Expectation-Maximization (Contd) and Introduction to Variational Inference

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Recap: The Expectation Maximization (EM) Algorithm

Used for doing parameter estimation in latent variable models

$$\Theta_{MLE} = \arg\max_{\Theta} \log p(\mathbf{X}|\Theta) = \arg\max_{\Theta} \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\Theta)$$

The EM Algorithm

- Initialize Θ as $\Theta^{(0)}$, set $t = 1$
- Step 1: Compute conditional posterior of latent vars given current params $\Theta^{(t-1)}$

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

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

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

- If not yet converged, set $t = t + 1$ and go to Step 1.

Making EM Faster: Online EM

- Needn't compute $p(\boldsymbol{z}_n|\boldsymbol{x}_n)$ for every $\boldsymbol{x}_n$ in each EM iteration (computational/storage efficiency)
  - Recall that the expected CLL is often a sum over all data points

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

  - Can compute this quantity recursively using small minibatches of data

$$\mathcal{Q}_t = (1-\gamma_t)\mathcal{Q}_{t-1} + \gamma_t \left[\sum_{n=1}^{N_t} \mathbb{E}[\log p(\boldsymbol{x}_n|\boldsymbol{z}_n, \theta)] + \mathbb{E}[\log p(\boldsymbol{z}_n|\phi)]\right]$$

    .. where $\gamma_t = (1+t)^{-\kappa}, 0.5 < \kappa \leq 1$ is a decaying learning rate

  - Requires computing $p(\boldsymbol{z}_n|\boldsymbol{x}_n)$ only for data in current mini-batch (computational/storage efficiency)
  - MLE on above $\mathcal{Q}_t$ can be shown to be equivalent to a simple recursive updates for Θ

$$\Theta^{(t)} = (1-\gamma_t) \times \Theta^{(t-1)} + \gamma_t \times \arg\max_{\Theta} \underbrace{\mathcal{Q}(\Theta, \Theta^{t-1})}_{\text{computed using only the } N_t \text{ examples from this minibatch}}$$

How M Step uses Sufficient Statistics

- First recall the **batch EM** algorithm for a K component Gaussian mixture model
  - Cluster id $\boldsymbol{z}_n$ s.t. $z_{nk} = 1$ if $\boldsymbol{x}_n$ belongs to cluster k, and zero otherwise
  - The conditional posterior of z_{nk} is $p(z_{nk} = 1|\boldsymbol{x}_n, \Theta) \propto \pi_k \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$
- Denoting current iteration by t, and the expectation computed in E step: $\mathbb{E}[z_{nk}^{(t)}] = \gamma_{nk}^{(t)}$
- The M step updates for params $\Theta = \{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$ are

$$\begin{aligned}
\boldsymbol{\mu}_k^{(t)} &= \frac{1}{N_k}\sum_{n=1}^N \gamma_{nk}^{(t)} \boldsymbol{x}_n \\
\boldsymbol{\Sigma}_k^{(t)} &= \frac{1}{N_k}\sum_{n=1}^N \gamma_{nk}^{(t)} (\boldsymbol{x}_n - \boldsymbol{\mu}_k^{(t)})(\boldsymbol{x}_n - \boldsymbol{\mu}_k^{(t)})^\top \\
\pi_k^{(t)} &= \frac{\sum_{n=1}^N \gamma_{nk}^{(t)}}{N}
\end{aligned}$$

- Each update depends on sum of expected sufficient statistics (ESS). For each data point $\boldsymbol{x}_n, \boldsymbol{z}_n$
  - ESS for $\boldsymbol{\mu}_k$ is $\gamma_{nk}^{(t)} \boldsymbol{x}_n$; ESS for $\boldsymbol{\Sigma}_k$ is $\gamma_{nk}^{(t)} (\boldsymbol{x}_n - \boldsymbol{\mu}_k^{(t)})(\boldsymbol{x}_n - \boldsymbol{\mu}_k^{(t)})^\top$; ESS for π_k is $\gamma_{nk}^{(t)}$

Batch EM Algorithm in terms of Sufficient Statistics

- Denote the sum of ESS as $\mathbf{S} = \sum_{n=1}^{N} \boldsymbol{s}_n$ where each ESS $\boldsymbol{s}_n = \sum_{\boldsymbol{z}_n} p(\boldsymbol{z}_n|\boldsymbol{x}_n, \Theta)\phi(\boldsymbol{x}_n, \boldsymbol{z}_n)$
- Here $\phi(\boldsymbol{x}_n, \boldsymbol{z}_n)$ is the SS associated with one observation $\boldsymbol{x}_n$ and its latent variable $\boldsymbol{z}_n$
- M step updates of Θ are like computing a function of $\mathbf{S}$, i.e., $\Theta = f(\mathbf{S})$

Batch EM in terms of ESS

- Initialize $\mathbf{S}$ and compute parameters $\Theta = f(\mathbf{S})$
- For $t = 1 : T$ (or until convergence)
  - $\mathbf{S}^{new} = 0$ (fresh sum of ESS; will be computed in this iteration)
  - For $n = 1 : N$

$$
\begin{aligned}
\boldsymbol{s}_n &= \sum_{\boldsymbol{z}_n} p(\boldsymbol{z}_n|\boldsymbol{x}_n, \Theta)\phi(\boldsymbol{x}_n, \boldsymbol{z}_n) = \mathbb{E}[\phi(\boldsymbol{x}_n, \boldsymbol{z}_n)] \\
\mathbf{S}^{new} &= \mathbf{S}^{new} + \boldsymbol{s}_n
\end{aligned}
$$

  - $\mathbf{S} = \mathbf{S}^{new}$
  - Recompute parameters $\Theta = f(\mathbf{S})$

- Note: In general, there may be more than one sum of ESS (one for each parameter update)

Online EM Algorithm in terms of Sufficient Statistics

- Works in a similar way as batch EM except we need an online way to update $\mathbf{S}$
- Can be done in one of the two manners (Liang and Klein, 2009)
  - Stepwise EM (based on recursively updating the sum of ESS)
  - Incremental EM (based on deleting old and adding new ESS of each data point)

Online EM as Stepwise EM

- Initialize the sum of ESS $\mathbf{S}$ and compute $\Theta = f(\mathbf{S})$
- For $t = 1 : T$ (or until convergence)
  - Set "learning rate" γ_t, pick a random example n and compute its sufficient statistics

$$\begin{aligned} \boldsymbol{s}_n &= \sum_{\boldsymbol{z}_n} p(\boldsymbol{z}_n | \boldsymbol{x}_n, \Theta)\phi(\boldsymbol{x}_n, \boldsymbol{z}_n) \\ \mathbf{S} &= (1 - \gamma_t)\mathbf{S} + \gamma_t \boldsymbol{s}_n \end{aligned}$$

  - Recompute $\Theta = f(\mathbf{S})$

Online EM Algorithm in terms of Sufficient Statistics

- The other Online EM approach "Incremental EM" needs no learning rate (unlike "Stepwise EM")

Online EM as Incremental EM

- Initialize each ESS $\boldsymbol{s}_n$, $n = 1, \ldots, N$, $\mathbf{S} = \sum_{n=1}^{N} \boldsymbol{s}_n$, and compute $\Theta = f(\mathbf{S})$
- For $t = 1 : T$ (or until convergence)
  - Pick a random example n and update its exp. sufficient statistics

$$\begin{aligned}
\boldsymbol{s}_n^{new} &= \sum_{\boldsymbol{z}_n} p(\boldsymbol{z}_n | \boldsymbol{x}_n, \Theta) \phi(\boldsymbol{x}_n, \boldsymbol{z}_n) \\
\mathbf{S} &= \mathbf{S} + \boldsymbol{s}_n^{new} - \boldsymbol{s}_n \\
\boldsymbol{s}_n &= \boldsymbol{s}_n^{new}
\end{aligned}$$

  - Recompute $\Theta = f(\mathbf{S})$

- However, incremental EM requires keeping a track of sum of ESS $\mathbf{S}$ as well as each $\boldsymbol{s}_n$
- In practice, stepwise EM outperforms batch EM as well as incremental EM on many problems (can refer to Liang and Klein, 2009 for some examples of models where these algos were tried)

EM vs Gradient-based Methods

- Can also estimate params use gradient-based optimization (or backprop in general) instead of EM
  - Reason: We can usually explicitly sum over or integrate out the latent variables $\mathbf{Z}$, 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 the form of updates
  - In some cases[†], EM usually converges faster (and often like second-order methods like Newton's)
    - Example: Mixture of Gaussians with when the data is reasonably well-clustered
  - EM applies even when the explicit summing over is expensive or integrating out isn't tractable
  - EM also provides the conditional posterior over the latent variables $\mathbf{Z}$ (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)

Variational Bayes (VB)
a.k.a. Variational Inference (VI)

(Note: "variational" here refers to optimization of functions of distributions)

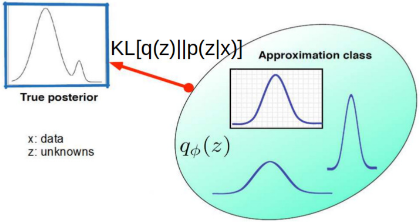
- Origins of VB/VI were in Statistical Physics (mainly "mean-field" methods; early 80s)
- Some of the early applications of VB/VI were for neural networks (late 80s)
- Became very popular in ML community in late 90s (and continues to remain so)
  - Primary reason: Faster than MCMC methods
- An aside: Statistics researchers were somewhat skeptical of VB/VI (but that is changing now) and continued their allegiance towards MCMC methods for approximate posterior inference

Variational Bayes (VB) or Variational Inference (VI)

- Consider a model with data $\mathbf{X}$ and unknowns $\mathbf{Z}$. Goal: Compute the posterior $p(\mathbf{Z}|\mathbf{X})$
- Suppose $p(\mathbf{Z}|\mathbf{X})$ is intractable. VB/VI approximates it using a distribution $q(\mathbf{Z}|\phi)$ or $q_\phi(\mathbf{Z})$
- VB/VI finds the $q(\mathbf{Z}|\phi)$ that is "closest" to $p(\mathbf{Z}|\mathbf{X})$ by finding the "optimal" value of ϕ

$$\phi^* = \arg\min_{\phi} \text{KL}[q_\phi(\mathbf{Z})||p(\mathbf{Z}|\mathbf{X})]$$

- This amounts of finding the best distribution from a class of distributions parametrized by ϕ



- VB/VI refers to the free parameters ϕ as variational parameters (w.r.t. which we optimize)
- **But wait!** If $p(\mathbf{Z}|\mathbf{X})$ itself is intractable, can we (easily) solve the above KL minimization problem?

Variational Bayes (VB) or Variational Inference (VI)

- The following holds for any q: $\log p(\mathbf{X}|m) = \mathcal{L}(q) + \text{KL}(q||p)$ where

$$\begin{aligned}\mathcal{L}(q) &= \int q(\mathbf{Z}) \log\left[\frac{p(\mathbf{X},\mathbf{Z})}{q(\mathbf{Z})}\right] d\mathbf{Z} \\ \text{KL}(q||p) &= -\int q(\mathbf{Z}) \log\left[\frac{p(\mathbf{Z}|\mathbf{X})}{q(\mathbf{Z})}\right] d\mathbf{Z}\end{aligned}$$

- Above is similar to what we had in EM, but now no Θ (param) vs $\mathbf{Z}$ (latent var) distinction
- We would like to infer the posterior for all the unknowns (denoted collectively as $\mathbf{Z}$)
- Since $\log p(\mathbf{X})$ is a constant w.r.t. $\mathbf{Z}$, the following must hold

$$\arg\min_q \text{KL}(q||p) = \arg\max_q \mathcal{L}(q)$$

- Since $\text{KL}(q||p) \geq 0$, $\log p(\mathbf{X}) \geq \mathcal{L}(q)$
- $\mathcal{L}(q)$ is also known as the **Evidence Lower Bound (ELBO)**
  - Reason for the name "ELBO": $\log p(\mathbf{X})$ or $\log p(\mathbf{X}|m)$ is the log-evidence of model m

VB/VI = Maximizing the ELBO

- Notation: $q(\mathbf{Z})$, $q(\mathbf{Z}|\phi)$, $q_\phi(\mathbf{Z})$, all will refer to the same thing
- VB/VI finds an approximating distribution $q(\mathbf{Z})$ that maximizes the ELBO

$$\mathcal{L}(q) = \int q(\mathbf{Z}) \log \left[\frac{p(\mathbf{X}, \mathbf{Z})}{q(\mathbf{Z})} \right] d\mathbf{Z}$$

- Since $q(\mathbf{Z})$ depends on ϕ, the ELBO is essentially a function of ϕ

$$\mathcal{L}(q) = \mathcal{L}(\phi) = \mathbb{E}_q[\log p(\mathbf{X}, \mathbf{Z})] - \mathbb{E}_q[\log q(\mathbf{Z})] = \mathbb{E}_q[\log p(\mathbf{X}|\mathbf{Z})] - \mathrm{KL}(q(\mathbf{Z})||p(\mathbf{Z}))$$

- Makes sense: Maximizing $\mathcal{L}(q)$ will give a q that explains data well and is close to the prior
- Maximizing $\mathcal{L}(q)$ w.r.t. q can still be hard in general (note the expectation w.r.t. q)
- Some of the ways to make this problem easier
  1. Restricting the form of our approximation $q(\mathbf{Z})$, e.g., mean-field VB (today's discussion)
  2. Using Monte-Carlo approximation of the expectation/gradient of the ELBO (later)
- For locally conjugate models VB/VI is particularly easy to derive

Mean-Field VB

- One of the simplest ways of doing VB
- In mean-field VB, we define a partition of the latent variables $\mathbf{Z}$ into M groups $\mathbf{Z}_1, \ldots, \mathbf{Z}_M$
- Assume our approximation $q(\mathbf{Z})$ factorizes over these groups

$$q(\mathbf{Z}|\phi) = \prod_{i=1}^{M} q(\mathbf{Z}_i|\phi_i)$$

- As a short-hand, sometimes we write $q = \prod_{i=1}^{M} q_i$ where $q_i = q(\mathbf{Z}_i|\phi_i)$
- In mean-field VB, learning the optimal q reduces to learning the optimal $q_1, \ldots, q_M$
- The groups are usually chosen based on the model's structure, e.g., in Bayesian linear regression

$$q(\mathbf{Z}|\phi) = q(\boldsymbol{w}, \lambda, \beta|\phi) = q(\boldsymbol{w}|\phi_w)q(\lambda|\phi_\lambda)q(\beta|\phi_\beta)$$

- Note: Mean-field is quite a strong assumption (can destroy structure among latent variables)

Deriving Mean-Field VB Updates

- With $q = \prod_{i=1}^{M} q_j$, what's each optimal q_i equal to when we do $\arg\max_q \mathcal{L}(q)$?
- Note that under this mean-field assumption, the ELBO simplifies to

$$\mathcal{L}(q) = \int q(\mathbf{Z}) \log \left[\frac{p(\mathbf{X},\mathbf{Z})}{q(\mathbf{Z})} \right] d\mathbf{Z} = \int \prod_i q_i \left[\log p(\mathbf{X},\mathbf{Z}) - \sum_i \log q_i \right] d\mathbf{Z}$$

- Suppose we wish to find the optimal q_j given all other q_i $(i \neq j)$. Let's re-express $\mathcal{L}(q)$ as

$$\begin{aligned}
\mathcal{L}(q) &= \int q_j \left[\int \log p(\mathbf{X},\mathbf{Z}) \prod_{i \neq j} q_i d\mathbf{Z}_i \right] d\mathbf{Z}_j - \int q_j \log q_j d\mathbf{Z}_j \quad + \quad \text{consts w.r.t. } q_j \\
&= \int q_j \log \tilde{p}(\mathbf{X},\mathbf{Z}_j) d\mathbf{Z}_j - \int q_j \log q_j d\mathbf{Z}_j
\end{aligned}$$

where $\log \tilde{p}(\mathbf{X},\mathbf{Z}_j) = \mathbb{E}_{i \neq j}[\log p(\mathbf{X},\mathbf{Z})] + \text{const}$

- Note that $\mathcal{L}(q) = -KL(q_j || \tilde{p}) + \text{const}$. Which q_j will maximize it?

$$\boxed{q_j = \tilde{p}(\mathbf{X},\mathbf{Z}_j)}$$

Deriving Mean-Field VB Updates

- Since $\log q_j^*(\mathbf{Z}_j) = \log \tilde{p}(\mathbf{X}, \mathbf{Z}_j) = \mathbb{E}_{i \neq j}[\ln p(\mathbf{X}, \mathbf{Z})] + \text{const}$, we have

$$q_j^*(\mathbf{Z}_j) = \frac{\exp(\mathbb{E}_{i \neq j}[\ln p(\mathbf{X}, \mathbf{Z})])}{\int \exp(\mathbb{E}_{i \neq j}[\ln p(\mathbf{X}, \mathbf{Z})]) d\mathbf{Z}_j} \qquad \forall j$$

- Note: Only need to compute the numerator. Denominator can usually be recognized by inspection
- For locally-conjugate models, $q_j^*(\mathbf{Z}_j)$ will have the same form as the prior $p(\mathbf{Z}_j)$
- Important: For estimating q_j, the required expectation depends on other $\{q_i\}_{i \neq j}$
- Thus we need to cycle through updating each q_j in turn (similar to co-ordinate ascent, alternating optimization, Gibbs sampling, etc.)
- Guaranteed to converge (to a local optima)
  - We are basically solving a sequence of concave maximization problems
  - Reason: $\mathcal{L}(q) = \int q_j \ln \tilde{p}(\mathbf{X}, \mathbf{Z}_j)\mathbf{Z}_j - \int q_j \ln q_j d\mathbf{Z}_j + \text{const}$ is concave w.r.t. each q_j

The Mean-Field VB Algorithm

- Also known as Co-ordinate Ascent Variational Inference (CAVI) Algorithm
- Input: Model $p(\mathbf{X}, \mathbf{Z})$, Data $\mathbf{X}$
- Output: A variational distribution $q(\mathbf{Z}) = \prod_{j=1}^{M} q_j(\mathbf{Z}_j)$
- Initialize: Variational distributions $q_j(\mathbf{Z}_j)$, $j = 1, \ldots, M$
- While the ELBO has not converged
  - For each $j = 1, \ldots, M$, set

$$q_j(\mathbf{Z}_j) \propto \exp(\mathbb{E}_{i \neq j}[\log p(\mathbf{X}, \mathbf{Z})])$$

  - Compute ELBO $\mathcal{L}(q) = \mathbb{E}_q[\log p(\mathbf{X}, \mathbf{Z})] - \mathbb{E}_q[\log q(\mathbf{Z})]$

Next Class

- Continue the discussion on mean-field VI
- Some examples of mean-field VI
- Mean-field VI for models with exponential family distributions
- Some properties of VI
- More general forms of VI (modern VI methods)