{n} w_j^{(i)} x^{(i)}}{\sum_{i=1}^{n} w_j^{(i)}}, \\ \Sigma_j &:= \frac{\sum_{i=1}^{n} w_j^{(i)} (x^{(i)} - \mu_j)(x^{(i)} - \mu_j)^T}{\sum_{i=1}^{n} w_j^{(i)}} \end{aligned}$$

update parameters using current p(z|x)

}

Expectation Maximization

- Why does it work?
- What is its relation to MLE estimation?
- How is convergence guaranteed?
- When we perform EM, what is the real objective that we are optimizing?

General EM Algorithm

$$p(x;\theta) = \sum_z p(x,z;\theta)$$

$$\begin{aligned}\ell(\theta) &= \sum_{i=1}^{n} \log p(x^{(i)};\theta) \\ &= \sum_{i=1}^{n} \log \sum_{z^{(i)}} p(x^{(i)}, z^{(i)};\theta).\end{aligned}$$

This lower bound holds for any Q(z)

Let Q to be a distribution over z

$$\begin{aligned}\log p(x;\theta) &= \log \sum_z p(x,z;\theta) \\ &= \log \sum_z Q(z) \frac{p(x,z;\theta)}{Q(z)} \\ &\geq \sum_z Q(z) \log \frac{p(x,z;\theta)}{Q(z)}\end{aligned}$$

Jensen inequality

Jensen Inequality

For a convex function f, and $t \in [0,1]$

$$f(tx_1 + (1-t)x_2) \leq tf(x_1) + (1-t)f(x_2)$$

In probability:

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

If f is strictly convex, then equality holds only when X is a constant

Evidence Lower Bound (ELBO)

$$\begin{aligned}\log p(x;\theta) &= \log \sum_z p(x,z;\theta) \\ &= \log \sum_z Q(z) \frac{p(x,z;\theta)}{Q(z)} \\ &\geq \sum_z Q(z) \log \frac{p(x,z;\theta)}{Q(z)}\end{aligned}$$

ELBO

Because the log likelihood is intractable, people often optimize its lower bound instead

Why optimizing lower bound works? How to choose Q(z), why we computed posterior in the E step, what is the benefit?

Thank You!
Q & A