Abstract

This paper introduces a variational approximation framework using direct optimization of what is known as the scale invariant Alpha-Beta divergence (sAB divergence). This new objective encompasses most variational objectives that use the Kullback-Leibler, the Rényi or the gamma divergences. It also gives access to objective functions never exploited before in the context of variational inference. This is achieved via two easy to interpret control parameters, which allow for a smooth interpolation over the divergence space while trading-off properties such as mass-covering of a target distribution and robustness to outliers in the data. Furthermore, the sAB variational objective can be optimized directly by repurposing existing methods for Monte Carlo computation of complex variational objectives, leading to estimates of the divergence instead of variational lower bounds. We show the advantages of this objective on Bayesian models for regression problems.

1. Introduction

Modern probabilistic machine learning relies on complex models for which the exact computation of the posterior distribution is intractable. This has motivated the need for scalable and flexible approximation methods. Research on this topic belongs mainly to two families, sampling based methods constructed around Markov Chain Monte Carlo (MCMC) approximations (Robert & Casella, 2004), or optimization based approximations collectively known under the name of variational inference (VI) (Jordan et al., 1999). In this paper, we focus on the latter, although with the aid of Monte Carlo methods.

The quality of the posterior approximation is a core question in variational inference. When using the KL-divergence (Kullback & Leibler, 1951) averaging with respect to the approximate distribution, standard VI methods such as mean-field underestimate the true variance of the target distribution. In this scenario, such behavior is sometimes known as mode-seeking (Minka, 2005). On the other end, by (approximately) averaging over the target distribution as in Expectation-Propagation, we might assign much mass to low-probability regions (Minka, 2005). In an effort to smoothly interpolate between such behaviors, some recent contributions have exploited parameterized families of divergences such as the alpha-divergence (Amari, 2012; Minka, 2005; Hernández-Lobato et al., 2016), and the Rényi-divergence (Li & Turner, 2016). Another fundamental property of an approximation is its robustness to outliers. To that end, divergences such as the beta (Basu et al., 1998) or the gamma-divergences (Fujisawa & Eguchi, 2008) have been developed and widely used in fields such as matrix factorization (Févotte & Idier, 2011; Cichocki & Amari, 2010). Recently, they have been used to develop a robust pseudo variational inference method (Futami et al., 2017). A cartoon depicting stylized examples of these different types of behavior is shown in Figure 1.

We propose here a variational objective to simultaneously trade-off effects of mass-covering, spread and outlier robustness. This is done by developing a variational inference objective using an extended version of the alpha-beta (AB) divergence (Cichocki et al., 2011), a family of divergence governed by two parameters and covering many of the divergences already used for VI as special cases. After reviewing some basic concepts of VI and some useful divergences, we extend it to what we will call the scale invariant AB (sAB) divergence and explain the influence of each parameter. We then develop a framework to perform direct optimization of the divergence measure which can leverage most of the modern methods to ensure scalability of VI. Finally, we demonstrate the interesting properties of the resulting approximation on regression tasks with outliers.
Figure 1: Illustration of the robustness/efficiency properties (left) and mass-covering/mode-seeking (right). The red region is a stylized representation of a high probability region of a model approximated to fit training data (blue points). Mass-covering and mode-seeking are well-established concepts described by (Minka, 2005). Efficiency refers to the ability of capturing the correct distribution from data, including tail behavior. Robustness is defined here as the ability of ignoring points contaminated with noise that are judged not to be representative of test-time behavior if their probability is too small, according to a problem-dependent notion of outliers.

2. Background

This section briefly reviews the basis of variational inference. It also introduces some divergence measures which have been used before in the context of VI, and which will be used as baselines in this paper.

2.1. Variational Inference

We first review the variational inference method for posterior approximation, as typically required in Bayesian inference tasks. Unless stated otherwise, the notation defined in this section will be used throughout this document.

Let us consider a set of $N$ i.i.d samples $X = \{x_n\}_{n=1}^N$ observed from a probabilistic model $p(x|\theta)$ parametrized by a random variable $\theta$ that is drawn from a prior $p_0(\theta)$. Bayesian inference involves computing the posterior distribution of the unknowns given the observations:

$$p(\theta|X) = \frac{p_0(\theta) \prod_{n=1}^N p(x_n|\theta)}{p(X)}$$

This posterior is in general intractable due to the normalizing constant. The idea behind variational inference is to reduce the inference task to an optimization problem rather than an integration problem. To do so, it introduces a probability distribution $q(\theta)$ from a tractable family $Q$, optimized to approximate the true posterior to an acceptable standard. The approximation is found by minimizing a divergence $D[q(\theta)||p(\theta|X)]$ between the approximation and the true posterior. For the vast majority of divergences, this objective remains intractable as it usually involves computing $p(X)$. VI circumvents the issue by considering the equivalent maximization a lower-bound (“ELBO,” short for evidence lower-bound) of that objective,

$$\mathcal{L}_D(q, X, \varphi) \equiv \log p(X|\varphi) - D[q(\theta)||p(\theta|X, \varphi)]$$

where $D(., ||.)$ is a divergence measure and $\mathcal{L}_D(.)$ denotes the objective function associated with $D$.

2.2. Notable Divergences and their Families

A key component for successful variational inference lies in the choice of the divergence metric used in Equation (2). A different divergence means a different optimization objective and results in the approximation having different properties. Over the years, several have been proposed. The review below here does not intend to be exhaustive, but focuses only on the divergences of interest in the context of this paper.

Arguably, the most famous divergence within the VI community is the Kullback-Leibler divergence (Jordan et al., 1999),

$$D_{KL}(q||p) = \int q(\theta) \log \left( \frac{q(\theta)}{p(\theta)} \right) d\theta.$$ 

It offers a relatively simple to optimize objective. However, because the KL-divergence considers the log-likelihood ratio $p/q$, it tends to penalize more the region where $q > p$—i.e., for any given region over-estimating the true posterior is penalized more than underestimating it. The approximation derived tends to poorly cover regions of small probability in the target model (Turner & Sahani, 2011) while focusing on a number of modes according to what is allowed by the constraints of $Q$.

To mitigate this issue, efforts have been made to use broader families of divergences, where one meta-parameter can be tuned to modify the mass-covering...
behavior of the approximation. In the context of variational inference, the alpha-divergence (Amari, 2012) has been used to develop power EP (Minka, 2005) and the black-box alpha divergence (Hernández-Lobato et al., 2016). In this paper, however, we focus on the Rényi divergence (Rényi et al., 1961; Van Erven & Harremos, 2014),

\[ D^R_\alpha(p||q) = \frac{1}{\alpha - 1} \log \int p(\theta)^\alpha q(\theta)^{1-\alpha} d\theta, \tag{4} \]

used in Rényi VI (Li & Turner, 2016). For this family, the meta-parameter \( \alpha \) can be used to control the influence granted to likelihood ratio \( p/q \) on the objective in regions of over/under estimation. This flexibility has allowed for improvements on traditional VI on complex models, by fine-tuning the meta-parameter to the problem (Depeweg et al., 2016).

KL-divergence also suffers from the presence of outliers in the training data (Ghosh et al., 2017). To perform robust distribution approximation, families of divergences such as the beta-divergence (Basu et al., 1998) have been developed and used to define a pseudo variational objective (Ghosh & Basu, 2016). Instead of solving the optimization problem defined in Equation (2), they use a surrogate objective function motivated by the beta-divergence. In this paper, however, we focus on the gamma-divergence (Fujisawa & Eguchi, 2008),

\[ D^\beta_\alpha(p||q) = \frac{1}{\beta(\beta + 1)} \log \int p(\theta)^\beta q(\theta)^{\beta+1} d\theta \]

\[ + \frac{1}{\beta+1} \log \int q(\theta)^{\beta+1} d\theta - \frac{1}{\beta} \log \int p(\theta)q(\theta)^\beta d\theta. \tag{5} \]

In this family, the parameter \( \beta \) controls how much importance is granted to elements of small probability. The upshot is that in the case the data is contaminated in the approximation to the posterior.

As flexible as the divergences defined in Equations (4) and (5) are, they control only either the mass-covering property or the robustness property, respectively. The AB-divergence (Cichocki et al., 2011) allows for both properties to be tuned independently, but to the best of our knowledge it has not yet been used in the context of variational inference.

3. Scale invariant AB Divergence

In this section, we extend the definition of the scale invariant AB-divergence (Cichocki et al., 2011) (sAB), as well as defining it for continuous distributions. We also describe how it compares to other commonly used divergence measures.

3.1. A two degrees of freedom family of divergences

Under its simplest form, the AB-divergence cannot be used for variational inference as it does not provide any computationally tractable form for the loss function \( \mathcal{L}_{AB}(\cdot) \) as defined in Equation (2) as one cannot isolate the terms involving computing the marginal likelihood \( p(X) \). Detailed computations are available in Appendix A. One could use the AB-divergence to perform pseudo variational updates as described in (Futami et al., 2017). However, in that case we would lose the guarantees of divergence minimization.

Consider instead, as our primary divergence of interest, the scale invariant version of the AB-divergence. This concept was briefly introduced by (Cichocki et al., 2011):

\[ D_{sAB}^{\alpha,\beta}(p||q) \equiv \frac{1}{\beta(\alpha + \beta)} \log \int p(\theta)^{\alpha+\beta} d\theta \]

\[ + \frac{1}{\alpha(\alpha + \beta)} \log \int q(\theta)^{\alpha+\beta} d\theta \]

\[ - \frac{1}{\alpha\beta} \log \int p(\theta)^\alpha q(\theta)^\beta d\theta, \tag{6} \]

for \( (\alpha, \beta) \in \mathbb{R}^2 \) such that \( \alpha \neq 0, \beta \neq 0 \) and \( \alpha + \beta \neq 0 \).

3.2. Extension by continuity

In Equation (6), the sAB divergence is not defined on the complete \( \mathbb{R}^2 \) space. We extend this definition to cover all values \((\alpha, \beta) \in \mathbb{R}^2 \) for the purpose of compar-
When $\alpha = 1$ and $\beta \in \mathbb{R}$, Equation (7) becomes

$$D_{sAB}^{\alpha=1, \beta}(p||q) = \frac{1}{\beta(\beta + 1)} \log \int p(\theta)^{\beta+1} d\theta$$

$$+ \frac{1}{\beta + 1} \log \int q(\theta)^{\beta+1} d\theta - \frac{1}{\beta} \log \int p(\theta)q(\theta)^{\beta} d\theta,$$

and the sAB-divergence is equivalent to gamma-divergence.

A mapping of the $(\alpha, \beta)$ space is shown in Figure 2. To summarize, the sAB-divergence allows smooth interpolation between many known divergences.

### 3.3. Special cases

In this section, we describe how some specific choice of parameters $(\alpha, \beta)$ simplifies the sAB-divergence into some known divergences or families of divergences.

When $\alpha = 0$ and $\beta = 1$, the sAB-divergence reduces down to the Kullback-Leibler divergence as defined in Equation (3). By symmetry, the reverse KL is obtained for $\alpha = 1$ and $\beta = 0$.

More generally, when $\alpha + \beta = 1$, Equation (7) becomes

$$D_{sAB}^{\alpha+\beta=1}(p||q) = \frac{1}{\alpha(\alpha - 1)} \log \int p(\theta)^{\alpha} q(\theta)^{1-\alpha} d\theta,$$

and the sAB-divergence is proportional to the Rényi-divergence defined in Equation (4).

| $D_{\alpha,\beta}$ | $D_{sAB}$ | $D_{K\ell}$ | $D_{KL}$ |
|---------------------|---------------------|---------------------|---------------------|
| $D_{\alpha,\beta}$ | $D_{sAB}$ | $D_{K\ell}$ | $D_{KL}$ |
| $p \| q$ | $q \| p$ | $p \| q$ | $q \| p$ |
| $D_{\alpha,\beta}$ | $D_{sAB}$ | $D_{K\ell}$ | $D_{KL}$ |

| Figure 2: Mapping of the $(\alpha, \beta)$ space. The sAB-divergence reduces down to many known divergences but also interpolates smoothly in between them and cover a much broader spectrum than the Rényi or the gamma-divergence. For $(\alpha, \beta)$ equals $(0.5, 0.5)$ and $(2, -1)$ the sAB divergence is proportional to respectively the Hellinger and the Chi-square divergences. Detailed expressions for the divergences mentioned in that Figure are available in Appendix C. |

### 3.4. Robustness of the divergence

To develop a better understanding on why using the sAB-divergence might be good as a variational objective, we describe how the governing parameters affect the optimization problem for various divergences. Let us assume here that the approximation $q$ is a function of a vector of parameters $\varphi$. Detailed computations are available in Appendix D.

Let us first consider as a baseline the usual KL-divergence $D_{KL}(q||p)$. Its derivative with regard to
\[ \varphi \] is

\[
\frac{d}{d\varphi} D_{KL}(q||p) = - \int \frac{dq(\theta)}{d\varphi} \left( \log \frac{p(\theta)}{q(\theta)} - 1 \right) d\theta. \tag{10}
\]

The log-term in Equation (10) increases with the cost over-estimating \( p \) and hence causes the underestimation of the posterior variance (Turner & Sahani, 2011).

In order to gain more flexibility in the approximation behavior, some have suggested using broader families of divergences to formulate the variational objective. The Rényi divergence (Li & Turner, 2016) is one of them and differentiating it with regard to \( \varphi \) yields,

\[
\frac{d}{d\varphi} D_{K}(q||p) = \frac{1}{1 - \alpha} \int \frac{dq(\theta)}{d\varphi} \left( \frac{p(\theta)}{q(\theta)} \right)^{1-\alpha} d\theta. \tag{11}
\]

When using the Rényi-divergence as an objective, the influence of the ratio of \( p/q \) is deformed by a factor \( \alpha \). This allows the practitioner to select whether to emphasize the relative importance of the large ratios (i.e. set \( \alpha < 0 \)) or on the small ones (i.e. set \( \alpha > 0 \)), thus going from respectively mass-covering to mode-seeking behavior. This does not, however, provide any mechanism to handle outliers or rare events.

In the case of the gamma-divergence discussed by (Futami et al., 2017), its derivative with regard to \( \varphi \) is

\[
\frac{d}{d\varphi} D_{\gamma}(q||p) = - \frac{1}{\beta} \left( \int \frac{dq(\theta)}{d\varphi} q(\theta)^{\alpha} \frac{p(\theta)}{q(\theta)} d\theta - \beta \int \frac{dq(\theta)}{d\varphi} q(\theta)^{\beta} d\theta \right). \tag{12}
\]

When using the gamma-divergence, the influence of the ratio \( p/q \) in the gradient is weighted by the factor \( q(\theta)^{\beta} \). For \( \beta < 1 \), its influence is reduced for small values of \( q \) causing robustness to outliers. For \( \beta > 1 \), the influence of ratios where \( q \) is large is reduced instead causing a focus on outliers. By setting \( \beta \) to values slightly below 1, one can achieve robustness to outliers whilst maintaining the efficiency of the objective (Fujisawa & Eguchi, 2008).

Finally differentiating the sAB-divergence with regard to \( \varphi \) yields

\[
\frac{d}{d\varphi} D_{sAB}^\alpha\beta(q||p) =
- \frac{1}{\beta} \left( \int \frac{dq(\theta)}{d\varphi} q(\theta)^{\alpha+\beta-1} \frac{p(\theta)}{q(\theta)} d\theta - \alpha \beta \int \frac{dq(\theta)}{d\varphi} q(\theta)^{\alpha+\beta-1} d\theta \right). \tag{13}
\]

The two meta-parameters of the sAB-divergence allow us to combine the effects of both the gamma and the Rényi divergences. All the terms similar to Equation (12) are controlled by the parameter \( \alpha + \beta - 1 \). For the sake of clarity, in the reminder of the paper we will use the expression \( \lambda = \alpha + \beta \) and parameterize the AB divergence in terms of \( \lambda \) and \( \beta \). One can control the robustness of the objective by varying \( \lambda \). By setting it to small values below 2, one can achieve robustness to outliers while maintaining the efficiency of the objective. The terms responsible for the “mode-seeking” behavior as seen in Equation (11) are here governed by the term \( 1 - \beta \). Thus, for \( \beta > 1 \), one gets the objective to promote a mass-covering behavior. For \( \beta < 1 \), it promotes mode-seeking behaviors. Figure 3 provides a visual explanation of the influence of each parameters.

![Figure 3: Graphical illustration of the influence of the set control parameters (\( \alpha, \beta \)). The red line < \( \alpha + \beta = 2 \) > shows the region where the robustness factor \( q(\theta)^{\alpha+\beta-1} \) in Equation (13) is uniform. The blue line < \( \beta = 1 \) > shows the region where the ratio \( p/q \) in the mass-seeking term \( (p(\theta)/q(\theta))^\beta \) is constant and equal to that of the standard Kullback-Leibler divergence.](image)
used to instantiate the sAB-divergence using \( \lambda = \alpha + \beta \) instead of \( \alpha \) to get a direct understanding in terms of robustness and mass covering properties.

To further illustrate the flexibility offered by the two control parameters of the sAB-divergence, Figure 4 shows the approximation \( q \) minimizing \( D_{sAB}(\alpha, \beta)(q||p) \). Here \( p \) is set to be a mixture of two skewed unimodal densities — a tall and narrow one combined with a short and wide density. Density \( q \) is required to be a single (non skewed) Gaussian with arbitrary mean and variance.

\[
\begin{align*}
\lambda = 2.4, \beta = -1.0 & \quad \lambda = 2.4, \beta = 2.0 \\
\lambda = 1.8, \beta = -1.0 & \quad \lambda = 1.8, \beta = 2.0
\end{align*}
\]

Figure 4: Approximation of a mixture of 2 skewed densities \( p \) by a Gaussian \( q \) for various parameters \( \lambda \) and \( \beta \). \( \lambda < 2 \) causes the objective to be robust to outliers, while \( \lambda > 2 \) increases their weight. \( \beta > 1 \) causes the objective to have a mass-covering property, whilst \( \beta < 1 \) enforce mode-seeking.

The sAB divergence allows to smoothly tune the properties of the objective between “mass covering” and “robustness to outliers.” In this sense, it is a richer objective than either the Rényi or the gamma divergences, which can only affect respectively the “mass covering” or the “robustness” properties.

4. sAB-divergence Variational Inference

Let us consider a posterior distribution of interest \( p(\theta | X) \) as well as a probability distribution \( q(\theta) \) set to approximate the true posterior and let us derive the associated sAB variational objective.

4.1. sAB Variational Objective

As seen in Section 2.1, the variational approximation is fitted by minimizing the divergence between the true distribution and the approximated posterior. Using the sAB-divergence defined in Equation (7) we get the following objective,

\[
D_{sAB}^{\alpha, \beta}(q(\theta)||p(\theta|X)) = \frac{1}{\alpha(\alpha + \beta)} \log E_q \left[ \frac{p(\theta, X)^{\alpha+\beta}}{q(\theta)} \right] + \frac{1}{\beta(\alpha + \beta)} \log E_q \left[ q(\theta)^{\alpha+\beta-1} \right] - \frac{1}{\alpha \beta} \log E_q \left[ q(\theta)^{\alpha+\beta-1} \left( \frac{p(\theta, X)}{q(\theta)} \right)^\beta \right]
\]

Equation (14) has three main components,

- The first term ensures the objective satisfies the properties of a divergence. \( D_{sAB} \) is always positive and it is equal to 0 if and only if \( p = q \).
- The second element and the weighting of the ratio \( p(\theta, X)/q(\theta) \) in the third element by \( q(\theta)^{\alpha+\beta-1} \) control the sensibility to outliers. As seen in Section 3.4, by setting \( \lambda = \alpha + \beta \) to small values below 2, one can achieve robustness to outliers whilst maintaining the efficiency of the objective.
- The scaling on the ratio \( p(\theta, X)/q(\theta) \) by a power \( \beta \) in the last element is similar to the bound objective of (Li & Turner, 2016) and favors the mass-covering property.
4.2. Optimization framework

Unfortunately, in general the objective defined in Equation (14) still remains intractable and further approximations need to be made. As observed in Section 3.3, the sAB-divergence has a form very similar to the Renyi divergence, so we here use the same approximations as in (Li & Turner, 2016). Theoretically, however, this objective could be used with any optimization method as long we are able to compute \( p(\theta, X) \) and \( q(\theta) \) independently (i.e. not computing the ratio of the two).

To simplify the computation of the objective, a simple Monte Carlo (MC) method is deployed, which uses finite samples \( \theta_k \sim q(\theta) \), \( k = 1, \ldots, K \) to approximate \( D_{sAB}^{\alpha, \beta} \approx \hat{D}_{sAB}^{\alpha, \beta, K} \),

\[
\hat{D}_{sAB}^{\alpha, \beta, K}(q(.)||p(.|X)) = \frac{1}{\alpha(\alpha + \beta)} \log \frac{1}{K} \sum_{k=1}^{K} p(\theta_k, X)^{\alpha + \beta} \\
+ \frac{1}{\beta(\alpha + \beta)} \log \frac{1}{K} \sum_{k=1}^{K} q(\theta_k|X)^{\alpha + \beta - 1} \\
- \frac{1}{\alpha \beta} \log \frac{1}{K} \sum_{k=1}^{K} \left[ q(\theta_k|X)^{\alpha + \beta - 1} \left( \frac{p(\theta_k, X)}{q(\theta_k|X)} \right)^{\beta} \right] .
\]

(15)

We also use the reparametrization trick (Kingma & Welling, 2013), along with gradient based methods as explained in the next section.

5. Experiments

To demonstrate the advantages of the sAB-divergence over a simpler objective, we use it to train variational models on regression tasks on both synthetic and real dataset corrupted with outliers. The following experiments have been implemented using tensorflow and Edward (Tran et al., 2016) and the code is publicly available at github.com\(^2\).

5.1. Regression on synthetic dataset

First, similarly to (Futami et al., 2017), we fit a Bayesian linear regression model (Murphy, 2012) to a two-dimensional toy dataset where 5% of the data points are corrupted and observe how the generalization performances are affected for various training objectives on a non corrupted test set. We use a fully factorized Gaussian approximation to the true posterior \( q(\theta) \). A detailed experimental setup is provided in Appendix F.

The mean of the predictive distributions for various values of \((\alpha, \beta)\) are displayed in Figure 5 and Table 2. As expected, the network trained with standard VI is highly sensitive to outliers and thus has poor predictive abilities at test time, where contamination did not happen. On the other end, when trained with \((\lambda, \beta) = (1.8, 0.8)\) —for this values the sAB-divergence is equivalent to a gamma distribution set up to be robust to outliers—, the predictive distribution ignores the corrupted values. More complex behavior can be obtained by tuning the values of the pair \((\alpha, \beta)\) but only yield little improvement on such a simple problem.

| \((\lambda, \beta)\) | MAE       | MSE       |
|-------------------|-----------|-----------|
| (1, 0.0) (KL)     | 0.58 ± 0.001 | 0.53 ± 0.003 |
| (1.0, 0.3) (Renyi) | 0.58 ± 0.003 | 0.51 ± 0.007 |
| (1.8, 0.8) (Gamma) | 0.34 ± 0.025 | 0.21 ± 0.030 |
| (1.9, -0.3) (sAB) | 0.34 ± 0.025 | 0.21 ± 0.030 |

Table 2: Average Mean Square Error and Mean Absolute Error over 40 regression experiments on the same toy dataset where the training data contain a 5% proportion of corrupted values.

Figure 5: Bayesian linear regression fitted to a dataset containing outliers using several sAB objectives. The parameters \(\alpha\) and \(\beta\) can be used to ensure robustness to outliers.

5.2. UCI datasets regression

In this section, we show that cross validation can be used to fine-tune the parameters \((\alpha, \beta)\) to outperform standard variational inference with a KL-objective.

We use here a Bayesian neural network regression model (Neal, 2012) with Gaussian likelihood on data-
sets collected from the UCI dataset repository (Lichman, 2013). We also artificially corrupt part of the outputs in the training data to test the influence of outliers.

For all the experiments, we use a two-layers neural network with 50 hidden units with ReLUs activation functions. We use a fully factorized Gaussian approximation to the true posterior $q(\theta)$. Independent standard Gaussian priors are given to each of the network weights. The model is optimized using ADAM (Kingma & Ba, 2014) with learning rate of 0.01 and the standard settings for the other parameters. We perform nested cross-validations (Cawley & Talbot, 2010) where the inner validation is used to select the optimal parameters $\alpha$ and $\beta$ within the $[-0.5, 2.5] \times [-1.5, 1.5]$ (with step 0.25). Table 3 reports the Root Mean Squared Error (RMSE) for the two best pairs $(\alpha, \beta)$ and for the KL (i.e. $(\alpha, \beta) = (1,0)$).

| $(\alpha + \beta, \beta)$ | RMSE  |
|---------------------------|-------|
| **Boston housing - $p_{\text{outliers}} = 0\%$** |       |
| $(1.0, 0.0)$ (KL)         | 0.99 ± 0.031 |
| $(1.0, 0.25)$ (sAB)       | 1.01 ± 0.015 |
| $(0.0, -0.75)$ (sAB)      | 1.03 ± 0.021 |
| **Boston housing - $p_{\text{outliers}} = 10\%$** |       |
| $(1.0, 0.0)$ (KL)         | 1.13 ± 0.043 |
| $(1.25, -0.5)$ (sAB)      | 1.07 ± 0.016 |
| $(1.75, -0.25)$ (sAB)     | 1.12 ± 0.029 |
| **Concrete - $p_{\text{outliers}} = 0\%$** |       |
| $(1.0, 0.0)$ (KL)         | 1.01 ± 0.002 |
| $(1.0, -1.0)$ (sAB)       | 0.99 ± 0.001 |
| $(1.5, -0.5)$ (sAB)       | 1.02 ± 0.003 |
| **Concrete - $p_{\text{outliers}} = 10\%$** |       |
| $(1.0, 0.0)$ (KL)         | 1.16 ± 0.002 |
| $(1.5, -0.25)$ (sAB)      | 1.07 ± 0.008 |
| $(1.25, -0.5)$ (sAB)      | 1.08 ± 0.003 |
| **Yacht - $p_{\text{outliers}} = 0\%$** |       |
| $(1.0, 0.0)$ (KL)         | 0.98 ± 0.021 |
| $(1.0, 0.5)$ (sAB)        | 1.00 ± 0.011 |
| $(1.0, -1.0)$ (sAB)       | 1.01 ± 0.003 |
| **Yacht - $p_{\text{outliers}} = 10\%$** |       |
| $(1.0, 0.0)$ (KL)         | 1.09 ± 0.025 |
| $(1.25, -0.25)$ (sAB)     | 1.05 ± 0.011 |
| $(1.75, -0.5)$ (sAB)      | 1.06 ± 0.017 |

Table 3: Regression accuracy of a two layer Bayesian neural network trained on datasets from the UCI bank of datasets with corrupted by $p_{\text{outliers}}\%$ training points. The flexibility offered by the sAB-objective allows us to outperform KL-VI in most of the cases where there is noise contamination.

In the case of uncorrupted data, KL-divergence is often the best choice of objective though other set of values for $(\alpha, \beta)$ geared toward mode seeking can yield comparable predictive performances. As expected when contaminated with outliers, a carefully selected set of parameters such that $\alpha + \beta < 2$ allows achieving better generalization performances on a non corrupted test set compared to VI with KL. In most of the cases —with and without outliers— the best test score is achieved with $\beta < 1$, corresponding to a mode-seeking type of objective.

### 6. Conclusion

We introduced the extended sAB divergence and its associated variational objective. This objective minimize directly the divergence and does not require to define an equivalent objective via a lower bound. Furthermore, this family of divergence covers most of the already known methods and extend them into a more general framework which taps into the growing literature of Monte Carlo methods for complex variational objectives. As the resulting objective functions are not bounds, they provide a way of directly comparing different approximating posterior families, provided that the Monte Carlo error is not difficult to control.

We show that the two governing meta-parameters of the objective allow to control independently the mass-covering character and the robustness of the approximation. Experimental results point out the interest of this flexible objective over the already existing ones for data corrupted with outliers.

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Alpha-Beta Variational Inference - Appendix

The appendix is organised as follows. Section A, we review why it was not possible to use the AB-divergence for VI. Section B develops the computations to extend the sAB-divergence by continuity to \((\alpha, \beta) \in \mathbb{R}^2\). Section D provides the mathematical details fo the computation of the influence of each parameter. Section C lists and describes all the divergences encompassed within the sAB-divergence. Section E, we provide a more detailed derivation of the sAB-variational objective. Finally, Section F details the experimental setups used in the core paper.

A. AB variational Inference:
In the core paper, we use the scale invariant version of the AB-divergence (sAB-divergence) to derive the variational objective. We here show why the simple AB-divergence cannot be used for this.

In (Cichocki et al., 2011) the AB-divergence is defined as,

\[
D_{\alpha, \beta}^{\alpha, \beta}(p || q) = -\frac{1}{\alpha \beta} \int \left( (\theta)^{\alpha} q(\theta)^{\beta} - \frac{\alpha}{\alpha + \beta} p(\theta)^{\alpha + \beta} - \frac{\beta}{\alpha + \beta} q(\theta)^{\alpha + \beta} \right) d\theta.
\]  

(16)

Let us try to derive the ELBO associated with this divergence,

\[
D_{\alpha, \beta}^{\alpha, \beta}(q(\theta) || p(\theta | X)) = -\frac{1}{\alpha \beta} \int \left( (\theta)^{\alpha} p(\theta | X)^{\beta} - \frac{\alpha}{\alpha + \beta} q(\theta)^{\alpha + \beta} - \frac{\beta}{\alpha + \beta} p(\theta | X)^{\alpha + \beta} \right) d\theta
\]

\[
= -\frac{1}{\alpha \beta} \int \left( (\theta)^{\alpha} \left( \frac{p(\theta, X)}{p(X)} \right)^\beta - \frac{\alpha}{\alpha + \beta} q(\theta)^{\alpha + \beta} - \frac{\beta}{\alpha + \beta} \left( \frac{p(\theta, X)}{p(X)} \right)^{\alpha + \beta} \right) d\theta
\]

\[
= -\frac{1}{\alpha \beta} \left( p(X)^{-\beta} \int q(\theta)^{\alpha} p(\theta, X)^{\beta} d\theta - \frac{\alpha}{\alpha + \beta} \int q(\theta)^{\alpha + \beta} d\theta - \frac{\beta}{\alpha + \beta} \int p(X)^{(\alpha + \beta)} \int p(\theta, X)^{\alpha + \beta} d\theta \right)
\]

At that step for the KL-divergence or the Renyi-divergence, one can use the log term to separate the products in sums and isolate the likelihood of the data \(p(X)\) from the rest of the equation (i.e. the ELBO). For the AB-divergence, however, we cannot apply this and isolate the intractable terms. This makes using the AB-divergence for variational inference impossible. We will see in section E that this is not the case for the scale invariant AB-divergence.

B. Extension by continuity of the sAB-divergence
We here provide details of the extension by continuity of the sAB-divergence.

In (Cichocki et al., 2011) they define the scale invariant AB-divergence as,

\[
D_{sAB}^{\alpha, \beta}(p || q) = \frac{1}{\beta(\alpha + \beta)} \log \int p(\theta)^{\alpha + \beta} d\theta
\]

\[
+ \frac{1}{\alpha(\alpha + \beta)} \log \int q(\theta)^{\alpha + \beta} d\theta - \frac{1}{\alpha \beta} \log \int p(\theta)^{\alpha} q(\theta)^{\beta} d\theta,
\]  

(17)

for \((\alpha, \beta) \in \mathbb{R}^2\) such that \(\alpha \neq 0\), \(\beta \neq 0\) and \(\alpha + \beta \neq 0\).
We here provide detailed computation of the extension of the domain of definition to $\mathbb{R}^2$. For simplicity we authorize ourselves to use some shortcuts in the notations of undetermined forms.

**B.1. $\alpha + \beta = 0$**

In that case $\beta \to -\alpha$ and Equation 17 becomes,

$$D_{sAB}^{\alpha+\beta=0}(p||q) = \frac{1}{\beta(\alpha + \beta)} \log \int p(\theta)^{\alpha} q(\theta)^{\beta} d\theta$$

$$= \frac{1}{\beta(\alpha + \beta)} \log \left( \int p(\theta)^{\alpha} q(\theta)^{\beta} d\theta \right) - \frac{1}{\alpha \beta} \log \left( \int p(\theta)^{\alpha} q(\theta)^{\beta} d\theta \right)$$

In that case Equation 17 becomes,

$$\beta(\alpha + \beta) \int p(\theta)^{\alpha} q(\theta)^{\beta} d\theta$$

$$= \frac{1}{\beta(\alpha + \beta)} \log \int p(\theta)^{\alpha} q(\theta)^{\beta} d\theta$$

$$= -\frac{1}{\alpha} \log \int p(\theta)^{\alpha} q(\theta)^{\beta} d\theta + \frac{1}{\alpha} \int \log q(\theta)d\theta$$

So finally we get

$$D_{sAB}^{\alpha+\beta=0}(p||q) = \frac{1}{\alpha^2} \left( \log \int \left( \frac{p(\theta)}{q(\theta)} \right)^{\alpha} d\theta - \int \log \left( \frac{p(\theta)}{q(\theta)} \right)^{\alpha} d\theta \right)$$

(19)

**B.2. $\alpha = 0$ and $\beta \neq 0$**

In that case Equation 17 becomes,

$$D_{sAB}^{\alpha=0,\beta}(p||q)$$

$$= \frac{1}{\beta^2} \log \int p(\theta)^{\beta} d\theta + \frac{1}{\alpha(\alpha + \beta)} \log \int q(\theta)^{\beta} (1 + \alpha \log q(\theta)) d\theta$$

$$= \frac{1}{\beta^2} \log \left( \int p(\theta)^{\beta} d\theta \right) + \frac{1}{\alpha(\alpha + \beta)} \log \left( \int q(\theta)^{\beta} (1 + \alpha \log q(\theta)) d\theta \right)$$

The first approximation uses $x^a = 1 + a \log x$ when $a \approx 0$, the second uses $\log x \approx x$ when $x \to 1$.

So finally we get

$$D_{sAB}^{\alpha,\beta}(p||q) = \frac{1}{\beta^2} \left( \log \int p(\theta)^{\beta} d\theta - \log \int q(\theta)^{\beta} d\theta - \beta \log \int q(\theta)^{\beta} \frac{p(\theta)}{q(\theta)} d\theta \right)$$

(21)
B.3. \( \alpha \neq 0 \) and \( \beta = 0 \)

In that case Equation 17 becomes,

\[
D_{sAB}^{\alpha,\beta \to 0}(p|q) = \frac{1}{\beta(\alpha + \beta)} \log \int p(\theta)^{\alpha} (1 + \beta \log p(\theta)) d\theta + \frac{1}{\alpha \beta} \log \int q(\theta)^{\alpha} d\theta \\
- \frac{1}{\alpha^2} \log \int p(\theta)^{\alpha} (1 + \beta \log q(\theta)) d\theta
\]

\[
= \frac{1}{\beta(\alpha + \beta)} \log \int p(\theta)^{\alpha} d\theta + \frac{1}{\alpha + \beta} \log \int p(\theta)^{\alpha} \log p(\theta) d\theta + \frac{1}{\alpha^2} \log \int q(\theta)^{\alpha} d\theta \\
- \frac{1}{\alpha \beta} \log \int p(\theta)^{\alpha} d\theta - \frac{1}{\alpha} \int p(\theta)^{\alpha} \log q(\theta) d\theta
\]

\[
= - \frac{1}{\alpha(\alpha + \beta)} \log \int p(\theta)^{\alpha} d\theta + \frac{1}{\alpha + \beta} \log \int p(\theta)^{\alpha} \log(\theta) d\theta + \frac{1}{\alpha^2} \log \int q(\theta)^{\alpha} d\theta \\
- \frac{1}{\alpha} \int p(\theta)^{\alpha} \log q(\theta) d\theta
\]

The first approximation uses \( x^a = 1 + a \log x \) when \( a \approx 0 \), the second uses \( \log x \approx x \) when \( x \to 1 \).

So finally we get

\[
D_{sAB}^{\alpha,0}(p|q) = \frac{1}{\alpha^2} \left( \log \int q(\theta)^{\alpha} d\theta - \log \int p(\theta)^{\alpha} d\theta - \alpha \log \int p(\theta)^{\alpha} \log \frac{q(\theta)}{p(\theta)} d\theta \right) 
\]

B.4. \( \alpha = 0 \) and \( \beta = 0 \)

In that case Equation 17 becomes,

\[
D_{sAB}^{\alpha \to 0,\beta \to 0}(p|q) = \frac{1}{\beta(\alpha + \beta)} \log \int (1 + (\alpha + \beta) \log p(\theta)) d\theta + \frac{1}{\alpha \beta} \log \int (1 + (\alpha + \beta) \log q(\theta)) d\theta \\
- \frac{1}{\alpha^2} \log \int p(\theta)^{\alpha} (1 + \beta \log q(\theta)) d\theta
\]

\[
= \frac{1}{\beta(\alpha + \beta)} \log \int (1 + (\alpha + \beta) \log p(\theta)) d\theta + \frac{1}{\alpha(\alpha + \beta)} \log \int (1 + (\alpha + \beta) \log p(\theta)) d\theta \\
- \frac{1}{\alpha \beta} \log \int (1 + \alpha \log p(\theta)) \log q(\theta) d\theta - \alpha \log \int p(\theta)^{\alpha} \log q(\theta) d\theta
\]

\[
= \frac{1}{\beta(\alpha + \beta)} \int (\alpha + \beta) \log p(\theta) d\theta + \frac{1}{\alpha(\alpha + \beta)} \int (\alpha + \beta) \log q(\theta) d\theta
\\
- \frac{1}{\alpha \beta} \int (\alpha \log p(\theta) + \beta \log q(\theta) + \alpha \beta \log p(\theta) \log q(\theta)) d\theta
\]

\[
= - \int \log p(\theta) \log q(\theta) d\theta
\]

The first approximation uses \( x^a = 1 + a \log x \) when \( a \approx 0 \), the second uses \( \log x \approx x \) when \( x \to 1 \).

So finally we get

\[
D_{sAB}^{0,0}(p|q) = \frac{1}{2} \int (\log p(\theta) - \log q(\theta))^2 d\theta
\]
C. Special cases of the sAB-divergence

We here provide a more complete list of the known divergences included in the sAB-divergence.

For \((\alpha, \beta) = (1, 0)\), the sAB-divergence reduces down to the KL-divergence (Kullback & Leibler, 1951),
\[
D^{(1,0)}_{sAB}(q||p) = \int q(\theta) \log \left( \frac{q(\theta)}{p(\theta)} \right) d\theta.
\] (26)

For \((\alpha, \beta) = (0, 1)\), the sAB-divergence reduces down to the reverse KL-divergence,
\[
D^{(1,0)}_{sAB}(q||p) = \int p(\theta) \log \left( \frac{p(\theta)}{q(\theta)} \right) d\theta.
\] (27)

For \((\alpha, \beta) = (0.5, 0.5)\), the sAB-divergence is a function of the Hellinger-distance (Lindsay, 1994),
\[
D^{(0.5,0.5)}_{sAB}(q||p) = -4 \log \int \sqrt{p(\theta)} \sqrt{q(\theta)} d\theta
\]
\[
= -4 \log \int \left( 1 - \frac{1}{2} \left( \sqrt{p(\theta)} - \sqrt{q(\theta)} \right)^2 \right) d\theta
\]
\[
= -4 \log(1 - D_H(p||q))
\] (28)

For \((\alpha, \beta) = (2, -1)\), the sAB-divergence is a function of the \(\chi^2\)-divergence (Nielsen & Nock, 2014),
\[
D^{(2,-1)}_{sAB}(q||p) = \frac{1}{2} \log \int \frac{p(\theta)^2}{q(\theta)} d\theta
\]
\[
= \frac{1}{2} \log(1 - D_{\chi^2}(p||q))
\] (29)

For \((\alpha, \beta) = (0, 0)\), the sAB-divergence is equal to the log-euclidean divergence \(D_E\) (Huang et al., 2015),
\[
D^{0,0}_{sAB}(p||q) = \frac{1}{2} \int (\log p(\theta) - \log q(\theta))^2 d\theta
\] (30)

When \(\alpha + \beta = 1\), the sAB-divergence is proportional to the Rényi-divergence (Rényi et al., 1961)
\[
D^{\alpha+\beta=1}_{sAB}(p||q) = \frac{1}{\alpha(\alpha-1)} \log \int p(\theta)^\alpha q(\theta)^{1-\alpha} d\theta.
\] (31)

When \(\alpha = 1\) and \(\beta \in \mathbb{R}\), the sAB-divergence is equivalent to gamma-divergence (Fujisawa & Eguchi, 2008),
\[
D^{\alpha=1,\beta}_{sAB}(p||q) = \frac{1}{\beta(\beta+1)} \log \int p(\theta)^{\beta+1} d\theta + \frac{1}{\beta+1} \log \int q(\theta)^{\beta+1} d\theta - \frac{1}{\beta} \log \int p(\theta)q(\theta)^\beta d\theta.
\] (32)

D. Robustness the sAB-divergence

We here provide detailed computation of the derivative of various divergences with regard to the governing parameters of the approximation. Let us here assume we approximate the distribution \(p\) by \(q\) a function of the vector of parameters \(\varphi\).
D.1. Kullback-Leibler divergence

For the Kullback-Leibler divergence, we get the following results,

\[
\frac{d}{d\varphi} D_{KL}(q||p) = - \frac{d}{d\varphi} \left( \int q(\theta) \log \frac{p(\theta)}{q(\theta)} d\theta \right) \\
= - \int \left( \frac{dq(\theta)}{d\varphi} \log \frac{p(\theta)}{q(\theta)} + q(\theta) \frac{d}{d\varphi} \log \frac{p(\theta)}{q(\theta)} \right) d\theta \\
= - \int \frac{dq(\theta)}{d\varphi} \left( \log \frac{p(\theta)}{q(\theta)} - 1 \right) d\theta. 
\]

(33)

D.2. Rényi-divergence

For the Rényi-divergence, we get the following results,

\[
\frac{d}{d\varphi} D_\alpha^\alpha(q||p) = - \frac{d}{d\varphi} \left( \frac{1}{\alpha - 1} \log \int q(\theta)^\alpha p(\theta)^{1-\alpha} d\theta \right) \\
= - \frac{1}{\alpha - 1} \int \frac{dq(\theta)}{d\varphi} q(\theta)^{\alpha-1} p(\theta)^{1-\alpha} d\theta \\
= - \frac{\alpha}{1 - \alpha} \int \frac{dq(\theta)}{d\varphi} \left( \frac{p(\theta)}{q(\theta)} \right)^{1-\alpha} d\theta. 
\]

(34)

D.3. Gamma-divergence

For the Gamma-divergence, we get the following results,

\[
\frac{d}{d\varphi} D_\gamma^\beta(q||p) = \frac{d}{d\varphi} \left( \frac{1}{1 + \beta} \log \int q(\theta)^{\beta+1} d\theta + \frac{1}{\beta(1 + \beta)} \log \int p(\theta)^{\beta+1} d\theta \\
- \log \int q(\theta)^{\beta} p(\theta) d\theta \right) \\
= \frac{1}{1 + \beta} \frac{d}{d\varphi} \int q(\theta)^{\beta+1} d\theta - \frac{d}{d\varphi} \int q(\theta)^{\beta} p(\theta) d\theta \\
= - \frac{\beta}{1 + \beta} \frac{dq(\theta)}{d\varphi} q(\theta)^{\beta} d\theta - \frac{d}{d\varphi} \int q(\theta)^{\beta} p(\theta) d\theta \\
= - \frac{1}{\beta} \left( \int \frac{dq(\theta)}{d\varphi} q(\theta)^{\beta} \frac{p(\theta)}{q(\theta)} d\theta \right) - \frac{d}{d\varphi} \int q(\theta)^{\beta+1} d\theta. 
\]

(35)
For the sAB-divergence, we get the following results,

\[
\frac{d}{d\phi} D^{\alpha, \beta}_{sAB} (q || p) = \frac{d}{d\phi} \left( \frac{1}{\beta (\alpha + \beta)} \log \int q(\theta)^{\alpha + \beta} d\theta + \frac{1}{\alpha (\alpha + \beta)} \log \int p(\theta)^{\alpha + \beta} d\theta \right) \\
- \log \int q(\theta)^{\alpha} p(\theta)^{\beta} d\theta
\]

\[
= \frac{1}{\beta (\alpha + \beta)} \int q(\theta)^{\alpha + \beta} d\theta - \frac{1}{\alpha (\alpha + \beta)} \int p(\theta)^{\alpha + \beta} d\theta \\
= \frac{1}{\beta} \int \frac{dq(\theta)}{d\phi} q(\theta)^{\alpha + \beta - 1} d\theta - \alpha \int \frac{dq(\theta)}{d\phi} q(\theta)^{\alpha - 1} p(\theta)^{\beta} d\theta \\
= -\frac{1}{\beta^2} \left( \int \frac{dq(\theta)}{d\phi} q(\theta)^{\alpha + \beta - 1} \left( \frac{p(\theta)}{q(\theta)} \right)^{\beta} d\theta - \beta \int \frac{dq(\theta)}{d\phi} q(\theta)^{\alpha + \beta - 1} d\theta \right) .
\]

E. sAB-divergence Variational Inference

We here provide detailed computation of the variational objective using the sAB-divergence. We also detail the extension of this objective to the complete domain of definition.
E.1. sAB variational objective

We are interested in minimizing the divergence $D_{sAB}^{\alpha,\beta}(q(\theta)||p(\theta|X))$, this yields,

\[
D_{sAB}^{\alpha,\beta}(q(\theta)||p(\theta|X)) = \frac{1}{\alpha \beta} \left[ \log \left( \int q(\theta)^{\alpha+\beta} d\theta \right)^{\frac{\alpha}{\alpha+\beta}} + \log \left( \int \left( \frac{p(\theta, X)}{p(X)} \right)^{\alpha+\beta} d\theta \right)^{\frac{\beta}{\alpha+\beta}} \right] - \log \left( \int q(\theta)^{\alpha} p(\theta, X)^{\beta} d\theta \right) - \log \left( \int q(\theta)^{\alpha} p(\theta) d\theta \right) - \log \left( \int q(\theta)^{\alpha+\beta} d\theta \right) - \log \left( \int q(\theta) d\theta \right)
\]

Finally rewriting this expression to make expectations over $q(\theta)$ appears yields,

\[
D_{sAB}^{\alpha,\beta}(q(\theta)||p(\theta|X)) = \frac{1}{\alpha(\alpha+\beta)} \log \mathbb{E}_q \left[ \frac{p(\theta, X)^{\alpha+\beta}}{q(\theta)} \right] + \frac{1}{\beta(\alpha+\beta)} \log \mathbb{E}_q \left[ q(\theta)^{\alpha+\beta-1} \right] - \frac{1}{\alpha \beta} \log \mathbb{E}_q \left[ \frac{p(\theta, X)^{\beta}}{q(\theta)^{1-\alpha}} \right]
\]
E.2. Extension by continuity

Computation very similar to those in Section B yields,

\[
D_{sAB}^{\alpha,\beta}(q(\theta)||p(\theta|X)) = \begin{cases}
\frac{1}{\alpha(\alpha + \beta)} \log \int q(\theta)^{\alpha + \beta} d\theta + \frac{1}{\beta(\alpha + \beta)} \log \int p(\theta, X)^{\alpha + \beta} d\theta - \frac{1}{\alpha \beta} \log \int q(\theta)^{\alpha} p(\theta, X)^{\beta} d\theta & \text{for } \alpha, \beta, \alpha + \beta \neq 0 \\
\frac{1}{\alpha^2} \left( \log \int \left( \frac{q(\theta)}{p(\theta, X)} \right)^\alpha d\theta - \int \log \left( \frac{q(\theta)}{p(\theta, X)} \right)^\alpha d\theta \right) & \text{for } \alpha = -\beta \neq 0 \\
\frac{1}{\beta^2} \left( \log \int p(\theta, X)^\beta d\theta - \int \log p(\theta, X)^\beta d\theta - \beta \log \int q(\theta)^\beta \log \frac{p(\theta, X)}{q(\theta)} d\theta \right) & \text{for } \alpha \neq 0, \beta = 0 \\
\frac{1}{\alpha} \left( \log \int q(\theta)^\alpha d\theta - \log \int p(\theta, X)^\alpha d\theta - \alpha \log \int p(\theta, X)^\beta \log \frac{q(\theta)}{p(\theta, X)} d\theta \right) & \text{for } \alpha = 0, \beta \neq 0 \\
\frac{1}{2} \int (\log q(\theta) - \log p(\theta, X))^2 d\theta, & \text{for } \alpha, \beta = 0 
\end{cases}
\]  

(39)

F. Experiments

We here provide a more detailed description of our experimental setups. The following experiments have been implemented using tensorflow (ten) and Edward (Tran et al., 2016).

F.1. Regression on synthetic dataset

In this experiment we create a toy dataset to showcase the strength of the sAB variational objective.

The non-corrupted data are generated by the following process,

\[
y = \mathbf{wX} + \mathcal{N}(0, 0.1) \tag{40}
\]

with \( \mathbf{w} = [1/2...1/2] \) a \( D \)-dimensional vector and \( \mathbf{b} = \{\text{a set of points randomly distributed between } [-1, 1]^D\} \).

A given percentage \( p_{\text{outliers}} \) of the data are corrupted and follows the process,

\[
y = 5 + \mathbf{wX} + \mathcal{N}(0, 0.1) \tag{41}
\]

with \( \mathbf{w} = [1/2...1/2] \) and \( \mathbf{X} \) is sampled from \( \mathcal{N}(0, 0.2) \).

For \( N \) such data points \([\{\mathbf{x}_n, y_n\}]_{n \in [1,N]}\), we uses the following distributions,

\[
p(\mathbf{w}) = \mathcal{N}(\mathbf{w} | 0, \sigma_w^2 \mathbf{I}_D), \\
p(\mathbf{b}) = \mathcal{N}(\mathbf{b} | 0, \sigma_b^2), \tag{42}
\]

and

\[
p(y | \mathbf{w}, \mathbf{b}, \mathbf{X}) = \prod_{n=1}^{N} \mathcal{N}(y_n | \mathbf{x}_n^\top \mathbf{w} + b, \sigma_y^2). \tag{43}
\]

We define the variational model to be a fully factorized normal across the weights.

For the experiments presented in the paper we use \( N = 1000, D = 4 \) and \( p_{\text{outliers}} = 5\% \).

We train the model using ADAM (Kingma & Ba, 2014) with learning rate of 0.01 for 1000 steps. We use 5 MC samples to evaluate the divergence.
F.2. UCI datasets regression

We use here a Bayesian neural network regression model with Gaussian likelihood on datasets collected from the UCI dataset repository (Lichman, 2013). We also artificially corrupt part of the outputs in the training data to test the influence of outliers. The corruption is achieved by randomly adding 5 standard deviation to $p_{\text{outliers}}\%$ of the points after normalization.

For all the experiments, we use a two-layers neural network with 50 hidden units with ReLUs activation functions. We use a fully factorized Gaussian approximation to the true posterior $q(\theta)$. Independent standard Gaussian priors are given to each of the network weights. The model is optimized using ADAM (Kingma & Ba, 2014) with learning rate of 0.01 and the standard settings for the other parameters for 500 epochs. We perform nested cross-validations (Cawley & Talbot, 2010) where the inner validation is used to select the optimal parameters $\alpha$ and $\beta$ within the $[-0.5, 2.5] \times [-1.5, 1.5]$ (with step 0.25). The best model selected from the inner loop is then re-trained on the complete outer split. We use 25 MC samples to evaluate the divergence. The outer cross validation used $K_1 = 10$ folds and the inner one uses $K_2 = 2$ folds.
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