CS 446/ECE 449: Machine Learning

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Gaussian Mixture Models

Recall: Linear regression (discriminative)

$$p(y^{(i)}|x^{(i)}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(y^{(i)} - \boldsymbol{w}^\top \phi(x^{(i)}))^2\right)$$

Now: (generative)

$$p(x^{(i)}|\underbrace{\mu, \sigma}_{\theta \text{ or } \boldsymbol{w}}) = \mathcal{N}(x^{(i)}|\mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x^{(i)} - \mu)^2\right)$$

Important difference: we are now interested in modeling the distribution of the data $x^{(i)}$ and not the class labels $y^{(i)}$. Though it is sometimes ambiguous what you call data or labels.

Given a dataset $\mathcal{D} = \{(x^{(i)})\}$ how to find $\theta = (\mu, \sigma)$ of

$$p(x^{(i)}|\mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x^{(i)} - \mu)^2\right)$$

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Minimize negative log-likelihood

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Minimize negative log-likelihood

Program:

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Minimize negative log-likelihood

Program:

$$\min_{\mu,\sigma} -\log \prod_{i \in \mathcal{D}} p(x^{(i)}|\mu, \sigma) := \sum_{i \in \mathcal{D}} \frac{1}{2\sigma^2}(x^{(i)} - \mu)^2 + \frac{N}{2}\log(2\pi\sigma^2)$$

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Optimality condition:

Program:

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Optimality condition:

$$\frac{\partial}{\partial\mu}: \quad \frac{1}{\sigma^2}\sum_{i\in\mathcal{D}}(x^{(i)}-\mu) = 0 \quad \Longrightarrow$$

$$\frac{\partial}{\partial\sigma}: \quad \frac{-1}{\sigma^3}\sum_{i\in\mathcal{D}}(x^{(i)}-\mu)^2 + \frac{N}{\sigma} = 0 \quad \Longrightarrow$$

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$$\frac{\partial}{\partial\sigma}: \quad \frac{-1}{\sigma^3}\sum_{i\in\mathcal{D}}(x^{(i)}-\mu)^2 + \frac{N}{\sigma} = 0 \quad \Longrightarrow$$

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$$\frac{\partial}{\partial\sigma}: \quad \frac{-1}{\sigma^3}\sum_{i\in\mathcal{D}}(x^{(i)}-\mu)^2 + \frac{N}{\sigma} = 0 \quad \Longrightarrow \quad \sigma^2 = \frac{1}{N}\sum_{i\in\mathcal{D}}(x^{(i)}-\mu)^2$$

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$$\min_{\mu,\sigma} - \log \prod_{i \in \mathcal{D}} p(x^{(i)}|\mu,\sigma) := \sum_{i \in \mathcal{D}} \frac{1}{2\sigma^2}(x^{(i)} - \mu)^2 + \frac{N}{2}\log(2\pi\sigma^2)$$

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Issue:

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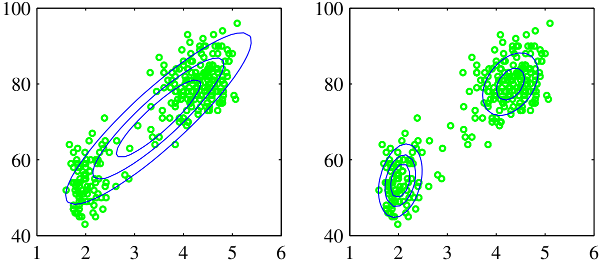
Issue: single Gaussian isn't that flexible


100
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6

Goals of this lecture

- Understanding Gaussian mixture models
- Getting to know more details about generative modeling
- Learning the relationship between Gaussian mixture models and kMeans

Reading material:

- K. Murphy; Machine Learning: A Probabilistic Perspective; Chapter 11

Fix: linear superposition of Gaussians

$$p(x^{(i)}| \underbrace{\pi, \mu, \sigma}_{\text{all components}}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x^{(i)}|\mu_k, \sigma_k)$$

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Constraints:

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Constraints:

$$\sum_{k=1}^{K} \pi_k = 1 \qquad \pi_k \geq 0$$

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How to optimize:

Fix: linear superposition of Gaussians

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How to optimize:

No closed form solution. Gradient descent is possible.

Alternative:

Alternative: auxiliary/latent variable $z_{ik} \in \{0, 1\}$ with $\sum_{k=1}^{K} z_{ik} = 1 \; \forall i$

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$$p(z_{ik} = 1) = \pi_k \qquad p(\boldsymbol{z}_i) = \prod_{k=1}^{K} \pi_k^{z_{ik}} \text{ where } \boldsymbol{z}_i = [z_{i1}, \ldots, z_{iK}]^\top$$

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Conditional

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Posterior:

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Posterior:

$$r_{ik} = p(z_{ik} = 1 | x^{(i)}) = \frac{p(z_{ik} = 1) p(x^{(i)} | z_{ik} = 1)}{\sum_{\hat{k}=1}^{K} p(z_{i\hat{k}} = 1) p(x^{(i)} | z_{i\hat{k}} = 1)} =$$

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With all those definitions at hand, minimize negative log-likelihood:

$$\min_{\pi,\mu,\sigma} -\log \prod_{i \in \mathcal{D}} p(x^{(i)}|\pi,\mu,\sigma) := -\sum_{i \in \mathcal{D}} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(x^{(i)}|\mu_k,\sigma_k) \ \text{ s.t. } \sum_{k=1}^{K} \pi_k = 1$$

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Stationary point: (per cluster weight $N_k = \sum_{i \in \mathcal{D}} r_{ik}$)

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$$\frac{\partial}{\partial\mu_k}: \quad -\sum_{i\in\mathcal{D}} r_{ik} \left(-\frac{1}{2\sigma^2}(x^{(i)} - \mu_k)\right) = 0 \quad \Longrightarrow$$

$$\frac{\partial}{\partial\sigma_k}:$$

$$\frac{\partial}{\partial\pi_k}:$$

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Stationary point: (per cluster weight $N_k = \sum_{i \in \mathcal{D}} r_{ik}$)

$$\frac{\partial}{\partial \mu_k} : \quad - \sum_{i \in \mathcal{D}} r_{ik} \left(-\frac{1}{2\sigma^2}(x^{(i)} - \mu_k)\right) = 0 \quad \Longrightarrow \quad \mu_k = \frac{1}{N_k} \sum_{i \in \mathcal{D}} r_{ik} x^{(i)}$$

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Stationary point: (per cluster weight $N_k = \sum_{i\in\mathcal{D}} r_{ik}$)

$$\frac{\partial}{\partial\mu_k}: \quad -\sum_{i\in\mathcal{D}} r_{ik} \left(-\frac{1}{2\sigma^2}(x^{(i)}-\mu_k)\right) = 0 \quad \Longrightarrow \quad \mu_k = \frac{1}{N_k}\sum_{i\in\mathcal{D}} r_{ik} x^{(i)}$$

$$\frac{\partial}{\partial\sigma_k}: \sum_{i\in\mathcal{D}} r_{ik} \left(\frac{1}{\sigma} - \frac{1}{\sigma^3}(x^{(i)}-\mu_k)^2\right) = 0 \Longrightarrow$$

$$\frac{\partial}{\partial\pi_k}:$$

With all those definitions at hand, minimize negative log-likelihood:

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Stationary point: (per cluster weight $N_k = \sum_{i\in\mathcal{D}} r_{ik}$)

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Not a closed form solution

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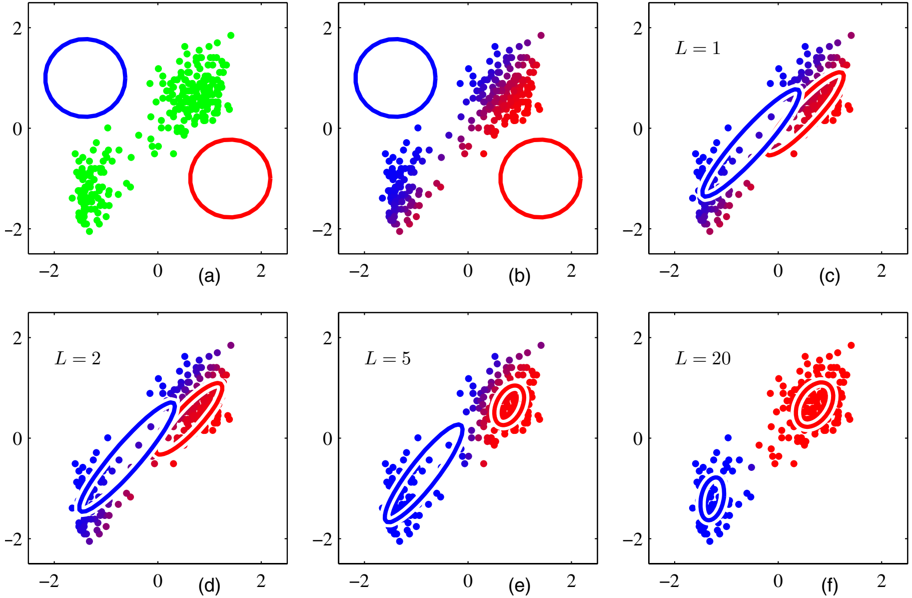
\end{aligned}$$



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

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Can we make this similarity formal?

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What happens for $\epsilon \rightarrow 0$?

- In the denominator the term for which $(x^{(i)} - \mu_{\hat{k}})^2$ is smallest goes to zero slowest
- All responsibilities will go to zero except the one for which $(x^{(i)} - \mu_{\hat{k}})^2$ is smallest, which will go to unity

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- Cost function can be shown to be identical in the limit

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- How do we find the means, variances and responsibilities of the Gaussian mixture model?

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What's next

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What's next

- Generalizing the Gaussian mixture model concept