# Expectation-Maximization (Contd) and Introduction to Variational Inference

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Topics in Probabilistic Modeling and Inference (CS698X)

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# Recap: The Expectation Maximization (EM) Algorithm

Used for doing parameter estimation in latent variable models

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

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## The EM Algorithm

- Initialize $\Theta$ 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. $\Theta$

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

- 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

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

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  - Can compute this quantity recursively using small minibatches of data

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  - 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 $\Theta$

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

# How M Step uses Sufficient Statistics

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

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- 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 $\Theta$ 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)

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- 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

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- 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

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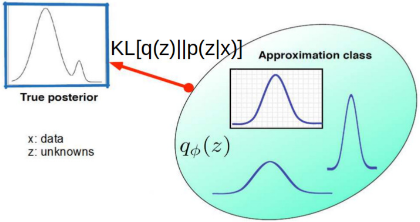

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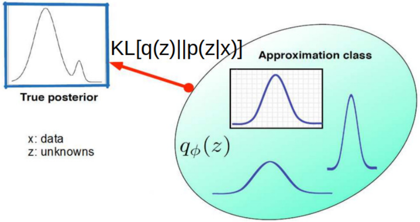


- VB/VI refers to the free parameters $\phi$ as variational parameters (w.r.t. which we optimize)

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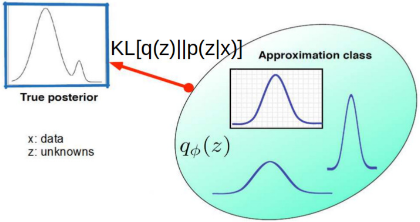
- VB/VI finds the $q(\mathbf{Z}|\phi)$ that is "closest" to $p(\mathbf{Z}|\mathbf{X})$ by finding the "optimal" value of $\phi$

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

- This amounts of finding the best distribution from a class of distributions parametrized by $\phi$




- VB/VI refers to the free parameters $\phi$ 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

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    - Reason for the name "ELBO": $\log p(\mathbf{X})$ or $\log p(\mathbf{X}|m)$ is the log-evidence of model $m$

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- For locally conjugate models VB/VI is particularly easy to derive

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

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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

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  - 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)