

# Computational Statistics II

Unit D.1: Laplace approximation, Variational Bayes, and Expectation Propagation

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# Unit D.1

## Main concepts

- Laplace approximation;
- Variational Bayes;
- Expectation propagation.

## Main references

- Bishop, C. M. (2006). Pattern Recognition and Machine Learning (Chapter 9-10). Springer.
- Blei, D. M., Kucukelbir A., and McAuliffe, J. D. (2017). Variational inference: a review for statisticians. *JASA*, **112**(518), 859–877.
- Tierney, L. and Kadane, J. (1987). Accurate approximations for posterior moments and marginal densities. *JASA*, **81**(393), 82–86.

# Motivations

- MCMC methods could be expensive to compute, especially for large sample sizes  $n$ .
- Moreover, many MCMC algorithms require a rough estimate of some key posterior quantities, such as the posterior variance. Recall e.g. the MALA example of **unit B.2**.
- These issues motivates the development of **deterministic approximations** of the posterior distribution.
- Compared to MCMC methods, the accuracy of this class of approximations can not be reduced by running the algorithm longer.
- On the other hand, deterministic approximations are typically **very fast** to compute and sufficiently reliable in several applied contexts.

# The Laplace approximation

- Let  $\pi(\boldsymbol{\theta} \mid \mathbf{X})$  be a **continuous** and **differentiable** posterior density in  $\Theta \subseteq \mathbb{R}^p$ .
- The **Laplace** approximation is one of the first approximation methods that has been proposed. It was known even before the advent of MCMC.
- The key idea is approximating the log-posterior density  $\log \pi(\boldsymbol{\theta} \mid \mathbf{X})$  using a **Taylor expansion** around the mode  $\hat{\boldsymbol{\theta}}_{\text{MAP}}$ , yielding

$$\log \pi(\boldsymbol{\theta} \mid \mathbf{X}) \approx \log \pi(\hat{\boldsymbol{\theta}}_{\text{MAP}} \mid \mathbf{X}) - \frac{1}{2}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}_{\text{MAP}})^\top \hat{\mathbf{M}}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}_{\text{MAP}}) + \text{const},$$

where  $\hat{\mathbf{M}}$  is the **negative Hessian** of  $\log \pi(\boldsymbol{\theta} \mid \mathbf{X})$  evaluated at  $\hat{\boldsymbol{\theta}}_{\text{MAP}}$ , that is

$$\hat{\mathbf{M}} = - \frac{\partial^2}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^\top} \log \pi(\boldsymbol{\theta} \mid \mathbf{X}) \Big|_{\boldsymbol{\theta} = \hat{\boldsymbol{\theta}}_{\text{MAP}}}.$$

- Hence, the above quadratic expansion leads to the following **multivariate Gaussian** approximate posterior

$$\pi(\boldsymbol{\theta} \mid \mathbf{X}) \approx \mathcal{N}_p(\boldsymbol{\theta} \mid \hat{\boldsymbol{\theta}}_{\text{MAP}}, \hat{\mathbf{M}}^{-1}).$$

# Bernstein–von Mises theorem (a rough intuition)

- A fairly strong **asymptotic** justification of the Laplace approximation is based on the **Bernstein–von Mises** theorem.
- Suppose the data  $X_1, \dots, X_n$  are iid from a “true” model  $P_{\theta_0}$ .

- Very **roughly speaking**, under suitable regularity and sampling conditions

$$\|\pi(\boldsymbol{\theta} \mid \mathbf{X}) - N_p(\boldsymbol{\theta} \mid \hat{\boldsymbol{\theta}}_{\text{MAP}}, \hat{\mathbf{M}}^{-1})\| \xrightarrow{P_{\theta_0}} 0, \quad n \rightarrow \infty,$$

meaning that the total variation distance between the posterior and the Laplace approximation weakly converges to 0 w.r.t. to the law of the sampling process  $P_{\theta_0}$ .

- Here we are also assuming that  $\hat{\boldsymbol{\theta}}_{\text{MAP}}$  and  $n\hat{\mathbf{M}}^{-1}$  are consistent estimators for the “true” parameter value  $\boldsymbol{\theta}_0$  and for the inverse Fisher information matrix, respectively.
- Hence, in several cases and for  $n$  large enough, the law  $\pi(\boldsymbol{\theta} \mid \mathbf{X})$  is roughly a Gaussian centered at the mode and with variance depending on the Fisher information.

## Main reference

- van der Vaart, A. W. (1998). Asymptotic Statistics. Cambridge University Press.

# Laplace approximation: considerations

- The Laplace approximation is an old and simple method that has appealing asymptotic guarantees. Moreover, it only requires the computation of the Hessian and the MAP.
- Refined **higher order improvements** of expected posterior functionals can be obtained as in Tierney and Kadane (1987).
- On the other hand, especially when the sample size  $n$  is relatively small, the quadratic approximation of  $\log \pi(\theta \mid \mathbf{X})$  may perform poorly.
- For example, if the posterior is not symmetric and unimodal, the MAP is not a good estimate for the posterior mean, thus leading to inaccurate Gaussian approximations.
- Furthermore, if the **parameter space**  $\Theta$  is **bounded**, a Gaussian approximation could be quite problematic  $\implies$  a reparametrization should be considered.
- Finally, it is unclear how to handle **discrete parameter** spaces.

# Approximation methods

- Let  $\pi(\boldsymbol{\theta} \mid \mathbf{X})$  be the intractable posterior distribution and let  $q(\boldsymbol{\theta})$  be a density belonging to  $\mathbb{Q}$ , where  $\mathbb{Q}$  is a general class of tractable densities.

- An optimal approximation  $\hat{q}(\boldsymbol{\theta}) \in \mathbb{Q}$  of the posterior distribution is defined as

$$\hat{q}(\boldsymbol{\theta}) = \arg \min_{q \in \mathbb{Q}} \mathcal{D}\{q(\boldsymbol{\theta}), \pi(\boldsymbol{\theta} \mid \mathbf{X})\},$$

where  $\mathcal{D}(\cdot, \cdot)$  is some divergence or metric over the space of probability distributions.

- An example is the Kullback-Leibler divergence  $\mathcal{D}(\cdot, \cdot) = \text{KL}(\cdot \parallel \cdot)$ .
- Depending on the choice of the divergence  $\mathcal{D}(\cdot, \cdot)$  and of the space of approximating densities  $\mathbb{Q}$ , the problem could be computationally feasible or not.
- Clearly, the posterior  $\pi(\boldsymbol{\theta} \mid \mathbf{X})$  should not be included in the space of tractable densities  $\mathbb{Q}$ , otherwise we would get  $\hat{q}(\boldsymbol{\theta}) = \pi(\boldsymbol{\theta} \mid \mathbf{X})$  for any reasonable divergence  $\mathcal{D}(\cdot, \cdot)$ .

# Approximation methods

- As for the choice of  $\mathcal{D}(\cdot, \cdot)$ , it would be theoretically appealing to consider metrics such as the Hellinger distance, the total variation distance or the Wasserstein distance.
- Unfortunately, even when we let  $\mathbb{Q}$  be the space of multivariate Gaussians, finding the optimal density  $\hat{q}(\theta)$  could be problematic.
- A basic requirement is that the optimization procedure should not depend on the intractable normalizing constant of the posterior.
- We will consider two different though quite related divergences.
- The  $\text{KL}\{q(\theta) \parallel \pi(\theta \mid \mathbf{X})\}$  divergence, leading to the **variational Bayes** method.
- The  $\text{KL}\{\pi(\theta \mid \mathbf{X}) \parallel q(\theta)\}$  divergence, leading to the **expectation propagation** method.



# A summary about variational Bayes (VB)

- The variational Bayes (VB) approach aims at minimizing  $\text{KL}\{q(\theta) \parallel \pi(\theta \mid \mathbf{X})\}$  divergence.
- The VB approach “works well” whenever the class of tractable densities  $\mathbb{Q}$  admits a factorized representation, called **mean-field approximation**.
- The literature about mean-field VB flourished because whenever the full conditionals are known distribution, then it is often possible to obtain a fast VB approximation.
- The main algorithm for obtaining mean-field approximations is called **coordinate ascent variational inference** (CAVI).
- The main drawback of VB approximations is their tendency to **underestimate** the **posterior variability**, often by a substantial margin.

# The evidence lower bound (ELBO)

- In first place, let us note that the following decomposition hold

$$\log \pi(\mathbf{X}) = \text{KL}\{q(\boldsymbol{\theta}) \parallel \pi(\boldsymbol{\theta} \mid \mathbf{X})\} + \text{ELBO}\{q(\boldsymbol{\theta})\},$$

- Recall that the **Kullback-Leibler divergence** is

$$\text{KL}\{q(\boldsymbol{\theta}) \parallel \pi(\boldsymbol{\theta} \mid \mathbf{X})\} = - \int_{\Theta} q(\boldsymbol{\theta}) \log \frac{\pi(\boldsymbol{\theta} \mid \mathbf{X})}{q(\boldsymbol{\theta})} d\boldsymbol{\theta}.$$

- The **evidence lower bound**  $\text{ELBO}\{q(\boldsymbol{\theta})\}$  is instead defined as

$$\text{ELBO}\{q(\boldsymbol{\theta})\} = \int_{\Theta} q(\boldsymbol{\theta}) \log \frac{\pi(\boldsymbol{\theta}, \mathbf{X})}{q(\boldsymbol{\theta})} d\boldsymbol{\theta}.$$

- **Key property.** Since  $\log \pi(\mathbf{X})$  does not depend on  $\boldsymbol{\theta}$ , we obtain that

$$\hat{q}(\boldsymbol{\theta}) = \arg \min_{q \in \mathbb{Q}} \text{KL}\{q(\boldsymbol{\theta}) \parallel \pi(\boldsymbol{\theta} \mid \mathbf{X})\} = \arg \max_{q \in \mathbb{Q}} \text{ELBO}\{q(\boldsymbol{\theta})\},$$

therefore the optimization does not depend on the intractable normalizing constant.

# Evidence lower bound (ELBO)

- The ELBO is indeed a **lower bound** of the marginal likelihood, because the divergence  $\text{KL}\{q(\theta) \parallel \pi(\theta \mid \mathbf{X})\} \geq 0$ , implying that

$$\text{ELBO}\{q(\theta)\} \leq \log \pi(\mathbf{X}).$$

- This property of the ELBO has led to using the variational bound as a model selection criterion, on the assumption that the ELBO is a good approximation of the marginal.
- **Remark.** Even when the optimal distribution  $\hat{q}(\theta)$  can be found, there is no guarantee that the minimized KL

$$\text{KL}\{\hat{q}(\theta) \parallel \pi(\theta \mid \mathbf{X})\} \geq 0$$

will be small in absolute terms.

- Moreover, quantifying the value of  $\text{KL}\{\hat{q}(\theta) \parallel \pi(\theta \mid \mathbf{X})\} = \log \pi(\mathbf{X}) - \text{ELBO}\{q(\theta)\}$  would require the knowledge of the normalizing constant, which is intractable.
- Essentially, it is currently hard to **assess the quality** of the obtained **approximation** without comparing it with some “gold standard” such as MCMC.

# Mean-field approximation

- The VB optimization problem is ill-posed if we do not specify a tractable class  $\mathbb{Q}$ .
- For reasons that will become clear later on, a convenient assumption is restricting the focus on the class  $\mathbb{Q}$  of **mean-field approximations**, in which we assume

$$q(\theta) = \prod_{b=1}^B q(\theta_b),$$

implying that we are forcing **independence** among  $B$  groups of parameters.

- It is important to notice that dependence is preserved within each block of parameters.
- Moreover, note that we are not forcing  $q(\theta)$  to belong to any known parametric family of distributions. The only assumption we are making is independence.

# Derivation of the CAVI algorithm

- Under the mean-field assumption, the optimization of the ELBO can be written as

$$\text{ELBO}\{q(\boldsymbol{\theta})\} = \int_{\Theta} \prod_{b=1}^B \{q(\boldsymbol{\theta}_b) \log \pi(\boldsymbol{\theta}, \mathbf{X})\} d\boldsymbol{\theta} - \int_{\Theta} \prod_{b=1}^B \{q(\boldsymbol{\theta}_b) \log q(\boldsymbol{\theta}_b)\} d\boldsymbol{\theta}.$$

- We aim at maximizing the  $b$ th component  $q(\boldsymbol{\theta}_b)$ , keeping the others fixed. Thus, we express the ELBO isolating the term  $q(\boldsymbol{\theta}_b)$ , obtaining

$$\int q(\boldsymbol{\theta}_b) \left\{ \int \log \pi(\boldsymbol{\theta}, \mathbf{X}) \prod_{j \neq b} q(\boldsymbol{\theta}_j) d\boldsymbol{\theta}_{-b} \right\} d\boldsymbol{\theta}_b - \int q(\boldsymbol{\theta}_b) \log q(\boldsymbol{\theta}_b) d\boldsymbol{\theta}_b + c_b,$$

where  $c_b$  denotes a term not depending on  $\boldsymbol{\theta}_b$ .

- Defining the density  $\log \tilde{\pi}(\boldsymbol{\theta}_b, \mathbf{X}) = \mathbb{E}_{-b}\{\log \pi(\boldsymbol{\theta}, \mathbf{X})\} + \text{const}$  and re-arranging the terms, we get

$$\text{ELBO}\{q(\boldsymbol{\theta})\} = \int q(\boldsymbol{\theta}_b) \log \frac{\tilde{\pi}(\boldsymbol{\theta}_b, \mathbf{X})}{q(\boldsymbol{\theta}_b)} d\boldsymbol{\theta}_b + \tilde{c}_b = -\text{KL}\{q(\boldsymbol{\theta}_b) \parallel \tilde{\pi}(\boldsymbol{\theta}_b, \mathbf{X})\} + \tilde{c}_b.$$

# Derivation of the CAVI

- The above previous chain of equations implies that the **local maximization** of the  $\text{ELBO}(q(\theta))$  with respect to the  $b$ th term of  $q(\theta_b)$  is obtained by setting

$$\hat{q}(\theta_b) \propto \exp \left[ \mathbb{E}_{-b} \{ \log \pi(\theta, \mathbf{X}) \} \right],$$

for any  $b = 1, \dots, B$ .

- In practice, the above expectation is often straightforward to compute and usually some **known kernel** can be recognized (as in the Gibbs sampling).
- In the CAVI algorithm, we iteratively update the factors  $q(\theta_b)$  by using the locally maximized terms given the others.
- By construction, this produces a **monotonic sequence** that converges to a local optimum of the ELBO.

# Properties and convergence

- The CAVI is an appealing algorithm for maximizing the ELBO under the mean-field assumption, but in principle one could use any other optimizer.
- The necessary computations and expectations are usually doable if the full conditional distributions belong to some **exponential family**.
- The algorithm stops whenever the ELBO sequence has reached convergence.
- Moreover, checking that the ELBO is indeed monotone is a common practice to verify the correctness of the implementation.
- Although not shown here, a common application of the CAVI algorithm is indeed the case of Bayesian **mixture models**.

# The CAVI for a Gaussian example

- As in **unit A.2**, let us assume the observations  $(x_1, \dots, x_n)$  are draws from

$$(x_i \mid \mu, \tau) \stackrel{\text{iid}}{\sim} \mathcal{N}(\mu, \tau^{-1}), \quad i = 1, \dots, n,$$

with independent priors  $\mu \sim \mathcal{N}(\mu_\mu, \sigma_\mu^2)$  and  $\tau \sim \text{Ga}(a_\tau, b_\tau)$ .

- Assuming a mean-field approximation  $q(\mu, \tau) = q(\mu)q(\tau)$ , the CAVI algorithm iterates between the following steps simple steps.

- **Update  $q(\mu)$ .** The locally optimal variational distribution for  $q(\mu)$  is

$$q(\mu) = \mathcal{N}(\mu \mid \mu_n, \sigma_n^2), \quad \mu_n = \sigma_n^2 \left( \frac{\mu_\mu}{\sigma_\mu^2} + \mathbb{E}_q(\tau) \sum_{i=1}^n x_i \right), \quad \sigma_n^2 = \left( n \mathbb{E}_q(\tau) + \frac{1}{\sigma_\mu^2} \right)^{-1}.$$

- **Update  $q(\tau)$ .** The locally optimal variational distribution for  $q(\tau)$  is

$$q(\tau) = \text{Ga}(\tau \mid a_n, b_n), \quad a_n = a_\tau + n/2, \quad b_n = b_\tau + \frac{1}{2} \sum_{i=1}^n \mathbb{E}_q\{(x_i - \mu)^2\}.$$



# Underestimation of the variability

- As previously mentioned, the combination of mean-field assumption + VB approach typically leads to a sensible **underestimation of the variability**.
- In first place, this is a consequence of the **insufficient flexibility** of the mean-field class of approximating densities.
- Indeed, if the densities in  $\mathbb{Q}$  were arbitrarily close to the posterior, this phenomenon would be negligible in practice.
- In second place, this is a consequence of the chosen divergence. Indeed, the quantity

$$\text{KL}\{q(\boldsymbol{\theta}) \parallel \pi(\boldsymbol{\theta} \mid \mathbf{X})\} = - \int_{\Theta} q(\boldsymbol{\theta}) \log \frac{\pi(\boldsymbol{\theta} \mid \mathbf{X})}{q(\boldsymbol{\theta})}, d\boldsymbol{\theta}$$

favors the choice of densities  $q(\boldsymbol{\theta})$  which are included in the support of  $\pi(\boldsymbol{\theta} \mid \mathbf{X})$ .

- Indeed, there is a large positive contribution to the above KL for those values of  $\boldsymbol{\theta}$  such that  $\pi(\boldsymbol{\theta} \mid \mathbf{X}) \approx 0$ , unless  $q(\boldsymbol{\theta}) \approx 0$  as well.

# Expectation propagation (EP)

- The **Expectation Propagation** algorithm (EP) has been proposed by Minka (2001).
- The EP approach aims at minimizing the divergence  $\text{KL}\{\pi(\boldsymbol{\theta} \mid \mathbf{X}) \parallel q(\boldsymbol{\theta})\}$ , which is the reversed situation compared to the VB.
- At least in principle, the EP is expected to **overestimate** the variability of the posterior, but this is not a big concern in practice.
- Indeed, the EP does not rely on the mean-field approximation for  $\mathbb{Q}$ . In contrast, the class  $\mathbb{Q}$  will be some **parametric exponential family of distributions**.
- The EP is essentially a **heuristic method** for minimizing  $\text{KL}\{\pi(\boldsymbol{\theta} \mid \mathbf{X}) \parallel q(\boldsymbol{\theta})\}$ , as there are little theoretical guarantees that this is indeed occurring.
- On the other hand, in specific contexts the EP approach outperforms other approaches.

# EP and exponential families

- Let us assume  $\mathbb{Q}$  is an **exponential family of distributions**, with natural parameters  $\boldsymbol{\eta} \in \mathbb{R}^p$ , so that

$$q(\boldsymbol{\theta} \mid \boldsymbol{\eta}) = h(\boldsymbol{\theta}) \exp \{ \boldsymbol{\theta}^\top \boldsymbol{\eta} - K(\boldsymbol{\eta}) \}.$$

- Then, it can be shown that the minimum of the KL divergence is such that

$$\min_{q \in \mathbb{Q}} \text{KL} \{ \pi(\boldsymbol{\theta} \mid \mathbf{X}) \parallel q(\boldsymbol{\theta} \mid \boldsymbol{\eta}) \} = \min_{\boldsymbol{\eta} \in \mathbb{R}^p} \text{KL} \{ \pi(\boldsymbol{\theta} \mid \mathbf{X}) \parallel q(\boldsymbol{\theta} \mid \boldsymbol{\eta}) \},$$

where the optimal set of parameters  $\hat{\boldsymbol{\eta}}$  minimizing the divergence is such that

$$\mathbb{E}_q(\boldsymbol{\theta}) = \mathbb{E}(\boldsymbol{\theta} \mid \mathbf{X}).$$

- In words, the optimal parameter  $\hat{\boldsymbol{\eta}}$  is the one **matching** the true posterior mean of the **natural parameter**  $\mathbb{E}(\boldsymbol{\theta} \mid \mathbf{X})$ , with the mean  $\mathbb{E}_q(\boldsymbol{\theta})$  under the variational distribution.
- In the multivariate Gaussian case, this implies that both the **mean** and the **variance** are matched.

# The EP procedure

- The moment-matching procedure we just described is not directly applicable, because the posterior mean of the natural parameter  $\theta$  is unknown.
- The EP seeks for an heuristic procedure that iteratively minimize the KL using the principle of **moment-matching** local components.
- In first place, let us assume that the **joint likelihood factorizes** as follows

$$\pi(\theta, \mathbf{X}) = \prod_{i=0}^n \pi_i(\theta, \mathbf{X}),$$

the first term corresponds to the prior, so that  $\pi_0(\theta, \mathbf{X}) = \pi(\theta)$ .

- This is a common **modelling assumption**, which is satisfied for example if the data are conditionally independent (i.e. regression).

# The EP procedure

- In second place, note that the **exponential family** assumption for  $\mathbb{Q}$  guarantees that there exists a **decomposition** of the form

$$q(\boldsymbol{\theta} \mid \boldsymbol{\eta}) = \frac{1}{K} \prod_{i=0}^n q_i(\boldsymbol{\theta} \mid \boldsymbol{\eta}_i),$$

with  $\boldsymbol{\eta} = \sum_{i=0}^n \boldsymbol{\eta}_i$  and  $K$  being the normalizing constant, and where the  $q_i(\boldsymbol{\theta} \mid \boldsymbol{\eta}_i)$  is proportional to an exponential family of distributions.

- For example, if we consider a Gaussian kernel

$$q_i(\boldsymbol{\beta} \mid \mathbf{r}_i, \mathbf{M}_i) = \exp \left\{ -\frac{1}{2} \boldsymbol{\beta}^\top \mathbf{M}_i \boldsymbol{\beta} + \boldsymbol{\beta}^\top \mathbf{r}_i \right\} \implies q(\boldsymbol{\theta} \mid \boldsymbol{\eta}) \propto \exp \left\{ -\frac{1}{2} \boldsymbol{\beta}^\top \mathbf{M} \boldsymbol{\beta} + \boldsymbol{\beta}^\top \mathbf{r} \right\},$$

with  $\mathbf{r} = \sum_{i=0}^n \mathbf{r}_i$  and  $\mathbf{M} = \sum_{i=0}^n \mathbf{M}_i$ .

# The EP procedure

- Recall that the goal is obtaining the value  $\hat{\eta}$  minimizing the following KL

$$\min_{\eta \in \mathbb{R}^p} \text{KL}\{\pi(\theta | \mathbf{X}) \parallel q(\theta | \eta)\} = \min_{\eta \in \mathbb{R}^p} \text{KL}\left\{ \frac{1}{\pi(\mathbf{X})} \prod_{i=0}^n \pi_i(\theta, \mathbf{X}) \parallel \frac{1}{K} \prod_{i=0}^n q_i(\theta | \eta_i) \right\}.$$

- Unfortunately, this is unfeasible so we proceed by iteratively updating each factor  $q_j(\theta | \eta_j)$ , for  $j = 0, \dots, n$ , keeping the other fixed.
- Hence, we iteratively update **only the  $j$ th factor**  $q_j(\theta | \eta_j)$  so that

$$\min_{\eta_j \in \mathbb{R}^p} \text{KL}\left\{ \frac{1}{K_j} \pi_j(\theta, \mathbf{X}) \prod_{i \neq j} q_i(\theta | \eta_i) \parallel \frac{1}{K} q_j(\theta | \eta_j) \prod_{i \neq j} q_i(\theta | \eta_i) \right\},$$

where  $K_j$  is the normalizing constant.

- The minimizer  $\hat{\eta}_j$  of the above KL is indeed solved by **moment-matching**, possibly leveraging on a well-behaved numerical integration step.

# The EP procedure

- The minimization of the previously considered local KL takes advantage of several recursive formulas, speeding up computations.
- There is no guarantee this algorithm is going to converge at all, especially if the target density is not log-concave.
- Moreover, the moment-matching step often involves **numerical integration**, which could be computationally delicate.
- Finally, the EP approach requires a particular likelihood structure and only works using exponential families.
- That said, when considering well-behaved posteriors (such as logistic regression), the EP strategy is very effective and often numerically stable.