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- The marginal distribution over $\mathbf{z}$ is specified in terms of the mixing coefficients:

$$p(z_k = 1) = \pi_k \tag{8}$$

And, recall, $0 \leq \pi_k \leq 1$ and $\sum_k \pi_k = 1$.

- Since $\mathbf{z}$ has a 1-of-K representation, we can also write this distribution as

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- The conditional distribution of $\mathbf{x}$ given $\mathbf{z}$ is a Gaussian:

$$p(\mathbf{x}|z_k = 1) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \tag{10}$$

or

$$p(\mathbf{x}|\mathbf{z}) = \prod_{k=1}^{K} \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{z_k} \tag{11}$$

- We are interested in the marginal distribution of $\mathbf{x}$:

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- So, given our latent variable $\mathbf{z}$, the marginal distribution of $\mathbf{x}$ is a Gaussian mixture.
- If we have N observations $\mathbf{x}_1, \ldots, \mathbf{x}_N$, then because of our chosen representation, it follows that we have a latent variable $\mathbf{z}_n$ for each observed data point $\mathbf{x}_n$.

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$$\gamma(z_k) \doteq p(z_k = 1|\mathbf{x}) = \frac{p(z_k = 1)p(\mathbf{x}|z_k = 1)}{\sum_{j=1}^{K} p(z_j = 1)p(\mathbf{x}|z_j = 1)} \tag{16}$$

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- View π_k as the prior probability of $z_k = 1$ and the quantity $\gamma(z_k)$ as the corresponding posterior probability once we have observed $\mathbf{x}$.
- $\gamma(z_k)$ can also be viewed as the responsibility that component k takes for explaining the observation $\mathbf{x}$.

Sampling from the GMM

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- The figure below-left shows samples from a three-mixture and colors the samples based on their $\mathbf{z}$. The figure below-middle shows samples from the marginal $p(\mathbf{x})$ and ignores $\mathbf{z}$. On the right, we show the $\gamma(z_k)$ for each sampled point, colored accordingly.

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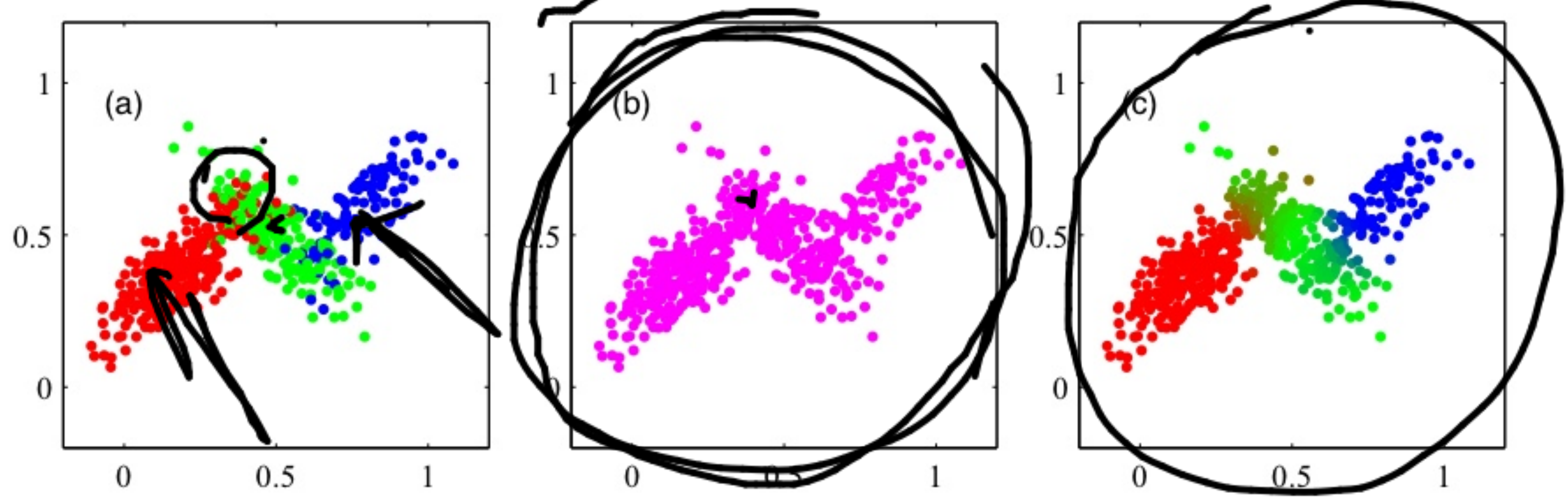

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- Ultimately, we want to find the values of the parameters $\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}$ that maximize this function.

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- The difficulty arises from the sum over k inside of the log-term. The log function no longer acts directly on the Gaussian, and no closed-form solution is available.

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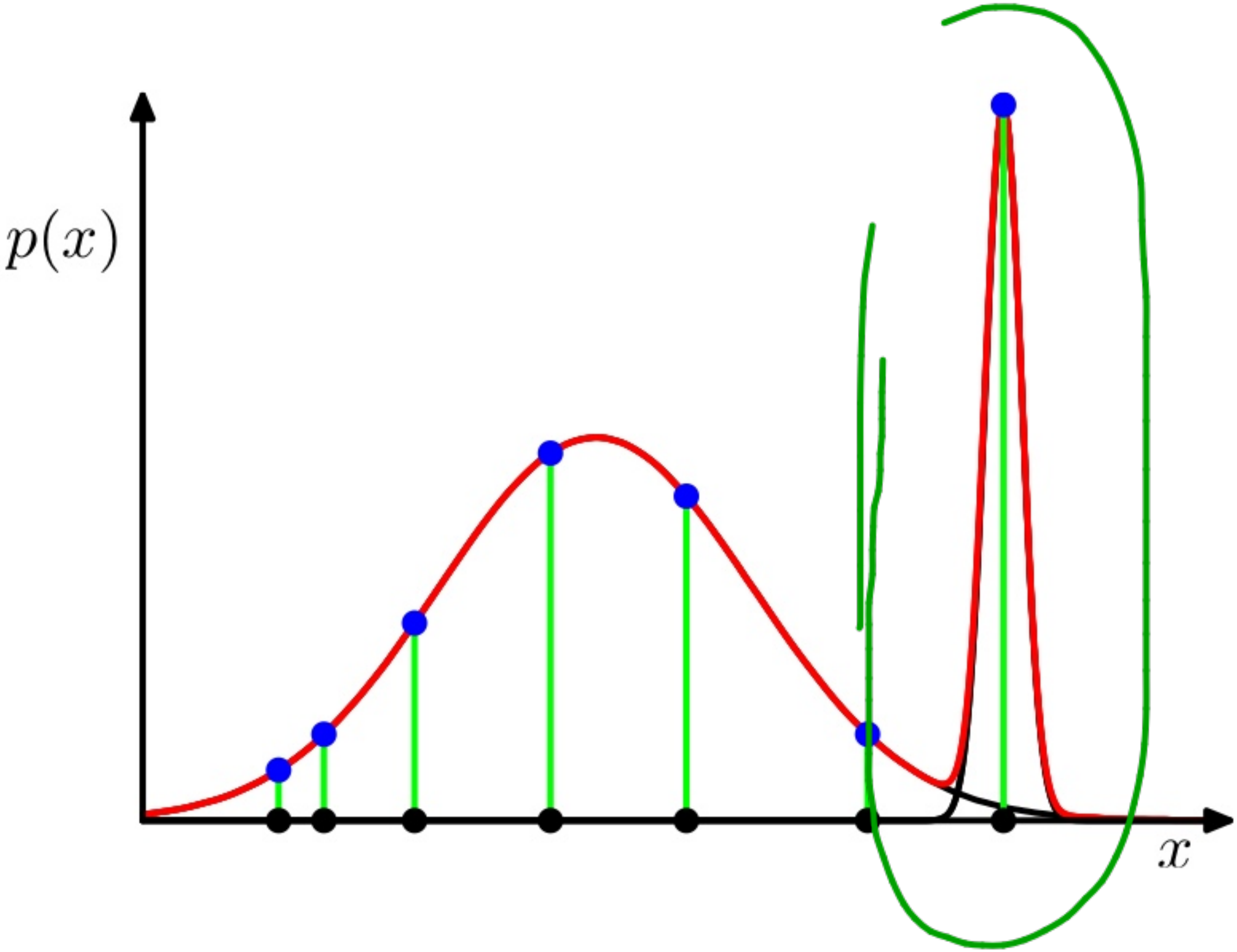
- Consider the limit $\sigma_j \rightarrow 0$ to see that this term goes to infinity and hence the log-likelihood will also go to infinity.
- **Thus, the maximization of the log-likelihood function is not a well posed problem because such a singularity will occur whenever one of the components collapses to a single, specific data point.**


$p(x)$
x

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- Recall the conditions that must be satisfied at a maximum of the likelihood function.
- For the mean $\boldsymbol{\mu}_k$, setting the derivatives of $\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$ w.r.t. $\boldsymbol{\mu}_k$ to zero yields

$$0 = -\sum_{n=1}^{N} \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} \boldsymbol{\Sigma}_k(\mathbf{x}_n - \boldsymbol{\mu}_k) \quad (20)$$

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- Note the natural appearance of the responsibility terms on the RHS.

- Multiplying by $\boldsymbol{\Sigma}_k^{-1}$, which we assume is non-singular, gives

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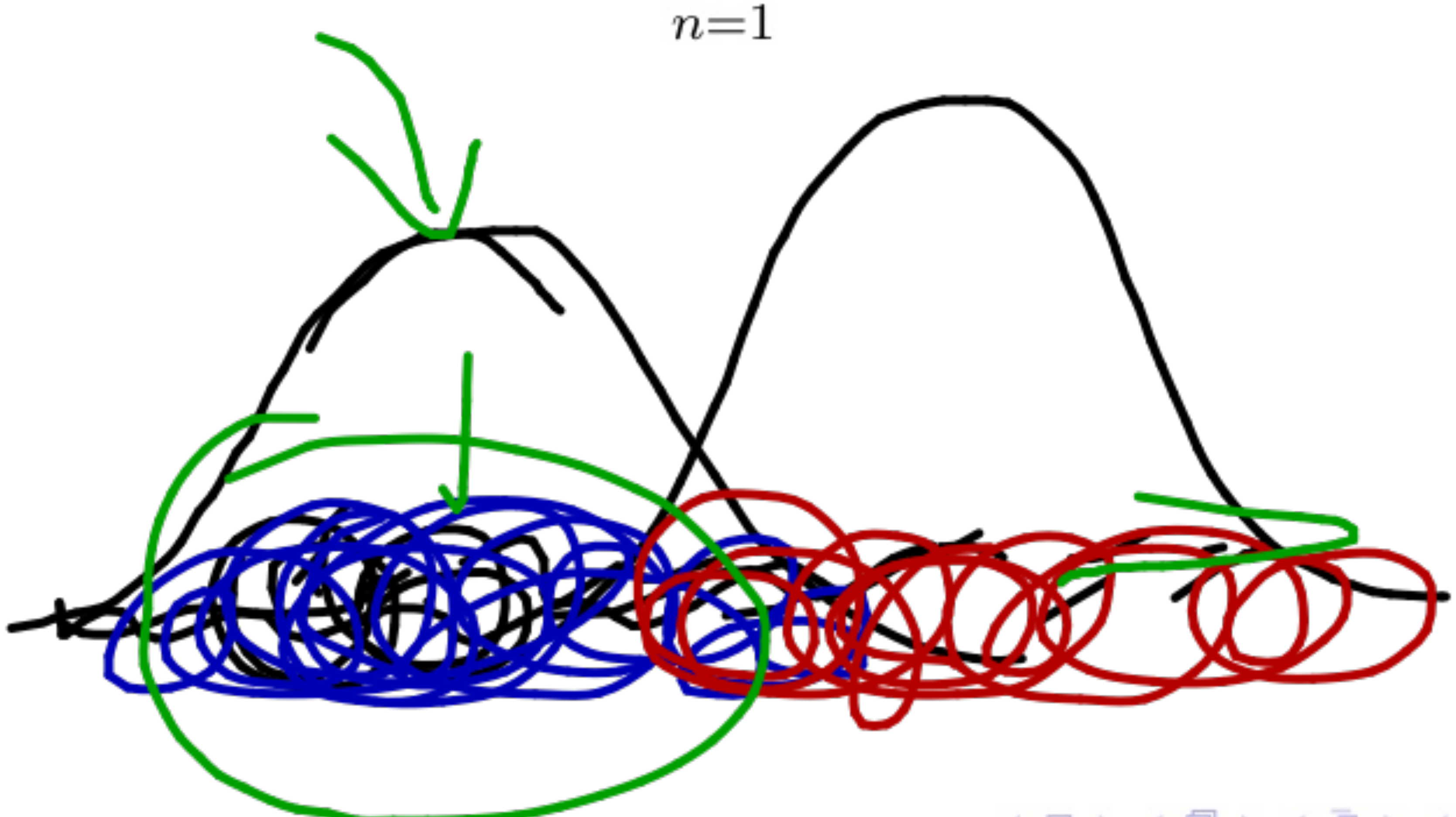

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- We find a similar result for the covariance matrix:

$$\boldsymbol{\Sigma}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) (x_n - \boldsymbol{\mu}_k)(x_n - \boldsymbol{\mu}_k)^{\mathsf{T}} \ . \tag{24}$$

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- Eliminate λ and rearrange to obtain:

$$\pi_k = \frac{N_k}{N} \tag{28}$$

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- The responsibility terms depend on these parameters in an intricate way:

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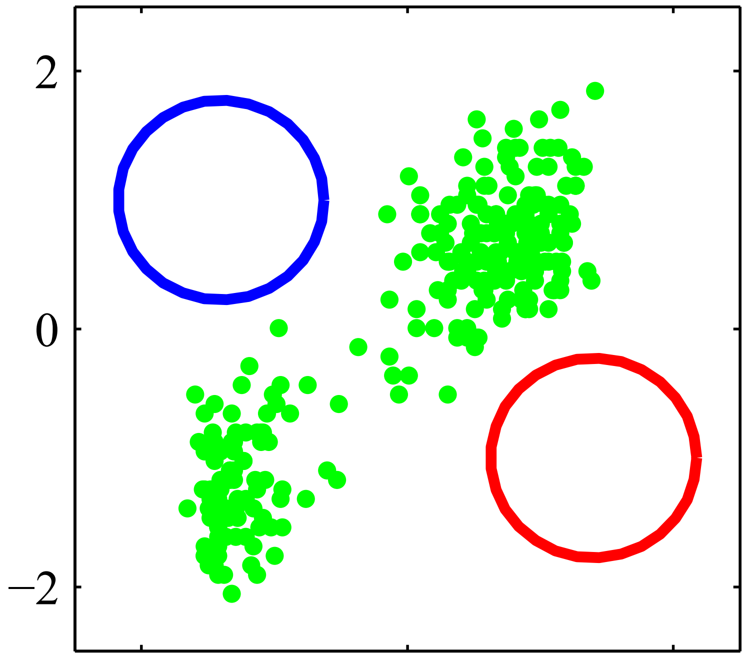
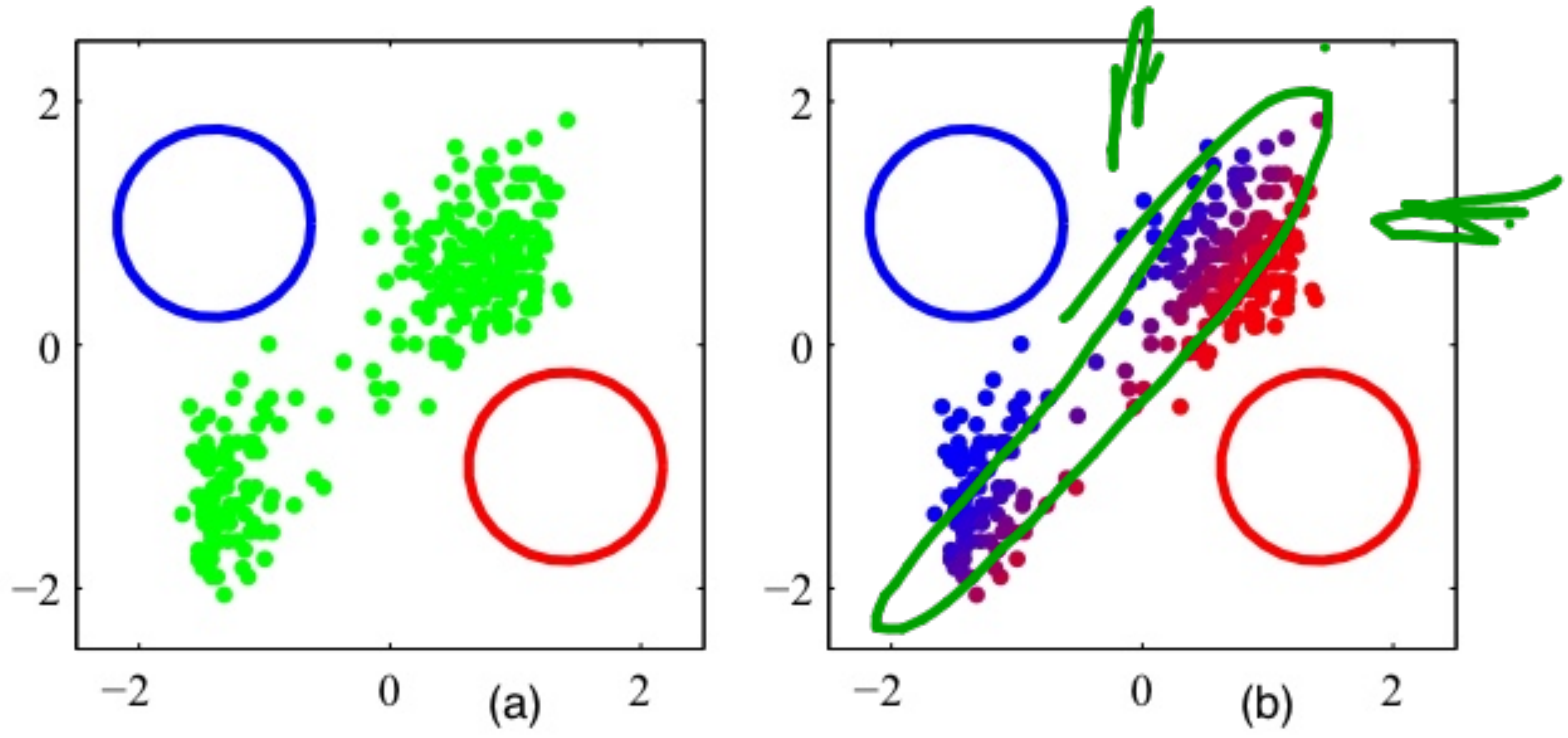
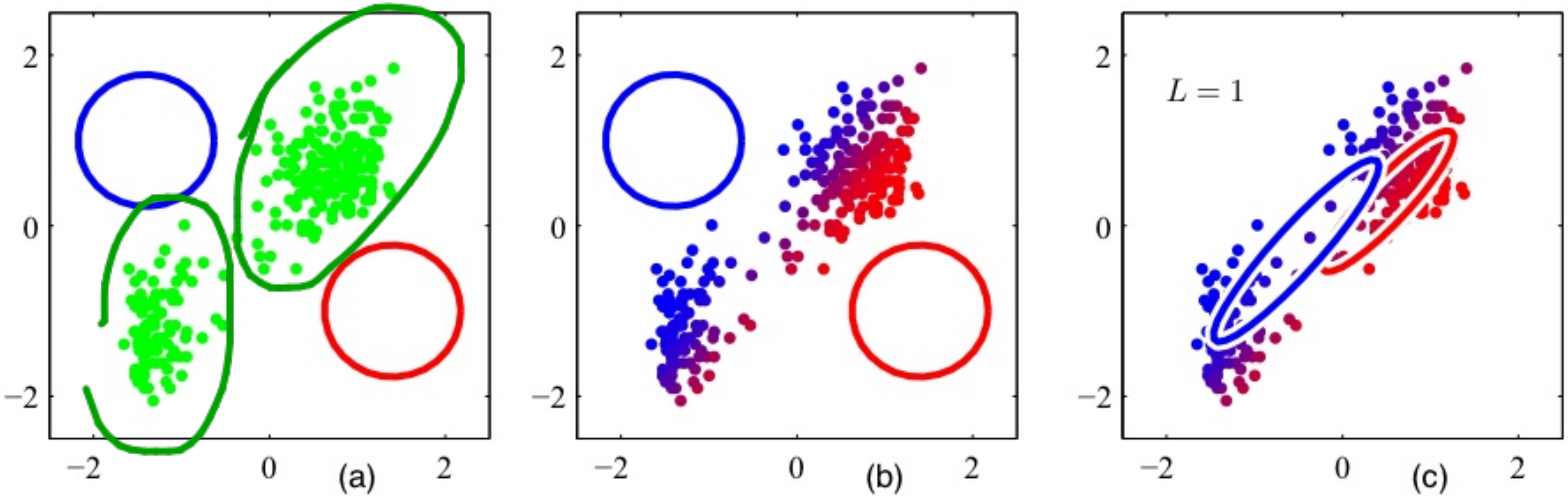
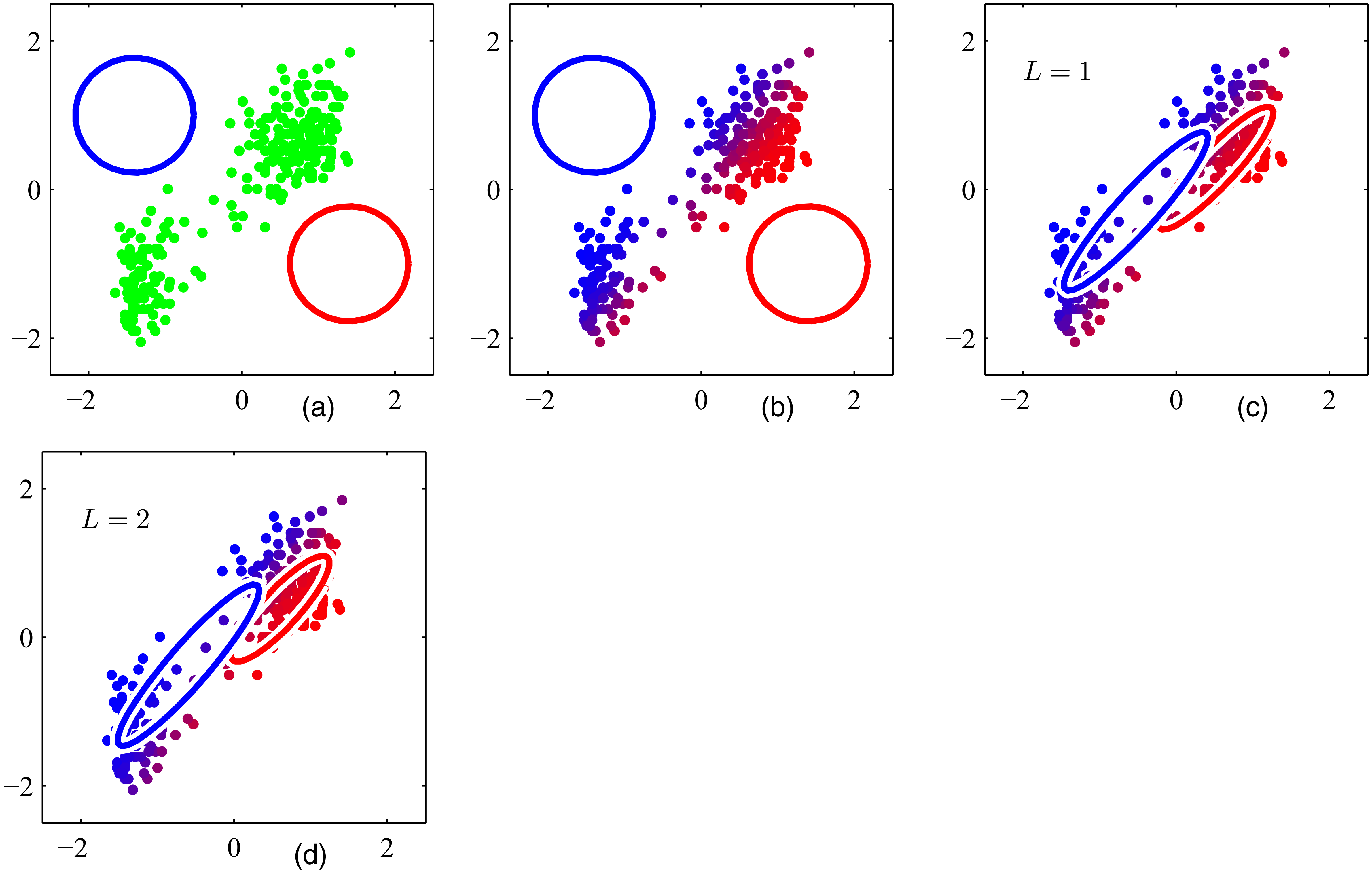
- But, these results do suggest an iterative scheme for finding a solution to the maximum likelihood problem.
  1. Chooce some initial values for the parameters, $\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}$.
  2. Use the current parameters estimates to compute the posteriors on the latent terms, i.e., the responsibilities.
  3. Use the responsibilities to update the estimates of the parameters.
  4. Repeat 2 and 3 until convergence.

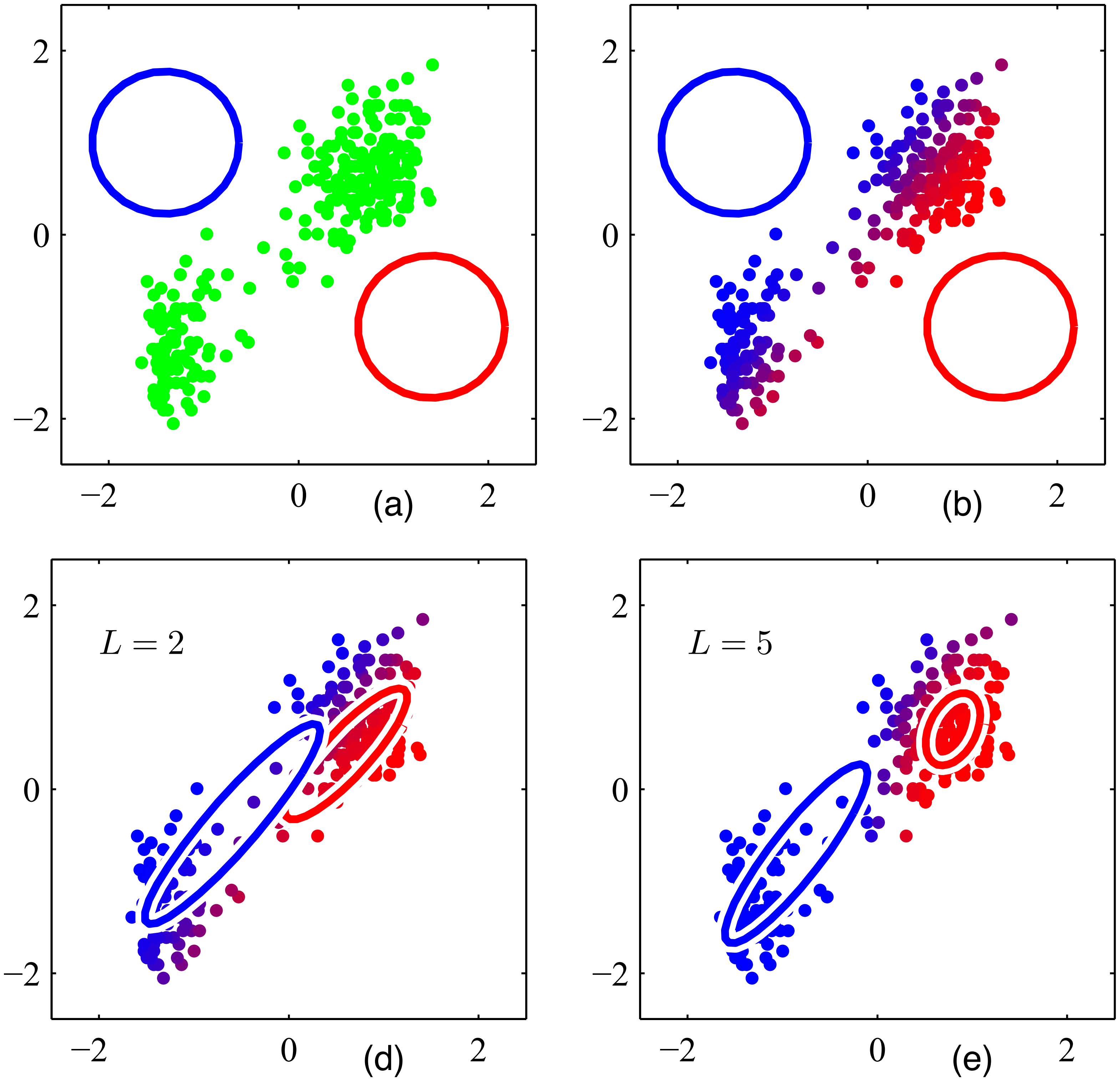


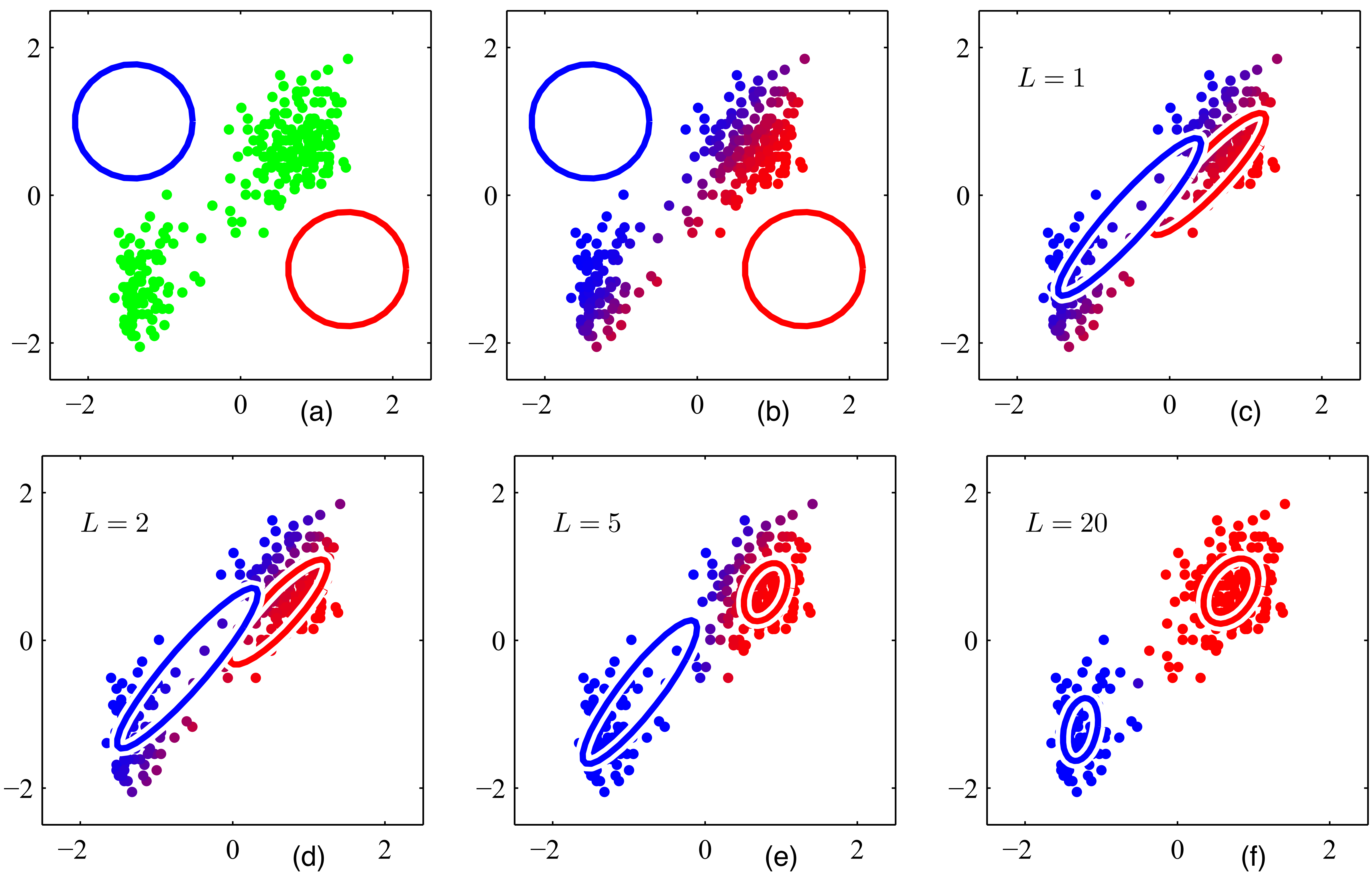
(a)


2
0
−2
−2
0
2
(a)
2
0
−2
−2
0
2
(b)


2
0
−2
−2
0
2
(a)
2
0
−2
−2
0
2
(b)
2
0
−2
−2
0
2
(c)
$L = 1$


2
0
−2
−2
0
2
(a)
(b)
L = 1
(c)
L = 2
(d)


2
0
−2
−2
0
2
(a)
(b)
L = 1
(c)
L = 2
(d)
L = 5
(e)


2
0
−2
−2
0
(a)
2
(b)
L = 1
(c)
L = 2
(d)
L = 5
(e)
L = 20
(f)

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- So, one commonly computes K-Means first and then initializes EM from the resulting clusters.
- Care must be taken to avoid singularities in the MLE solution.
- There will generally be multiple local maxima of the likelihood function and EM is not guaranteed to find the largest of these.

Given a GMM, the goal is to maximize the likelihood function with respect to the parameters (the means, the covarianes, and the mixing coefficients).

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3. **M-Step** Update the parameters using the current responsibilities

$$\boldsymbol{\mu}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n \tag{29}$$

$$\boldsymbol{\Sigma}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) (\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}})(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}})^{\mathsf{T}} \tag{30}$$

$$\pi_k^{\text{new}} = \frac{N_k}{N} \tag{31}$$

where

$$N_k = \sum_{n=1}^{N} \gamma(z_{nk}) \tag{32}$$

4. Evaluate the log-likelihood

$$\ln p(\mathbf{X}|\boldsymbol{\mu}^{\text{new}}, \boldsymbol{\Sigma}^{\text{new}}, \boldsymbol{\pi}^{\text{new}}) = \sum_{n=1}^{N} \ln \left[\sum_{k=1}^{K} \pi_k^{\text{new}} \mathcal{N}\left(\mathbf{x}_n | \boldsymbol{\mu}_k^{\text{new}}, \boldsymbol{\Sigma}_k^{\text{new}}\right) \right] \quad (33)$$

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5. Check for convergence of either the parameters of the log-likelihood. If the convergence is not satisfied, set the parameters:

$$\boldsymbol{\mu} = \boldsymbol{\mu}^{\text{new}} \tag{34}$$

$$\boldsymbol{\Sigma} = \boldsymbol{\Sigma}^{\text{new}} \tag{35}$$

$$\boldsymbol{\pi} = \boldsymbol{\pi}^{\text{new}} \tag{36}$$

and goto step 2.

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  - Even if the joint distribution $p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})$ belongs to the exponential family, the marginal $p(\mathbf{X}|\boldsymbol{\theta})$ typically does not.
- If, for each sample $\mathbf{x}_n$ we were given the value of the latent variable $\mathbf{z}_n$, then we would have a **complete** data set, $\{\mathbf{X}, \mathbf{Z}\}$, with which maximizing this likelihood term would be straightforward.

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- Then, in the M-step, we revise the parameters to $\boldsymbol{\theta}^{\text{new}}$ by maximizing this function:

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- Note that the log acts directly on the joint distribution $p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})$ and so the M-step maximization will likely be tractable.

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