

Advanced Section: Gaussian Mixture Models

CS 109B

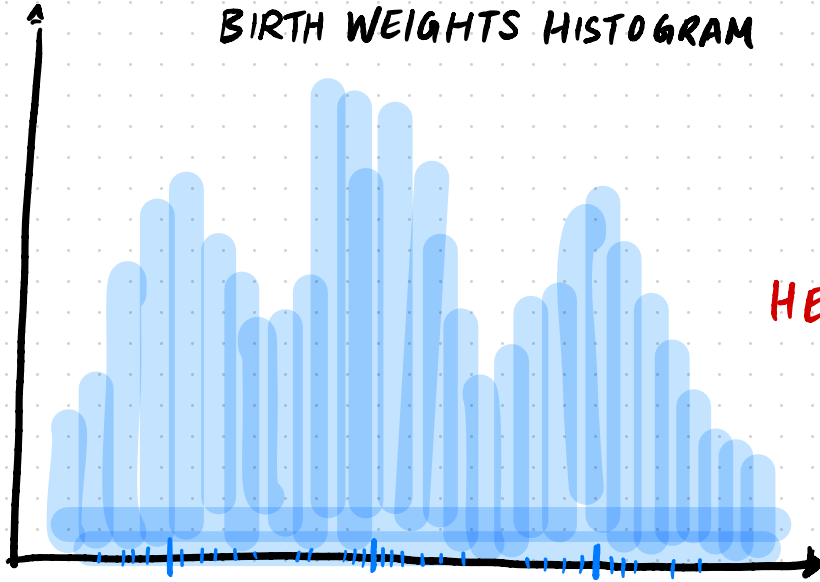
Spring, 2021





NON (PROBABILISTIC) MODEL BASED CLUSTERING

BIRTH WEIGHTS HISTOGRAM



- How many clusters are there?
- How do we find them?

HEURISTIC

K-MEANS:

1. Assign points to clusters based on cluster means
 2. Based on point assignments update cluster means
- How do we evaluate the quality of the clusters?

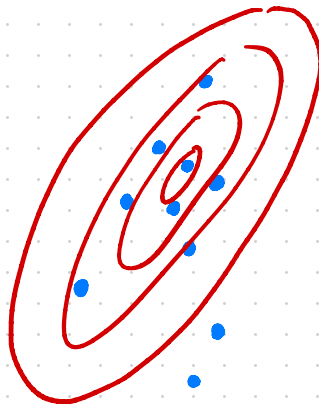
PROBABILISTIC VS NON-PROBABILISTIC APPROACHES

IS THIS ONE CLUSTER?



ASSUMPTIONS ABOUT
CLUSTERS UNSTATED

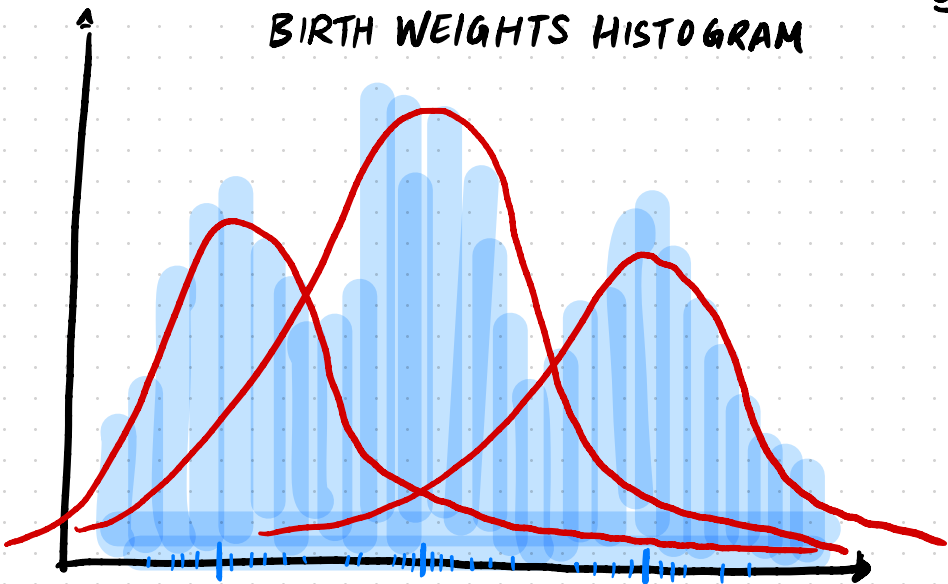
DOES THE DATA COME FROM $N(\mu, \Sigma)$?



ASSUMPTIONS ABOUT CLUSTERS
EXPLICITLY STATED

PROBABILISTIC MODELS FOR CLUSTERING

BIRTH WEIGHTS HISTOGRAM



GAUSSIAN MIXTURE MODEL (GMM)

$$l = \pi_1 N(y_n; \mu_1, \sigma_1^2) + \\ \pi_2 N(y_n; \mu_2, \sigma_2^2) + \\ \pi_3 N(y_n; \mu_3, \sigma_3^2)$$

ASSUMPTIONS

- Each cluster is a Gaussian
- clusters are "mixed" as Gaussians overlap

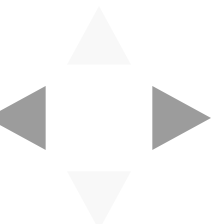
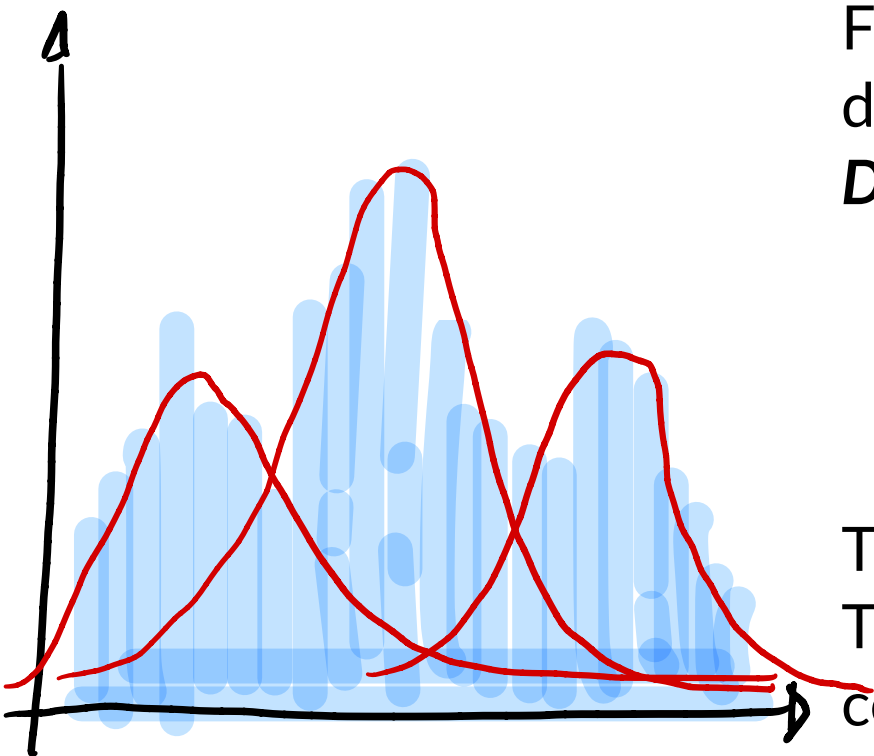
A Similarity Measure for Distributions: Kullback–Leibler Divergence

Visually comparing models to the *empirical distribution* of the data is impractical. Fortunately, there are a large number of quantitative measures for comparing two distributions, these are called *divergence measures*. For example, the *Kullback–Leibler (KL) Divergence* is defined for two distributions $p(\theta)$ and $q(\theta)$ supported on Θ as:

$$D_{\text{KL}}[q \parallel p] = \int_{\Theta} \log \left[\frac{q(\theta)}{p(\theta)} \right] q(\theta) d\theta$$

The KL-divergence $D_{\text{KL}}[q \parallel p]$ is bounded below by 0, which happens if and only if $q = p$. The KL-divergence has information theoretic interpretations that we will explore later in the course.

Note: The KL-divergence is defined in terms of the pdf's of p and q . If p is a distribution from which we only have samples and not the pdf (like the empirical distribution), we can nonetheless estimate $D_{\text{KL}}[q \parallel p]$. Techniques that estimate the KL-divergence from samples are called *non-parametric*. We will use them later in the course.



INFERENCE FOR GMM'S: LIKELIHOOD MAXIMIZATION

$$\begin{aligned} \underbrace{\ell(\pi_k, \mu_k, \sigma_k^2)}_{\text{joint likelihood of the data set}} &= \log \prod_{n=1}^N \sum_{k=1}^K \pi_k N(y_n; \mu_k, \sigma_k^2) \\ &= \sum_{n=1}^N \log \underbrace{\sum_{k=1}^K \pi_k N(y_n; \mu_k, \sigma_k^2)}_{\text{likelihood of each point}} \end{aligned}$$

GOAL: find π_k, μ_k, σ_k^2 to maximize the likelihood of the dataset.

HOW: Want to do gradient descent: Want:

$$\hookrightarrow \nabla_{\pi_k, \mu_k, \sigma_k^2} \ell$$

BUT: • Gradient seems complicated
• This is secretly a constrained opt problem

$$\hookrightarrow \sigma_k > 0$$

$$\hookrightarrow \sum_{k=1}^K \pi_k = 1$$

1. Guess which Gaussians gets which points

2. Then it's easy to compute MLE of π_k, μ_k, σ_k^2

EX: μ_k is empirical mean of pts in k -th Gaussian

Class Membership as a Latent Variable

We observe that there are three *clusters* in the data. We posit that there are three *classes* of infants in the study: infants with low birth weights, infants with normal birth weights and those with high birth weights. The numbers of infants in the classes are not equal.

OBSERVED DATA LOG-
LIKELIHOOD

For each observation Y_n , we model its class membership Z_n as a categorical variable,

$$Z_n \sim \text{Cat}(\pi),$$

$$P(y_n) = \int P(y_n | z_n) p(z_n) dz_n$$

$$= \sum_{k=1}^K P(z_n=k) P(y_n | z_n)$$

where π_i in $\pi = [\pi_1, \pi_2, \pi_3]$ is the class proportion. Note that we don't have the class membership Z_n in the data! So Z_n is called a *latent variable*.

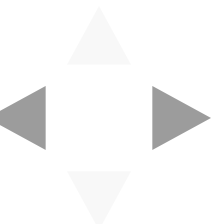
$$= \sum_{k=1}^K \pi_{1k} P(y_n | z_n)$$

Depending on the class, the n -th birth weight Y_n will have a different normal distribution,

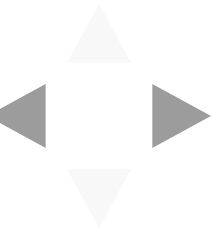
$$= \sum_{k=1}^K \pi_{1k} N(y_n; \mu_{1k}, \sigma_{1k}^2)$$

$$Y_n | Z_n \sim \mathcal{N}(\mu_{Z_n}, \sigma_{Z_n}^2)$$

where μ_{Z_n} is one of the three class means $[\mu_1, \mu_2, \mu_3]$ and $\sigma_{Z_n}^2$ is one of the three class variances $[\sigma_1^2, \sigma_2^2, \sigma_3^2]$.

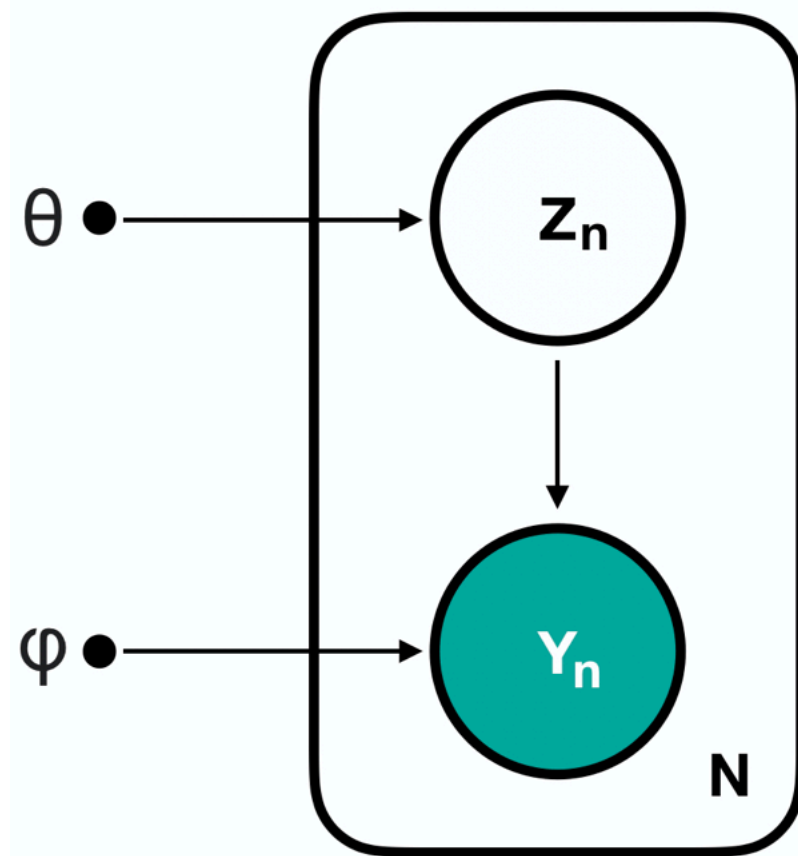


Common Latent Variable Models

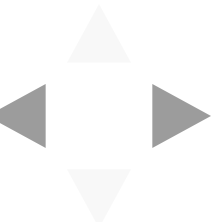


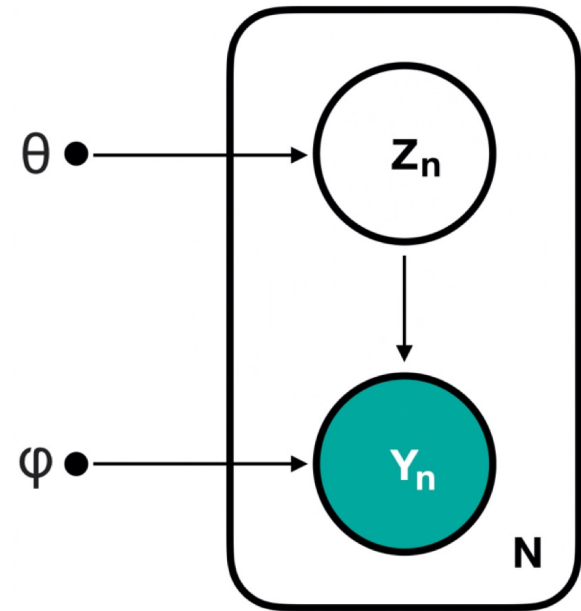
Latent Variable Models

Models that include an observed variable Y and at least one unobserved variable Z are called *latent variable models*. In general, our model can allow Y and Z to interact in many different ways. Today, we will study models with one type of interaction:



$$\begin{aligned} Z_n &\sim p(Z|\theta) \\ Y_n|Z_n &\sim p(Y|Z, \phi) \\ n &= 1, \dots, N \end{aligned}$$





Item-Response Models

In *item-response models*, we measure an real-valued unobserved trait Z of a subject by performing a series of experiments with binary observable outcomes, Y :

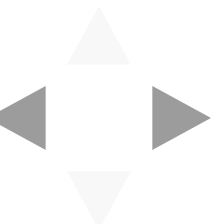
$$\begin{aligned} Z_n &\sim \mathcal{N}(\mu, \sigma^2), \\ \theta_n &= g(Z_n) \\ Y_n | Z_n &\sim \text{Ber}(\theta_n), \end{aligned}$$

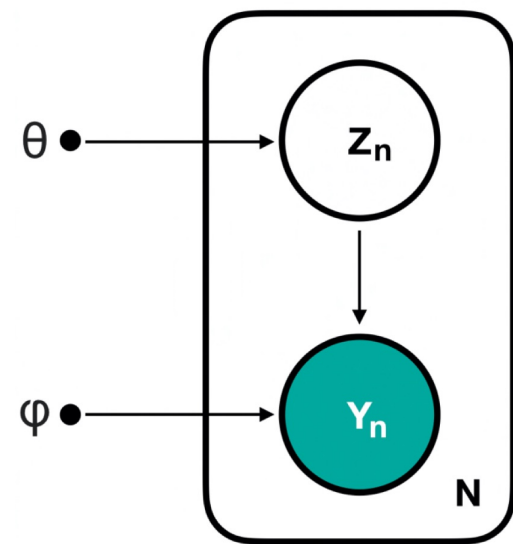
where $n = 1, \dots, N$ and g is some fixed function of Z_n .

Applications

Item response models are used to model the way "underlying intelligence" Z relates to scores Y on IQ tests.

Item response models can also be used to model the way "suicidality" Z relates to answers on mental health surveys. Building a good model may help to infer when a patient is at psychiatric risk based on in-take surveys at points of care through out the health-care system.





Factor Analysis Models

In *factor analysis models*, we posit that the observed data Y with many measurements is generated by a small set of unobserved factors Z :

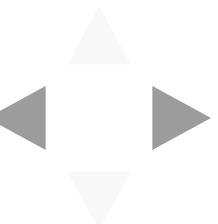
$$Z_n \sim \mathcal{N}(0, I),$$

$$Y_n | Z_n \sim \mathcal{N}(\mu + \Lambda Z_n, \Phi),$$

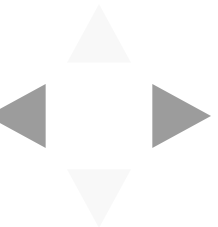
where $n = 1, \dots, N$, $Z_n \in \mathbb{R}^{D'}$ and $Y_n \in \mathbb{R}^D$. We typically assume that D' is much smaller than D .

Applications

Factor analysis models are useful for biomedical data, where we typically measure a large number of characteristics of a patient (e.g. blood pressure, heart rate, etc), but these characteristics are all generated by a small list of health factors (e.g. diabetes, cancer, hypertension etc). Building a good model means we may be able to infer the list of health factors of a patient from their observed measurements.



Maximum Likelihood Estimation for Latent Variable Models: Expectation Maximization



MODEL



$y \sim p(y|z, \theta)$
 $z \sim p(z|\theta)$
 parameters: θ, ϕ

Calculus facts we need:

1. $E[f(x)] = \int f(x)p(x) dx$

2. properties of E :

A. $E[z + \sum_{i=1}^n f_i(x)] = z + \sum_{i=1}^n E[f_i(x)]$

(Jensen's inequality) $\rightarrow B. \log E[f(x)] \geq E[\log f(x)]$

C. $\nabla_x E[f(x)] = E[\nabla_x f(x)]$

3. $D_{KL}[q(x)||p(x)] = \int \log \left[\frac{q(x)}{p(x)} \right] q(x) dx$
 $= E \left[\log \left(\frac{q(x)}{p(x)} \right) \right]$

Likelihood over $q(z)$:

$$\log \prod_{n=1}^N p(y_n|z_n, \theta) p(z_n|\theta) = \sum_{n=1}^N \log p(y_n|z_n, \theta) + \log p(z_n|\theta)$$

can we evaluate this?

Likelihood over observed data:

$$\log \prod_{n=1}^N p(y_n|\theta, \phi) = \sum_{n=1}^N \log p(y_n|\theta, \phi)$$

does the log help?

$$= \sum_{n=1}^N \log \int p(y_n|z_n, \theta) p(z_n|\theta) dz_n$$

$$= \sum_{n=1}^N \log E_{z_n \sim p(z_n|\theta)} [p(y_n|z_n, \theta)]$$

The maximum likelihood objective:

$$\theta_{ML}, \phi_{ML} = \underset{\theta, \phi}{\text{argmax}} \ell(\theta, \phi) = \underset{\theta, \phi}{\text{argmax}} \sum_{n=1}^N \log E_{z_n \sim p(z_n|\theta)} [p(y_n|z_n, \theta)]$$

is this hard?

Trying out the optimization:

$$\nabla_{\theta, \phi} \ell(\theta, \phi) = \nabla_{\theta, \phi} \sum_{n=1}^N \log E_{z_n \sim p(z_n|\theta)} [p(y_n|z_n, \theta)]$$

$$= \sum_{n=1}^N \nabla_{\theta, \phi} \log E_{z_n \sim p(z_n|\theta)} [p(y_n|z_n, \theta)]$$

$$\stackrel{a.}{=} \sum_{n=1}^N \frac{\nabla_{\theta, \phi} E_{z_n \sim p(z_n|\theta)} [p(y_n|z_n, \theta)]}{E_{z_n \sim p(z_n|\theta)} [p(y_n|z_n, \theta)]}$$

can we MC estimate this?



An objective we can actually work with:

$$\max_{\theta, \phi} \ell(\theta, \phi) = \max_{\theta, \phi} \sum_{n=1}^N \log E_{z_n \sim p(z_n|\theta)} [p(y_n|z_n, \theta)]$$

$$= \max_{\theta, \phi} \sum_{n=1}^N \log \int p(y_n|z_n, \theta) p(z_n|\theta) dz_n$$

$$= \max_{\theta, \phi} \sum_{n=1}^N \log \int \frac{p(y_n|z_n, \theta) p(z_n|\theta)}{q(z_n)} q(z_n) dz_n$$

introduce auxiliary variables $q(z)$!
 q is some distr. of your choice.

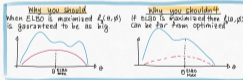
$$= \max_{\theta, \phi} \sum_{n=1}^N \log E_{z_n \sim q(z_n)} \left[\frac{p(y_n|z_n, \theta) p(z_n|\theta)}{q(z_n)} \right]$$

is the log helping? does $\nabla_{\theta, \phi}$ commute with $E_{q(z)}$?

$$\geq \max_{\theta, \phi, q} \sum_{n=1}^N E_{z_n \sim q(z_n)} \left[\log \left(\frac{p(y_n|z_n, \theta) p(z_n|\theta)}{q(z_n)} \right) \right]$$

The Evidence Lower Bound ELBO(θ, ϕ, q)

Idea: Instead of maximizing the log-likelihood, we maximize the lower bound ELBO.



How to maximize ELBO: coordinate ascent

I. Maximize θ, ϕ , fixing q^*

$$\theta^*, \phi^* = \underset{\theta, \phi}{\text{argmax}} \text{ELBO}(\theta, \phi, q^*)$$

$$= \underset{\theta, \phi}{\text{argmax}} \sum_{n=1}^N E_{z_n \sim q^*(z_n)} \left[\log \left(\frac{p(y_n|z_n, \theta) p(z_n|\theta)}{q^*(z_n)} \right) \right]$$

$$(M\text{-step}) = \underset{\theta, \phi}{\text{argmax}} \sum_{n=1}^N \left(E_{z_n \sim q^*(z_n)} \left[\log [p(y_n|z_n, \theta) p(z_n|\theta)] \right] \right)$$

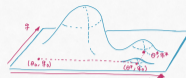
$$- E_{z_n \sim q^*(z_n)} [q^*(z_n)]$$

irrelevant for $\max_{\theta, \phi}$

$$\equiv \underset{\theta, \phi}{\text{argmax}} \sum_{n=1}^N E_{z_n \sim q^*(z_n)} \left[\log [p(y_n|z_n, \theta) p(z_n|\theta)] \right]$$

is this problem easier?

Are we done?



Maximizing each coordinate once is not sufficient! we need to iterate!

II. Maximize q , fixing θ^*, ϕ^*

$$q^* = \underset{q}{\text{argmax}} \text{ELBO}(\theta^*, \phi^*, q)$$

NOTE: $\ell(\theta^*, \phi^*) - \text{ELBO}(\theta^*, \phi^*, q) = \sum_{n=1}^N \left[\log p(y_n|\theta^*, \phi^*) - E_{z_n \sim q(z_n)} \left[\log \frac{p(y_n, z_n|\theta^*, \phi^*)}{q(z_n)} \right] \right]$

$$= \sum_{n=1}^N \left[E_{z_n \sim q(z_n)} \left[\log p(y_n|\theta^*, \phi^*) \right] - E_{z_n \sim q(z_n)} \left[\log \frac{p(y_n, z_n|\theta^*, \phi^*)}{q(z_n)} \right] \right]$$

$$= \sum_{n=1}^N \left[E_{z_n \sim q(z_n)} \left[\log p(y_n|\theta^*, \phi^*) - \log \frac{p(y_n, z_n|\theta^*, \phi^*)}{q(z_n)} \right] \right]$$

$$= \sum_{n=1}^N \left[E_{z_n \sim q(z_n)} \left[\log \left(\frac{p(y_n|\theta^*, \phi^*) q(z_n)}{p(z_n|y_n, \theta^*, \phi^*)} \right) \right] \right]$$

$$= \sum_{n=1}^N \left[E_{z_n \sim q(z_n)} \left[\log \left(\frac{q(z_n)}{p(z_n|y_n, \theta^*, \phi^*)} \right) \right] \right]$$

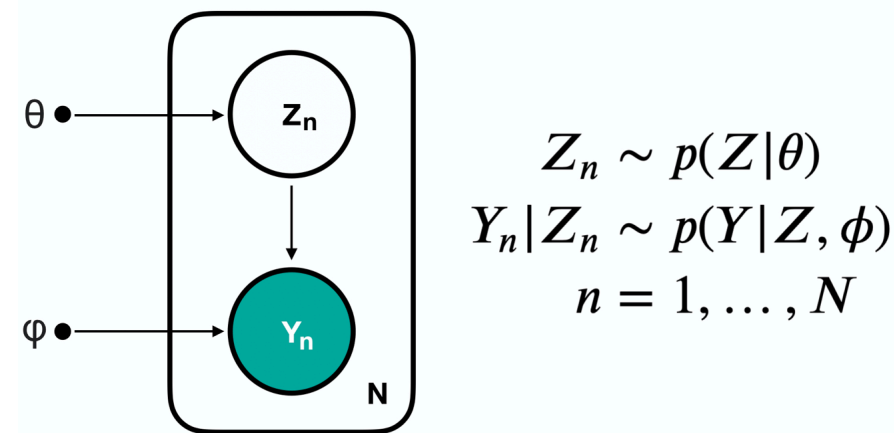
$$= \sum_{n=1}^N D_{KL} [q(z_n) || p(z_n|y_n, \theta^*, \phi^*)]$$

$$q^* = \underset{q}{\text{argmax}} \text{ELBO}(\theta^*, \phi^*, q) = \underset{q}{\text{argmin}} D_{KL} [q(z_n) || p(z_n|y_n, \theta^*, \phi^*)]$$

$$q^* = p(z_n|y_n, \theta^*, \phi^*)$$

The Expectation Maximization Algorithm

The *expectation maximization (EM) algorithm* maximize the ELBO of the model,



1. **Initialization:** Pick θ_0, ϕ_0 .
2. Repeat $i = 1, \dots, I$ times:

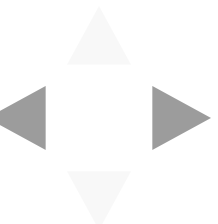
E-Step:

$$q_{\text{new}}(Z_n) = \operatorname{argmax}_q ELBO(\theta_{\text{old}}, \phi_{\text{old}}, q) = p(Z_n|Y_n, \theta_{\text{old}}, \phi_{\text{old}})$$

M-Step:

$$\theta_{\text{new}}, \phi_{\text{new}} = \operatorname{argmax}_{\theta, \phi} ELBO(\theta, \phi, q_{\text{new}})$$

$$= \operatorname{argmax}_{\theta, \phi} \sum_{n=1}^N \mathbb{E}_{Z_n \sim p(Z_n|Y_n, \theta_{\text{old}}, \phi_{\text{old}})} [\log(p(y_n, Z_n|\phi, \theta))] .$$



Example: EM for the Gaussian Mixture Model of Birth Weight

The Gaussian mixture model for the birth weight data has 3 Gaussians with mean $\mu = [\mu_1, \mu_2, \mu_3]$ and variances $\sigma^2 = [\sigma_1^2, \sigma_2^2, \sigma_3^2]$, and the model is defined as:

$$\begin{aligned}Z_n &\sim \text{Cat}(\pi), \\Y_n|Z_n &\sim \mathcal{N}(\mu_{Z_n}, \sigma_{Z_n}^2),\end{aligned}$$

where $n = 1, \dots, N$ and $\sum_{k=1}^3 \pi_k = 1$.

The E-Step

The E-step in EM computes the distribution:

$$q_{\text{new}}(Z_n) = \underset{q}{\operatorname{argmax}} \text{ELBO}(\mu_{i-1}, \sigma_{i-1}^2, \pi_{i-1}, q) = p(Z_n|Y_n, \mu_{\text{old}}, \sigma_{\text{old}}^2, \pi_{\text{old}}).$$

Since Z_n is a label, $p(Z_n|Y_n, \dots)$ is a categorical distribution, with the probability of $Z_n = k$ given by:

$$p(Z_n = k|Y_n, \mu_{\text{old}}, \sigma_{\text{old}}^2, \pi_{\text{old}}) = \frac{p(y_n|Z_n = k, \mu_{\text{old}}, \sigma_{\text{old}}^2)p(Z_n = k|\pi_{\text{old}})}{\sum_{k=1}^K p(y|Z_n = k, \mu_{\text{old}}, \sigma_{\text{old}}^2)p(Z_n = k|\pi_{\text{old}})} = \underbrace{\frac{\pi_{k,\text{old}} \mathcal{N}(y_n; \mu_{k,\text{old}}, \sigma_{k,\text{old}}^2)}{\mathcal{Z}}}_{r_{n,k}},$$

where $\mathcal{Z} = \sum_{k=1}^K \pi_{k,\text{old}} \mathcal{N}(y_n; \mu_{k,\text{old}}, \sigma_{k,\text{old}}^2)$.

Example: EM for the Gaussian Mixture Model of Birth Weight

Setting Up the M-Step

The M-step in EM maximize the following:

$$\operatorname{argmax}_{\mu, \sigma^2, \pi} ELBO(\mu, \sigma^2, \pi, q_{\text{new}}) = \operatorname{argmax}_{\mu, \sigma^2, \pi} \sum_{n=1}^N \mathbb{E}_{Z_n \sim p(Z_n | Y_n, \mu_{k, \text{old}}, \sigma_{k, \text{old}}^2)} [\log(p(y_n, Z_n | \mu, \sigma^2, \pi))].$$

If we expand the expectation a little, we get:

$$\begin{aligned} \sum_{n=1}^N \mathbb{E}_{Z_n \sim p(Z_n | Y_n, \mu_{\text{old}}, \sigma_{\text{old}}^2, \pi_{\text{old}})} [\log(p(y_n, Z_n | \mu, \sigma^2, \pi))] &= \underbrace{\sum_{n=1}^N \sum_{k=1}^K \log \left(\underbrace{p(y_n | Z_n = k, \mu, \sigma^2) p(Z_n = k | \pi)}_{\text{factoring the joint } p(y_n, Z_n | \dots)} \right)}_{\text{expanding the expectation}} p(Z_n = k | y_n, \theta_{\text{old}}, \phi_{\text{old}}) \\ &= \sum_{n=1}^N \sum_{k=1}^K \underbrace{r_{n,k}}_{p(Z_n = k | y_n, \theta_{\text{old}}, \phi_{\text{old}})} \left[\underbrace{\log \mathcal{N}(y_n; \mu_k, \sigma_k^2)}_{p(y_n | Z_n = k, \mu, \sigma^2)} + \log \underbrace{\pi_k}_{p(Z_n = k | \pi)} \right] \\ &= \underbrace{\sum_{n=1}^N \sum_{k=1}^K r_{n,k} \log \mathcal{N}(y_n; \mu_k, \sigma_k^2)}_{\text{Term \#1}} + \underbrace{\sum_{n=1}^N \sum_{k=1}^K r_{n,k} \pi_k}_{\text{Term \#2}} \end{aligned}$$

We can maximize each Term #1 and Term #2 individually.

Example: EM for the Gaussian Mixture Model of Birth Weight

Solving the M-Step

We see that the optimization problem in the M-step:

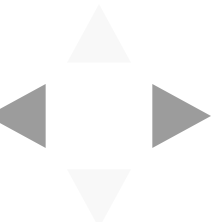
$\mu_{\text{new}}, \sigma_{\text{new}}^2, \pi_{\text{new}} = \underset{\mu, \sigma^2, \pi}{\operatorname{argmax}} ELBO(\mu, \sigma^2, \pi, q_{\text{new}})$ is equivalent to two problems

$$1. \quad \underset{\mu, \sigma^2}{\operatorname{argmax}} \sum_{n=1}^N \sum_{k=1}^K r_{n,k} \log \mathcal{N}(y_n; \mu_k, \sigma_k^2)$$

$$2. \quad \underset{\pi}{\operatorname{argmax}} \sum_{n=1}^N \sum_{k=1}^K r_{n,k} \pi_k$$

We can solve each optimization problem analytically by finding stationary points of the gradient (or the Lagrangian):

- $\mu_{\text{new}} = \frac{1}{\sum_{n=1}^N r_{n,k}} \sum_{n=1}^N r_{n,k} y_n$
- $\sigma_{\text{new}}^2 = \frac{1}{\sum_{n=1}^N r_{n,k}} \sum_{n=1}^N r_{n,k} (y_n - \mu_{\text{new}})^2$
- $\pi_{\text{new}} = \frac{\sum_{n=1}^N r_{n,k}}{N}$



Example: EM for the Gaussian Mixture Model of Birth Weight

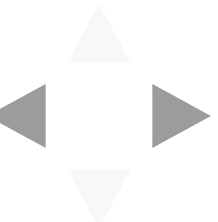
All Together

Initialization: Pick any π, μ, σ^2

E-Step: Compute $r_{n,k} = \frac{\pi_{k,\text{old}} \mathcal{N}(y_n; \mu_{k,\text{old}}, \sigma_{k,\text{old}}^2)}{\mathcal{Z}}$, where
 $\mathcal{Z} = \sum_{k=1}^K \pi_{k,\text{old}} \mathcal{N}(y_n; \mu_{k,\text{old}}, \sigma_{k,\text{old}}^2)$.

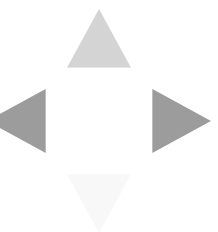
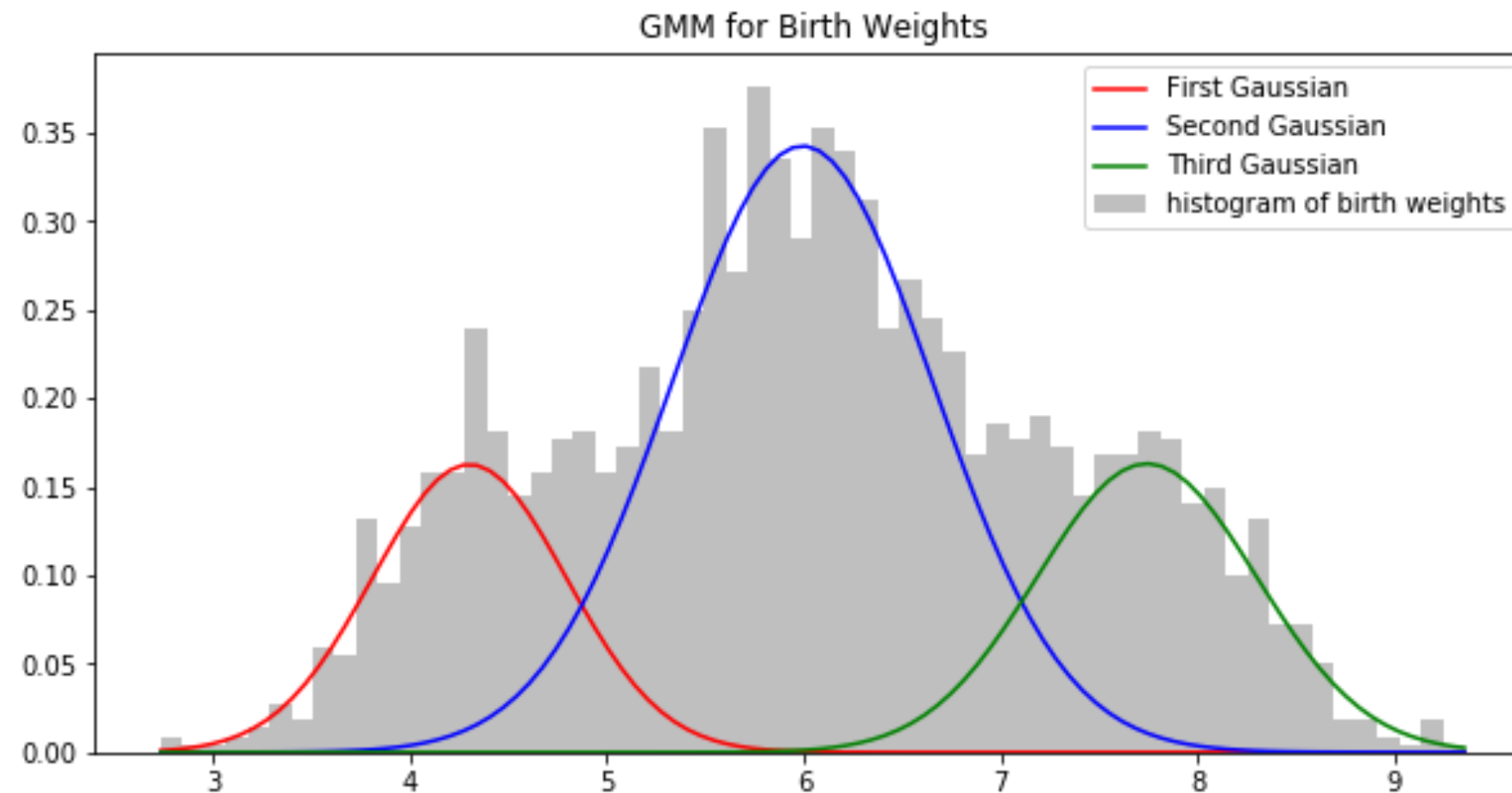
M-Step: Compute model parameters:

- $\mu_{\text{new}} = \frac{1}{\sum_{n=1}^N r_{n,k}} \sum_{n=1}^N r_{n,k} y_n$
- $\sigma_{\text{new}}^2 = \frac{1}{\sum_{n=1}^N r_{n,k}} \sum_{n=1}^N r_{n,k} (y_n - \mu_{\text{new}})^2$
- $\pi_{\text{new}} = \frac{\sum_{n=1}^N r_{n,k}}{N}$



Implementing EM for the Gaussian Mixture Model of Birth Weight

```
In [3]: fig, ax = plt.subplots(1, 1, figsize=(10, 5))
ax.hist(y, bins=60, density=True, color='gray', alpha=0.5, label='histogram of b
irth weights')
ax.plot(x, pi_current[0] * sp.stats.norm(mu_current[0], sigma_current[0]**0.5).p
df(x), color='red', label='First Gaussian')
ax.plot(x, pi_current[1] * sp.stats.norm(mu_current[1], sigma_current[1]**0.5).p
df(x), color='blue', label='Second Gaussian')
ax.plot(x, pi_current[2] * sp.stats.norm(mu_current[2], sigma_current[2]**0.5).p
df(x), color='green', label='Third Gaussian')
ax.set_title('GMM for Birth Weights')
ax.legend(loc='best')
plt.show()
```



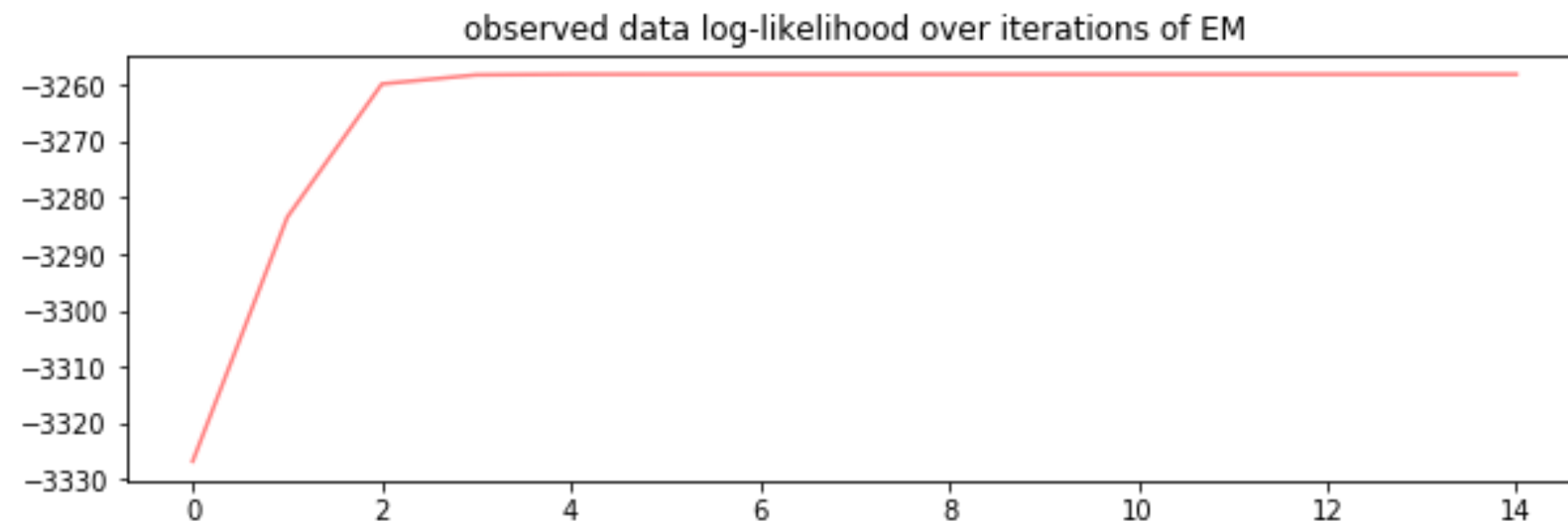
Sanity Check: Log-Likelihood During Training

Remember that plotting the MLE model against actual data is not always an option (e.g. high-dimensional data).

A sanity check for that your EM algorithm has been implemented correctly is to plot the observed data log-likelihood over the iterations of the algorithm:

$$\ell_y(\mu, \sigma^2, \pi) = \sum_{n=1}^N \log \sum_{k=1}^K \mathcal{N}(y_n; \mu_k, \sigma_k^2) \pi_k$$

```
In [4]: fig, ax = plt.subplots(1, 1, figsize=(10, 3))
ax.plot(range(len(log_lkhd)), log_lkhd, color='red', alpha=0.5)
ax.set_title('observed data log-likelihood over iterations of EM')
plt.show()
```



Expectation Maximization versus Gradient-based Optimization

Pros of EM:

1. No learning rates to adjust
2. Don't need to worry about incorporating constraints (i.e. $p(Z_n | Y_n)$ is between 0 and 1)
3. Each iteration is guaranteed to increase or maintain observed data log-likelihood
4. Is guaranteed to converge to local optimum
5. Can be very fast to converge (when parameters are fewer)

Cons of EM:

1. Can get stuck in local optima
2. May not maximize observed data log-likelihood (the ELBO is just a lower bound)
3. Requires you to do math - you need analytic solutions for E-step and M-step
4. May be much slower than fancier gradient-based optimization

