Expectation Maximization

CS771: Introduction to Machine Learning

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Building intuition for EM: a case study

Let events be "grades in a class"

w_1 = Gets an A — P(A) = ½

w_2 = Gets a B — P(B) = μ

w_3 = Gets a C — P(C) = 2μ

w_4 = Gets a D — P(D) = ½-3μ

(Note $0 \leq \mu \leq 1/6$)

Assume we want to estimate μ from data. In a given class there were

a A's
b B's
c C's
d D's

What's the maximum likelihood estimate of μ given a,b,c,d ?

Max likelihood solution

P(A) = ½ P(B) = μ P(C) = 2μ P(D) = ½-3μ

P(*a,b,c,d* | μ) = $K(½)^{a}(μ)^{b}(2μ)^{c}(½-3μ)^{d}$

log P(*a,b,c,d* | μ) = log K + *a*log ½ + *b*log μ + *c*log 2μ + *d*log (½-3μ)

$$\text{FOR MAX LIKE } \mu, \text{ SET } \frac{\partial \text{LogP}}{\partial \mu} = 0$$

$$\frac{\partial \text{LogP}}{\partial \mu} = \frac{b}{\mu} + \frac{2c}{2\mu} - \frac{3d}{1/2 - 3\mu} = 0$$

$$\text{Gives max like } \mu = \frac{b+c}{6(b+c+d)}$$

So if class got

A	B	C	D
14	6	9	10

$$\text{Max like } \mu = \frac{1}{10}$$

Same Problem with Hidden Information

Someone tells us that

Number of High grades (A's + B's) = h

Number of C's = c

Number of D's = d

What is the max. like estimate of μ now?

REMEMBER
P(A) = ½
P(B) = μ
P(C) = 2μ
P(D) = ½-3μ

Same Problem with Hidden Information

Someone tells us that

Number of High grades (A's + B's) = h

Number of C's = c

Number of D's = d

What is the max. like estimate of μ now?

We can answer this question circularly:

REMEMBER
P(A) = ½
P(B) = μ
P(C) = 2μ
P(D) = ½-3μ

EXPECTATION

If we know the value of μ we could compute the expected value of *a* and *b*

Since the ratio a:b should be the same as the ratio ½ : μ

$$a = \frac{\frac{1}{2}}{\frac{1}{2} + \mu} h \qquad b = \frac{\mu}{\frac{1}{2} + \mu} h$$

MAXIMIZATION

If we know the expected values of *a* and *b* we could compute the maximum likelihood value of μ

$$\mu = \frac{b + c}{6(b + c + d)}$$

EM for our problem

REMEMBER
P(A) = ½
P(B) = μ
P(C) = 2μ
P(D) = ½-3μ

We begin with a guess for μ

We iterate between EXPECTATION and MAXIMIZATION to improve our estimates of μ and *a* and *b*.

Define μ(t) the estimate of μ on the t'th iteration

b(t) the estimate of *b* on t'th iteration

$$\mu(0) = \text{initial guess}$$

$$b(t) = \frac{\mu(t) h}{\frac{1}{2} + \mu(t)} = \mathrm{E}[b \mid \mu(t)]$$

E -step

$$\mu(t+1) = \frac{b(t) + c}{6(b(t) + c + d)}$$

$$= \text{max like est of } \mu \text{ given } b(t)$$

M -step

EM Convergence

- Convergence proof based on fact that Prob(data | μ) must increase or remain same between each iteration [NOT OBVIOUS]
- But it can never exceed 1 [OBVIOUS]

So it must therefore converge [OBVIOUS]

In our example, suppose we had

$h = 20$

$c = 10$

$d = 10$

$\mu(0) = 0$

t	μ(t)	b(t)
0	0	0
1	0.0833	2.857
2	0.0937	3.158
3	0.0947	3.185
4	0.0948	3.187
5	0.0948	3.187
6	0.0948	3.187

Convergence is generally linear: error decreases by a constant factor each time step.

ALT-OPT/EM for Gaussian Mixture Model

MLE for Gaussian Discriminant Analysis

- Assume a K class generative classification model with Gaussian class-conditionals
- Assume class $k = 1,2,\ldots,K$ is modeled by a Gaussian with mean μ_k and cov matrix Σ_k
- Can assume label y_n to be one-hot and then $y_{nk} = 1$ if $y_n = k$, and $y_{nk} = 0$, o/w
- Assuming class prior as $p(y_n = k) = \pi_k$, the model has params $\Theta = \{\pi_k, \mu_k, \Sigma_k\}_{k=1}^{K}$
- Given training data $\{\boldsymbol{x}_n, y_n\}_{n=1}^{N}$, the MLE solution will be

$$\hat{\pi}_k = \frac{1}{N}\sum_{n=1}^{N} y_{nk}$$

Same as $\frac{N_k}{N}$ where N_k is # of training ex. for which $y_n = k$

$$\hat{\mu}_k = \frac{1}{N_k}\sum_{n=1}^{N} y_{nk}\boldsymbol{x}_n$$

Same as $\frac{1}{N_k}\sum_{n:y_n=k}^{N} \boldsymbol{x}_n$

$$\hat{\Sigma}_k = \frac{1}{N_k}\sum_{n=1}^{N} y_{nk}(\boldsymbol{x}_n - \hat{\mu}_k)(\boldsymbol{x}_n - \hat{\mu}_k)^\top$$

Same as $\frac{1}{N_k}\sum_{n:y_n=k}^{N}(\boldsymbol{x}_n - \hat{\mu}_k)(\boldsymbol{x}_n - \hat{\mu}_k)^\top$

See here for a derivation of the MLE for GDA

Observations on the GDA objective function

- Here is a formal derivation of the MLE solution for $\Theta = \{\pi_k, \mu_k, \Sigma_k\}_{k=1}^{K}$

$$\hat{\Theta} = \text{argmax}_\Theta\, p(\boldsymbol{X}, \boldsymbol{y}|\Theta) = \text{argmax}_\Theta \prod_{n=1}^{N} p(\boldsymbol{x}_n, y_n|\Theta)$$

multinoulli — Gaussian

$$= \text{argmax}_\Theta \prod_{n=1}^{N} p(y_n|\Theta)\, p(x_n|y_n, \Theta)$$

$$= \text{argmax}_\Theta \prod_{n=1}^{N} \prod_{k=1}^{K} \pi_k^{y_{nk}} \prod_{k=1}^{K} p(x_n|y_n = k, \Theta)^{y_{nk}}$$

$$= \text{argmax}_\Theta \prod_{n=1}^{N} \prod_{k=1}^{K} [\pi_k p(x_n|y_n = k, \Theta)]^{y_{nk}}$$

$$= \text{argmax}_\Theta \log \prod_{n=1}^{N} \prod_{k=1}^{K} [\pi_k p(x_n|y_n = k, \Theta)]^{y_{nk}}$$

$$= \text{argmax}_\Theta \sum_{n=1}^{N} \sum_{k=1}^{K} y_{nk}[\log \pi_k + \log \mathcal{N}(\boldsymbol{x}_n|\mu_k, \Sigma_k)]$$

In general, in models with probability distributions from the **exponential family**, the MLE problem will usually have a simple analytic form

Also, due to the form of the likelihood (Gaussian) and prior (multinoulli), the MLE problem had a nice separable structure after taking the log

Can see that, when estimating the parameters of the k^{th} Gaussian (π_k, μ_k, Σ_k), we only will only need training examples from the k^{th} class, i.e., examples for which $y_{nk} = 1$

The form of this expression is important; will encounter this in GMM too

Need for EM/ALT-OPT: Two Equivalent Perspectives

1. Consider an LVM with latent variables and parameters. Trying to estimate parameters without also estimating the latent variables (by marginalizing them) is difficult

A Gaussian Mixture Model (GMM)

$$p(\boldsymbol{x}_n|\Theta) = \sum_{k=1}^{K} p(\boldsymbol{x}_n, \boldsymbol{z}_n = k|\Theta) = \sum_{k=1}^{K} p(\boldsymbol{z}_n = k|\phi)p(\boldsymbol{x}_n|\boldsymbol{z}_n = k, \theta) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\boldsymbol{x}_n|\mu_k, \Sigma_k)$$

MLE for GMM with cluster ids marginalized/summed/integrated out

$$\Theta_{MLE} = \underset{\Theta}{\operatorname{argmax}} \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(\boldsymbol{x}_n|\mu_k, \Sigma_k)$$

Can't get closed form expressions for the π_k, μ_k, Σ_k due to "log of sum". Have to use gradient based methods

This issue not just for MLE for GMM but MLE for other LVMs too

If we knew the $\boldsymbol{z}_n$'s, the problem will be much simpler; just like MLE for generative classification with Gaussian class-conditional

Since no marginalization of the $\boldsymbol{z}_n$'s required

EM/ALT-OPT will help us "simulate" this condition by making guesses about the values of $\boldsymbol{z}_n$'s

2. Consider a complex prob. density (without any latent vars) for which MLE is hard

Directly defining a probability density as a mixture of Gaussians ($\boldsymbol{x}_n$ is generated by the k^{th} Gaussian with probability π_k) without any reference to any latent variable whatsoever (we didn't define it as an LVM)

$$p(\boldsymbol{x}_n|\Theta) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\boldsymbol{x}_n|\mu_k, \Sigma_k)$$

MLE for the params Θ of this distribution will again be hard (as we already saw above). However, we can artificially introduce a latent variable z_n with each data point $\boldsymbol{x}_n$, denoting which Gaussian generated $\boldsymbol{x}_n$

Can now apply ALT-OPT/EM to estimate parameters Θ + we get the latent variables z_n as a "by-product" (though we may not be interested in learning z_n's if our goal is just density estimation, not clustering)

Even though we didn't need the artificially introduced z_n's, their presence and doing ALT-OPT/EM made our job of estimating Θ easier!

Also in any LVM, given Θ, you can always estimate z_n's. Likewise, given z_n, you can always estimate Θ

MLE for GMM

- Already saw that MLE is hard for GMM

$$\Theta_{MLE} = \arg\max_{\Theta} \log p(\boldsymbol{X}|\Theta) = \arg\max_{\Theta} \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(\boldsymbol{x}_n|\mu_k, \Sigma_k)$$

- Two possible ways to solve this MLE problem

Will soon see how to get these guesses

1. If someone gave us optimal "point" guesses $\hat{\boldsymbol{z}}_n$'s of cluster ids $\boldsymbol{z}_n$'s, we could do MLE for the parameters just like we did for generative classification with Gaussian class-conditionals

$$\Theta_{MLE} = \arg\max_{\Theta} \log p(\boldsymbol{X}, \hat{\boldsymbol{Z}}|\Theta) = \arg\max_{\Theta} \sum_{n=1}^{N} \sum_{k=1}^{K} \hat{z}_{nk}[\log \pi_k + \log \mathcal{N}(\boldsymbol{x}_n|\mu_k, \Sigma_k)]$$

In form of a probability distribution instead of a singe "optimal" guess

2. Alternatively, if someone gave a "probabilistic" guess of $\boldsymbol{z}_n$'s, we can do MLE for $\boldsymbol{\Theta}$ as follows

$$\Theta_{MLE} = \arg\max_{\Theta} \mathbb{E}[\log p(\boldsymbol{X}, \boldsymbol{Z}|\Theta)] = \arg\max_{\Theta} \sum_{n=1}^{N} \sum_{k=1}^{K} \mathbb{E}[z_{nk}][\log \pi_k + \log \mathcal{N}(\boldsymbol{x}_n|\mu_k, \Sigma_k)]$$

Similar to Approach 1 but maximizes an expectation

The expectation is w.r.t a distribution of Z which we will see shortly

- Approach 1 is ALT-OPT and Approach 2 is Expectation Maximization ("soft" ALT-OPT). Both require alternating between estimating $\boldsymbol{Z}$ and $\boldsymbol{\Theta}$ until convergence

ALT-OPT for GMM

Keep in mind: In LVMs, assuming i.i.d. data, the quantity $\log p(\boldsymbol{X}|\Theta) = \sum_{n=1}^{N} \log p(\boldsymbol{x}_n|\Theta)$ is called incomplete data log-likelihood (ILL) whereas $\log p(\boldsymbol{X}, \boldsymbol{Z}|\Theta) = \sum_{n=1}^{N} \log p(\boldsymbol{x}_n, \boldsymbol{z}_n|\Theta)$ is called complete data log-likelihood (CLL). Goal is to maximize ILL but ALT-OPT maximizes CLL (EM too will maximize the expectation of CLL). The latent vars z_n's "complete" the data $\boldsymbol{x}_n$ ☺

- We will assume we have a "hard" (most probable) guess of z_n, say $\hat{z}_n$
- Then ALT-OPT would look like this
  - Initialize $\Theta = \{\pi_k, \mu_k, \Sigma_k\}_{k=1}^{K}$ as $\hat{\Theta}$
  - Repeat the following until convergence
    - For each n, compute most probable value (our best guess) of z_n as

$$\hat{z}_n = \text{argmax}_{k=1,2,\ldots,K}\, p(z_n = k|\hat{\Theta}, \boldsymbol{x}_n)$$

Proportional to prior prob times likelihood, i.e., $p(z_n = k|\Theta)\, p(x_n|z_n = k, \Theta) = \pi_k\, \mathcal{N}(\boldsymbol{x}_n|\mu_k, \Sigma_k)$

Posterior probability of point $\boldsymbol{x}_n$ belonging to cluster k

    - Solve MLE problem for Θ using most probable z_n's

$$\hat{\Theta} = \text{argmax}_{\Theta} \sum_{n=1}^{N} \sum_{k=1}^{K} \hat{z}_{nk}[\log \pi_k + \log \mathcal{N}(\boldsymbol{x}_n|\mu_k, \Sigma_k)]$$

Same objective function as generative K-class classification with Gaussian class-conditionals

Note: The objective function is $\sum_{n=1}^{N} \log p(\boldsymbol{x}_n, \hat{\boldsymbol{z}}_n|\Theta) = \sum_{n=1}^{N} \log p(\hat{\boldsymbol{z}}_n|\Theta) + \log p(\boldsymbol{x}_n|\hat{\boldsymbol{z}}_n, \Theta)$

$$\hat{\pi}_k = \frac{1}{N}\sum_{n=1}^{N} \hat{z}_{nk} \qquad \hat{\mu}_k = \frac{1}{N_k}\sum_{n=1}^{N} \hat{z}_{nk}\boldsymbol{x}_n$$

$$\hat{\Sigma}_k = \frac{1}{N_k}\sum_{n=1}^{N} \hat{z}_{nk}(\boldsymbol{x}_n - \hat{\mu}_k)(\boldsymbol{x}_n - \hat{\mu}_k)^\top$$

N_k : Effective number of points in cluster k

Does that matter? Should we worry that we aren't solving the actual problem anymore?

Not really; will see the justification soon ☺

But wait! This is not the same as $\sum_{n=1}^{N} \log p(\boldsymbol{x}_n|\Theta)$ which was the original MLE objective for this LVM ☹

Expectation-Maximization (EM) for GMM

Expectation of CLL

.. which we maximized in ALT-OPT

- EM finds Θ_{MLE} by maximizing $\mathbb{E}[\log p(\boldsymbol{X},\boldsymbol{Z}|\Theta)]$ rather than $\log p(\boldsymbol{X},\hat{\boldsymbol{Z}}|\Theta)$
- Note: Expectation will be w.r.t. the conditional posterior distribution of $\boldsymbol{Z}$, i.e., $p(\boldsymbol{Z}|\boldsymbol{X},\Theta)$

It is "conditional" posterior because it is also conditioned on Θ, not just data X

Why w.r.t. this distribution? Will see justification in a bit

- The EM algorithm for GMM operates as follows
  - Initialize $\Theta = \{\pi_k,\mu_k,\Sigma_k\}_{k=1}^{K}$ as $\hat{\Theta}$
  - Repeat until convergence

Requires knowing Θ

Needed to get the expected CLL

    - Compute conditional posterior $p(\boldsymbol{Z}|\boldsymbol{X},\hat{\Theta})$. Since obs are i.i.d, compute separately for each n (and for $k=1,2,..K$)

Same as $p(z_{nk}=1|\boldsymbol{x}_n,\hat{\Theta})$, just a different notation

$$p(\boldsymbol{z}_n=k|\boldsymbol{x}_n,\hat{\Theta}) \propto p(\boldsymbol{z}_n=k|\hat{\Theta})\, p(\boldsymbol{x}_n|\boldsymbol{z}_n=k,\hat{\Theta}) = \hat{\pi}_k \mathcal{N}(x_n|\hat{\mu}_k,\hat{\Sigma}_k)$$

    - Update Θ by maximizing the expected complete data log-likelihood

Solution has a similar form as ALT-OPT (or gen. class.), except we now have the expectation of z_{nk} being used

$$\hat{\Theta} = \text{argmax}_{\Theta}\mathbb{E}_{p(\boldsymbol{Z}|\boldsymbol{X},\hat{\Theta})}[\log p(\boldsymbol{X},\boldsymbol{Z}|\Theta)] = \sum_{n=1}^{N}\mathbb{E}_{p(\boldsymbol{z}_n|\boldsymbol{x}_n,\hat{\Theta})}[\log p(\boldsymbol{x}_n,\boldsymbol{z}_n|\Theta)]$$

$$= \text{argmax}_{\Theta}\ \mathbb{E}\left[\sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk}[\log \pi_k + \log \mathcal{N}(\boldsymbol{x}_n|\mu_k,\Sigma_k)]\right]$$

$$= \text{argmax}_{\Theta}\sum_{n=1}^{N}\sum_{k=1}^{K}\mathbb{E}[z_{nk}][\log \pi_k + \log \mathcal{N}(\boldsymbol{x}_n|\mu_k,\Sigma_k)]$$

$$\hat{\pi}_k = \frac{1}{N}\sum_{n=1}^{N}\mathbb{E}[z_{nk}] \qquad \hat{\mu}_k = \frac{1}{N_k}\sum_{n=1}^{N}\mathbb{E}[z_{nk}]\boldsymbol{x}_n$$

N_k : Effective number of points in cluster k

$$\hat{\Sigma}_k = \frac{1}{N_k}\sum_{n=1}^{N}\mathbb{E}[z_{nk}](\boldsymbol{x}_n-\hat{\mu}_k)(\boldsymbol{x}_n-\hat{\mu}_k)^\top$$

EM for GMM (Contd)

- The EM algo for GMM required $\mathbb{E}[z_{nk}]$. Note $z_{nk} \in \{0,1\}$

Need to normalize: $\mathbb{E}[z_{nk}] = \frac{\hat{\pi}_k \mathcal{N}(x_n|\hat{\mu}_k,\hat{\Sigma}_k)}{\sum_{\ell=1}^K \hat{\pi}_\ell \mathcal{N}(x_n|\hat{\mu}_\ell,\hat{\Sigma}_\ell)}$

Reason: $\sum_{k=1}^K \gamma_{nk} = 1$

$$\mathbb{E}[z_{nk}] = \gamma_{nk} = 0 \times p(z_{nk} = 0|x_n, \hat{\Theta}) + 1 \times p(z_{nk} = 1|x_n, \hat{\Theta}) = p(z_{nk} = 1|x_n, \hat{\Theta}) \propto \hat{\pi}_k \mathcal{N}(x_n|\hat{\mu}_k, \hat{\Sigma}_k)$$

EM for Gaussian Mixture Model

1. Initialize $\Theta = \{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$ as $\Theta^{(0)}$, set $t = 1$
2. E step: compute the expectation of each $\boldsymbol{z}_n$ (we need it in M step)

$$\mathbb{E}[z_{nk}^{(t)}] = \gamma_{nk}^{(t)} = \frac{\pi_k^{(t-1)} \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_k^{(t-1)}, \boldsymbol{\Sigma}_k^{(t-1)})}{\sum_{\ell=1}^K \pi_\ell^{(t-1)} \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_\ell^{(t-1)}, \boldsymbol{\Sigma}_\ell^{(t-1)})} \quad \forall n, k$$

Accounts for fraction of points in each cluster

Accounts for cluster shapes (since each cluster is a Gaussian

Soft K-means, which are more of a heuristic to get soft-clustering, also gave us probabilities but didn't account for cluster shapes or fraction of points in each cluster

3. Given "responsibilities" $\gamma_{nk} = \mathbb{E}[z_{nk}]$, and $N_k = \sum_{n=1}^N \gamma_{nk}$, re-estimate Θ via MLE

Effective number of points in the k^{th} cluster

M-step:

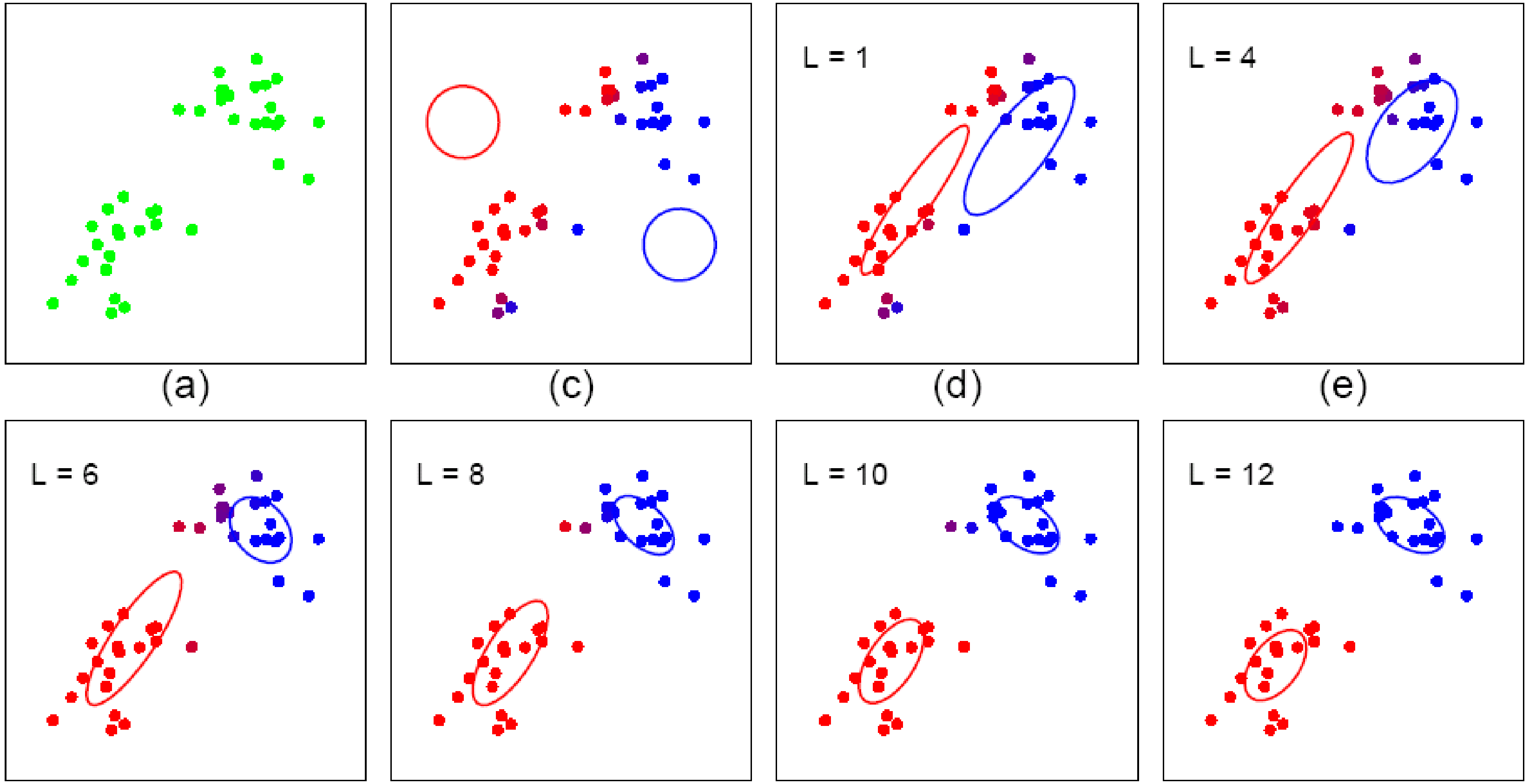
$$\boldsymbol{\mu}_k^{(t)} = \frac{1}{N_k} \sum_{n=1}^N \gamma_{nk}^{(t)} \boldsymbol{x}_n$$

$$\boldsymbol{\Sigma}_k^{(t)} = \frac{1}{N_k} \sum_{n=1}^N \gamma_{nk}^{(t)} (\boldsymbol{x}_n - \boldsymbol{\mu}_k^{(t)})(\boldsymbol{x}_n - \boldsymbol{\mu}_k^{(t)})^\top$$

$$\pi_k^{(t)} = \frac{N_k}{N}$$

4. Set $t = t + 1$ and go to step 2 if not yet converged

EM for GMM in action



(a) (c) (d) (e)
(f) (g) (h) (i)

Note: Just like with k-means, cluster initialization matters. EM only finds local optima.