Abstract

This report provides an in-depth overview over the implications and novelty Generalized Variational Inference (GVI) \[22\] brings to Deep Gaussian Processes (DGP) \[9\]. Specifically, robustness to model misspecification as well as principled alternatives for uncertainty quantification are motivated with an information-geometric view. These modifications have clear interpretations and can be implemented in less than 100 lines of Python code. Most importantly, the corresponding empirical results show that DGP can greatly benefit from the presented enhancements.

1 Introduction

Deep Gaussian Processes (DGP) were introduced by Damianou and Lawrence \[9\] and extend the logic of deep learning to the nonparametric Bayesian setting. The principal idea is to iteratively place Gaussian Process (GP) priors over emerging latent spaces. More specifically, given observations \((X, Y)\) where \(X \in \mathbb{R}^{n \times D}\) and \(Y \in \mathbb{R}^{n \times p}\), a DGP of \(L\) layers introduces the additional collection of latent functions \(\{F_l\}_{l=1}^L\). Here, \(F_l\) is a matrix of dimension \(D_l \times D_{l+1}\). Setting \(F_0 = X\), \(D_0 = D\) and \(D_{l+1} = p\) for notational convenience, one can now write the hierarchical DGP construction as

\[
\begin{align*}
Y | F_L & \sim p (Y | F_L) \\
F_L | F_{L-1} = f^L(F_{L-1}) & \sim \text{GP} (\mu^L(F_{L-1}), \kappa^L(F_{L-1}, F_{L-1})) \\
F_{L-1} | F_{L-2} = f^{L-1}(F_{L-2}) & \sim \text{GP} (\mu^{L-1}(F_{L-2}), \kappa^{L-1}(F_{L-2}, F_{L-2})) \\
& \vdots \\
F_1 | F_0 = f^1(F_0) & \sim \text{GP} (\mu^1(F_0), \kappa^1(F_0, F_0)),
\end{align*}
\]

where the mean and covariance functions are of form \(\mu^l : \mathbb{R}^{D_l} \to \mathbb{R}^{D_{l+1}}\) and \(\kappa^l : \mathbb{R}^{D_l \times D_l} \to \mathbb{R}^{D_{l+1} \times D_{l+1}}\). Scalable inference in this construction is obviously a challenge. In principle, the attempts at tackling this problem rely on Variational inference (VI) strategies \[9\] \[8\] \[27\] \[13\], Monte Carlo methods \[29\] \[30\] or more specialized approaches \[5\] \[7\]. In the remainder, we will focus on VI strategies for DGP inference. To keep things as simple as possible, we discuss the implications of Generalized Variational Inference (GVI) only in relation to the arguably most promising VI approach of Salimbeni and Deisenroth \[27\] which encodes conditional dependence into the variational family \(\mathcal{Q}\). We note in passing however that due to GVI’s versatility, the same logic applies to any other variational family \(\mathcal{Q}\).

The rest of this report is structured as follows: First, we give a brief recap of the variational families for DGP proposed by Salimbeni and Deisenroth \[27\]. Next, we give a brief overview of GVI as introduced in Knoblauch et al. \[22\]. Lastly, we give the necessary derivations necessary to apply GVI to DGPs and investigate the performance gains.

\[1\]If you cite this report, it is appropriate to cite these two papers, too.
2 Variational inference for Deep Gaussian Processes

This report focuses on the variational family $Q$ for DGP s geared towards large-scale inference introduced by Salimbeni and Deisenroth [27]. Unlike competing VI approaches for DGP s, this family encodes some part of the conditional dependence structure of the DGP. This comes at the expense of losing a tractable closed form lower bound [as in [9]], but makes DGP s more flexible and adaptable.

2.1 The conditionally dependent variational family for DGP s

Including the inducing point framework for GP inference [see [28, 14, 13]], we now introduce the exact Bayesian posterior arising from the DGP construction. First, define the set of $m$ additional inducing points $Z^l = (z^{l}_1, z^{l}_2, \ldots, z^{l}_m)^T$ and their function values $U^l = (f^l(z^{l}_{1}), f^l(z^{l}_{2}), \ldots, f^l(z^{l}_{m}))^T$. For better readability, we will often drop $X$ and $Z^l$ from the conditioning sets. Further, note that we will denote the $i$-th row of the $D^l \times D^{l+1}$ latent functions $F^l$ as $f^{l}_{i}$. With this in place, the joint distribution of the DGP construction is

$$p(Y, \{F^l\}_{l=1}^{L}, \{U^l\}_{l=1}^{L}) = \prod_{l=1}^{n} p(y_i | f^l_i) \times \prod_{l=1}^{L} p(F^l | U^l, F^{l-1}, Z^{l-1}) p(U^l | Z^{l-1}).$$

Thus, the posteriors $p(\{F^l\}_{l=1}^{L}, \{U^l\}_{l=1}^{L})$ and $p(\{F^l\}_{l=1}^{L})$ are intractable due to the required normalizing constants required for their computation. To overcome this, different variational approximations have been proposed. Here, we focus on the variational family proposed in Salimbeni and Deisenroth [27] given by

$$q(\{F^l\}_{l=1}^{L}) = \prod_{l=1}^{L} q(F^l | U^l, F^{l-1}, Z^{l-1}) q(U^l),$$

where the posterior $q(F^l)$ is chosen because it allows for exact integration over the inducing points $Z^{l-1}$, yielding the closed form variational posterior

$$q(\{F^l\}_{l=1}^{L}) = \prod_{l=1}^{L} \mathcal{N}(F^l | \mu^l, \Sigma^l),$$

where the parameters of the posterior are available in closed form as

$$[\mu^l]_i = \mu_{m^l, Z^{l-1}}(f^l_i) = \mu^l(f^l_i) + a(f^l_i)^T (m^l - \mu^l(Z^{l-1}))$$

$$[\Sigma^l]_{i,j} = \Sigma_{S_l, Z^{l-1}}(f^l_i, f^l_j) = \kappa^l(f^l_i, F^{l-1}) - a(f^l_i)^T (\kappa^l(Z^{l-1}, Z^{l-1}) - S_l) a(F^{l-1}),$$

where as usual we define $a(f^l_i) = \kappa^l(Z^{l-1}, Z^{l-1})^{-1} \kappa^l(Z^{l-1}, f^l_i)$. Note the attractive feature of the family specified via eqs. (1) - (2): At each layer $l$, the output $f^l_i$ only depends on the corresponding input $f^{l-1}_i$. This property is a direct consequence of setting every layer up exactly as a sparse GP [see, e.g. [28, 14, 13]]. This enables efficient probabilistic backpropagation [15] with the reparameterization trick [e.g. [26, 20]] and makes the approach scalable.

In particular, Salimbeni and Deisenroth [27] propose a doubly stochastic minimization of the negative Evidence Lower Bound (ELBO) given by

$$\mathcal{L}(q | Y, X) = - \sum_{i=1}^{n} \mathbb{E}_{q(f^l_i)} [\log p(y_i | f^l_i)] - \sum_{l=1}^{L} \text{KLD}(q(F^l, U^l) || p(F^l, U^l | Z^{l-1})).$$

The Kullback-Leibler divergence (KLD) terms of this bound further simplify because by eq. (1), $q$ is designed to cancel the conditional over $F^l$ with $p$. This finally leads to the bound

$$\mathcal{L}(q | Y, X) = - \sum_{i=1}^{n} \mathbb{E}_{q(f^l_i)} [\log p(y_i | f^l_i)] - \sum_{l=1}^{L} \text{KLD}(q(U^l) || p(U^l | Z^{l-1})).$$


where for optimization the samples for $F^l$ are drawn using the variational posteriors from the previous layers. Because $F^l$ only depends on the corresponding input $F^{n,l-1}$, this can be done using univariate Gaussians and thus does not involve matrix operations. Approximating the expectation over $q(\theta)$ induces the first layer of stochasticity in this model. The second layer is due to drawing a mini-batches from $X = F^0$ and $Y$ at each iteration. Because of this degree of stochasticity, it is an appealing feature that the expectations $\mathbb{E}_{q(f^l)} \log p(y_i|f^L)$ are available in closed form for some choices of $p$. This is for instance the case for the regression setting, where $p$ is a normal likelihood. Later on, we also derive such closed forms for a new class of alternatives for $p$ geared towards robustness and derived from normal likelihoods.

2.2 An alternative problem representation

We now decompose the components of the DGP model. Specifically, we define the collection of likelihood terms as

$$
\ell_n \left( \{ (F^l)_{i=1}^L, \{U^l\}_{i=1}^L \}, Y \right) = \sum_{i=1}^n \ell \left( f^L_i, y_i \right) \quad \text{for} \quad \ell \left( f^L_i, y_i \right) = - \log p(y_i|f^L_i)
$$

and the layered DGP prior via

$$
p \left( \{ (F^l)_{i=1}^L, \{U^l\}_{i=1}^L \}, \{ Z^l \}_{i=1}^L \right) = \prod_{l=1}^L p_l \left( F^l, U^l | F^{l-1}, U^{l-1}, Z^{l-1} \right)
$$

$$
p_l \left( F^l, U^l | F^{l-1}, U^{l-1}, Z^{l-1} \right) = p \left( F^l | F^{l-1}, U^l, Z^{l-1} \right) p \left( U^l | Z^{l-1} \right).
$$

With this, one can rewrite the sought-after posterior as

$$
p \left( \{ F^l \}_{l=1}^L, \{ U^l \}_{l=1}^L | Y, X \right) = \frac{\exp \left\{ -\ell_n \left( \{ (F^l)_{i=1}^L, \{U^l\}_{i=1}^L \}, Y \right) \right\} \pi \left( \{ (F^l)_{i=1}^L, \{U^l\}_{i=1}^L \}, \{ Z^l \}_{i=1}^L \right) \pi \left( \{ F^l \}_{l=1}^L, \{ U^l \}_{l=1}^L | \{ Z^l \}_{i=1}^L \right)}{\int_Y \exp \left\{ -\ell_n \left( \{ (F^l)_{i=1}^L, \{U^l\}_{i=1}^L \}, Y \right) \right\} \pi \left( \{ (F^l)_{i=1}^L, \{U^l\}_{i=1}^L \}, \{ Z^l \}_{i=1}^L \right) \pi \left( \{ F^l \}_{l=1}^L, \{ U^l \}_{l=1}^L | \{ Z^l \}_{i=1}^L \right) dY}
$$

This representation gives a generalized Bayesian distribution associated with a general loss function $\ell$. For the standard DGP, the loss function is the negative log likelihood $\ell(f^L, y_i) = - \log p(y_i|f^L_i)$, which is the loss traditionally associated with the Bayesian paradigm. As part of this report, we explain alternative losses $\ell_n$ for the probabilistic DGP model as in [22]. However, unlike the log likelihood these losses will be robust to model misspecification and outliers. Note that the variational methods outlined in the previous section still apply to any new additive loss $\ell$. In fact, one only needs to replace $- \log(p(y_i|f^L_i))$ in eq. (7) with the alternative loss $\ell(f^l_i, y_i)$.

3 Generalized Variational Inference

Unlike VI where the quality of the posterior is controlled only via the variational family $Q$, Generalized Variational Inference (GVI) allows for adapting two additional objects: The loss used for inference and the manner of uncertainty quantification. For notational convenience, we formulate GVI in full generality for a generic parameter $\theta$ of interest for inference. For the purposes of this report, this parameter indexes a DGP and is $\theta = \{ (F^l)_{i=1}^L, \{U^l\}_{i=1}^L \}$.

In a nutshell, GVI is the natural methodological outgrowth arising from the study of a generalized representation of Bayesian inference. This representation recovers standard Bayesian inference, VI and many other methods as special cases. Specifically, Knoblauch et al. [22] axiomatically derive Bayesian inference as the triplet $P(\ell_n, D, \Pi)$ given by

$$
q^*(\theta) = \arg \min_{q \in \Pi} \{ \mathcal{L}(q(Y, X, \ell_n, D)) \}; \quad \mathcal{L}(q(Y, X, \ell_n, D)) = \mathbb{E}_{q(\theta)} \left[ \ell_n(\theta, Y) \right] + D(q||p).
$$

where $D(q||p)$ depends on $X$ for the DGP. Denoting by $\mathcal{P}(\Theta)$ the space of all probability distributions over $\Theta$, the constituent parts of the form $P(\ell_n, D, \Pi)$ are given by

- a loss $\ell_n$ linking a parameter of interest $\theta$ to the observations $Y = y_{1:n}$. This loss is assumed to be additive throughout, i.e. $\ell_n(\theta, Y) = \sum_{i=1}^n \ell(\theta, y_i)$ for some $\ell$.

- a divergence $D : \mathcal{P}(\Theta) \times \mathcal{P}(\Theta) \to \mathbb{R}_+$ regularizing the posterior with respect to the prior. As $D$ determines how the prior $p$ quantifies uncertainty, it is called uncertainty quantifier.

Note that for the DGP, $X$ enters eq. (12) via $D(q||p)$.
a set of admissible posteriors $\Pi \subseteq \mathcal{P}(\Theta)$ the regularized expected loss is minimized over.

The seminal paper of Zellner [32] shows that standard Bayesian inference solves $P(- \sum_{i=1}^{n} \log(p(\theta|y_i)), \text{KLD}, \mathcal{P}(\Theta))$. This is extended in Bissiri et al. [3], who show that for an additive loss function $\ell_n$, the Gibbs-posterior is the solution to $P(- \sum_{i=1}^{n} \log(p(\theta|y_i)), \text{KLD}, \mathcal{P}(\Theta))$. Further, for $Q$ a variational family, the objective of $P(- \sum_{i=1}^{n} \log(p(\theta|y_i)), \text{KLD}, \mathcal{Q})$ in eq. (12) is the Evidence Lower Bound (ELBO) of VI. This observation is the inspiration to call any problem of form $P(\ell_n, D, Q)$ a Generalized Variational Inference (GV1) problem. Perhaps the most interesting aspect of GV1 lies in its modularity. Roughly speaking, once $Q$ is fixed, this modularity allows one to prove that (i) robustness to model misspecification should enter the Bayesian inference problem via $\ell_n$ and that (ii) a change in the posterior shape should enter via $D$ [see Thm. 5 in [22]].

4 Generalized Variational Inference for Deep Gaussian Processes

With $\theta = \{\{F_i\}_{i=1}^{L}, \{U_i\}_{i=1}^{L}\}$, it is clear that (12) allows for tractable alternatives of eq. (7). This section explains which roles $\ell$ and $D$ take in the GV1 formulation and derive appropriate choices for robust DGP's. We do not discuss $\Pi$, since throughout, we focus on the case where $\Pi = \mathcal{Q}$ using the variational family $\mathcal{Q}$ of Salimbeni and Deisenroth [27] introduced above.

4.1 Model-agnostic and likelihood-based losses for robustness against misspecification

In traditional Bayesian inference, the loss term $\ell_n$ is a sum over negative log likelihoods. Yet, this is just a special case [3] and $\ell_n(\theta, Y)$ can be any additive loss about whose optimum $\theta^*$ one wishes to learn in a Bayesian manner. In fact, using the notation introduced above, Bissiri et al. [3] show that for the exact Bayesian inference problem $P(\ell_n, \text{KLD}, \mathcal{P}(\Theta))$, one recovers the generalized Bayes Theorem

$$q^*(\theta) = \frac{p(\theta) \exp \{ \sum_{i=1}^{n} -\ell(\theta, y_i) \}}{\int_\Theta p(\theta) \exp \{ \sum_{i=1}^{n} -\ell(\theta, y_i) \} d\theta},$$

which mirrors the form in eq. (11). We note that updating rules of this kind have been studied under the name of Gibbs- or Pseudo-posteriors before, but Bissiri et al. [3] show that they are indeed valid and coherent posterior beliefs about $\theta$ in their own right.

Inspired by this insight, various authors have proposed likelihood-based losses replacing the negative log likelihood $-\log p(\theta|y_i)$ but enabling inference in the same model described by the likelihood $p$ and the same parameter $\theta$. Usually, this is done for robust inference and a recent overview is provided for in Jewson et al. [13]. The recipe for deriving these alternative losses derives from geometric considerations. In particular, when minimizing $\sum_{i=1}^{n} -\log p(y_i|\theta)$ to conduct inference on $\theta$, one implicitly minimizes the (non-robust) KLD in the space of densities. To see that this is the case, denote by $g$ the data-generating probability density (i.e., $y_1, y_2, \ldots, y_n \sim g$) and observe that

$$\frac{1}{n} \sum_{i=1}^{n} -\log(p(y_i|\theta)) \approx \mathbb{E}_g[-\log(p(y_i|\theta))] = \text{KLD}(g||p(\cdot|\theta)) + \mathbb{E}_g[\log(g(y))].$$

Since the entropy term $\mathbb{E}_g[\log(g(y))]$ does not depend on $\theta$, minimizing the negative log likelihood thus amounts to (approximately) minimizing the KLD between the true data generating mechanism and the model as parameterized by $\theta$. While the KLD is a good measure of discrepancy if the model is an appropriate description for the data-generating mechanism, this no longer holds under moderate model misspecification or outliers. In traditional statistical inference, this is usually not a problem: A lot of effort is typically expanded in order to investigate the data patterns and adapt $p$ to be a better description of $g$. In modern statistical machine learning and its accompanying black box methods and variational approximations, this is no longer the case: Moderate, even severe misspecification is the norm.

In these circumstances, using the KLD as a measure of discrepancy can often adversely affect inference outcomes. An information-geometrically elegant solution to this conundrum is changing the measure of discrepancy in the space of probability measures. Numerous authors have pursued this idea [see e.g. [16] [2] [17] [10] [18]. For the robust DGP, we focus on the $\beta$-divergences $(D_B^\beta)$ and $\gamma$-divergences $(D_\gamma^\gamma)$ [see also [12] [18] [21] [11]. The logic is analogous to eq. (14) and leads to alternative loss
functions. For example, the $\beta$-divergence is given by

$$D_{\beta}^{(g)}(g||p(\cdot|\theta)) = \frac{1}{\beta(\beta - 1)} \mathbb{E}_g[g(y)^{\beta - 1}] + \frac{1}{\beta} \int p(y|\theta)^{\beta - 1} dy = \frac{1}{\beta - 1} \mathbb{E}_g[p(y|\theta)^{\beta - 1}],$$

and it is obvious that the first term does not depend on $\theta$. Thus, using the natural approximation of the expectation over $g$, one can target this divergence via $\frac{1}{\beta} \sum_{i=1}^{n} L_{\beta}(\theta, y_i)$, where

$$L_{\beta}(\theta, y_i) = -\frac{1}{\beta - 1} p(y_i|\theta)^{\beta - 1} + \frac{I_{p,\beta}(\theta)}{\beta}$$

and $I_{p,\gamma}(\theta) = \int p(y|\theta)^{\gamma} dy$. The derivation for the $\gamma$-divergence is similar [17] and yields

$$L_{\gamma}(\theta, y_i) = -\frac{1}{\gamma - 1} p(y_i|\theta)^{\gamma - 1} \cdot \frac{\gamma}{I_{p,\gamma}(\theta)^{-\gamma}}.$$

For the DGP, these losses simplify as $p(y_i|\theta) = p(y_i|\{f_i\}_{i=1}^T, \{U_i\}_{i=1}^T) = \frac{p(y_i|f_i)}{p(f_i)}$. For clarity and brevity, this report thus uses $L_{\beta}(\theta, y_i) = L_{\beta}^p(f_i, y_i)$ and $L_{\gamma}(\theta, y_i) = L_{\gamma}^p(f_i, y_i)$.

Through tedious but straightforward calculation, one can show that the corresponding expectations $\mathbb{E}_q(f_i^L) [L_{\beta}^q(f_i^L, y_i)]$ and $\mathbb{E}_q(f_i^L) [L_{\gamma}^q(f_i^L, y_i)]$ are available in closed form for the regression setting where $p$ is a normal likelihood [see supplementary material of 22].

**Theorem 1** (Closed form for robust regression). If it holds that $y_i \in \mathbb{R}^d$,

$$p(y_i|f_i) = \mathcal{N}(y_i; f_i, \Sigma); \quad q(f_i) = \mathcal{N}(f_i; \mu, \Sigma),$$

then for the quantities given by

$$\tilde{\Sigma}^{-1} = \left( \frac{C}{\sigma^2} I_d + \Sigma^{-1} \right); \quad \tilde{\mu} = \left( \frac{C}{\sigma^2} y_i + \Sigma^{-1} \mu \right); \quad I(c) = (2\pi\sigma^2)^{-0.5}c^{-0.5}d$$

and for

$$E(c) = \frac{1}{c} (2\pi\sigma^2)^{-0.5}c^0.5 \exp \left\{ -\frac{1}{2} \left( \frac{C}{\sigma^2} y_i^T \mu \Sigma^{-1} \mu - \tilde{\mu}^T \tilde{\Sigma} \tilde{\mu} \right) \right\}.$$
the following expectations are available in closed form:

\begin{align}
\mathbb{E}_{q(f^l)} \left[ \mathcal{L}^\alpha_p (f^l, y_i) \right] &= -E(\beta - 1) + \frac{I(\beta)}{\beta} \\
\mathbb{E}_{q(f^l)} \left[ \mathcal{L}^\beta_p (f^l, y_i) \right] &= -E(\gamma - 1) \cdot \frac{\gamma}{I(\gamma)^{\gamma - 1}}
\end{align}

(20) (21)

Fig. [1] demonstrates that misspecification can be a severe detriment for inference with the negative log likelihood. It also uses influence functions to showcase how the alternative model-based losses \( \mathcal{L}^\alpha_p \) and \( \mathcal{L}^\beta_p \) can avoid suffering under model misspecification. We note in passing that for numerical stability, \( \mathcal{L}^\beta_p \) is the preferable loss since it is multiplicative and unlike \( \mathcal{L}^\alpha_p \) never changes sign. Thus, it can be processed and stored entirely in log form.

4.2 Alternative uncertainty quantification for prior robustness and marginal variances

In contrast to Maximum Likelihood inference, Bayesian methods provide uncertainty quantification about \( \theta \). Specifically, uncertainty about \( \theta \) is quantified by penalizing how far the posterior \( q \) diverges from the prior \( \pi \). GVI is the first method relaxing the constraint that \( D = \text{KLD} \). Specifically, Knoblauch et al. [22] study robust alternatives to the GVI. While GVI is not limited to other divergences, in this report we focus on Rényi’s \( \alpha \)-divergence \( D^{(\alpha)}_{AR} \) (with the parameterization of Cichocki and Amari [6]) given by

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

(22)

This divergence is available in closed form for the variational families and priors on DGP of [27] for \( \alpha \in (0, 1) \). More importantly, it provides larger marginal variances than VI for \( \alpha \in (0, 1) \), tighter marginal variances than VI for \( \alpha > 1 \) and is robust to badly specified priors. We refer to Fig. 2 for an illustration of both properties. We note that the supplementary material of [22] contains a much wider selection of pictorial examples that also encompass other divergences.

As a second alternative to \( D^{(\alpha)}_{AR} \)-uncertainty quantification, we also consider \( D = \frac{1}{\alpha} \text{KLD} \) [see also [51]]. Note that this has an intimate relationship to power likelihoods. In particular, using the negative power log likelihood \(- \log p(y_i|\theta)^w = -\log p(y_i|\theta)\) as the loss in eq. (12) gives the same solution as using the standard log likelihood together with \( D = \frac{1}{\alpha} \text{KLD} \). More generally and using the notation introduced above, \( P(w\ell_n, D, \Pi) = P(\ell_n, \frac{1}{\alpha} \text{KLD}, \Pi). \) We note in passing that for \( w \in (0, 1) \) this choice of \( D \) places more weight on the prior. Thus, contrary to \( D^{(\alpha)}_{AR} \) it is anti-robust to the prior. For \( D = \text{KLD}, \) \( D(q||p) \) has closed form if both \( q \) and \( p \) are (multivariate) normal densities. Next, we show that this discrepancy is available in closed form for \( D = D^{(\alpha)}_{AR} \), too [see also [22]].

**Theorem 2** (closed forms for \( D = D^{(\alpha)}_{AR} \)). For \( q(\theta) = \mathcal{N}(\theta; \mu^q, \Sigma_q) \) and \( p(\theta) = \mathcal{N}(\theta; \mu^p, \Sigma_p) \) and

\[
(\Sigma^*)^{-1} = \alpha \Sigma_q^{-1} + (1 - \alpha) \Sigma_p^{-1}; \quad \mu^* = \Sigma^* (\alpha \Sigma_q^{-1} \mu^q + (1 - \alpha) \Sigma_p^{-1} \mu^p)
\]

it holds that for \( \alpha \in (0, 1) \),

\[
D^{(\alpha)}_{AR} (q(\theta)||p(\theta)) = \frac{1}{2\alpha(1 - \alpha)} \left\{ -\alpha \left[ \mu^q \Sigma_q^{-1} \mu^q + \ln |\Sigma_q| \right] - (1 - \alpha) \left[ \mu^p \Sigma_p^{-1} \mu^p + \ln |\Sigma_p| \right] + \left[ \mu^* \Sigma^* \right]^{-1} \mu^* + \ln |\Sigma^*| \right\}
\]

(23)

Notice that computing this is of the same order as computing the KLD uncertainty quantifier. In particular, one needs to perform a cholesky decomposition of \( \Sigma_q \) and \( \Sigma_q \) for either choice of \( D \).

4.3 GVI objectives for DGP

Using the layer-specific uncertainty quantifier \( D^l \in \{ D^{(\alpha)}_{AR}, \frac{1}{\alpha} \text{KLD} \} \) for the DGP layer with index \( l \), the GVI formulations of robust DGPs within this report have the generalized form of eq. (6) given by

\[
\mathcal{L}(q(Y, X, l, \{D^l\}_{l=1}^L) = \sum_{i=1}^n \mathbb{E}_{q(f^l_i)} \left[ \ell(f^l_i, y_i) \right] + \sum_{i=1}^L D^l(q(F^l_i, U^l)||p(F^l, U^l|Z^{l-1})).
\]

(24)
The answer to (II) is less obvious and requires the following technical result [see 22].

This clearly holds for the special case of the GVI, $\alpha = 0.5$, $\alpha = 0.025$, and MLE. Depicted are approximate marginals for two different priors $\pi \in \{N(-30, 2^2), N(-5, 2^2)\}$. VI is sensitive to the badly specified prior. GVI can avoid this.

For the DGP, Thms. [1] and [2] show that the relevant quantities of this objective will be available in closed form. Conceptually, the extension to generalized losses is straightforward [3]. Moreover, the same cannot be said about the new uncertainty quantifier. In particular, two important questions arise at this point:

(I) Will the divergence term simplify to $\sum_{l=1}^{L} D'(q(U_l)||p(U_l|Z^{l-1}))$ as in eq. (7)?

(II) Is $\sum_{l=1}^{L} D'(q(F_l, U_l)||p(F_l, U_l|Z^{l-1}))$ a valid divergence between the full prior $\pi$ of eq. (9) and the variational posterior $q$ of eq. (1)?

4.3.1 Does the layer-specific divergence define a valid divergence?

To see that (I) can be answered positively, one simply needs to re-examine eq. (10) – (12) in Bonilla et al. [4]. In particular, note that for any divergence $D'(q||p)$ that can be written as $D'(q||p) = g(D(q||p))$ for some function $g(x)$ such that $g(x) \geq 0$ and $g(x) = 0$ if and only if $x = 0$ and for some f-divergence $D'(q||p) = \int_{p(F_l, U_l)} q(F_l, U_l) f \left( \frac{q(F_l, U_l)}{p(F_l, U_l|Z^{l-1})} \right) d(F_l, U_l)$, it holds that

$$D'(q(F_l, U_l)||p(F_l, U_l|Z^{l-1})) = g \left( \mathbb{E}_{q(F_l, U_l)} \left[ f \left( \frac{q(F_l, U_l)}{p(F_l, U_l|Z^{l-1})} \right) \right] \right) = g \left( \mathbb{E}_{p(F_l, U_l|Z^{l-1})} q(F_l, U_l) \mathbb{E}_{q(U_l)} \left[ f \left( \frac{q(U_l)}{p(U_l|Z^{l-1})} \right) \right] \right) = D'(q(U_l)||p(U_l|Z^{l-1})).$$

This clearly holds for the special case of the $D_{AR}^{(U)}$ with $g(x) = \frac{1}{\alpha(1-\alpha)} \log(x + 1)$ and $f(x) = x^{1-\alpha}$.

4.3.2 Does the layer-specific divergence simplify?

The answer to (II) is less obvious and requires the following technical result [see 22].
Figure 3: Comparing performance in DGP s with \( L \) layers for \( \text{DGP-GVI} \) with \( \ell_{\gamma}(\theta, x) = \sum_{i=1}^{n} L^i(\theta(x_i)) \) and \( \text{DGP-VI} \). Benchmark performance is the DGP with three layers as in [27]. Top row: Negative test log likelihoods. Bottom row: Test RMSE. The lower the better.

**Theorem 3** (Divergence recombination). Let \( D^l \) be divergences and \( c_l \geq 0 \) scalars for \( l = 1, 2, \ldots, L \). Moreover, denote \( \theta = (\theta_1, \theta_2, \ldots, \theta_L)^T, \theta_{-i} = (\theta_1, \theta_2, \ldots, \theta_{i-1}, \theta_{i+1}, \ldots, \theta_L)^T \). Further, define the conditionally independent densities

\[
p(\theta) = \prod_{l=1}^{L} p_l(\theta_l|\theta_{-i})\text{ and } q(\theta) = \prod_{l=1}^{L} q_l(\theta_l|\theta_{-i})\text{ and the conditioning-set dependent function } D^\theta_{-1;L}(q|p) = \sum_{l=1}^{L} c_l D^\theta_{-1;L}(q_l|p_l(\theta_l|\theta_{-i})).\]

Then, \( D^\theta_{-1;L}(q|p) \) defines a divergence between \( q \) and \( p \) if (i) a version of the Hammersley-Clifford Theorem holds for \( \{ q_l, p_l : l = 1, 2, \ldots, L \} \) and (ii) \( D^\theta_{-1;L}(q|p) \) for any fixed pair of conditioning sets \( \theta_{-(1;L)}^p, \theta_{-(1;L)}^q \).

Since conditions (i) and (ii) of this Theorem are easily verified for the DGP as long as \( D^l \in \{ D_{AR}, \text{KLD} \} \) for all \( l = 1, 2, \ldots, L \), the answer to (I) is also positive.

5 Experiments

This section restates the experiments reported in Knoblauch et al. [22]. As in Salimbeni and Deisenroth [27], the method of choice is doubly stochastic (generalized) black box VI/GVI. Note that the supplementary material of [22] contains more detail on the experimental setup as well as additional results. The code will be available publicly upon publication of Knoblauch et al. [22].

**Setup:** Test set likelihoods and RMSEs are reported by averaging over 50 random splits with 90% training and 10% test data. The GVI methods provide robustness via \( L^l(\theta(x_i)) \) rather than \( L^l(\theta(x_i)) \) as \( L^l > 0 \), which allows for a log representation. This is especially attractive on DGP s due to the importance of numerical stability. We use the variational family and code base of Salimbeni and Deisenroth [27]. Except for choosing 50 (instead of 20) -fold cross validation with a 10% randomly selected held out test set, all settings are the same as in Salimbeni and Deisenroth [27]. As in their paper, each experiment runs with ADAM [19] and a learning rate of 0.01 with 20,000 iterations. For the kernel, we choose the RBF kernel with a lengthscale for each dimension. The number of inducing points is 100 for all settings, and they are run after normalization with a whitened representation. The batch size is min(1000, \( n \)), where \( n \) is the number of observations in the training set. Each layer has min(30, \( D \)) latent functions, that is to say \( D^l = \text{min}(30, D) \) for all \( l \). The Python implementation extends the one of [27] and is based on tensorflow [11] and gpfow [25].

**Results & Interpretation:** The results for using \( L^l(\theta(x_i)) \) are shown in Fig. 3. We find that DGP s can benefit substantially from robust losses. This true for both the test RMSE and the test.
likelihoods, giving a strong indication that information-geometric considerations are of considerable importance when dealing with large-scale, black-box type Bayesian models. Moreover, Fig. 2 gives an overview over alternative uncertainty quantifiers $D$ as well as alternative losses $L$. While the results indicate that similarly to Bayesian Neural Networks [see 22], enforcing more conservative uncertainty quantification typically does not lead to better test scores. In fact, the contrary is the case. This finding is explained by noting that any kind of deep architecture is likely to have an extremely adaptable mean function. Thus, inflating the variance around this very informative mean function amounts to unwarranted uncertainty quantification.

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