CSCI567 Machine Learning (Spring 2021)

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Outline

1. Review of last lecture
2. Gaussian mixture models

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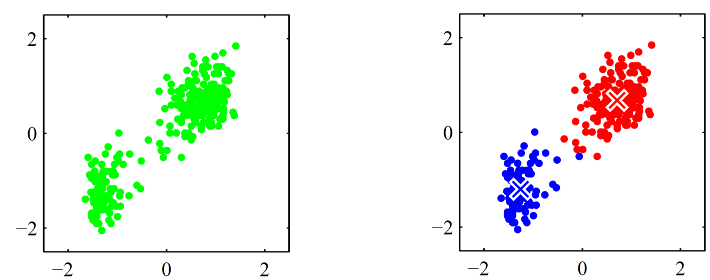
Clustering: formal definition

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

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

Outline

Gaussian mixture models

Gaussian mixture models (GMMs) are a probabilistic approach for clustering

- more explanatory than minimizing the K-means objective
- can be seen as a soft version of K-means

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

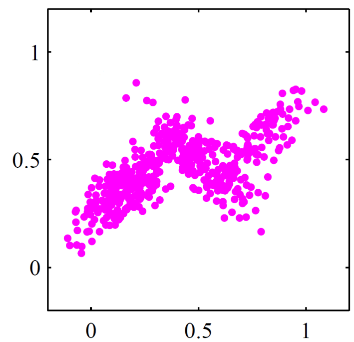
A generative model

For classification, we discussed the sigmoid model to "explain" how the labels are generated.

Similarly, for clustering, we want to come up with a probabilistic model p to **"explain" how the data is generated**.

That is, each point is an independent sample of $\boldsymbol{x} \sim p$.

What probabilistic model generates data like this?

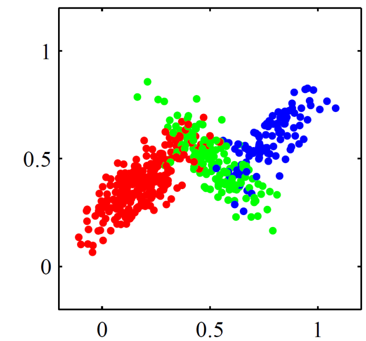


GMM: intuition

GMM is a natural model to explain such data

Assume there are 3 ground-truth Gaussian models. To generate a point, we

- first **randomly pick one of the Gaussian models**,
- then **draw a point according this Gaussian**.



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

GMM: formal definition

A GMM has the following density function:

$$p(\boldsymbol{x}) = \sum_{k=1}^{K} \omega_k N(\boldsymbol{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

where

- K: the number of Gaussian components (same as #clusters we want)
- $\omega_1, \ldots, \omega_K$: mixture weights, a distribution over K components
- $\boldsymbol{\mu}_k$ and $\boldsymbol{\Sigma}_k$: mean and covariance matrix of the k-th Gaussian
- N: the density function for a Gaussian

Another view

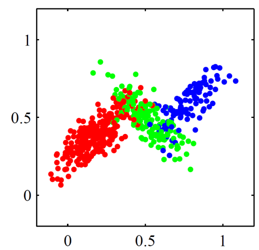
By introducing a **latent variable** $z \in [K]$, which indicates cluster membership, we can see p as a **marginal distribution**

$$p(\boldsymbol{x}) = \sum_{k=1}^{K} p(\boldsymbol{x}, z = k) = \sum_{k=1}^{K} p(z = k) p(\boldsymbol{x} | z = k) = \sum_{k=1}^{K} \omega_k N(\boldsymbol{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

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

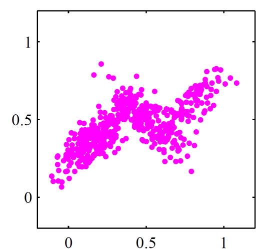
- $\boldsymbol{x}$ is observed
- z is unobserved/latent

An example



The conditional distributions are

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



The marginal distribution is

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

Learning GMMs

Learning a GMM means finding all the parameters $\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$.

In the process, we will learn the latent variable z_n as well:

$$p(z_n = k \mid \boldsymbol{x}_n) \triangleq \gamma_{nk} \in [0, 1]$$

i.e. "soft assignment" of each point to each cluster, as opposed to "hard assignment" by K-means.

GMM is more explanatory than K-means

- 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

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

This is called incomplete log-likelihood (since z_n's are unobserved), and is *intractable in general* (non-concave problem).

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

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

Step 1 (E-Step) **update the "soft assignment"** (fixing parameters)

$$\gamma_{nk} = p(z_n = k \mid \boldsymbol{x}_n) \propto \omega_k N(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

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

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

Demo

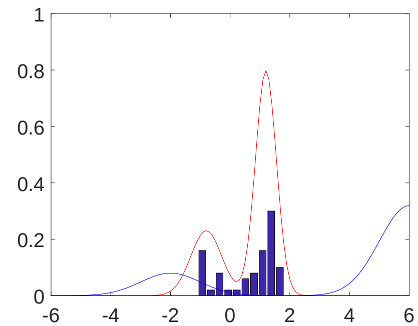
Generate 50 data points from a mixture of 2 Gaussians with

- $\omega_1 = 0.3, \mu_1 = -0.8, \Sigma_1 = 0.52$
- $\omega_2 = 0.7, \mu_2 = 1.2, \Sigma_2 = 0.35$

histogram represents the data

red curve represents the ground-truth density $p(\boldsymbol{x}) = \sum_{k=1}^{K} \omega_k N(\boldsymbol{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$

blue curve represents the learned density for a specific round



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

EM algorithm

In general EM is **a heuristic to solve MLE with latent variables** (not just GMM), i.e. find the maximizer of

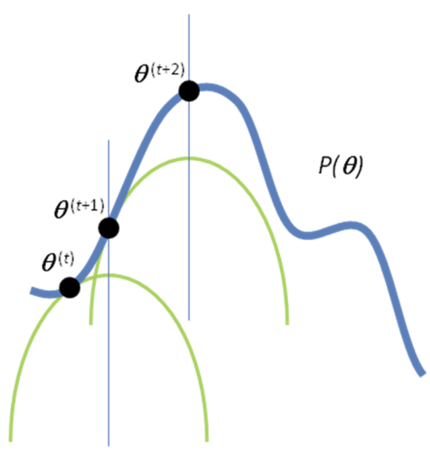
$$P(\boldsymbol{\theta}) = \sum_{n=1}^{N} \ln p(\boldsymbol{x}_n \,; \boldsymbol{\theta}) = \sum_{n=1}^{N} \ln \int_{z_n} p(\boldsymbol{x}_n, z_n \,; \boldsymbol{\theta}) dz_n$$

- $\boldsymbol{\theta}$ is the parameters for a general probabilistic model
- $\boldsymbol{x}_n$'s are observed random variables
- z_n's are latent variables

Again, directly solving the objective is intractable.

High level idea

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



Derivation of EM

Finding the lower bound of P:

$$\begin{aligned}
\ln p(\boldsymbol{x} \,; \boldsymbol{\theta}) &= \ln \int_z p(\boldsymbol{x}, z \,; \boldsymbol{\theta}) dz \\
&= \ln \int_z q(z) \frac{p(\boldsymbol{x}, z \,; \boldsymbol{\theta})}{q(z)} dz && \text{(true for any dist. } q\text{)} \\
&= \ln \mathbb{E}_{z\sim q}\left[\frac{p(\boldsymbol{x}, z \,; \boldsymbol{\theta})}{q(z)}\right] \\
&\geq \mathbb{E}_{z\sim q}\left[\ln \frac{p(\boldsymbol{x}, z \,; \boldsymbol{\theta})}{q(z)}\right] && \text{(Jensen's inequality)} \\
&= \mathbb{E}_{z\sim q}\left[\ln p(\boldsymbol{x}, z \,; \boldsymbol{\theta})\right] + H(q)
\end{aligned}$$

where, $H(q) = -\mathbb{E}_{z\sim q}[\ln q(z)]$ 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

$$\begin{aligned} P(\boldsymbol{\theta}) &= \sum_{n=1}^{N} \ln p(\boldsymbol{x}_n\,; \boldsymbol{\theta}) \\ &\geq \sum_{n=1}^{N} \left(\mathbb{E}_{z_n \sim q_n} \left[\ln p(\boldsymbol{x}_n, z_n\,; \boldsymbol{\theta}) \right] + H(q_n) \right) = F(\boldsymbol{\theta}, \{q_n\}) \end{aligned}$$

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.

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

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

So at $\boldsymbol{\theta}^{(t)}$, we found the tightest lower bound $F\left(\boldsymbol{\theta}, \{q_n^{(t)}\}\right)$:

- $F\left(\boldsymbol{\theta}, \{q_n^{(t)}\}\right) \leq P(\boldsymbol{\theta})$ for all $\boldsymbol{\theta}$.
- $F\left(\boldsymbol{\theta}^{(t)}, \{q_n^{(t)}\}\right) = P(\boldsymbol{\theta}^{(t)})$ (verify using Slide 20 and MLaPP 11.4.7)

Maximizing over $\boldsymbol{\theta}$

Fix $\{q_n^{(t)}\}$, maximize over $\boldsymbol{\theta}$:

$$\begin{aligned} &\operatorname*{argmax}_{\boldsymbol{\theta}} F\left(\boldsymbol{\theta}, \{q_n^{(t)}\}\right) \\ &= \operatorname*{argmax}_{\boldsymbol{\theta}} \sum_{n=1}^{N} \mathbb{E}_{z_n \sim q_n^{(t)}} \left[\ln p(\boldsymbol{x}_n, z_n\,; \boldsymbol{\theta}) \right] \qquad (H(q_n^{(t)}) \text{ is independent of } \boldsymbol{\theta}) \\ &\triangleq \operatorname*{argmax}_{\boldsymbol{\theta}}\ Q(\boldsymbol{\theta}\,; \boldsymbol{\theta}^{(t)}) \qquad (\{q_n^{(t)}\} \text{ are computed via } \boldsymbol{\theta}^{(t)}) \end{aligned}$$

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

General EM algorithm

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

Step 1 (E-Step) **update the posterior of latent variables**

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

and obtain **Expectation** of complete likelihood

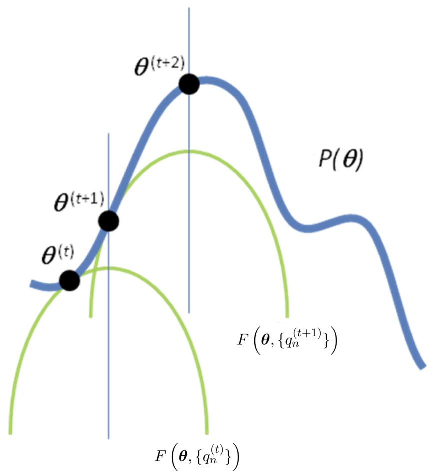
$$Q(\boldsymbol{\theta}\,; \boldsymbol{\theta}^{(t)}) = \sum_{n=1}^{N} \mathbb{E}_{z_n \sim q_n^{(t)}} \left[\ln p(\boldsymbol{x}_n, z_n\,; \boldsymbol{\theta}) \right]$$

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.

$$\begin{aligned} P(\boldsymbol{\theta}^{(t+1)}) &\geq F\left(\boldsymbol{\theta}^{(t+1)} ; \{q_n^{(t)}\}\right) \\ &\geq F\left(\boldsymbol{\theta}^{(t)} ; \{q_n^{(t)}\}\right) \\ &= P(\boldsymbol{\theta}^{(t)}) \end{aligned}$$

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:

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

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.

Apply EM to learn GMMs

M-Step:

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

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

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

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

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

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

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

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

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

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 $k \in [K]$

Step 1 (E-Step) **update the "soft assignment"** (fixing parameters)

$$\gamma_{nk} = p(z_n = k \mid \boldsymbol{x}_n) \propto \omega_k N(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

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

Connection to K-means

K-means is in fact a special case of EM for (a simplified) GMM:

- assume $\boldsymbol{\Sigma}_k = \sigma^2 \boldsymbol{I}$ for some fixed σ so only ω_k and $\boldsymbol{\mu}_k$ are parameters
- when $\sigma \to 0$, EM becomes K-means

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.