CSCI567 Machine Learning (Spring 2021)

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Outline

1. Review of last lecture
2. Gaussian mixture models

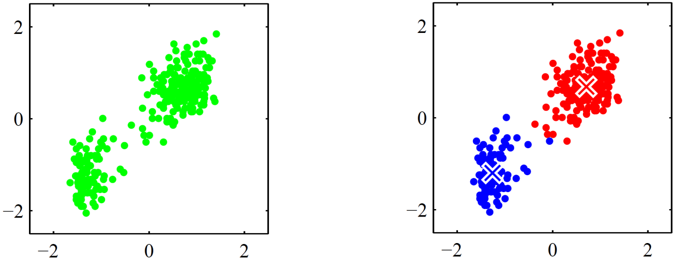
Outline

Clustering: formal definition

Given: data points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \in \mathbb{R}^{\mathsf{D}}$ and #clusters K we want

Output: group the data into K clusters, which means

- find assignment $\gamma_{nk} \in \{0, 1\}$ for each data point $n \in [N]$ and $k \in [K]$ s.t. $\sum_{k \in [K]} \gamma_{nk} = 1$ for any fixed n
- find the cluster centers $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K \in \mathbb{R}^{\mathsf{D}}$



Alternating minimization

Instead, use a heuristic that alternatingly minimizes over $\{\gamma_{nk}\}$ and $\{\boldsymbol{\mu}_k\}$:

Initialize $\{\boldsymbol{\mu}_k^{(1)}\}$

For $t = 1, 2, \ldots$

- find
$$\{\gamma_{nk}^{(t+1)}\} = \underset{\{\gamma_{nk}\}}{\operatorname{argmin}} F\left(\{\gamma_{nk}\}, \{\boldsymbol{\mu}_k^{(t)}\}\right)$$

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The K-means algorithm

Step 0 Initialize $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$

Step 1 Fix the centers $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$, assign each point to the closest center:

$$\gamma_{nk} = \mathbb{I}\left[k == \operatorname*{argmin}_c \|\boldsymbol{x}_n - \boldsymbol{\mu}_c\|_2^2\right]$$

Step 2 Fix the assignment $\{\gamma_{nk}\}$, update the centers

$$\boldsymbol{\mu}_k = \frac{\sum_n \gamma_{nk}\boldsymbol{x}_n}{\sum_n \gamma_{nk}}$$

Step 3 Return to Step 1 if not converged

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To solve GMM, we will introduce a powerful method for learning probabilistic model: **Expectation–Maximization (EM) algorithm**

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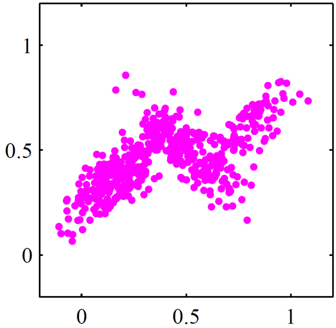

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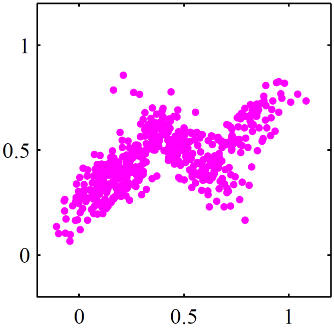
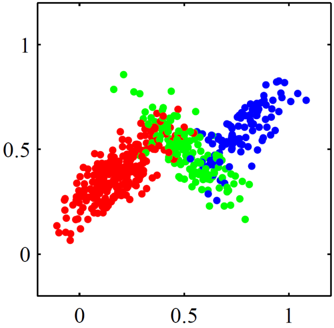
What probabilistic model generates data like this?



GMM: intuition

GMM is a natural model to explain such data

Assume there are 3 ground-truth Gaussian models.



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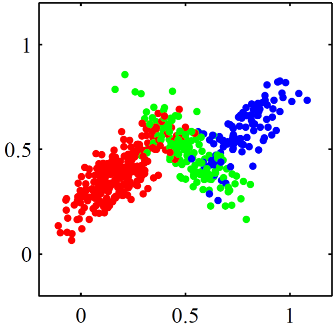

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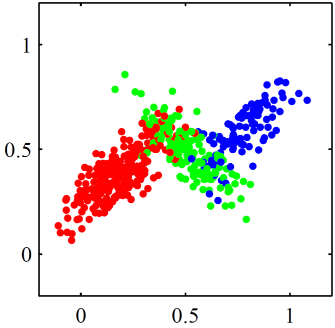

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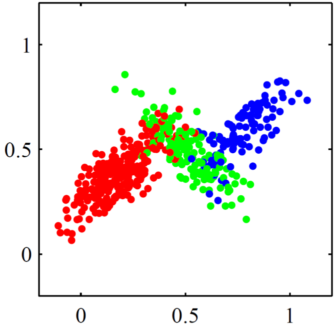

Hence the name "**Gaussian mixture model**".

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- N: the density function for a Gaussian

Another view

By introducing a **latent variable** $z \in [K]$, which indicates cluster membership, we can see p as a **marginal distribution**

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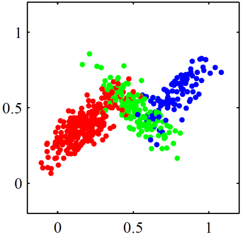
$\boldsymbol{x}$ and z are both random variables drawn from the model

- $\boldsymbol{x}$ is observed
- z is unobserved/latent

An example



The conditional distributions are

$$p(\boldsymbol{x} \mid z = \text{red}) = N(\boldsymbol{x} \mid \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)$$
$$p(\boldsymbol{x} \mid z = \text{blue}) = N(\boldsymbol{x} \mid \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)$$
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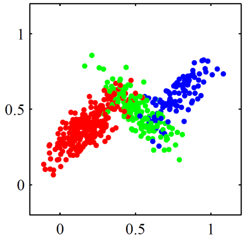

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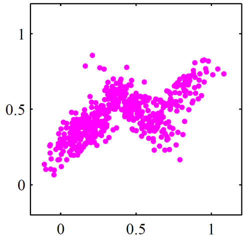

The marginal distribution is

$$p(\boldsymbol{x}) = p(\text{red}) N(\boldsymbol{x} \mid \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) + p(\text{blue}) N(\boldsymbol{x} \mid \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) + p(\text{green}) N(\boldsymbol{x} \mid \boldsymbol{\mu}_3, \boldsymbol{\Sigma}_3)$$

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- both learn the cluster centers $\boldsymbol{\mu}_k$'s
- in addition, GMM learns cluster weight ω_k and covariance $\boldsymbol{\Sigma}_k$, thus
  - we can *predict probability of seeing a new point*
  - we can *generate synthetic data*

How to learn these parameters?

An obvious attempt is **maximum-likelihood estimation (MLE)**: find

$$\underset{\boldsymbol{\theta}}{\operatorname{argmax}} \; \ln \prod_{n=1}^{N} p(\boldsymbol{x}_n \; ; \boldsymbol{\theta}) = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \sum_{n=1}^{N} \ln p(\boldsymbol{x}_n \; ; \boldsymbol{\theta}) \triangleq \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \, P(\boldsymbol{\theta})$$

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One solution is to still apply GD/SGD, but a much more effective approach is the **Expectation–Maximization (EM) algorithm**.

Preview of EM for learning GMMs

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$$\omega_k = \frac{\sum_n \gamma_{nk}}{N} \qquad \boldsymbol{\mu}_k = \frac{\sum_n \gamma_{nk}\boldsymbol{x}_n}{\sum_n \gamma_{nk}}$$

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We will see how this is a special case of EM.

Demo

Generate 50 data points from a mixture of 2 Gaussians with

- $\omega_1 = 0.3, \mu_1 = -0.8, \Sigma_1 = 0.52$
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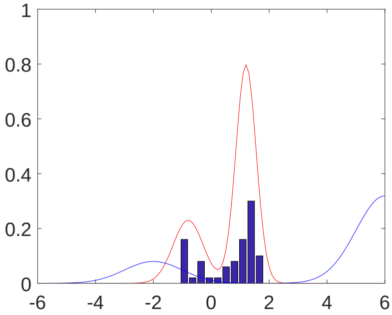

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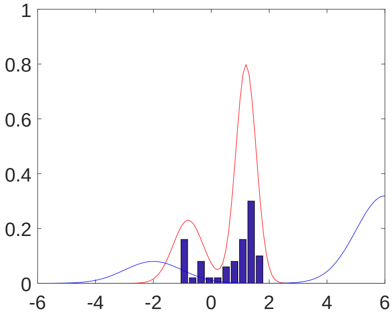

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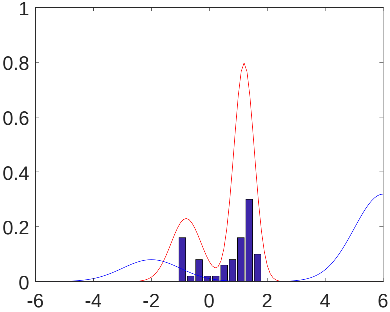

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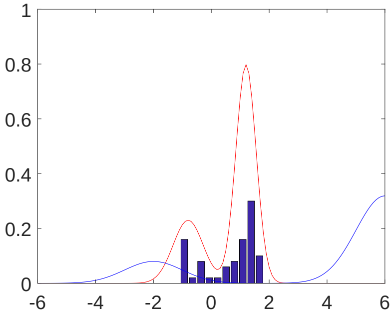

EM_demo.pdf shows how the blue curve moves towards red curve quickly via EM

EM algorithm

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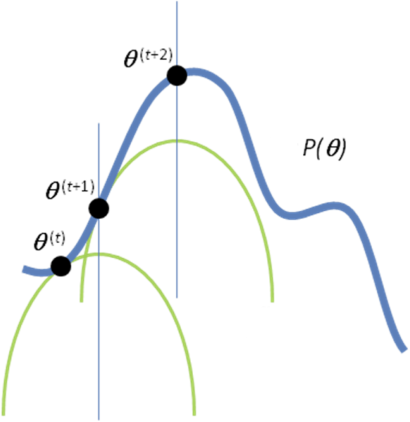
Again, directly solving the objective is intractable.

High level idea

Keep maximizing **a lower bound of P that is more manageable**



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&\geq \mathbb{E}_{z\sim q}\left[\ln \frac{p(\boldsymbol{x}, z\,;\boldsymbol{\theta})}{q(z)}\right] && \text{(Jensen's inequality)}
\end{aligned}$$

Derivation of EM

Finding the lower bound of P:

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\begin{aligned}
\ln p(\boldsymbol{x}\,;\boldsymbol{\theta}) &= \ln \int_z p(\boldsymbol{x}, z\,;\boldsymbol{\theta})dz \\
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where, $H(q) = -\mathbb{E}_{z\sim q}\left[\ln q(z)\right]$ is the Entropy. Therefore, for an observation $\boldsymbol{x}$ we have

$$\ln p(\boldsymbol{x}\,;\boldsymbol{\theta}) \geq \mathbb{E}_{z\sim q}\left[\ln p(\boldsymbol{x}, z\,;\boldsymbol{\theta})\right] + H(q)$$

Alternatively maximize the lower bound

Therefore, we obtain a lower bound for the log-likelihood function

$$
\begin{aligned}
P(\boldsymbol{\theta}) &= \sum_{n=1}^{N} \ln p(\boldsymbol{x}_n \,; \boldsymbol{\theta}) \\
&\geq \sum_{n=1}^{N} \left(\mathbb{E}_{z_n \sim q_n} \left[\ln p(\boldsymbol{x}_n, z_n \,; \boldsymbol{\theta}) \right] + H(q_n) \right) = F(\boldsymbol{\theta}, \{q_n\})
\end{aligned}
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This holds for *any* $\{q_n\}$, so how do we choose?

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This holds for *any* $\{q_n\}$, so how do we choose? Naturally, *the one that maximizes the lower bound* (i.e. the tightest lower bound)!

Equivalently, this is the same as alternatingly maximizing F over $\{q_n\}$ and $\boldsymbol{\theta}$ (similar to K-means).

Maximizing over $\{q_n\}$

Fix $\boldsymbol{\theta}^{(t)}$, the solution to

$$\operatorname*{argmax}_{q_n} \mathbb{E}_{z_n \sim q_n}\left[\ln p(\boldsymbol{x}_n, z_n \,; \boldsymbol{\theta}^{(t)})\right] + H(q_n)$$

is $q_n^{(t)}$ s.t.

$$q_n^{(t)}(z_n) = p(z_n \mid \boldsymbol{x}_n \,; \boldsymbol{\theta}^{(t)})$$

i.e., the *posterior distribution of z_n* given $\boldsymbol{x}_n$ and $\boldsymbol{\theta}^{(t)}$. (See MLaPP 11.4.7)

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Q is the (expected) **complete likelihood** and is usually more tractable.

General EM algorithm

Step 0 Initialize $\boldsymbol{\theta}^{(1)}$, $t = 1$

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and obtain **Expectation** of complete likelihood

$$Q(\boldsymbol{\theta} \,; \boldsymbol{\theta}^{(t)}) = \sum_{n=1}^{N} \mathbb{E}_{z_n \sim q_n^{(t)}} \left[\ln p(\boldsymbol{x}_n, z_n \,; \boldsymbol{\theta}) \right]$$

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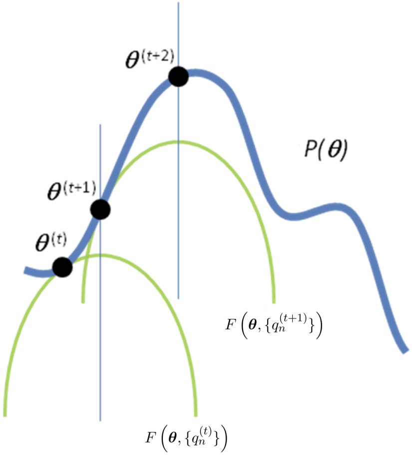
Step 2 (M-Step) **update the model parameter** via **Maximization**

$$\boldsymbol{\theta}^{(t+1)} \leftarrow \operatorname*{argmax}_{\boldsymbol{\theta}} Q(\boldsymbol{\theta} \,; \boldsymbol{\theta}^{(t)})$$

Step 3 $t \leftarrow t + 1$ and return to Step 1 if not converged

Pictorial explanation



$P(\boldsymbol{\theta})$ is non-concave, but $Q(\boldsymbol{\theta}; \boldsymbol{\theta}^{(t)})$ often is concave and easy to maximize.

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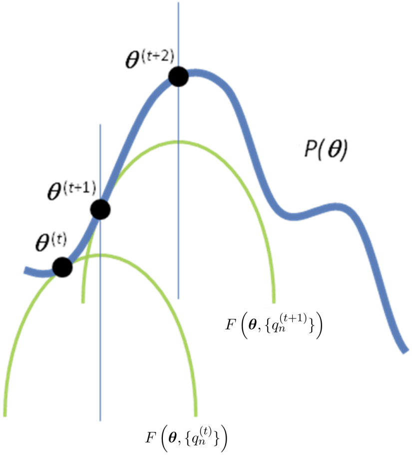

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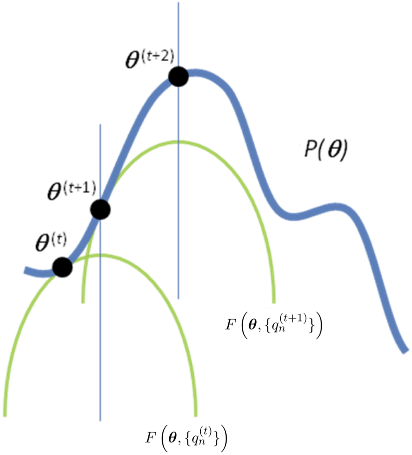

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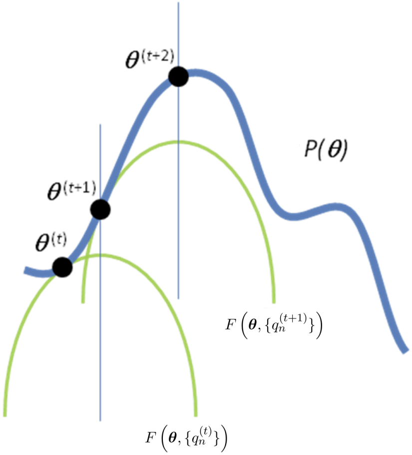

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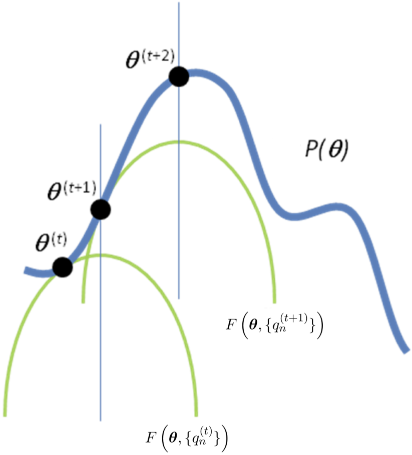

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&= P(\boldsymbol{\theta}^{(t)})
\end{aligned}
$$

So EM always increases the objective value and will converge to some local maximum (similar to K-means).

Apply EM to learn GMMs

E-Step:

$$q_n^{(t)}(z_n = k) = p\left(z_n = k \mid \boldsymbol{x}_n \,; \boldsymbol{\theta}^{(t)}\right)$$
$$\propto p\left(\boldsymbol{x}_n, z_n = k \,; \boldsymbol{\theta}^{(t)}\right)$$

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&= p\left(z_n = k ; \boldsymbol{\theta}^{(t)}\right) p(\boldsymbol{x}_n \mid z_n = k ; \boldsymbol{\theta}^{(t)}\Big) \\
&= \omega_k^{(t)} N\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)}\right)
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\end{aligned}
$$

This computes the "soft assignment" $\gamma_{nk} = q_n^{(t)}(z_n = k)$, i.e. conditional probability of $\boldsymbol{x}_n$ belonging to cluster k.

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$$\operatorname*{argmax}_{\boldsymbol{\theta}} Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}) = \operatorname*{argmax}_{\boldsymbol{\theta}} \sum_{n=1}^{N} \mathbb{E}_{z_n \sim q_n^{(t)}} \left[\ln p(\boldsymbol{x}_n, z_n \; ; \boldsymbol{\theta}) \right]$$

Apply EM to learn GMMs

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&= \operatorname*{argmax}_{\boldsymbol{\theta}} \sum_{n=1}^{N} \mathbb{E}_{z_n \sim q_n^{(t)}} \left[\ln p(z_n \, ; \boldsymbol{\theta}) + \ln p(\boldsymbol{x}_n | z_n \, ; \boldsymbol{\theta}) \right]
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&= \operatorname*{argmax}_{\{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}} \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_{nk} \left(\ln \omega_k + \ln N(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\right)
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To find $\omega_1, \ldots, \omega_K$, solve

$$\operatorname*{argmax}_{\boldsymbol{\omega}} \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_{nk} \ln \omega_k$$

Apply EM to learn GMMs

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\end{aligned}$$

To find $\omega_1, \ldots, \omega_K$, solve

$$\underset{\boldsymbol{\omega}}{\operatorname{argmax}} \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_{nk} \ln \omega_k$$

To find each $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k$, solve

$$\underset{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k}{\operatorname{argmax}} \sum_{n=1}^{N} \gamma_{nk} \ln N(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

M-Step (continued)

Solutions to previous two problems are very natural, for each k

$$\omega_k = \frac{\sum_n \gamma_{nk}}{N}$$

i.e. (weighted) fraction of examples belonging to cluster k

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$$\boldsymbol{\Sigma}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}}$$

i.e (weighted) covariance of examples belonging to cluster k

Putting it together

EM for learning GMMs:

Step 0 Initialize $\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k$ for each $k \in [K]$

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$$\omega_k = \frac{\sum_n \gamma_{nk}}{N} \qquad \boldsymbol{\mu}_k = \frac{\sum_n \gamma_{nk}\boldsymbol{x}_n}{\sum_n \gamma_{nk}}$$

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Step 2 (M-Step) **update the model parameter** (fixing assignments)

$$\omega_k = \frac{\sum_n \gamma_{nk}}{N} \qquad \boldsymbol{\mu}_k = \frac{\sum_n \gamma_{nk} \boldsymbol{x}_n}{\sum_n \gamma_{nk}}$$

$$\boldsymbol{\Sigma}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}}$$

Step 3 return to Step 1 if not converged

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GMM is a soft version of K-means and it provides a probabilistic interpretation of the data, which means we can predict and generate data after learning.