

Data Modelling Methods-II

CS771: Introduction to Machine Learning
Purushottam Kar

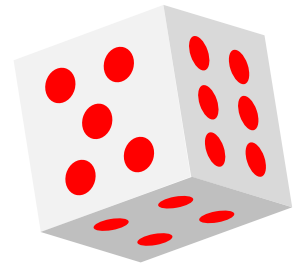
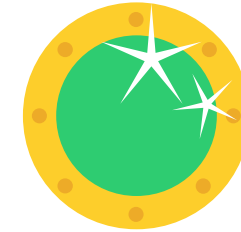


Outline of today's discussion

- Revise Naïve Bayes method
- Feature modelling methods for unlabelled data
- Gaussian mixture Models (GMMs)
- The alternating optimization approach to learning GMMs
- The k-means approach to learning GMMs

The Multinoulli Distribution

- Also known as categorical distribution
- Generalizes the Bernoulli distribution
 - Bernoulli models a coin with two outcomes (call them head and tail)
 - ... using one “bias” parameter p (taken to be the probability of heads)
- Multinoulli models a K -sided dice
 - ... using a K -dimensional vector π
 - π_k is taken to denote the probability of the k -th side turning up
 - $\pi_k \geq 0$ and $\sum_{k=1}^K \pi_k = 1$
- Conjugate prior for Bernoulli: Beta $\mathbb{P}[p; \alpha, \beta] = \frac{1}{B(\alpha, \beta)} p^{\alpha-1} (1-p)^{\beta-1}$
- Conjugate prior for Multinoulli: Dirichlet $\mathbb{P}[\boldsymbol{\pi}; \boldsymbol{\alpha}] = \frac{1}{B(\boldsymbol{\alpha})} \prod_{i=1}^L \pi_i^{\alpha_i-1}$



App: Email Categorizer using Naïve Bayes

Sept 6, 2017



App: Email Categorizer using Naïve Bayes

HEC			DoSA	Supervisor
<input type="checkbox"/>	☆	➤	HallPresi	Awesome talk at eSumm
<input type="checkbox"/>	☆	➤	HEC	Urgent! Mess bill overdue
<input type="checkbox"/>	☆	➤	HEC	Urgent! Canteen bill over

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X

talk	meet	project	wake	meeting	wallet	keys	awesome	lost	trip	lost	mess	report

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talk meet project wake meeting wallet keys awesome lost trip lost mess report

$y \in \{ \text{red circle}, \text{green circle}, \text{blue circle} \}$

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Bag of words feature
can record just
occurrence or count

X

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x	1	0	0	0	0	0	0	1	0	0	0	0	0
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Choice of words crucial
– stemming, throw
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Commonly used in NLP

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Usually very high dimensional

App: Email Categorizer using Naïve Bayes

HEC	DoSA	Supervisor
<input type="checkbox"/> ☆ ▷ HallPresi		Awesome talk at eSumm
<input type="checkbox"/> ☆ ▷ HEC		Urgent! Mess bill overdue
<input type="checkbox"/> ☆ ▷ HEC		Urgent! Canteen bill over

Commonly used in NLP

Choice of words crucial
– stemming, throw away articles etc

Bag of words feature can record just occurrence or count

x	1	0	0	0	0	0	0	1	0	0	0	0	0
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$y \in \{ \text{red circle}, \text{green circle}, \text{blue circle} \}$

Usually very high dimensional

Usually very very sparse

App: Email Categorizer using Naïve Bayes

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At test time ...

App: Email Categorizer using Naïve Bayes

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$$\mathbb{P}[\mathbf{x}^t, \bullet] = \mathbb{P}[\bullet] \cdot \prod_{j=1}^d \mathbb{P}[\mathbf{x}_j^t \mid \bullet]$$

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At test time ...

$$\begin{aligned}\mathbb{P}[\text{awesome} = 0 \mid \bullet] \\ = 1 - \mathbb{P}[\text{awesome} = 1 \mid \bullet]\end{aligned}$$

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$$\hat{y}^t = \arg \max \{ \mathbb{P}[\mathbf{x}^t, \text{red}], \mathbb{P}[\mathbf{x}^t, \text{green}], \mathbb{P}[\mathbf{x}^t, \text{blue}] \}$$

App: Email Categorizer using Naïve Bayes

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$$\mathbb{P}[\mathbf{x}^t, \bullet] = \mathbb{P}[\bullet] \cdot \prod_{j=1}^d \mathbb{P}[\mathbf{x}_j^t \mid \bullet]$$

Will give the same result as
 $\arg \max\{\mathbb{P}[\text{red} \mid \mathbf{x}^t], \mathbb{P}[\text{green} \mid \mathbf{x}^t], \mathbb{P}[\text{blue} \mid \mathbf{x}^t]\}$

$$\hat{y}^t = \arg \max\{\mathbb{P}[\mathbf{x}^t, \text{red}], \mathbb{P}[\mathbf{x}^t, \text{green}], \mathbb{P}[\mathbf{x}^t, \text{blue}]\}$$

App: Automatic Email Generator!

Class proportions

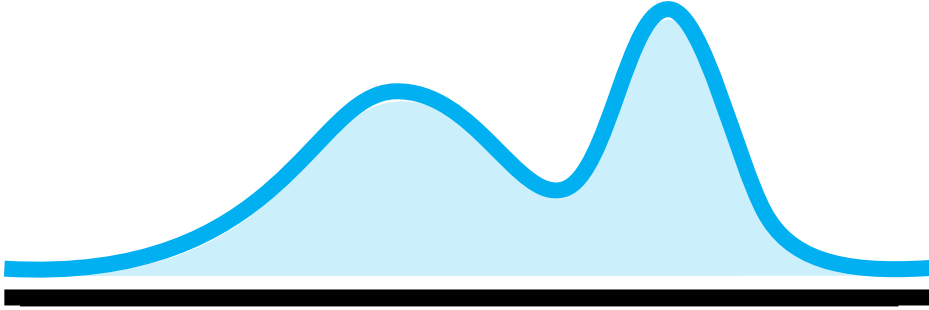
- Choose a category from {HEC, DoSA, Supervisor}
 - Toss a 3-sided "coin" aka categorical/multinoulli distribution using $\mathbb{P}[\bullet]$
 - Say we chose DoSA
- For each word in your dictionary of d words, toss a Bernoulli coin to decide whether to include that word in the mail or not
 - For $j \in [d]$, toss a coin that lands heads with probability $\mathbb{P}[x_j = 1 \mid \bullet]$
- Collect all words for which the toss landed heads
- Compose an email using only those words (and maybe a few articles, prepositions etc)
- Congratulations, you can now ask the dean to stop sending you emails – you will generate them yourself!

Already learnt from training data!

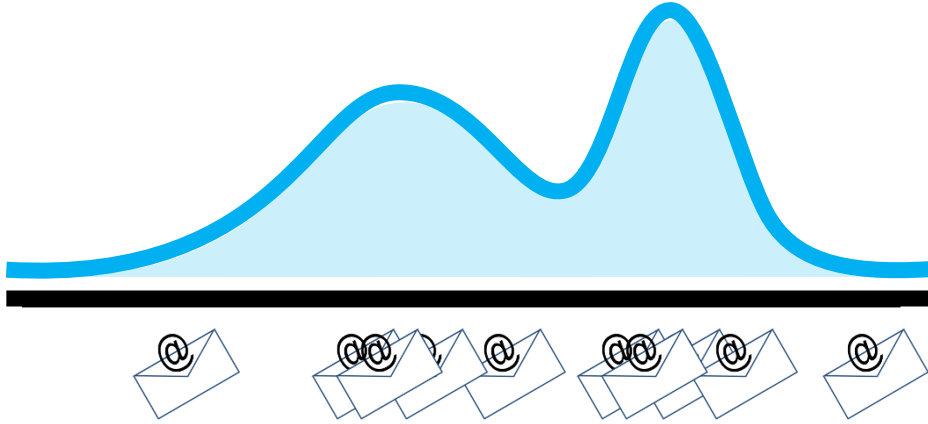


The generative story for unlabelled data??

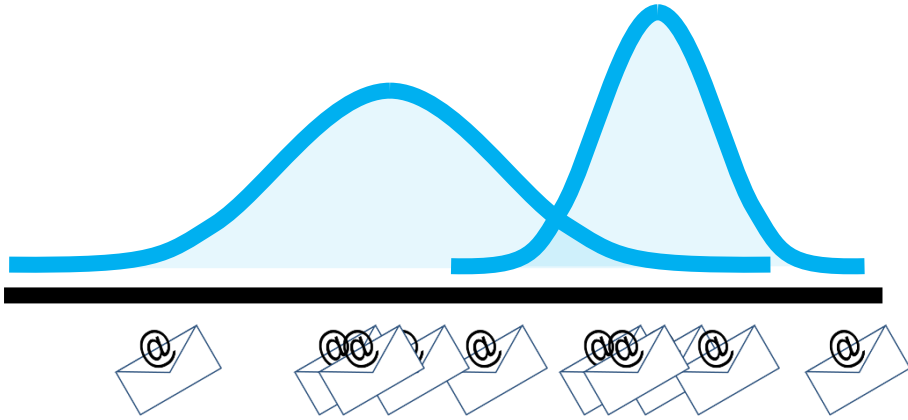
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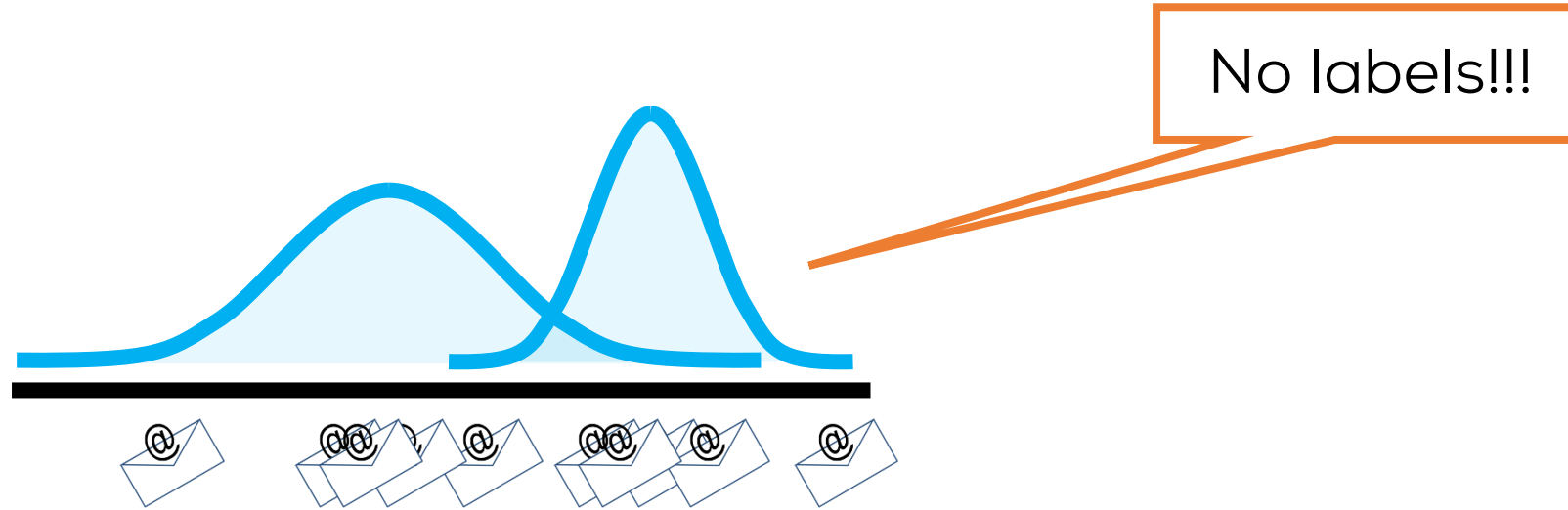
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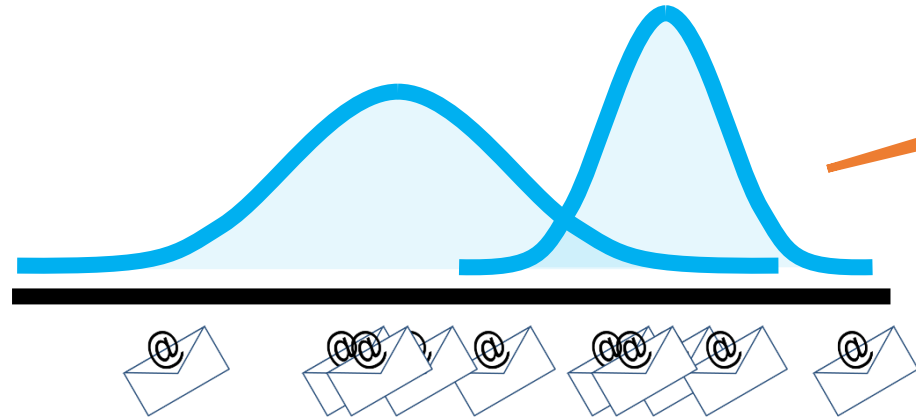
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The generative story for unlabelled data??



No labels!!!

Can we still recover the two Gaussian components in the mixture??

How to grade a CS771 exam??

Sept 8, 2017



CS771: Intro to ML

How to grade a CS771 exam??

 gradescope

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Q1. $\int x = ?$
5 marks

How to grade a CS771 exam??

 gradescope

Q1. $\int x = ?$
5 marks

$$\begin{array}{ccc} \frac{x^2}{2} + b & x^2 + d & \frac{x^2}{2} \\ x^2/2 & x^2/2 & \\ x^2 + C & & \frac{x^2}{2} + C \\ x^2/2 & \frac{x^2}{2} + a & x^2 + e \end{array}$$

How to grade a CS771 exam??

 gradescope

Q1. $\int x = ?$
5 marks

$$x^2/2$$
$$x^2/2 \quad x^2/2$$

$$x^2/2 + a$$
$$\frac{x^2}{2} + b \frac{x^2}{2} + c$$

$$x^2 + C x^2 + d$$
$$x^2 + e$$

How to grade a CS771 exam??

 gradescope

Q1. $\int x = ?$
5 marks

$$\begin{array}{l} x^2/2 \\ x^2/2 \quad x^2/2 \end{array}$$

$$\begin{array}{l} x^2/2 + a \\ \frac{x^2}{2} + b \quad \frac{x^2}{2} + c \end{array}$$

$$\begin{array}{l} x^2 + C \quad x^2 + d \\ x^2 + e \end{array}$$

How to grade a CS771 exam??

 gradescope

Q1. $\int x = ?$
5 marks

$x^2 / 2$
4/5
 $x^2 / 2$

$x^2 / 2 + a$
5/5
 $x^2 / 2 + b$
 $x^2 / 2 + c$

$x^2 + c$
2/5
 $x^2 + d$
 $x^2 + e$

How to grade a CS771 exam??

 gradescope

Q1. $\int x = ?$
5 marks

Clustering!

$x^2/2$
4/5
 $x^2/2$

$x^2/2 + a$
5/5
 $x^2/2 + b$
 $x^2/2 + c$

$x^2 + c$
2/5
 $x^2 + d$
 $x^2 + e$

How to grade a CS771 exam??

 gradescope

Q1. $\int x = ?$
5 marks

Clustering!

Like classification
without labels ☺

Sept 8, 2017

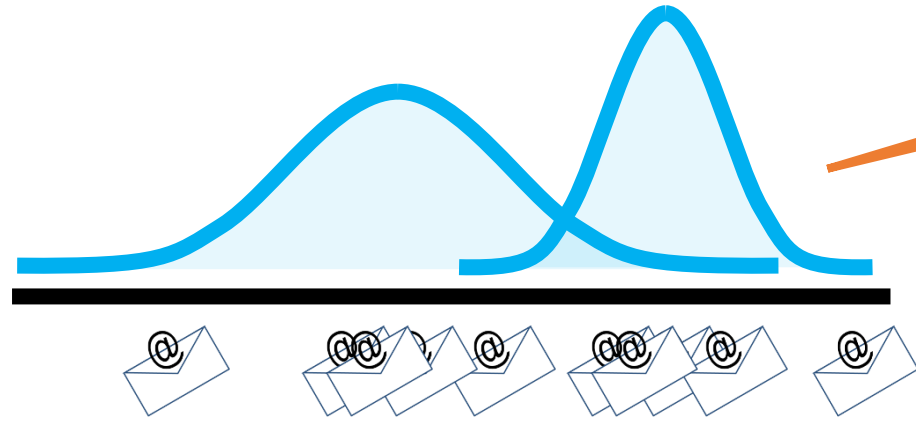
$$\frac{x^2}{2} + a$$

$$\frac{x^2}{2} + b$$

$$\frac{x^2}{2} + c$$



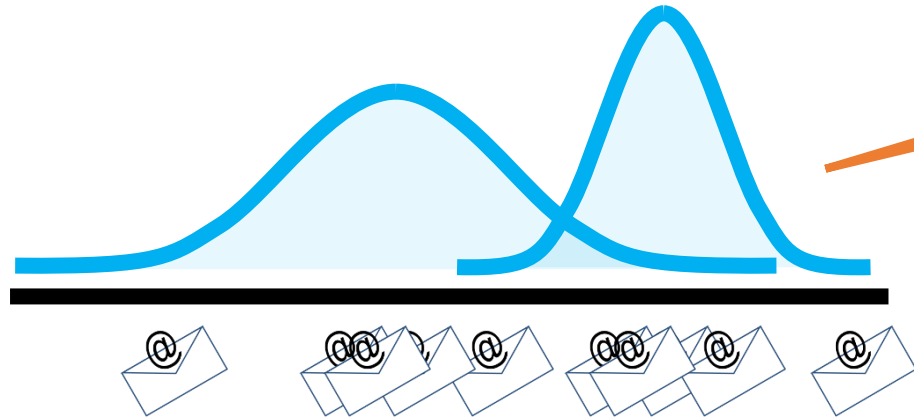
The generative story for unlabelled data??



No labels!!!

Can we still recover the two Gaussian components in the mixture??

The generative story for unlabelled data??

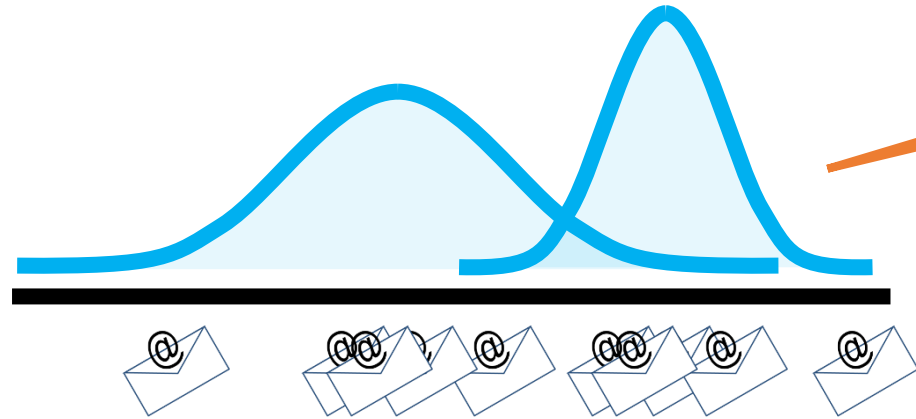


No labels!!!

Can we still recover the two Gaussian components in the mixture??

How do we know there are only two Gaussians?

The generative story for unlabelled data??



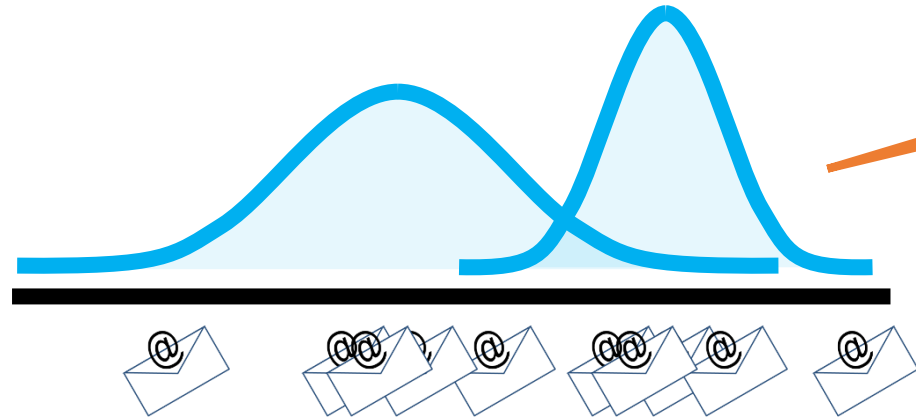
No labels!!!

Gaussians can be
a hyper-parameter
 K you can tune

Can we still recover
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mixture??

How do we know there
are only two Gaussians?

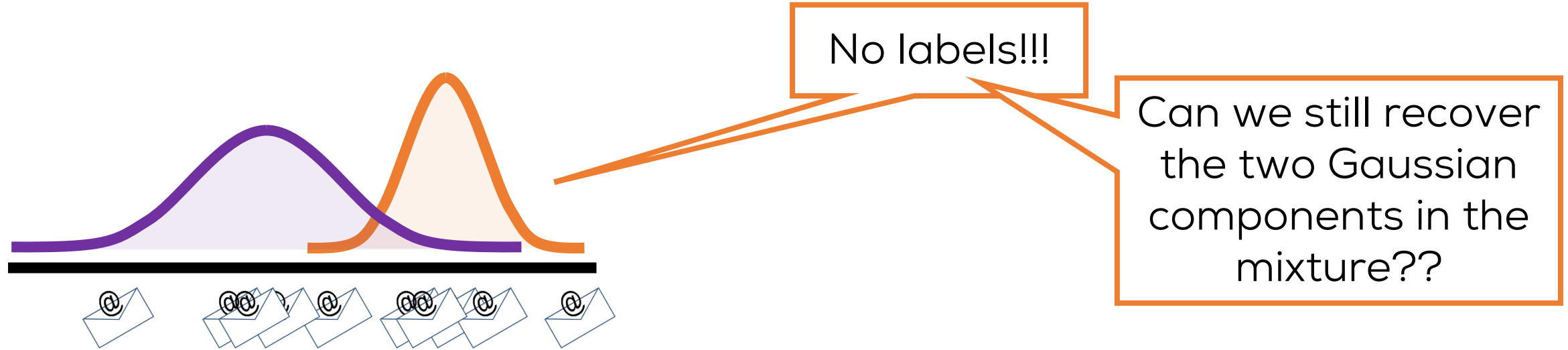
The generative story for unlabelled data??



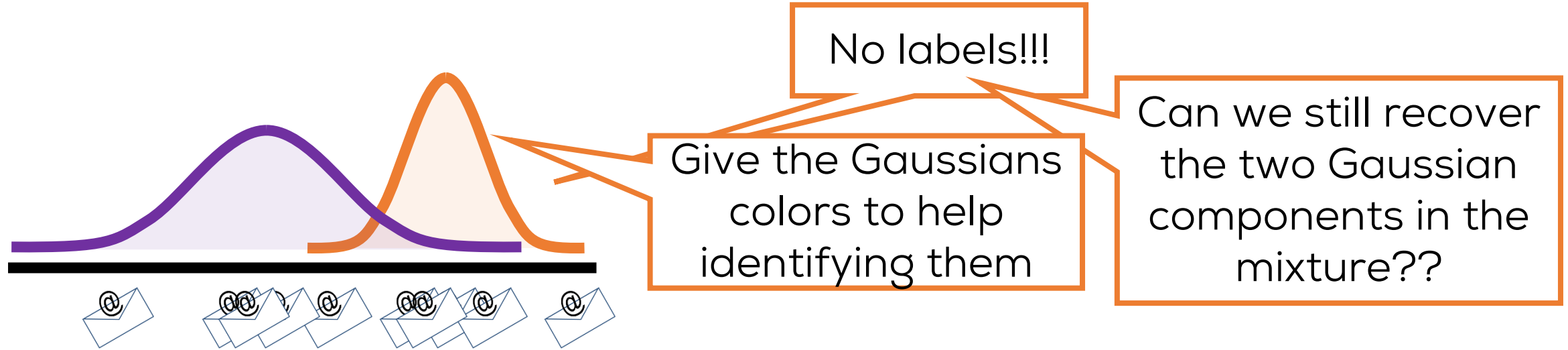
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The generative story for unlabelled data??



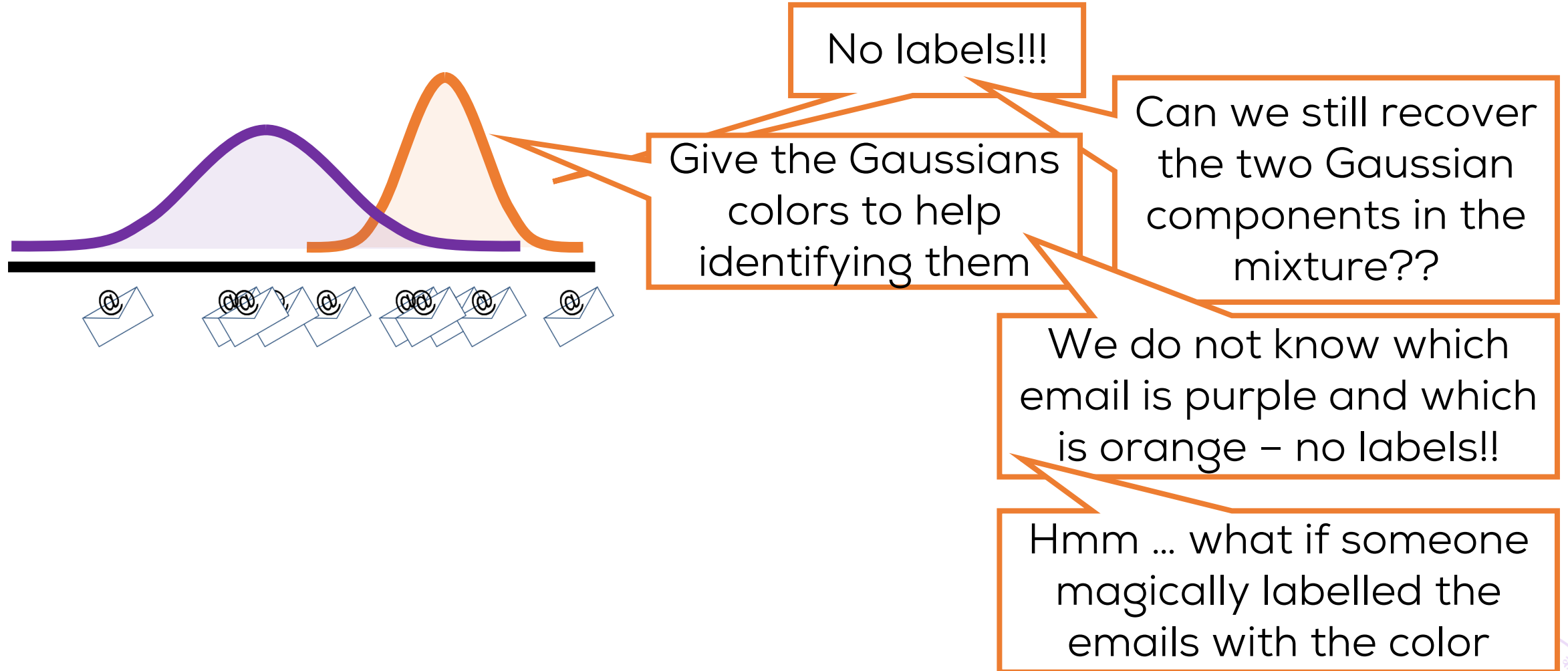
The generative story for unlabelled data??



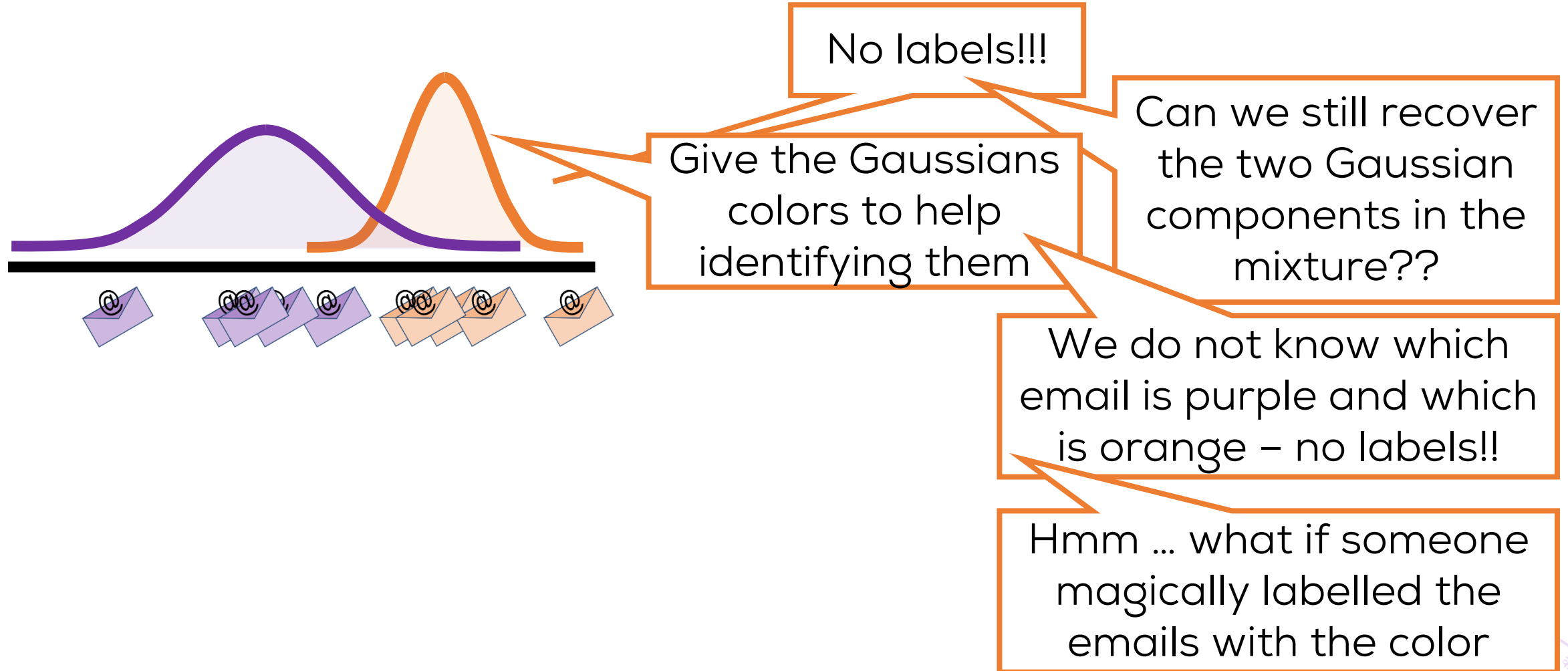
The generative story for unlabelled data??



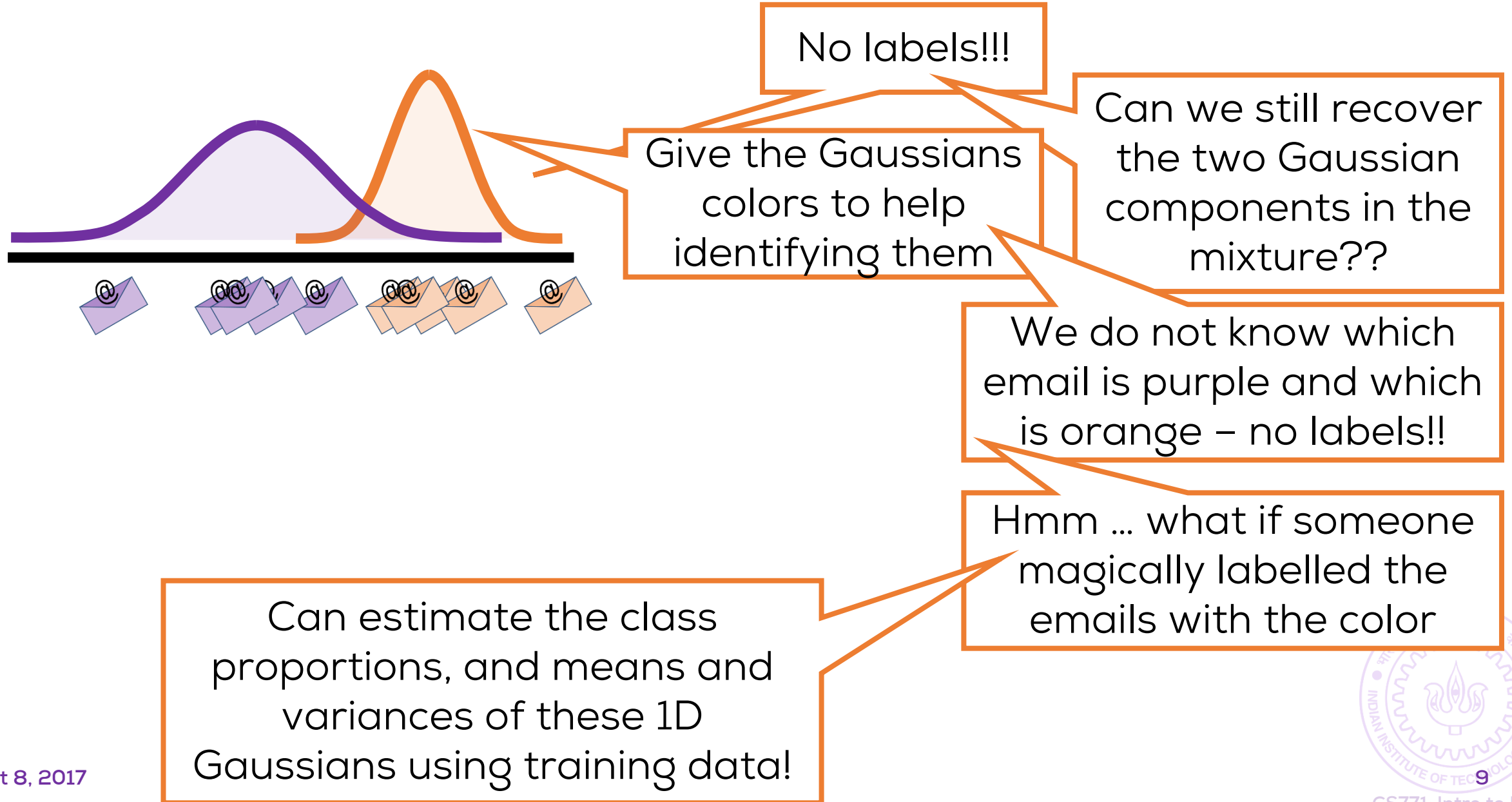
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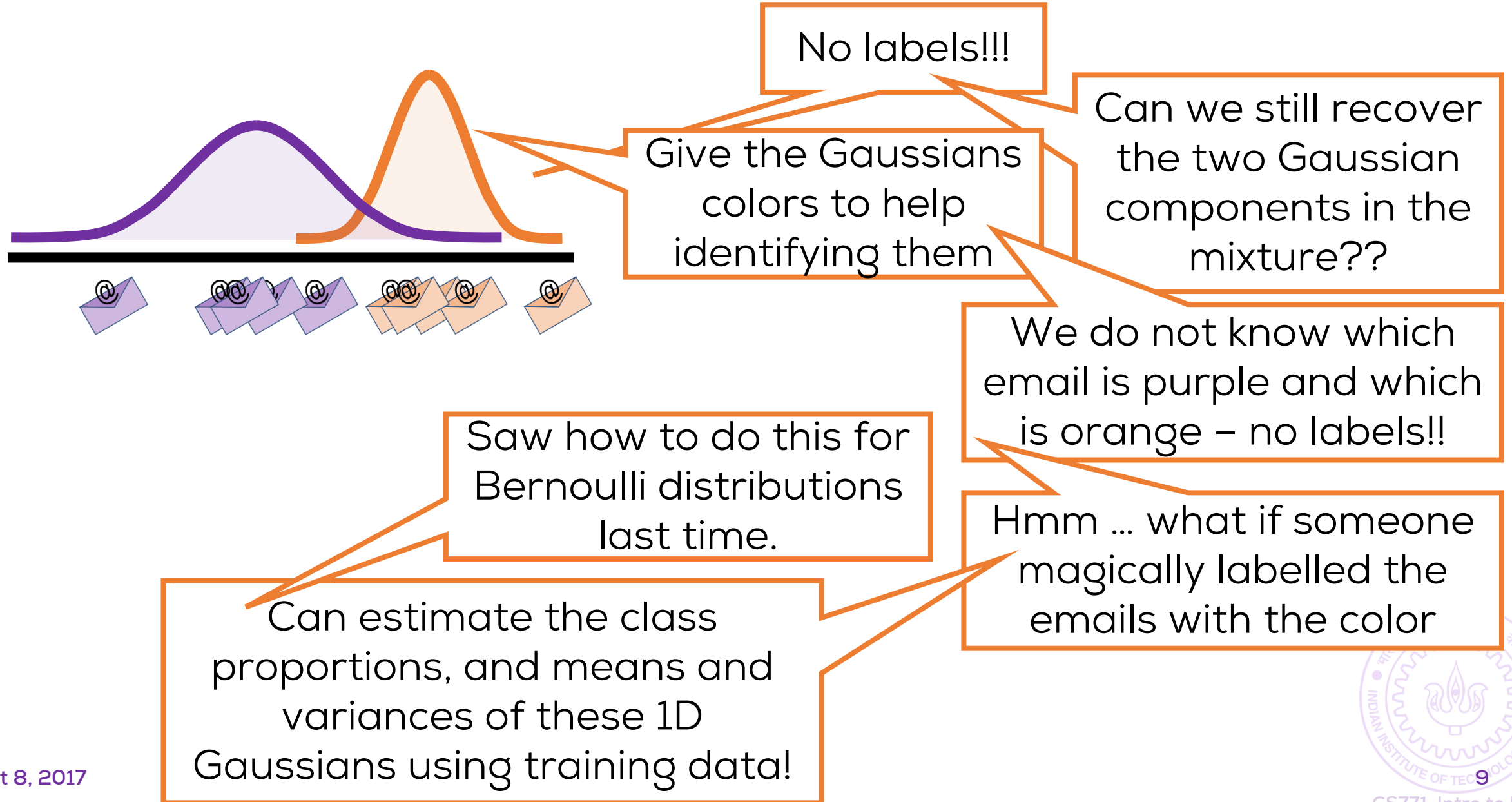
The generative story for unlabelled data??



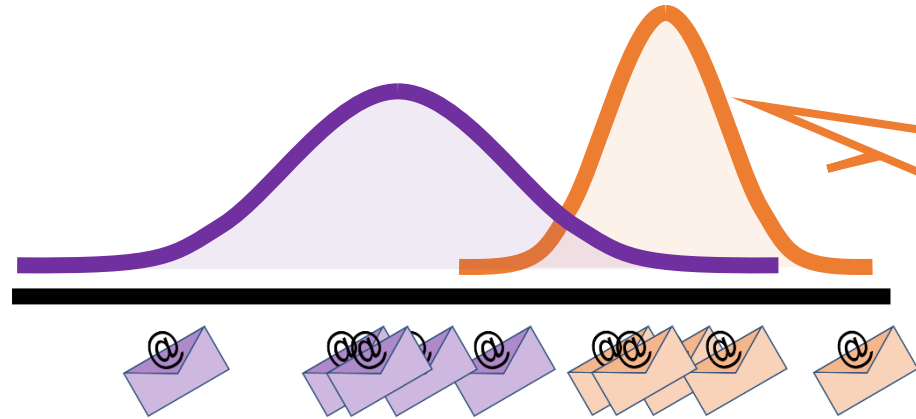
The generative story for unlabelled data??



The generative story for unlabelled data??



The generative story for unlabelled data??



No labels!!!

Give the Gaussians colors to help identifying them

Can we still recover the two Gaussian components in the mixture??

We do not know which email is purple and which is orange – no labels!!

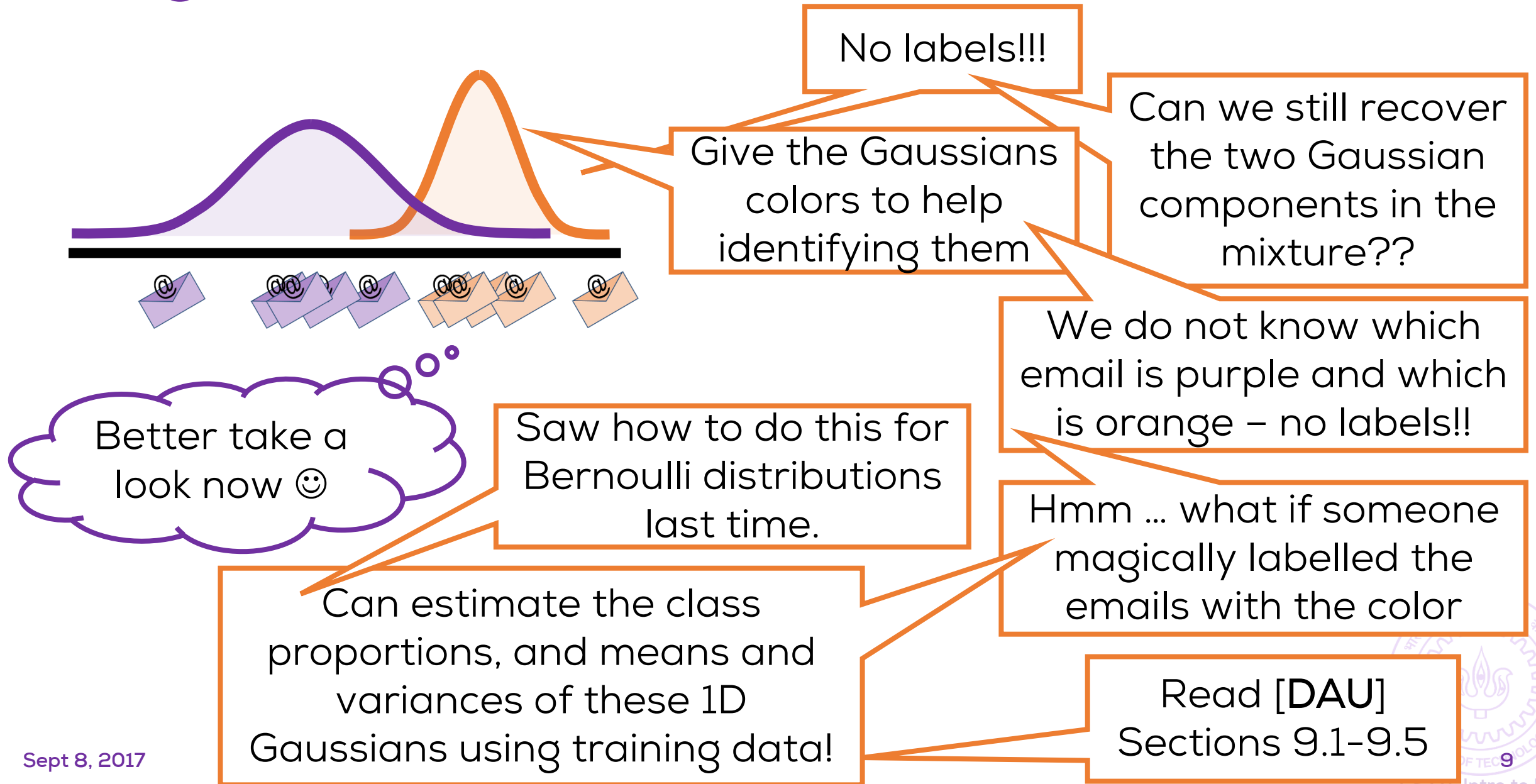
Saw how to do this for Bernoulli distributions last time.

Hmm ... what if someone magically labelled the emails with the color

Can estimate the class proportions, and means and variances of these 1D Gaussians using training data!

Read [DAU] Sections 9.1-9.5

The generative story for unlabelled data??

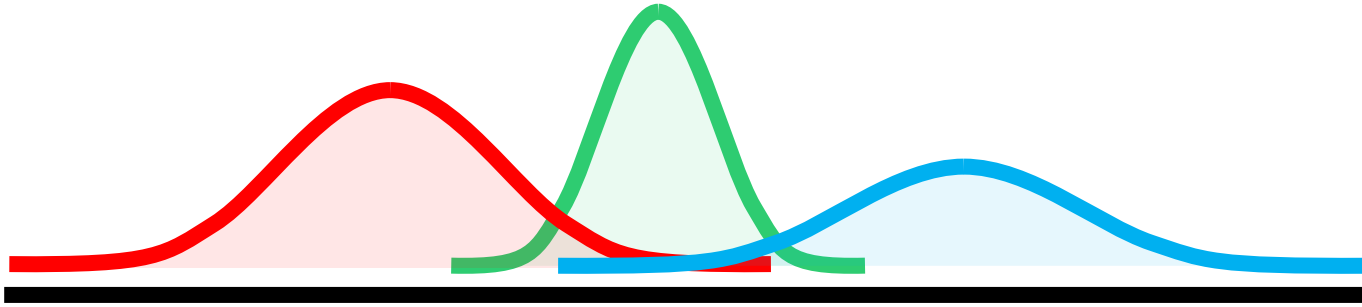


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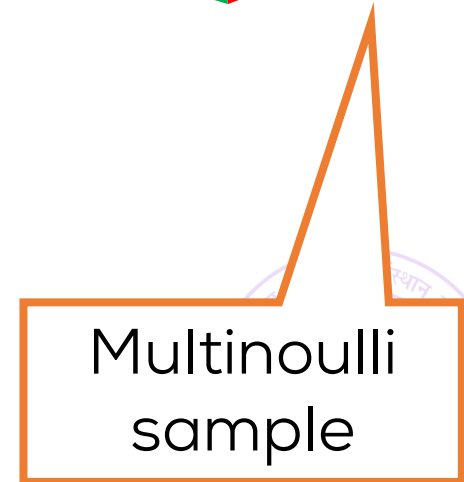
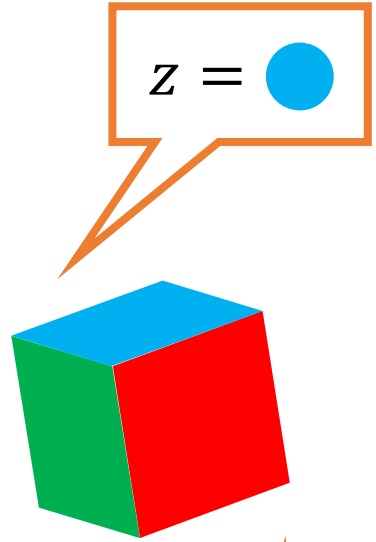
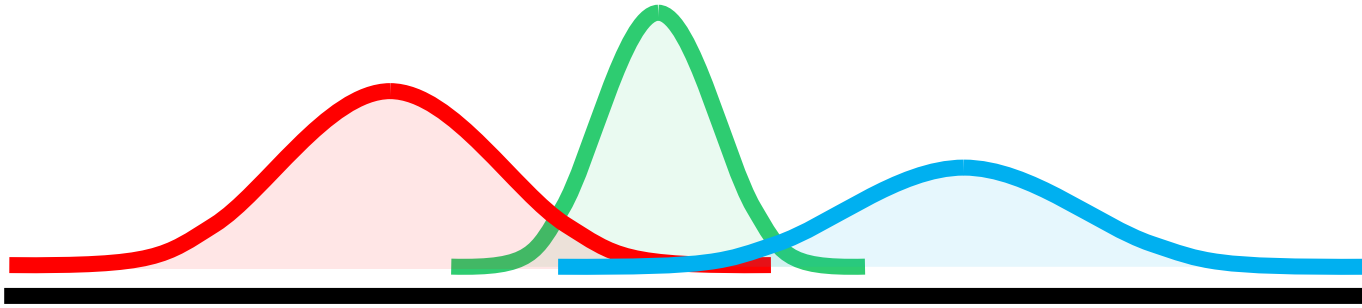
Learning a mixture of Gaussians in presence of labels

The generative story for labelled data

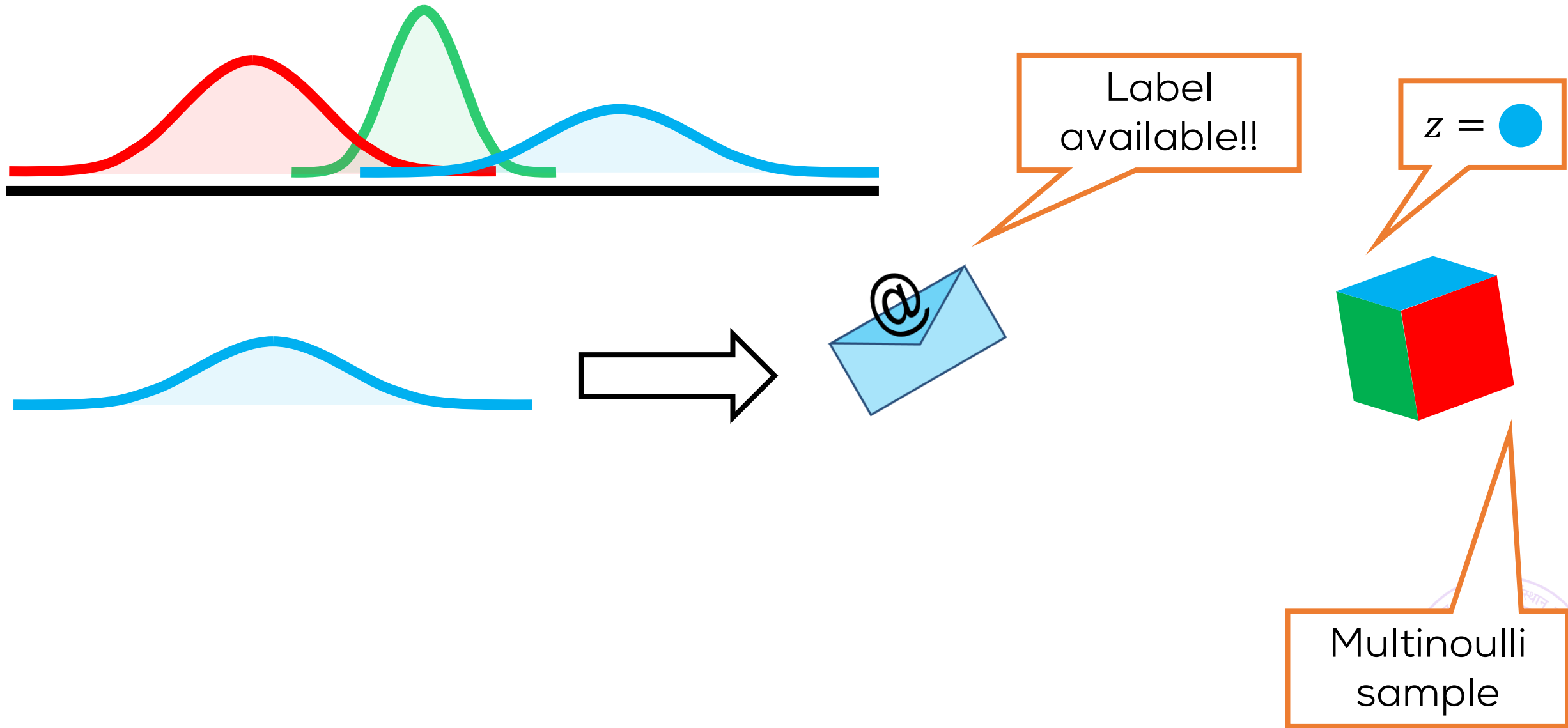
The generative story for labelled data



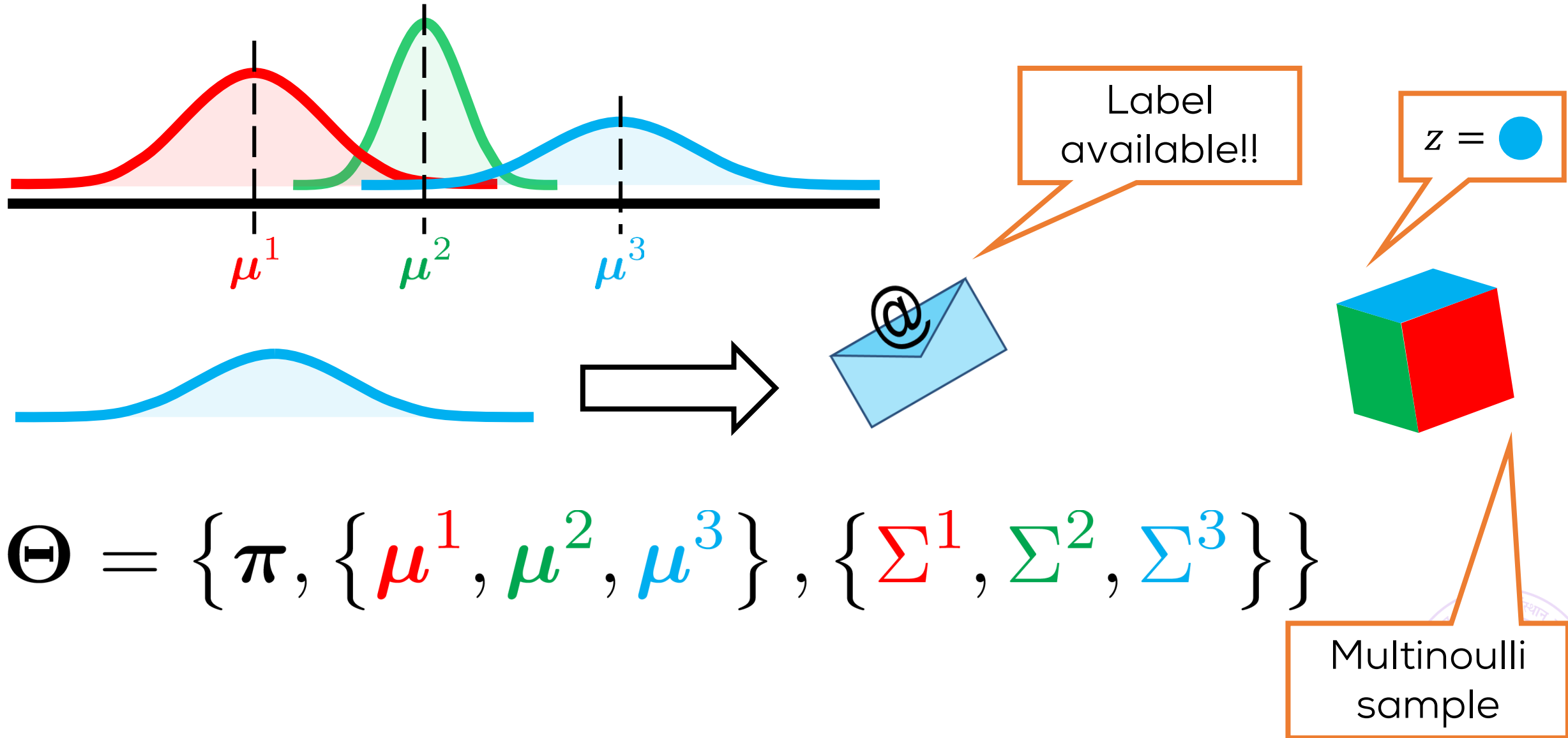
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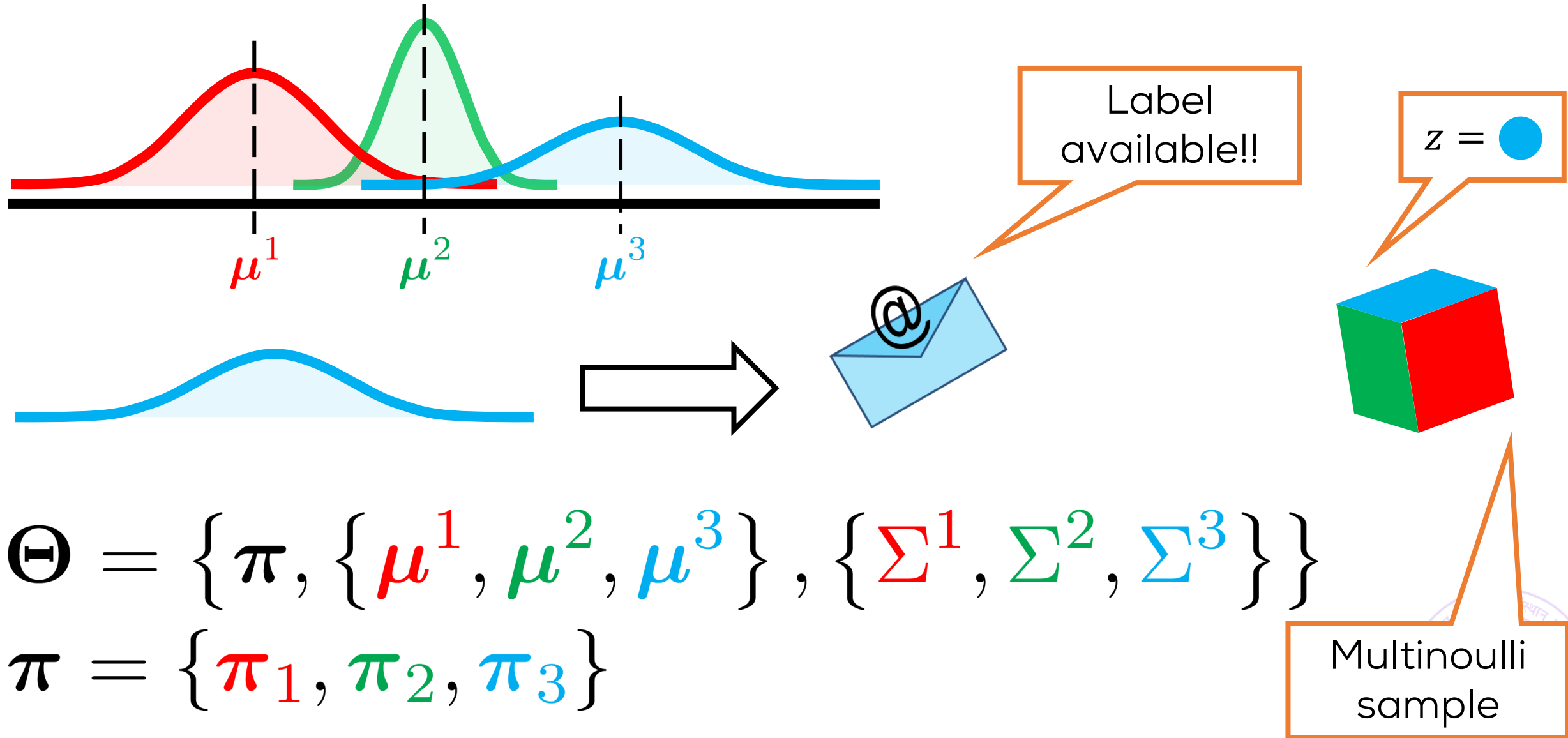
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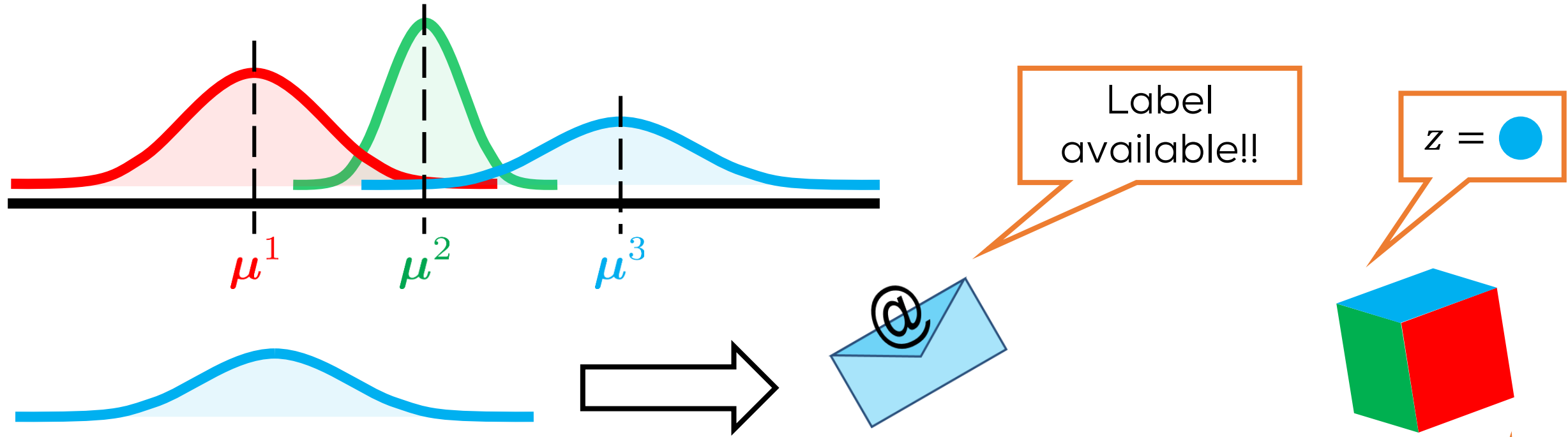
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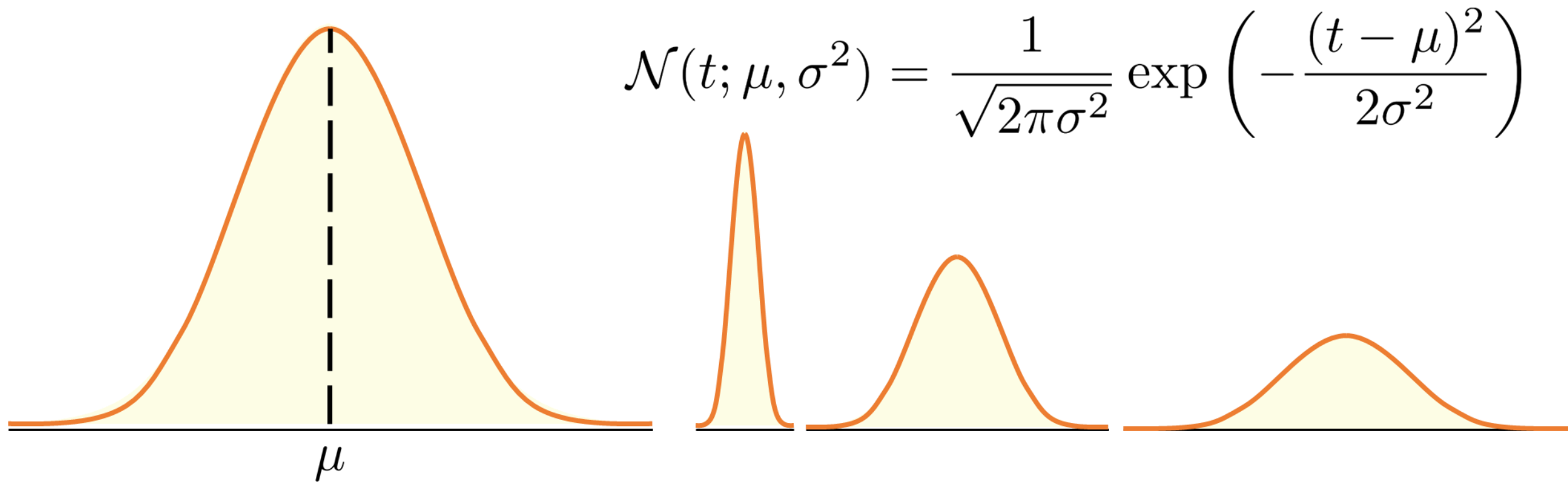
The generative story for labelled data



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

$$\pi = \left\{ \pi_1, \pi_2, \pi_3 \right\} \quad \pi_1 = \mathbb{P} \left[z = \bullet \right]$$

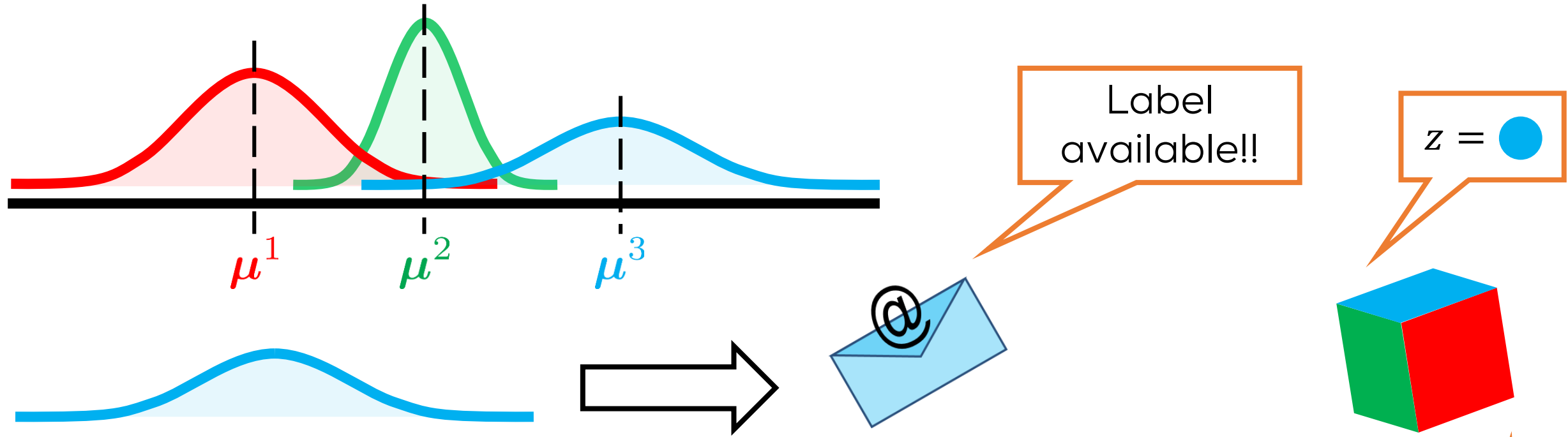
The Gaussian Distribution



Multivariate Gaussian

$$\mathcal{N}(\mathbf{v}; \boldsymbol{\mu}, \Sigma) = \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} \exp\left(-\frac{1}{2}(\mathbf{v} - \boldsymbol{\mu})^\top \Sigma^{-1}(\mathbf{v} - \boldsymbol{\mu})\right)$$

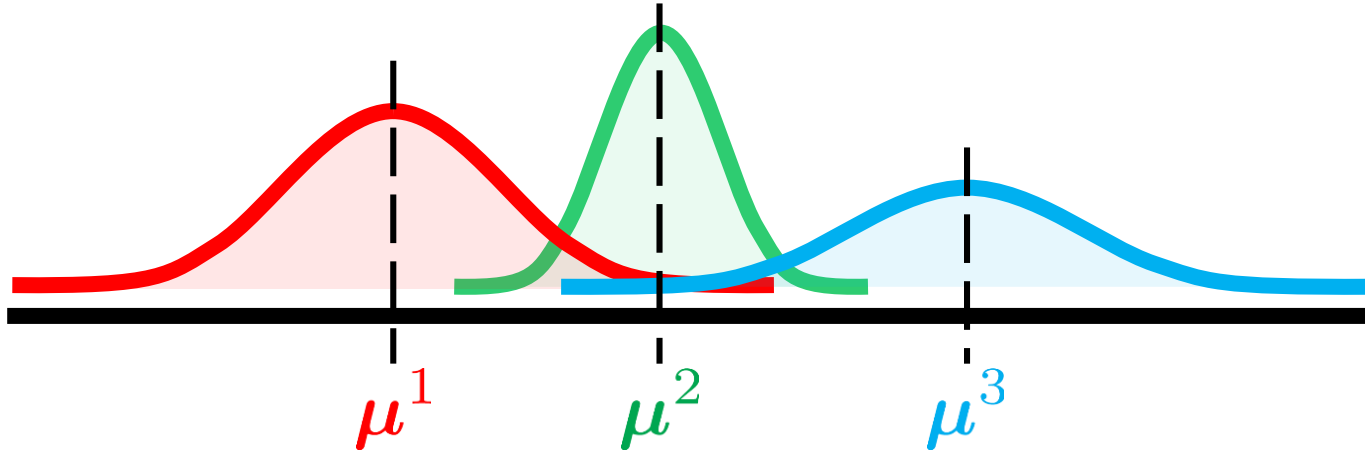
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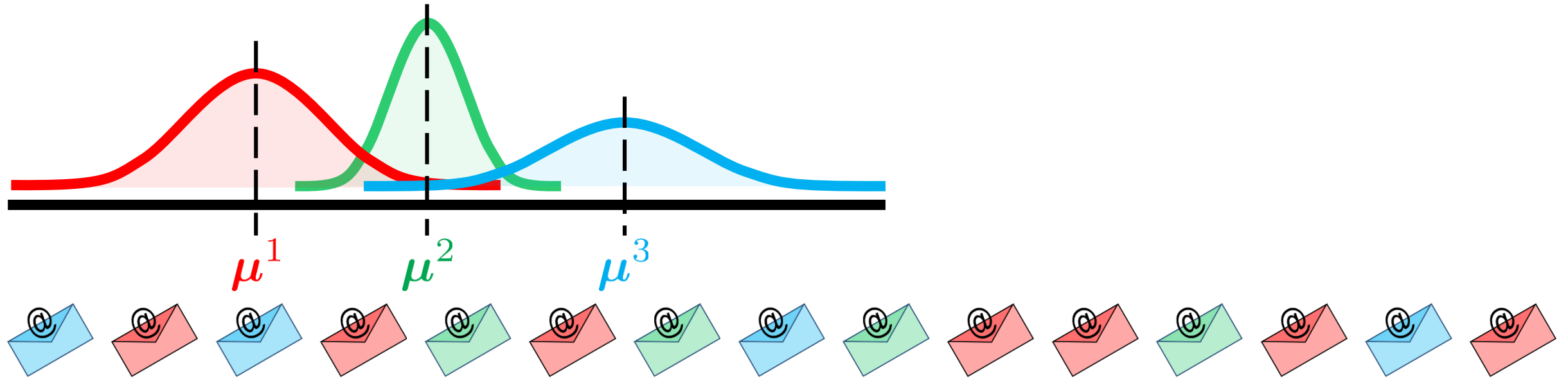
$$\Theta = \left\{ \pi, \left\{ \mu^1, \mu^2, \mu^3 \right\}, \left\{ \Sigma^1, \Sigma^2, \Sigma^3 \right\} \right\}$$

$$\pi = \left\{ \pi_1, \pi_2, \pi_3 \right\} \quad \pi_1 = \mathbb{P} \left[z = \bullet \right]$$

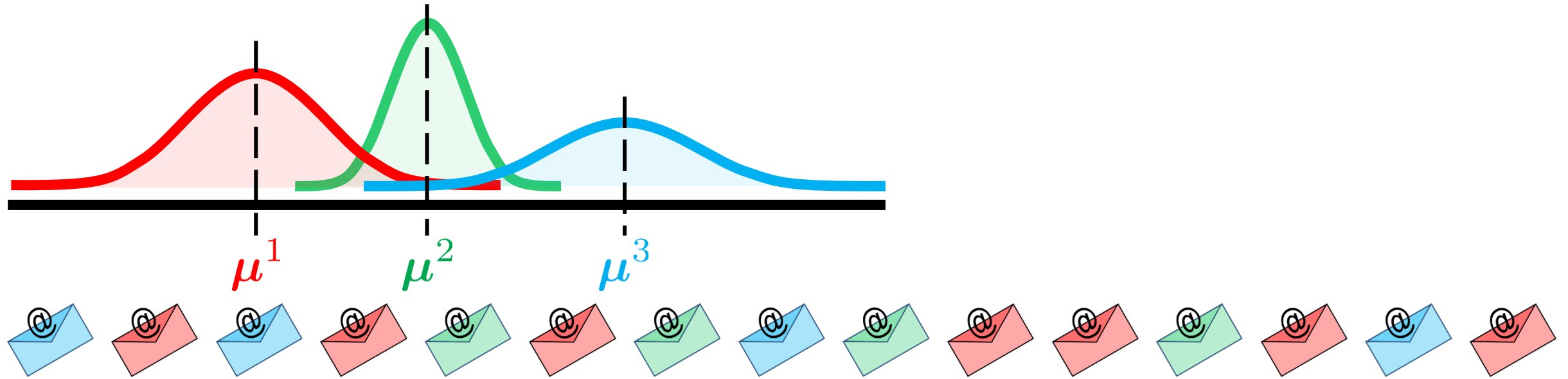
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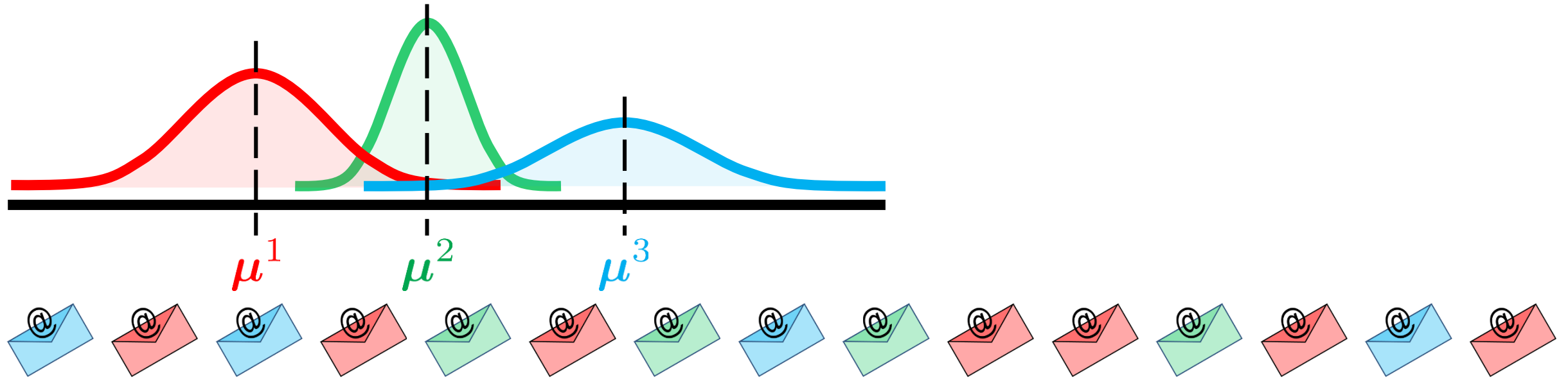


The generative story for labelled data



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

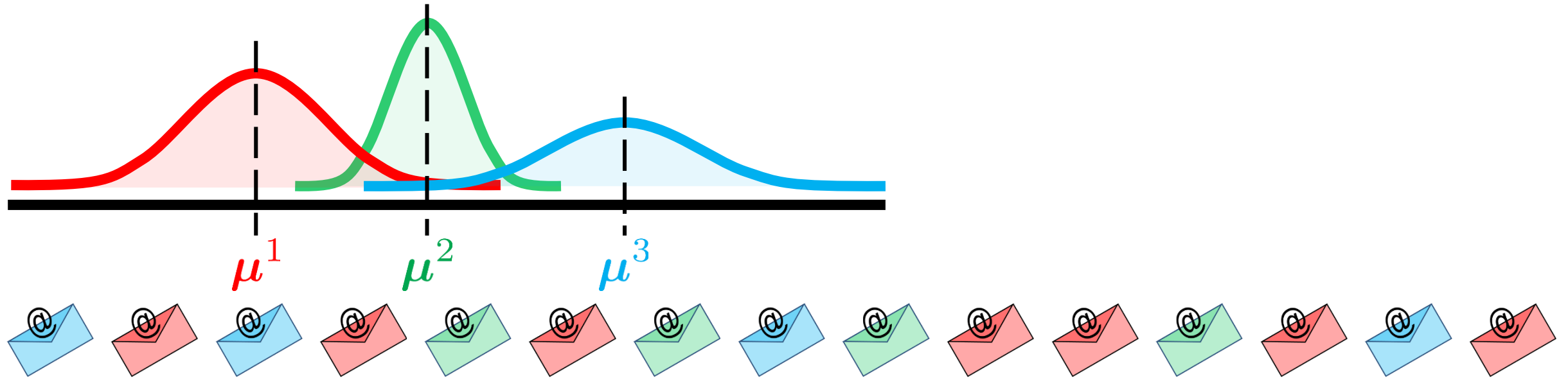
The generative story for labelled data



$$\mathbb{P}[\mathbf{x}^i, z^i \mid \Theta] = \mathbb{P}[z^i \mid \Theta] \cdot \mathbb{P}[\mathbf{x}^i \mid z^i, \Theta] = \pi_{z^i} \cdot \mathcal{N}(\mathbf{x}^i \mid \mu^{z^i}, \Sigma^{z^i})$$

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

The generative story for labelled data

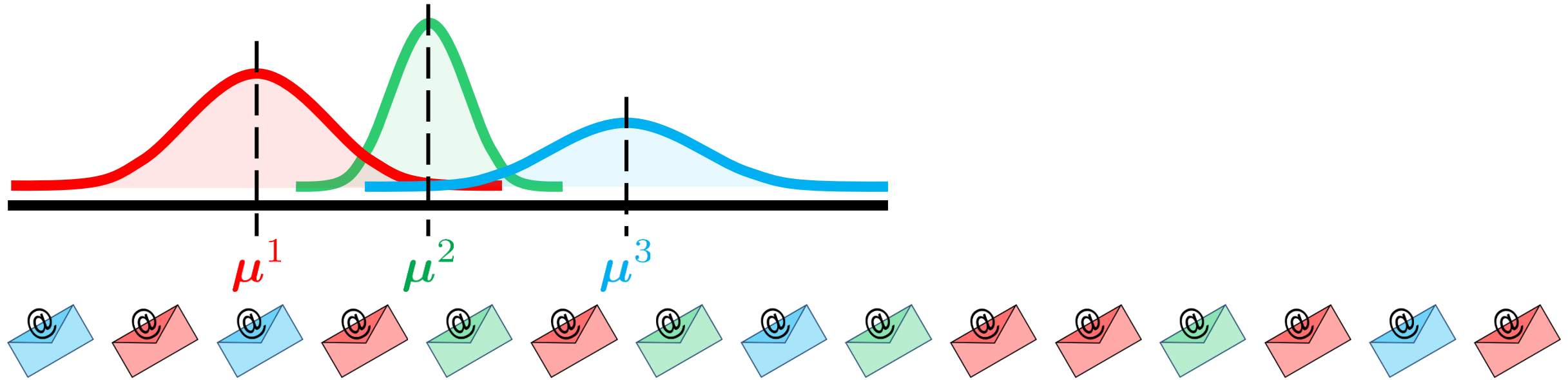


$$\mathbb{P}[\mathbf{x}^i, z^i \mid \Theta] = \mathbb{P}[z^i \mid \Theta] \cdot \mathbb{P}[\mathbf{x}^i \mid z^i, \Theta] = \pi_{z^i} \cdot \mathcal{N}(\mathbf{x}^i \mid \mu^{z^i}, \Sigma^{z^i})$$

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

The generative story for labelled data



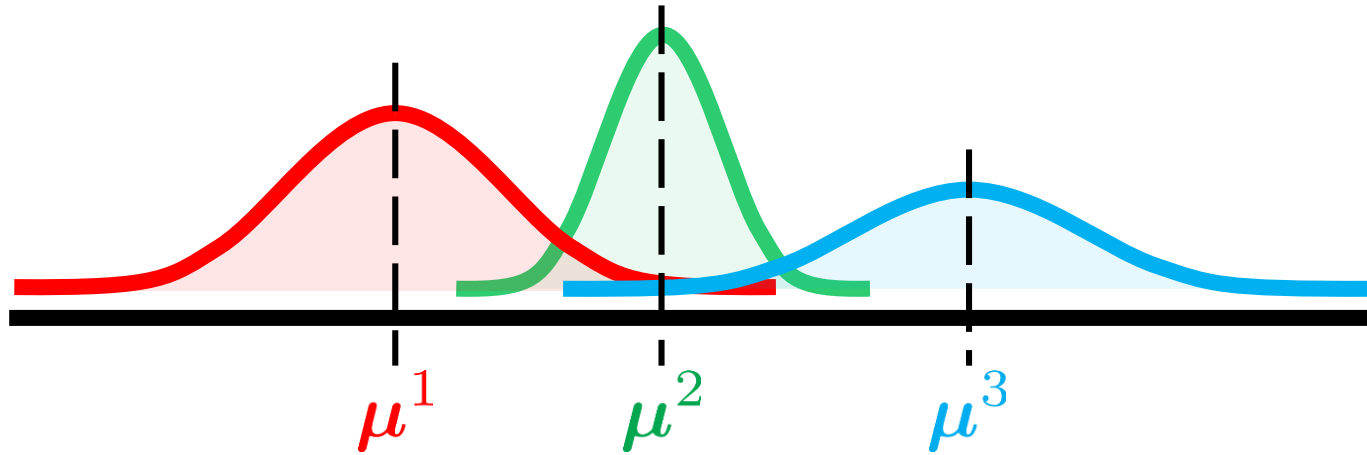
$$\mathbb{P}[\mathbf{x}^i, z^i | \Theta] = \mathbb{P}[z^i | \Theta] \cdot \mathbb{P}[\mathbf{x}^i | z^i, \Theta] = \pi_{z^i} \cdot \mathcal{N}(\mathbf{x}^i | \mu^{z^i}, \Sigma^{z^i})$$

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

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

Take log and apply 1st
order optimality

The generative story for labelled data



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

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

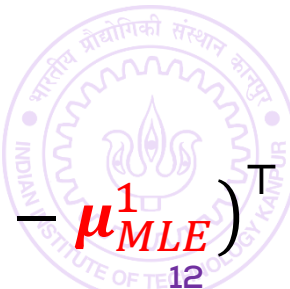
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Take log and apply 1st order optimality

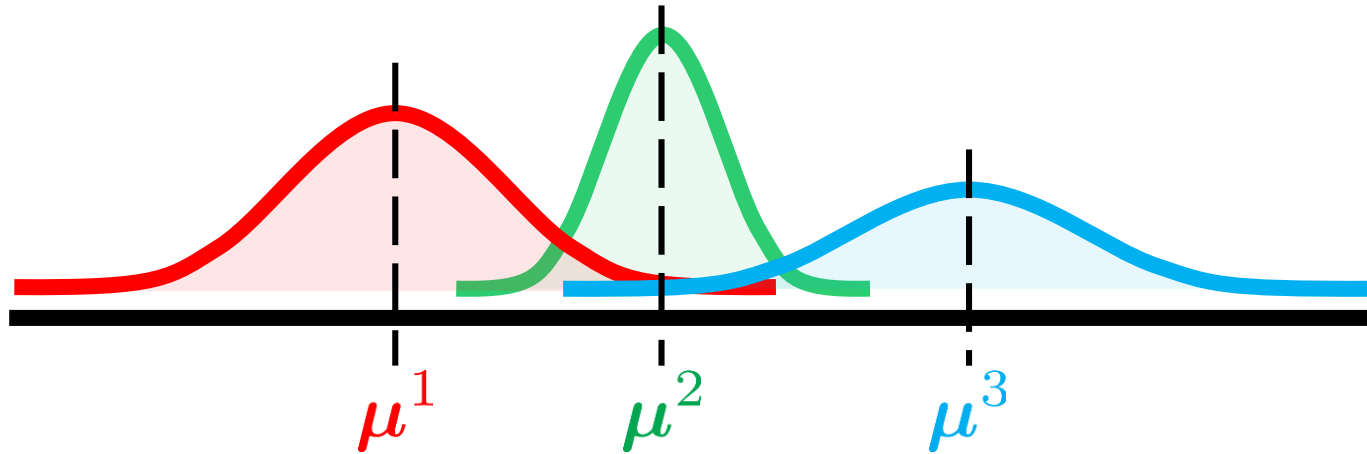
$$\pi_1^{\text{MLE}} = \frac{\# \text{ red emails}}{\# \text{ total emails}} = \frac{n_r}{n}$$

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

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



The generative story for labelled data



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

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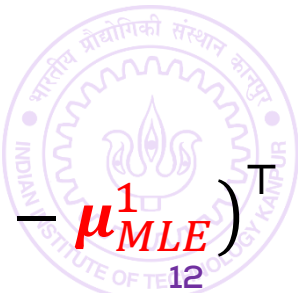
Take log and apply 1st order optimality

Read [DAU]
Sections 9.1-9.5

$$\pi_1^{\text{MLE}} = \frac{\# \text{ red emails}}{\# \text{ total emails}} = \frac{n_r}{n}$$

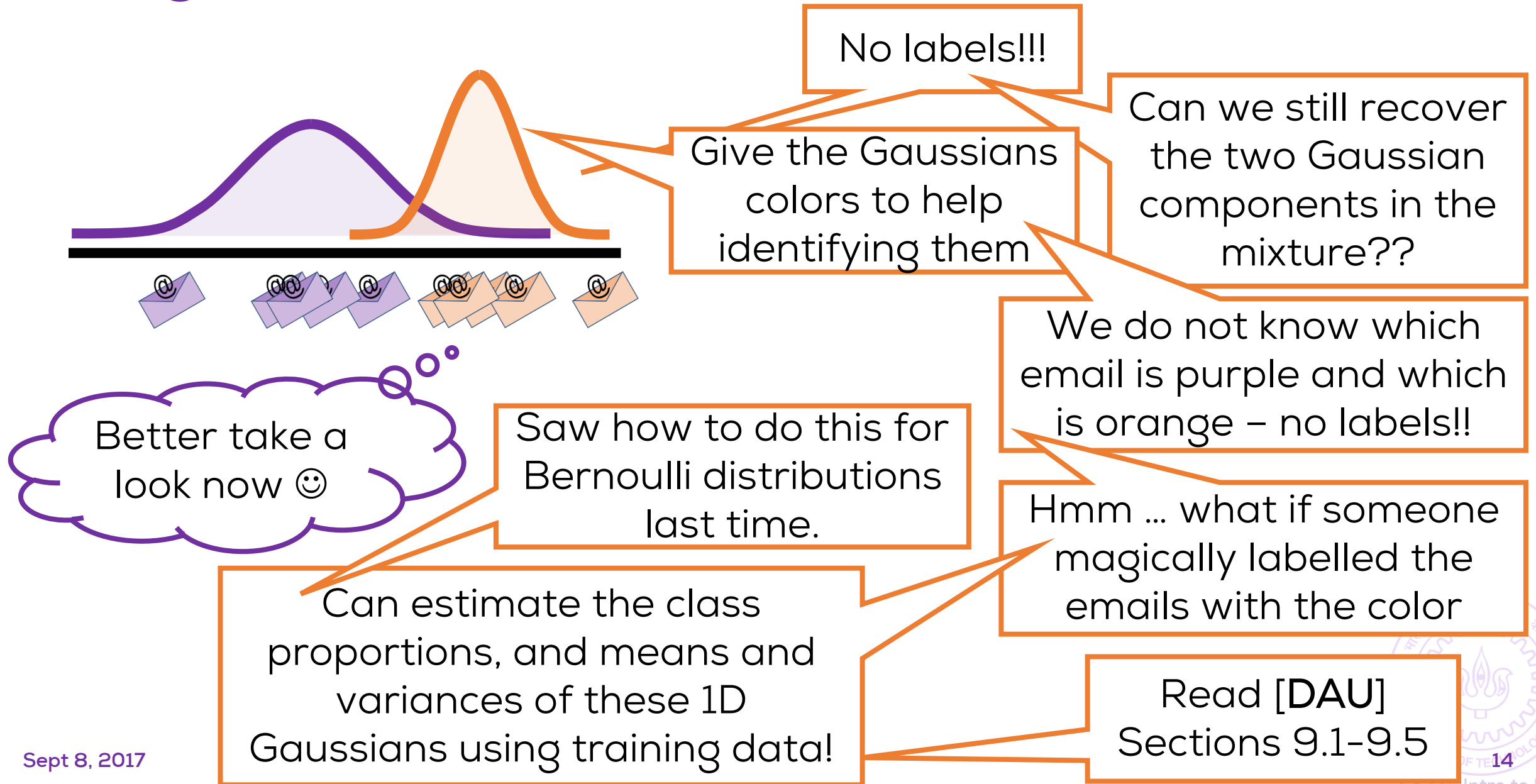
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</detour>

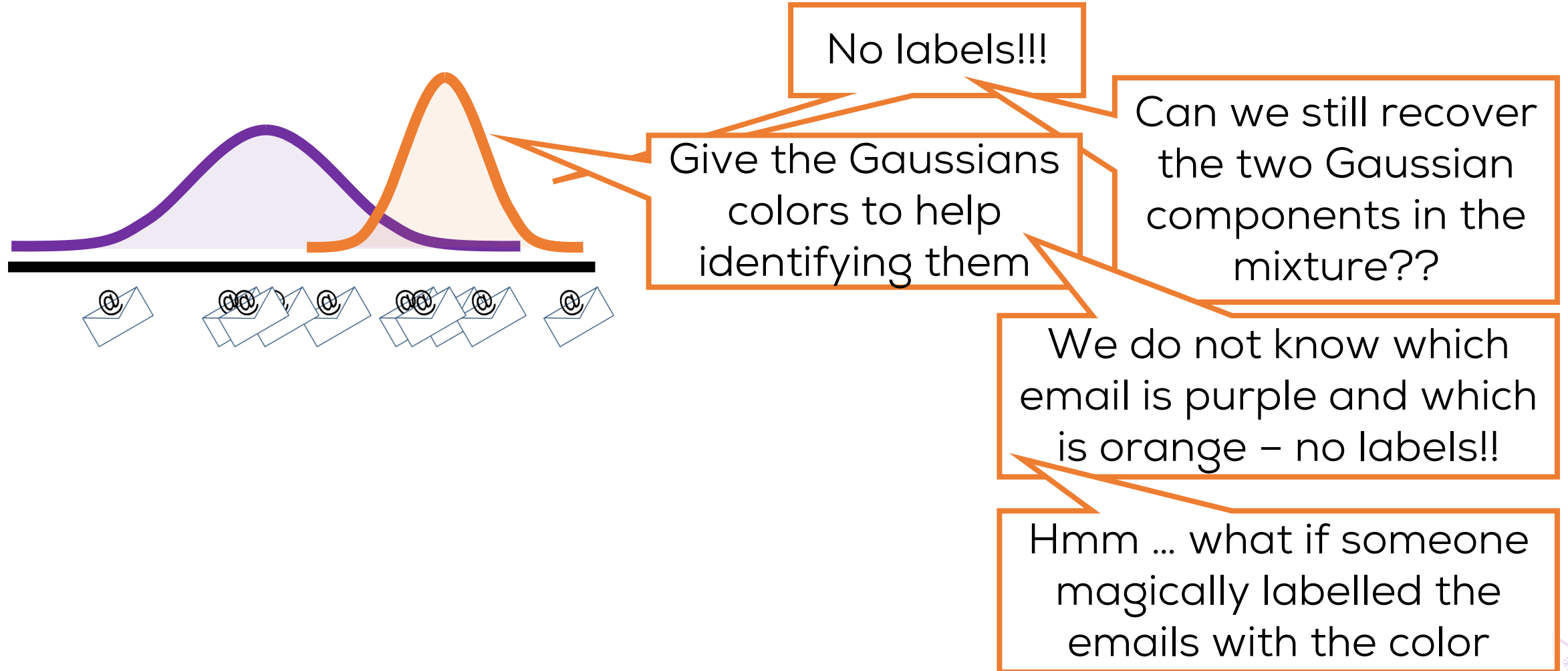
The generative story for unlabelled data??



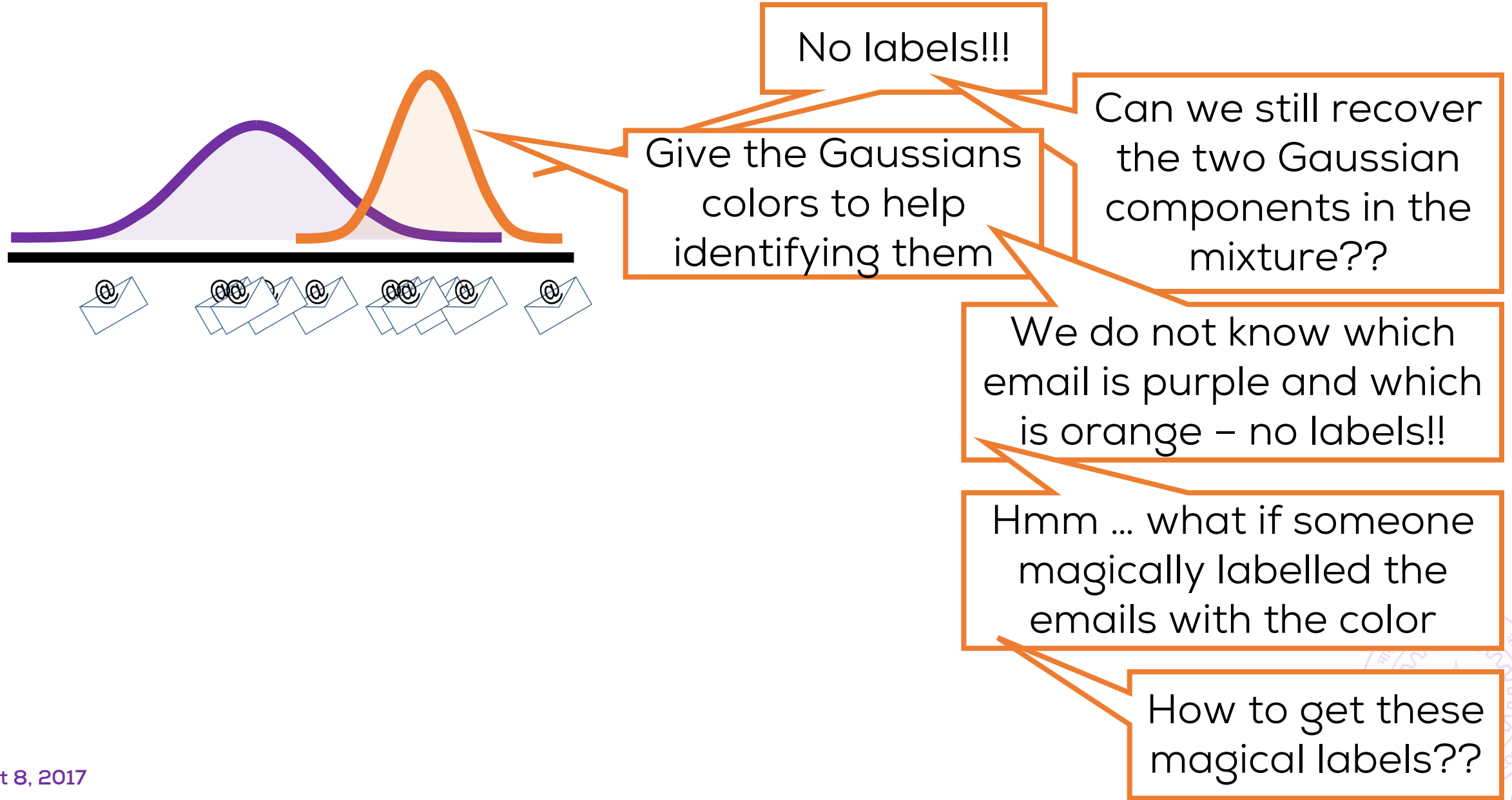
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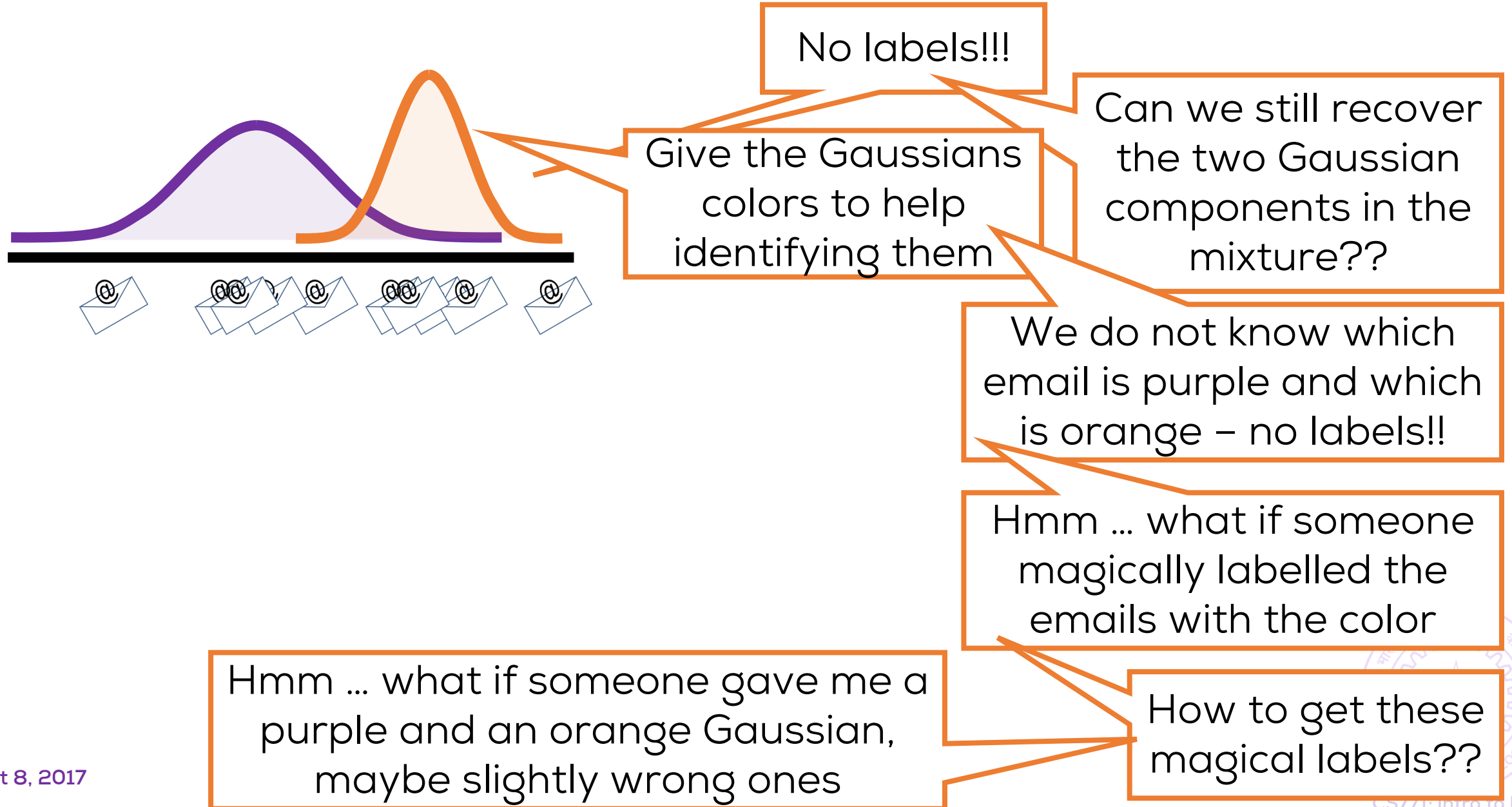
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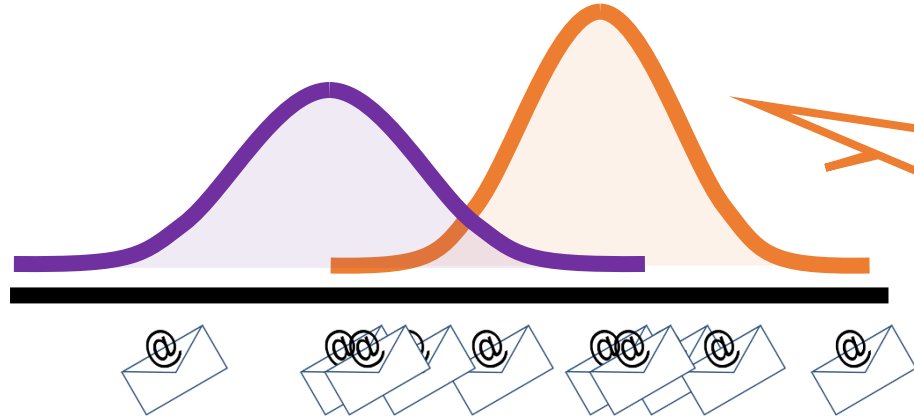
The generative story for unlabelled data??



The generative story for unlabelled data??



The generative story for unlabelled data??



No labels!!!

Give the Gaussians colors to help identifying them

Can we still recover the two Gaussian components in the mixture??

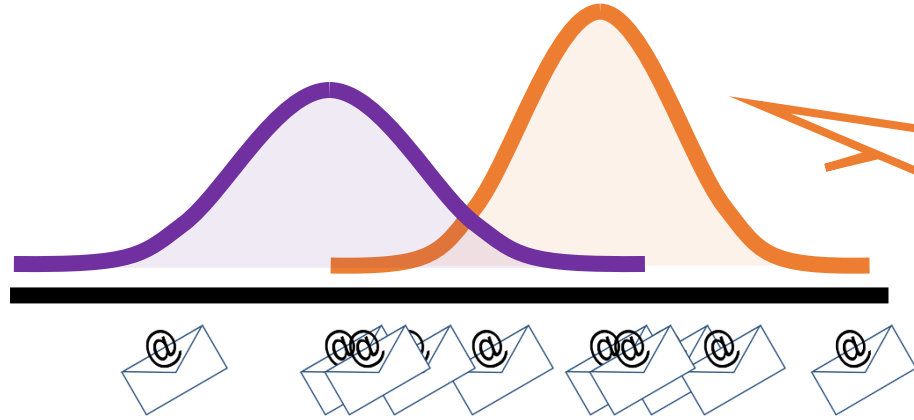
We do not know which email is purple and which is orange – no labels!!

Hmm ... what if someone magically labelled the emails with the color

Hmm ... what if someone gave me a purple and an orange Gaussian, maybe slightly wrong ones

How to get these magical labels??

The generative story for unlabelled data??



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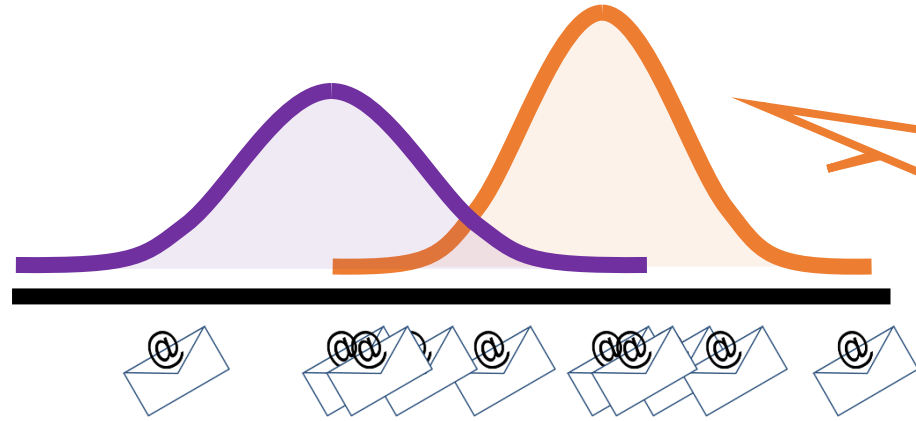
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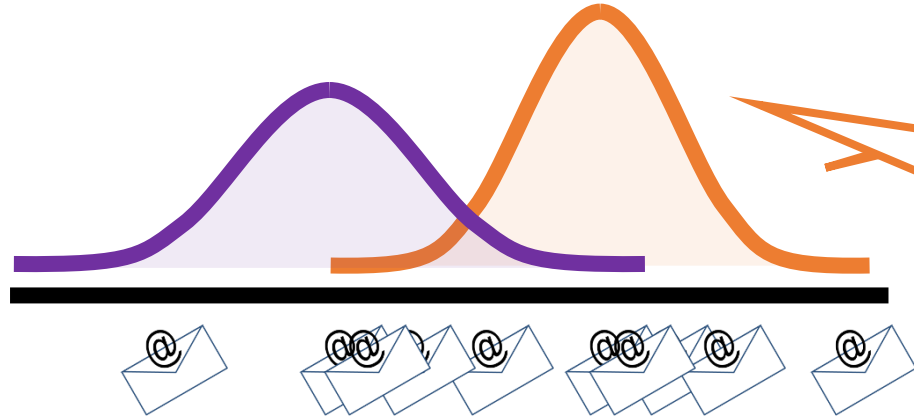
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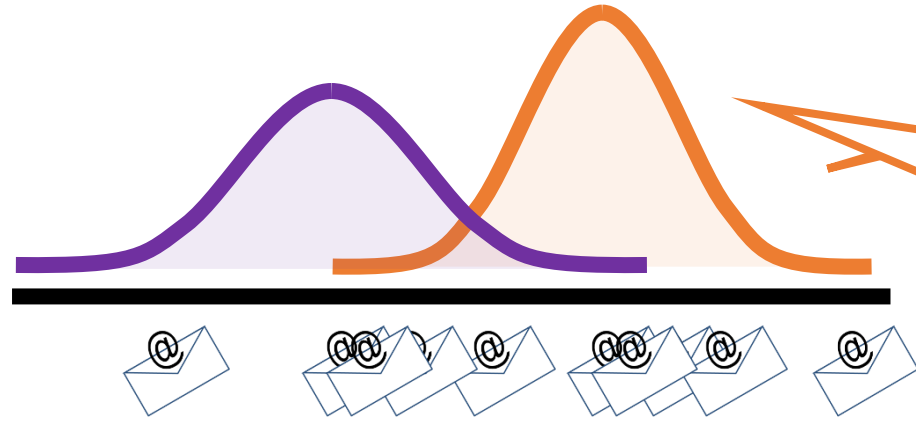
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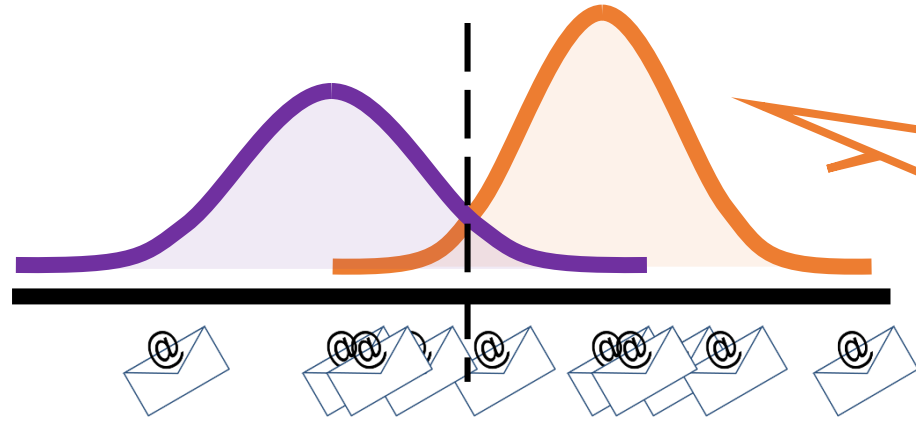
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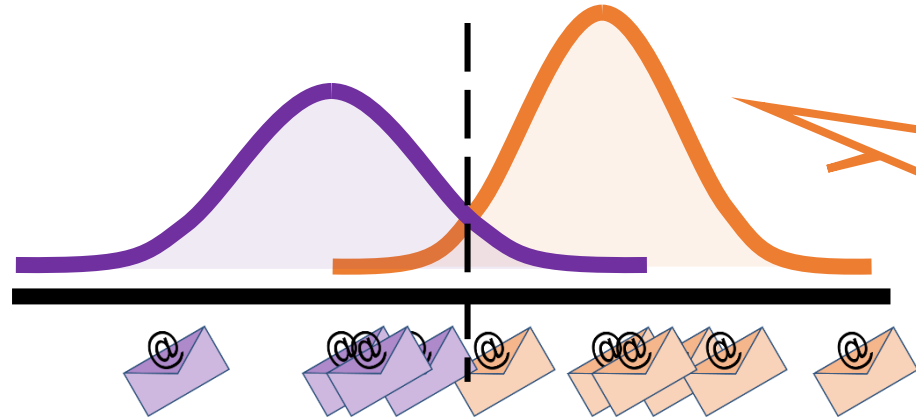
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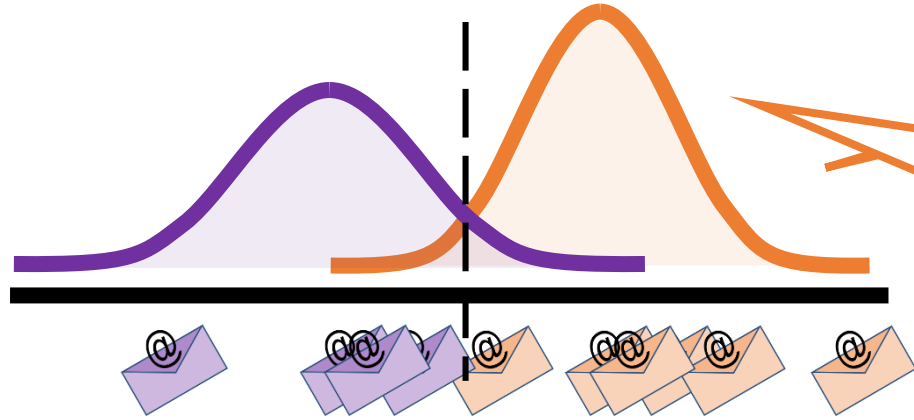
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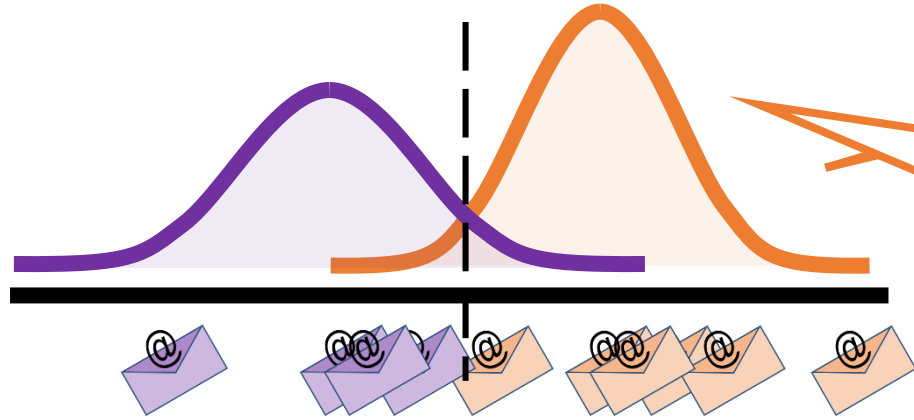
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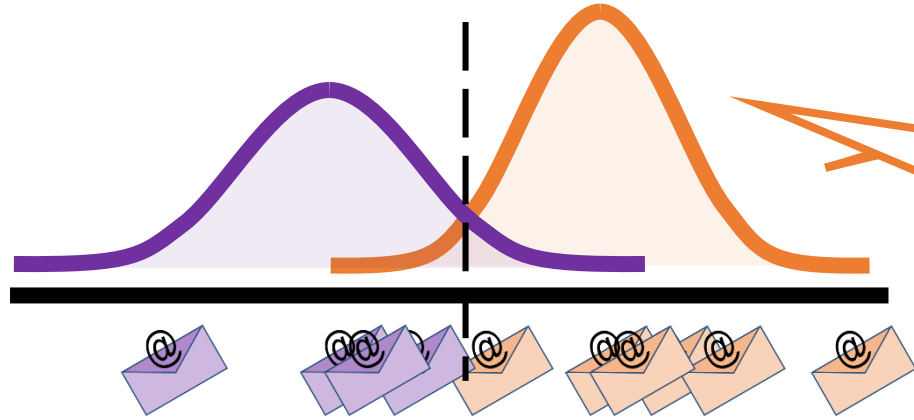
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The generative story for unlabelled data??



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Won't I just learn the wrong ones that generated the labels?

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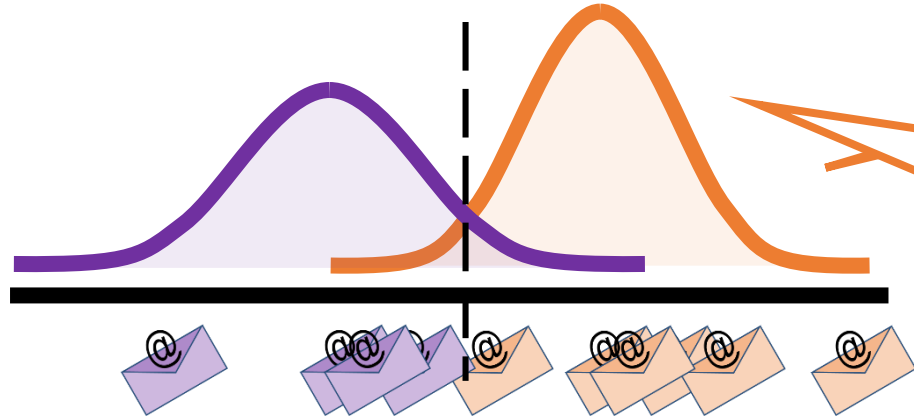
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The generative story for unlabelled data??



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Can we still recover the two Gaussian components in the mixture??

In practice: you will learn slightly "less wrong" ones ☺

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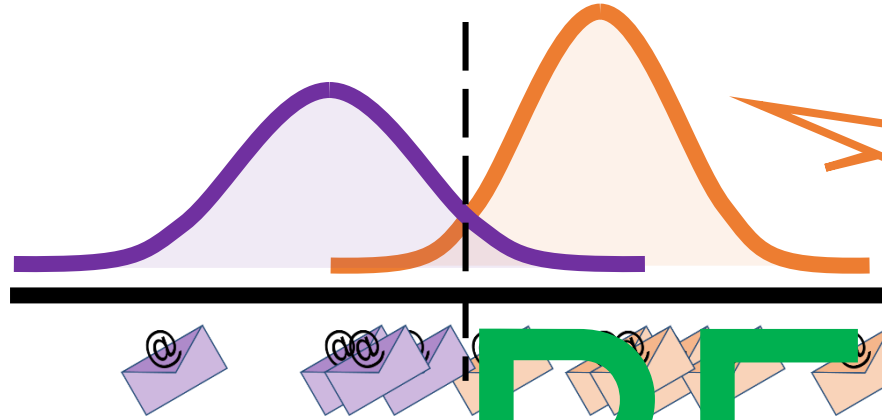
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The generative story for unlabelled data??



No labels!!!

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In practice: you will learn slightly "less wrong" ones ☺

Would it just learn the wrong ones that generated the labels?

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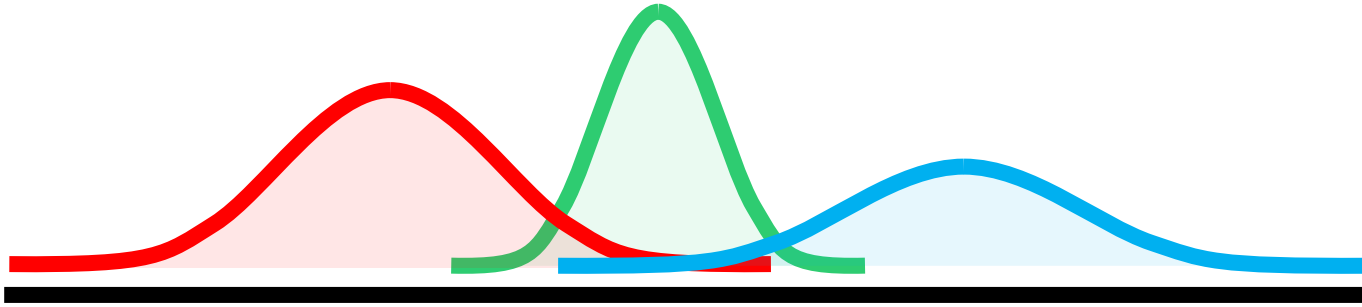
Hmm ... what if someone magically labelled the emails with the color

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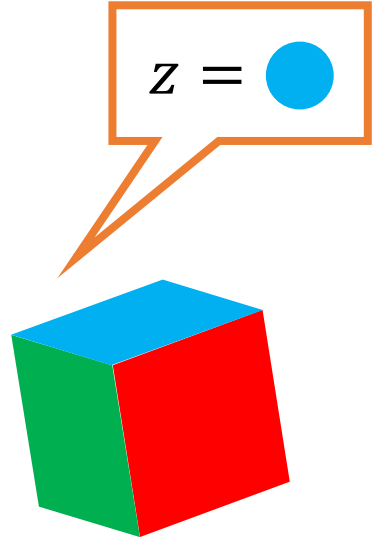
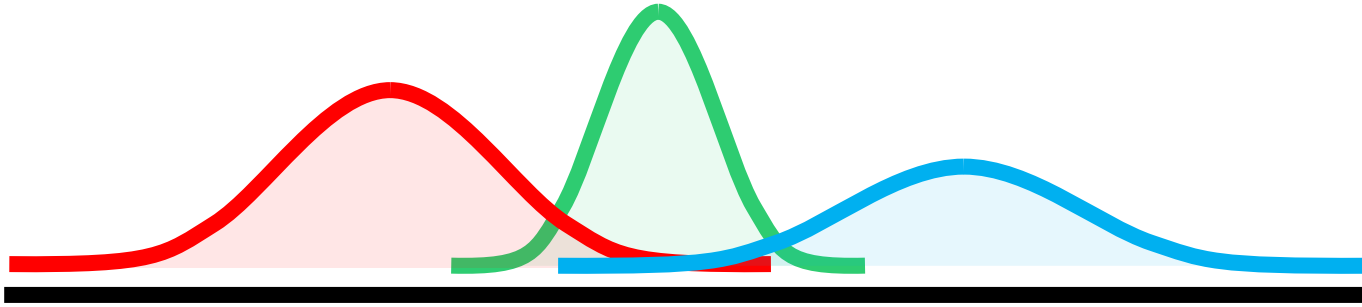
How to get these magical labels??

The generative story for unlabelled data

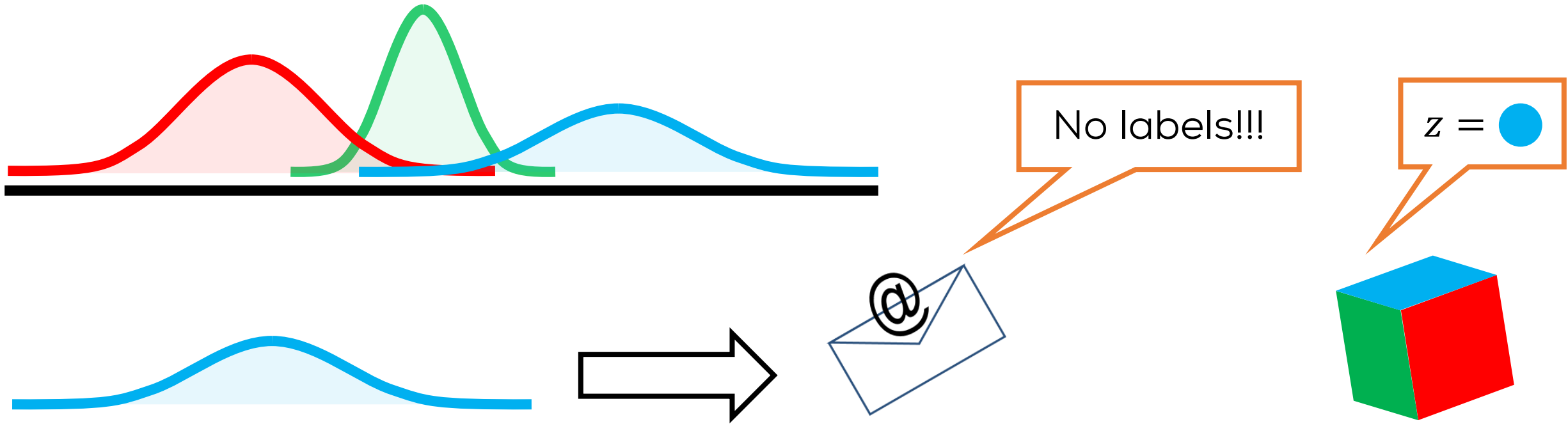
The generative story for unlabelled data



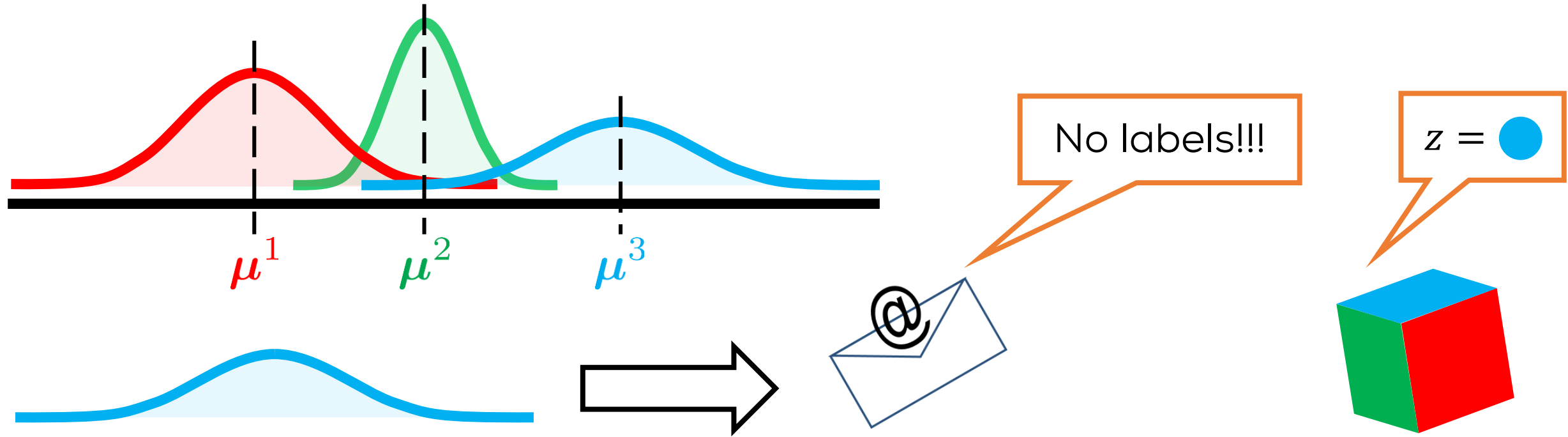
The generative story for unlabelled data



The generative story for unlabelled data

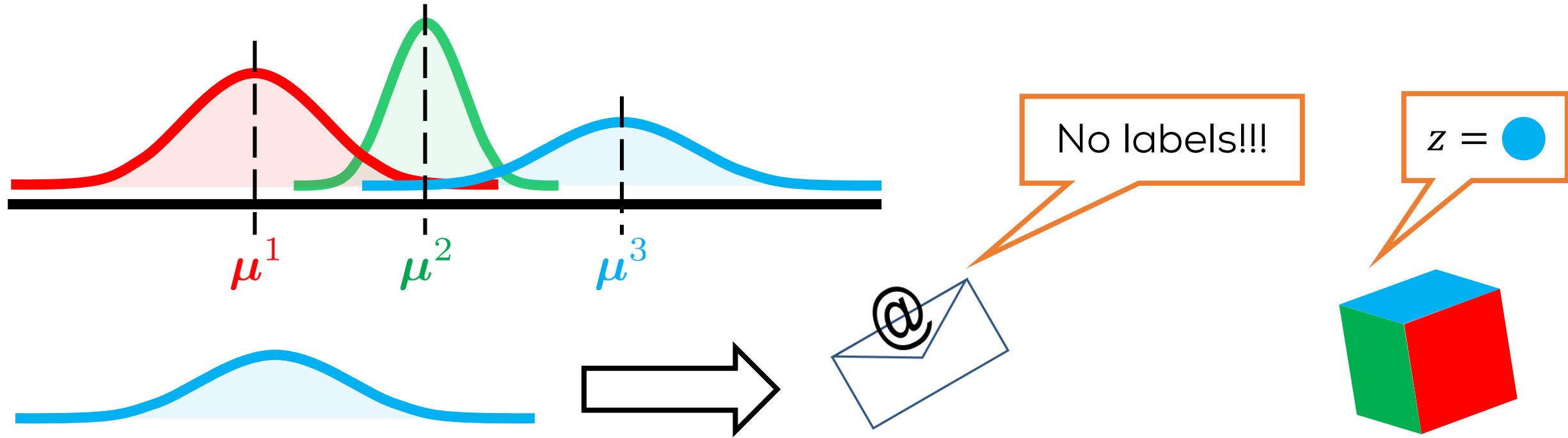


The generative story for unlabelled data



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

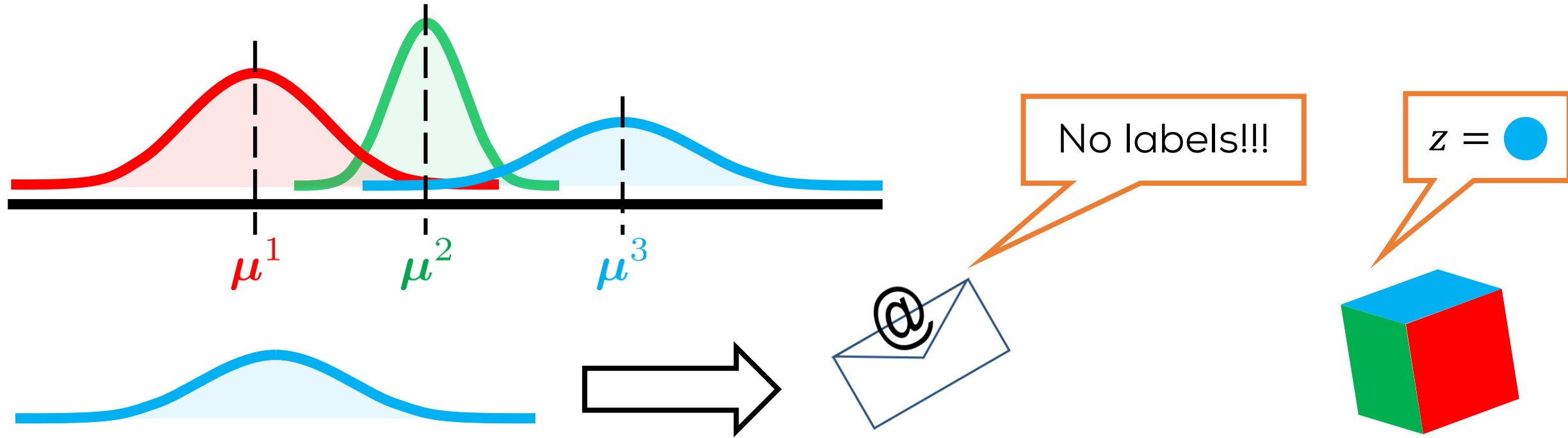
The generative story for unlabelled data



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$$\pi = \left\{ \pi_1, \pi_2, \pi_3 \right\}$$

The generative story for unlabelled data

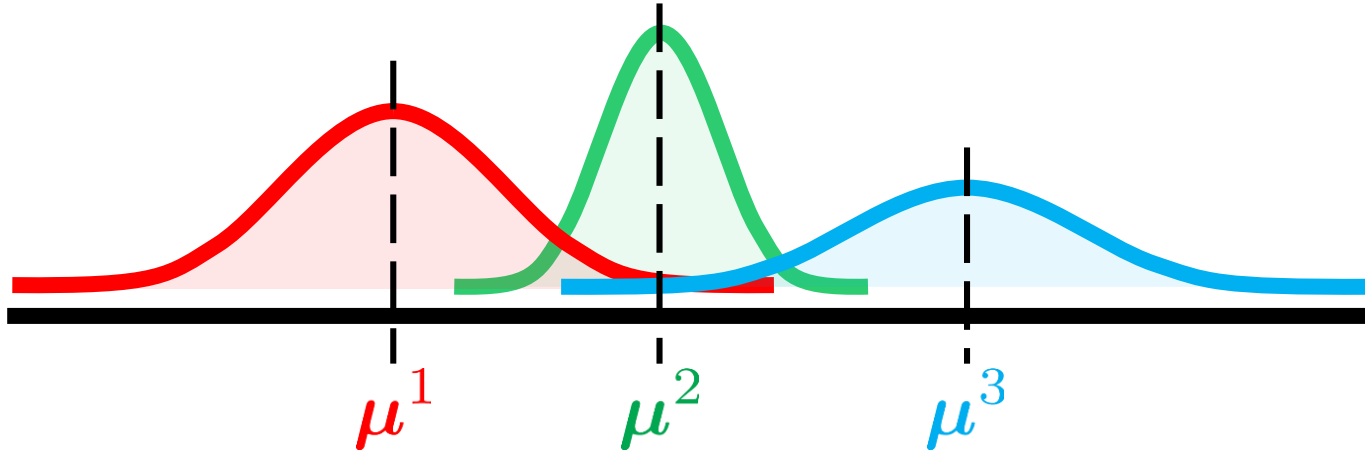


$$\Theta = \left\{ \pi, \left\{ \mu^1, \mu^2, \mu^3 \right\}, \left\{ \Sigma^1, \Sigma^2, \Sigma^3 \right\} \right\}$$

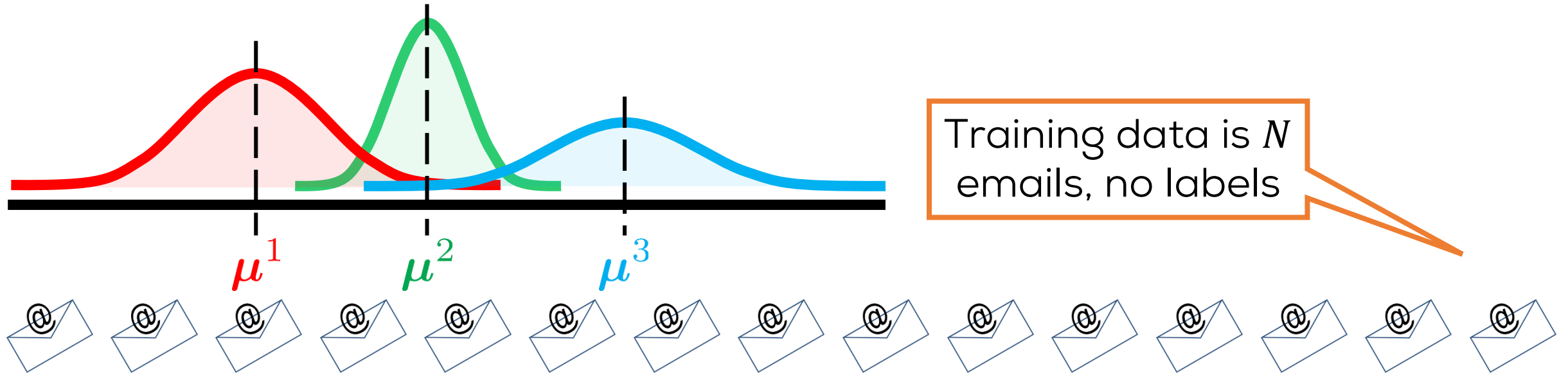
$$\pi = \left\{ \pi_1, \pi_2, \pi_3 \right\} \quad \pi_1 = \mathbb{P} \left[z = \bullet \right]$$

Just as before!

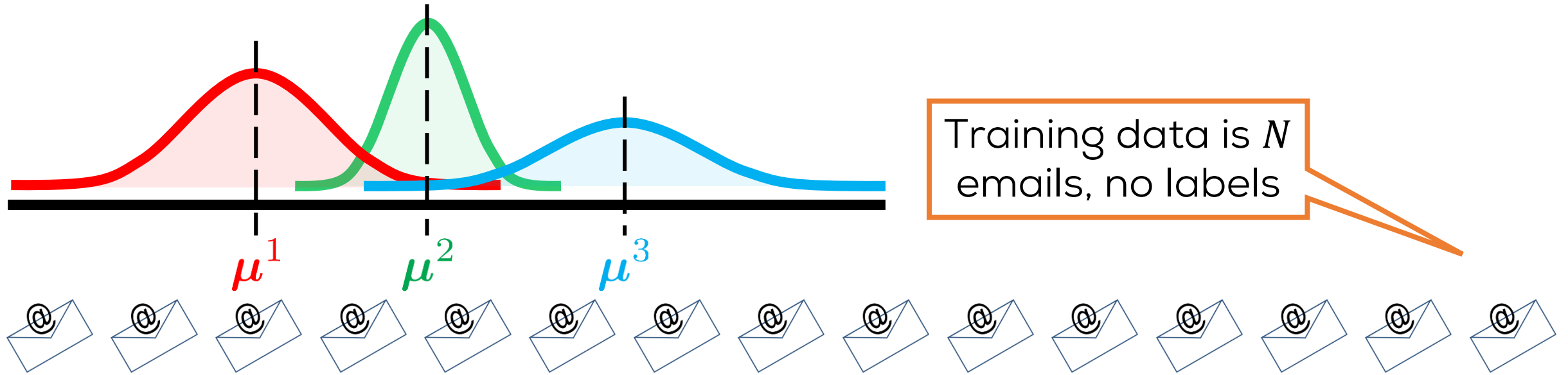
The generative story for unlabelled data



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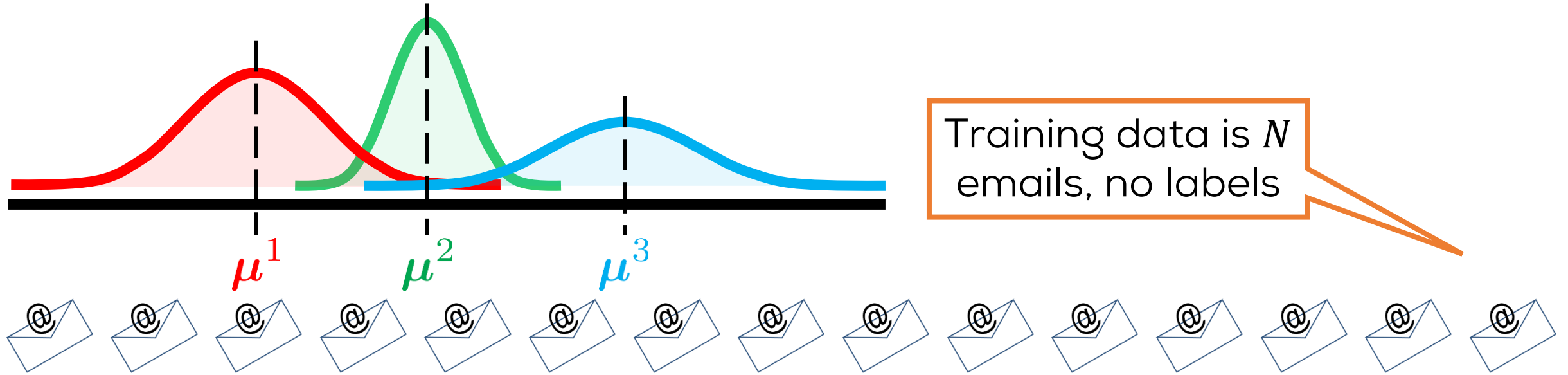


The generative story for unlabelled data



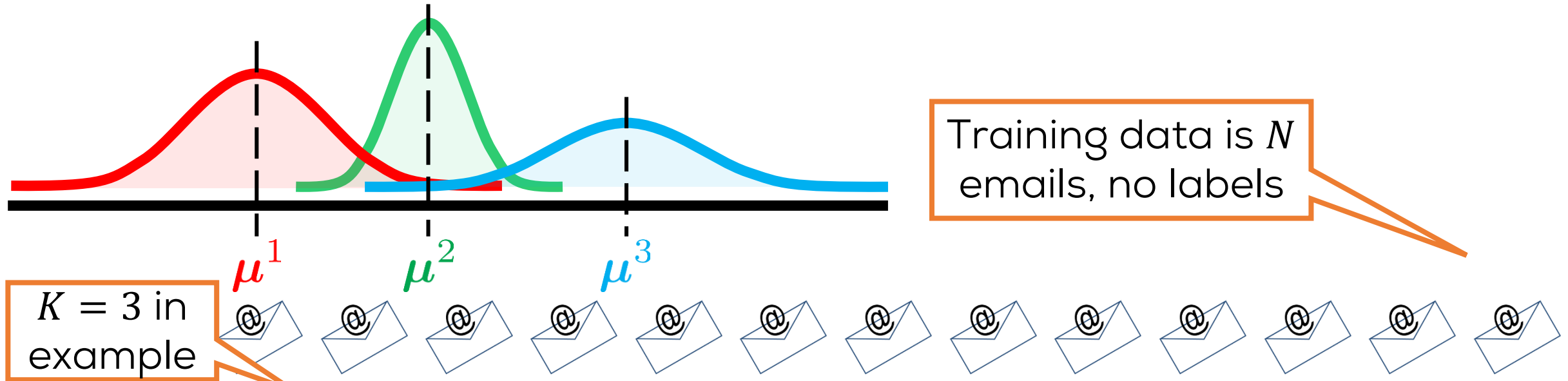
$$\mathbb{P} [\mathbf{x}^i \mid \Theta]$$

The generative story for unlabelled data



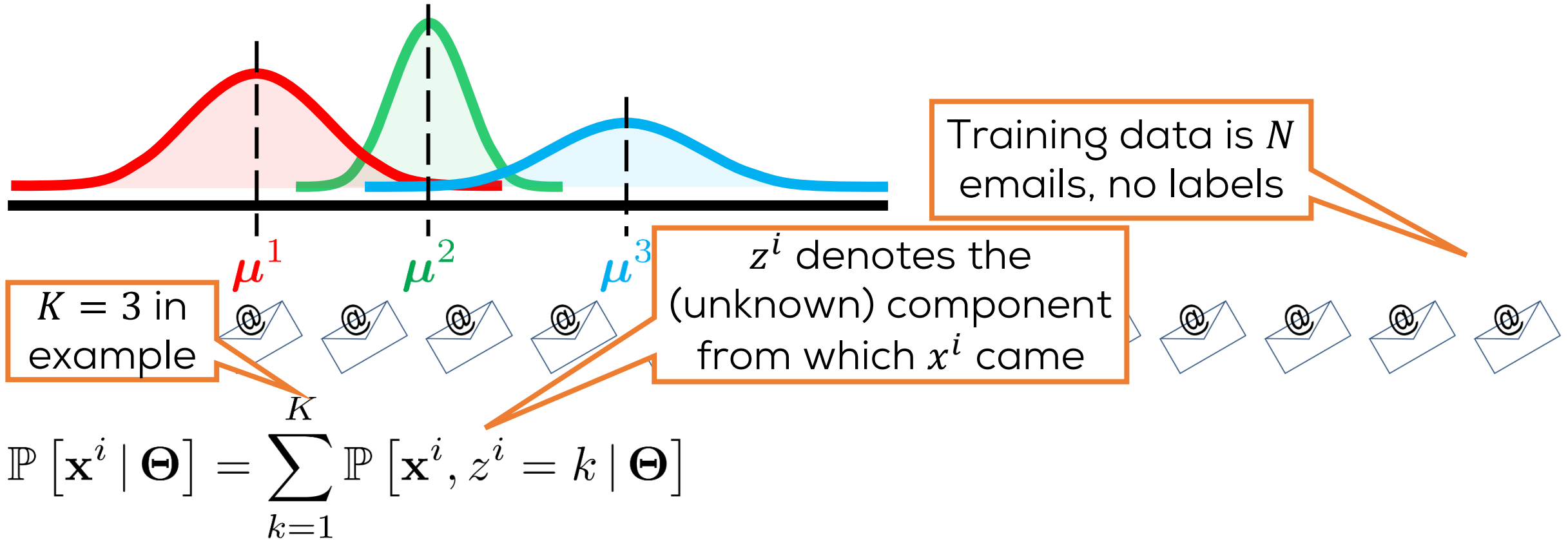
$$\mathbb{P} [\mathbf{x}^i \mid \Theta] = \sum_{k=1}^K \mathbb{P} [\mathbf{x}^i, z^i = k \mid \Theta]$$

The generative story for unlabelled data

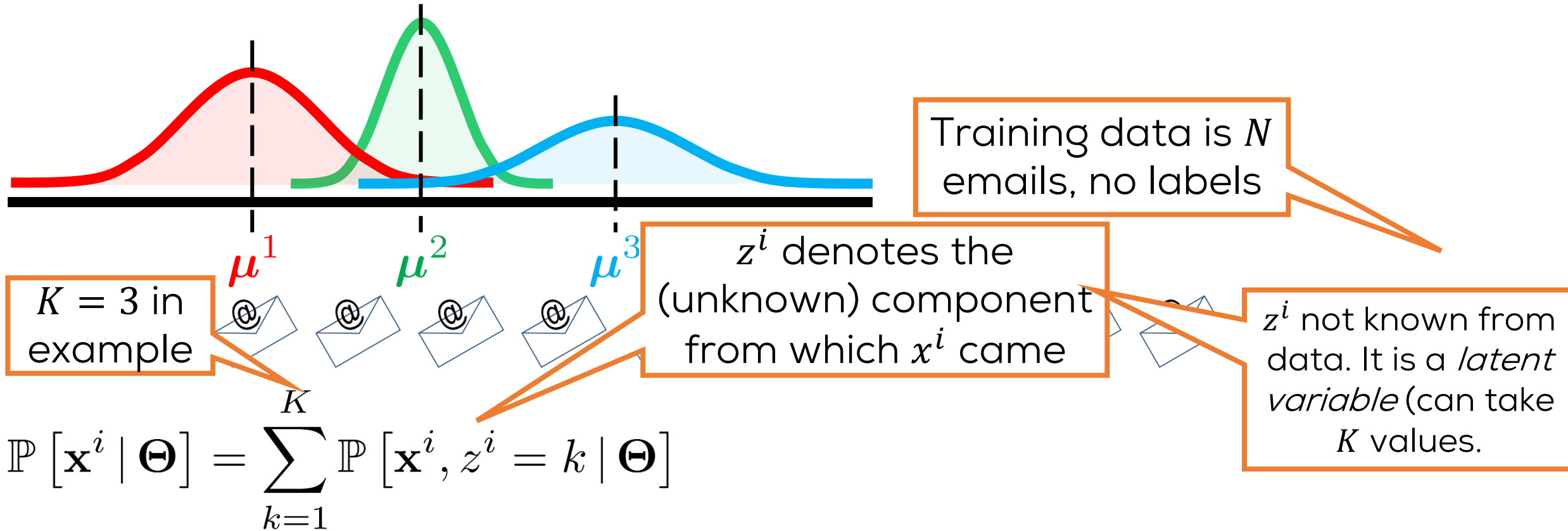


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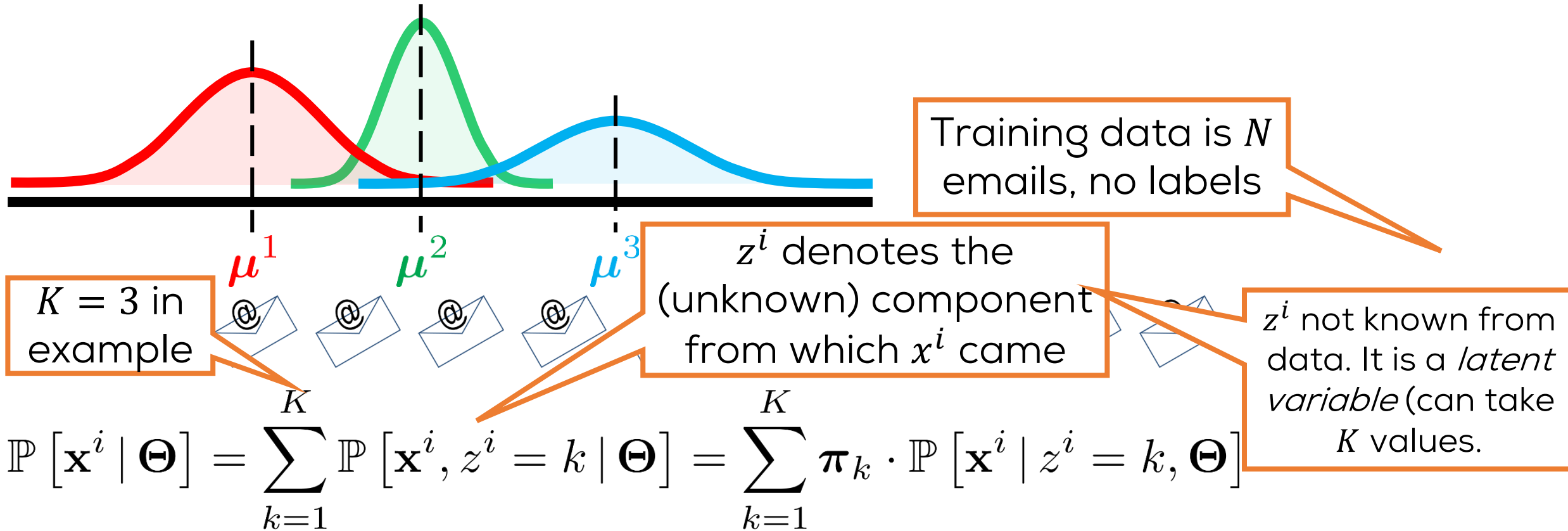
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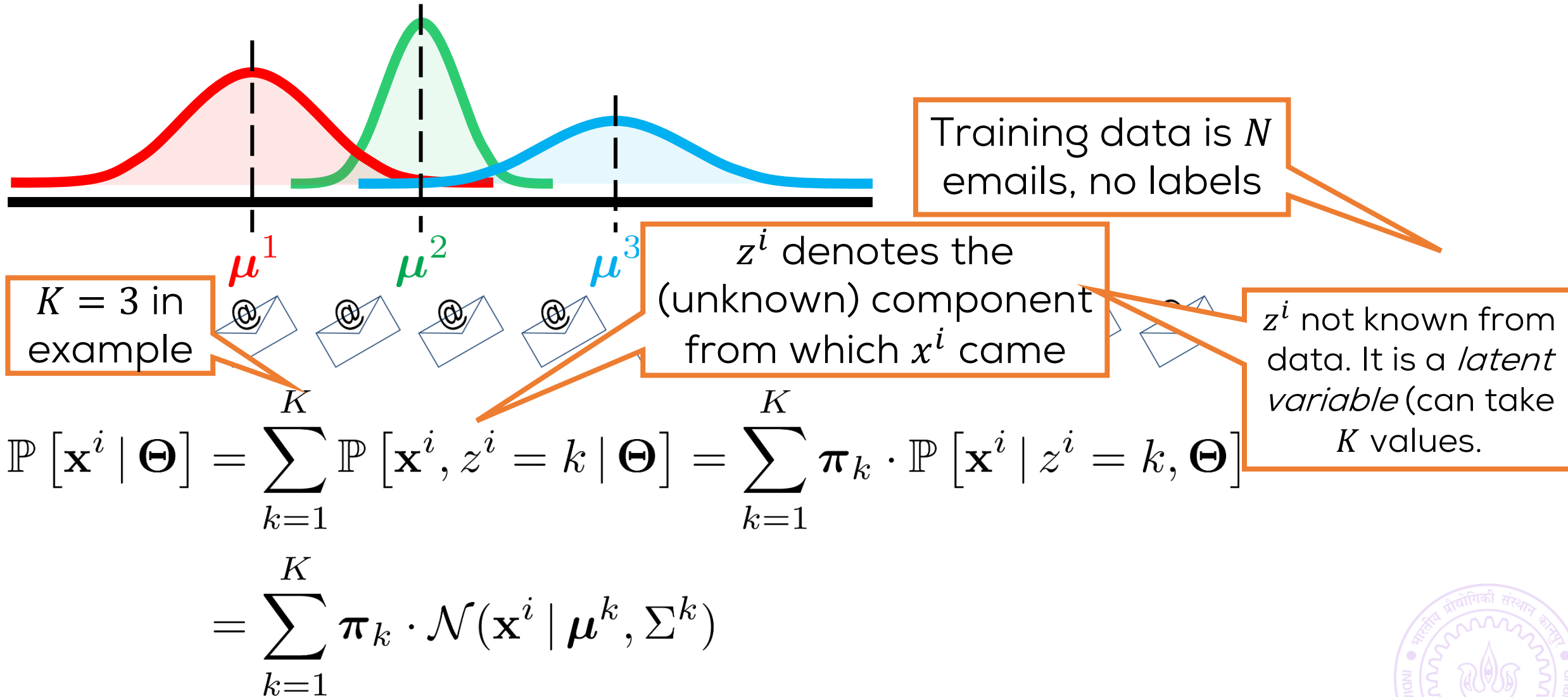
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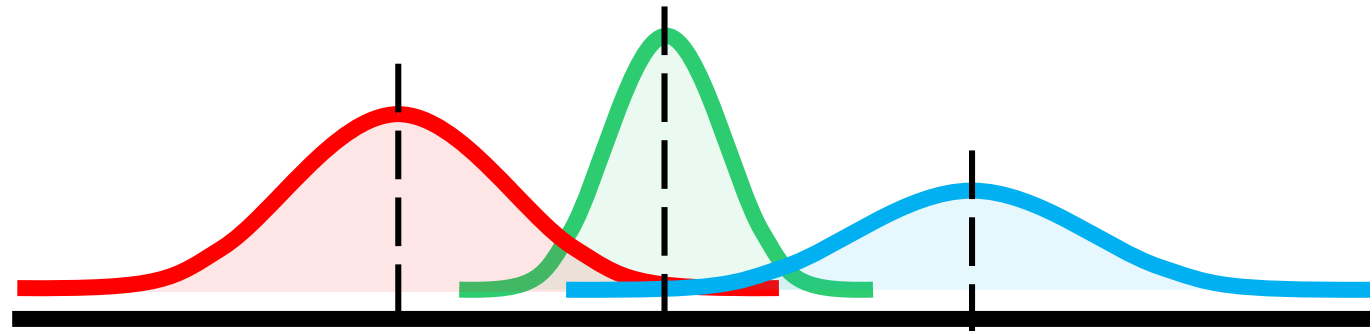
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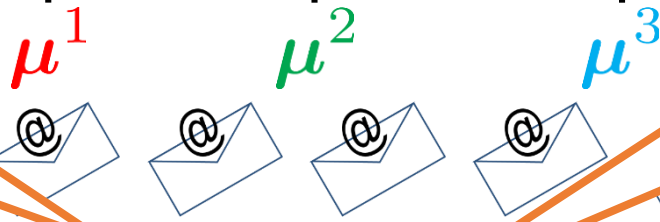


The generative story for unlabelled data



Training data is N emails, no labels

$K = 3$ in example



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

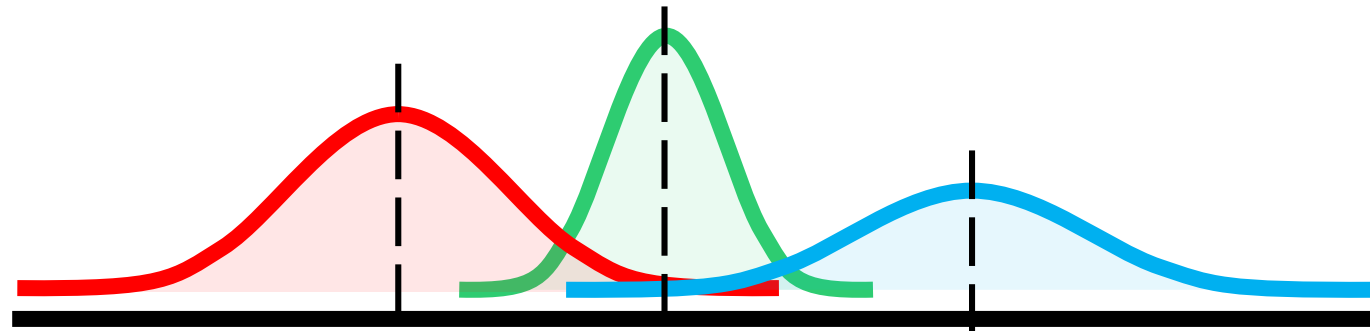
z^i not known from data. It is a *latent variable* (can take K values).

$$\mathbb{P}[\mathbf{x}^i | \Theta] = \sum_{k=1}^K \mathbb{P}[\mathbf{x}^i, z^i = k | \Theta] = \sum_{k=1}^K \pi_k \cdot \mathbb{P}[\mathbf{x}^i | z^i = k, \Theta]$$

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

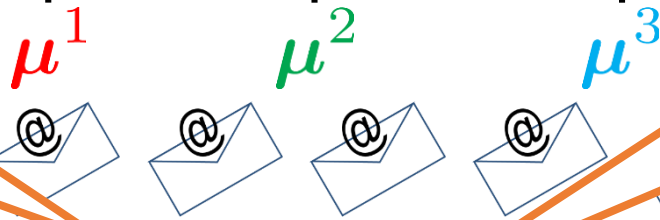
We assumed each component is a multidim. Gaussian

The generative story for unlabelled data



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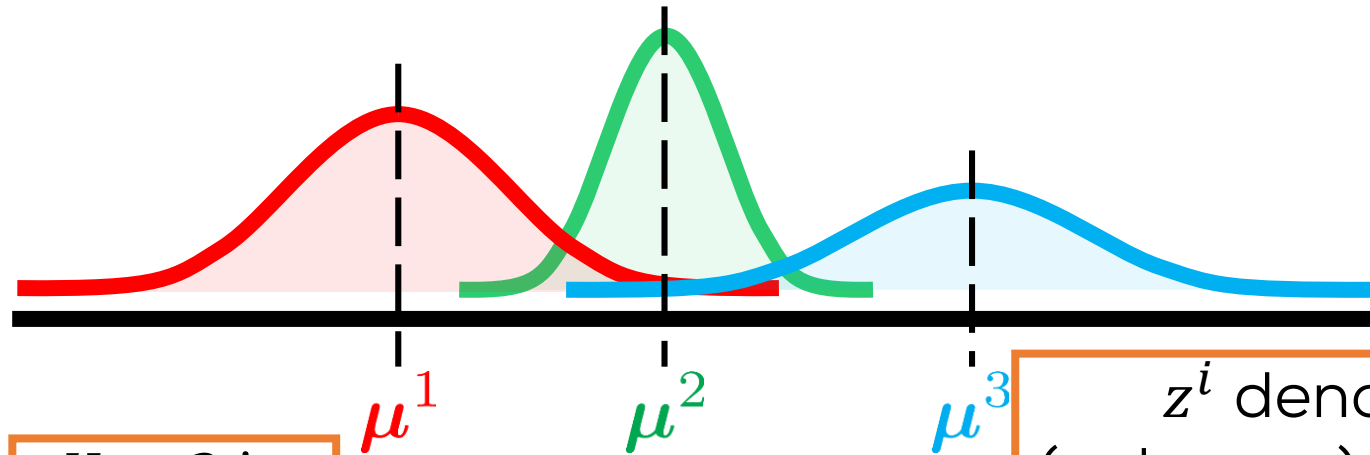
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$$\begin{aligned}\mathbb{P}[\mathbf{x}^i | \Theta] &= \sum_{k=1}^K \mathbb{P}[\mathbf{x}^i, z^i = k | \Theta] = \sum_{k=1}^K \pi_k \cdot \mathbb{P}[\mathbf{x}^i | z^i = k, \Theta] \\ &= \sum_{k=1}^K \pi_k \cdot \mathcal{N}(\mathbf{x}^i | \boldsymbol{\mu}^k, \Sigma^k)\end{aligned}$$

Gaussian Mixture Model (GMM) with K components

We assumed each component is a multidim. Gaussian

The generative story for unlabelled data



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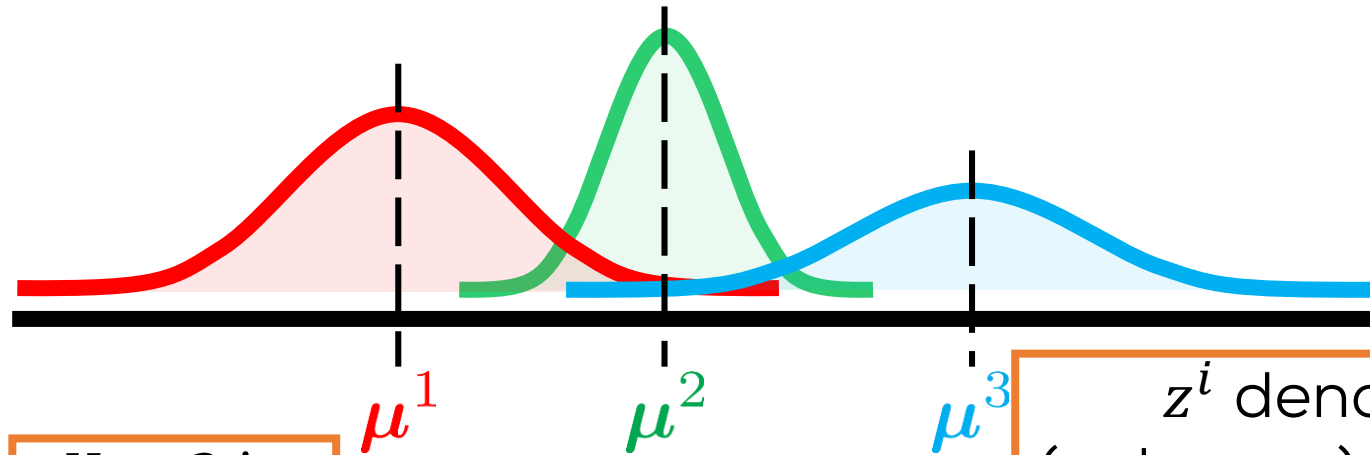
$$= \sum_{k=1}^K \pi_k \cdot \mathcal{N}(\mathbf{x}^i | \boldsymbol{\mu}^k, \Sigma^k)$$

Gaussian Mixture Model (GMM) with K components

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

We assumed each component is a multidim. Gaussian

The generative story for unlabelled data



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$K = 3$ in example

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

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

$$\mathbb{P}[\mathbf{x}^i | \Theta] = \sum_{k=1}^K \mathbb{P}[\mathbf{x}^i, z^i = k | \Theta] = \sum_{k=1}^K \pi_k \cdot \mathbb{P}[\mathbf{x}^i | z^i = k, \Theta]$$

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

Gaussian Mixture Model (GMM) with K components

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

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

We assumed each component is a multidim. Gaussian

The Likelihood Expression

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$$\mathbb{P} [\mathbf{x}^i \mid \Theta] = \sum_{k=1}^K \pi_k \cdot \mathcal{N}(\mathbf{x}^i \mid \boldsymbol{\mu}^k, \Sigma^k)$$

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$$= \arg \max_{\Theta} \prod_{i=1}^n \sum_{k=1}^K \pi_k \cdot \mathcal{N}(\mathbf{x}^i \mid \boldsymbol{\mu}^k, \Sigma^k)$$

The Likelihood Expression

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Cannot apply first order Optimality to get solution

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Horribly non-convex problem. Initialization matters!

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Things were so nice
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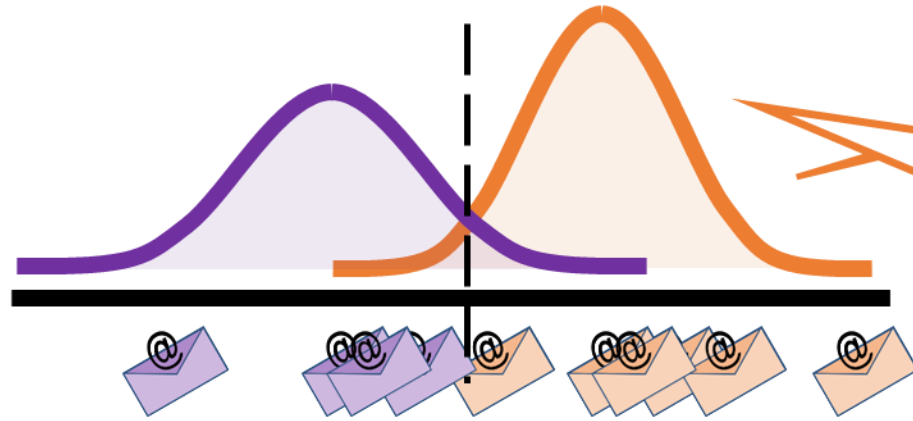
wait ...

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The generative story for unlabelled data??



No labels!!!

Give the Gaussians colors to help identifying them

Can we still recover the two Gaussian components in the mixture??

In practice: you will learn slightly "less wrong" ones 😊

Won't I just learn the wrong ones that generated the labels?

We do not know which email is purple and which is orange – no labels!!

What if I use these "magical" labels to learn two Gaussians?

Can use these to label emails!

Hmm ... what if someone magically labelled the emails with the color

Hmm ... what if someone gave me a purple and an orange Gaussian, maybe slightly wrong ones

How to get these magical labels??

The Likelihood Expression

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A Ray of Hope

Sept 8, 2017



A Ray of Hope

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A Ray of Hope

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ALTERNATING OPTIMIZATION

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

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Can use a method like the one discussed in the “detour”!

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Various ways of
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$$\hat{\Theta}_{\text{MLE}} = \arg \max_{\Theta} \mathbb{P}[X | \Theta]$$

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

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Hard Assignment

The K-means algorithm

A Ray of Hope

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Bayes
Rule!

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

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Towards the K-Means Algorithm

ALTERNATING OPTIMIZATION

1. Initialize Θ^0
2. For $i \in [n]$, update $z^{i,t}$ using Θ^t
 1. Let $z^{i,t} = \arg \max_k \pi_k^t \cdot \mathcal{N}(\mathbf{x}^i \mid \boldsymbol{\mu}^{k,t}, \Sigma^{k,t})$
3. Update $\Theta^{t+1} = \arg \max_{\Theta} \mathbb{P}[X, \{z^{i,t}\} \mid \Theta]$
 1. Let $\pi_k^{t+1} = \frac{n_k^t}{n}$, where $n_k^t = |\{i: z^{i,t} = k\}|$
 2. Let $\boldsymbol{\mu}^{k,t+1} = \frac{1}{n_k^t} \sum_{i: z^{i,t}=k} \mathbf{x}^i$
 3. Let $\Sigma_k^{t+1} = \frac{1}{n_k^t} \sum_{i: z^{i,t}=k} (\mathbf{x}^i - \boldsymbol{\mu}^{k,t}) (\mathbf{x}^i - \boldsymbol{\mu}^{k,t})^\top$
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 $\{\boldsymbol{\mu}^{k,0}\}_{k=1,\dots,K}$
2. For $i \in [n]$, update $z^{i,t}$ using $\boldsymbol{\mu}^{k,t}$
 1. Let $z^{i,t} = \arg \max_k \mathcal{N}(\mathbf{x}^i \mid \boldsymbol{\mu}^{k,t}, I)$
3. Update $\boldsymbol{\mu}^{k,t+1} = \frac{1}{n_k^t} \sum_{i: z^{i,t}=k} \mathbf{x}^i$
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The K-Means Objective

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$$\hat{\Theta}_{\text{km}} = \arg \min_{\substack{\{\boldsymbol{\mu}^k\}_{k=1,\dots,K} \\ \{z^i\}_{i=1,\dots,n}}} \sum_{k=1}^K \sum_{i: z^i=k} \|\mathbf{x}^i - \boldsymbol{\mu}^k\|_2^2$$

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For cluster k , we have
cluster center $\boldsymbol{\mu}^k$

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For cluster k ,

$$\sum_{i:z^i=k} \|\mathbf{x}^i - \boldsymbol{\mu}^k\|_2^2$$

is a measure of how much variance is in the cluster

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For cluster k , we have cluster center $\boldsymbol{\mu}^k$

Want to minimize sum of variance across all clusters.
Want tight clusters

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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!

An FA approach to solving a data modelling task!

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

Very scalable but sensitive to initialization!

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k-means++ initialization

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

K-MEANS/LLOYD'S ALGORITHM

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K-Means Algorithm in action!

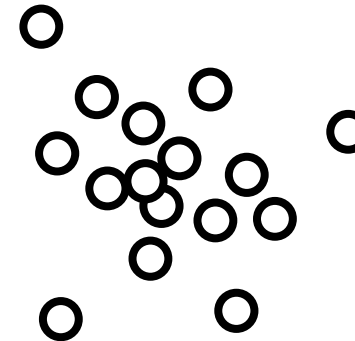
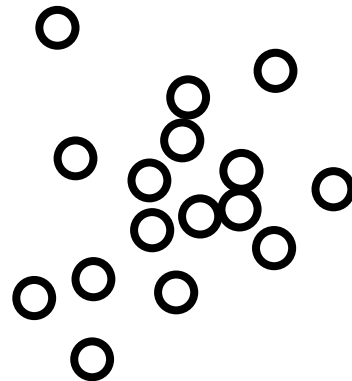
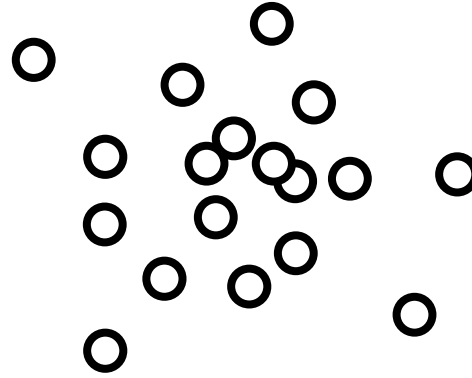
K-MEANS/LLOYD'S ALGORITHM

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4. Repeat until convergence

K-Means Algorithm in action!

K-MEANS/LLOYD'S ALGORITHM

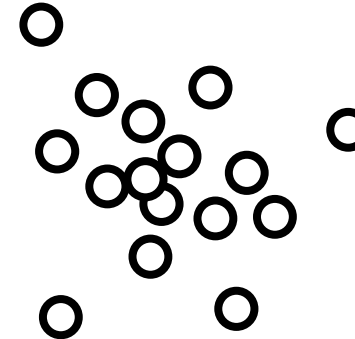
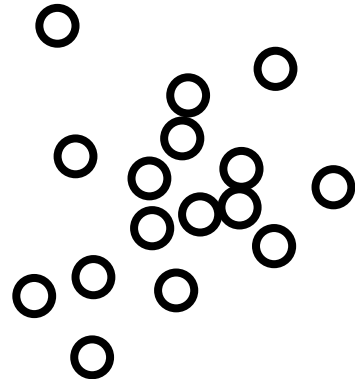
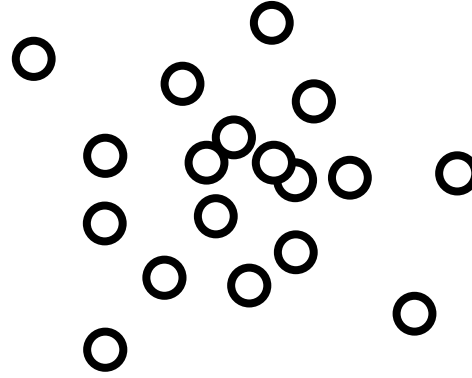
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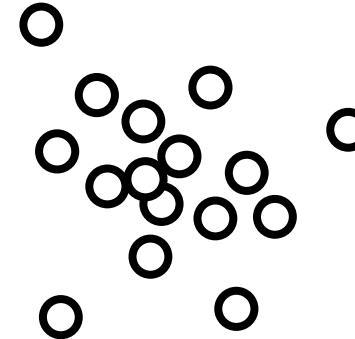
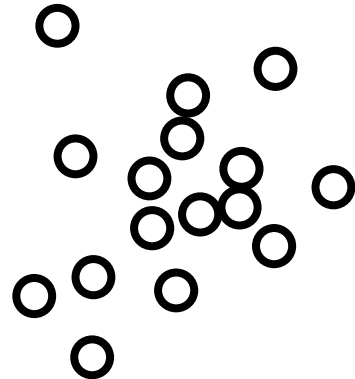
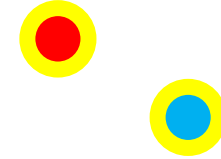
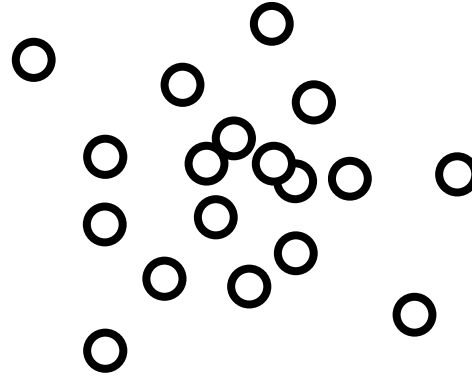
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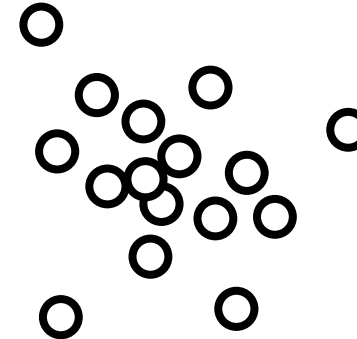
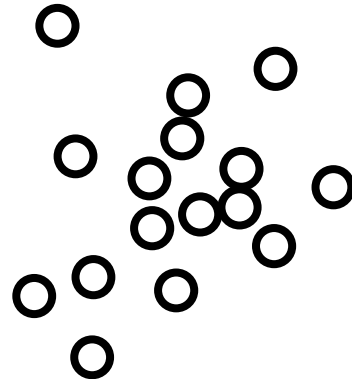
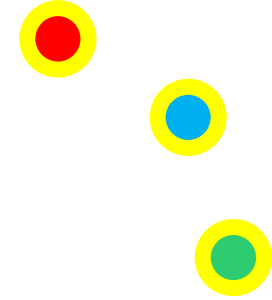
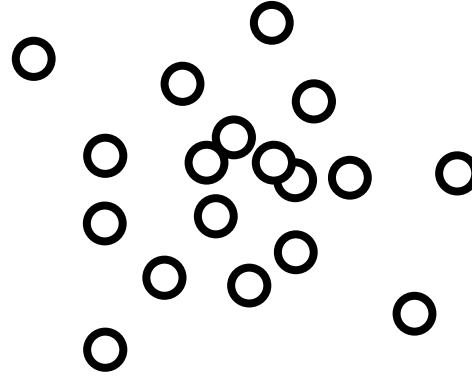
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K-Means Algorithm in action!

K-MEANS/LLOYD'S ALGORITHM

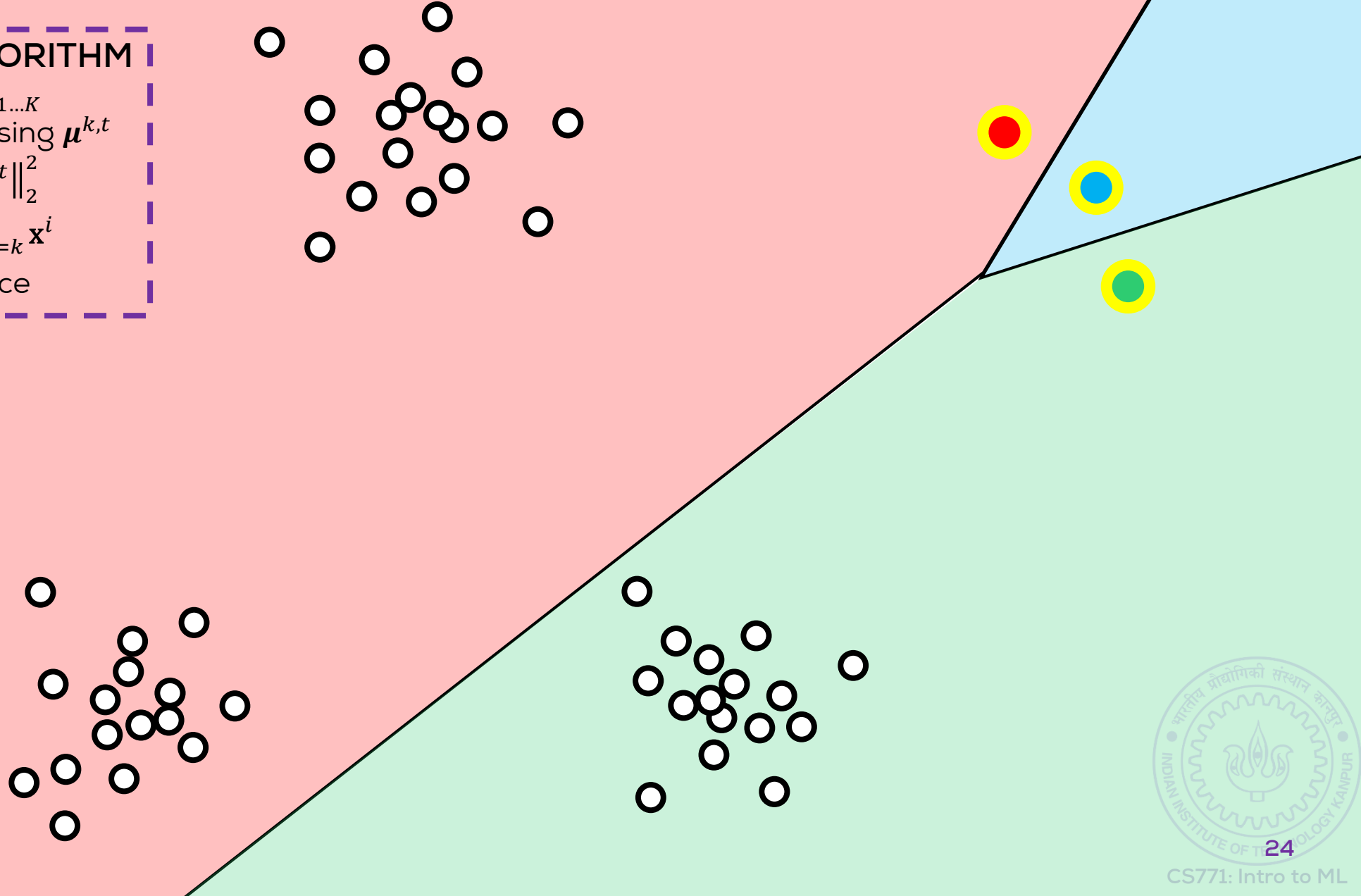
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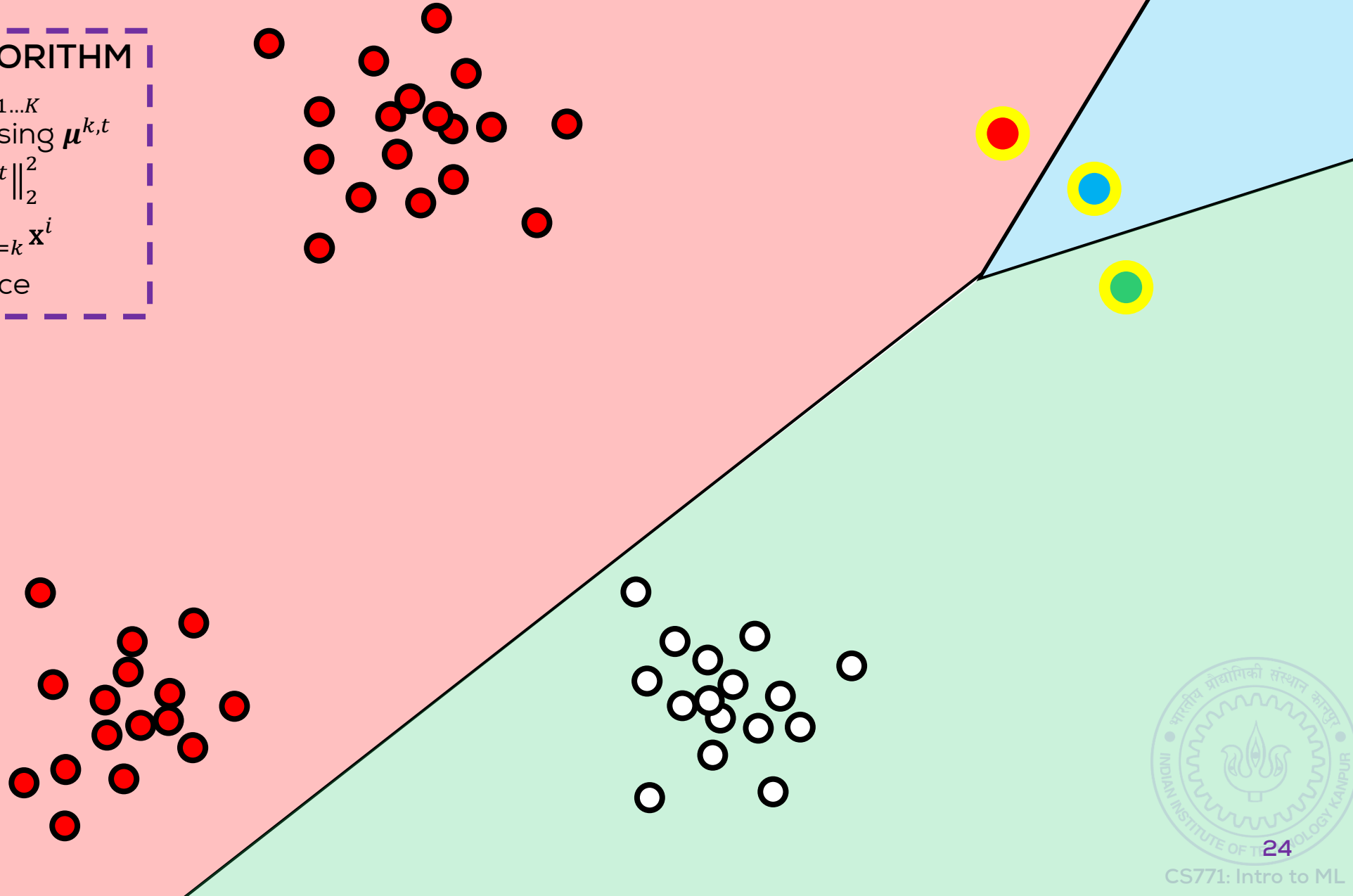
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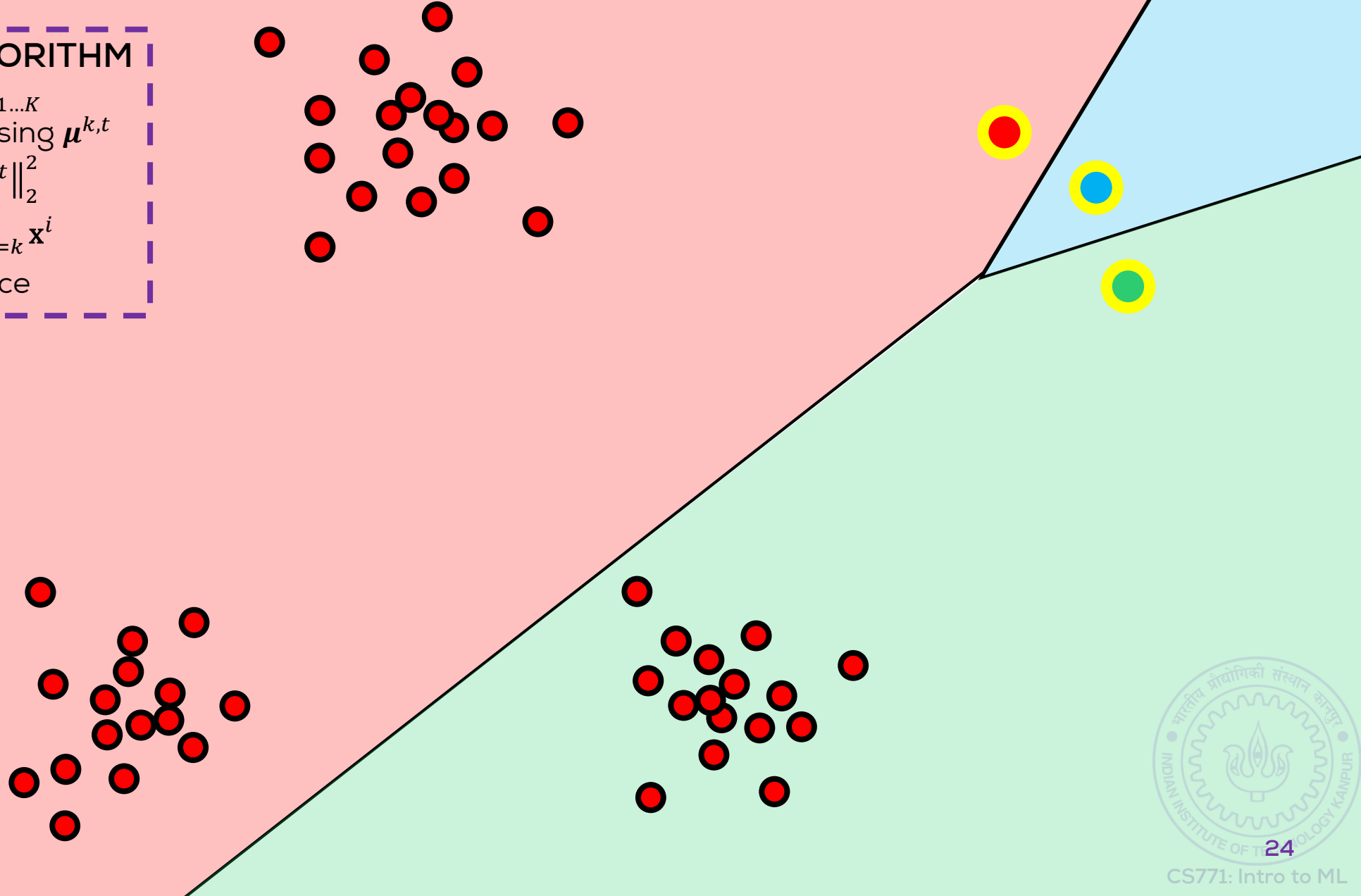
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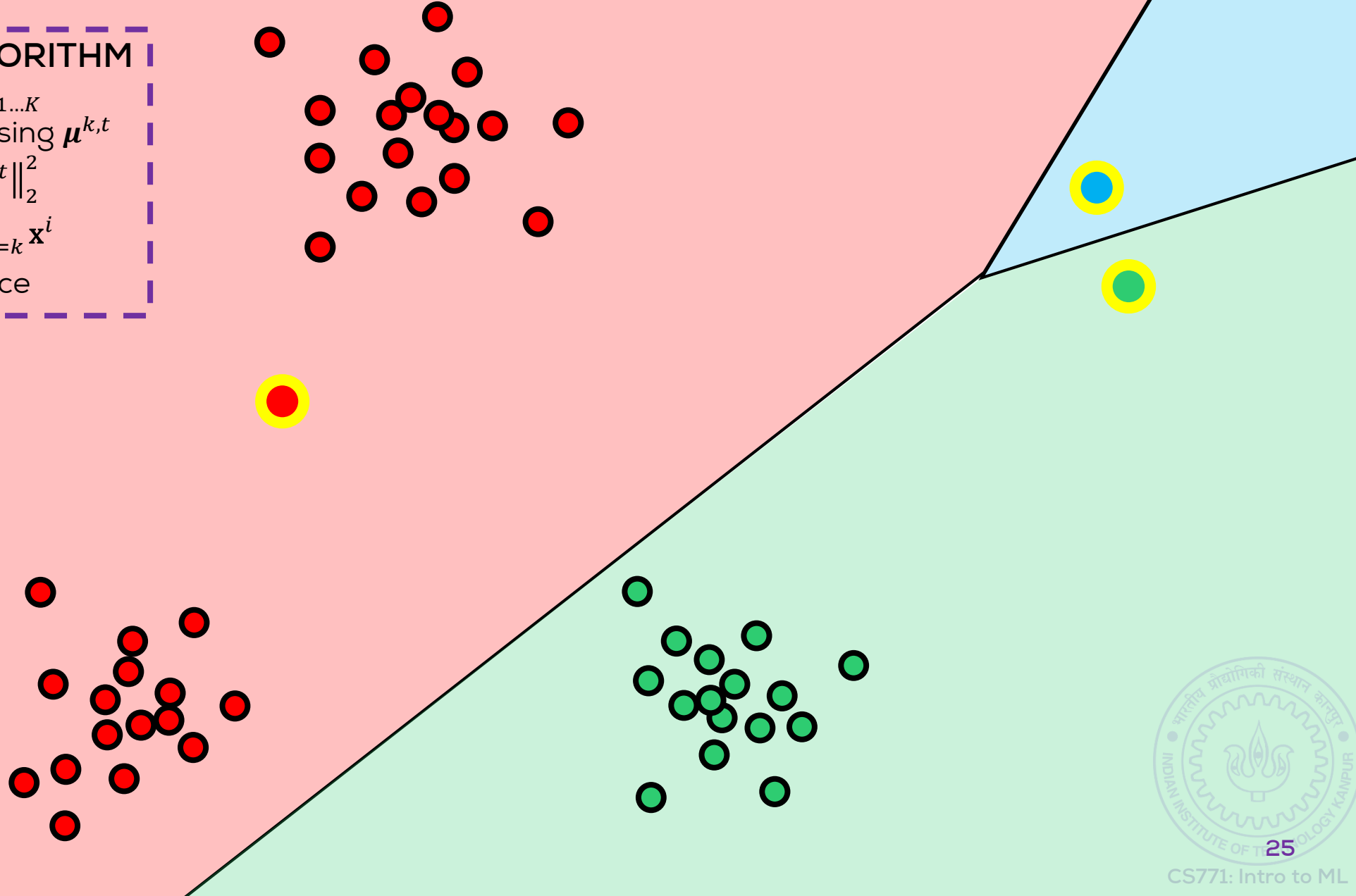
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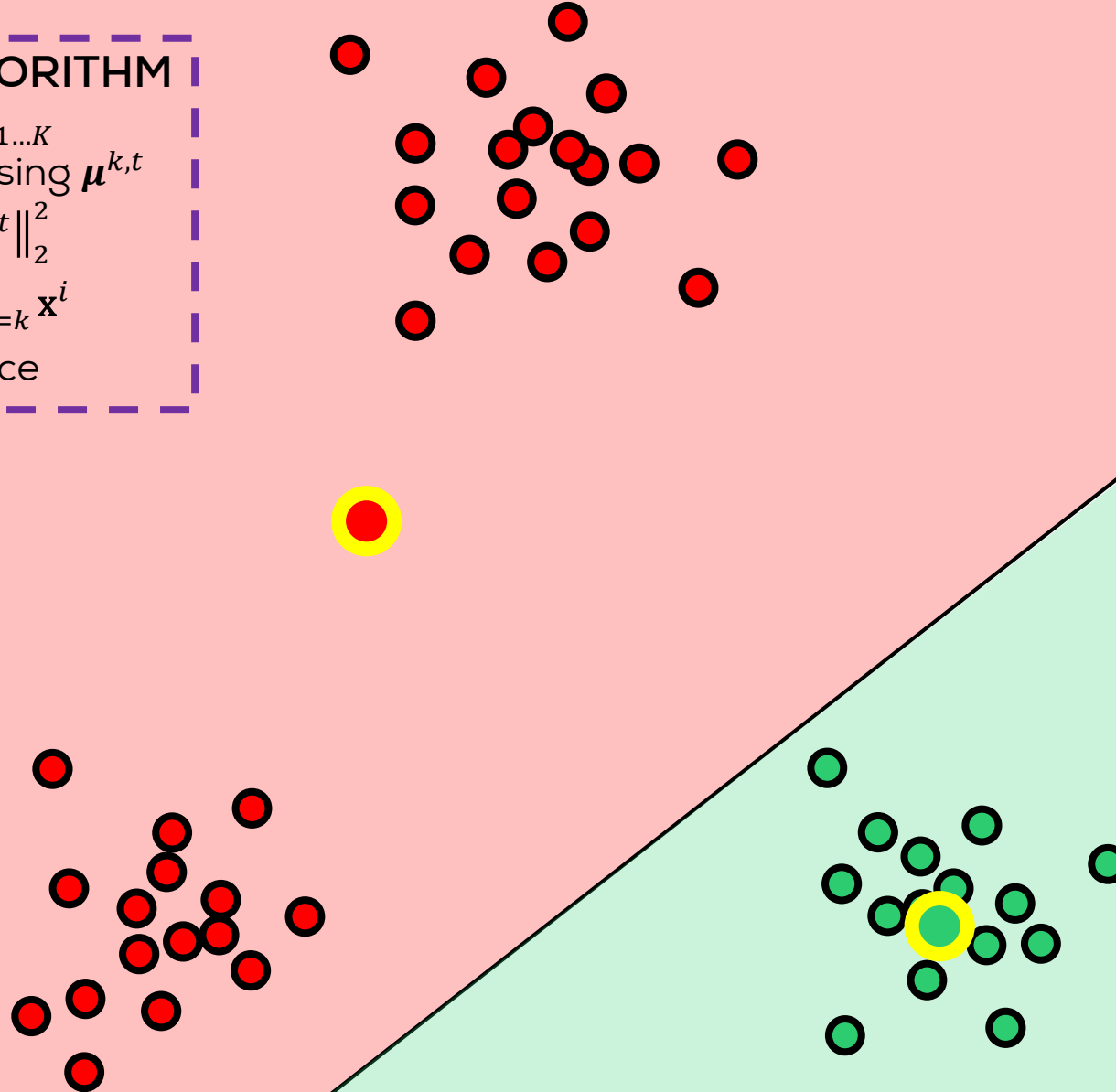
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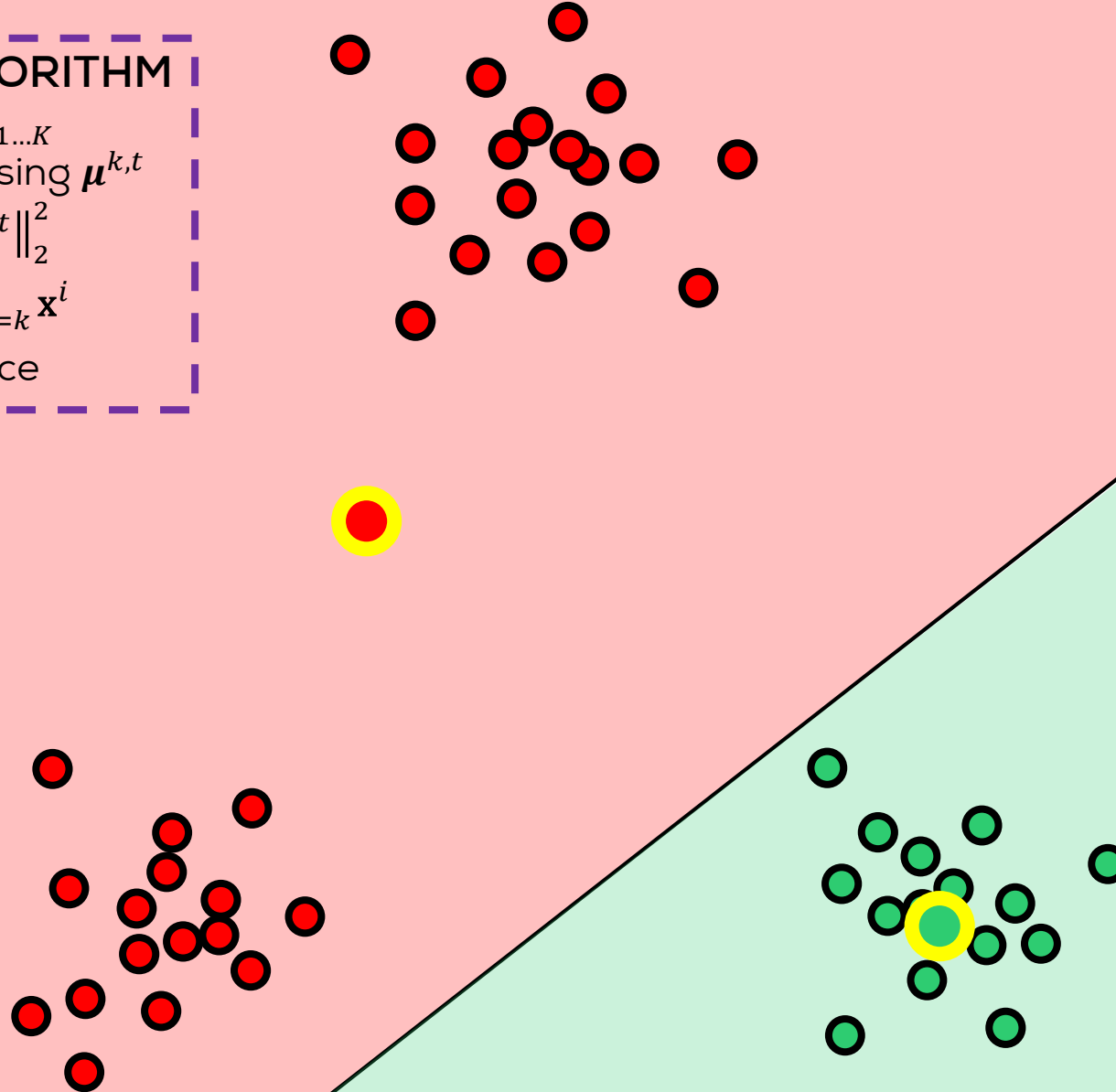
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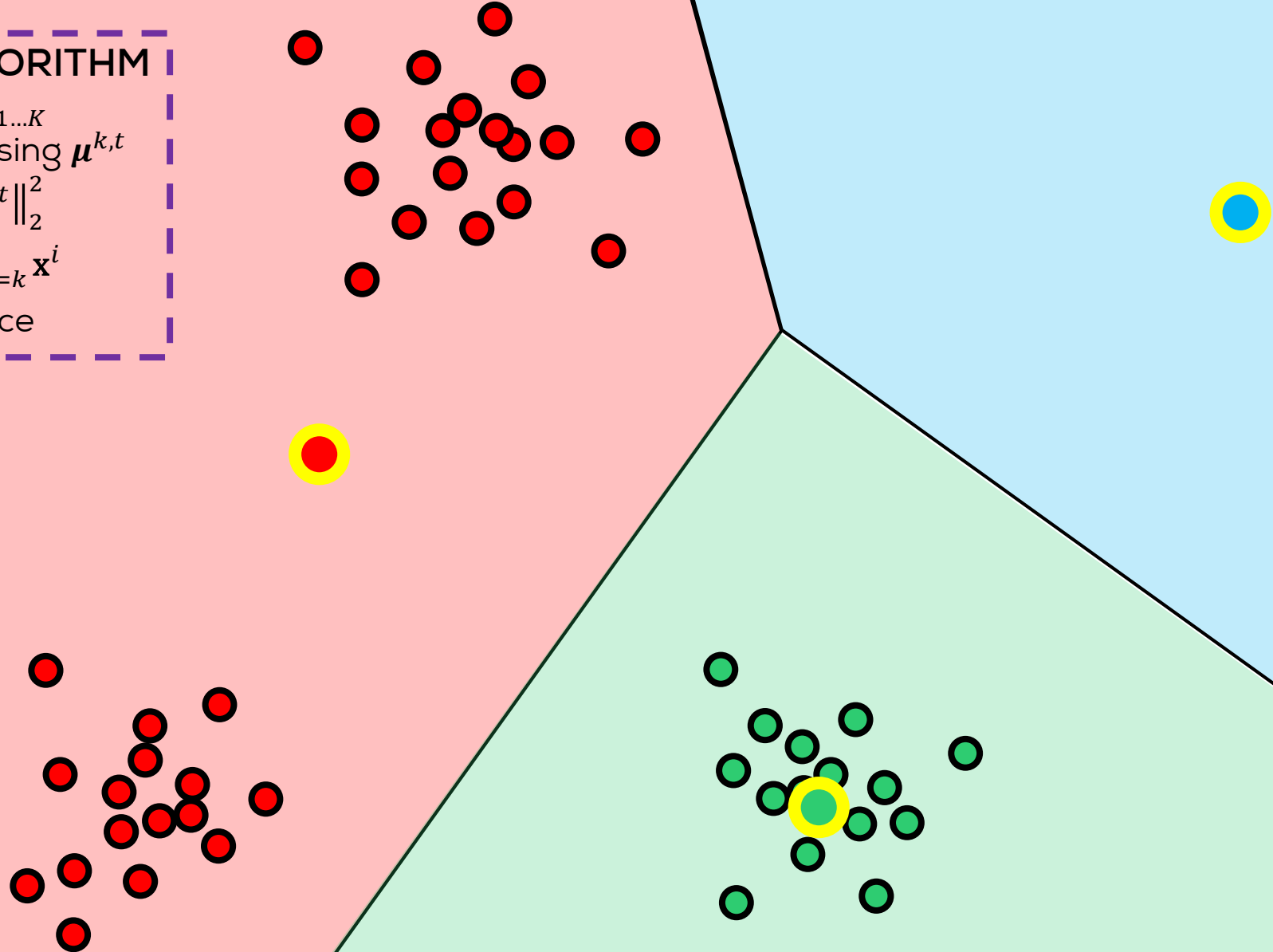
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Stuck!!!

K-Means Algorithm in action!

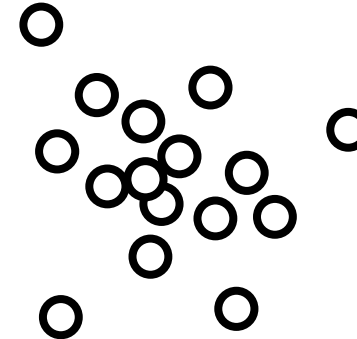
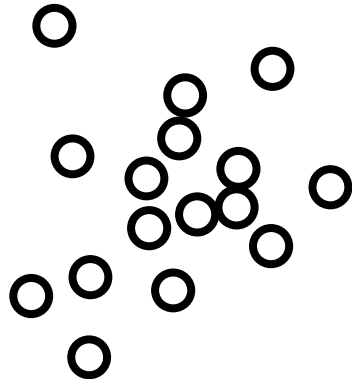
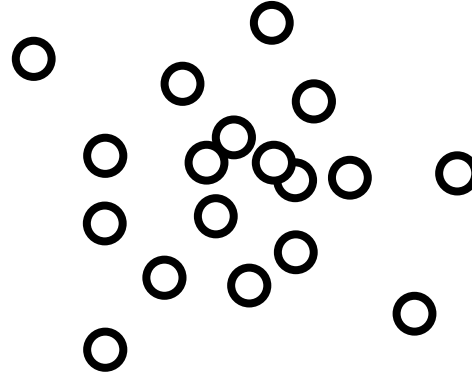
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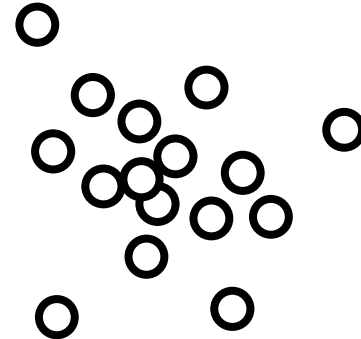
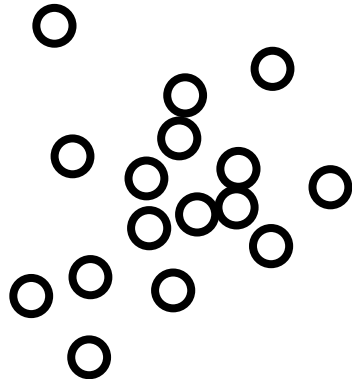
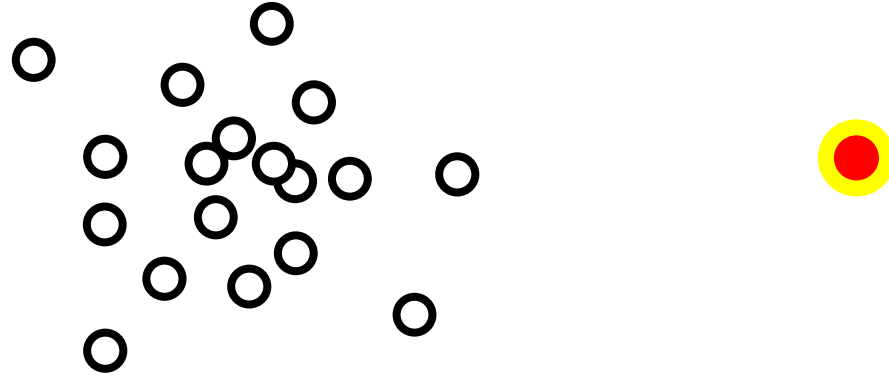
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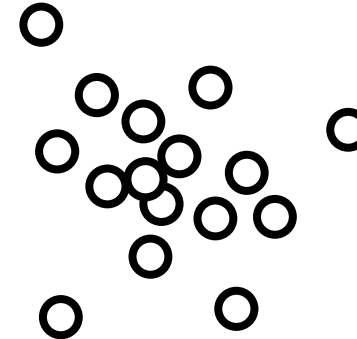
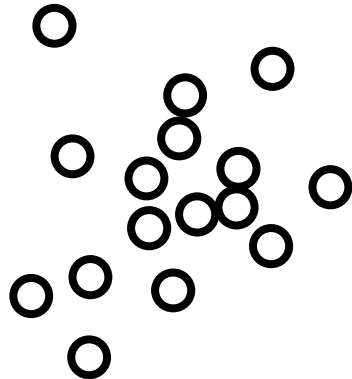
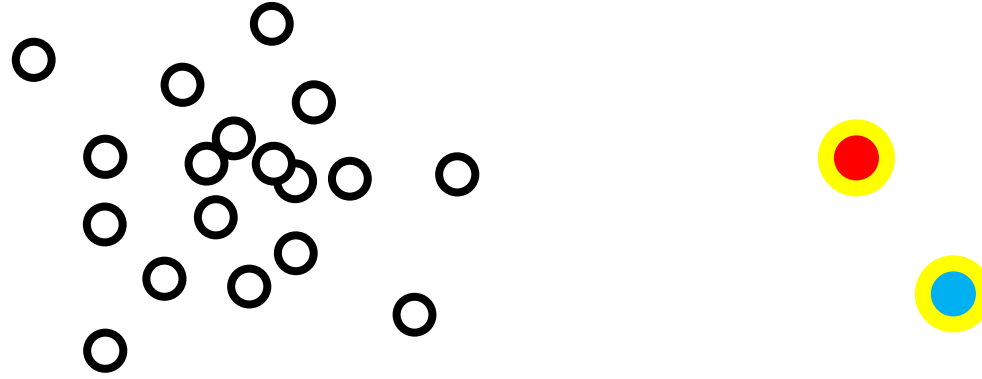
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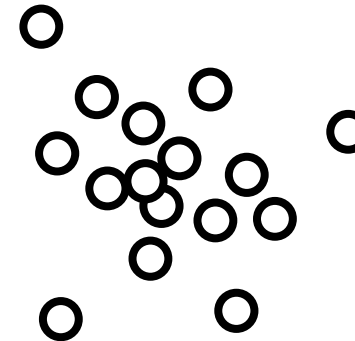
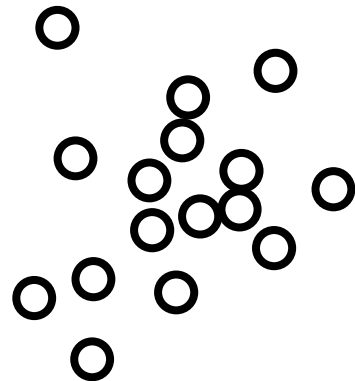
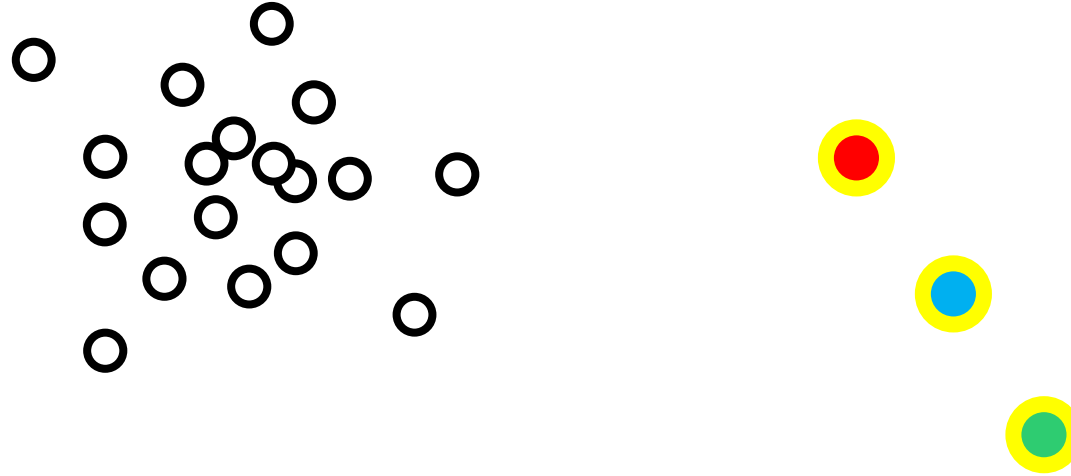
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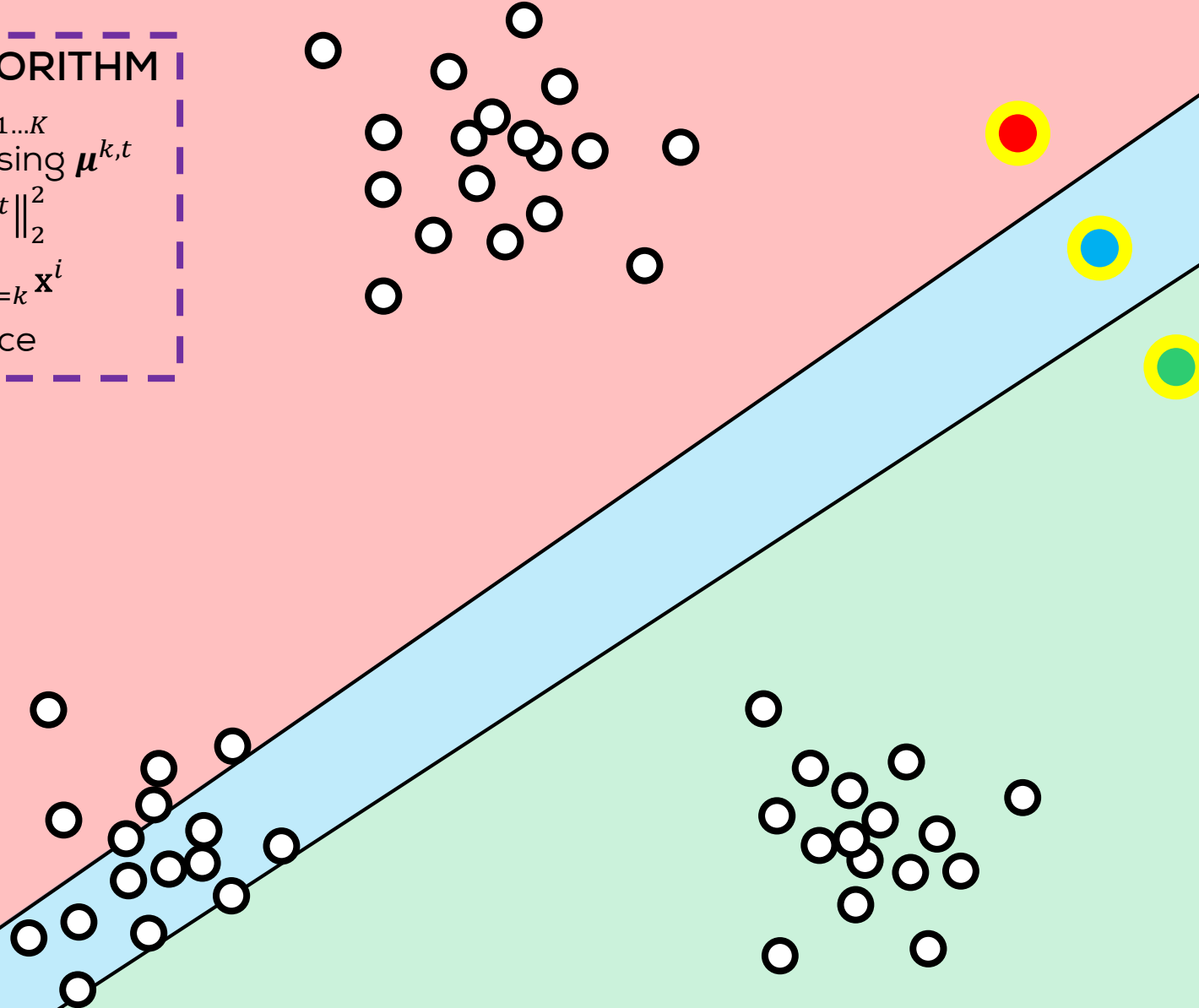
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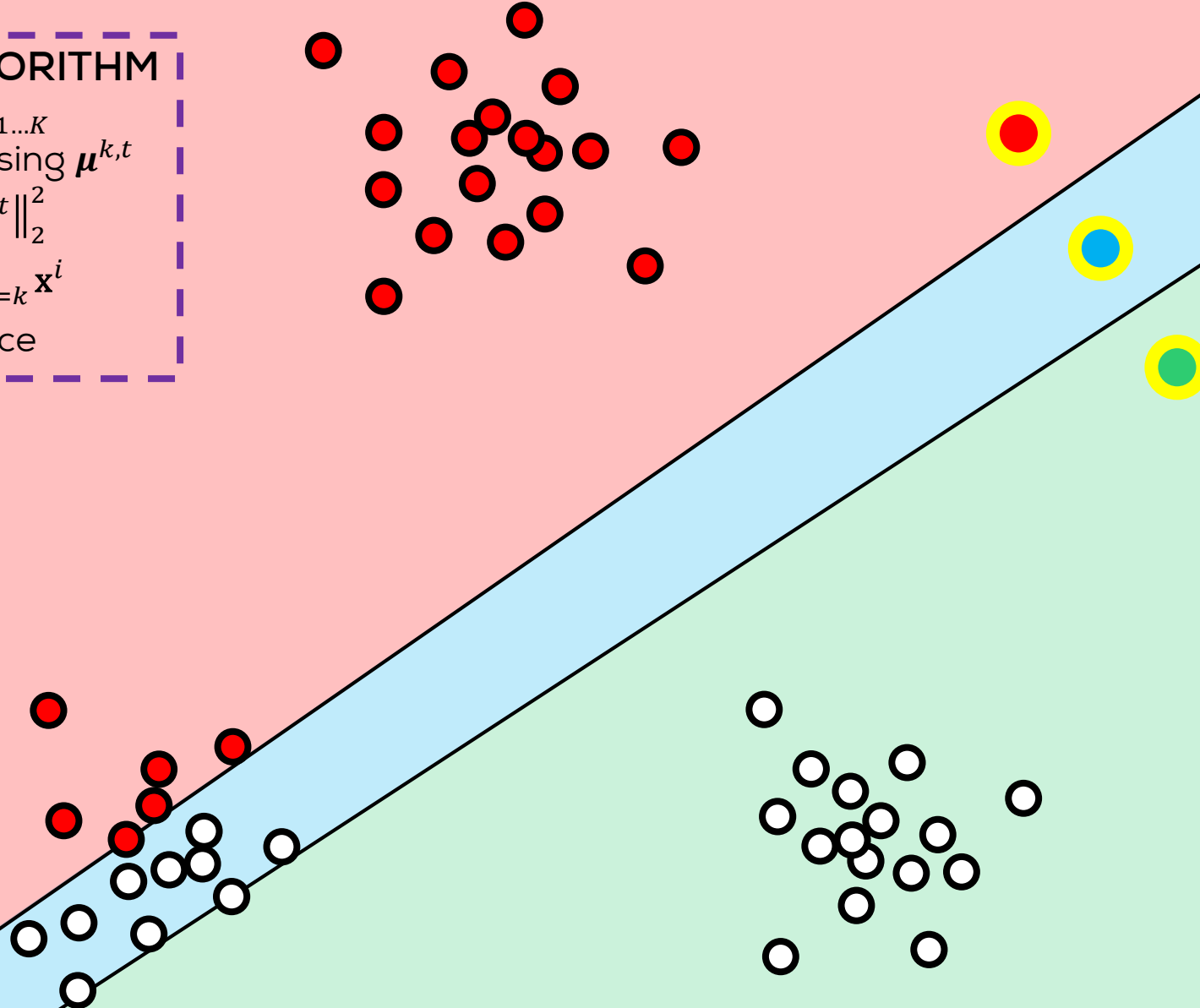
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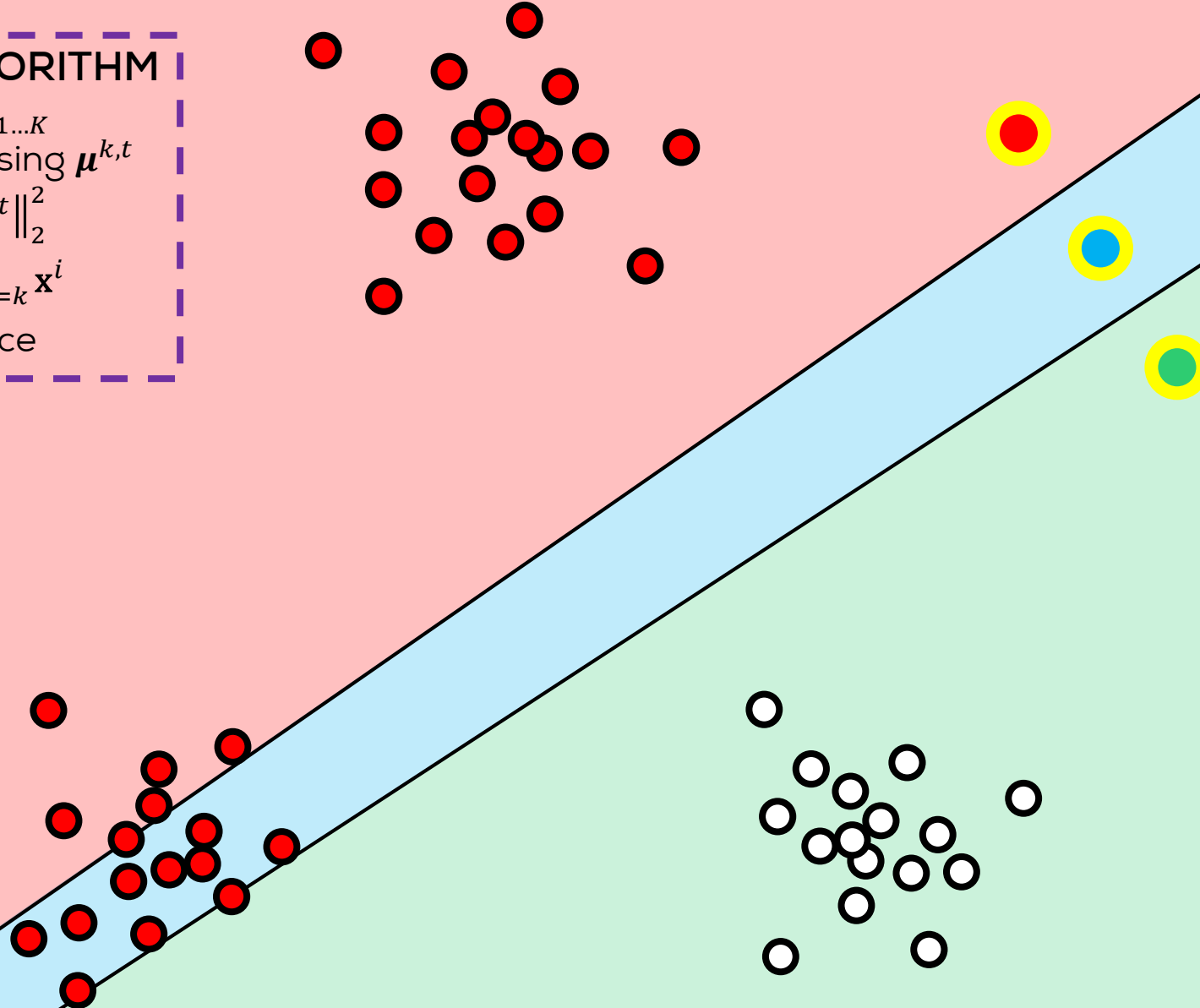
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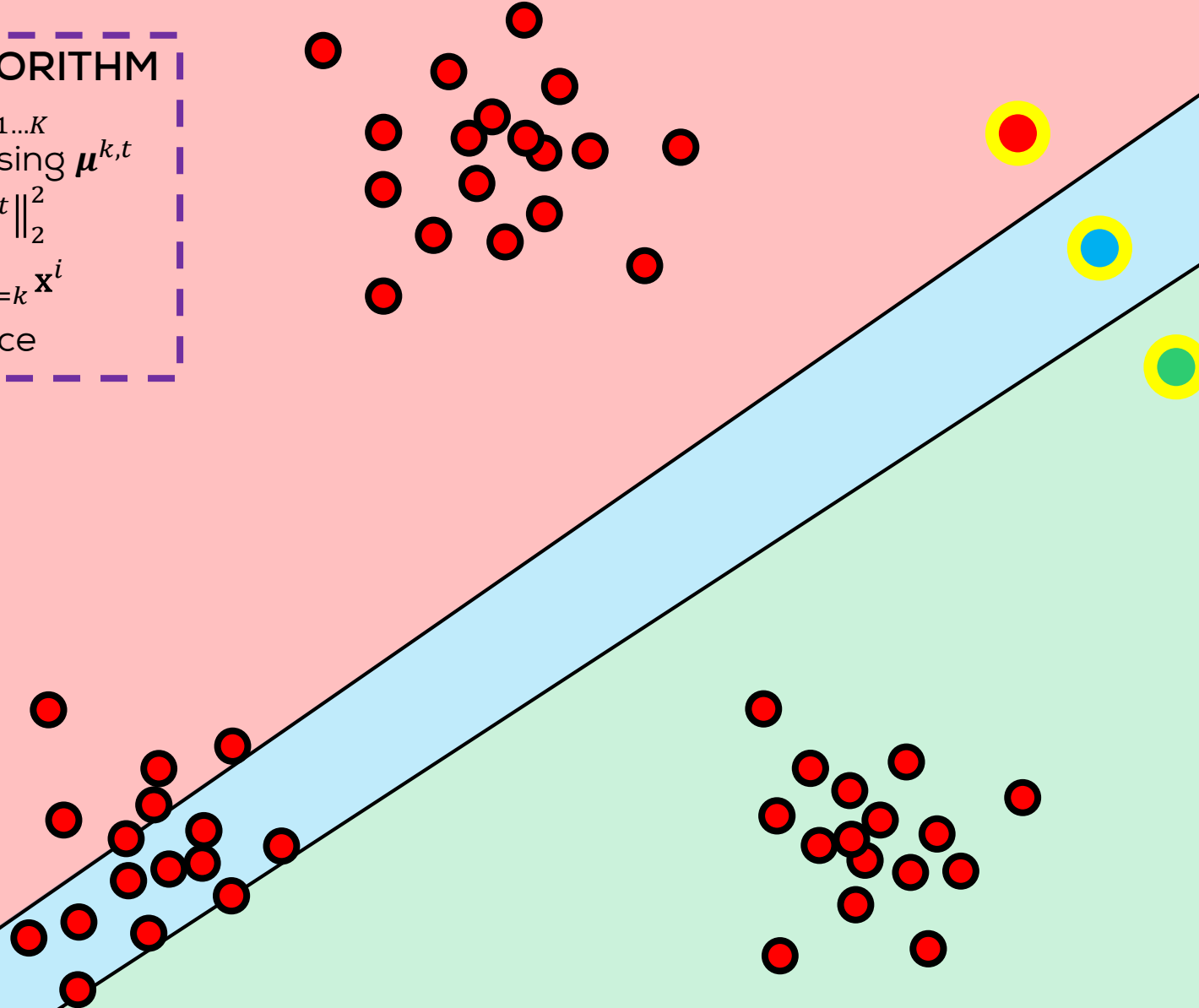
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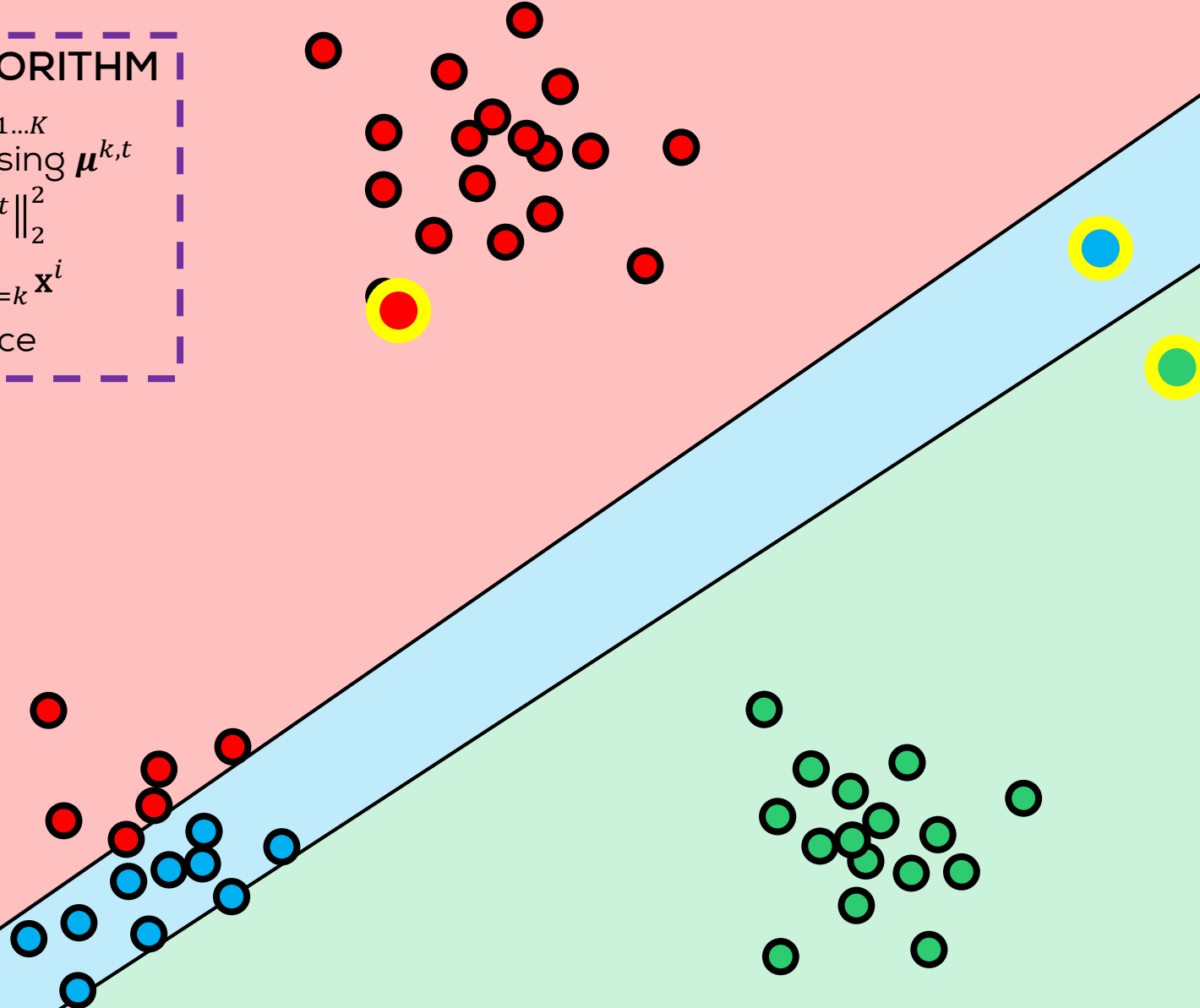
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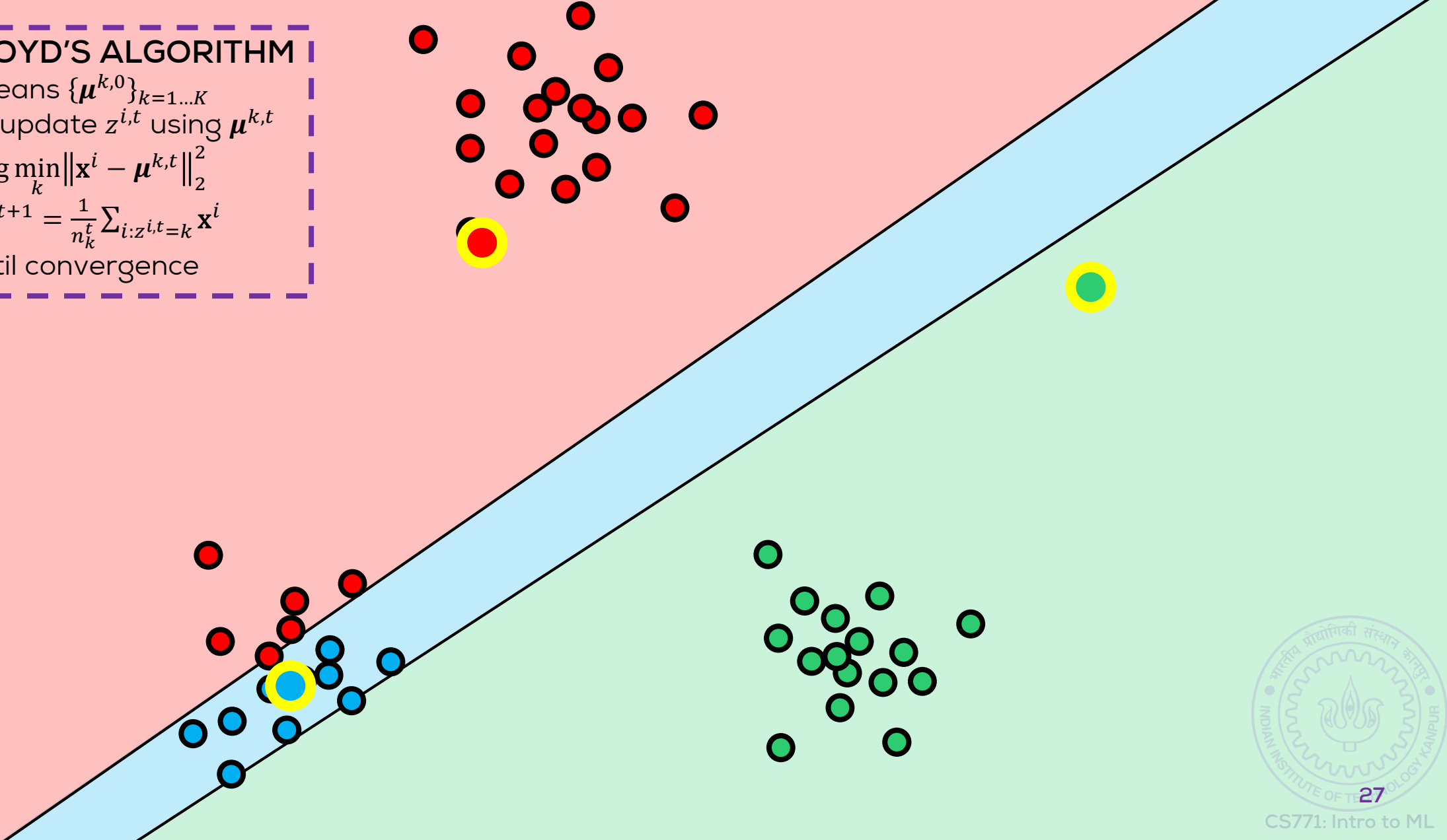
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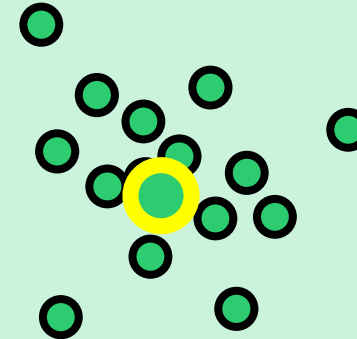
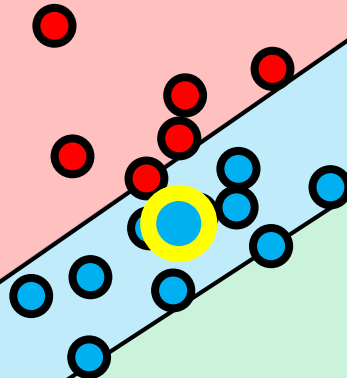
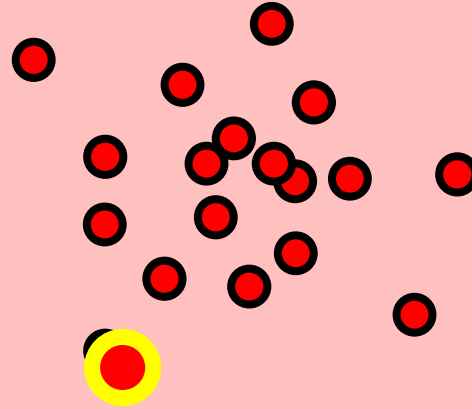
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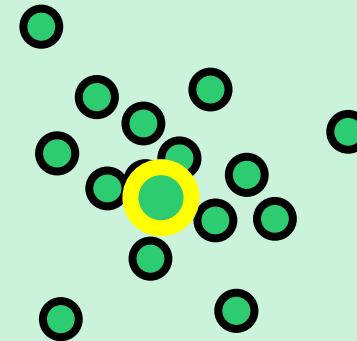
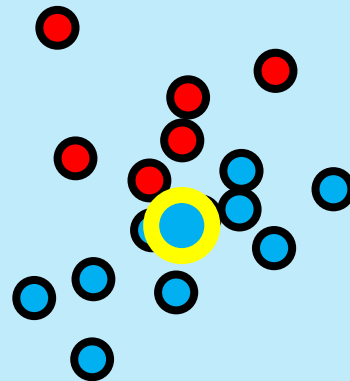
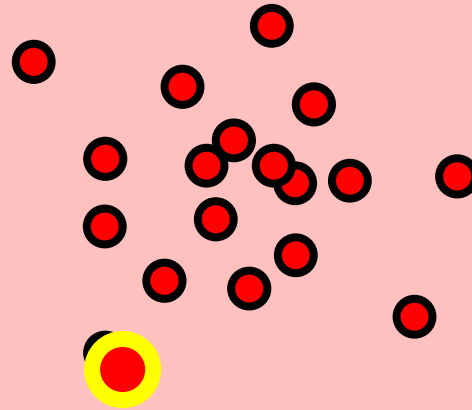
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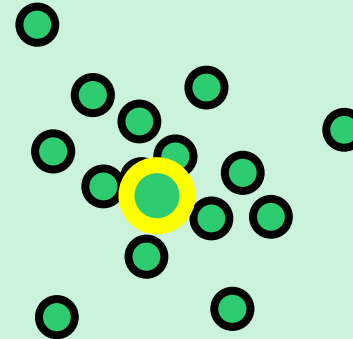
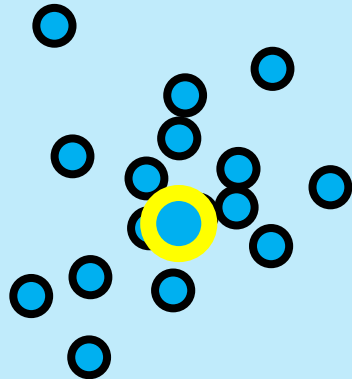
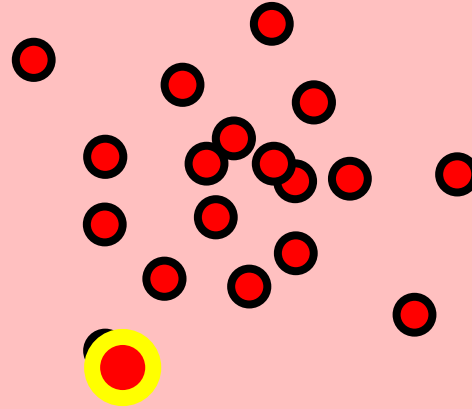
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K-Means Algorithm in action!

K-MEANS/LLOYD'S ALGORITHM

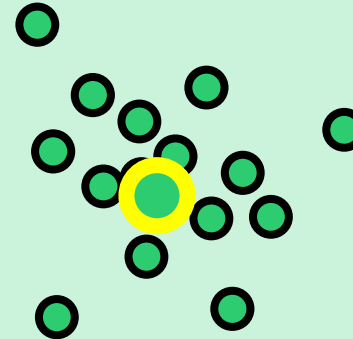
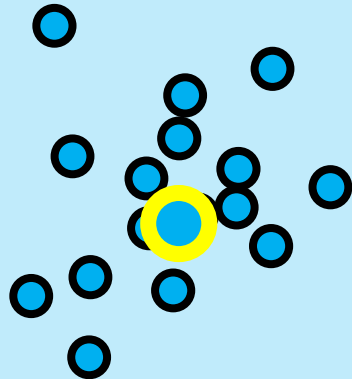
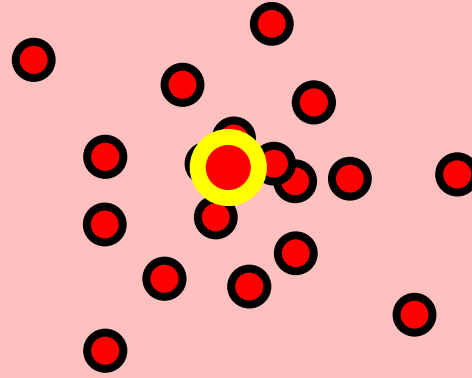
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2. For $i \in [n]$, update $z^{i,t}$ using $\mu^{k,t}$
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3. Update $\mu^{k,t+1} = \frac{1}{n_k^t} \sum_{i: z^{i,t}=k} \mathbf{x}^i$
4. Repeat until convergence



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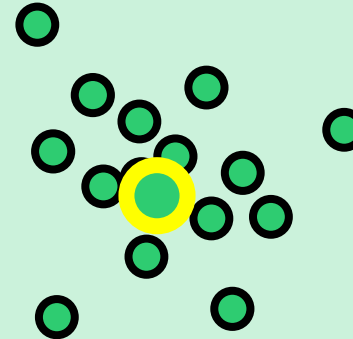
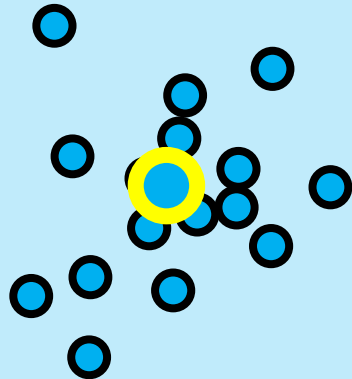
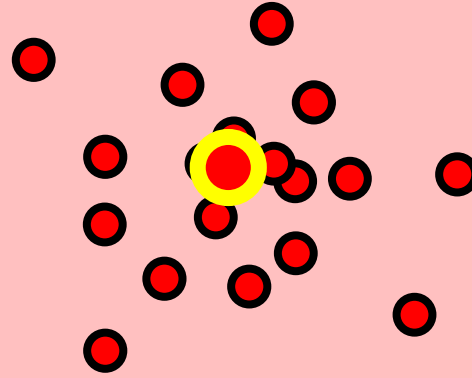
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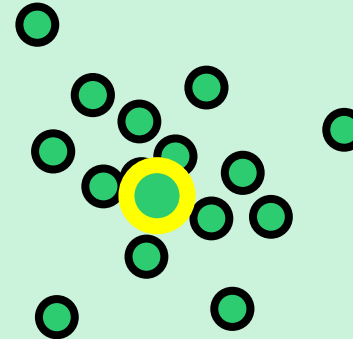
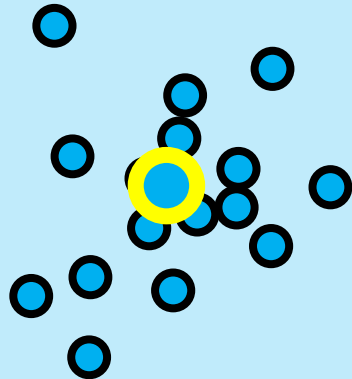
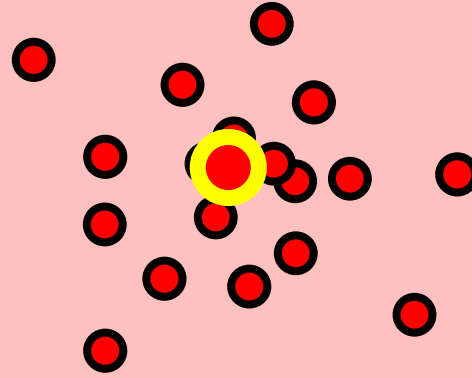
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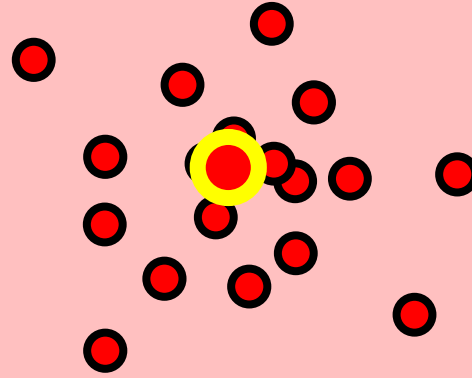
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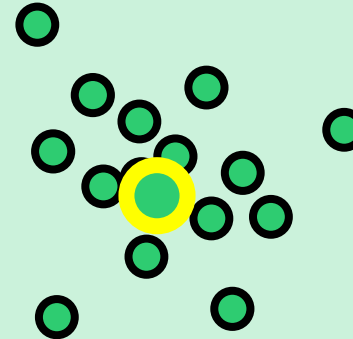
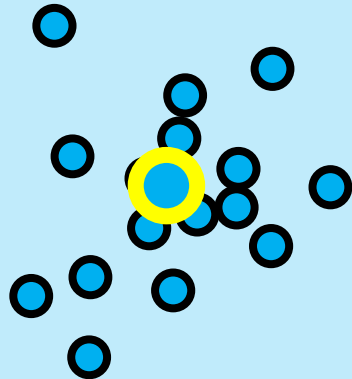
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Stuck!!! ... but
at the global
optimum 😊



Generating data from GMM learnt using Lloyd

- K clusters with means $\mu^1, \mu^2, \dots, \mu^K$ learnt using k-means
- To generate a data point from this GMM
 1. Select a cluster $k \sim [K]$ uniformly at random
 2. Select a point from the Gaussian $\mathcal{N}(\mu^k, I)$

K-means
uses $\pi_k = \frac{1}{K}$

K-means
use $\Sigma^k = I$

The K-means clustering algorithm

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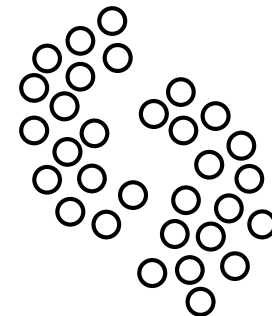
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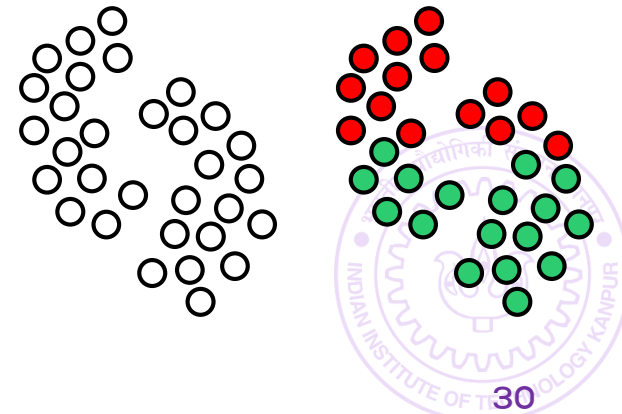
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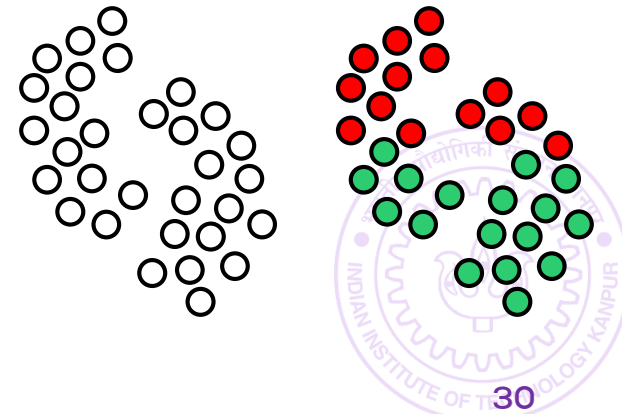
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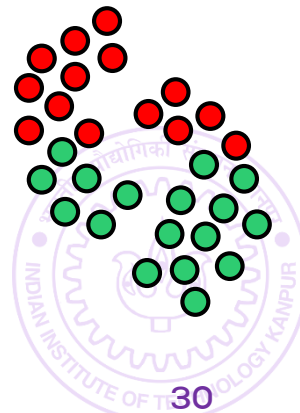
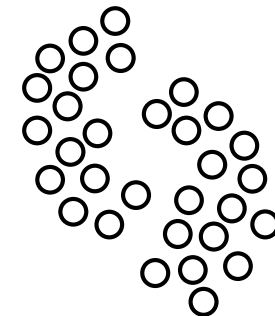
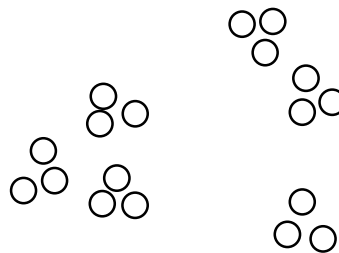
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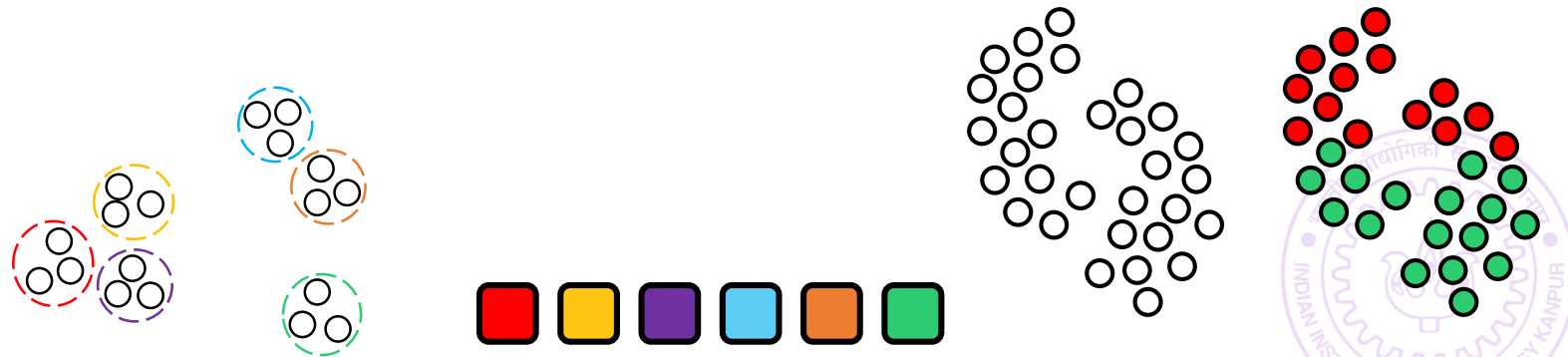
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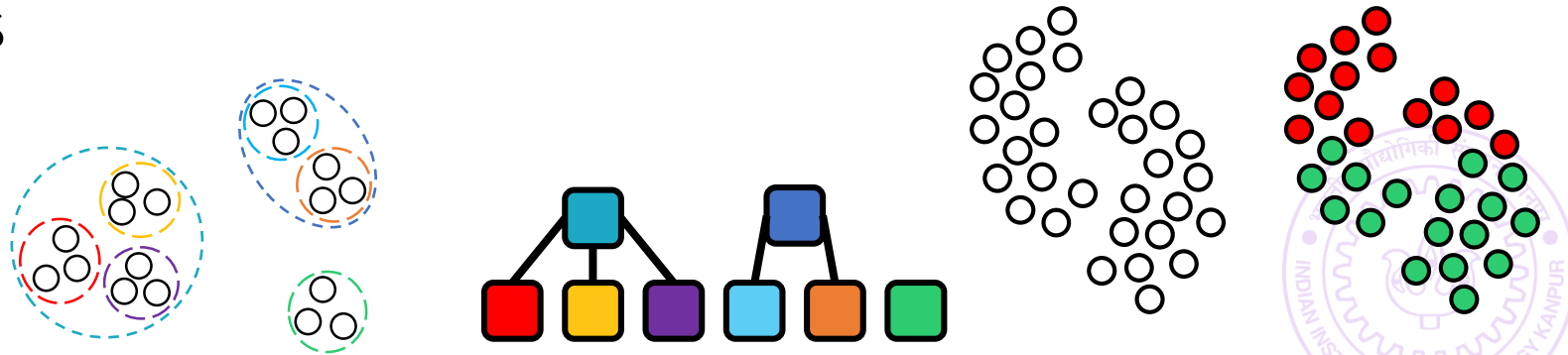
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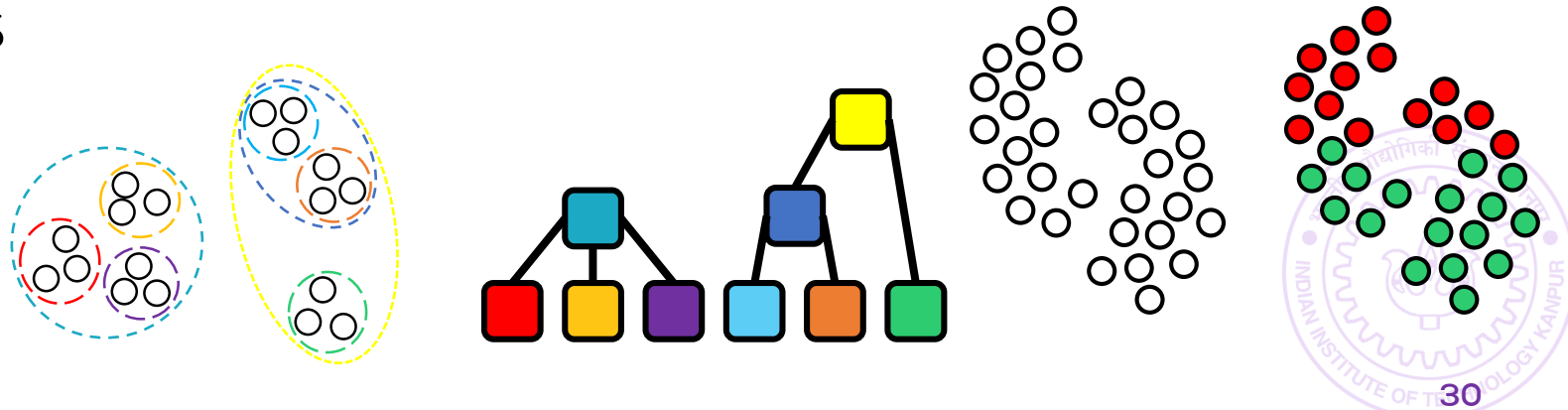
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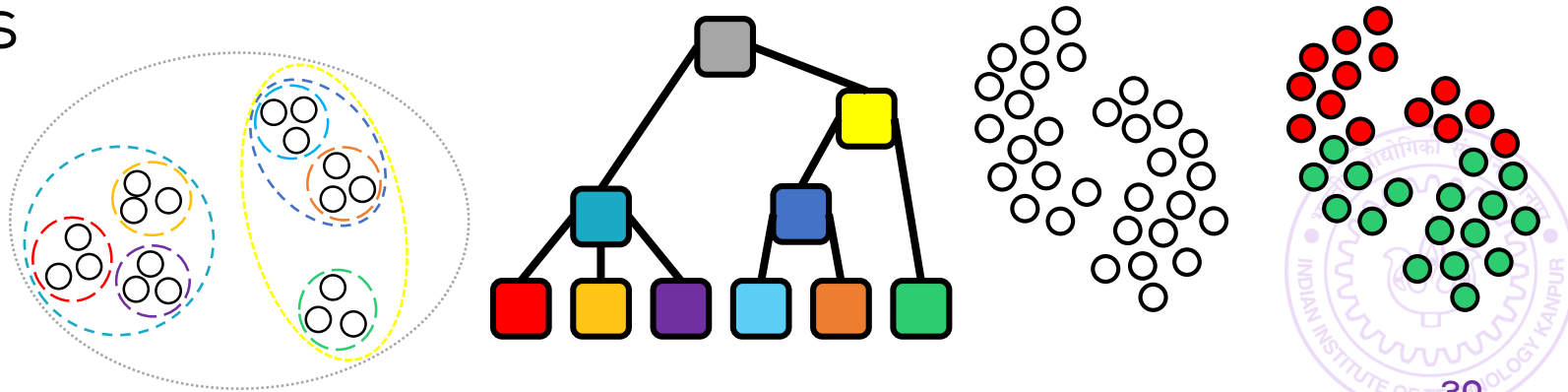
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Please give your Feedback

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