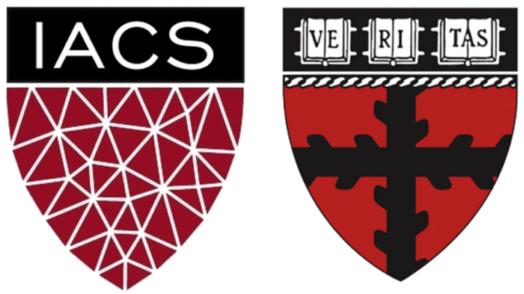
Lecture #9: Latent Variable Models and MLE

AM 207: Advanced Scientific Computing

Stochastic Methods for Data Analysis, Inference and Optimization

Fall, 2020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Outline

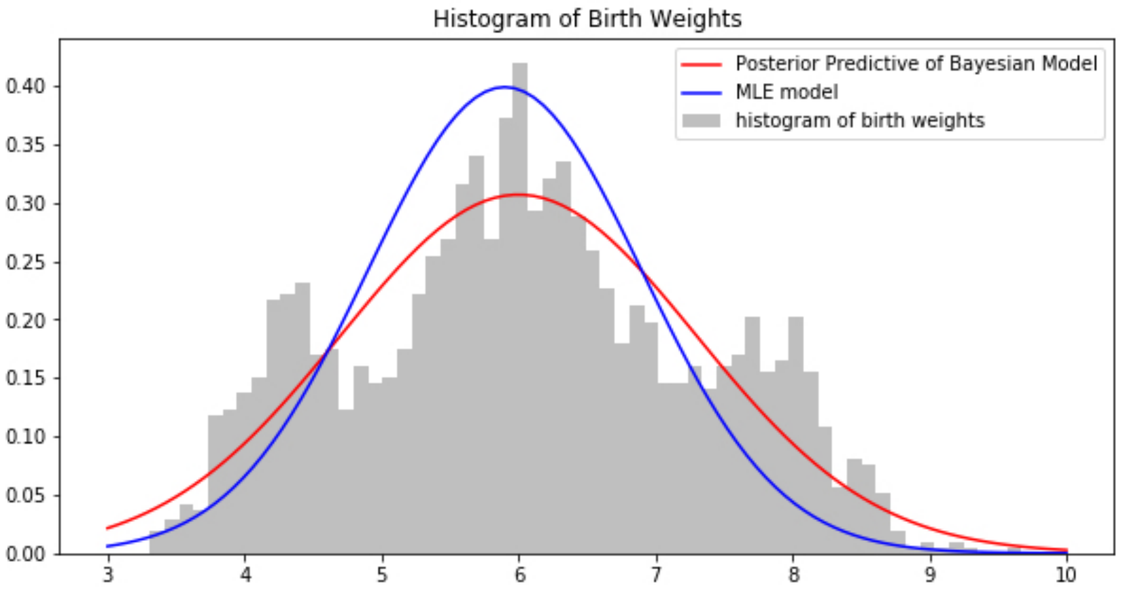
1. Motivation for Latent Variable Models
2. Common Latent Variable Models
3. Maximum Likelihood Estimation for Latent Variable Models: Expectation Maximization
4. Mixture of Gaussians

Motivation for Latent Variable Models

A Model for Birth Weights

Recall our model for birth weigths, $Y_1, \ldots, Y_N$. We *posited* that the birth weights are iid normally distributed with known σ^2, $Y_n \sim \mathcal{N}(\mu, 1)$.

Compare the maximum likelihood model and the Bayesian model for bith weight. Which model would you use to make clinical decisions? What's hard about this comparison?



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:

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

The KL-divergence $D_{\mathrm{KL}}[q \parallel p]$ 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 nontheless estimate $D_{\mathrm{KL}}[q \parallel p]$. Techniques that estimate the KL-divergence from samples are called ***non-parametric***. We will use them later in the course.

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.

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

$$Z_n \sim Cat(\pi),$$

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***.

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

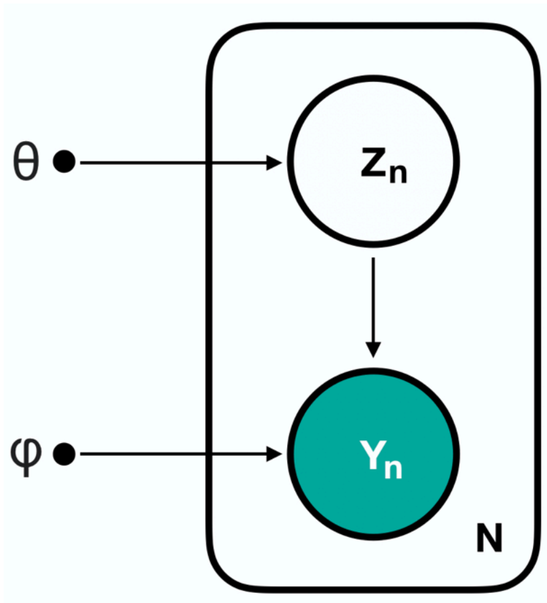
$$Y_n | Z_n \sim \mathcal{N}\left(\mu_{Z_n}, \sigma^2_{Z_n}\right)$$

where μ_{Z_n} is one of the three class means $[\mu_1, \mu_2, \mu_3]$ and $\sigma^2_{Z_n}$ is one of the three class variances $[\sigma^2_1, \sigma^2_2, \sigma^2_3]$.

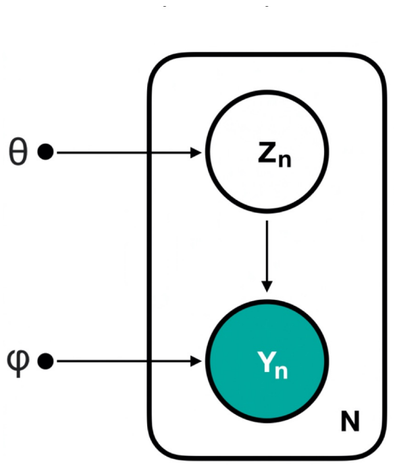
Common Latent Variable Models

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:



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



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:

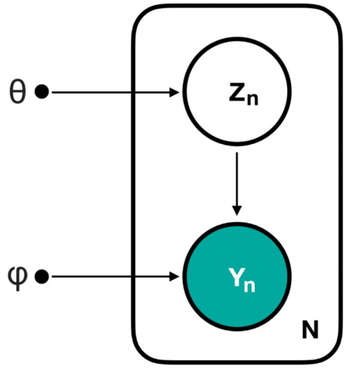
$$\begin{aligned} Z_n &\sim \mathcal{N}(\mu, \sigma^2), \\ \theta_n &= g(Z_n) \\ Y_n|Z_n &\sim Ber(\theta_n), \end{aligned}$$

where $n = 1, \ldots, N$ 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 $n = 1, \ldots, N, Z_n \in \mathbb{R}^{D'}$ 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

$x_n \sim p(x_n|z_n, \theta)$
$(x_n = f(z_n, \varepsilon_n, \theta))$
parameters: θ, β

Likelihood over q's:

$$\log \prod_{n=1}^{N} p(y_n|x_n, \beta)\, p(x_n|\theta) = \sum_{n=1}^{N} \log \underbrace{p(y_n|x_n, \beta) + \log p(x_n|\theta)}_{\text{can we evaluate this?}}$$

Likelihood over observed data:

$$\log \prod_{n=1}^{N} p(y_n|\theta, \beta) = \sum_{n=1}^{N} \log \int p(y_n|x_n, \beta)\, p(x_n|\theta)\, dx_n$$

$$= \sum_{n=1}^{N} \log \int p(y_n|x_n, \beta)\, \frac{p(x_n|\theta)}{q(x_n)}\, q(x_n)\, dx_n \quad \text{does the log hide?}$$

$$= \sum_{n=1}^{N} \log \underbrace{\mathbb{E}_{x_n \sim q(x_n)}\left[p(y_n|x_n, \beta)\, \frac{p(x_n|\theta)}{q(x_n)} \right]}_{\text{is this hard?}}$$

The maximum likelihood objective:

$$\theta_{ML}, \theta_{ML} = \arg\max_{\theta, \beta} \ell(\theta, \beta) = \arg\max_{\theta, \beta} \sum_{n=1}^{N} \log \underbrace{\mathbb{E}_{x_n \sim p(x_n|\theta)}\left[p(y_n|x_n, \beta) \right]}_{\text{is this hard?}}$$

Trying out the optimization:

$$\nabla_{\theta,\beta}\, \ell(\theta, \beta) = \sum_{n=1}^{N} \nabla_{\theta,\beta} \log \mathbb{E}_{x_n \sim p(x_n|\theta)}\left[p(y_n|x_n, \beta) \right]$$

$$= \sum_{n=1}^{N} \nabla_{\theta,\beta} \log \mathbb{E}_{x_n \sim p(x_n|\theta)}\left[p(y_n|x_n, \beta) \right]$$

$$\because \nabla_{\theta,\beta} \log f = \frac{\nabla_{\theta,\beta} f}{f}$$

$$= \sum_{n=1}^{N} \frac{\nabla_{\theta,\beta} \mathbb{E}_{x_n \sim p(x_n|\theta)}\left[p(y_n|x_n, \beta) \right]}{\mathbb{E}_{x_n \sim p(x_n|\theta)}\left[p(y_n|x_n, \beta) \right]}$$

can we MC estimate this?

Calculus Facts we need:

1. $\mathbb{E}_{x \sim p(x)}[f(x)] \rightarrow$ Footnote
2. Properties of $\mathbb{E}$:
   - A $\mathbb{E}_{x \sim p(x)}[a f(x)] = a \frac{1}{C} \sum_{x \sim p(x)} f(x) = a \sum_{x \sim p(x)} \mathbb{E}[f(x)]$
   - (Jensen's inequality) $\rightarrow$ B. $\log \mathbb{E}_{x \sim p(x)}[f(x)] \geq \mathbb{E}_{x \sim p(x)}[\log f(x)]$
   - C $\nabla_\theta \mathbb{E}_{x \sim p(x|\theta)}[f(x,w)] = \mathbb{E}_{x \sim p(x|\theta)}[\nabla_\theta f(x,w)]$
3. $D_{KL}[q(x) \| p(x)] = \left[\log \frac{q(x)}{p(x)}\right]$ Aside

$$= \mathbb{E}_{x \sim q(x)}\left[\log \frac{q(x)}{p(x)}\right]$$

An objective we can actually work with:

$$\max_{\theta,\beta} \ell(\theta, \beta) = \max_{\theta,\beta} \sum_{n=1}^{N} \log \mathbb{E}_{x_n \sim p(x_n|\theta)}\left[p(y_n|x_n, \beta) \right]$$

$$= \max_{\theta,\beta} \sum_{n=1}^{N} \log \int p(y_n|x_n, \beta)\, p(x_n|\theta)\, dx_n$$

$$= \max_{\theta,\beta} \sum_{n=1}^{N} \log \int p(y_n|x_n, \beta)\, \frac{p(x_n|\theta)}{q(x_n)}\, q(x_n)\, dx_n$$

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

$$= \max_{\theta,\beta} \sum_{n=1}^{N} \log \underbrace{\mathbb{E}_{x_n \sim q(x_n)}\left[p(y_n|x_n, \beta)\, \frac{p(x_n|\theta)}{q(x_n)} \right]}_{\text{is this log helping?}}$$

does $\nabla_{\theta,\beta}$ commute with $\mathbb{E}_{x \sim q(x)}$?

$$\geq \max_{\theta,\beta,q} \sum_{n=1}^{N} \underbrace{\mathbb{E}_{x_n \sim q(x_n)}\left[\log \left(p(y_n|x_n, \beta)\, \frac{p(x_n|\theta)}{q(x_n)} \right) \right]}_{\text{The Evidence Lower Bound ELBO}(\theta, \beta, q)}$$

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

Why you Should

When ELBO is maximized $\ell(\theta, \beta)$ is guaranteed to be as big.

Why you Shouldn't

If ELBO is maximized then $\ell(\theta, \beta)$ can be far from optimized

How to maximize ELBO: coordinate ascent

I. maximize θ, β, fixing q^t

$$\theta^*, \beta^* = \arg\max_{\theta,\beta} \text{ELBO}(\theta, \beta, q^t)$$

(M-step)

$$= \arg\max_{\theta,\beta} \sum_{n=1}^{N} \mathbb{E}_{x_n \sim q^t(x_n)}\left[\log \left(\frac{p(y_n|x_n, \beta)\, p(x_n|\theta)}{q^t(x_n)} \right) \right]$$

$$= \arg\max_{\theta,\beta} \sum_{n=1}^{N} \left(\mathbb{E}_{x_n \sim q^t(x_n)}\left[\log \left(p(y_n|x_n, \beta)\, p(x_n|\theta) \right) \right] - \mathbb{E}_{x_n \sim q^t(x_n)}\left[\log q^t(x_n) \right] \right)$$

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

$$\equiv \arg\max_{\theta,\beta} \sum_{n=1}^{N} \mathbb{E}_{x_n \sim q^t(x_n)}\left[\log \left(p(y_n|x_n, \beta)\, p(x_n|\theta) \right) \right]$$

is this problem easier?

II. maximize q, fixing θ^t, β^t

$$q^t = \arg\max_{q} \text{ELBO}(\theta^t, \beta^t, q)$$

Note $\ell(\theta^t, \beta^t) - \text{ELBO}(\theta^t, \beta^t, q) = \sum_{n=1}^{N} \left[\log p(y_n|\theta^t, \beta^t) - \mathbb{E}_{x_n \sim q(x_n)}\left[\log \frac{p(y_n, x_n|\theta^t, \beta^t)}{q(x_n)} \right] \right]$

$$= \sum_{n=1}^{N} \left[\mathbb{E}_{x_n \sim q(x_n)}\left[\log p(y_n|\theta^t, \beta^t) \right] - \mathbb{E}_{x_n \sim q(x_n)}\left[\log \frac{p(y_n, x_n|\theta^t, \beta^t)}{q(x_n)} \right] \right]$$

$$= \sum_{n=1}^{N} \left[\mathbb{E}_{x_n \sim q(x_n)}\left[\log \frac{p(y_n|\theta^t, \beta^t)\, q(x_n)}{p(y_n, x_n|\theta^t, \beta^t)} \right] \right]$$

$$= \sum_{n=1}^{N} \left[\mathbb{E}_{x_n \sim q(x_n)}\left[\log \frac{q(x_n)}{p(x_n|y_n, \theta^t, \beta^t)} \right] \right]$$

$$= \sum_{n=1}^{N} D_{KL}\left[q(x_n) \,\|\, p(x_n|y_n, \theta^t, \beta^t) \right]$$

$$q^t = \arg\max_{q} \text{ELBO}(\theta^t, \beta^t, q) = \arg\min_{q} D_{KL}[q(x_n) \,\|\, p(x_n|y_n, \theta^t, \beta^t)]$$

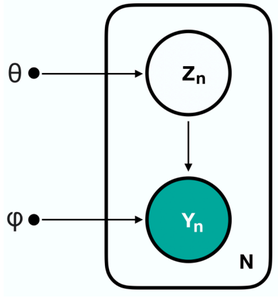
$$q^t = p(x_n|y_n, \theta^t, \beta^t)$$

Are we done?

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

The Expectation Maximization Algorithm

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



$$Z_n \sim p(Z|\theta)$$
$$Y_n|Z_n \sim p(Y|Z,\phi)$$
$$n = 1, \dots, N$$

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

   E-Step:
   $$q_{\text{new}}(Z_n) = \underset{q}{\text{argmax}}\ ELBO(\theta_{\text{old}}, \phi_{\text{old}}, q) = p(Z_n|Y_n, \theta_{\text{old}}, \phi_{\text{old}})$$

   M-Step:
   $$\theta_{\text{new}}, \phi_{\text{new}} = \underset{\theta,\phi}{\text{argmax}}\ ELBO(\theta, \phi, q_{\text{new}})$$
   $$= \underset{\theta,\phi}{\text{argmax}} \sum_{n=1}^{N} \mathbb{E}_{Z_n \sim p(Z_n|Y_n,\theta_{\text{old}},\phi_{\text{old}})} \left[\log(p(y_n, Z_n|\phi, \theta)\right].$$

Example: EM for the Gaussian Mixture Model of Birth Weight

Solving the M-Step

We see that the optimization problem in the M-step:
$\mu_{\text{new}}, \sigma^2_{\text{new}}, \pi_{\text{new}} = \underset{\mu,\sigma^2,\pi}{\text{argmax}}\ ELBO(\mu, \sigma^2, \pi, q_{\text{new}})$ is equivalent to two problems

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

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

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

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

Example: EM for the Gaussian Mixture Model of Birth Weight

All Together

Initialization: Pick any π, μ, σ^2

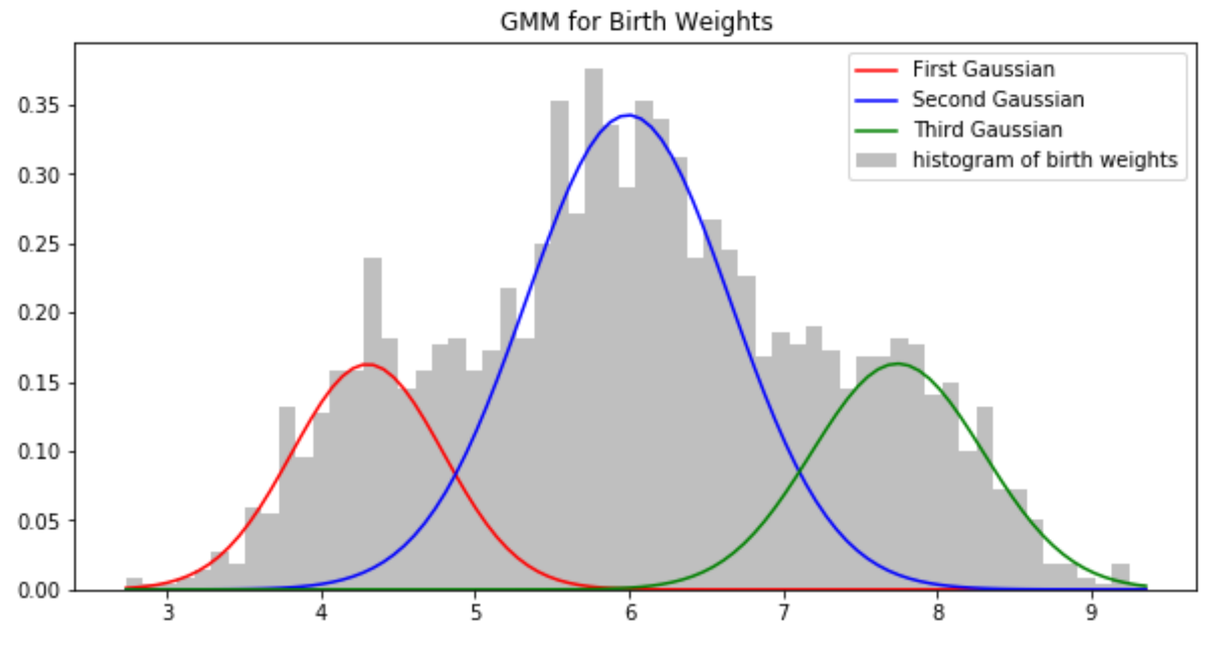
E-Step: Compute $r_{n,k} = \dfrac{\pi_{k,\text{old}}\ \mathcal{N}(y_n; \mu_{k,\text{old}}, \sigma^2_{k,\text{old}})}{\mathcal{Z}}$, where $\mathcal{Z} = \sum_{k=1}^{K} \pi_{k,\text{old}}\ \mathcal{N}(y_n; \mu_{k,\text{old}}, \sigma^2_{k,\text{old}})$.

M-Step: Compute model parameters:

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

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 ploting 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()
```