Title

Gian Carlo Diluvi
STAT 520C Final Project
April 2023

1 Introduction

The Bayesian statistical framework provides practitioners with a principled means to obtain finite-sample uncertainty quantification guarantees. Specifically, the posterior distribution encodes the uncertainty around the unobserved quantities given the observations and a prior distribution. Posterior credible intervals (CIs) or more general regions allow practitioners to quantify the accuracy of point estimates.

The quality of credible intervals can be measured by the proportion of times they contain the “true” value of the parameter. This is known as the frequentist coverage, and Bayesian credible intervals are asymptotically exact in this sense as a consequence of the Bernstein-von Mises theorem. Another way to assess the quality of an interval is via its *Bayesian* coverage, i.e., the proportion of times the interval contains the parameter value that generated the data and itself is a realization from the prior distribution. The Bayesian coverage of an interval leverages the fact that the prior distribution quantifies the uncertainty around the parameter before observing data.

In class, we showed that credible intervals attain nominal Bayesian coverage (i.e., their coverage is equal to the credibility level) for any sample size and without any regularity conditions. This follows from the definition of Bayesian coverage and credible intervals. However, this result assumes that we have access to *exact* credible intervals. For all but the simplest of models, however, the posterior distribution is intractable and has to be approximated numerically. In this setting, the resulting credible intervals are approximate and their Bayesian coverage need not be exact.

Variational inference (VI) is a scalable framework to learn posterior distributions. Succincly, VI casts inference as an optimization problem by approximating the posterior with an element of a family of candidate approximations that minimizes some divergence to the posterior. The quality of the approximation depends on the flexibility of the family of approximations, the divergence being minimized, and whether the optimization problem can be solved reliably. A simple instantiation of VI consists on finding the best Gaussian approximation to the posterior distribution (a framework called Gaussian VI). In this case, the optimization problem is usually amenable to off-the-shelf stochastic optimization algorithms for many common divergences.

In this work, I study the Bayesian coverage of credible intervals of Gaussian VI when minimizing the Kullback-Leibler (KL) divergence. Specifically, I focus on the impact of minimizing the reverse KL (from approximation to target) versus the forward KL (from target to approximation). The former is known to produce approximations that underestimate the posterior variance and viceversa. Through two simulation studies, I conclude that the forward KL tends to have better Bayesian coverage when the posterior has heavier-than-Gaussian tails, which is a common occurrence (e.g., in Bayesian logistic regression, see Section 3.2.)

2 Background: Variational Inference

Let $\pi(x)$ be a density that we are interested in approximating. In the Bayesian setting, $\pi(x) = p(x)/Z$ where $p(x) = \text{prior}(x)\mathcal{L}(y \mid x)$ combines the prior and likelihood (given data y) and $Z = \int p(\tilde{x})\mathrm{d}\tilde{x}$ is the (unknown) normalizing constant (or evidence). We assume that data have already been observed and we are just interested in estimating π as a function of x, so we omit y from notation.

Variational inference refers to approximating π with an element $q^\star \in \mathcal{Q} = \{q_\lambda \mid \lambda \in \Lambda\}$, where $\mathcal{Q}$ is a family of probability distributions parametrized by λ. In the remainder of this work, $\mathcal{Q}$ will be the family of Gaussian distributions: $\lambda = (\mu, \Sigma)$ and $\mathcal{Q} = \{q_\lambda = \mathcal{N}(\mu, \Sigma) \mid \mu \in \mathbb{R}^d, \Sigma \geq 0\}$. The approximation $q^\star$ is chosen to minimize some divergence D from elements in $\mathcal{Q}$ to π:

$$q_\star = q_{\lambda^\star}, \quad \lambda^\star = \operatorname*{arg\,min}_{\lambda \in \Lambda} \mathrm{D}\left(q_\lambda || \pi\right).$$

The choice of divergence can influence the geometry of the optimization problem as well as the characteristics of the optimal approximation $q^\star$. Arguably, the most popular choice of divergence is the Kullback-Leibler divergence from q to π, known as the *reverse* KL:

$$\mathrm{D}_{\mathrm{KL}}^{\mathrm{rev}}\left(q || \pi\right) = \int q(x) \log \frac{q(x)}{\pi(x)} \,\mathrm{d}x = \int q(x) \log \frac{q(x)}{p(x)} \,\mathrm{d}x + Z := -\mathcal{E}(q,p) + Z.$$

In the last equation, I factorized the evidence Z out of the integral and defined $\mathcal{E}(q,p)$ as the (negative) “unnormalized” KL. $\mathcal{E}(q,p)$ is known as the Evidence Lower BOund (ELBO). Since Z does not depend on λ, minimizing the KL divergence is equivalent to maximizing the ELBO.

We can solve this optimization problem through the use of gradient-based optimization algorithms. Specifically, the gradient of the ELBO is an expectation under the variational approximation q_λ:

$$\nabla_\lambda \mathcal{E}(q,p) = -\int q(x) \log \frac{q(x)}{p(x)} \nabla_\lambda q_\lambda(x) \,\mathrm{d}x.$$

We can approximate the ELBO gradient via Monte Carlo samples from q within a stochastics gradient ascent routine (black box vi cite).

The minimizer of the reverse KL, $q_{\mathrm{rev}}(x)$, is known to underestimate the variance of $\pi(x)$ (cite ML book). One way to address this is to minimize the *forward* KL divergence instead, i.e., the KL divergence from the posterior π to the approximation:

$$\mathrm{D}_{\mathrm{KL}}^{\mathrm{fwd}}\left(\pi || q\right) = \int \pi(x) \log \frac{\pi(x)}{q(x)}.$$

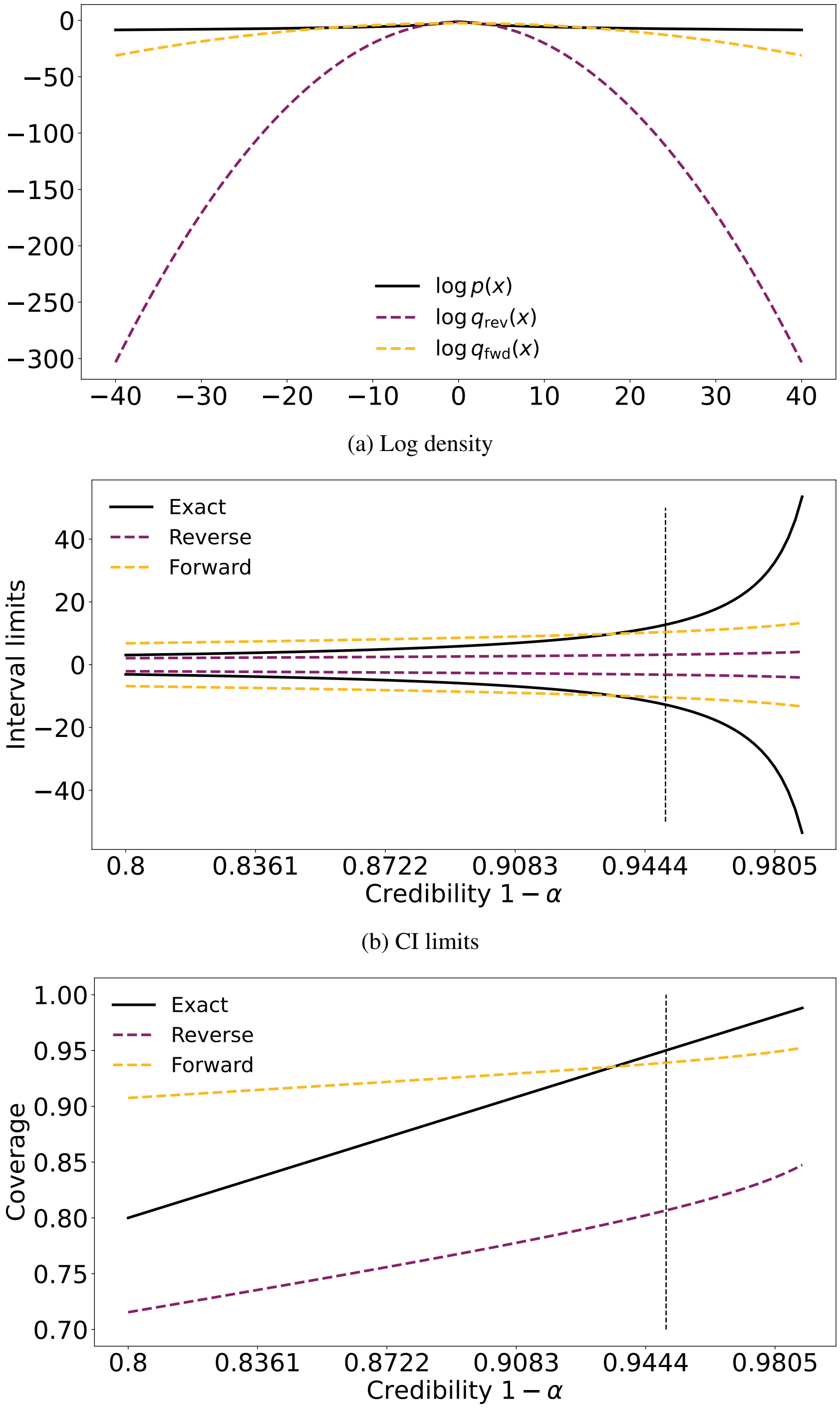
Common folk wisdom in the machine learning community suggests that $\mathrm{D}_{\mathrm{KL}}^{\mathrm{fwd}}\left(\pi || q\right)$ produces better approximations, but it is considerably more difficult to optimize. For example, its gradient can be expressed as an expectation but under the intractable π:

$$\nabla_\lambda \mathrm{D}_{\mathrm{KL}}^{\mathrm{fwd}}\left(q || \pi\right) = -\int \pi(x) \nabla_\lambda q(x) \,\mathrm{d}x.$$

Importance sampling can be numerically unstable for high-dimensional π, so recent work has attempted to estimate this gradient by running an MCMC chain in parallel to produce approximate samples from π (cite Markovian score climbing).

3 Experiments

3.1 Cauchy



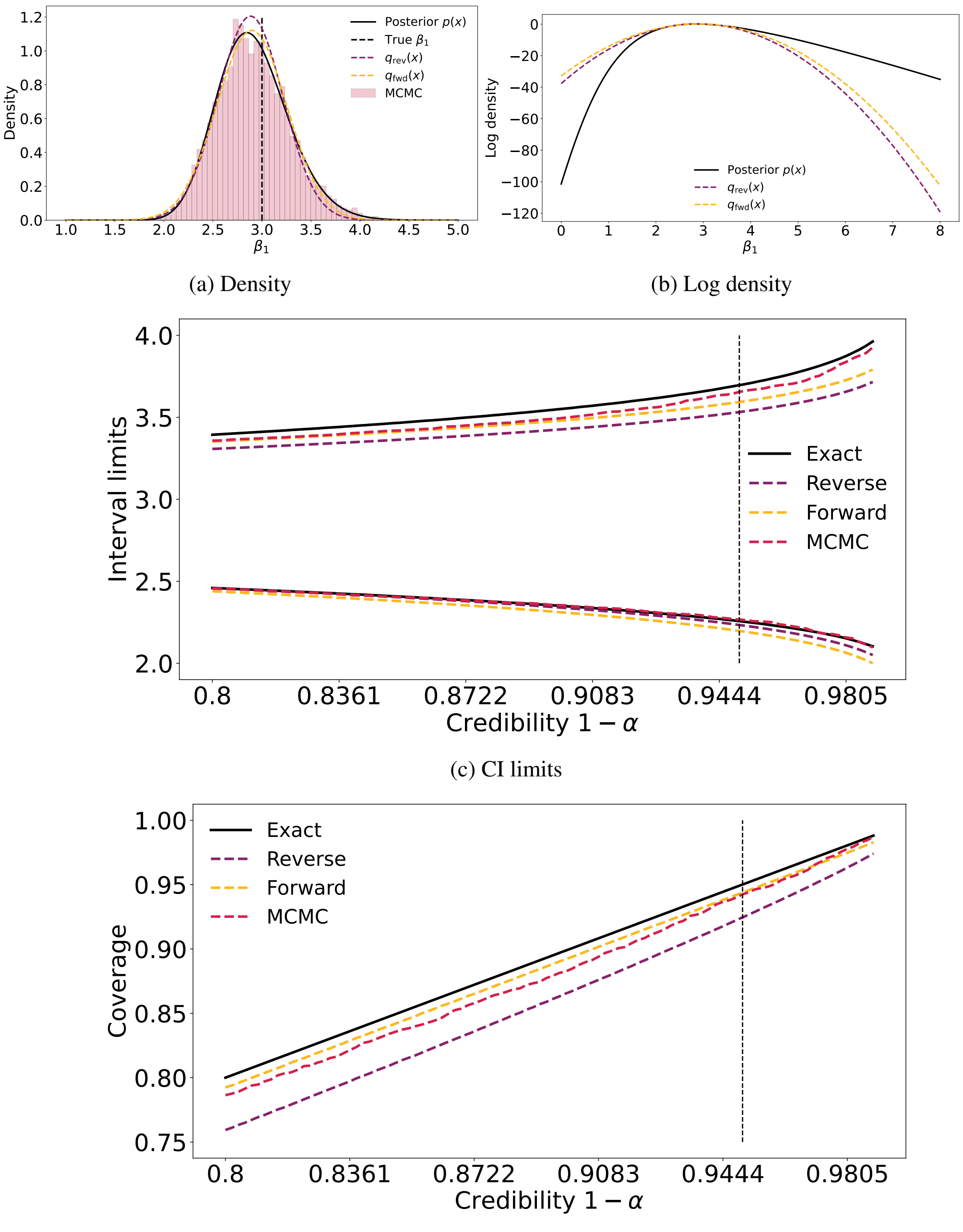
(a) Log density

(b) CI limits

(c) CI coverage

Figure 1: Results on the Cauchy distribution.

3.2 Logistics regression



(a) Density

(b) Log density

(c) CI limits

(d) CI coverage

Figure 2: Results on the logistic regression example.

References