Latent Variable Models and the EM Algorithm (Contd)

CS772A: Probabilistic Machine Learning

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Announcement

- Mid-sem exam on Sept 19, 1800-2000
- Venue: L17, ERES seating scheme
- Syllabus: Up to today's lecture
- Closed book exam
  - Necessary formulae/equations will be provided in the question paper

Plan Today

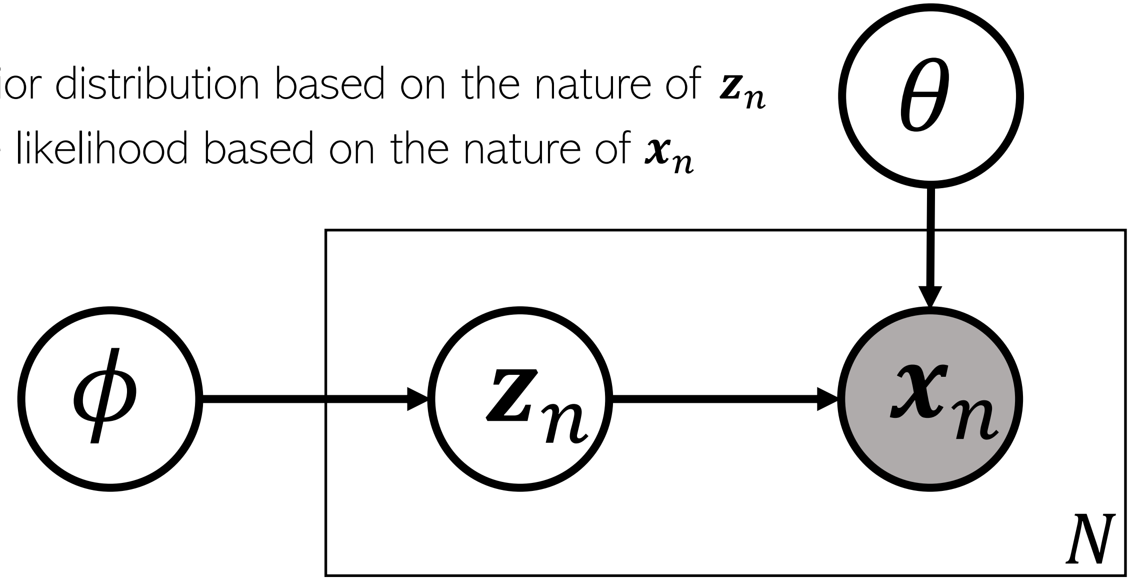
- Expectation Maximization (EM) algorithm for param-est/inference in LVMs

- An example of EM
  - Parameter estimation for Gaussian mixture models

Parameter Estimation in Latent Variable Models

- Assume each observation $\boldsymbol{x}_n$ to be associated with a "local" latent variable $\boldsymbol{z}_n$

$p(\boldsymbol{z}_n|\phi)$: A suitable prior distribution based on the nature of $\boldsymbol{z}_n$
$p(\boldsymbol{x}_n|\boldsymbol{z}_n, \theta)$: A suitable likelihood based on the nature of $\boldsymbol{x}_n$



- Although we can do fully Bayesian inference for all the unknowns, suppose we only want a point estimate of the "global" parameters $\boldsymbol{\Theta} = (\theta, \phi)$ via MLE/MAP
- Such MLE/MAP problems in LVMs are difficult to solve in a "clean" way
  - Can do gradient based opt on log-lik but usually won't get closed form updates for $\boldsymbol{\Theta}$
  - However, EM algo gives a clean way to obtain closed form updates for $\boldsymbol{\Theta}$ for such LVMs

Why MLE/MAP of Params is Hard for LVMs?

- Suppose we want to estimate parameters $\boldsymbol{\Theta}$ via MLE. If we knew $\boldsymbol{z}_n$, we could solve

$$\Theta_{MLE} = \arg\max_{\Theta} \sum_{n=1}^{N} \log p(\boldsymbol{x}_n, \boldsymbol{z}_n|\Theta) = \arg\max_{\Theta} \sum_{n=1}^{N} [\log p(\boldsymbol{z}_n|\phi) + \log p(\boldsymbol{x}_n|\boldsymbol{z}_n, \theta)]$$

Easy to solve

- Easy. Usually closed form if $p(\boldsymbol{z}_n|\phi)$ and $p(\boldsymbol{x}_n|\boldsymbol{z}_n, \theta)$ have simple forms

In particular, if they are exp-fam distributions

- However, since in LVMs, $\boldsymbol{z}_n$ is hidden, the MLE problem for $\boldsymbol{\Theta}$ will be the following

$$\Theta_{MLE} = \arg\max_{\Theta} \sum_{n=1}^{N} \log p(\boldsymbol{x}_n|\Theta) = \arg\max_{\Theta} \log p(\mathbf{X}|\Theta)$$

- $\log p(\boldsymbol{x}_n|\Theta)$ will not have a simple expression since $p(\boldsymbol{x}_n|\Theta)$ requires sum/integral

$$p(\boldsymbol{x}_n|\Theta) = \sum_{\boldsymbol{z}_n} p(\boldsymbol{x}_n, \boldsymbol{z}_n|\Theta) \quad \text{... or if } \boldsymbol{z}_n \text{ is continuous:} \quad p(\boldsymbol{x}_n|\Theta) = \int p(\boldsymbol{x}_n, \boldsymbol{z}_n|\Theta) d\boldsymbol{z}_n$$

- MLE now becomes difficult, no closed form expression for $\boldsymbol{\Theta}$

Can still use gradient based methods but won't get clean, closed-form updates for $\boldsymbol{\Theta}$

- Can we maximize some other quantity instead of $\log p(\boldsymbol{x}_n|\Theta)$ for this MLE?

An Important Identity

- Assume $p_Z = p(\boldsymbol{Z}|\boldsymbol{X},\Theta)$ and $q(\boldsymbol{Z})$ to be some prob distribution over $\boldsymbol{Z}$, then for all q

$$\log p(\boldsymbol{X}|\Theta) = \mathcal{L}(q,\Theta) + KL(q||p_Z)$$

Verify the identity

Assume $\boldsymbol{Z}$ discrete

- In the above $\mathcal{L}(q,\Theta) = \sum_Z q(Z)\log\left\{\frac{p(X,Z|\Theta)}{q(Z)}\right\}$

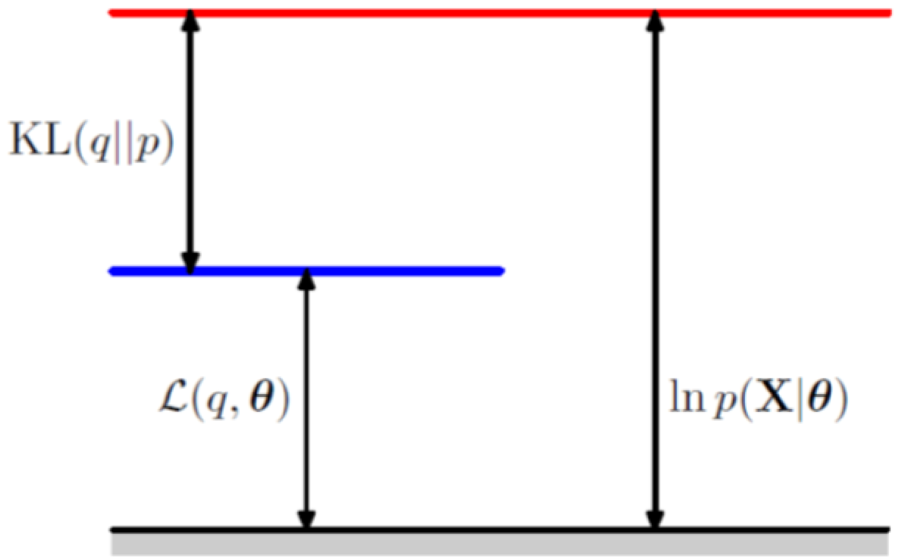
- $KL(q||p_z) = -\sum_Z q(\boldsymbol{Z})\log\left\{\frac{p(\boldsymbol{Z}|\boldsymbol{X},\Theta)}{q(\boldsymbol{Z})}\right\}$

- KL is always non-negative, so $\log p(\boldsymbol{X}|\Theta) \geq \mathcal{L}(q,\Theta)$

- Thus $\mathcal{L}(q,\Theta)$ is a lower-bound on $\log p(\boldsymbol{X}|\Theta)$

- Thus if we maximize $\mathcal{L}(q,\Theta)$, it will also improve $\log p(\boldsymbol{X}|\Theta)$

- Also, as we'll see, it's easier to maximize $\mathcal{L}(q,\Theta)$



Maximizing $\mathcal{L}(q,\Theta)$

$\log p(\boldsymbol{X}|\Theta)$ is called Incomplete-Data Log Likelihood (ILL)

- $\mathcal{L}(q,\Theta)$ depends on q and Θ. We'll use ALT-OPT to maximize it
- Let's maximize $\mathcal{L}(q,\Theta)$ w.r.t. q with Θ fixed at some Θ^{old}

Since $\log p(\boldsymbol{X}|\Theta) = \mathcal{L}(q,\Theta) + KL(q||p_z)$ is constant when Θ is held fixed at Θ^{old}

$$\hat{q} = \text{argmax}_q \mathcal{L}\left(q,\Theta^{\text{old}}\right) = \text{argmin}_q KL(q||p_z) = p_z = p(\boldsymbol{Z}|\boldsymbol{X},\Theta^{\text{old}})$$

The posterior distribution of Z given current parameters Θ^{old}

- Now let's maximize $\mathcal{L}(q,\Theta)$ w.r.t. Θ with q fixed at $\hat{q} = p_z = p(\boldsymbol{Z}|\boldsymbol{X},\Theta^{\text{old}})$

$$\Theta^{\text{new}} = \text{argmax}_\Theta \mathcal{L}(\hat{q},\Theta) = \text{argmax}_\Theta \sum_{\boldsymbol{Z}} p(\boldsymbol{Z}|\boldsymbol{X},\Theta^{\text{old}}) \log\left\{\frac{p(\boldsymbol{X},\boldsymbol{Z}|\Theta)}{p(\boldsymbol{Z}|\boldsymbol{X},\Theta^{\text{old}})}\right\}$$

$$= \text{argmax}_\Theta \sum_{\boldsymbol{Z}} p\left(\boldsymbol{Z}\middle|\boldsymbol{X},\Theta^{\text{old}}\right) \log p(\boldsymbol{X},\boldsymbol{Z}|\Theta)$$

$$= \text{argmax}_\Theta \, \mathbb{E}_{p\left(\boldsymbol{Z}\middle|\boldsymbol{X},\Theta^{\text{old}}\right)}[\log p(\boldsymbol{X},\boldsymbol{Z}|\Theta)]$$

$$= \text{argmax}_\Theta \, \mathcal{Q}(\Theta,\Theta^{\text{old}})$$

Complete-Data Log Likelihood (CLL)

Maximization of expected CLL where the expectation is w.r.t. the posterior distribution of Z given current parameters Θ^{old}

Much easier than maximizing ILL since CLL will have simple expressions (since it is kind of akin to knowing Z)

The Expectation-Maximization (EM) Algorithm

- ALT-OPT of $\mathcal{L}(q,\Theta)$ w.r.t. q and Θ gives the EM algorithm (Dempster, Laird, Rubin, 1977)

The EM Algorithm

Primarily designed for doing point estimation of the parameters Θ but also gives (CP of) latent variables z_n

Usually computing CP + expected CLL is referred to as the E step, and max. of exp-CLL w.r.t. Θ as the M step

1. Initialize Θ as $\Theta^{(0)}$, set $t=1$
2. Step 1: Compute posterior of latent variables given current parameters $\Theta^{(t-1)}$

Conditional posterior of each latent variable z_n

Latent variables also assumed indep. a priori

$$p(\boldsymbol{z}_n^{(t)}|\boldsymbol{x}_n,\Theta^{(t-1)}) = \frac{p(\boldsymbol{z}_n^{(t)}|\Theta^{(t-1)})p(\boldsymbol{x}_n|\boldsymbol{z}_n^{(t)},\Theta^{(t-1)})}{p(\boldsymbol{x}_n|\Theta^{(t-1)})} \propto \text{prior} \times \text{likelihood}$$

3. Step 2: Now maximize the expected complete data log-likelihood w.r.t. Θ

Assuming the (expected) CLL $\mathbb{E}_{p(\boldsymbol{Z}|\boldsymbol{X},\Theta^{\text{old}})}[\log p(\boldsymbol{X},\boldsymbol{Z}|\Theta)]$ factorizes over all observations

$$\Theta^{(t)} = \arg\max_{\Theta} \mathcal{Q}(\Theta,\Theta^{(t-1)}) = \arg\max_{\Theta} \sum_{n=1}^{N} \mathbb{E}_{p(\boldsymbol{z}_n^{(t)}|\boldsymbol{x}_n,\Theta^{(t-1)})}[\log p(\boldsymbol{x}_n,\boldsymbol{z}_n^{(t)}|\Theta)]$$

4. If not yet converged, set $t=t+1$ and go to step 2.

- Note: If we can take the MAP estimate $\hat{z}_n$ of z_n (not the CP) in Step 1 and maximize the CLL in Step 2 using that, i.e., do $\text{argmax}_{\Theta} \sum_{n=1}^{N}[\log p(\boldsymbol{x}_n,\hat{\boldsymbol{z}}_n^{(t)}|\Theta)]$ then this will be std ALT-OPT

The Expected CLL

- Expected CLL in EM is given by (assume observations are i.i.d.)

$$\mathcal{Q}(\Theta, \Theta^{old}) = \sum_{n=1}^{N} \mathbb{E}_{p(\boldsymbol{z}_n|\boldsymbol{x}_n,\Theta^{old})}[\log p(\boldsymbol{x}_n, \boldsymbol{z}_n|\Theta)]$$
$$= \sum_{n=1}^{N} \mathbb{E}_{p(\boldsymbol{z}_n|\boldsymbol{x}_n,\Theta^{old})}[\log p(\boldsymbol{x}_n|\boldsymbol{z}_n, \Theta) + \log p(\boldsymbol{z}_n|\Theta)]$$

- If $p(\boldsymbol{z}_n|\Theta)$ and $p(\boldsymbol{x}_n|\boldsymbol{z}_n, \Theta)$ are exp-family distributions, $\mathcal{Q}(\Theta, \Theta^{\text{old}})$ has a very simple form
- In resulting expressions, replace terms containing $\boldsymbol{z}_n$'s by their respective expectations, e.g.,
  - $\boldsymbol{z}_n$ replaced by $\mathbb{E}_{p(\boldsymbol{z}_n|\boldsymbol{x}_n,\hat{\Theta})}[\boldsymbol{z}_n]$
  - $\boldsymbol{z}_n\boldsymbol{z}_n^\top$ replaced by $\mathbb{E}_{p(\boldsymbol{z}_n|\boldsymbol{x}_n,\hat{\Theta})}[\boldsymbol{z}_n\boldsymbol{z}_n^\top]$
- However, in some LVMs, these expectations are intractable to compute and need to be approximated (will see some examples later), e.g., using MC integral approximation

What's Going On In EM?

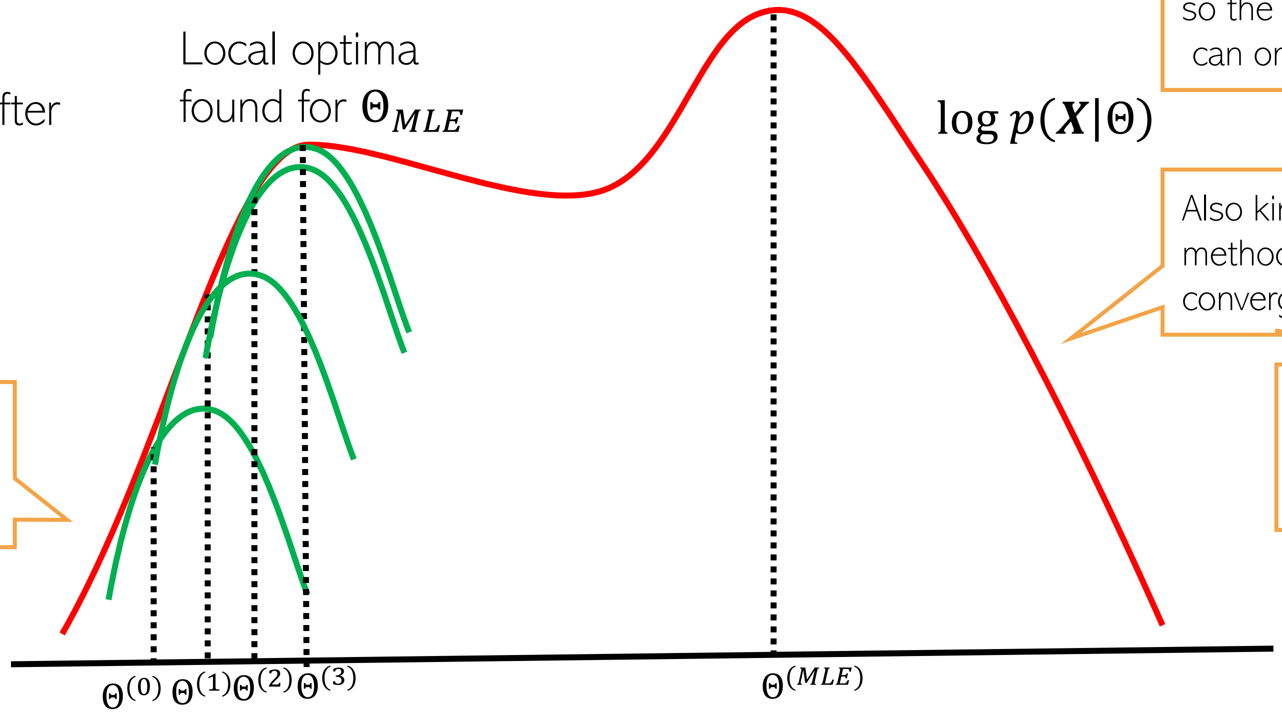
Alternating between them until convergence to some local optima

- As we saw, the maximization of lower bound $\mathcal{L}(q, \Theta)$ had two steps
- Step 1 finds the optimal q (call it $\hat{q}$) by setting it as the posterior of $\boldsymbol{Z}$ given current Θ
- Step 2 maximizes $\mathcal{L}(\hat{q}, \Theta)$ w.r.t. Θ which gives a new Θ.

KL becomes zero and $\mathcal{L}(q, \Theta)$ becomes equal to $\log p(\boldsymbol{X}|\Theta)$; thus their curves touch at current Θ

Note that Θ only changes in Step 2 so the objective $\log p(\boldsymbol{X}|\Theta)$ can only change in Step 2

Green curve: $\mathcal{L}(\hat{q}, \Theta)$ after setting q to $\hat{q}$



Good initialization matters; otherwise would converge to a poor local optima

Also kind of similar to Newton's method (and has second order like convergence behavior in some cases)

Unlike Newton's method, we don't construct and optimize a quadratic approximation, but a lower bound

Even though original MLE problem $\text{argmax}_{\Theta} \log p(\boldsymbol{X}|\Theta)$ could be solved using gradient methods, EM often works faster and has cleaner updates

Some Applications of EM

- Mixture Models (each data-point comes from one of K mixture components)
  - Examples: Mixture of Gaussians, Mixture of Experts, etc
- Latent variable models for dimensionality reduction or representation learning
  - Probabilistic PCA, Factor Analysis, Variational Autoencoders, etc
- Problems models with missing features/labels (treated as latent variables)
  - An example of problem with missing labels: Semi-supervised learning
- Hyperparameter estimation in probabilistic models (an alternative to MLE-II)
  - MLE-II estimates hyperparams by maximizing the marginal likelihood, e.g.,

$$\{\hat{\lambda}, \hat{\beta}\} = \text{argmax}_{\lambda,\beta}\, p(\boldsymbol{y}|\boldsymbol{X},\lambda,\beta) = \text{argmax}_{\lambda,\beta} \int p(\boldsymbol{y}|\boldsymbol{w},\boldsymbol{X},\beta)p(\boldsymbol{w}|\lambda)d\boldsymbol{w}$$

For a Bayesian linear regression model

  - With EM, can treat $\boldsymbol{w}$ as latent var, and $\boldsymbol{\lambda},\boldsymbol{\beta}$ as "parameters"
    - E step will estimate the CP of $\boldsymbol{w}$ given current estimates of $\boldsymbol{\lambda},\boldsymbol{\beta}$
    - M step will re-estimate $\boldsymbol{\lambda},\boldsymbol{\beta}$ by maximizing the expected CLL

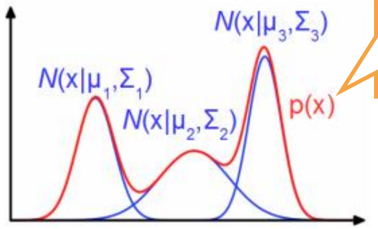
$$\mathbb{E}[\log p(\boldsymbol{y},\boldsymbol{w}|\mathbf{X},\beta,\lambda)] = \mathbb{E}[\log p(\boldsymbol{y}|\boldsymbol{w},\mathbf{X},\beta) + \log p(\boldsymbol{w}|\lambda)]$$

Expectations w.r.t. the CP of $\boldsymbol{w}$

An Example: Mixture Models

If the $\boldsymbol{z}_n$ were known, it just becomes **generative classification**, for which which we know how to estimate $\boldsymbol{\theta}$ and $\boldsymbol{\phi}$, given training data

- Assume K probability distributions (e.g., Gaussians), one for each cluster



$p(x)$ is a Gaussian mixture model (GMM)

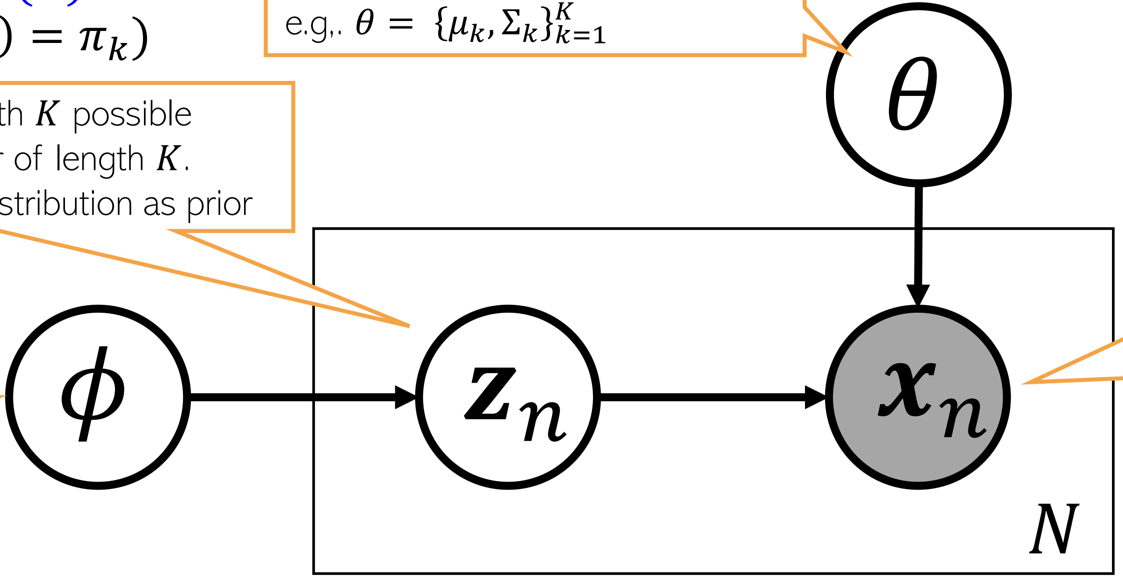
$p(z_n \,|\phi) = \text{multinoulli}(\boldsymbol{\pi})$

(also means $p(z_n = k \,|\phi) = \pi_k$)

Parameters of the K distributions, e.g,. $\theta = \{\mu_k, \Sigma_k\}_{k=1}^K$

Discrete latent variable (with K possible values) or a one-hot vector of length K. Modeled by a multinoulli distribution as prior

The parameter vector $\boldsymbol{\pi} = [\pi_1, \pi_2, \ldots, \pi_K]$ of the multinoulli distribution



Assumed generated from one of the K distributions depending on the true (but unknown) value of z_n (which clustering will find))

The likelihood distributions

$p(\boldsymbol{x}_n \,|\boldsymbol{z}_n = k, \theta) = \mathcal{N}(\mu_k, \Sigma_k)$

- The log-likelihood will be

$$\log p(\boldsymbol{x}_n|\Theta) = \log \sum_{k=1}^{K} p(\boldsymbol{x}_n, \boldsymbol{z}_n = k|\Theta)$$

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

MLE on this objective won't give closed form solution for the parameters

Detour: MLE for Generative Classification

- 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
- The labels $\boldsymbol{z}_n$ (known) are one-hot vecs. Also, $z_{nk} = 1$ if $\boldsymbol{z}_n = k$, and $\boldsymbol{z}_{nk} = \mathbf{0}$, o/w
- Assuming class prior as $p(\boldsymbol{z}_n = k) = \pi_k$, the model has params $\Theta = \{\pi_k, \mu_k, \Sigma_k\}_{k=1}^{K}$
- Given training data $\{\boldsymbol{x}_n, \boldsymbol{z}_n\}_{n=1}^{N}$, the MLE solution will be

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

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

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

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

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

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

Detour: MLE for Generative Classification

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

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

multinoulli

Gaussian

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

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

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

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

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

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 $z_{nk} = 1$

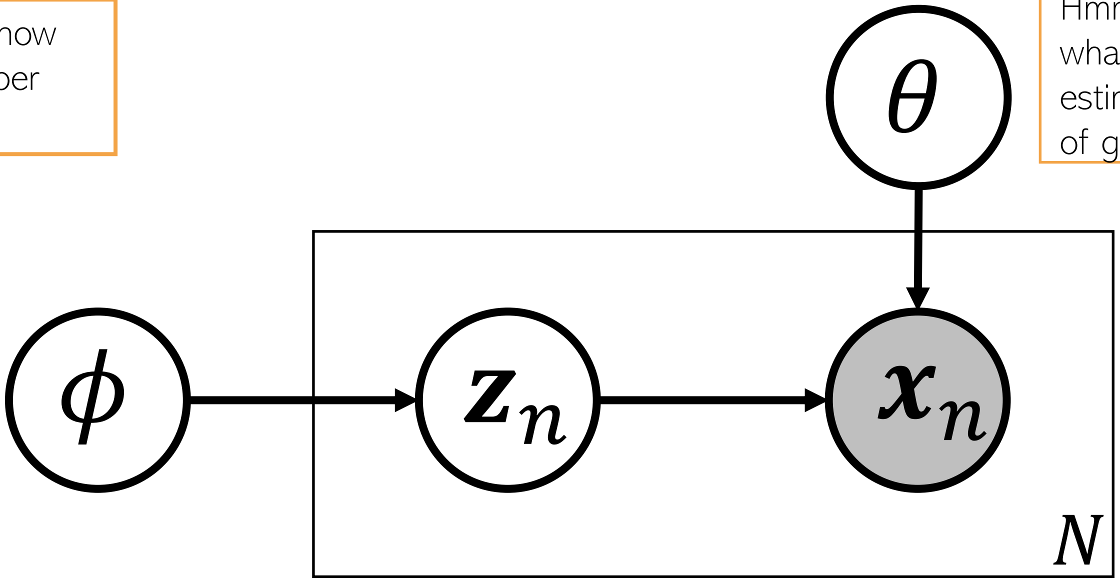
The form of this expression is important; will encounter this in GMM too

EM for Mixture Models

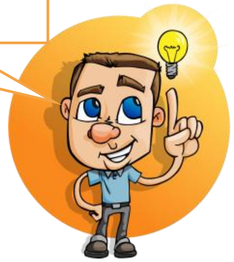
- So how do we estimate the parameters of a GMM where $\boldsymbol{z}_n$'s are <u>unknown</u>?

Well, you kind of already know how to do this. ☺ Remember generative classification?

Yes, exactly. ☺ However, just like in gen-class, you will need to repeat the guess and estimate them a few times until you converge



Hmmmm.. So can we make a guess what the value of each $\boldsymbol{z}_n$ and then estimate $\boldsymbol{\theta}$ and $\boldsymbol{\phi}$ as we do in case of generative classification??



- The guess about $\boldsymbol{z}_n$ can be in one of the two forms
  - A "hard" guess – a single best value $\hat{\boldsymbol{z}}_n$ (some "optimal" value of the random variable $\boldsymbol{z}_n$)
  - The "expected" value $\mathbb{E}[\boldsymbol{z}_n]$ of the random variable $\boldsymbol{z}_n$
- Using the hard guess $\hat{\boldsymbol{z}}_n$ of $\boldsymbol{z}_n$ will result in an ALT-OPT like algorithm
- Using the expected value of $\boldsymbol{z}_n$ will give the so-called Expectation-Maximization (EM) algo

EM is pretty much like ALT-OPT but with soft/expected values of the latent variables

EM for Gaussian Mixture Model (GMM)

Expectation of CLL

- 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 <u>conditional</u> posterior distribution of $\boldsymbol{Z}$, i.e., $p(\boldsymbol{Z}|\boldsymbol{X}, \Theta)$

It is "conditional" posterior because it is also conditioned on $\boldsymbol{\Theta}$, not just data $\boldsymbol{X}$

Requires knowing $\boldsymbol{\Theta}$

- 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

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 <u>expected</u> 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

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

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

N_k : Effective number of points in cluster k

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

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

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

EM for GMM (Contd)

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

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

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

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

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)

Accounts for fraction of points in each cluster

Accounts for cluster shapes (since each cluster is a Gaussian

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

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

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 vs Gradient-based Methods

- Can also estimate params using gradient-based optimization instead of EM
  - We can usually explicitly sum over or integrate out the latent variables $\boldsymbol{Z}$, e.g.,

$$\mathcal{L}(\Theta) = \log p(\mathbf{X}|\Theta) = \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\Theta)$$

  - Now we can optimize $\mathcal{L}(\Theta)$ using first/second order optimization to find the optimal Θ
- EM is usually preferred over this approach because
  - The M step has often simple closed-form updates for the parameters Θ
  - Often constraints (e.g., PSD matrices) are automatically satisfied due to form of updates
  - In some cases†, EM usually converges faster (and often like second-order methods)
    - E.g., Example: Mixture of Gaussians with when the data is reasonably well-clustered
  - EM also provides the conditional posterior over the latent variables Z (from E step)

†Optimization with EM and Expectation-Conjugate-Gradient (Salakhutdinov et al, 2003), On Convergence Properties of the EM Algorithm for Gaussian Mixtures (Xu and Jordan, 1996), Statistical guarantees for the EM algorithm: From population to sample-based analysis (Balakrishnan et al, 2017)

EM: Some Final Comments

- The E and M steps may not always be possible to perform exactly. Some reasons
  - The conditional posterior of latent variables $p(Z|X,\Theta)$ may not be easy to compute
    - Will need to approximate $p(Z|X,\Theta)$ using methods such as MCMC or variational inference

Results in
Monte-Carlo EM

  - Even if $p(Z|X,\Theta)$ is easy, the expected CLL may not be easy to compute

$$\mathbb{E}[\log p(\mathbf{X},\mathbf{Z}|\Theta)] = \int \log p(\mathbf{X},\mathbf{Z}|\Theta)p(\mathbf{Z}|\mathbf{X},\Theta)d\mathbf{Z}$$

Can often be approximated by Monte-Carlo using sample from the CP of Z

  - Maximization of the expected CLL may not be possible in closed form
- EM works even if the M step is only solved approximately (Generalized EM)
- If M step has multiple parameters whose updates depend on each other, they are updated in an alternating fashion - called Expectation Conditional Maximization (ECM)
- Other advanced probabilistic inference algos are based on ideas similar to EM
  - E.g., Variational EM, Variational Bayes (VB) inference, a.k.a. Variational Inference (VI)