Variational Inference

CS772A: Probabilistic Machine Learning Piyush Rai

Variational Bayes (VB) or Variational Inference (VI)²

- Consider a model with data X and unknowns Z. Goal: Compute the posterior p(Z|X)
- Z denotes all unknowns (params, latent vars, hyperparams of likelihood, prior, etc)

• Assuming $p(\pmb{Z}|\pmb{X})$ is intractable, VB/VI approximates it by a distr $q(\pmb{Z}|\pmb{\phi})$ or $q_{\pmb{\phi}}(\pmb{Z})$

Often called variational parameters

Defines a class of distributions

parametrized by ϕ

• We find the best approx. distr by finding ϕ s.t. its <u>distance</u> from p(Z|X) is minimized

But since we don't Other measures have also VI turns inference into optimization been used such as reverse know $p(\boldsymbol{Z}|\boldsymbol{X})$, can KL (KL[p||q]), and we easily solve Often, we will simply write various other divergence it as $\operatorname{argmin}_q \operatorname{KL}[q||p_z]$ this optimization functions defined for KL[q(z)||p(z|x)]Approximation class problem? distributions $\phi^* = \operatorname{argmin}_{\phi} \operatorname{KL}[q_{\phi}(Z)||p(Z|X)]$ **True posterior** x: data $q_{\phi}(z)$ z: unknowns Note: The name "variational" comes from Physics

Optimizing functions of distributions (KL is a func of distr)

Variational Bayes (VB) or Variational Inference (VI)³

• VB/VI is based on following identity for the log marg-lik (log evidence) of a model m

Similar as the identify we had in case of EM, which was defined for log of the ILL

$$\int \log p(\mathbf{X}|m) = \mathcal{L}(q) + \mathrm{KL}(q||p_z)^2$$

Also, unlike EM, here we don't have any distinction b/w latent variables Z and parameters Θ (all unknowns will be denoted by Z here, and we have $\mathcal{L}(q)$, not $\mathcal{L}(q, \Theta)$)

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

$$\mathrm{KL}(q||\mathbf{p}_{\mathbf{Z}}) = -\int q(\mathbf{Z})\log\left\{\frac{p(\mathbf{Z}|\mathbf{X})}{q(\mathbf{Z})}\right\}d\mathbf{Z}$$

• Since the log evidence $\log p(X|m)$ is constant w.r.t Z, we must have

$$\operatorname{argmin}_{q} \operatorname{KL}[q||p_{z}] = \operatorname{argmax}_{q} \mathcal{L}(q)$$

- Also note that since $KL[q||p_z] \ge 0$, we must have $\log p(X|m) \ge \mathcal{L}(q)$
- Therefore, $\mathcal{L}(q)$ is also known as Evidence Lower Bound (ELBO)
 - VB/VI finds the best q(Z) by maximizing the ELBO w.r.t. q



VB/VI = Maximizing the ELBO

- Notation: q(Z), $q(Z|\phi)$, $q_{\phi}(Z)$, all refer to the same thing (the approx. distr.)
- VB/VI finds an approximating distribution q(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 $\mathcal{L}(q) = \mathcal{L}(\phi) = \mathbb{E}_q[\log p(\mathbf{X}, \mathbf{Z})] - \mathbb{E}_q[\log q(\mathbf{Z})]$ $= \mathbb{E}_q[\log p(\mathbf{X}|\mathbf{Z})] - \mathrm{KL}[q(\mathbf{Z})||p(\mathbf{Z})]$
- ullet Thus maximizing the ELBO will give an approximating distr. q(Z) which
 - Explains the data **X** well, i.e., gives it large probability (large $\mathbb{E}_q[\log p(X|Z)]$)
 - Is close to the prior p(Z), i.e. is simple/regularized (small KL[log q(Z)||p(Z)])



Maximizing the ELBO

The goal is to maximize the ELBO

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

- This may still be hard because
 - ELBO expression has expectations, computed which may be intractable
 - Maximizing the ELBO will require computing gradients which may not always be easy
- Some of the ways to make this problem easier
 - Restricting the form of our approximation q(Z), e.g., mean-field VI
 - Using Monte-Carlo approximation of the expectation/gradient of the ELBO
- For locally conjugate models, ELBO maximization is easy
 - Closed form updates for q(Z)



E.g., part of the ELBO

may have terms that are not differentiable

Some Properties of VI

• Recall that VI approximates a posterior p by finding q that minimizes KL(q||p)

$$\mathsf{KL}(q||p) = \int q(\mathsf{Z}) \log\left[rac{q(\mathsf{Z})}{p(\mathsf{Z}|\mathsf{X})}
ight]$$

- $q(\mathbf{Z})$ will be small where $p(\mathbf{Z}|\mathbf{X})$ is small otherwise KL will blow up
- Thus $q(\mathbf{Z})$ avoids low-probability regions of the true posterior



ELBO for Model Selection

- Recall that ELBO is a <u>lower bound</u> on log of model evidence $\log p(X|m)$
- Can compute ELBO for each model m and choose the one with largest ELBO

Plot of the variational lower bound \mathcal{L} versus the number K of components in the Gaussian mixture model, for the Old Faithful data, showing a distinct peak at K =2 components. For each value of K, the model is trained from 100 different random starts, and the results shown as '+' symbols $p(\mathcal{D}|K)$ plotted with small random horizontal perturbations so that they can be distinguished. Note that some solutions find suboptimal local maxima, but that this happens infrequently.



CS772A: PML

Some criticism since we are using a lower-bound but often works well in practice

VI and Convergence

- VI is guaranteed to converge to a local optima (just like EM)
- Therefore proper initialization is important (just like EM)
 - Can sometimes run multiple times with different initializations and choose the best run



- ELBO increases monotonically with iterations
 - Can thus monitor the ELBO to assess convergence



Variational Inference and Expectation Maximization

- VI can be seen as a generalization of the EM algorithm
- In VI, there is no distinction between parameters Θ and latent variables Z
 - Also recall that EM finds CP of ${m Z}$ and point estimate for ${m \Theta}$
 - VI treats all unknowns identically and infers posterior for all
- VI can be used within an EM algorithm if the E step is intractable
- E step is intractable if the CP of latent variables given params is intractable
- This version of EM is known as Variational EM (VEM)
- If we only care about point estimates of the parameters, VEM is widely used if the CP of latent variables is intractable

Mean-Field VI



- One of the simplest ways for doing VB/VI
- Assumes unknowns Z can be partitioned into M groups Z_1, Z_2, \ldots, Z_M , s.t.,

$$q(\mathbf{Z}|\boldsymbol{\phi}) = \prod_{i=1}^{M} q(\mathbf{Z}_{i}|\boldsymbol{\phi}_{i}) \overset{\text{As a shorthand, often written as } q = \prod_{i=1}^{M} q_{i}}{\overset{\text{where } q_{i} = q(Z_{i}|\boldsymbol{\phi}_{i})}}$$

- Learning the optimal q reduces to learning the optimal q_1, q_2, \ldots, q_M
- Groups usually chosen based on model's structure, e.g., in Bayesian linear regression $p(w,\beta,\lambda|X,y) \approx q(Z|\phi) = q(w,\beta,\lambda|\phi) = q(w|\phi_w)p(\beta|\phi_\beta)p(\lambda|\phi_\lambda)$
- Mean-field is a very restrictive assumption. Ignores the correlations among unknowns
 - Less restrictive versions also exist, such as structured mean-field (factorization is still there but only among groups of unknowns)

Deriving Mean-Field VI Updates

- With $q = \prod_{i=1}^{M} q_i$, what's the optimal q_i when we do $\operatorname{argmax}_q \mathcal{L}(q)$?
- 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} 's $(i \neq j)$ as fixed, then
$$\mathcal{L}(q) = \int q_{j} \left[\int \log p(\mathbf{X}, \mathbf{Z}) \prod_{i \neq j} q_{i} d\mathbf{Z}_{i} \right] d\mathbf{Z}_{j} - \int q_{j} \log q_{j} d\mathbf{Z}_{j} + \text{const w.r.t. } q_{j}$$

$$= \int q_{j} \log \hat{p}(\mathbf{X}, \mathbf{Z}_{j}) d\mathbf{Z}_{j} - \int q_{j} \log q_{j} \mathbf{Z}_{j}$$

$$= -\text{KL}(q_{j} || \hat{p}) \log \hat{p}(\mathbf{X}, \mathbf{Z}_{j}) = \mathbb{E}_{i \neq j} [\log p(\mathbf{X}, \mathbf{Z})] + \text{const}$$

$$q_{j}^{*} = \operatorname{argmax}_{q_{j}} \mathcal{L}(q) = \operatorname{argmin}_{q_{j}} \text{KL}(q_{j} || \hat{p}) = \hat{p}(\mathbf{X}, \mathbf{Z}_{j})$$

$$(5772A; PML)$$

Deriving Mean-Field VI Updates

• So we saw that the optimal q_i when doing mean-field VI is

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

- Note: Can often just compute the numerator and recognize denominator by inspection
- Important: For locally conjugate models, $q_j^*(Z_j)$ will have the same form as prior $p(Z_j)$
 - Only the distribution parameters will be different
- Important: For estimating q_j the required expectation depends on other $\{q_i\}_{i\neq j}$
 - Thus we use an alternating update scheme for these (akin to ALT-OPT, Gibbs sampling, etc)
- Guaranteed to converge (to a local optima)
 - We are basically solving a sequence of concave maximization problems
 - Reason: $\mathcal{L}(q) = \int q_j \log \hat{p}(X, Z_j) Z_j \int q_j \log q_j Z_j$ is concave in q_j



The Mean-Field VI Algorithm

- Also known as Co-ordinate Ascent Variational Inference (CAVI) Algorithm
- Input: Model in form of priors and likelihood, or joint p(X, Z), Data X
- Output: A variational distribution $q(Z) = \prod_{j=1}^{M} q_j(Z_j)$
- Initialize: Variational distributions $q_j(\mathbf{Z}_j)$, j = 1, 2, ... M
- While the ELBO has not converged
 - For each j = 1, 2, ..., M, set

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

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



Mean-Field VI: A Simple Example

- Consider data $\mathbf{X} = \{x_1, x_2, \dots, x_N\}$ from a one-dim Gaussian $\mathcal{N}(\mu, \tau^{-1})$
- Assume the following normal-gamma prior on μ and au

 $p(\mu|\tau) = \mathcal{N}(\mu|\mu_0, (\lambda_0\tau)^{-1}) \quad p(\tau) = \text{Gamma}(\tau|a_0, b_0)$

- Posterior is also normal-gamma due to the jointly conjugate prior
- Let's anyway verify this by trying mean-field VI for this model
- With mean-field assumption on the variational posterior $q(\mu, \tau) = q_{\mu}(\mu)q_{\tau}(\tau)$

$$\log q_{\mu}^{*}(\mu) = \mathbb{E}_{q_{\tau}}[\log p(\mathbf{X}, \mu, \tau)] + \text{const}$$
$$\log q_{\tau}^{*}(\tau) = \mathbb{E}_{q_{\mu}}[\log p(\mathbf{X}, \mu, \tau)] + \text{const}$$

• In this example, the log-joint $\log p(\mathbf{X}, \mu, \tau) = \log p(\mathbf{X}|\mu, \tau) + \log p(\mu|\tau) + \log p(\tau)$. Thus

 $\log q_{\mu}^{*}(\mu) = \mathbb{E}_{q_{\tau}}[\log p(\mathbf{X}|\mu,\tau) + \log p(\mu|\tau)] + \text{const} \quad (\text{only keeping terms that involve } \mu)$ $\log q_{\tau}^{*}(\tau) = \mathbb{E}_{q_{\mu}}[\log p(\mathbf{X}|\mu,\tau) + \log p(\mu|\tau) + \log p(\tau)] + \text{const}$

Mean-Field VI: A Simple Example

• Substituting $p(\mathbf{X}|\mu,\tau) = \prod_{n=1}^{N} p(x_n|\mu,\tau)$ and $p(\mu|\tau)$, we get

$$\log q_{\mu}^{*}(\mu) = \mathbb{E}_{q_{\tau}}[\log p(\mathbf{X}|\mu,\tau) + \log p(\mu|\tau)] + \text{const}$$
$$= -\frac{\mathbb{E}_{q_{\tau}}[\tau]}{2} \left\{ \sum_{n=1}^{N} (x_{n}-\mu)^{2} + \lambda_{0}(\mu-\mu_{0})^{2} \right\} + \text{const}$$

• (Verify) The above is log of a Gaussian. This $q_{\mu}^* = \mathcal{N}(\mu | \mu_N, \lambda_N)$ with

$$\mu_N = rac{\lambda_0 \mu_0 + N ar{x}}{\lambda_0 + N}$$
 and $\lambda_N = (\lambda_0 + N) \mathbb{E}_{q_\tau} [\tau]^2$ This update depends on q_τ

• Proceeding in a similar way (verify), we can show that $q_{\tau}^* = \text{Gamma}(\tau | a_N, b_N)$

$$a_N = a_0 + rac{N+1}{2}$$
 and $b_N = b_0 + rac{1}{2} \mathbb{E}_{q_\mu} \left[\sum_{n=1}^N (x_n - \mu)^2 + \lambda_0 (\mu - \mu_0)^2 \right]^2$ This update depends on q_μ

• Note: Updates of q_{μ}^{*} and q_{τ}^{*} depend on each other (hence alternating updates needed)

Mean-Field VI: A Closer Look

- Since $\log q_j^*(Z_j) = \mathbb{E}_{i \neq j}[\log p(X, Z)] + \text{const} = \mathbb{E}_{i \neq j}[\log p(X, Z_j, Z_{-j})] + \text{const}$ $\log q_j^*(Z_j) = \mathbb{E}_{i \neq j}[\log p(Z_j | X, Z_{-j})] + \text{const}$
- Thus opt variational distr $q_j^*(Z_j)$ basically requires expectations of CP $p(Z_j|X,Z_{-j})$
- For locally conjugate models, CP can be easily found and is usually an exp-fam distr

$$p(\mathbf{Z}_j|\mathbf{X},\mathbf{Z}_{-j}) = h(\mathbf{Z}_j) \exp\left[\eta(\mathbf{X},\mathbf{Z}_{-j})^\top \mathbf{Z}_j - A(\eta(\mathbf{X},\mathbf{Z}_{-j}))\right]$$

• Using the above, we can rewrite the optimal variational distribution as follows $\log q_j^*(\mathbf{Z}_j) = \mathbb{E}_{i \neq j} \left[\log \left(h(\mathbf{Z}_j) \exp \left[\eta(\mathbf{X}, \mathbf{Z}_{-j})^\top \mathbf{Z}_j - A(\eta(\mathbf{X}, \mathbf{Z}_{-j})) \right] \right) \right] + \text{const}$ $\implies q_j^*(\mathbf{Z}_j) \propto h(\mathbf{Z}_j) \exp \left[\mathbb{E}_{i \neq j} [\eta(\mathbf{X}, \mathbf{Z}_{-j})]^\top \mathbf{Z}_j \right] \quad (\text{verify}) \quad \text{For locally} \text{conjugate} \text{model}$

- Thus, with local conj, we just require expectation of nat. params. of CP of Z_j

VI by Computing ELBO Gradients <

- Modern VI methods (e.g., those used in Bayesian deep learning) use this idea (more later)
- Can also do VI by computing <u>ELBO's gradient</u> and doing gradient ascent/descent
- Gradient based approach is broadly applicable, not just for mean-field VI
 - 1. Assume $q(\mathbf{Z})$ to be from some family of distributions with variational parameters ϕ
 - 2. Write down the full ELBO expression (will give us a function of var parameters ϕ)

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

- 3. Compute ELBO gradients, i.e., $abla_{\phi} \, \mathcal{L}(\phi)$ and use gradient methods to find optimal ϕ
- Step 2 may be simplified due to the problem structure or the form of $q(\mathbf{Z})$
 - i.i.d. observations simplify $\log p(X|Z)$; conditionally independent priors simplify $\log p(Z)$
 - Locally-conjugate models
 - The mean-field assumption simplifies $q(\mathbf{Z})$ as $q = \prod_{i=1}^{M} q_i$
 - Moreover, the last term reduces to sum of entropies of q_i 's (which usually has known forms)



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Mean-Field VI by Taking ELBO's Gradients

• Mean-field assumption $q(\mathbf{Z}|\phi) = \prod_{i=1}^{M} q(\mathbf{Z}_i|\phi_i)$ results in following optimal distribution

This approach is applicable even if we don't have mean-field assumption

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

Note that here we do not have to assume the form of this variational distribution. We simply compute the RHS and find what it is (in the locallyconjugate case, it will be the same distribution as the prior)

Prior on variance of

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- Alternatively, we can take ELBO's partial deriv w.r.t. $\phi_1, \phi_2, \dots, \phi_M$ to find their optimal values
- Consider a Bayesian linear regression model

Prior on
$$w$$
 assumed fixed Gaussian likelihood
Likelihood $y_i \sim \text{Normal}(x_i^T w, \alpha^{-1}), \quad w \sim \text{Normal}(0, \lambda^{-1}I), \quad \alpha \sim \text{Gamma}(a, b)$
Needed Joint distribution on data and unknowns $p(y, w, \alpha | x) = p(\alpha)p(w)\prod_{i=1}^N p(y_i | x_i, w, \alpha)$
Assumed variational posterior with mean-field assumption $q(w, \alpha) = q(\alpha)q(w) = \text{Gamma}(\alpha | a', b')\text{Normal}(w | \mu', \Sigma')$
Note that in this approach, we have to assume a form for each variational distribution. It is common to assume them to have the same form as the respective priors

• Now doing VI amounts to maximizing ELBO to find the optimal variational params a', b', μ', Σ'

Mean-Field VI by Taking ELBO's Gradients

The ELBO is For the Bayesian linear regression model, instead of p(X, Z), it will be of the form p(y, Z|X)

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

Thus the ELBO in the Bayesian linear regression model will be (assuming i.i.d. obs)

$$\mathcal{L}(a',b',\mu',\Sigma') = \int q(\alpha)\ln p(\alpha)d\alpha + \int q(w)\ln p(w)dw$$
Expectations of the log of the prior
$$\int q(\alpha)\ln p(\alpha)d\alpha + \int q(w)\ln p(w)dw$$
Expectations of the log of the likelihood
$$\int q(\alpha)d\alpha - \int q(w)\ln q(w)dw$$
Expectations of the log of the var. distributions (= their entropies)

Substituting the priors, likelihoods, and variational distributions

$$\mathcal{L}(a',b',\mu',\Sigma') = (a-1)(\psi(a') - \ln b') - b\frac{a'}{b'} + \text{constant} - \frac{\lambda}{2}(\mu'^T\mu' + \text{tr}(\Sigma')) + \text{constant} + \frac{N}{2}(\psi(a') - \ln b') - \sum_{i=1}^{N} \frac{1}{2}\frac{a'}{b'}\left((y_i - x_i^T\mu')^2 + x_i^T\Sigma'x_i\right) + \text{constant}$$

Digamma function (log of gamma function)
$$+a' - \ln b' + \ln \Gamma(a') + (1-a')\psi(a') + \frac{1}{2}\ln|\Sigma'| + \text{constant}$$

- Can now maximize the above ELBO w.r.t. a', b', μ' , Σ' in an alternating fashion
- For most models, ELBO or its gradients won't have a simple form (methods like BBVI, reparam trick etc will be needed in those cases)

Coming Up Next

- VI for latent variable models with local and global unknowns
- VI for non-conjugate models
 - Mostly such methods rely on computing approximations of ELBO and/or its gradients

