Data Modelling Methods-III

CS771: Introduction to Machine Learning

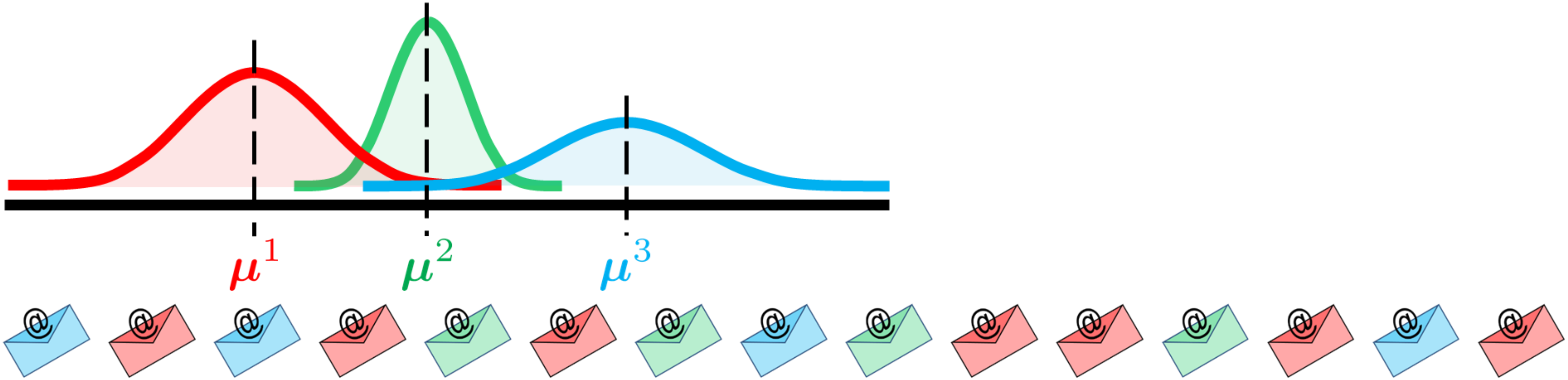
Purushottam Kar

Mid Semester Examination

- September 21st, 2017 (Thursday) 1300-1500 hrs
- Venue L18, 19, L20 (all OROS)
- Syllabus: till whatever we cover today
- Open notes (handwritten only)
- No printed/photocopied material
- No laptops, i-pads, mobile phones (switched off)
- Please bring a notepad with you for rough work
- Please bring a pencil/eraser with you – we will not provide these
- Answers will have to be written on the question paper itself

Recap

The generative story for labelled data



$$\mathbb{P}\left[\mathbf{x}^i, z^i \,|\, \boldsymbol{\Theta}\right] = \mathbb{P}\left[z^i \,|\, \boldsymbol{\Theta}\right] \cdot \mathbb{P}\left[\mathbf{x}^i \,|\, z^i, \boldsymbol{\Theta}\right] = \boldsymbol{\pi}_{z^i} \cdot \mathcal{N}(\mathbf{x}^i \,|\, \boldsymbol{\mu}^{z^i}, \Sigma^{z^i})$$

$$\mathbb{P}\left[X, \{z^i\} \,|\, \boldsymbol{\Theta}\right] = \prod_{i=1}^{n} \mathbb{P}\left[\mathbf{x}^i, z^i \,|\, \boldsymbol{\Theta}\right]$$

$$\hat{\boldsymbol{\Theta}}_{\text{MLE}} = \arg\max_{\boldsymbol{\Theta}} \mathbb{P}\left[X, \{z^i\} \,|\, \boldsymbol{\Theta}\right]$$

$$\boldsymbol{\pi}_1^{\text{MLE}} = \frac{\text{\# red emails}}{\text{\# total emails}} = \frac{n_r}{n}$$

$$\boldsymbol{\mu}^1_{\text{MLE}} = \frac{1}{n_r} \sum_{i:z^i=\bullet} \mathbf{x}^i$$

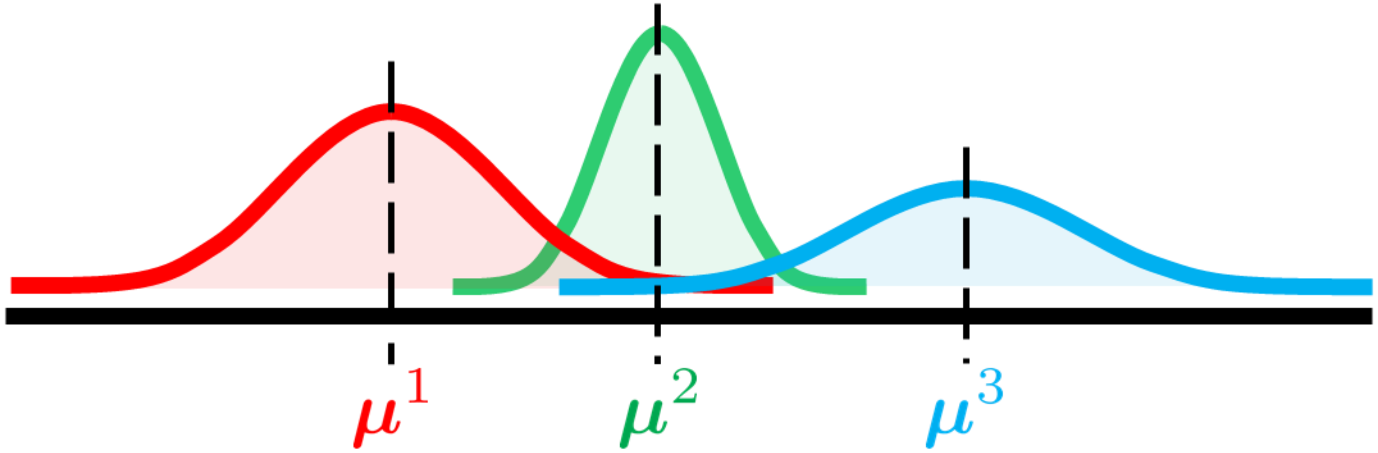
$$\Sigma^1_{\text{MLE}} = \frac{1}{n_r} \sum_{i:z^i=\bullet} (\mathbf{x}^i - \boldsymbol{\mu}^1_{MLE})(\mathbf{x}^i - \boldsymbol{\mu}^1_{MLE})^{\mathsf{T}}$$

Take log and apply 1st order optimality

Read [DAU] Sections 9.1-9.5

Recap

The generative story for unlabelled data



z^i denotes the (unknown) component from which x^i came

$$\mathbb{P}\left[\mathbf{x}^i \mid \boldsymbol{\Theta}\right] = \sum_{k=1}^{K} \mathbb{P}\left[\mathbf{x}^i, z^i = k \mid \boldsymbol{\Theta}\right] = \sum_{k=1}^{K} \boldsymbol{\pi}_k \cdot \mathbb{P}\left[\mathbf{x}^i \mid z^i = k, \boldsymbol{\Theta}\right]$$

z^i not known from data. It is a *latent variable* (can take K values.

$$= \sum_{k=1}^{K} \boldsymbol{\pi}_k \cdot \mathcal{N}(\mathbf{x}^i \mid \boldsymbol{\mu}^k, \Sigma^k)$$

Gaussian Mixture Model (GMM) with K components

Goal: incomplete data, learn $\boldsymbol{\mu}^k, \Sigma^k, \mathbb{P}[z = k]$

$\boldsymbol{\pi}_k = \mathbb{P}[z^i = k]$ prior prob. of $\mathbf{x}^i$ coming from k-th component

Recap

A Ray of Hope

$$\hat{\mathbf{\Theta}}_{\text{MLE}} = \arg\max_{\mathbf{\Theta}} \mathbb{P}\left[X \mid \mathbf{\Theta}\right]$$

Looks like block coordinate descent with $\Theta, \{z^i\}$ being two blocks of "coordinates"

ALTERNATING OPTIMIZATION

1. Initialize $\mathbf{\Theta}^0$
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Various ways of updating z^i

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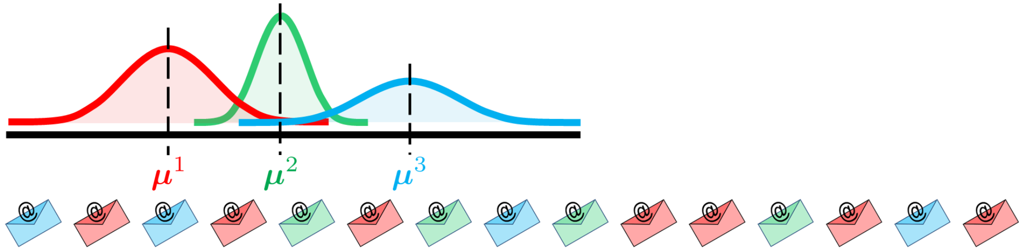

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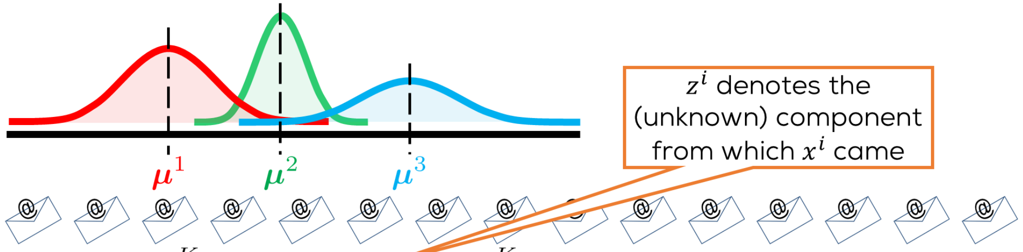
The generative story for unlabelled data



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Sept

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Various ways of updating z^i

Sept 8, 2017

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Hard Assignment

The K-means algorithm

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Bayes Rule!

$$z^{i,t} = \arg\max_{k \in [K]} \mathbb{P}\left[k \mid \mathbf{x}^i, \mathbf{\Theta}^t\right] = \arg\max_{k \in [K]} \mathbb{P}\left[k \mid \mathbf{\Theta}^t\right] \cdot \mathbb{P}\left[\mathbf{x}^i \mid k, \mathbf{\Theta}^t\right]$$

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Towards the K-Means Algorithm

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   1. Let $z^{i,t} = \arg\max_k \boldsymbol{\pi}_k^t \cdot \mathcal{N}\left(\mathbf{x}^i \mid \boldsymbol{\mu}^{k,t}, \Sigma^{k,t}\right)$
3. Update $\boldsymbol{\Theta}^{t+1} = \arg\max_{\boldsymbol{\Theta}} \mathbb{P}\left[X, \left\{z^{i,t}\right\} \mid \boldsymbol{\Theta}\right]$
   1. Let $\boldsymbol{\pi}_k^{t+1} = \frac{n_k^t}{n}$, where $\mathrm{n}_k^t = \left|\left\{i\colon z^{i,t} = k\right\}\right|$
   2. Let $\boldsymbol{\mu}^{k,t+1} = \frac{1}{n_k^t} \sum_{i:z^{i,t}=k} \mathbf{x}^i$
   3. Let $\Sigma_k^{t+1} = \frac{1}{n_k^t} \sum_{i:z^{i,t}=k} \left(\mathbf{x}^i - \boldsymbol{\mu}^{k,t+1}\right)\left(\mathbf{x}^i - \boldsymbol{\mu}^{k,t+1}\right)^\top$
4. Repeat until convergence

A few simplifications

- Fix $\boldsymbol{\pi}_k^t = \frac{1}{K}$ for all iterations. Don't update it.
- Fix $\boldsymbol{\Sigma}^{k,t} = I$ for all iterations. Don't update it.

K-MEANS/LLOYD'S ALGORITHM

1. Initialize means $\{\boldsymbol{\mu}^{k,0}\}_{k=1,\ldots K}$
2. For $i \in [n]$, update $z^{i,t}$ using $\boldsymbol{\mu}^{k,t}$
   1. Let $z^{i,t} = \arg\max_k \mathcal{N}\left(\mathbf{x}^i \mid \boldsymbol{\mu}^{k,t}, I\right)$
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$$\hat{\mathbf{\Theta}}_{\mathrm{km}} = \underset{\substack{\{\boldsymbol{\mu}^k\}_{k=1,\ldots,K} \\ \{z^i\}_{i=1,\ldots,n}}}{\arg\min} \sum_{k=1}^{K} \sum_{i:z^i=k} \left\|\mathbf{x}^i - \boldsymbol{\mu}^k\right\|_2^2$$

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Alternates between updating $\{z^i\}$ and $\{\mu^k\}$

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An FA approach to solving a data modelling task!

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NP-hard problem!

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Very scalable but sensitive to initialization!

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k-means++ initialization

1. Sample $i_1 \sim [n]$, let $\boldsymbol{\mu}^{1,0} = \mathbf{x}^{i_1}$
2. For k = 2,…K
   - Sample $i_k \propto$ min distance from $\{\boldsymbol{\mu}^{1,0}, \ldots, \boldsymbol{\mu}^{k-1,0}\}$
   - Let $\boldsymbol{\mu}^{k,0} = \mathbf{x}^{i_k}$

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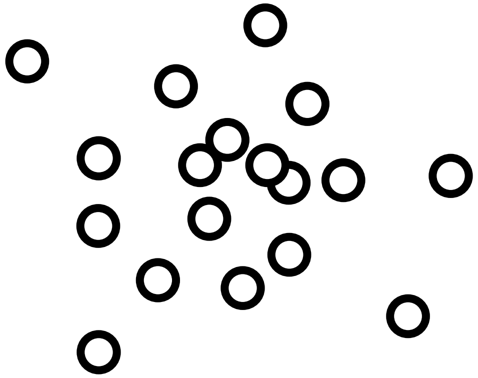

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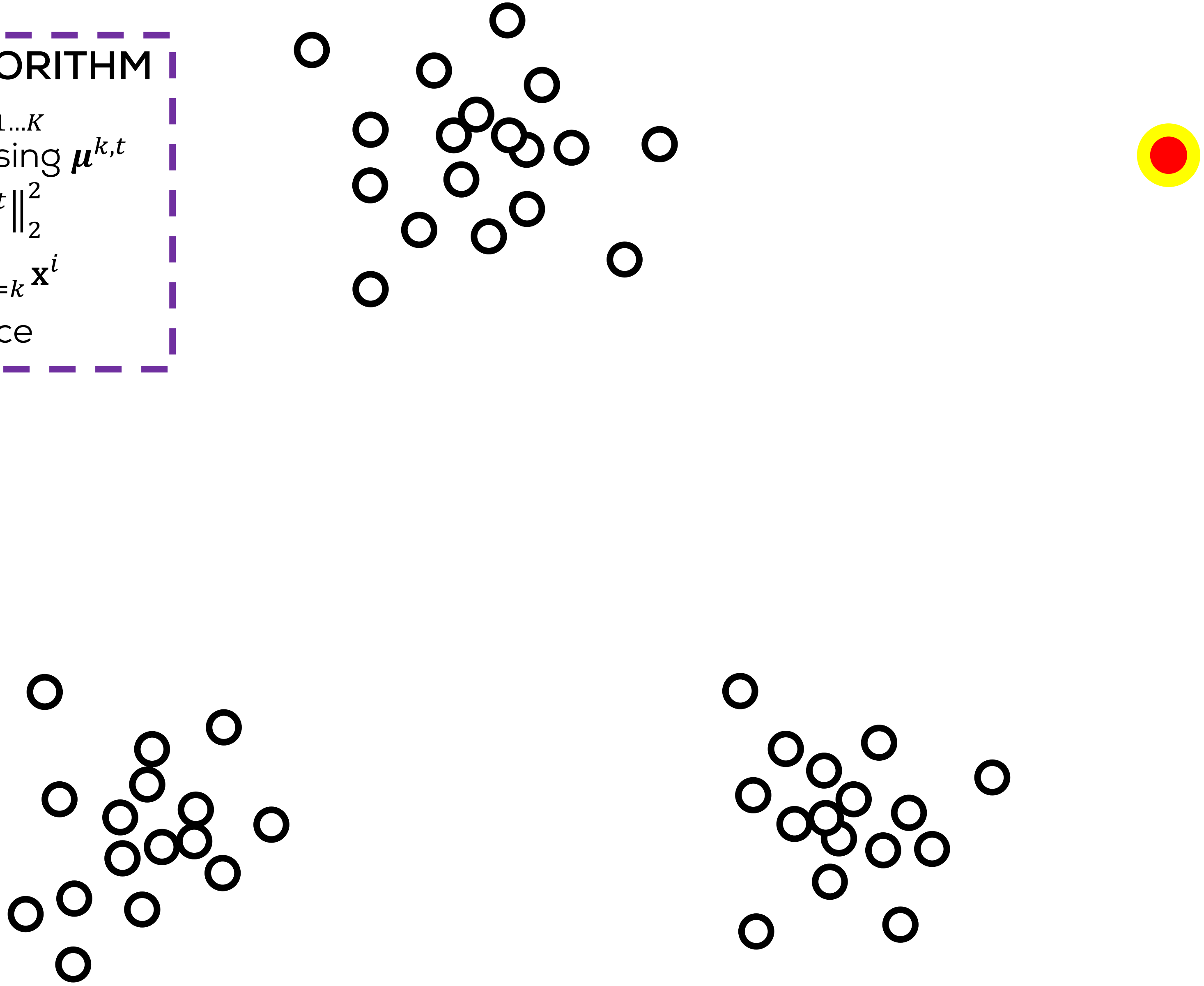

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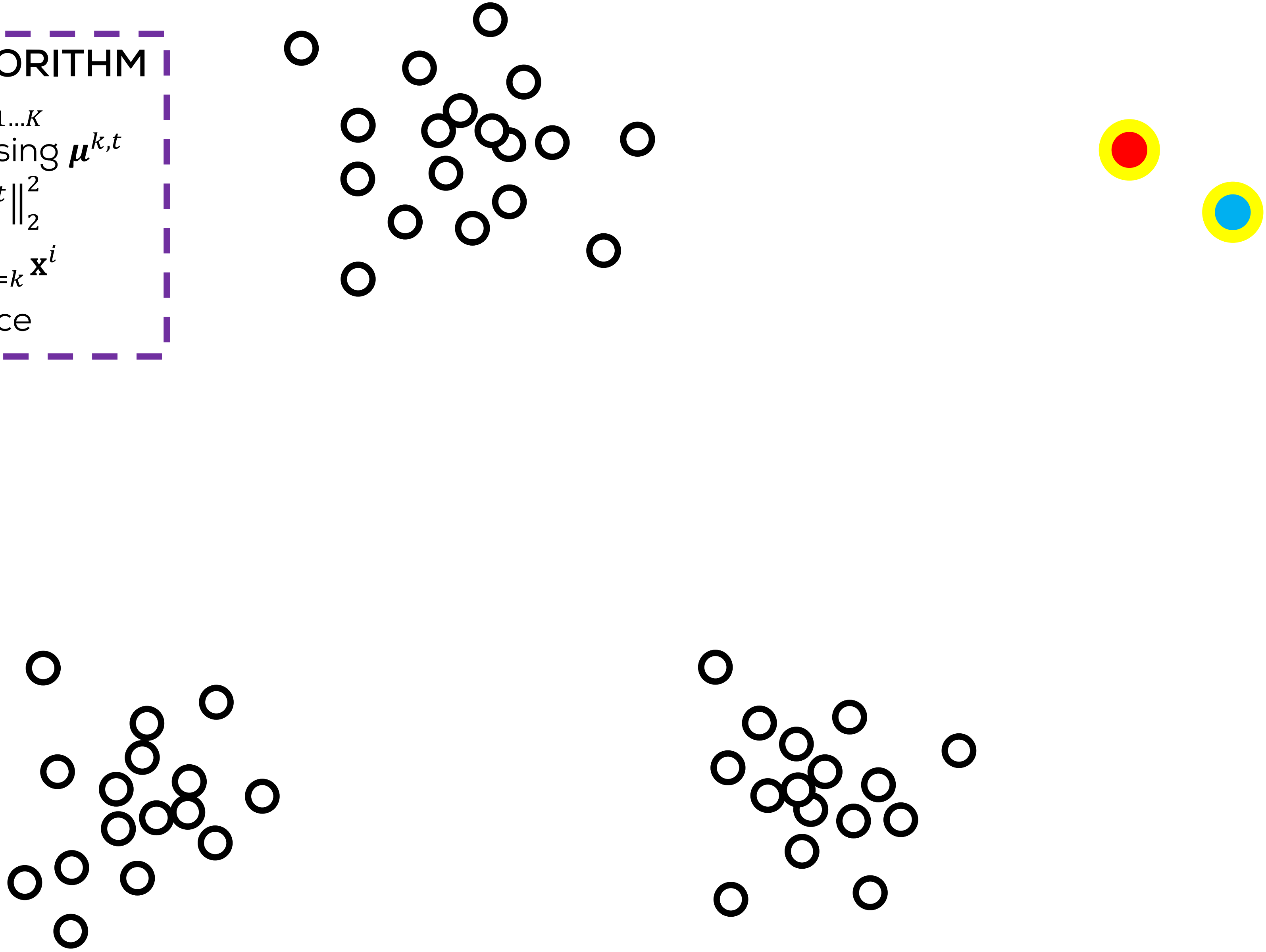

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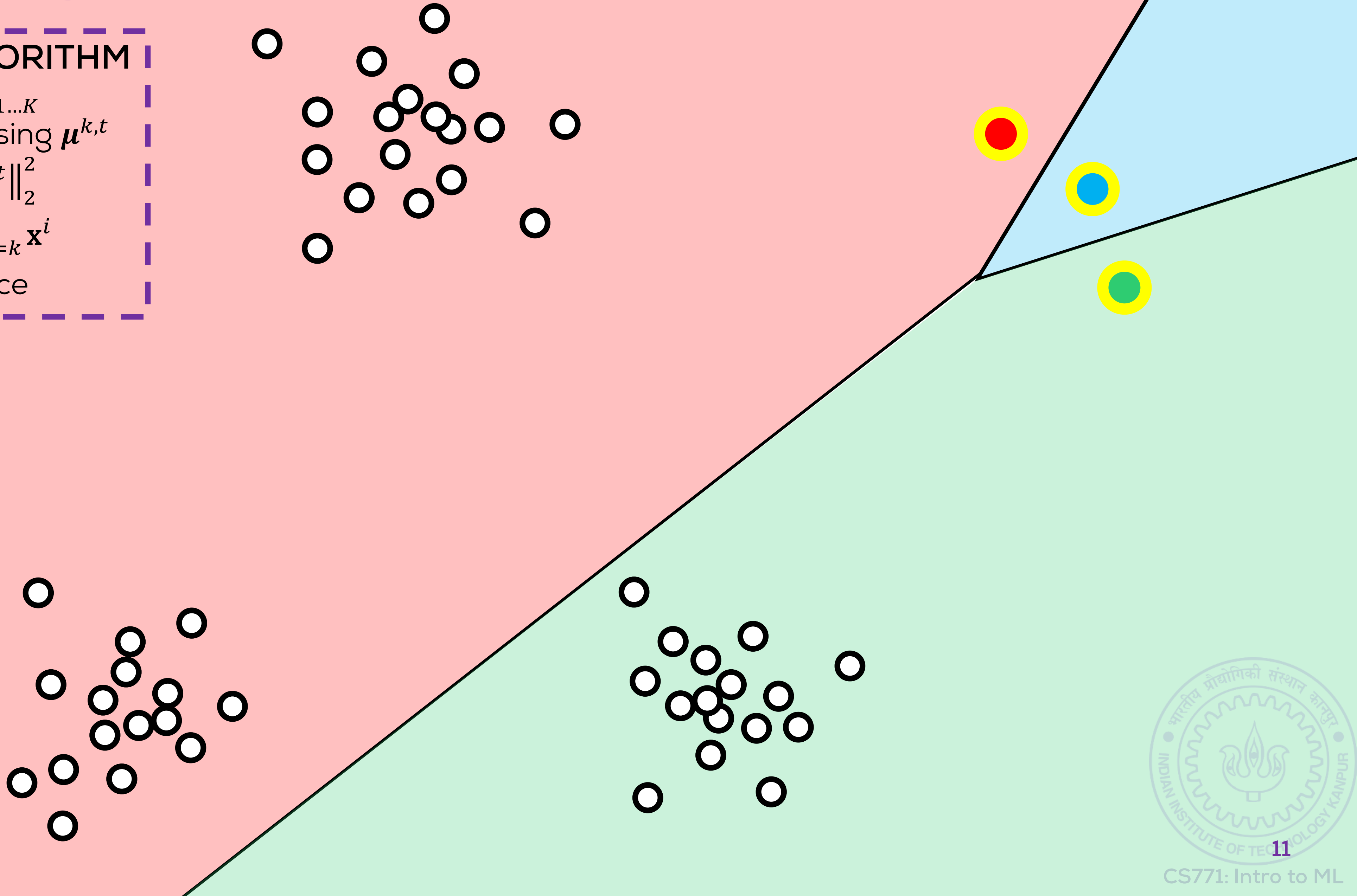

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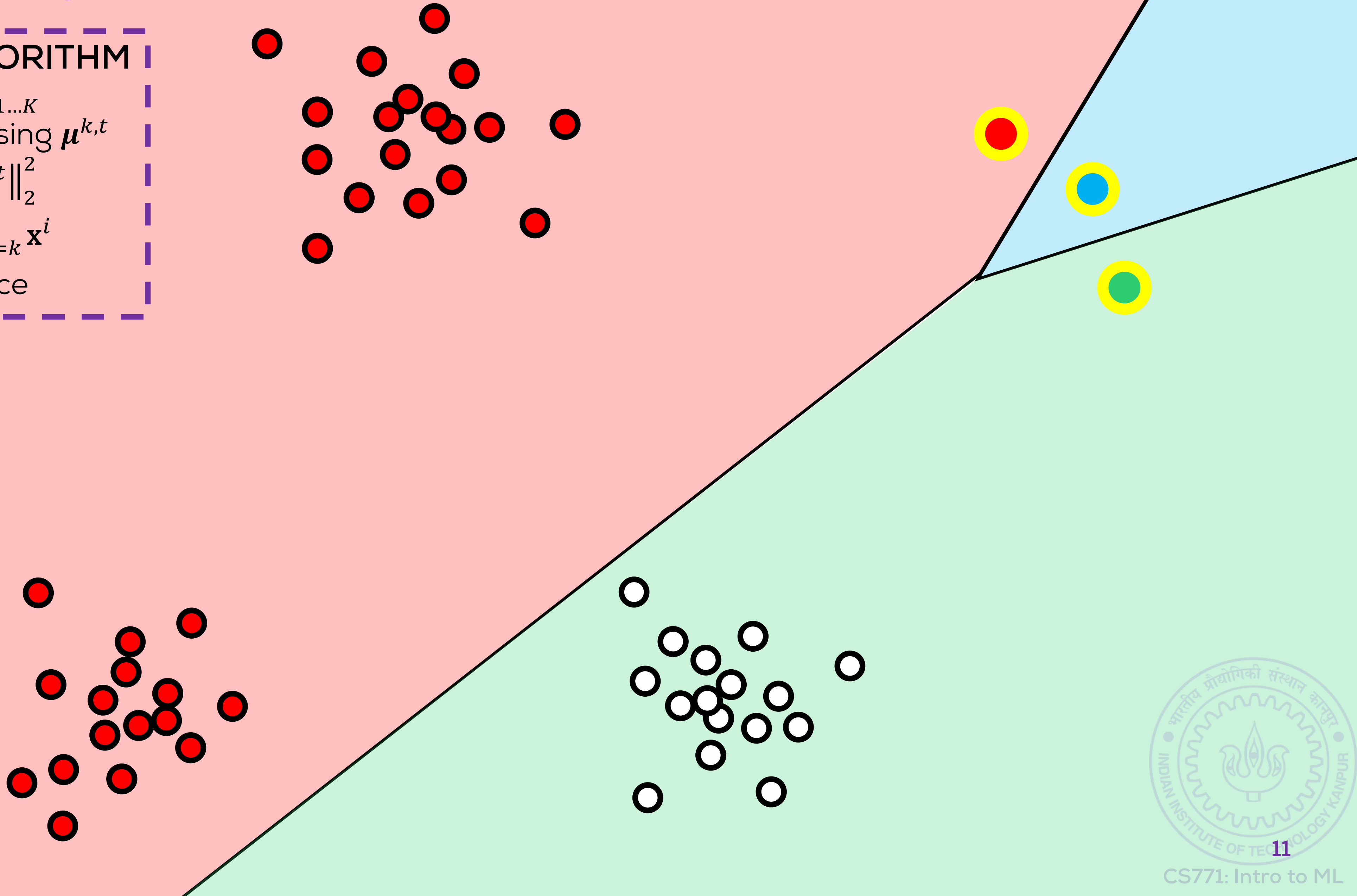

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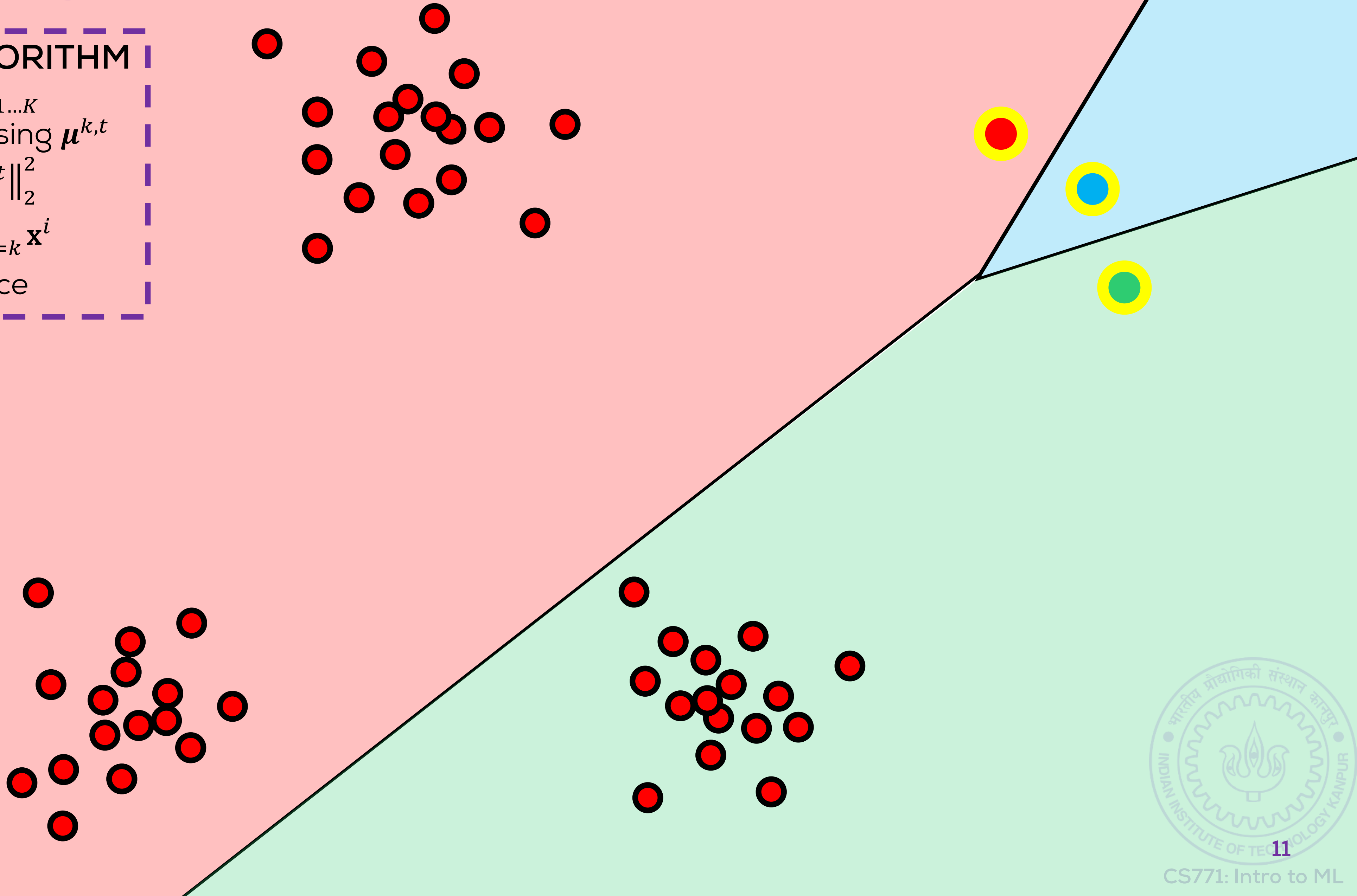

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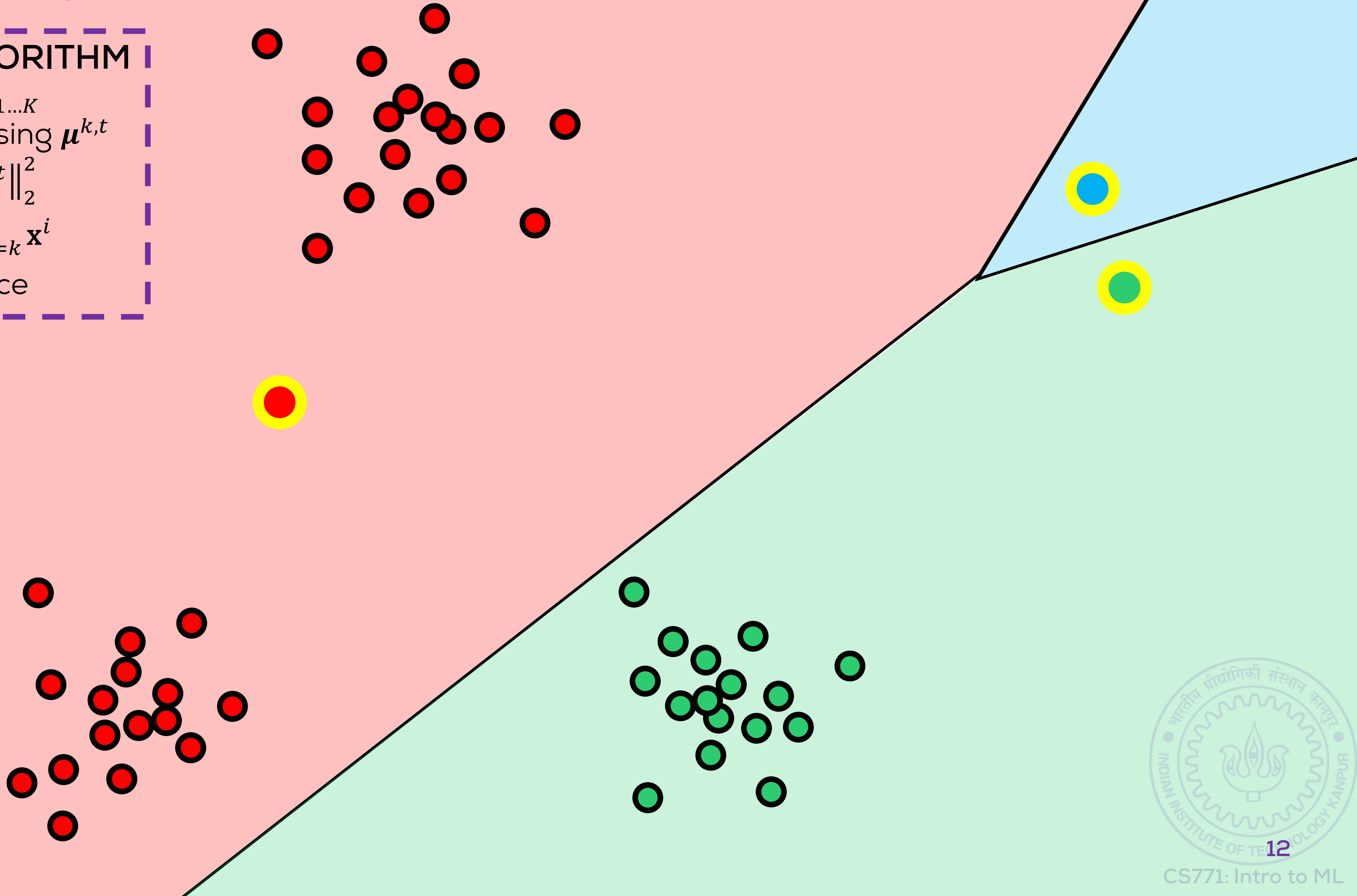

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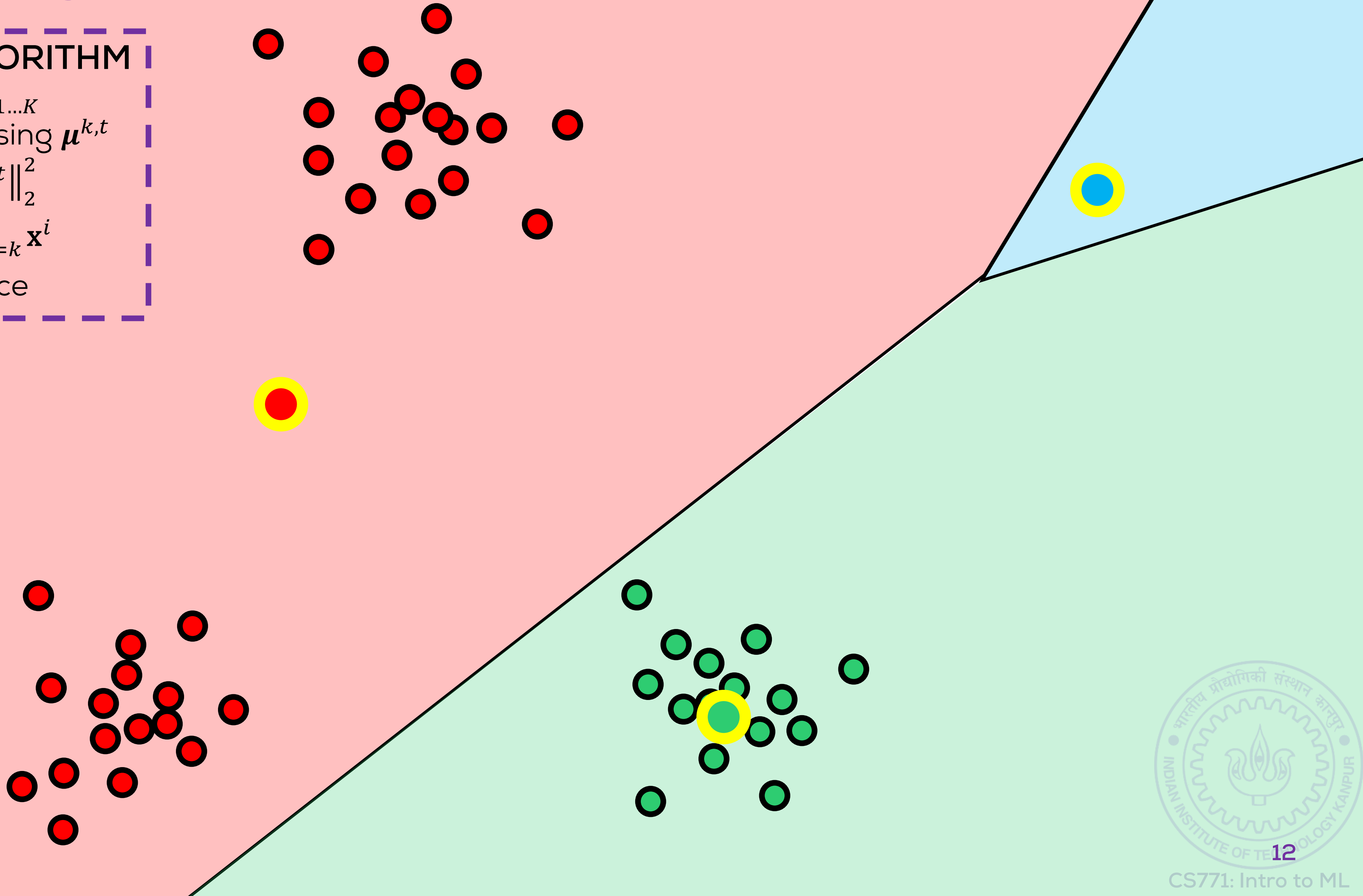

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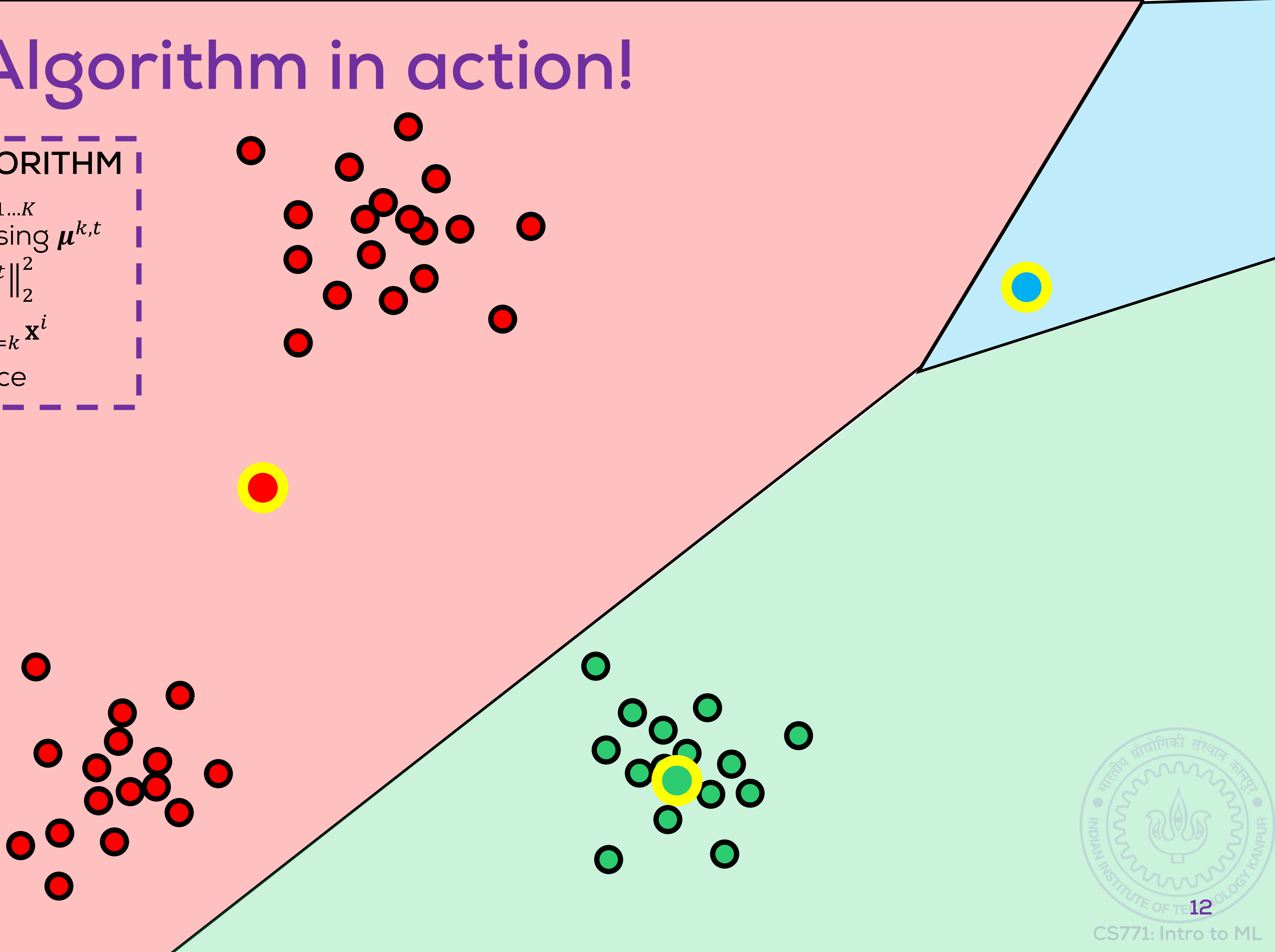

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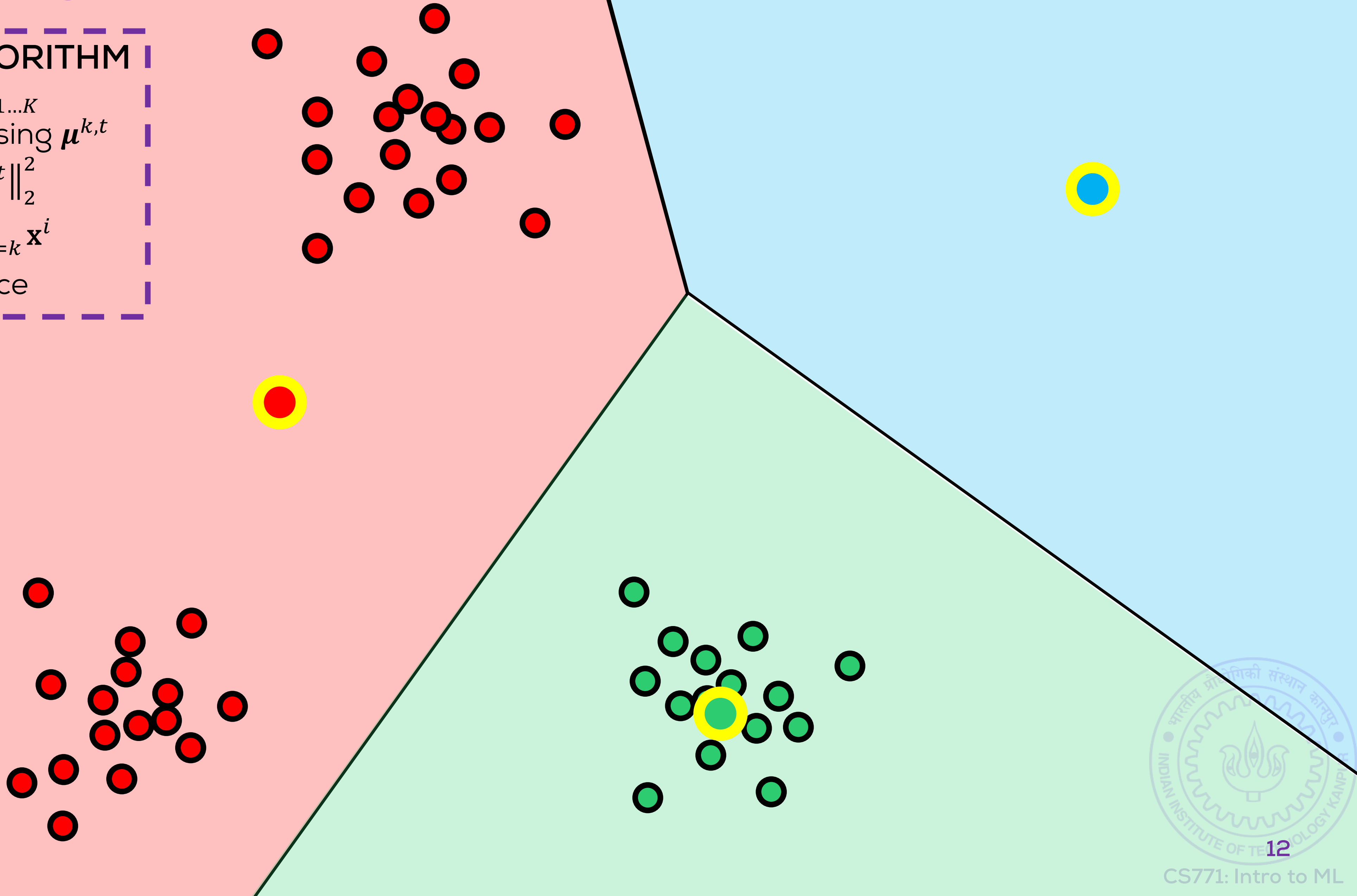

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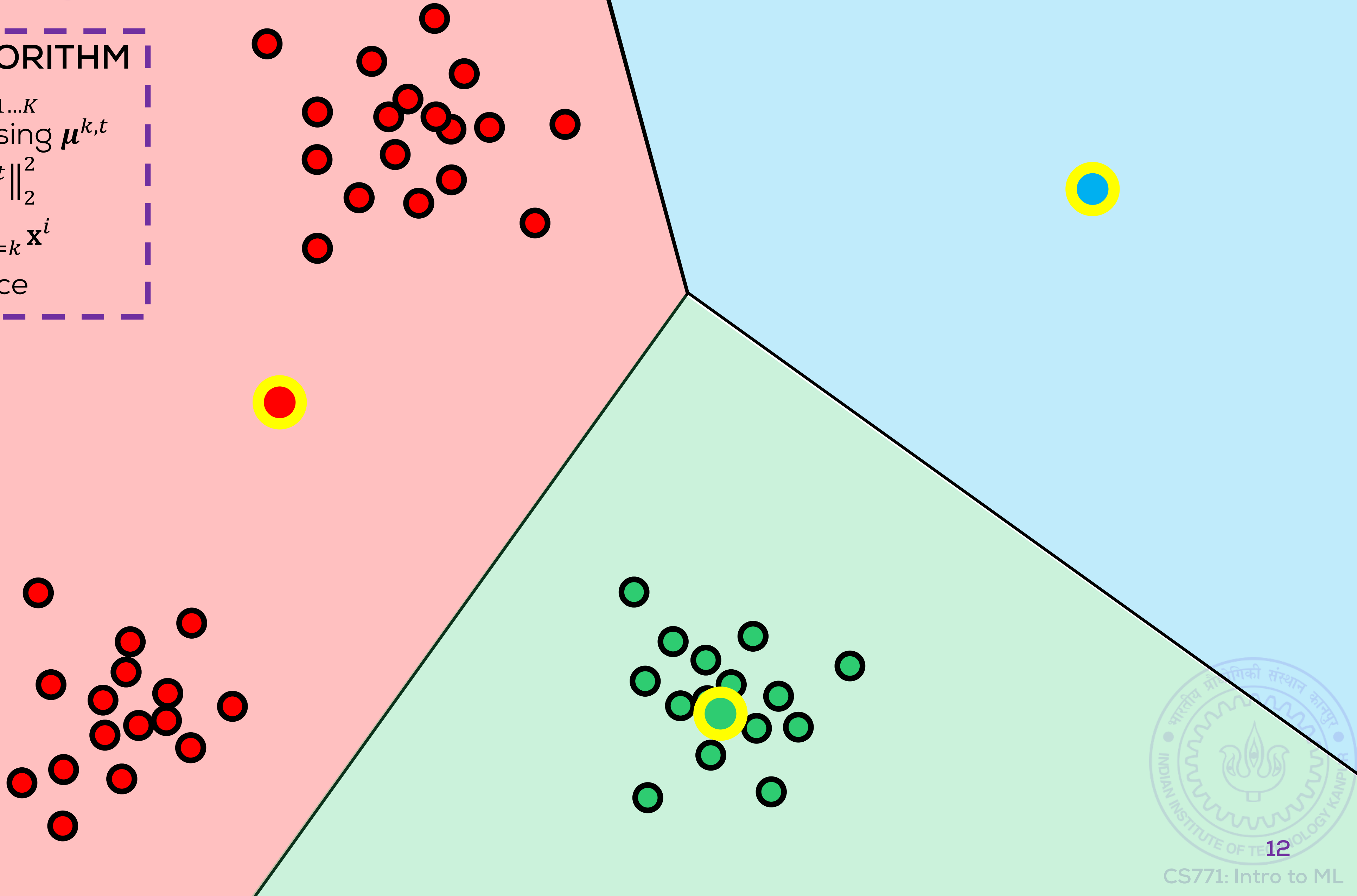

Stuck!!!

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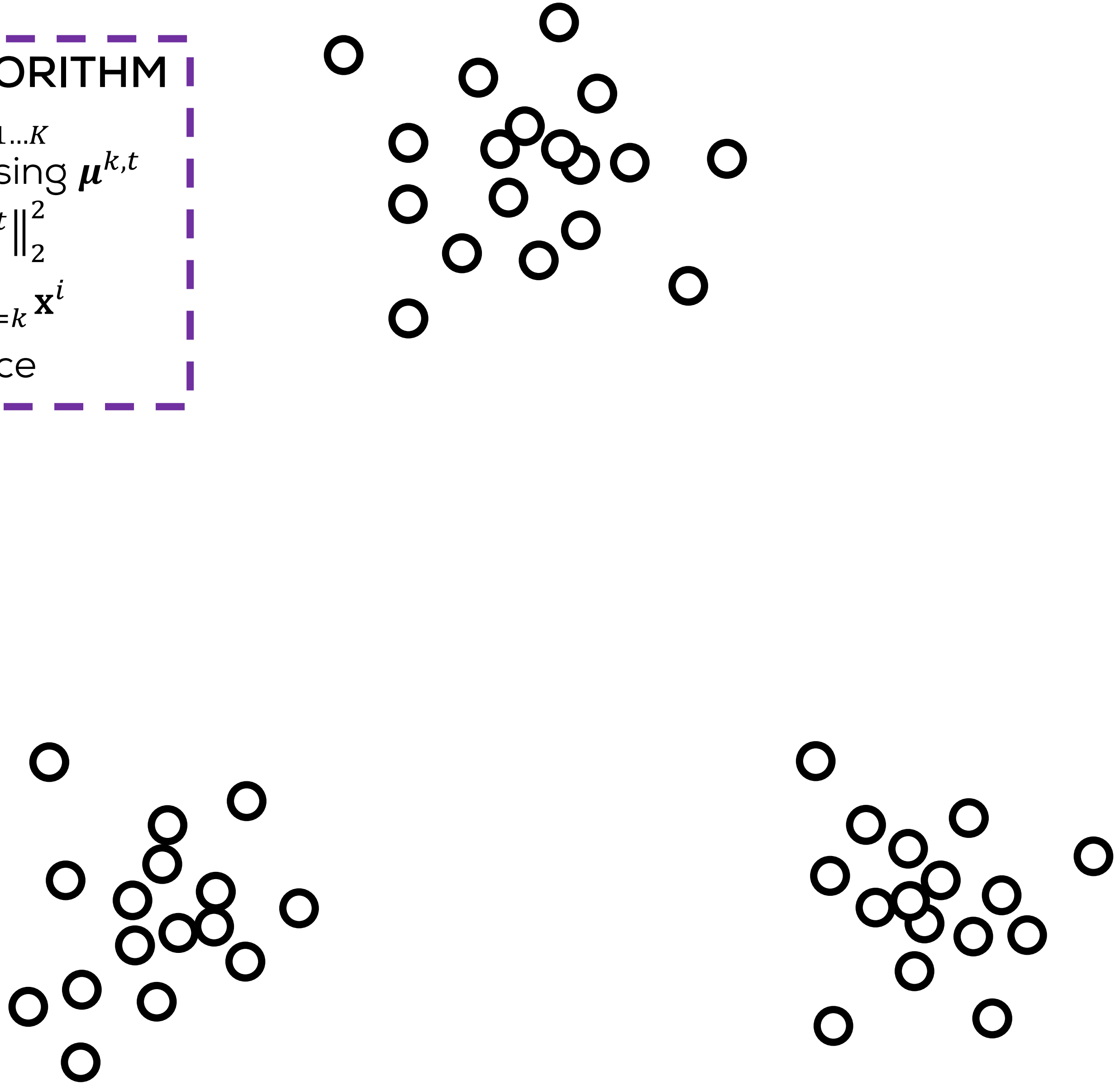

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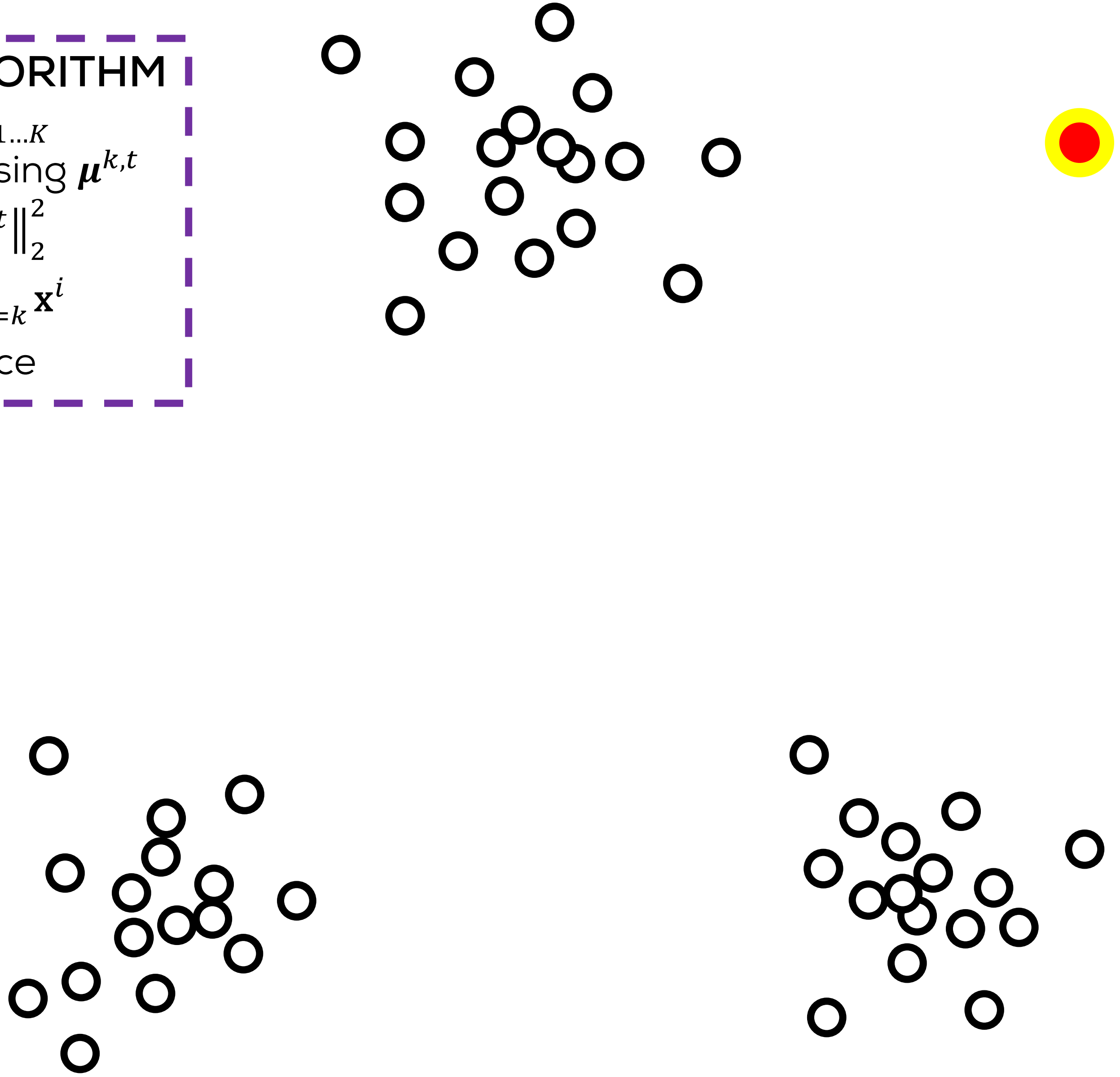

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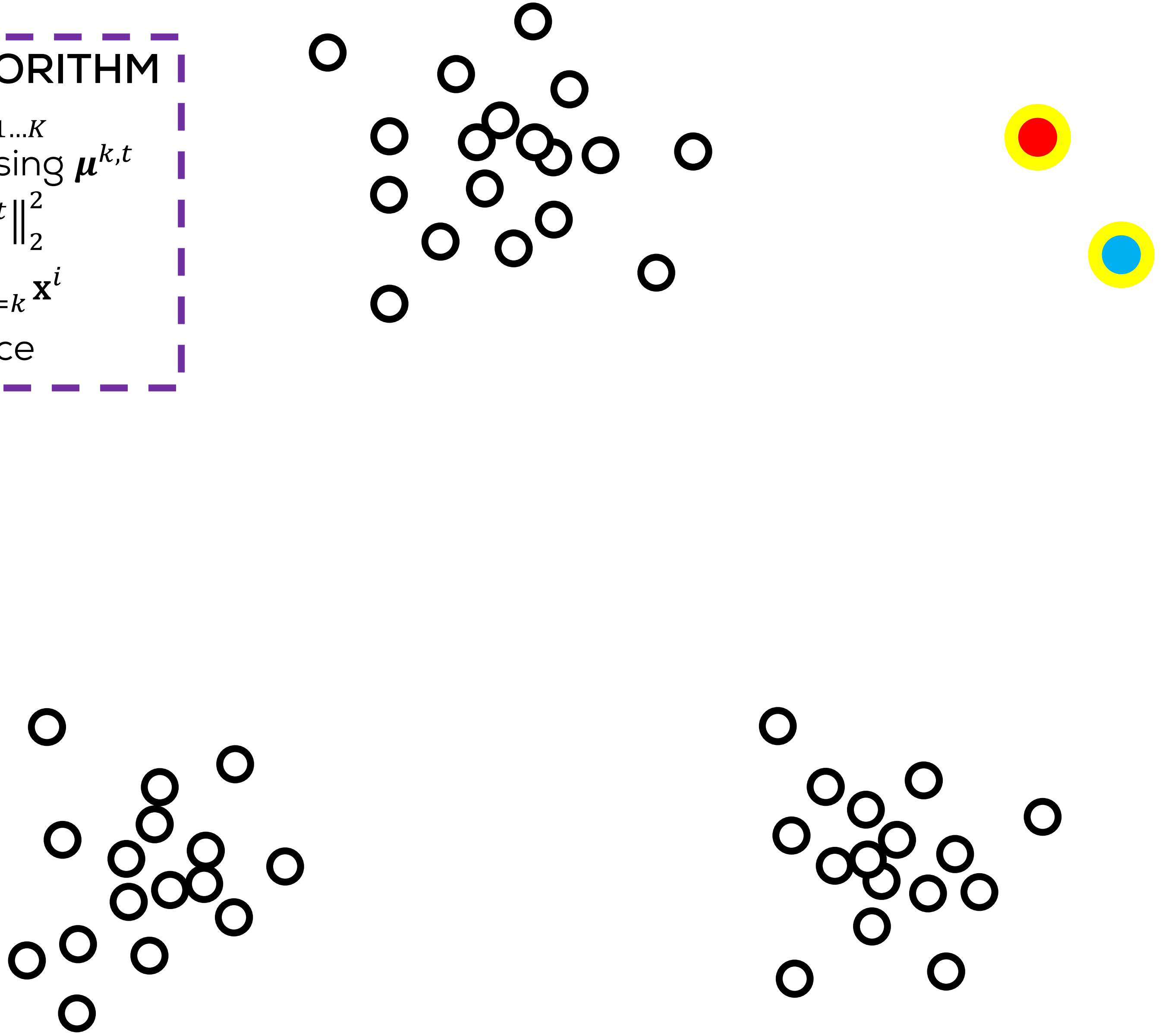

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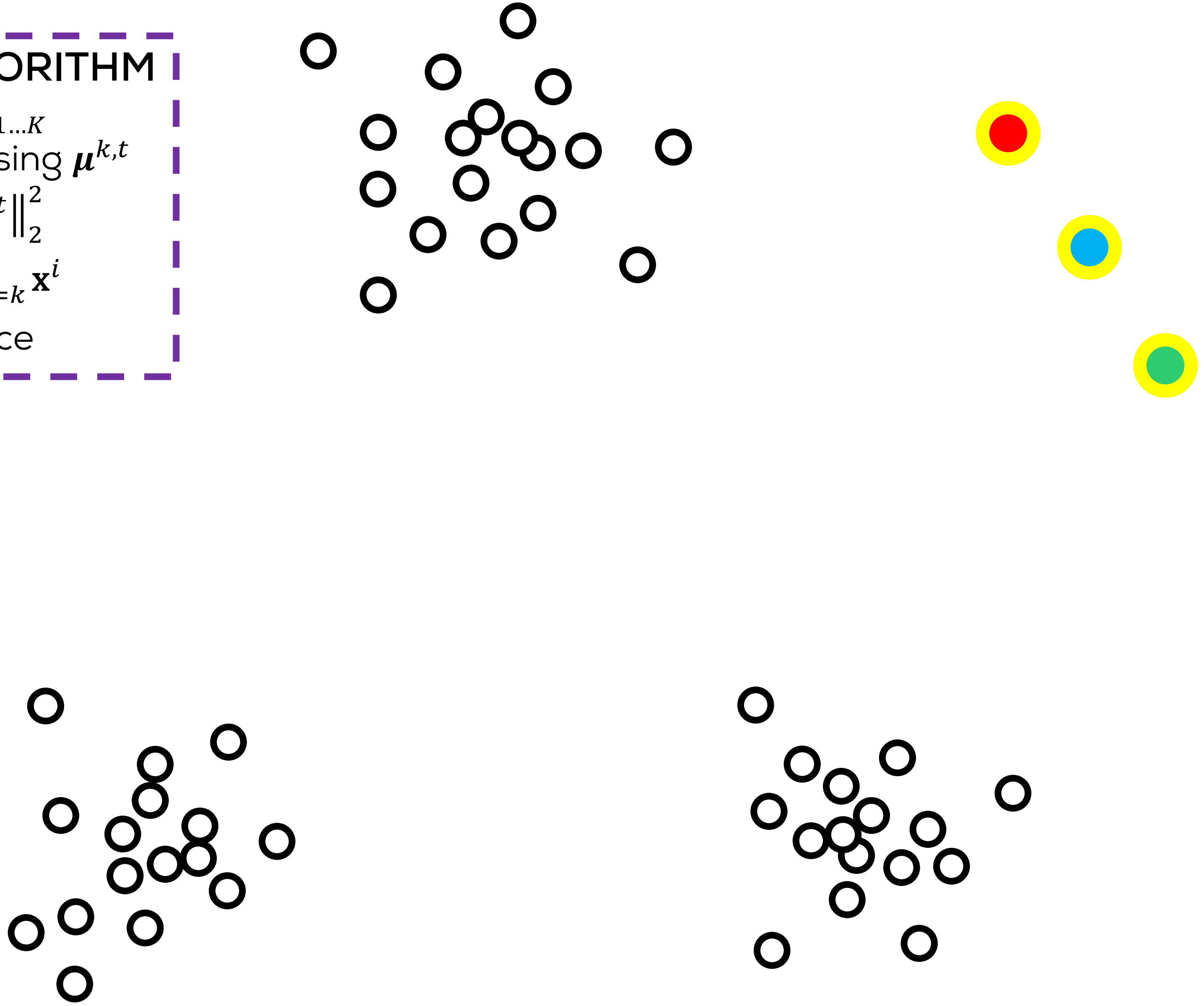

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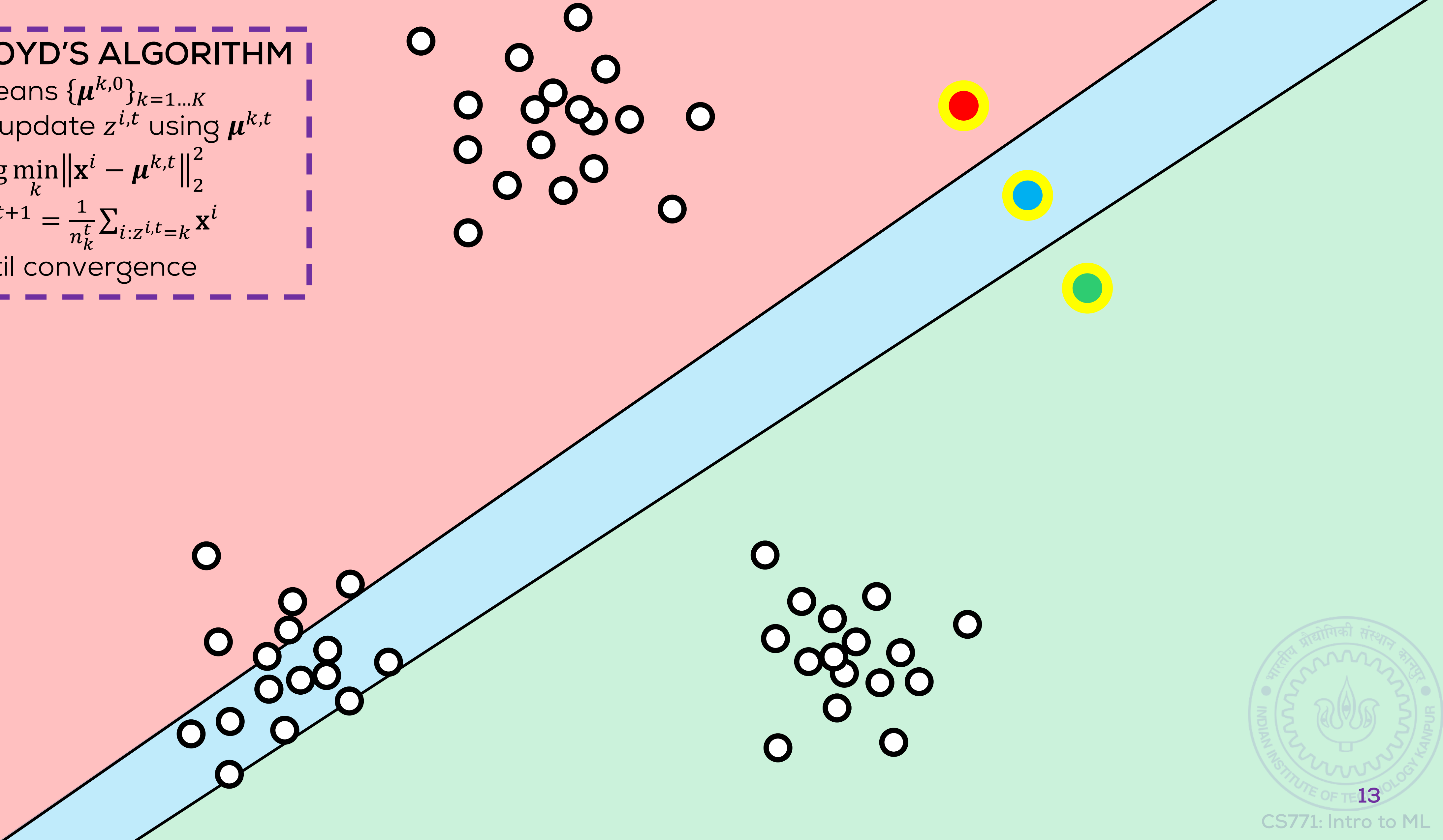

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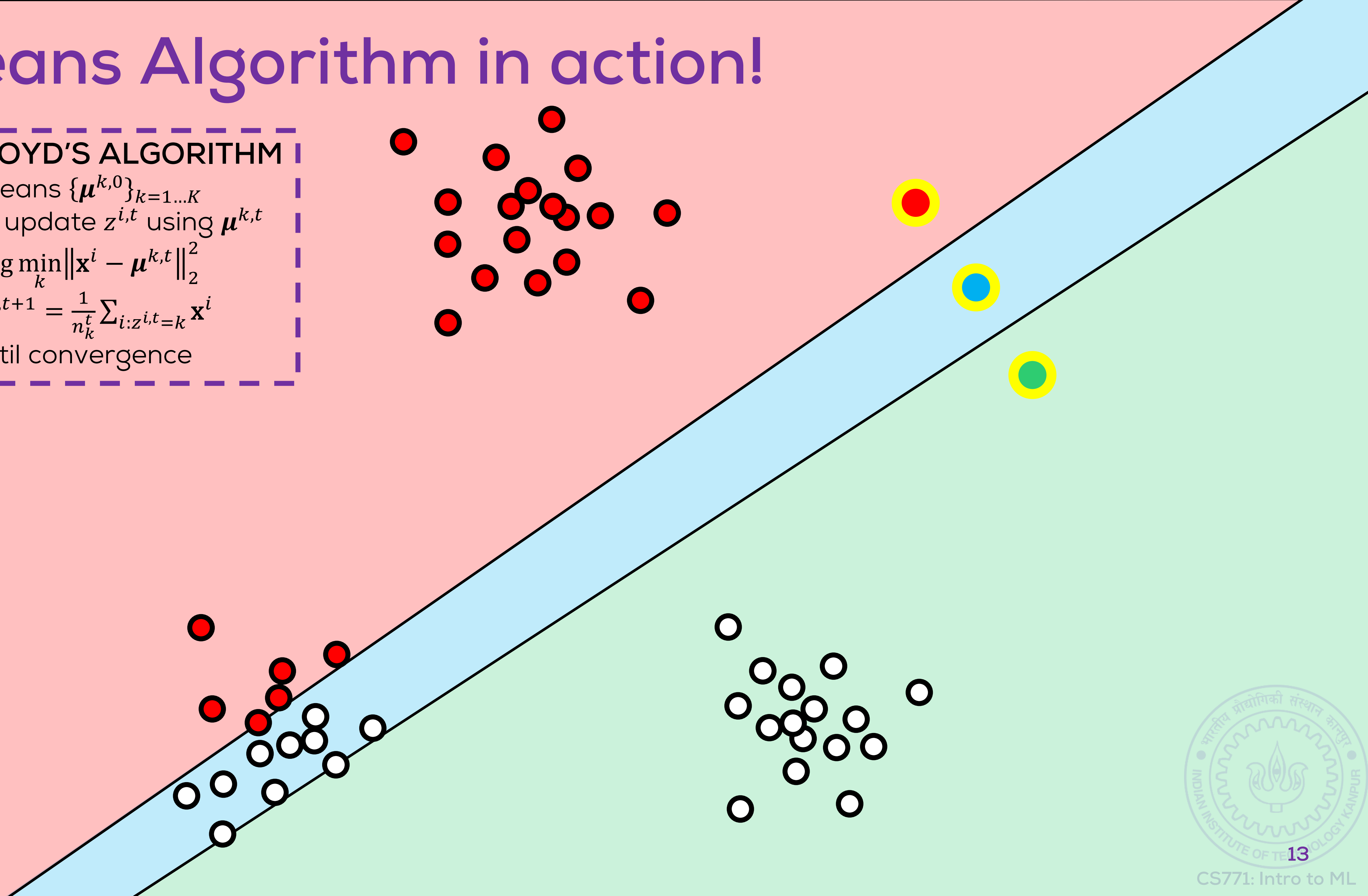

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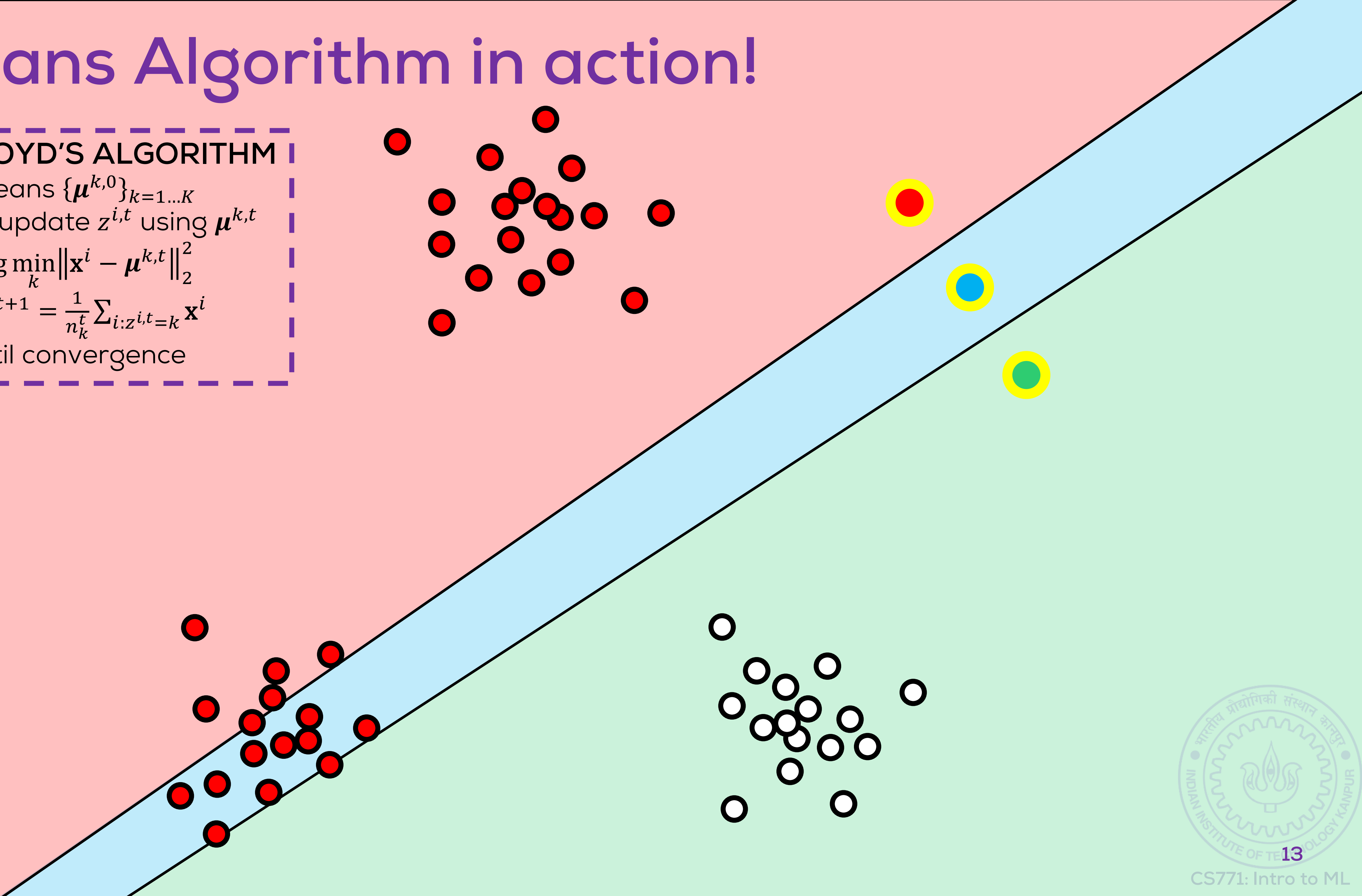

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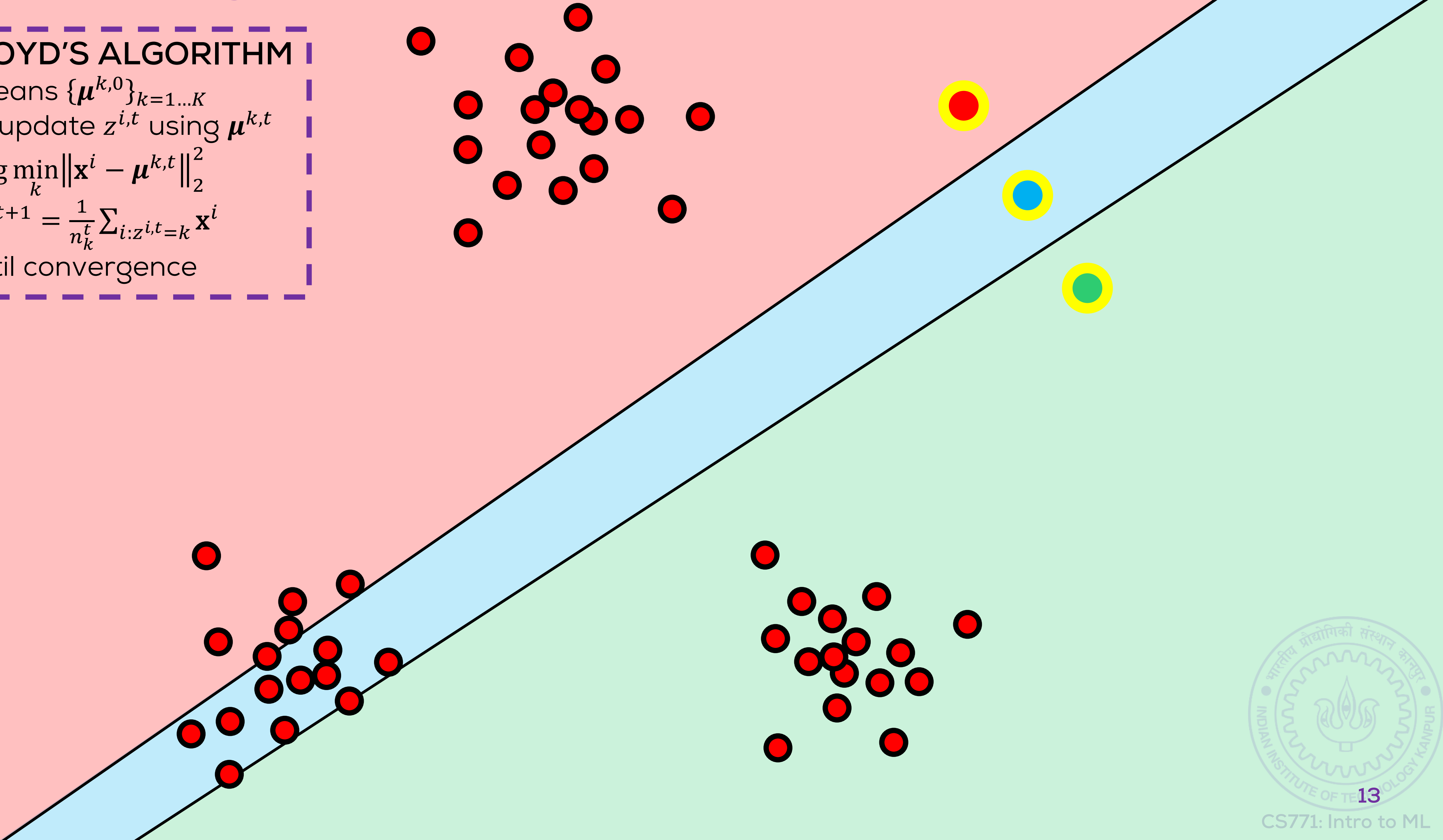

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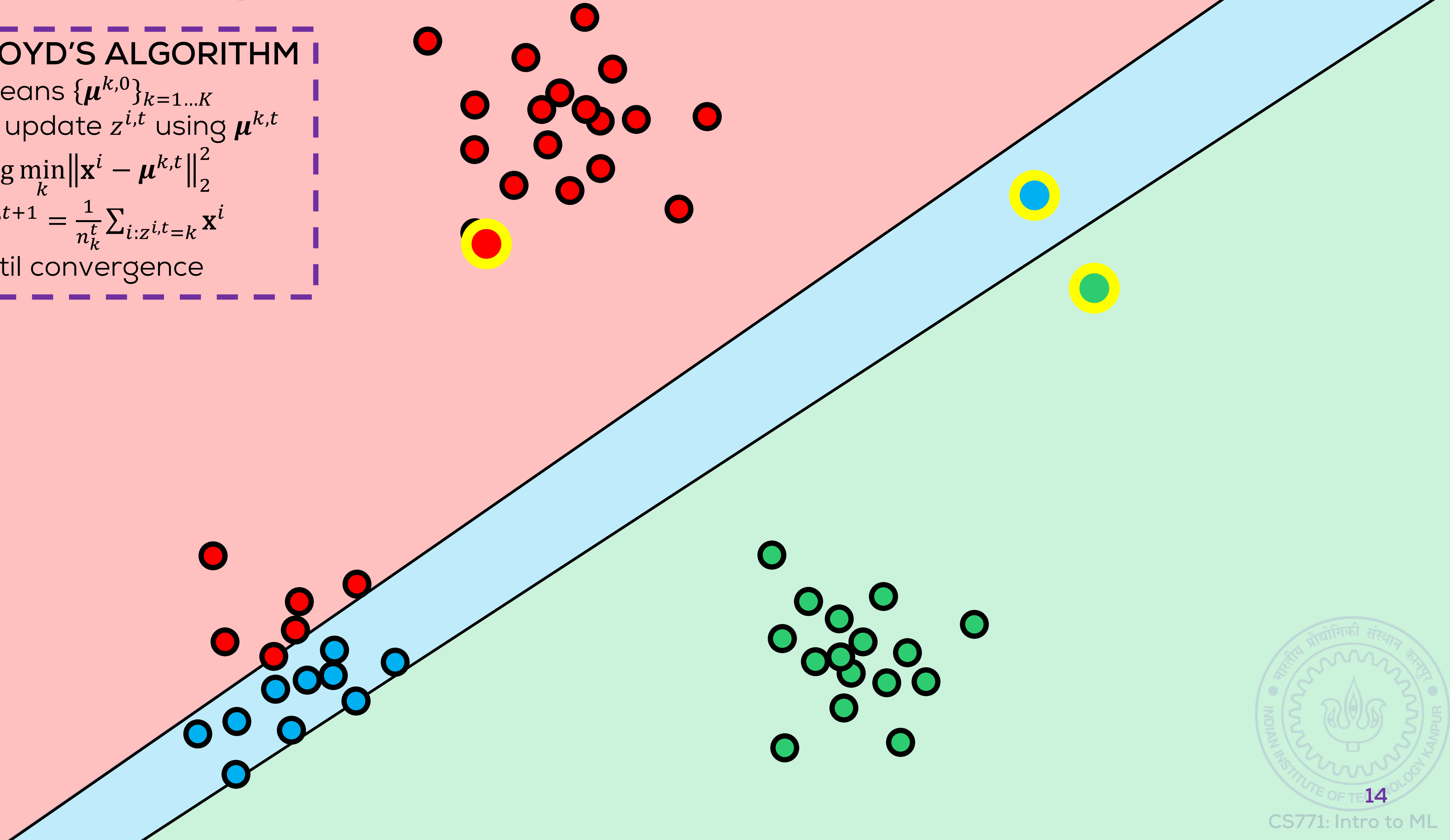

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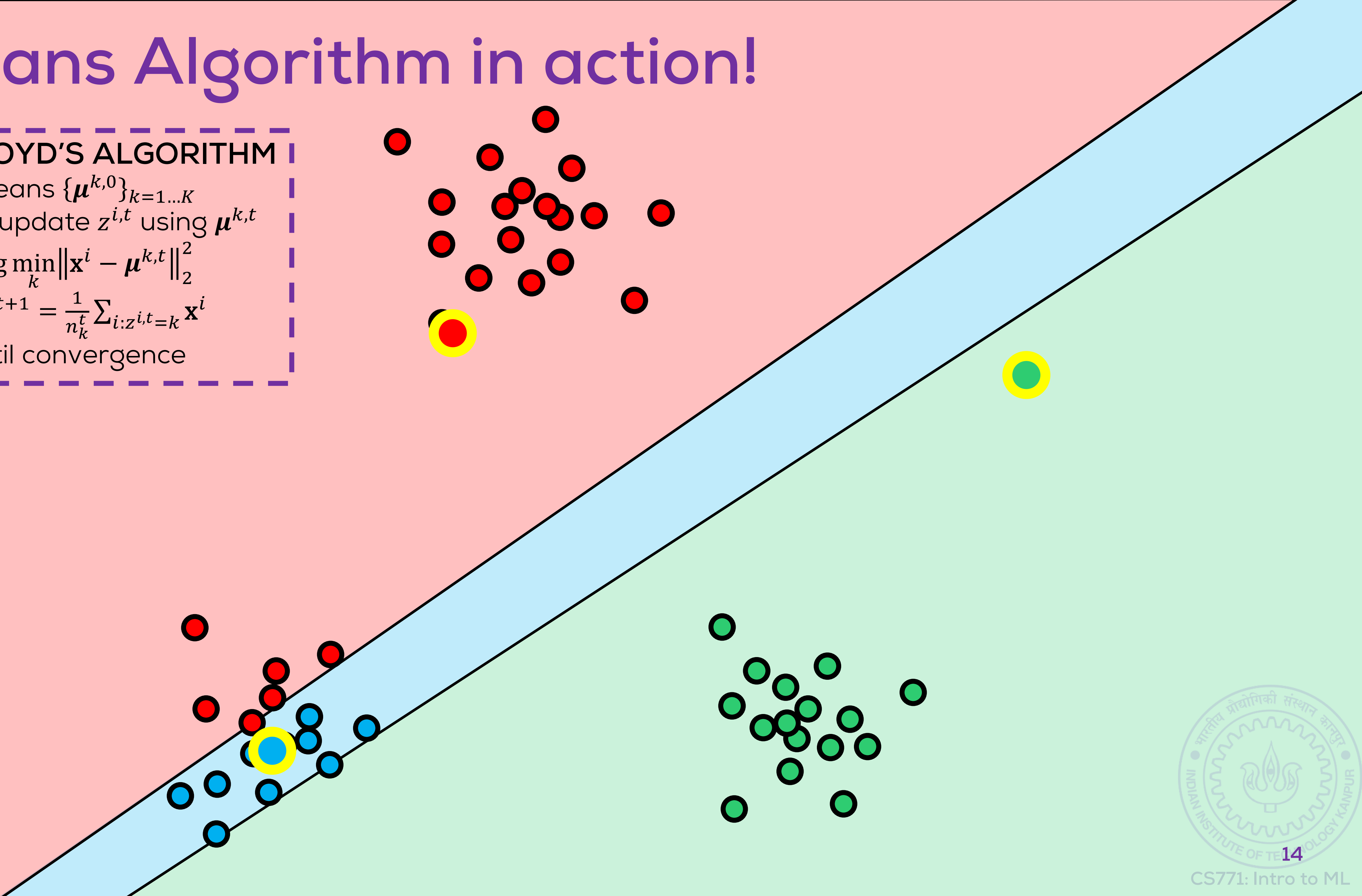

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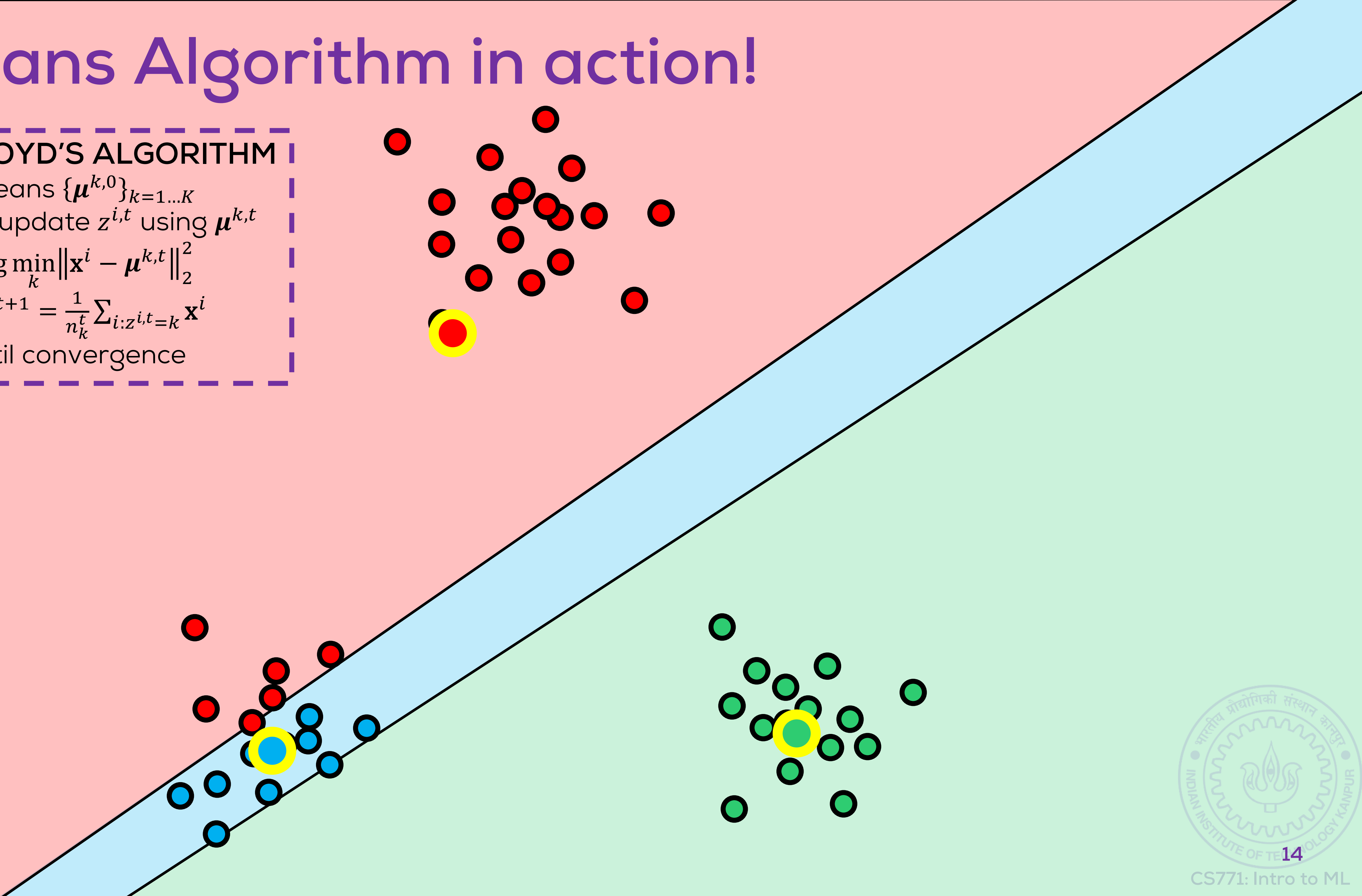

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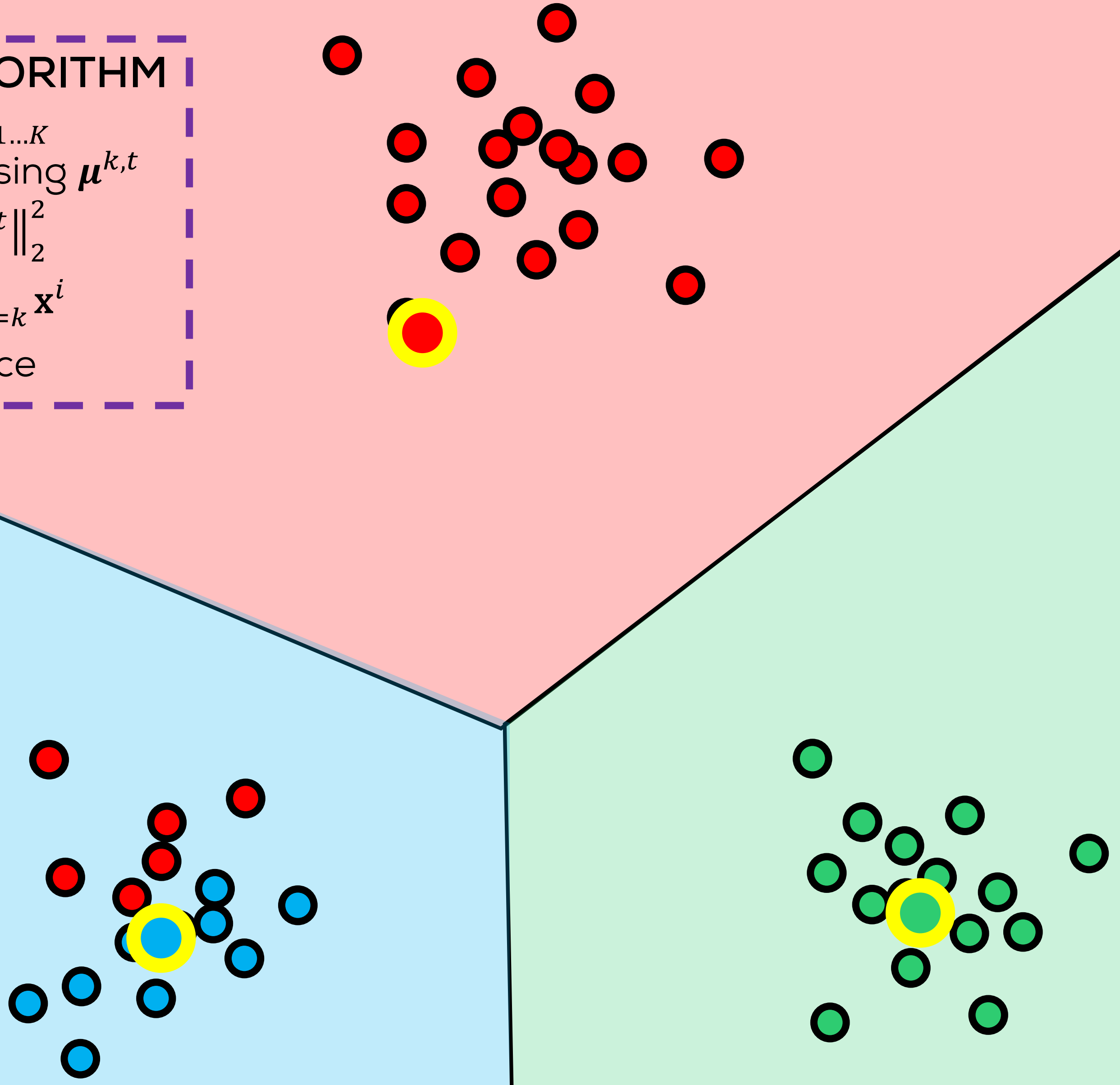

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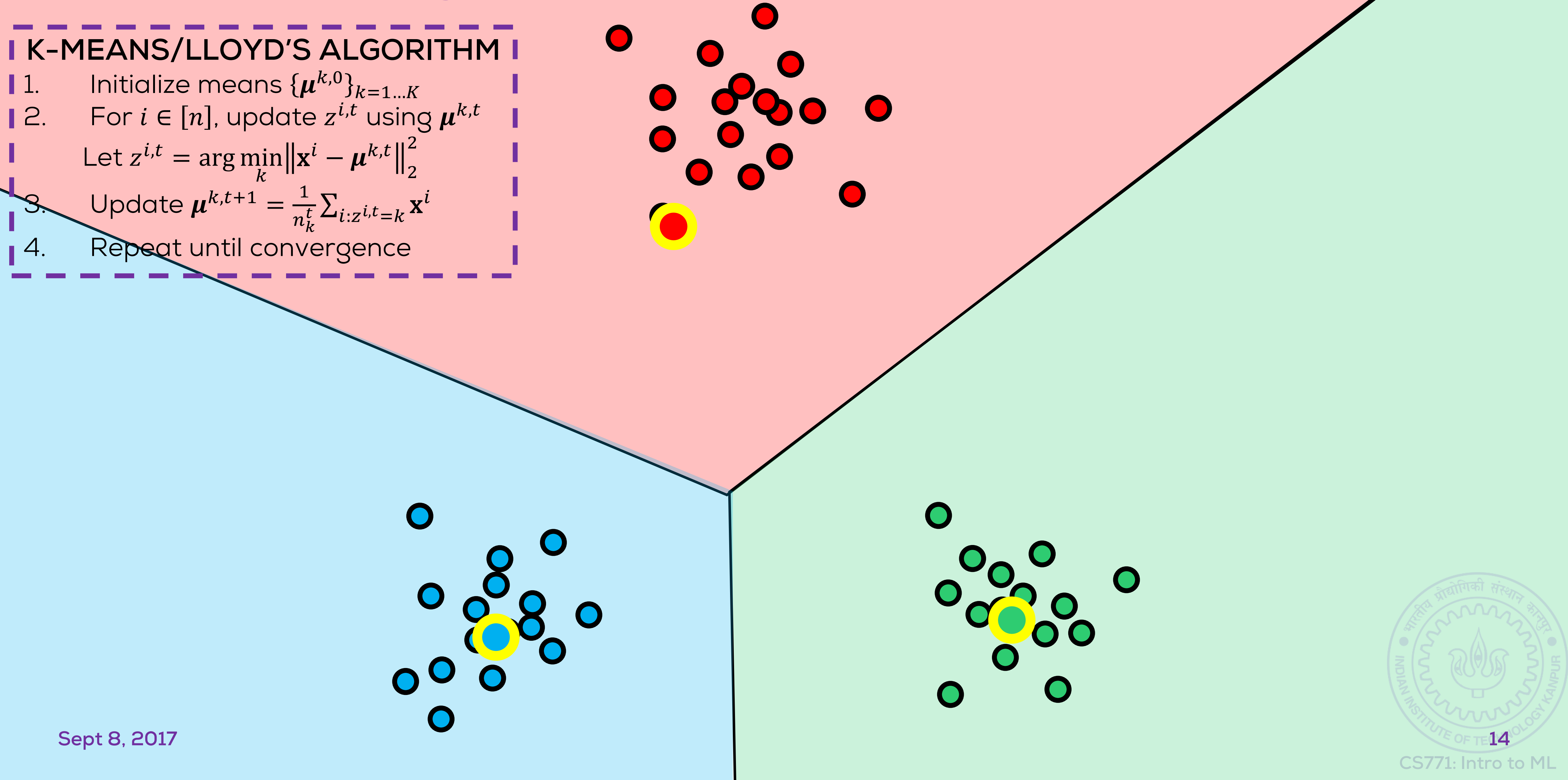

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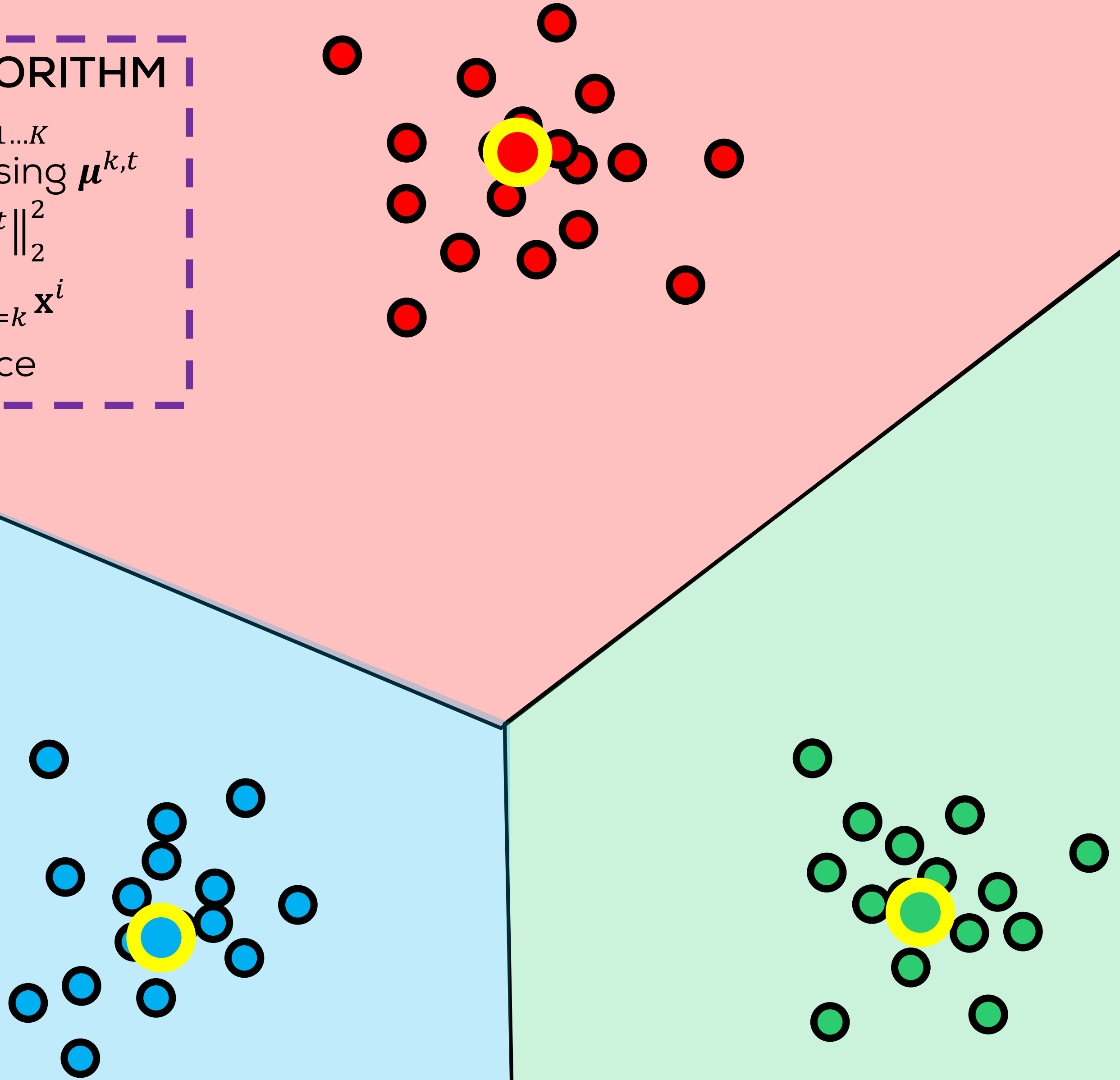

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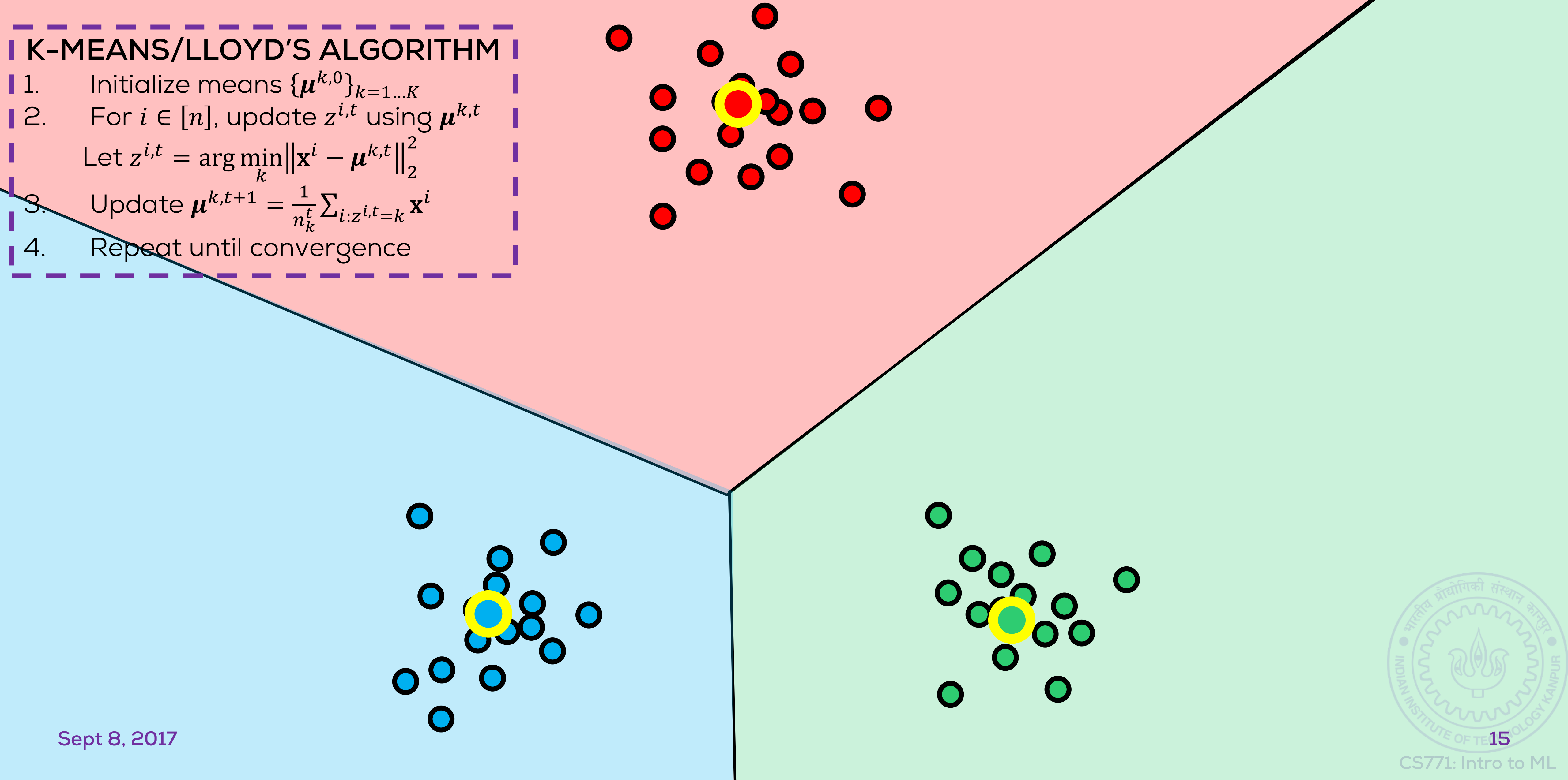

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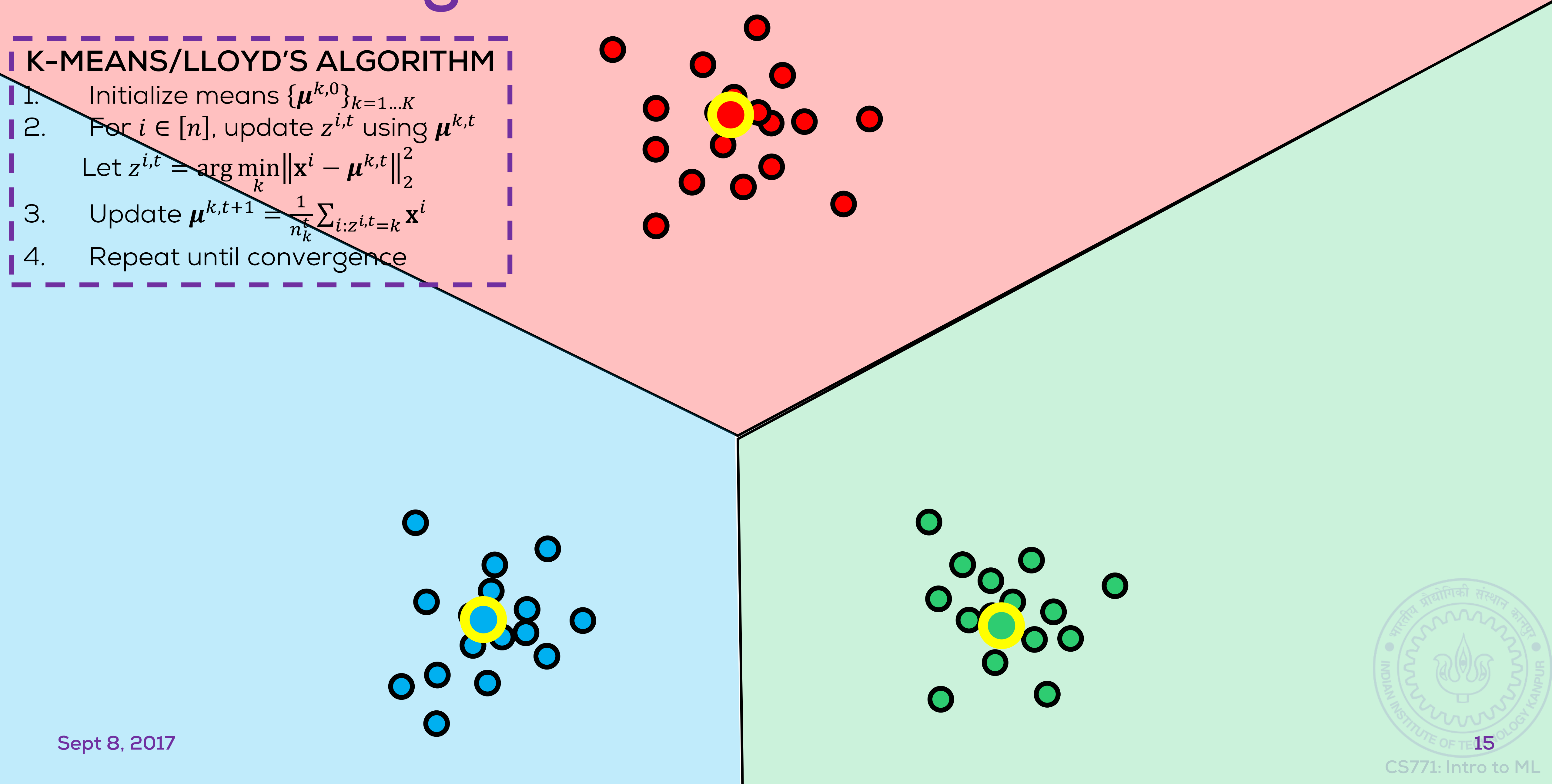

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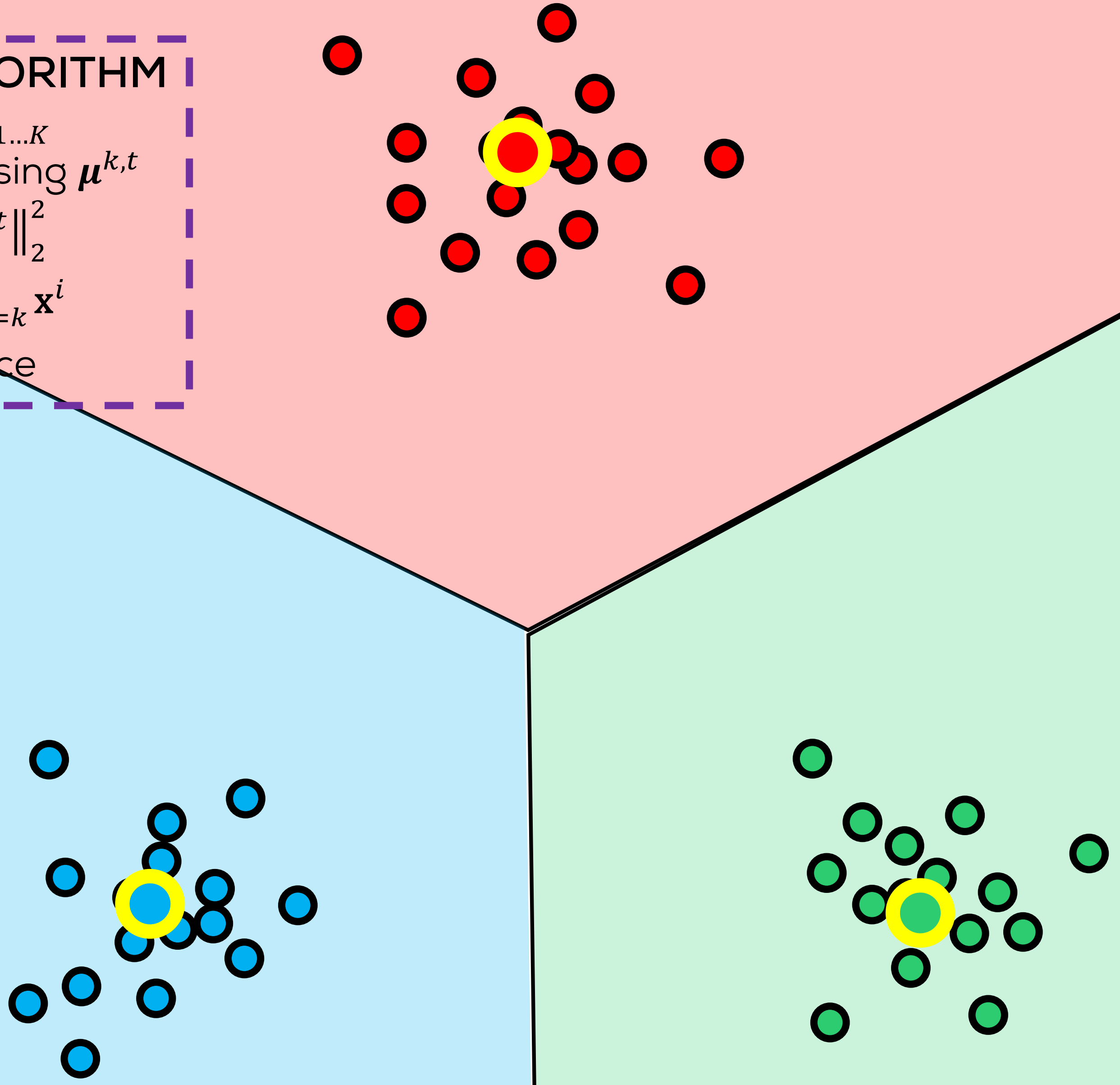

Stuck!!! … but at the global optimum ☺

The Magic is not Always very Useful!

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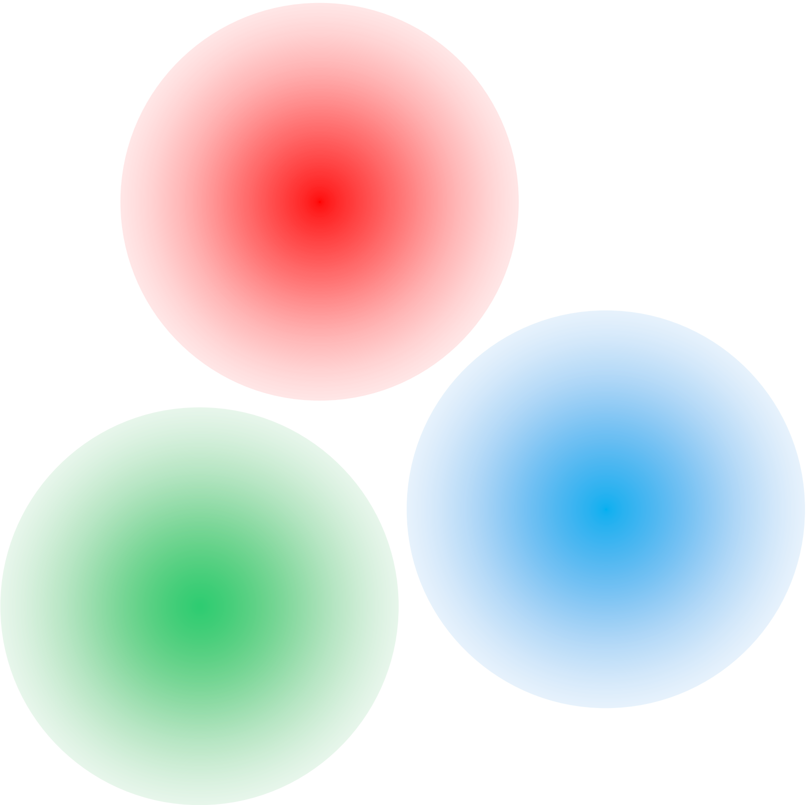

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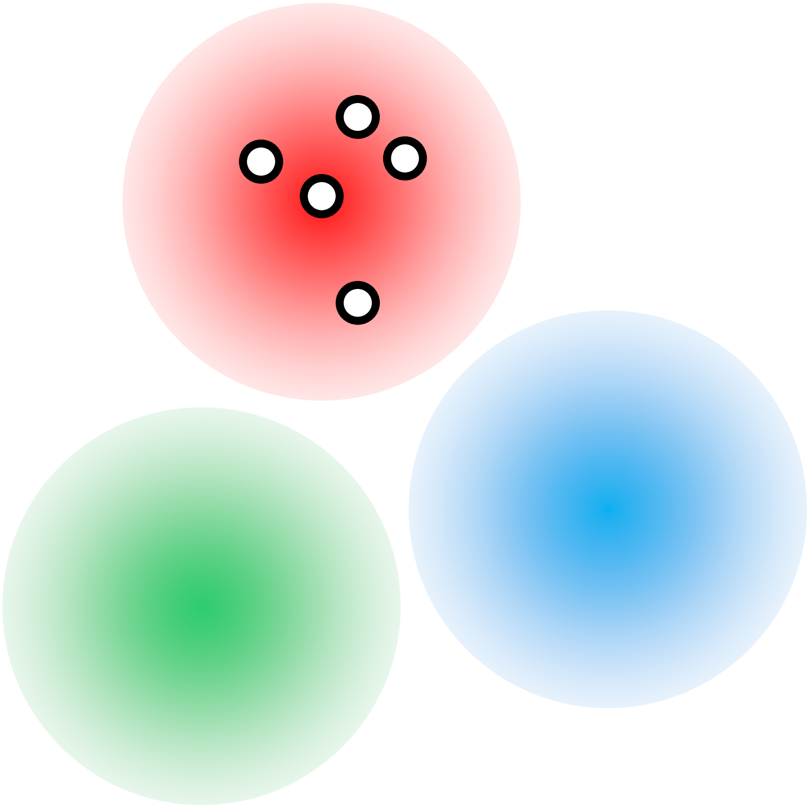

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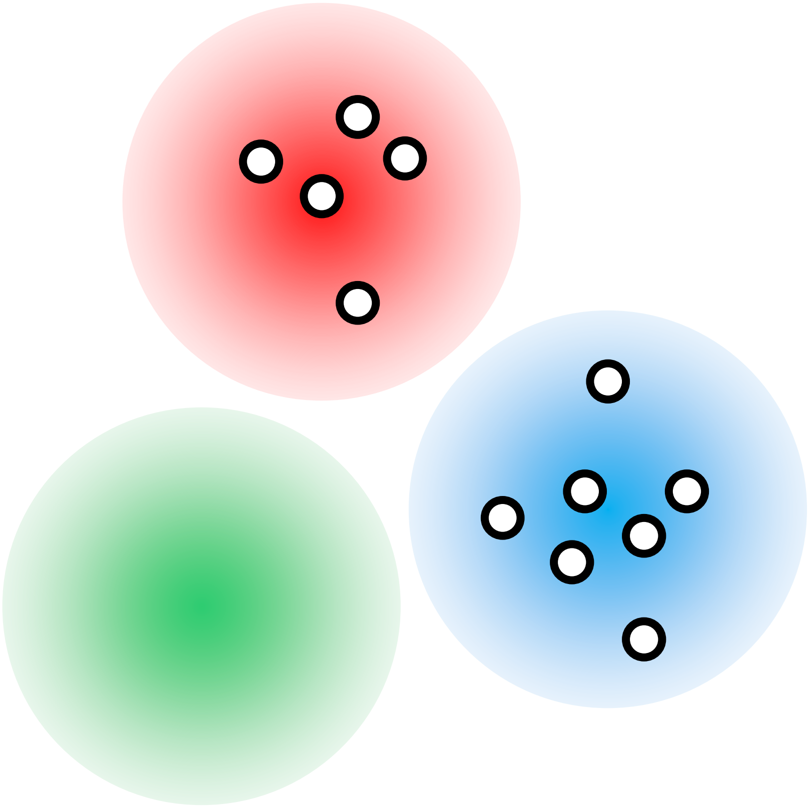

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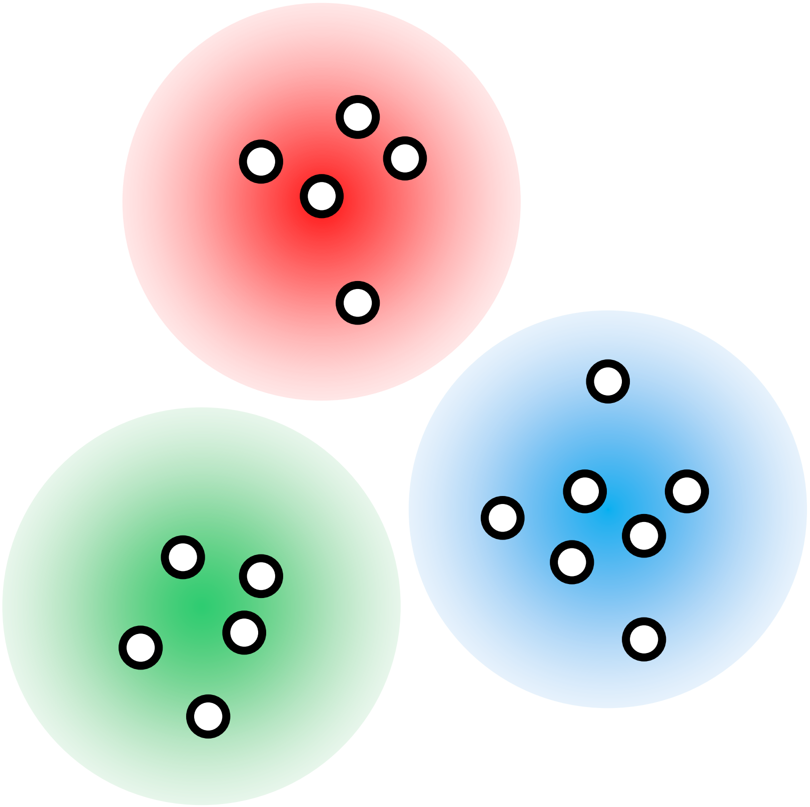

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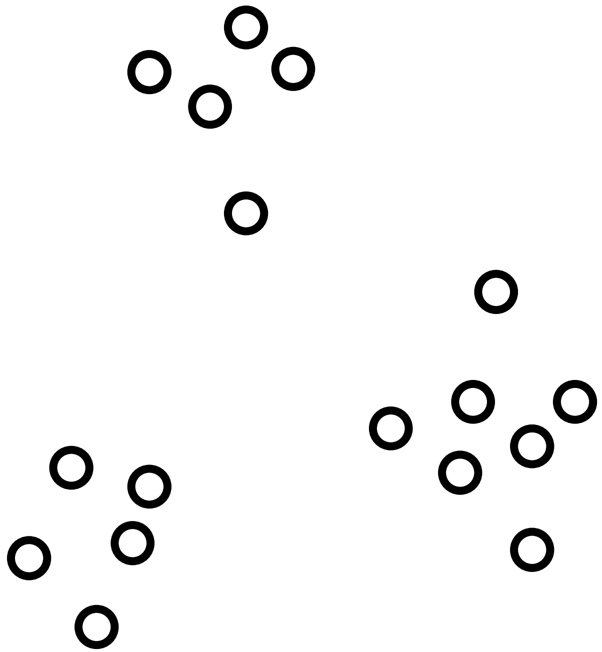

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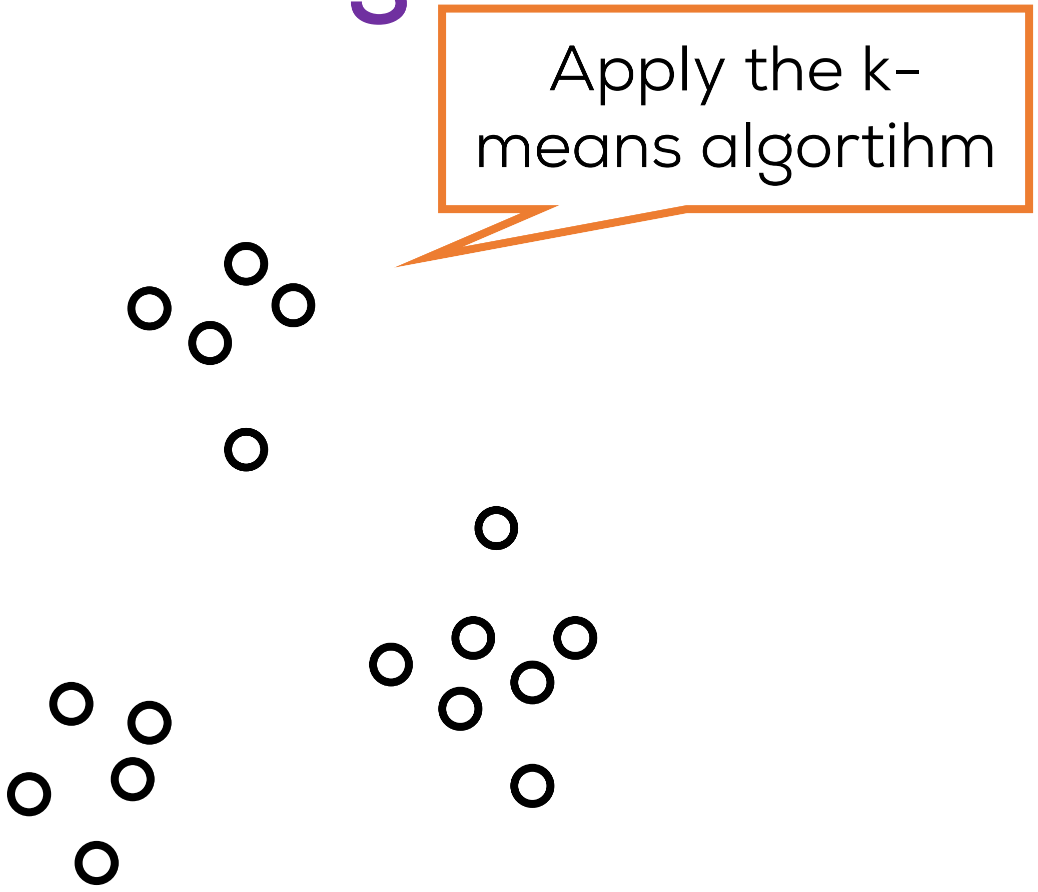

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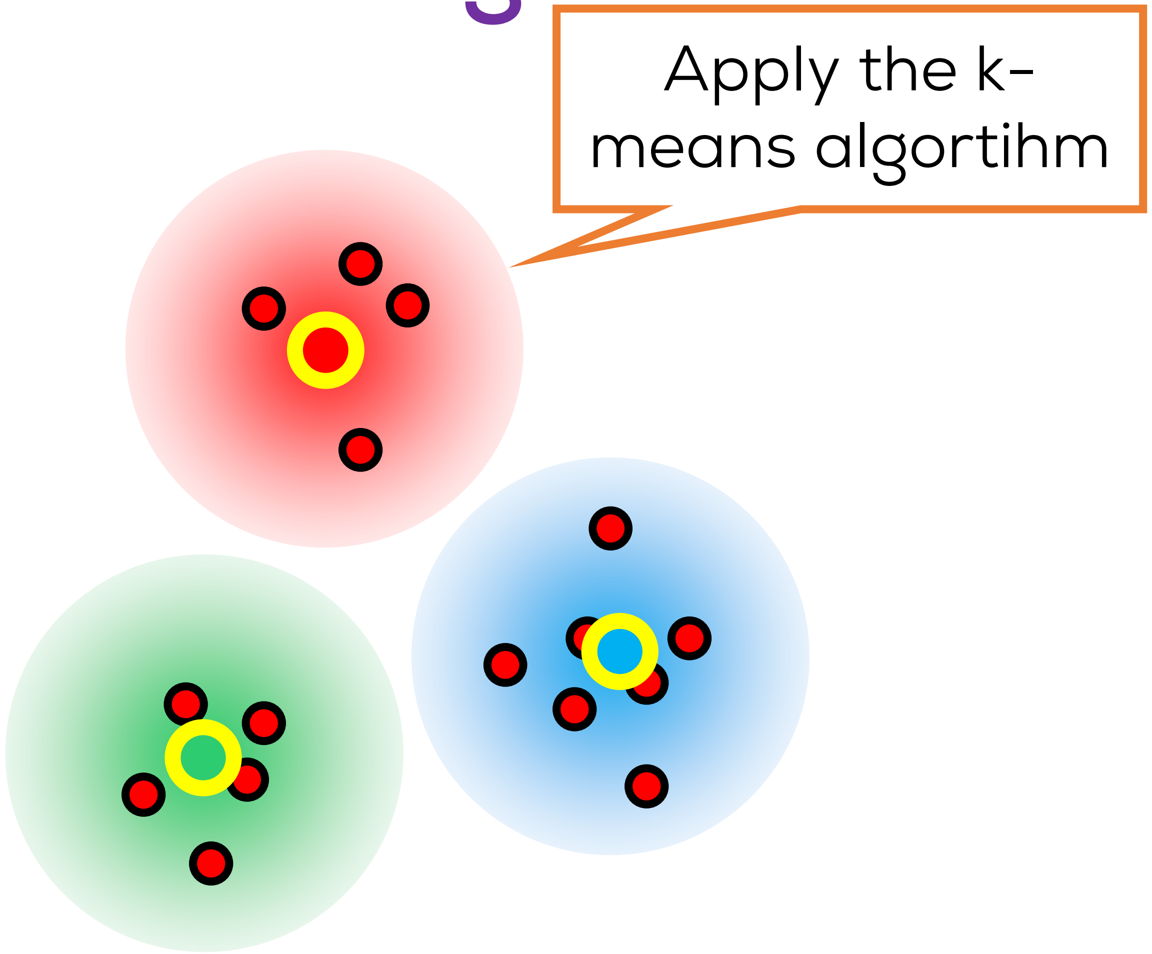

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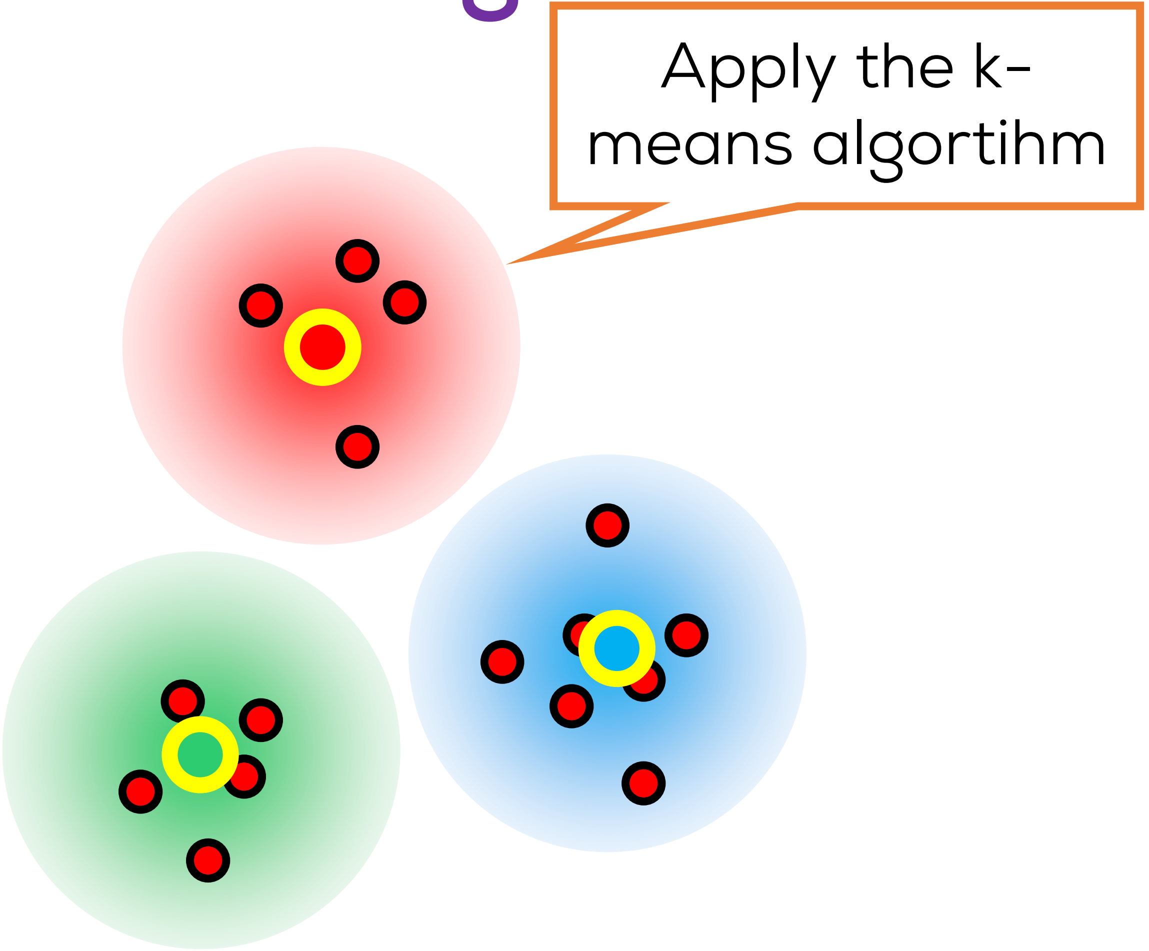
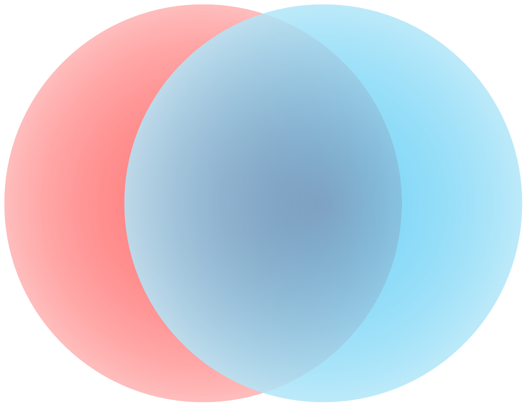
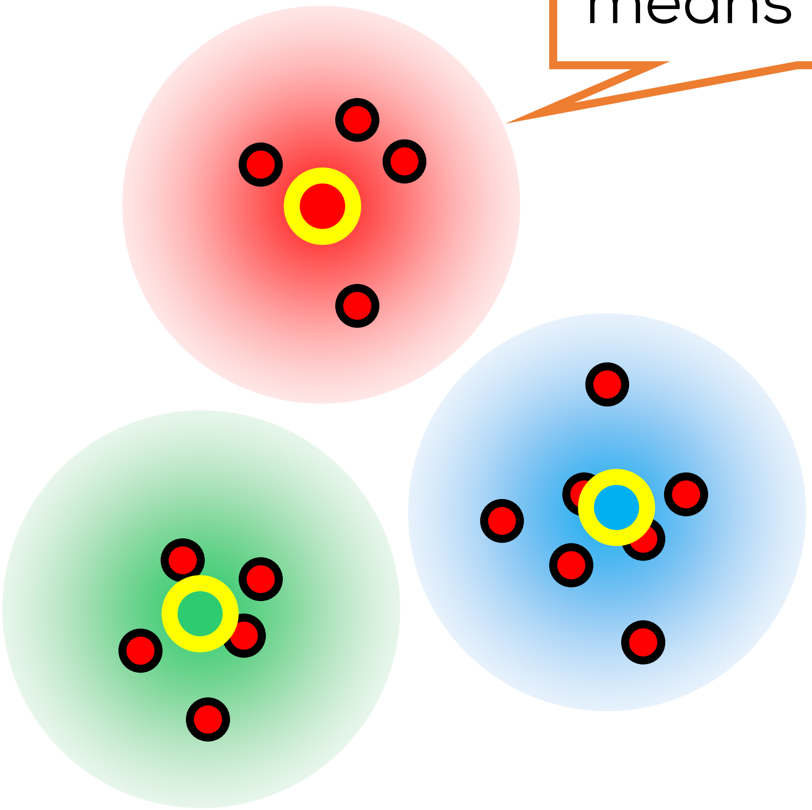
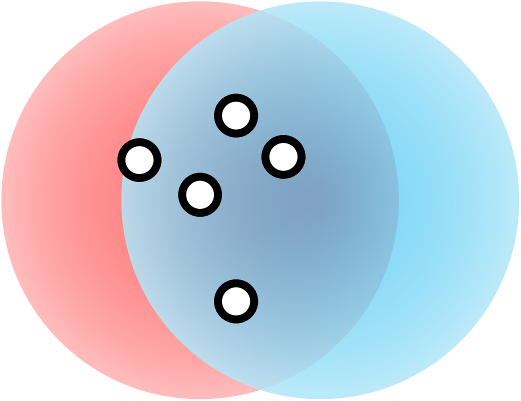




The Magic is not Always very Useful!

Apply the k-means algortihm





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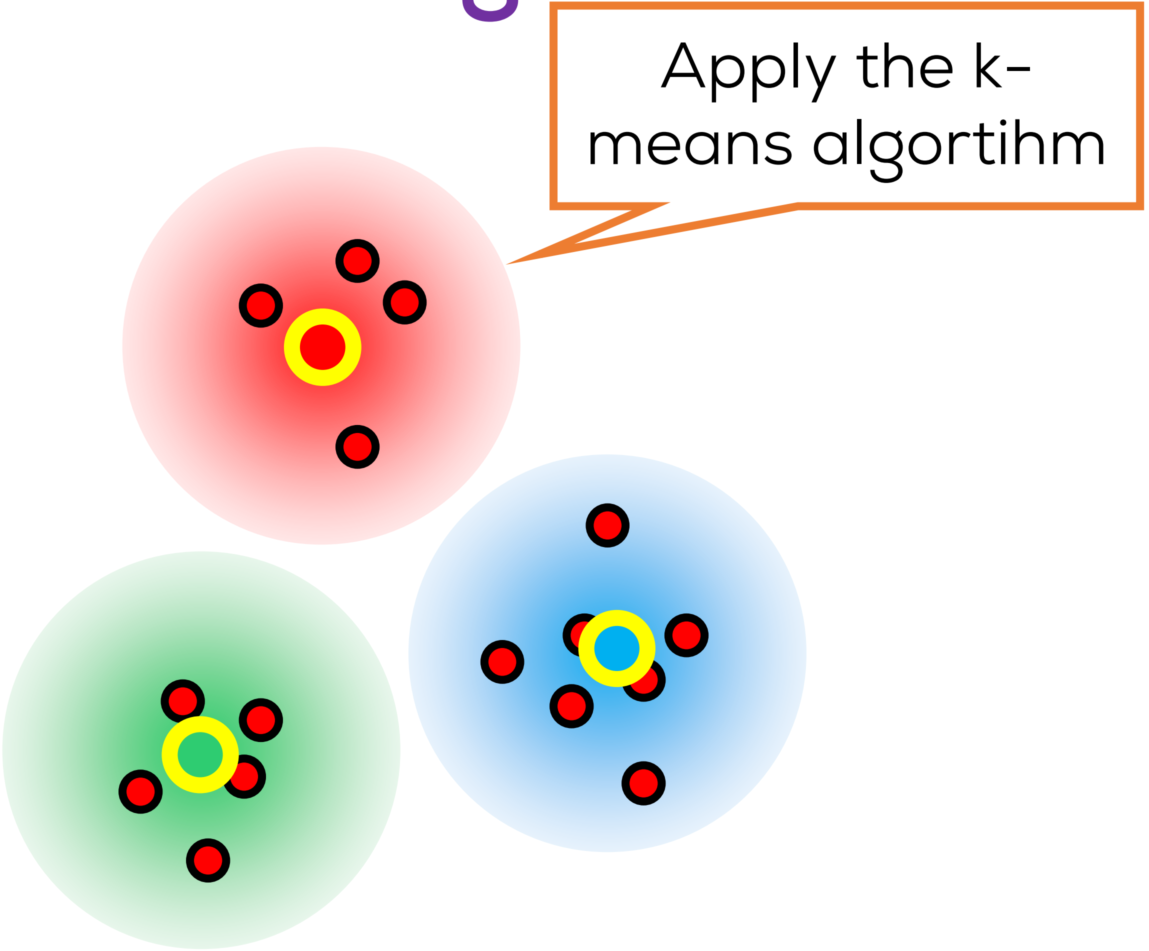

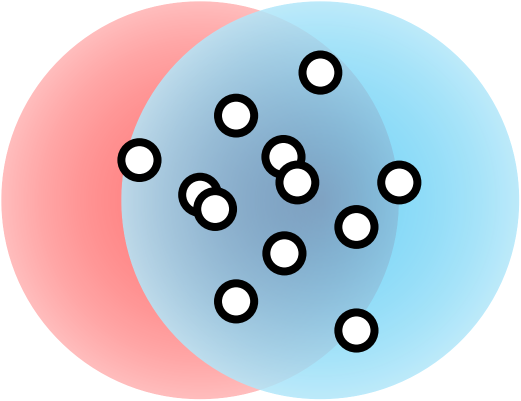

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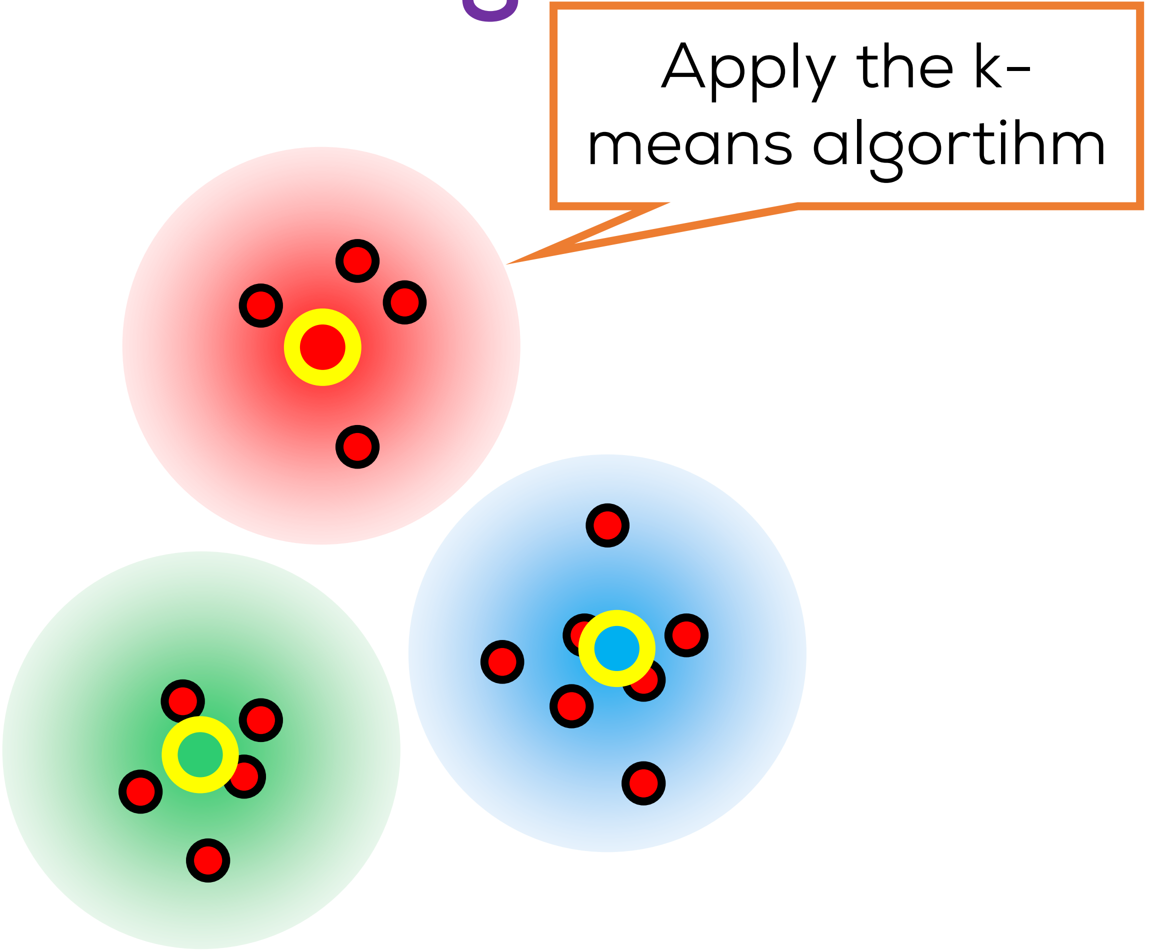

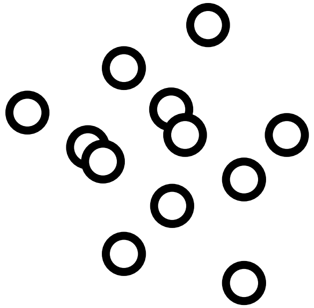

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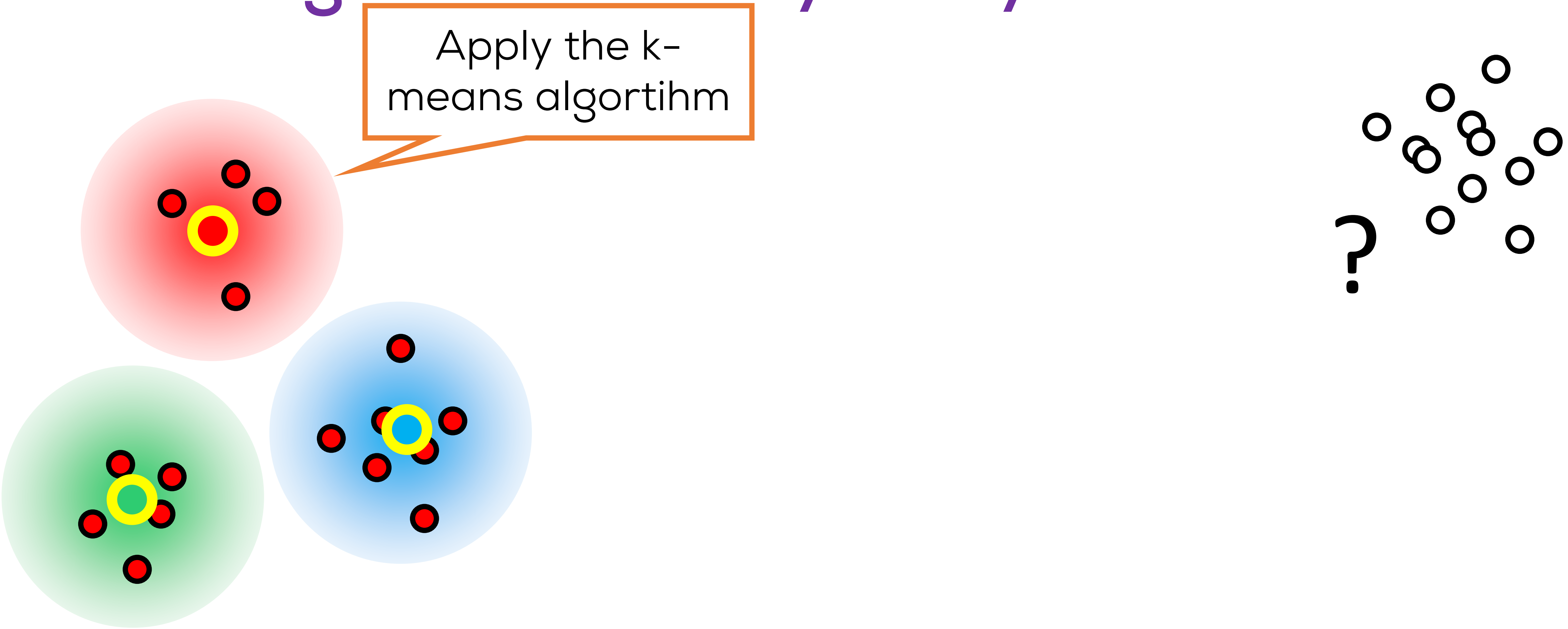

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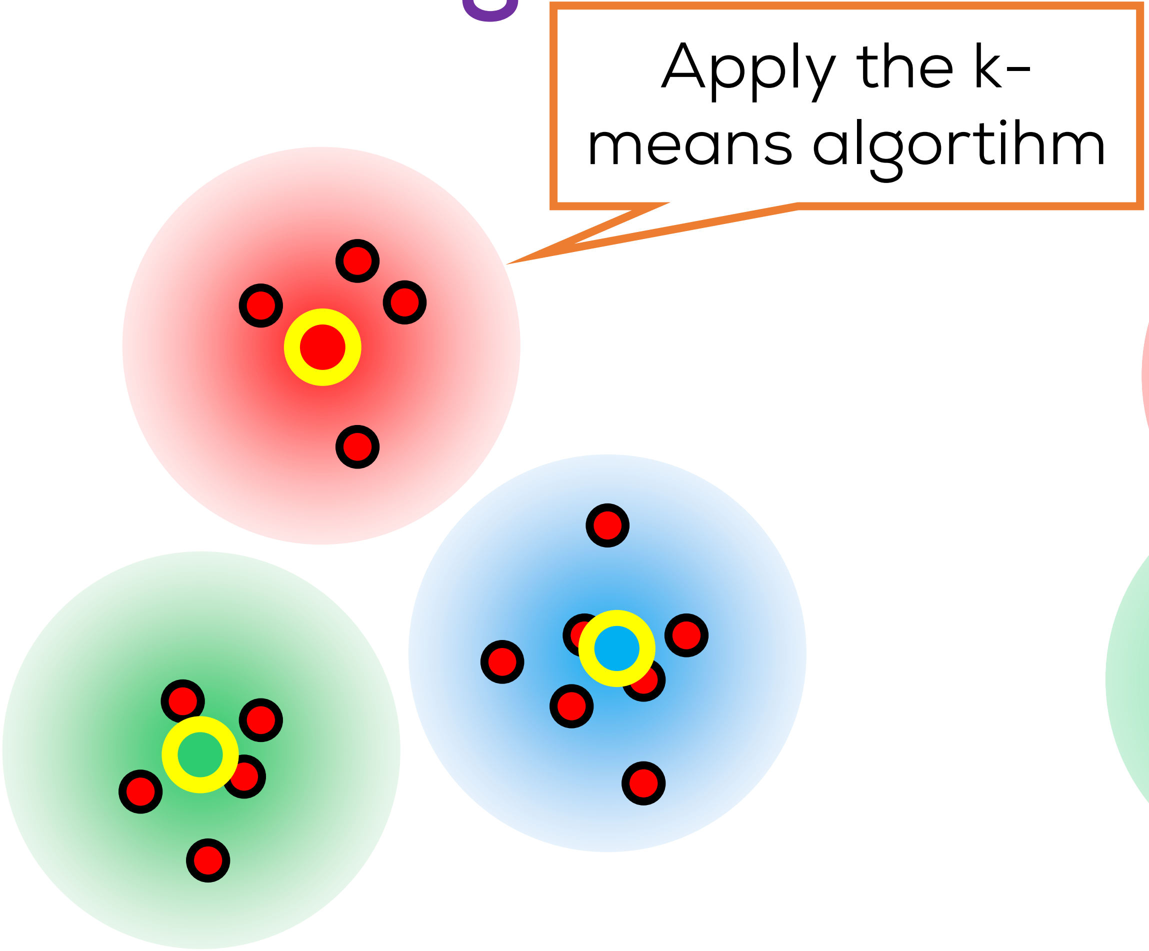

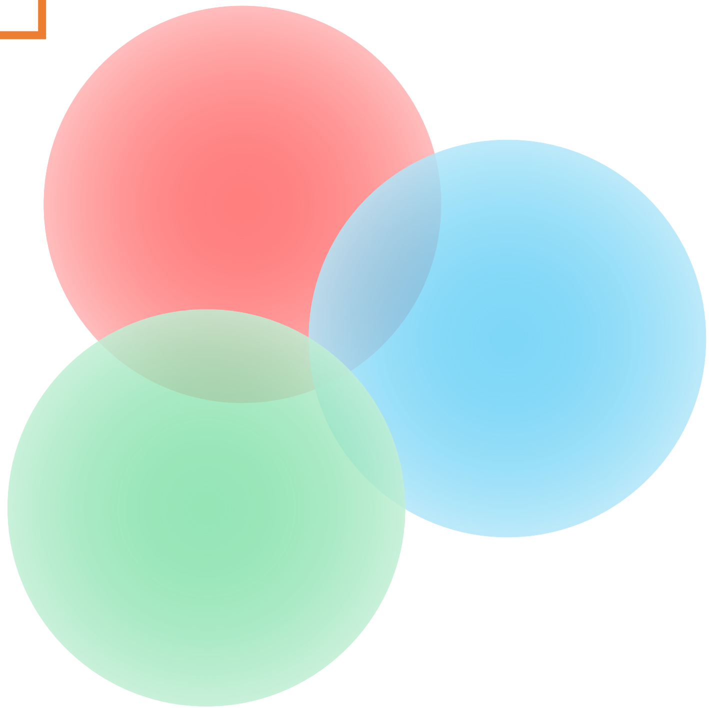

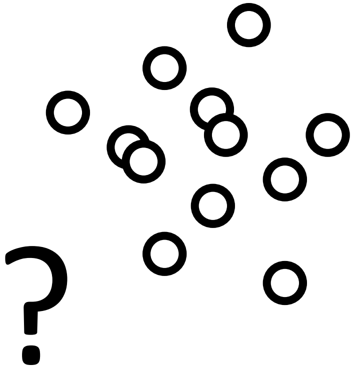

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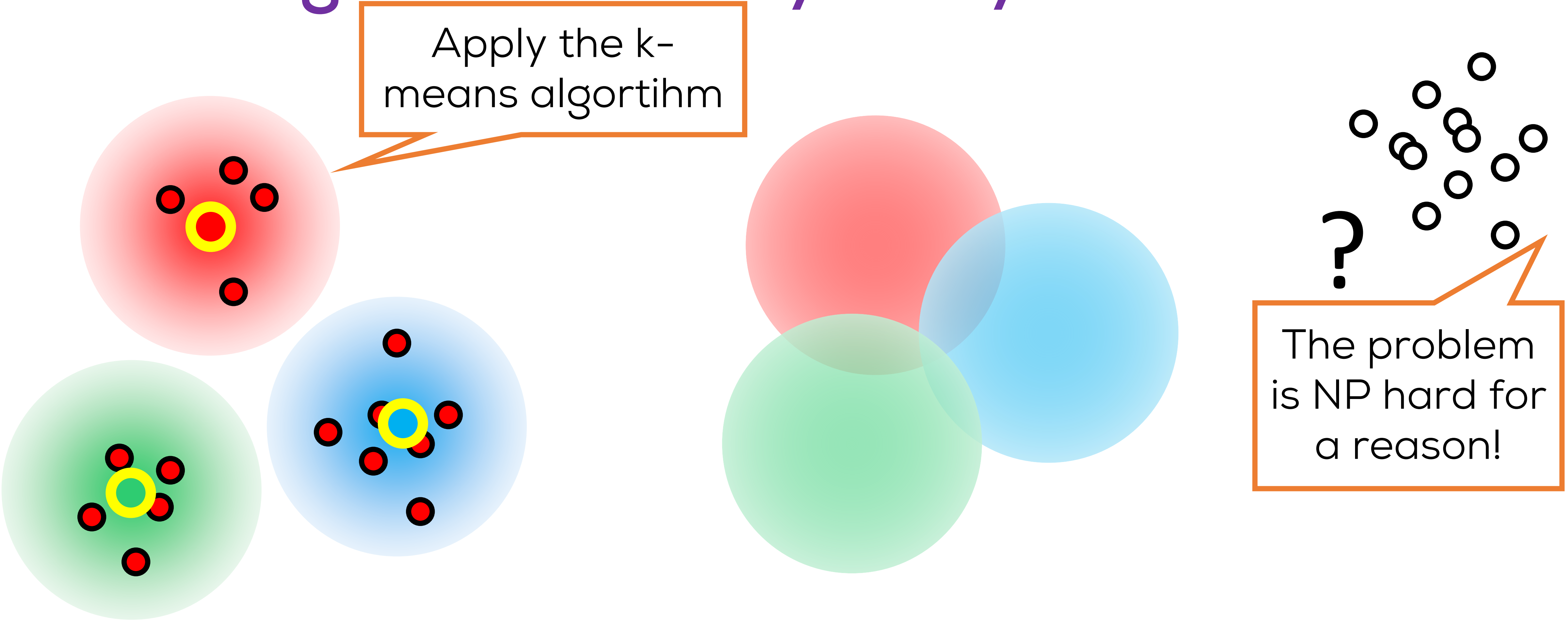

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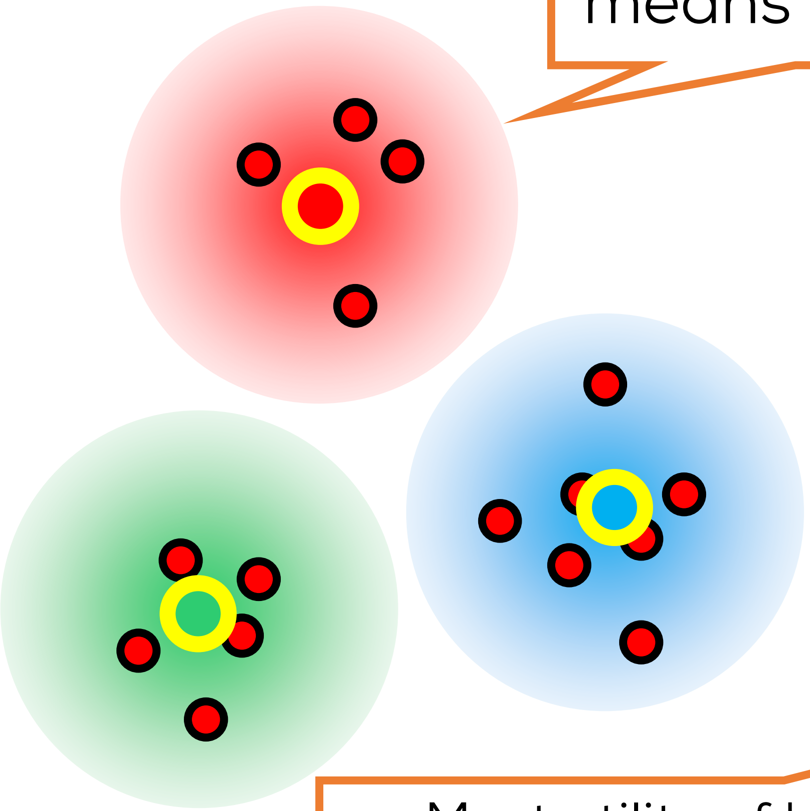
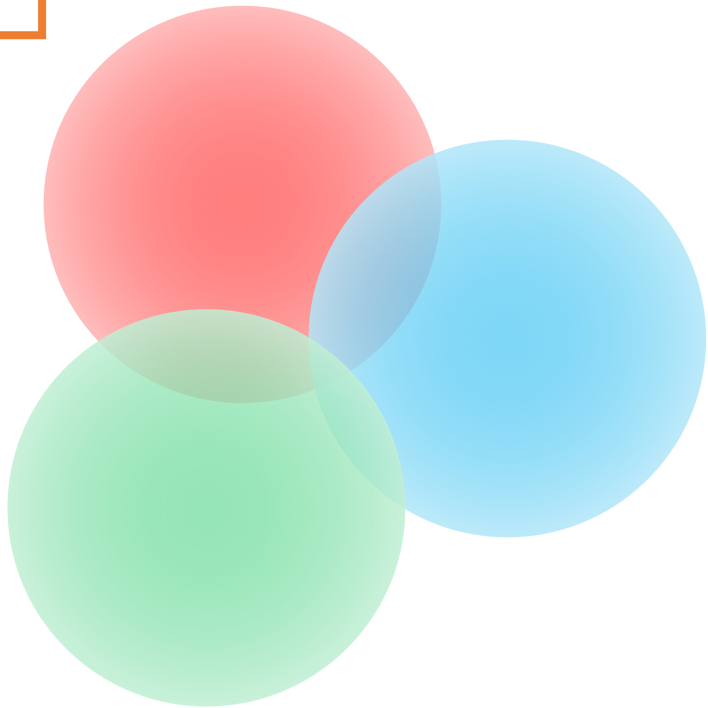
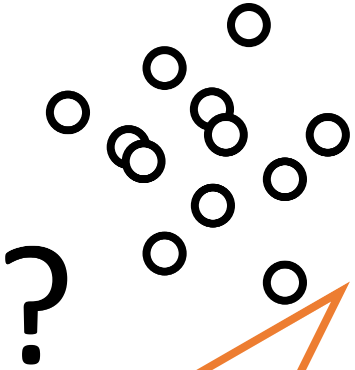
The Magic is not Always very Useful!

Apply the k-means algortihm



Most utility of k-means comes in problems that have some apparent stucture





The problem is NP hard for a reason!

Soft Assignment

The EM algorithm

A Ray of Hope

$$\hat{\mathbf{\Theta}}_{\text{MLE}} = \arg\max_{\mathbf{\Theta}} \mathbb{P}\left[X \mid \mathbf{\Theta}\right]$$

ALTERNATING OPTIMIZATION

1. Initialize $\mathbf{\Theta}^0$
2. For $i \in [n]$, update $z^{i,t}$ using $\mathbf{\Theta}^t$
3. Update $\mathbf{\Theta}^{t+1} = \arg\max_{\mathbf{\Theta}} \mathbb{P}\left[X, \left\{z^{i,t}\right\} \mid \mathbf{\Theta}\right]$
4. Repeat until convergence

A Ray of Hope

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$$z^{i,t} = \arg\max_{k \in [K]} \mathbb{P}\left[k \mid \mathbf{x}^i, \mathbf{\Theta}^t\right]$$

A Ray of Hope

$$\hat{\boldsymbol{\Theta}}_{\text{MLE}} = \arg\max_{\boldsymbol{\Theta}} \mathbb{P}\left[X \,|\, \boldsymbol{\Theta}\right]$$

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4. Repeat until convergence

$$z^{i,t} = \arg\max_{k \in [K]} \mathbb{P}\left[k \,|\, \mathbf{x}^i, \boldsymbol{\Theta}^t\right]$$

$$\boldsymbol{\Theta}^t = \left\{\boldsymbol{\pi}^t, \left\{\boldsymbol{\mu}^{1,t}, \boldsymbol{\mu}^{2,t}, \boldsymbol{\mu}^{3,t}\right\}, \left\{\Sigma^{1,t}, \Sigma^{2,t}, \Sigma^{3,t}\right\}\right\}$$

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4. Repeat until convergence

$$z^{i,t} = \arg\max_{k \in [K]} \mathbb{P}\left[k \mid \mathbf{x}^i, \boldsymbol{\Theta}^t\right] = \arg\max_{k \in [K]} \mathbb{P}\left[k \mid \boldsymbol{\Theta}^t\right] \cdot \mathbb{P}\left[\mathbf{x}^i \mid k, \boldsymbol{\Theta}^t\right]$$

$$\boldsymbol{\Theta}^t = \left\{\boldsymbol{\pi}^t, \left\{\boldsymbol{\mu}^{1,t}, \boldsymbol{\mu}^{2,t}, \boldsymbol{\mu}^{3,t}\right\}, \left\{\Sigma^{1,t}, \Sigma^{2,t}, \Sigma^{3,t}\right\}\right\}$$

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4. Repeat until convergence

$$z^{i,t} = \arg\max_{k \in [K]} \mathbb{P}\left[k \mid \mathbf{x}^i, \boldsymbol{\Theta}^t\right] = \arg\max_{k \in [K]} \boldsymbol{\pi}_k^t \cdot \mathbb{P}\left[\mathbf{x}^i \mid k, \boldsymbol{\Theta}^t\right]$$

$$\boldsymbol{\Theta}^t = \left\{\boldsymbol{\pi}^t, \left\{\boldsymbol{\mu}^{1,t}, \boldsymbol{\mu}^{2,t}, \boldsymbol{\mu}^{3,t}\right\}, \left\{\Sigma^{1,t}, \Sigma^{2,t}, \Sigma^{3,t}\right\}\right\}$$

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4. Repeat until convergence

Bayes Rule!

$$z^{i,t} = \arg\max_{k\in[K]} \mathbb{P}\left[k \mid \mathbf{x}^i, \boldsymbol{\Theta}^t\right] = \arg\max_{k\in[K]} \boldsymbol{\pi}_k^t \cdot \mathcal{N}(\mathbf{x}^i \mid \boldsymbol{\mu}^{k,t}, \Sigma^{k,t})$$

$$\boldsymbol{\Theta}^t = \left\{\boldsymbol{\pi}^t, \left\{\boldsymbol{\mu}^{1,t}, \boldsymbol{\mu}^{2,t}, \boldsymbol{\mu}^{3,t}\right\}, \left\{\Sigma^{1,t}, \Sigma^{2,t}, \Sigma^{3,t}\right\}\right\}$$

A Ray of Hope

$$\hat{\boldsymbol{\Theta}}_{\text{MLE}} = \underset{\boldsymbol{\Theta}}{\arg\max}\; \mathbb{P}\left[X \mid \boldsymbol{\Theta}\right]$$

ALTERNATING OPTIMIZATION

1. Initialize $\boldsymbol{\Theta}^0$
2. For $i \in [n]$, update $z^{i,t}$ using $\boldsymbol{\Theta}^t$

$^{+1} = \underset{\boldsymbol{\Theta}}{\arg\max}\, \mathbb{P}\left[X, \{z^{i,t}\} \mid \boldsymbol{\Theta}\right]$

il convergence

May be throwing away a lot of information!

Bayes Rule!

$$z^{i,t} = \underset{k \in [K]}{\arg\max}\; \mathbb{P}\left[k \mid \mathbf{x}^i, \boldsymbol{\Theta}^t\right] = \underset{k \in [K]}{\arg\max}\; \boldsymbol{\pi}_k^t \cdot \mathcal{N}(\mathbf{x}^i \mid \boldsymbol{\mu}^{k,t}, \Sigma^{k,t})$$

$$\boldsymbol{\Theta}^t = \left\{\boldsymbol{\pi}^t, \left\{\boldsymbol{\mu}^{1,t}, \boldsymbol{\mu}^{2,t}, \boldsymbol{\mu}^{3,t}\right\}, \left\{\Sigma^{1,t}, \Sigma^{2,t}, \Sigma^{3,t}\right\}\right\}$$

A Ray of Hope

$$\hat{\boldsymbol{\Theta}}_{\text{MLE}} = \arg\max_{\boldsymbol{\Theta}} \mathbb{P}\left[X \mid \boldsymbol{\Theta}\right]$$

E.g. $\mathbb{P}[\,{\color{red}\bullet} \mid \mathbf{x}^i, \boldsymbol{\Theta}^t] = 0.5$,
$\mathbb{P}[\,{\color{cyan}\bullet} \mid \mathbf{x}^i, \boldsymbol{\Theta}^t] = 0.4$,
$\mathbb{P}[\,{\color{green}\bullet} \mid \mathbf{x}^i, \boldsymbol{\Theta}^t] = 0.1$,

ERNATING OPTIMIZATION

alize $\boldsymbol{\Theta}^0$

2. For $i \in [n]$ update $z^{i,t}$ using $\boldsymbol{\Theta}^t$

$^{+1} = \arg\max_{\boldsymbol{\Theta}} \mathbb{P}\left[X, \{z^{i,t}\} \mid \boldsymbol{\Theta}\right]$

til convergence

May be throwing away a lot of information!

Bayes Rule!

$$z^{i,t} = \arg\max_{k \in [K]} \mathbb{P}\left[k \mid \mathbf{x}^i, \boldsymbol{\Theta}^t\right] = \arg\max_{k \in [K]} \boldsymbol{\pi}_k^t \cdot \mathcal{N}(\mathbf{x}^i \mid \boldsymbol{\mu}^{k,t}, \Sigma^{k,t})$$

$$\boldsymbol{\Theta}^t = \left\{\boldsymbol{\pi}^t, \left\{{\color{red}\boldsymbol{\mu}^{1,t}}, {\color{green}\boldsymbol{\mu}^{2,t}}, {\color{cyan}\boldsymbol{\mu}^{3,t}}\right\}, \left\{{\color{red}\Sigma^{1,t}}, {\color{green}\Sigma^{2,t}}, {\color{cyan}\Sigma^{3,t}}\right\}\right\}$$

A Ray of Hope

$$\hat{\mathbf{\Theta}}_{\text{MLE}} = \arg\max_{\mathbf{\Theta}} \mathbb{P}\left[X \mid \mathbf{\Theta}\right]$$

E.g. $\mathbb{P}[\,\text{red}\,|\mathbf{x}^i, \mathbf{\Theta}^t] = 0.5$,
$\mathbb{P}[\,\text{blue}\,|\mathbf{x}^i, \mathbf{\Theta}^t] = 0.4$,
$\mathbb{P}[\,\text{green}\,|\mathbf{x}^i, \mathbf{\Theta}^t] = 0.1$,

ERNA … ATION

…alize …

Can we use $\mathbb{P}[k|\mathbf{x}^i, \mathbf{\Theta}^t]$ as weights instead?

2. For $i \in [n]$, update $z^{i,t}$ using $\mathbf{\Theta}^t$

… $^{+1} = \arg\max_{\mathbf{\Theta}} \mathbb{P}\left[X, \{z^{i,t}\} \mid \mathbf{\Theta}\right]$

May be throwing away a lot of information!

…til convergence

Bayes Rule!

$$z^{i,t} = \arg\max_{k\in[K]} \mathbb{P}\left[k \mid \mathbf{x}^i, \mathbf{\Theta}^t\right] = \arg\max_{k\in[K]} \quad \boldsymbol{\pi}_k^t \cdot \mathcal{N}(\mathbf{x}^i \mid \boldsymbol{\mu}^{k,t}, \Sigma^{k,t})$$

$$\mathbf{\Theta}^t = \left\{\boldsymbol{\pi}^t, \left\{\boldsymbol{\mu}^{1,t}, \boldsymbol{\mu}^{2,t}, \boldsymbol{\mu}^{3,t}\right\}, \left\{\Sigma^{1,t}, \Sigma^{2,t}, \Sigma^{3,t}\right\}\right\}$$

A Ray of Hope

$$\hat{\mathbf{\Theta}}_{\mathrm{MLE}} = \arg\max_{\mathbf{\Theta}} \mathbb{P}\left[X \mid \mathbf{\Theta}\right]$$

E.g. $\mathbb{P}[\,\text{●}|\mathbf{x}^i, \mathbf{\Theta}^t] = 0.5$,
$\mathbb{P}[\,\text{●}|\mathbf{x}^i, \mathbf{\Theta}^t] = 0.4$,
$\mathbb{P}[\,\text{●}|\mathbf{x}^i, \mathbf{\Theta}^t] = 0.1$,

ERNA ... ZATION

...alize ...

2. For $i \in [n]$ update $z^{i,t}$ using $\mathbf{\Theta}^t$

... $^{+1} = \arg\max_{\mathbf{\Theta}} \mathbb{P}\left[X, \{z^{i,t}\} \mid \mathbf{\Theta}\right]$

... til convergence

Can we use $\mathbb{P}[k|\mathbf{x}^i, \mathbf{\Theta}^t]$ as weights instead?

Assign point $\mathbf{x}^i$ to cluster k with weight $\propto \mathbb{P}[k|\mathbf{x}^i, \mathbf{\Theta}^t]$

May be throwing away a lot of information!

Bayes Rule!

$$z^{i,t} = \arg\max_{k \in [K]} \mathbb{P}\left[k \mid \mathbf{x}^i, \mathbf{\Theta}^t\right] = \arg\max_{k \in [K]} \quad \boldsymbol{\pi}^t_k \cdot \mathcal{N}(\mathbf{x}^i \mid \boldsymbol{\mu}^{k,t}, \Sigma^{k,t})$$

$$\mathbf{\Theta}^t = \left\{\boldsymbol{\pi}^t, \left\{\boldsymbol{\mu}^{1,t}, \boldsymbol{\mu}^{2,t}, \boldsymbol{\mu}^{3,t}\right\}, \left\{\Sigma^{1,t}, \Sigma^{2,t}, \Sigma^{3,t}\right\}\right\}$$

A Ray of Hope

$$\hat{\Theta}_{\text{MLE}} = \arg\max_{\Theta} \mathbb{P}\left[X \mid \Theta\right]$$

Assign point $\mathbf{x}^i$ to cluster k with weight $\propto \mathbb{P}[k|\mathbf{x}^i, \Theta^t]$

E.g. $\mathbb{P}[\,\bullet|\mathbf{x}^i, \Theta^t] = 0.5,$
$\mathbb{P}[\,\bullet|\mathbf{x}^i, \Theta^t] = 0.4,$
$\mathbb{P}[\,\bullet|\mathbf{x}^i, \Theta^t] = 0.1,$

Can we use $\mathbb{P}[k|\mathbf{x}^i, \Theta^t]$ as weights instead?

Has a "Bayesian" feel to it – use all available posterior information

...ERNA... ...AT...

...alize ...

2. For $i \in [n]$, update $z^{i,t}$ using Θ^t

... $^{+1} = \arg\max_{\Theta} \mathbb{P}\left[X, \{z^{i,t}\} \mid \Theta\right]$

May be throwing away a lot of information!

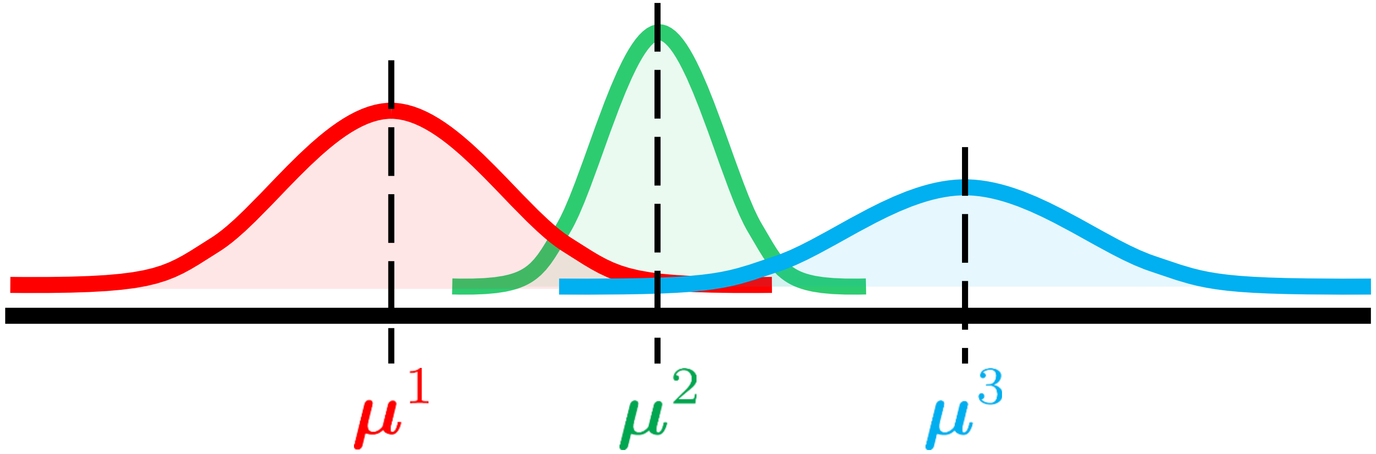
...peat until convergence

Bayes Rule!

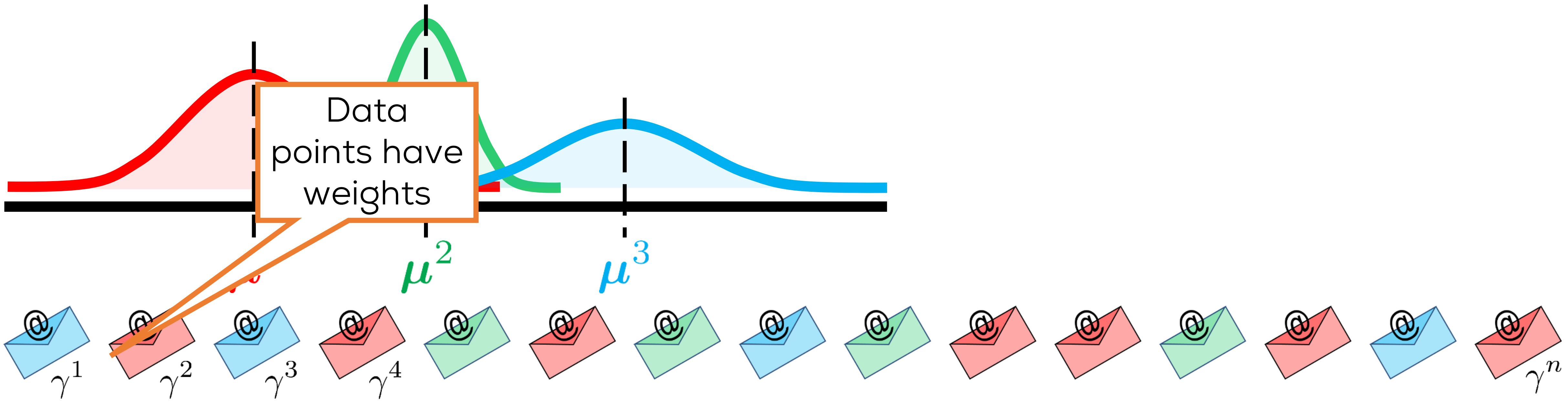
$$z^{i,t} = \arg\max_{k \in [K]} \mathbb{P}\left[k \mid \mathbf{x}^i, \Theta^t\right] = \arg\max_{k \in [K]} \quad \pi_k^t \quad \cdot \quad \mathcal{N}(\mathbf{x}^i \mid \mu^{k,t}, \Sigma^{k,t})$$

$$\Theta^t = \left\{\pi^t, \left\{\mu^{1,t}, \mu^{2,t}, \mu^{3,t}\right\}, \left\{\Sigma^{1,t}, \Sigma^{2,t}, \Sigma^{3,t}\right\}\right\}$$

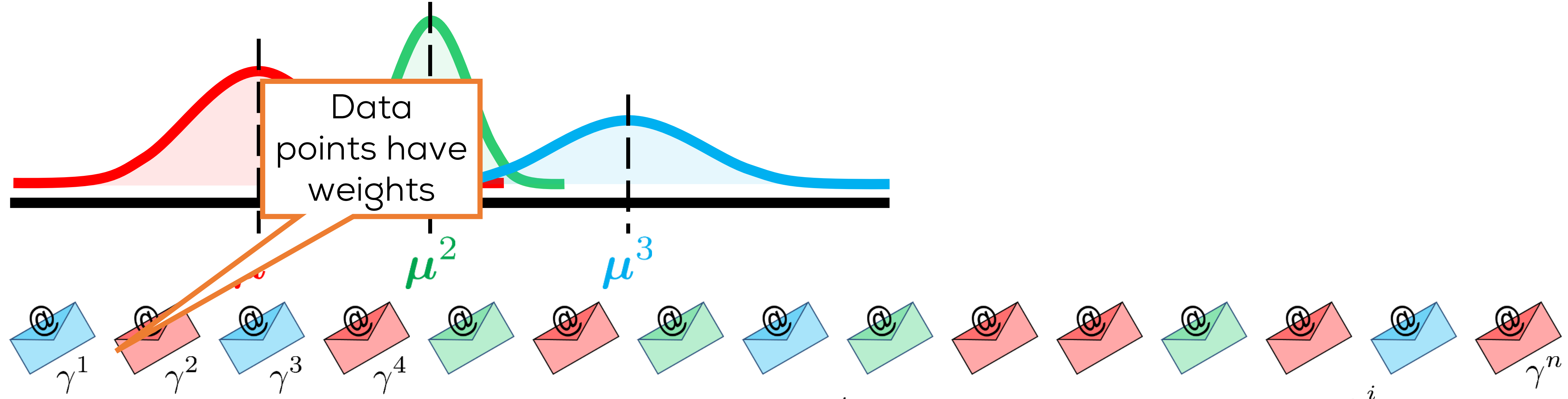
Weighted MLE



Weighted MLE

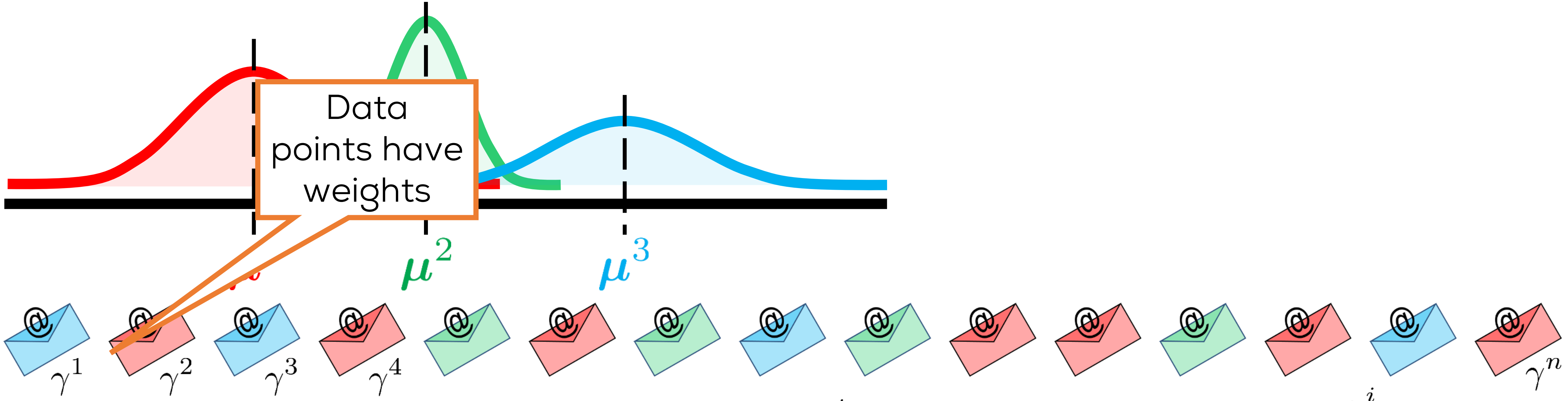


Weighted MLE



$$\mathbb{P}\left[\mathbf{x}^i, z^i, \gamma^i \mid \boldsymbol{\Theta}\right] = \left(\mathbb{P}\left[z^i \mid \boldsymbol{\Theta}\right] \cdot \mathbb{P}\left[\mathbf{x}^i \mid z^i, \boldsymbol{\Theta}\right]\right)^{\gamma^i} = \left(\boldsymbol{\pi}_{z^i} \cdot \mathcal{N}(\mathbf{x}^i \mid \boldsymbol{\mu}^{z^i}, \Sigma^{z^i})\right)^{\gamma^i}$$

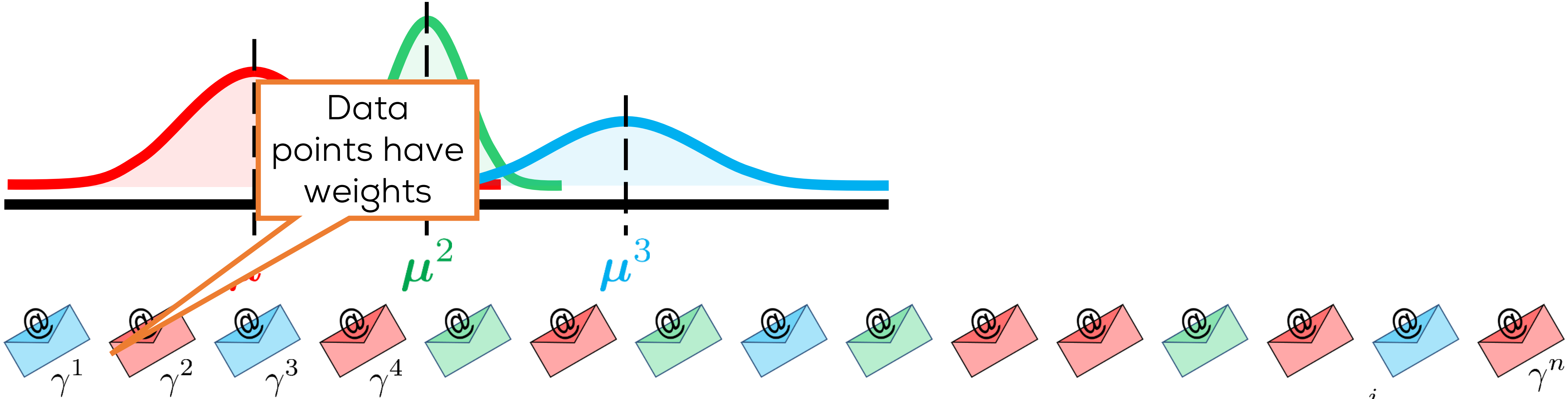
Weighted MLE



$$\mathbb{P}\left[\mathbf{x}^i, z^i, \gamma^i \,|\, \boldsymbol{\Theta}\right] = \left(\mathbb{P}\left[z^i \,|\, \boldsymbol{\Theta}\right] \cdot \mathbb{P}\left[\mathbf{x}^i \,|\, z^i, \boldsymbol{\Theta}\right]\right)^{\gamma^i} = \left(\boldsymbol{\pi}_{z^i} \cdot \mathcal{N}(\mathbf{x}^i \,|\, \boldsymbol{\mu}^{z^i}, \Sigma^{z^i})\right)^{\gamma^i}$$

$$\mathbb{P}\left[X, \{z^i\}, \{\gamma^i\} \,|\, \boldsymbol{\Theta}\right] = \prod_{i=1}^{n} \mathbb{P}\left[\mathbf{x}^i, z^i, \gamma^i \,|\, \boldsymbol{\Theta}\right]$$

Weighted MLE



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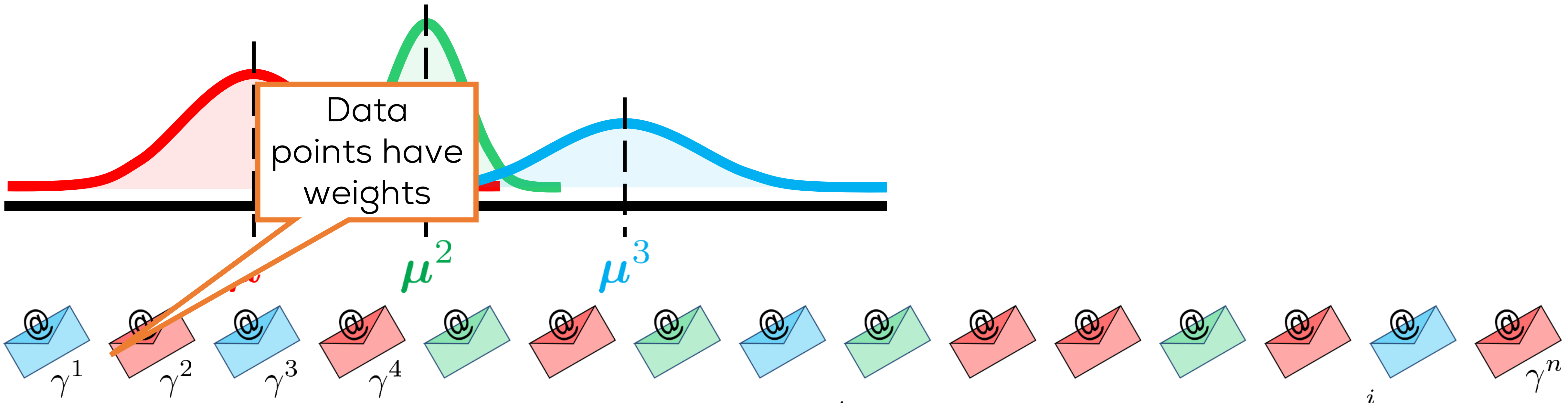
$$\hat{\boldsymbol{\Theta}}_{\text{MLE}} = \arg\max_{\boldsymbol{\Theta}} \mathbb{P}\left[X, \{z^i\}, \{\gamma^i\} \,|\, \boldsymbol{\Theta}\right]$$

Weighted MLE



$$\mathbb{P}\left[\mathbf{x}^i, z^i, \gamma^i \,|\, \boldsymbol{\Theta}\right] = \left(\mathbb{P}\left[z^i \,|\, \boldsymbol{\Theta}\right] \cdot \mathbb{P}\left[\mathbf{x}^i \,|\, z^i, \boldsymbol{\Theta}\right]\right)^{\gamma^i} = \left(\boldsymbol{\pi}_{z^i} \cdot \mathcal{N}(\mathbf{x}^i \,|\, \boldsymbol{\mu}^{z^i}, \Sigma^{z^i})\right)^{\gamma^i}$$

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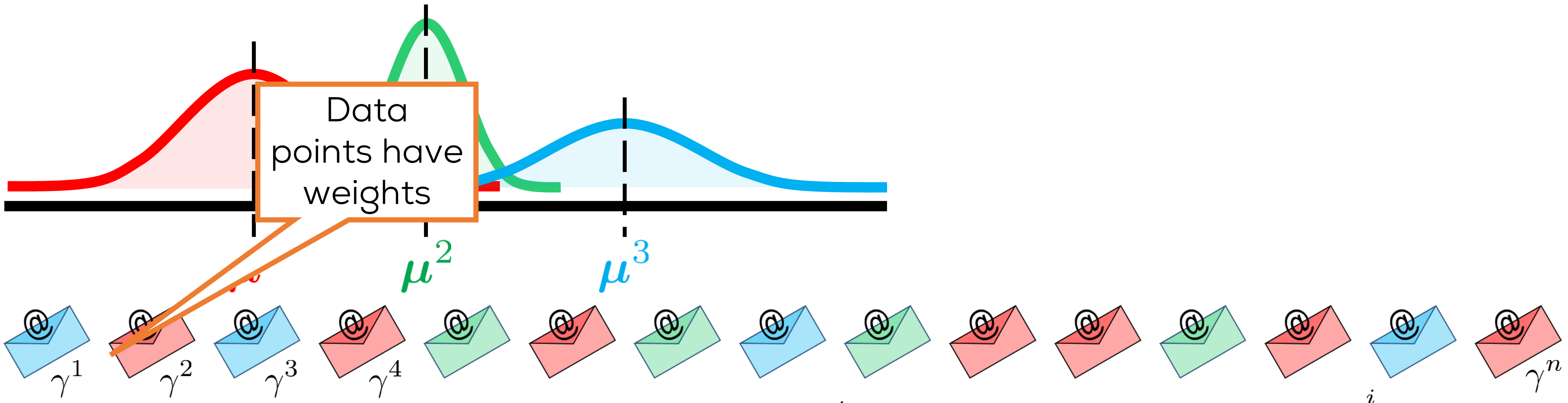
Take log and apply 1st order optimality

Weighted MLE



$$\mathbb{P}\left[\mathbf{x}^i, z^i, \gamma^i \mid \boldsymbol{\Theta}\right] = \left(\mathbb{P}\left[z^i \mid \boldsymbol{\Theta}\right] \cdot \mathbb{P}\left[\mathbf{x}^i \mid z^i, \boldsymbol{\Theta}\right]\right)^{\gamma^i} = \left(\boldsymbol{\pi}_{z^i} \cdot \mathcal{N}\left(\mathbf{x}^i \mid \boldsymbol{\mu}^{z^i}, \Sigma^{z^i}\right)\right)^{\gamma^i}$$

$$\mathbb{P}\left[X, \{z^i\}, \{\gamma^i\} \mid \boldsymbol{\Theta}\right] = \prod_{i=1}^{n} \mathbb{P}\left[\mathbf{x}^i, z^i, \gamma^i \mid \boldsymbol{\Theta}\right]$$

$$\hat{\boldsymbol{\Theta}}_{\mathrm{MLE}} = \arg\max_{\boldsymbol{\Theta}} \mathbb{P}\left[X, \{z^i\}, \{\gamma^i\} \mid \boldsymbol{\Theta}\right]$$

Take log and apply 1st order optimality

$$\boldsymbol{\pi}_1^{\mathrm{MLE}} = \frac{\text{\# eff. red emails}}{\text{\# eff. total emails}} = \frac{\tilde{n}_r}{n} = \frac{\sum_{i:z^i=\bullet} \gamma^i}{\sum_{j=1}^{n} \gamma^j}$$

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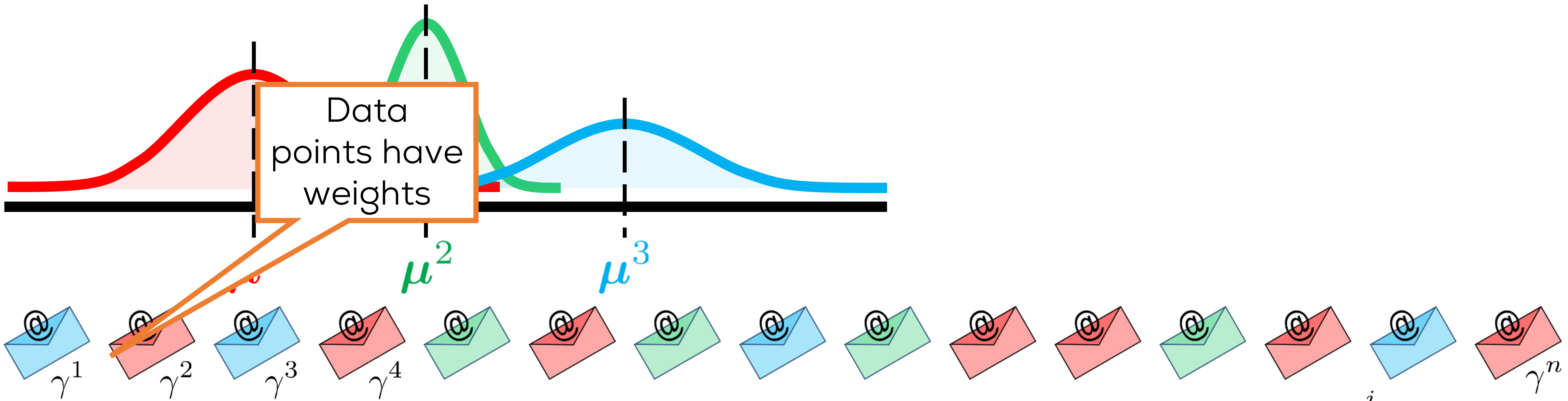
Weighted MLE



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Take log and apply 1st order optimality

$$\boldsymbol{\pi}_1^{\mathrm{MLE}} = \frac{\#\text{ eff. red emails}}{\#\text{ eff. total emails}} = \frac{\tilde{n}_r}{n} = \frac{\sum_{i:z^i={\color{red}\bullet}} \gamma^i}{\sum_{j=1}^{n} \gamma^j}$$

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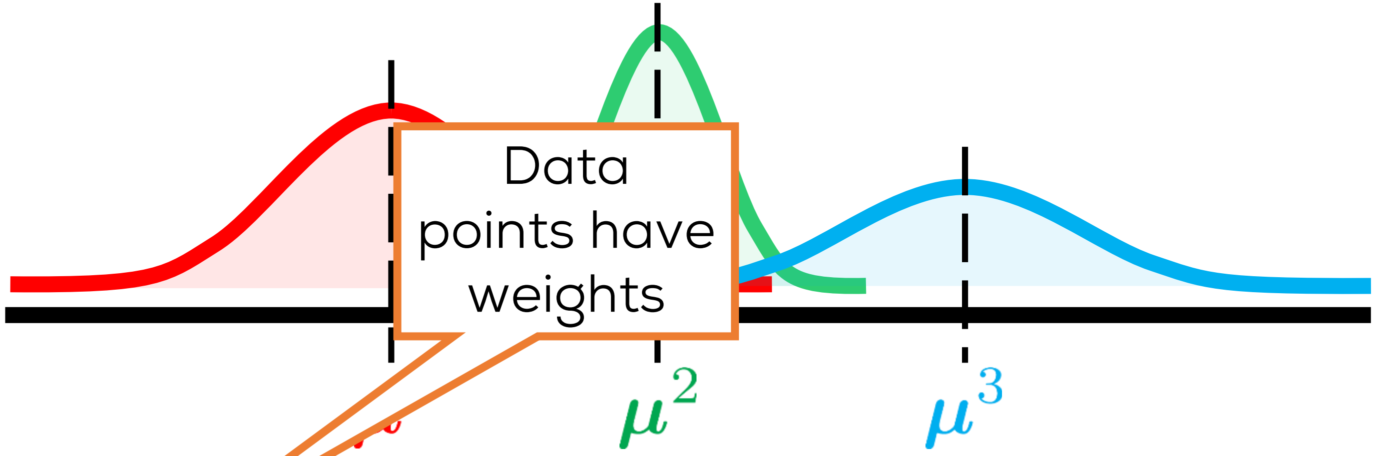
Exercise!

Weighted MLE



Reduces to normal MLE if $\gamma^i = 1$ for all i

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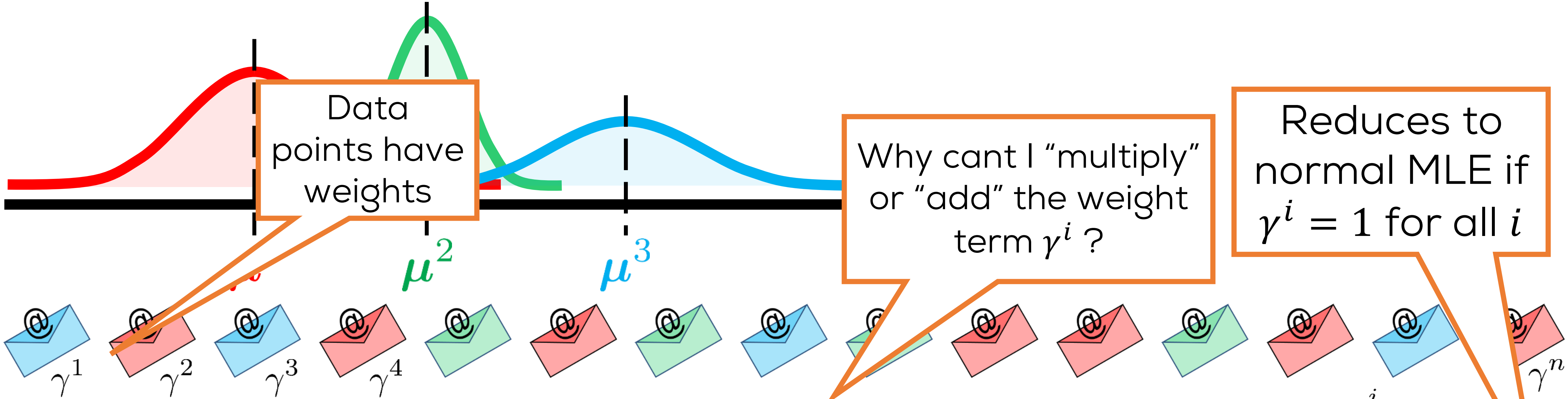
Take log and apply 1st order optimality

Exercise!

Weighted MLE



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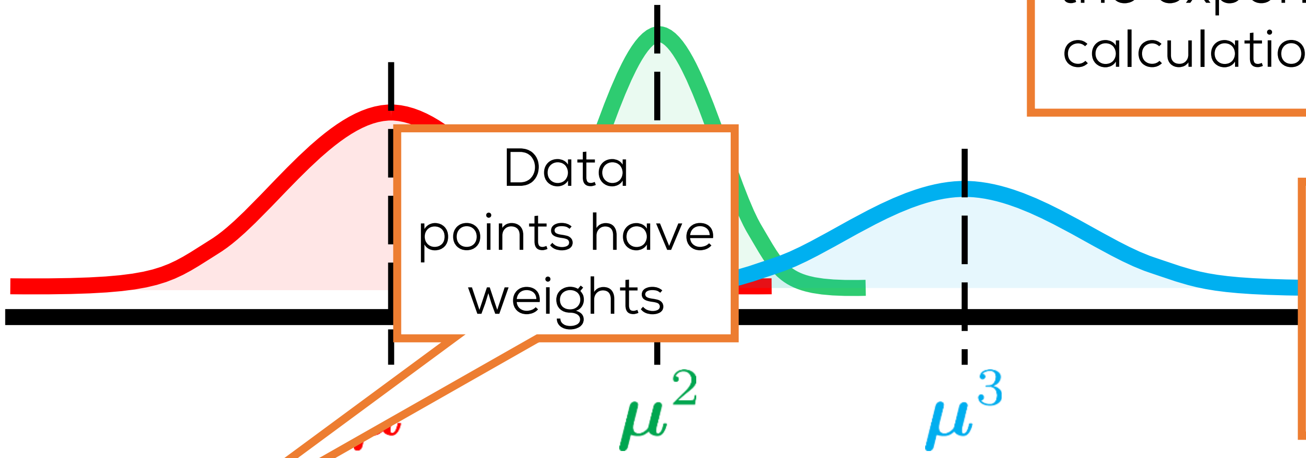
Exercise!

Weighted MLE



Data points have weights

Incorporating γ^i into the exponent makes calculations simpler

Why cant I "multiply" or "add" the weight term γ^i ?

Reduces to normal MLE if $\gamma^i = 1$ for all i

$$\mathbb{P}\left[\mathbf{x}^i, z^i, \gamma^i \mid \mathbf{\Theta}\right] = \left(\mathbb{P}\left[z^i \mid \mathbf{\Theta}\right] \cdot \mathbb{P}\left[\mathbf{x}^i \mid z^i, \mathbf{\Theta}\right]\right)^{\gamma^i} = \left(\boldsymbol{\pi}_{z^i} \cdot \mathcal{N}\left(\mathbf{x}^i \mid \boldsymbol{\mu}^{z^i}, \Sigma^{z^i}\right)\right)^{\gamma^i}$$

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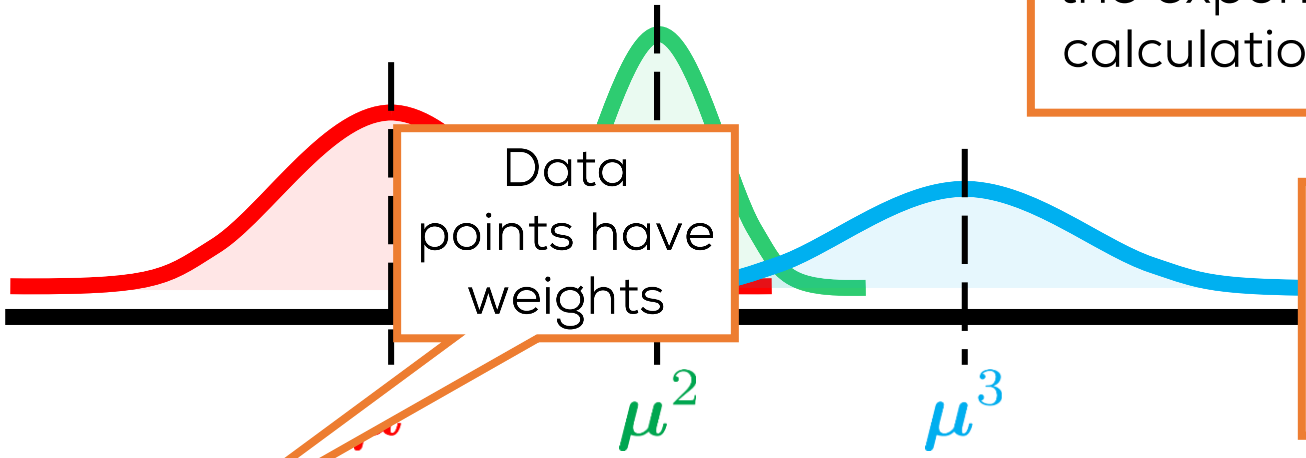
Exercise!

Weighted MLE



Data points have weights

Incorporating γ^i into the exponent makes calculations simpler

Also makes more sense (when we study the EM algo)

Why cant I "multiply" or "add" the weight term γ^i ?

Reduces to normal MLE if $\gamma^i = 1$ for all i

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Hard Alternating Minimization

ALTERNATING OPTIMIZATION

1. Initialize $\boldsymbol{\Theta}^0$
2. For $i \in [n]$, update $z^{i,t}$ using $\boldsymbol{\Theta}^t$
    1. Let $z^{i,t} = \arg\max_k \boldsymbol{\pi}_k^t \cdot \mathcal{N}\left(\mathbf{x}^i \mid \boldsymbol{\mu}^{k,t}, \Sigma^{k,t}\right)$
3. Update $\boldsymbol{\Theta}^{t+1} = \arg\max_{\boldsymbol{\Theta}} \mathbb{P}\left[X, \left\{z^{i,t}\right\} \mid \boldsymbol{\Theta}\right]$
4. Repeat until convergence

Soft Alternating Minimization

ALTERNATING OPTIMIZATION

1. For $i \in [n]$, create k copies of the data point
   1. Let $\mathbf{x}^i \to \left\{\mathbf{x}^{\{i,1\}}, \mathbf{x}^{\{i,2\}}, \dots, \mathbf{x}^{\{i,k\}}\right\}$
   2. Assign the k-th copy label k i.e. $z^{\{i,k\}} = k$
2. Initialize $\boldsymbol{\Theta}^0$
3. Update weights $\gamma^{i,k,t}$ using $\boldsymbol{\Theta}^t$
   1. Let $\gamma^{i,k,t} = \mathbb{P}[k \mid \mathbf{x}^i, \boldsymbol{\Theta}^t] = \dfrac{\boldsymbol{\pi}_k^t \cdot \mathcal{N}\left(\mathbf{X}^i \mid \boldsymbol{\mu}^{k,t}, \Sigma^{k,t}\right)}{\sum_j \boldsymbol{\pi}_j^t \cdot \mathcal{N}\left(\mathbf{X}^i \mid \boldsymbol{\mu}^{j,t}, \Sigma^{j,t}\right)}$
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$\sum_j \gamma^{\{i,j,t\}} = 1$ for all i and all t

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Distribute a unit weight across clusters

$\sum_j \gamma^{\{i,j,t\}} = 1$ for all i and all t

Soft Alternating Minimization

Hard-AM: all weight was on a single cluster

Distribute a unit weight across clusters

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ALTERNATING OPTIMIZATION

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Soft k-means Algorithm

- Fix $\boldsymbol{\pi}_k^t = \frac{1}{K}$ for all iterations. Don't update it.
- Fix $\boldsymbol{\Sigma}^{k,t} = I$ for all iterations. Don't update it.

K-MEANS ALGO

1. Initialize means $\{\boldsymbol{\mu}^{k,0}\}_{k=1,\ldots K}$
2. For all i, update $z^{i,t}$ using $\boldsymbol{\mu}^{k,t}$

   Let $z^{i,t} = \arg\min_k \left\|\mathbf{x}^i - \boldsymbol{\mu}^{k,t}\right\|_2^2$
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3. Let $\tilde{n}_k^t = \sum_i \gamma^{\{i,k,t\}}$
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Mixed Regression

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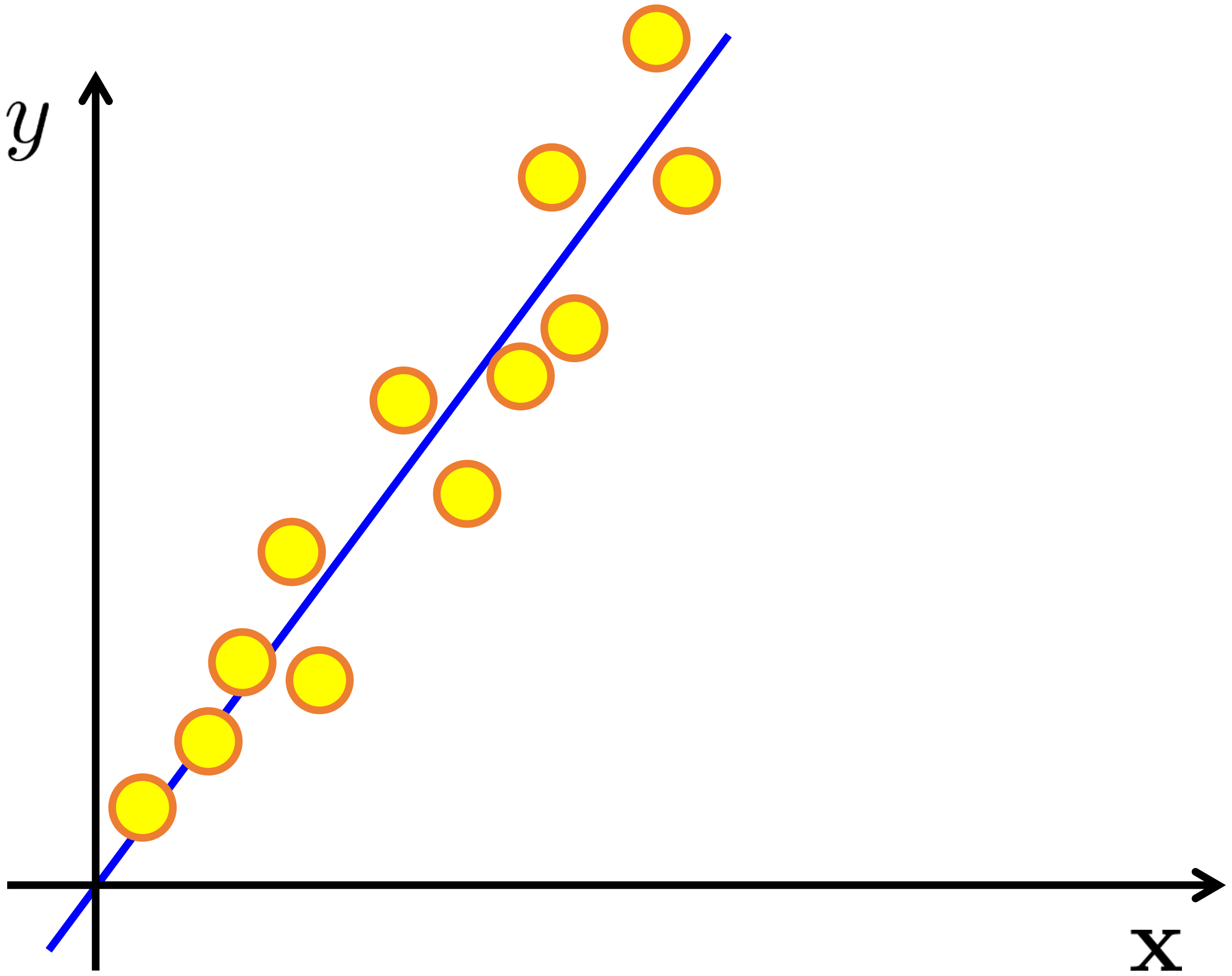
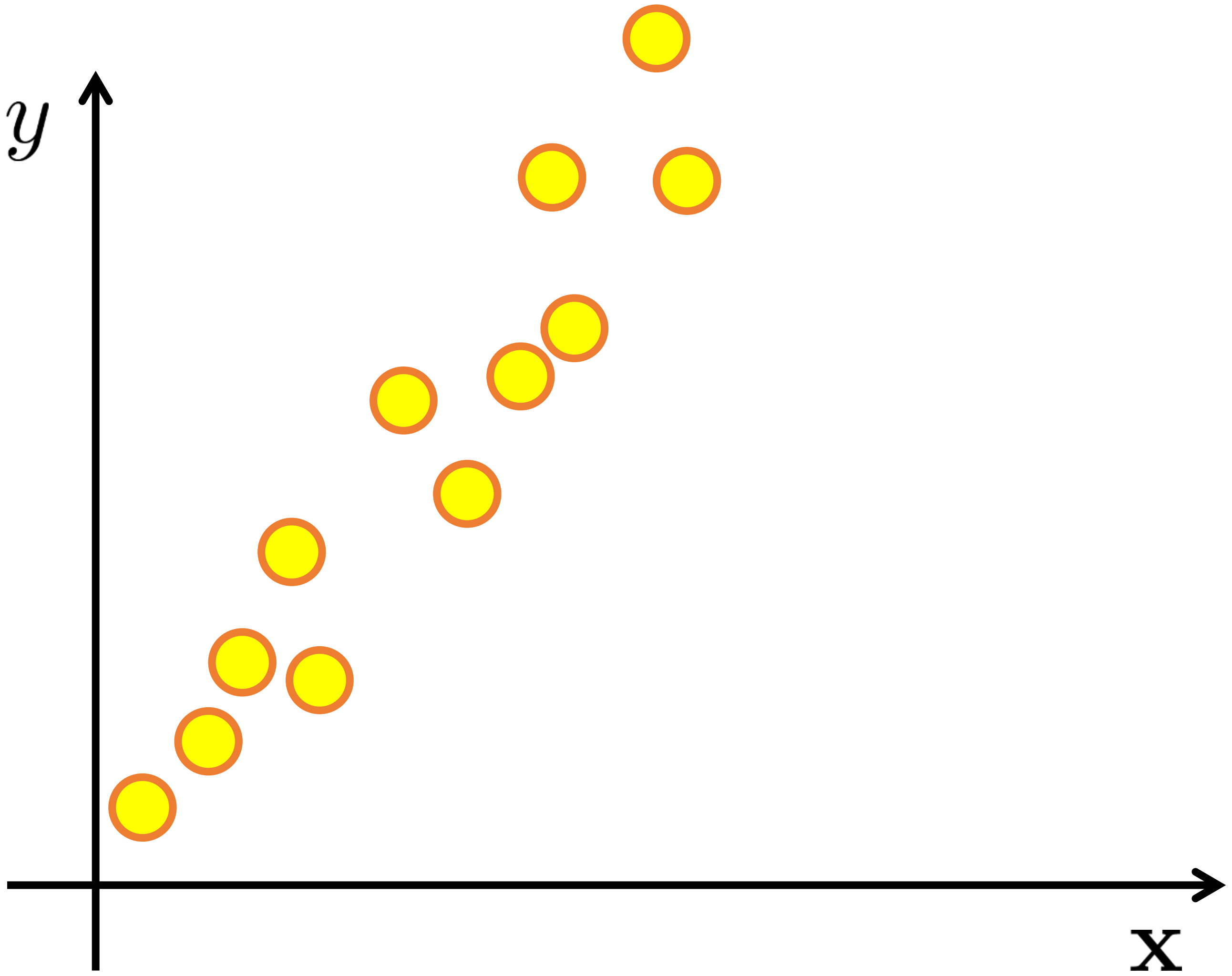


Mixed Regression



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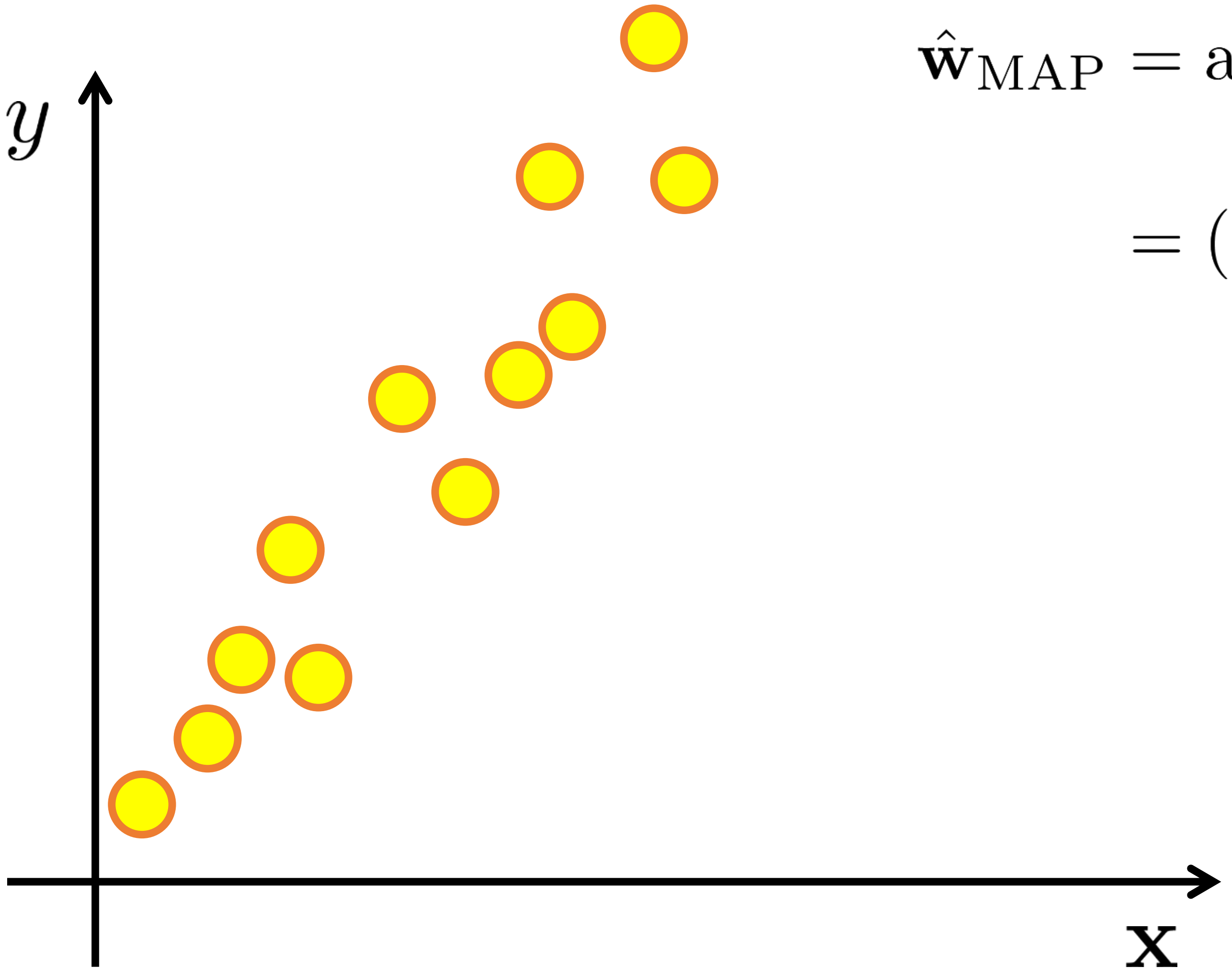
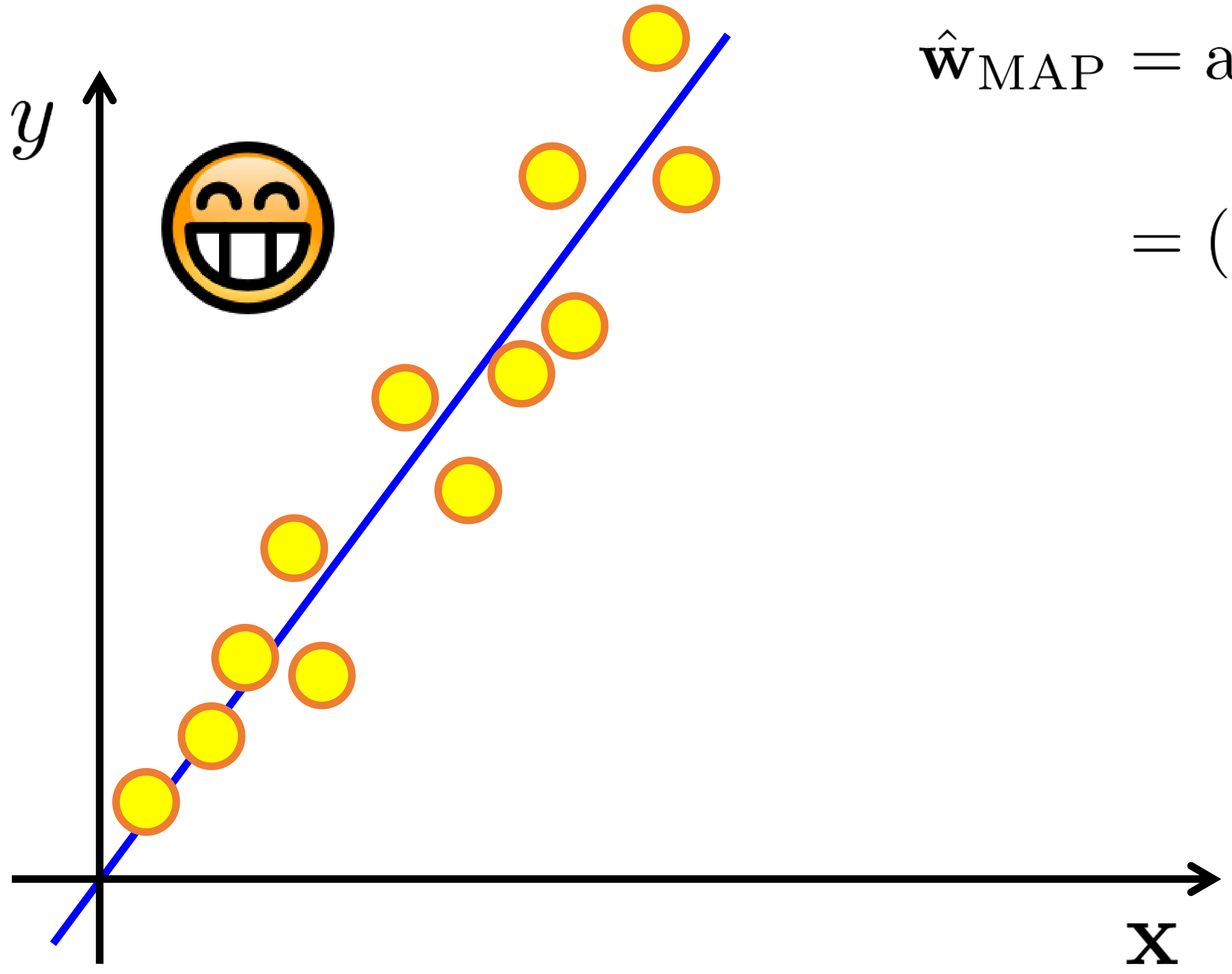


$$\hat{\mathbf{w}}_{\text{MAP}} = \arg\min \sum_{i=1}^{n} \left(y^i - \langle \mathbf{w}, \mathbf{x}^i \rangle\right)^2 + \lambda \cdot \|\mathbf{w}\|_2^2$$

$$= (\mathbf{X}\mathbf{X}^\top + \lambda \cdot I)^{-1}\mathbf{X}\mathbf{y}$$

Mixed Regression



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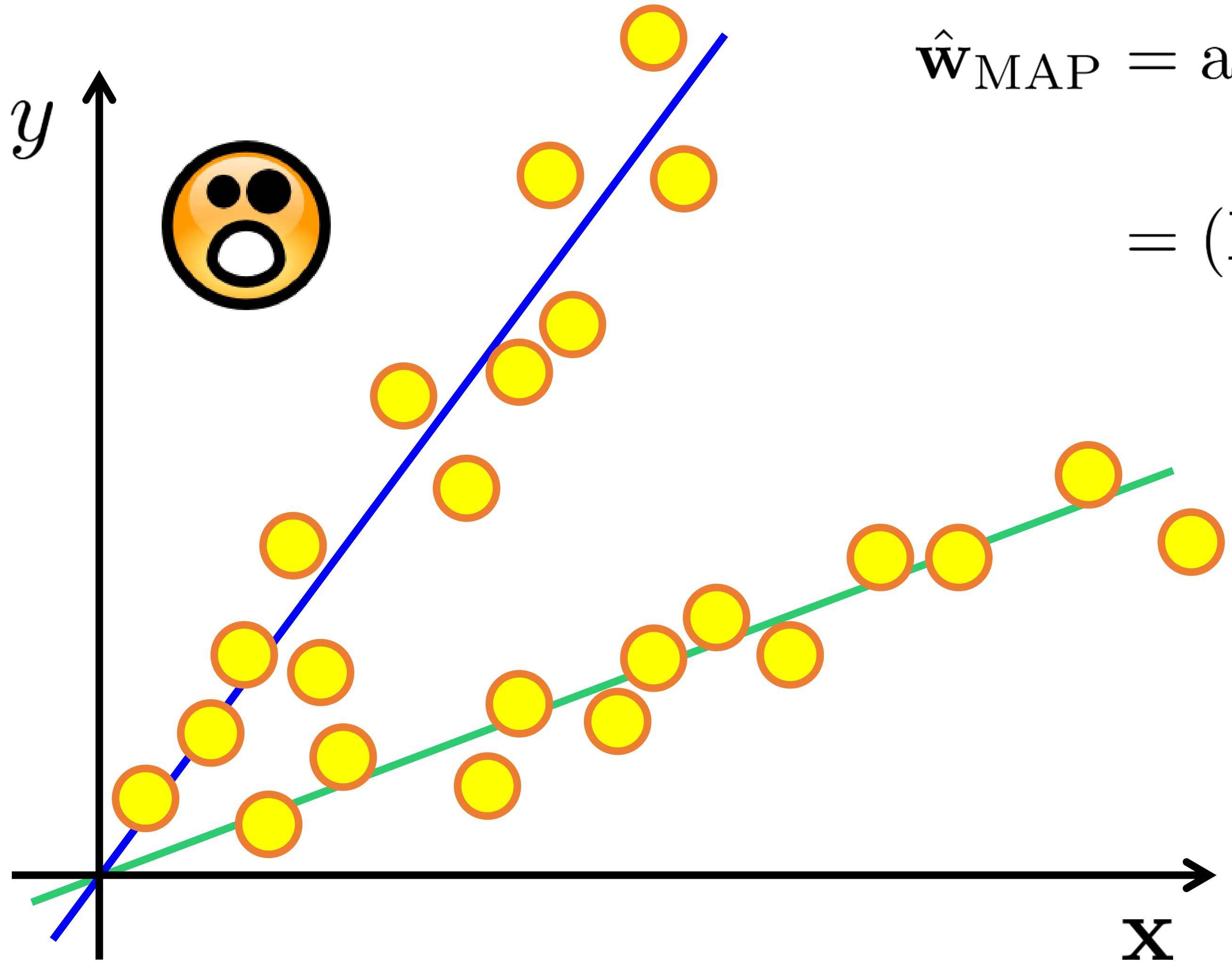

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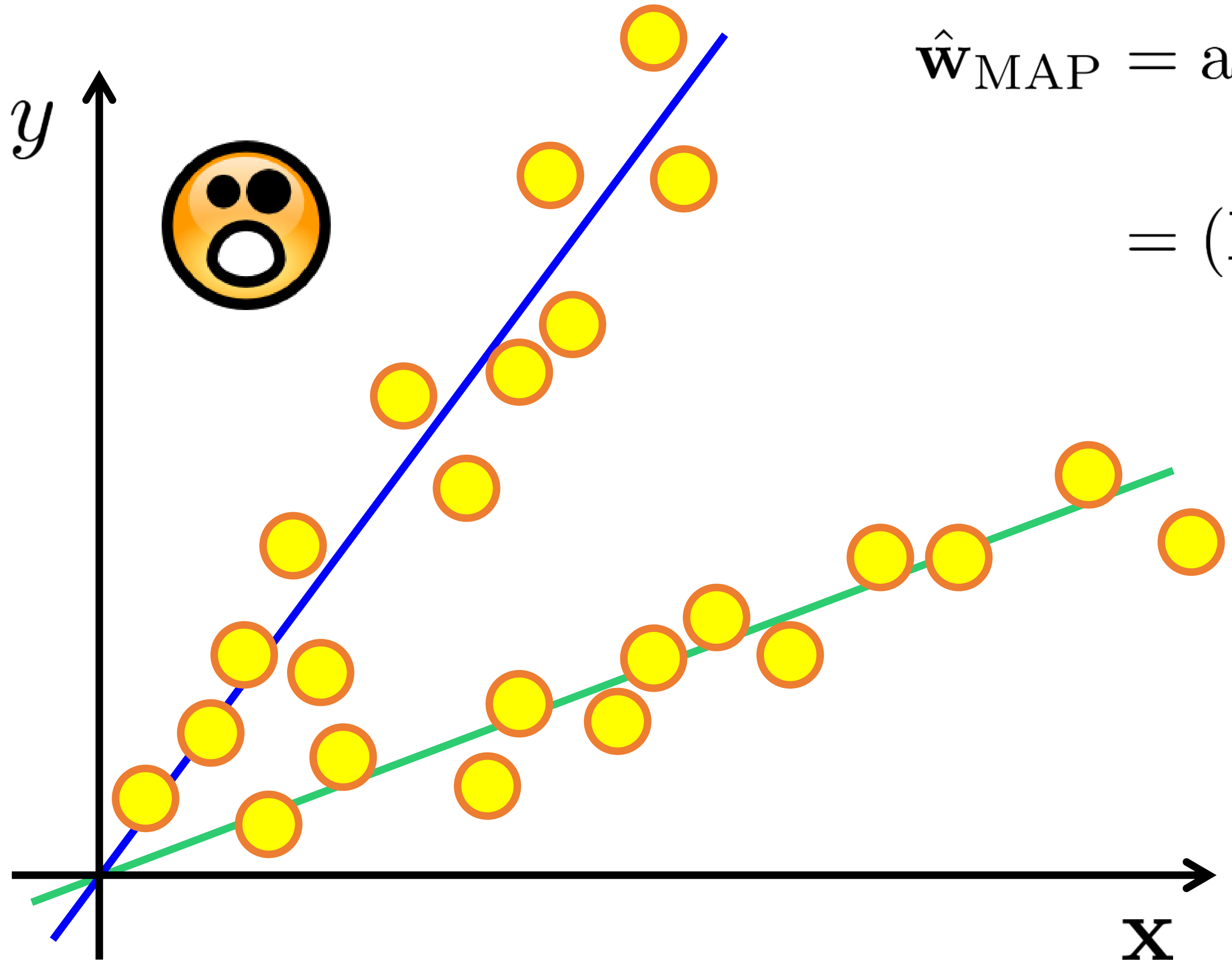

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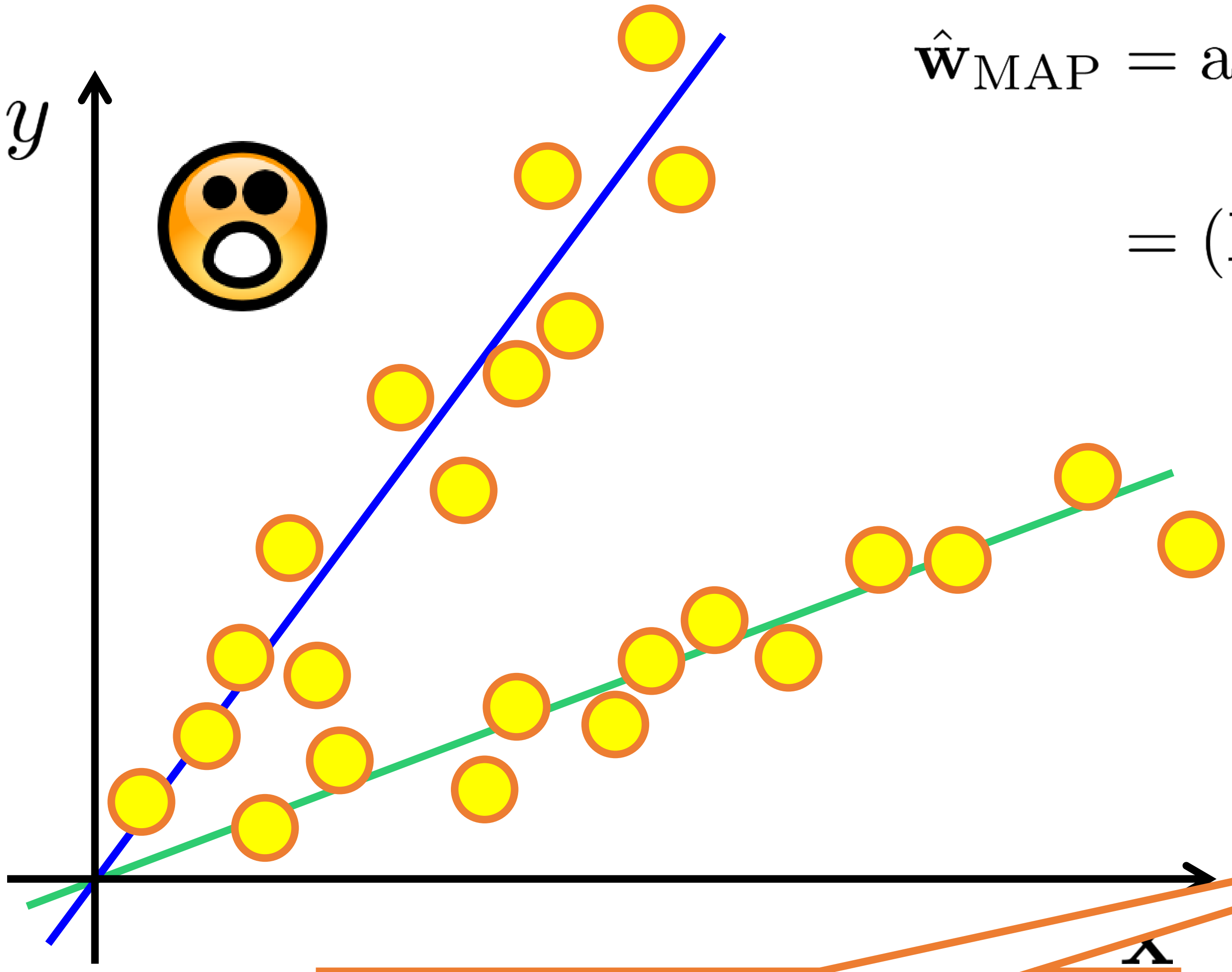
Regression with a classification touch ☺

E.g. recommendation systems, a different system might work for young and old but we don't know age of users

Mixed Regression



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Mixed models, Mixture of Experts

Mixed Regression

$$\mathbb{P}\left[y \,|\, \mathbf{x}^i, z^i, \mathbf{w}\right] = \mathcal{N}(\left\langle \mathbf{w}^{z^i}, \mathbf{x}^i \right\rangle, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y - \left\langle \mathbf{w}^{z^i}, \mathbf{x}^i \right\rangle)^2}{2\sigma^2}\right)$$

- Assume for sake of simplicity that both models are equally sampled $\mathbb{P}[z = 0] = \mathbb{P}[z = 1] = 0.5$
- Assume for sake of simplicity that Gaussian noise $\sigma_1 = \sigma_2 = 1$
- Only unknowns are the two linear models $\mathbf{w}^1, \mathbf{w}^2$

Mixed Regression

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$z^i \in \{0,1\}$ indicates which line generated the data

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Mixed Regression

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$z^i \in \{0,1\}$ indicates which line generated the data

z^i is a latent variable!

- Assume for sake of simplicity that both models are equally sampled $\mathbb{P}[z = 0] = \mathbb{P}[z = 1] = 0.5$
- Assume for sake of simplicity that Gaussian noise $\sigma_1 = \sigma_2 = 1$
- Only unknowns are the two linear models $\mathbf{w}^1, \mathbf{w}^2$

Hard Mixed Regression

ALTERNATING OPTIMIZATION

1. Initialize $\boldsymbol{\Theta}^0 = \left\{\mathbf{w}^{\{0,0\}}, \mathbf{w}^{\{0,1\}}\right\}$
2. For $i \in [n]$, update $z^{i,t}$ using $\boldsymbol{\Theta}^t$
   1. Let $z^{i,t} = \arg\max_{k \in \{0,1\}} \mathcal{N}\left(y^i \mid \mathbf{x}^i, \mathbf{w}^{k,t}\right)$
3. Update $\mathbf{w}^{\{t+1,k\}} = \arg\min_{\mathbf{w}} \sum_{i : z^{\{i,t\}} = k} \left(y^i - \langle \mathbf{w}, \mathbf{x}^i \rangle\right)^2 + \frac{1}{2}\|\mathbf{w}\|_2^2$
4. Set $\boldsymbol{\Theta}^{t+1} = \left\{\mathbf{w}^{\{t+1,0\}}, \mathbf{w}^{\{t+1,1\}}\right\}$
5. Repeat until convergence

Hard Mixed Regression

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Exercise: verify these updates

Hard Mixed Regression

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Exercise: verify these updates

Hard Mixed Regression

Assign to the "closest" line!

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5. Repeat until convergence

Assign to the “closest” line!

In k-means, we assigned to the closest mean

Exercise: verify these updates

Weighted Regression

Weighted Regression

$$\hat{\mathbf{w}}_{\mathrm{MAP}} = \arg\min \sum_{i=1}^{n} \left(y^i - \langle \mathbf{w}, \mathbf{x}^i \rangle\right)^2 + \lambda \cdot \|\mathbf{w}\|_2^2$$
$$= (\mathbf{X}\mathbf{X}^\top + \lambda \cdot I)^{-1}\mathbf{X}\mathbf{y}$$

Weighted Regression

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$$= (\mathbf{X}\mathbf{X}^\top + \lambda \cdot I)^{-1}\mathbf{X}\mathbf{y}$$

$$\hat{\mathbf{w}}_{\text{MAP}} = \arg\min \sum_{i=1}^{n} \gamma_i \cdot \left(y^i - \langle \mathbf{w}, \mathbf{x}^i \rangle\right)^2 + \lambda \cdot \|\mathbf{w}\|_2^2$$

$$= (M + \lambda \cdot I)^{-1}\mathbf{b}$$

$$M = \sum_{i=1}^{n} \gamma_i \mathbf{x}^i (\mathbf{x}^i)^\top$$

$$\mathbf{b} = \sum_{i=1}^{n} \gamma_i y_i \cdot \mathbf{x}^i$$

Weighted Regression

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Exercise

Soft Mixed Regression

SOFT ALTERNATING OPTIMIZATION

1. Initialize $\boldsymbol{\Theta}^0 = \left\{\mathbf{w}^{\{0,0\}}, \mathbf{w}^{\{0,1\}}\right\}$
2. For $i \in [n]$, update $\gamma^{\{i,k,t\}}$ using $\boldsymbol{\Theta}^t$
    1. Let $\mathrm{c}^{\{i,k,t\}} = \exp\left(-\frac{\left(y^i - \langle \mathbf{w}^{\{t,k\}}, \mathbf{x}^i \rangle\right)^2}{2}\right)$
    2. Let $\gamma^{\{i,k,t\}} = \frac{\mathrm{c}^{\{i,k,t\}}}{\mathrm{c}^{\{i,0,t\}} + \mathrm{c}^{\{i,1,t\}}}$
3. Update $\mathbf{w}^{\{t+1,k\}} = \arg\min_{\mathbf{w}} \sum_i \gamma^{\{i,k,t\}} \cdot \left(y^i - \langle \mathbf{w}, \mathbf{x}^i \rangle\right)^2 + \frac{1}{2}\|\mathbf{w}\|_2^2$
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5. Repeat until convergence

Soft Mixed Regression

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Exercise: derive these updates

Soft Mixed Regression

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5. Repeat until convergence

$\propto \mathbb{P}\left[k \mid y^i, \mathbf{x}^i, \boldsymbol{\Theta}^t\right]$

Exercise: derive these updates

Soft Mixed Regression

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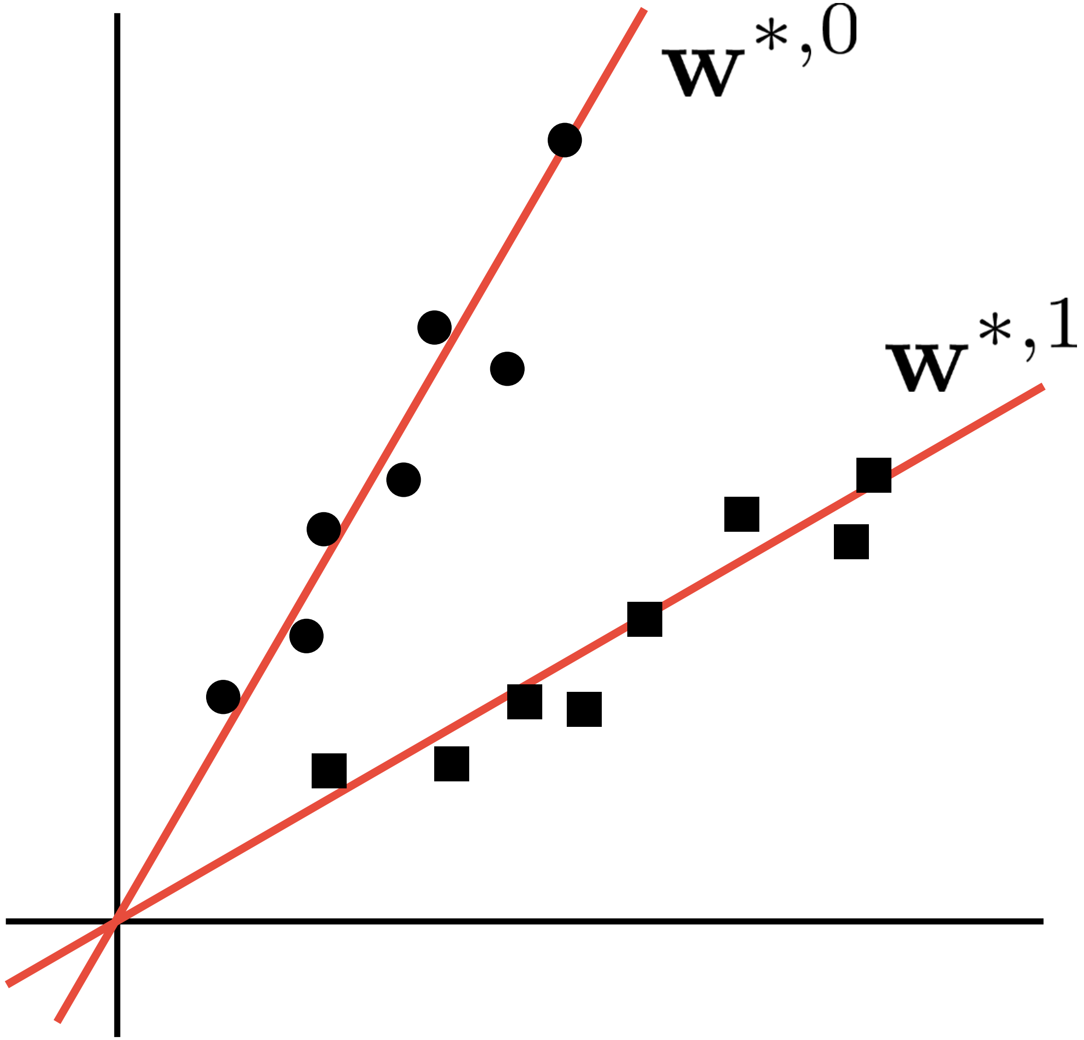
5. Repeat until convergence

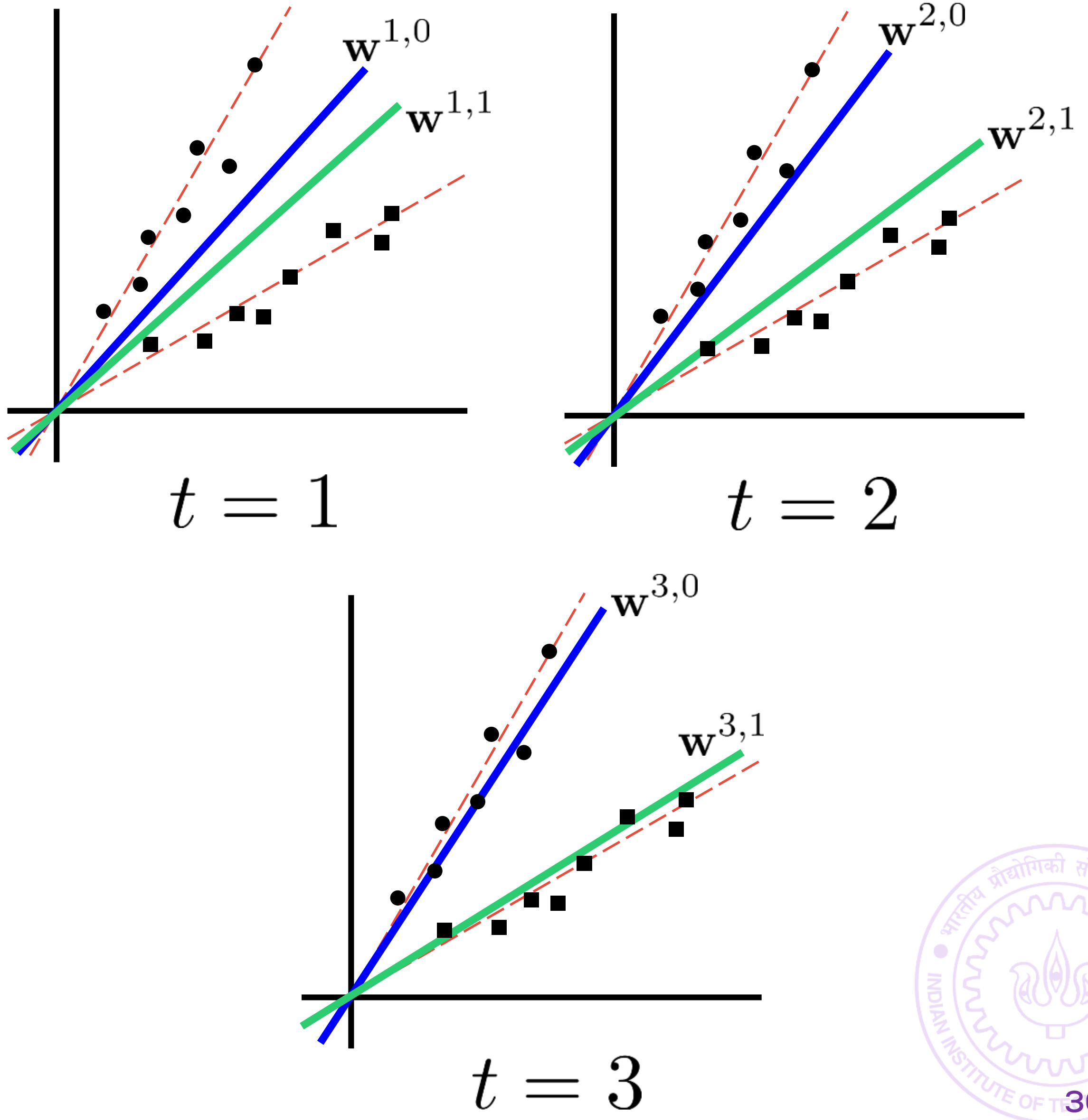
$\propto \mathbb{P}[k \mid y^i, \mathbf{x}^i, \boldsymbol{\Theta}^t]$

$= \mathbb{P}[k \mid y^i, \mathbf{x}^i, \boldsymbol{\Theta}^t]$

Exercise: derive these updates

Soft MR in action





The EM Algorithm

- Generalizes the notion of "soft" updates
- Very powerful algorithm
- Related to alternating minimization
- Will study this next time!

Please give your Feedback

http://tinyurl.com/ml17-18afb