A Unified Perspective on Natural Gradient Variational Inference with Gaussian Mixture Models

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Abstract

Variational inference with Gaussian mixture models (GMMs) enables learning of highly tractable yet multi-modal approximations of intractable target distributions with up to a few hundred dimensions. The two currently most effective methods for GMM-based variational inference, VIPS and iBayes-GMM, both employ independent natural gradient updates for the individual components and their weights. We show for the first time, that their derived updates are equivalent, although their practical implementations and theoretical guarantees differ. We identify several design choices that distinguish both approaches, namely with respect to sample selection, natural gradient estimation, stepsize adaptation, and whether trust regions are enforced or the number of components adapted. We argue that for both approaches, the quality of the learned approximations can heavily suffer from the respective design choices: By updating the individual components using samples from the mixture model, iBayes-GMM often fails to produce meaningful updates to low-weight components, and by using a zero-order method for estimating the natural gradient, VIPS scales badly to higher-dimensional problems. Furthermore, we show that information-geometric trust-regions (used by VIPS) are effective even when using first-order natural gradient estimates, and often outperform the improved Bayesian learning rule (iBLR) update used by iBayes-GMM. We systematically evaluate the effects of design choices and show that a hybrid approach significantly outperforms both prior works. Along with this work, we publish our highly modular and efficient implementation for natural gradient variational inference with Gaussian mixture models, which supports 432 different combinations of design choices, facilitates the reproduction of all our experiments, and may prove valuable for the practitioner.

1 Introduction

Many problems in machine learning involve inference from intractable distributions $p(\mathbf{x})$, that might further only be known up to a normalizing constant Z, that is, $p(\mathbf{x}) = \frac{1}{Z}\tilde{p}(\mathbf{x})$.

For example when learning latent variable models, $\tilde{p}(\mathbf{x})$ corresponds to the intractable distribution over the latent variable (Volpp et al., 2023); and in maximum entropy reinforcement learning, $\tilde{p}(\mathbf{x})$ corresponds to the exponentiated return, $\tilde{p}(\mathbf{x}) = \exp R(x)$ of trajectory $\mathbf{x}$ (Ziebart, 2010). Bayesian inference is another example, where the intractable, unnormalized target distribution $\tilde{p}(\mathbf{x})$ corresponds to the product of prior and likelihood, and the normalizing constant can not be computed in closed form. However, whereas in Bayesian inference, there is particular interest in scaling to high-dimensional problems and large datasets, we stress that our work considers problems of moderate dimensionality of up to a few hundred of dimensions, where modeling the full covariance matrix of Gaussian distributions is still tractable. Important applications can be found, for example, in robotics—where $p(\mathbf{x})$ could be a multimodal distribution over joint-configurations that reach the desired pose (Pignat et al., 2020) or over collision-free motions that reach a given goal (Ewerton et al., 2020)—, or in non-amortized variational inference for latent variable models (Volpp et al., 2023).

Variational inference (VI) aims to approximate the intractable target distribution $\tilde{p}(\mathbf{x})$ by means of a tractable, parametric model $\tilde{q}_{\boldsymbol{\theta}}(\mathbf{x})$, with parameters $\boldsymbol{\theta}$. Gaussian mixture models are a simple yet powerful choice for a model family since they can approximate arbitrary distributions when assuming a sufficiently

high number of components. Compared to more complex models, such as normalizing flows (Kobyzev et al., 2020), they are more interpretable and tractable since not only sampling and evaluating GMMs is cheap, but also marginalizations and certain expectations (of linear or quadratic functions) can be computed in closed form. Furthermore, the simplicity of GMMs allows for sample-efficient learning algorithms, that is, algorithms that require relatively few evaluations of the target distribution for learning the model parameters $\boldsymbol{\theta}$ (the weights, means, and covariance matrices of the GMM). GMM-based variational inference is, in particular, relevant for problem settings with up to a few hundred dimensions (Volpp et al., 2023; Ewerton et al., 2020; Pignat et al., 2020), where learning and storing of full covariance matrices is still tractable.

Arguably the two most effective algorithms for GMM-based VI, both apply independent natural gradient (NG) updates on each component as well as on the categorical distribution over weights (Arenz et al., 2018; Lin et al., 2019a). Yet, both algorithms were derived from a different perspective, have different theoretical guarantees, and even different objectives for the independent updates. Namely, iBayes-GMM (Lin et al., 2019a; 2020) uses the original GMM objective for each independent update to perform natural gradient descent also with respect to the full mixture model, whereas VIPS (Arenz et al., 2018; 2020) uses a lower bound for an expectation-maximization procedure, which yields independent objective functions for each component and the mixture weights. Their approach can be shown to converge, even when the M-Step does not consist of single natural gradient updates, however, it was not yet proven, that their proposed procedure, which does use single natural gradient steps, also performs natural gradient descent on the full mixture.

In this work, we show that the proposed updates of both procedures are in fact the same because, directly after the E-Step, the (natural) gradients of the lower bound objectives of VIPS momentarily match the gradients of the original objective. However, despite the theoretical equivalence of both updates, their reference implementations perform very differently due to several design choices, as we will show in our experiments. Namely, VIPS uses samples from the individual components to estimate the natural gradient using the policy search method MORE (Abdolmaleki et al., 2015), which is also applicable to non-differentiable target distributions, whereas iBayes-GMM (Lin et al., 2020) uses Stein's Lemma (Lin et al., 2019b), which makes use of gradients and is therefore less general, but more efficient. However, iBayes-GMM estimates the natural gradient for each component using samples from the mixture model (taking into account the components' weights) and, therefore, low-weight components get very noisy updates and fail to improve, which may even cause the mixture model to collapse, effectively learning a Gaussian approximation. Hence, it is not surprising that iBayes-GMM often works best, when not updating the uniformly-initialized weights (Lin et al. 2020), which, however, significantly impairs the capacity of the mixture model. Furthermore, iBayes-GMM directly controls the learning rates, whereas VIPS uses adaptive trust regions based on the Kullback-Leibler divergence (Kullback and Leibler, 1951) that may improve learning stability, and iBayes-GMM uses a fixed number of components, whereas VIPS adapts the number during optimization improving its ability to discover additional modes of the target distribution. We perform extensive ablations to evaluate the effects of these design choices on the quality of the learned approximations and show that a hybrid approach outperforms both previous methods significantly. We summarize our main contributions as follows:

- We improve our theoretical understanding of GMM-based VI by connecting two previously separated lines of research by Arenz et al. (2018; 2020) and Lin et al. (2019a; 2020). by showing that performing a single natural gradient step for updating each component as well as the mixture weights with respect to the lower bound objective of VIPS (Arenz et al., 2018) is equivalent to the iBayes-GMM (Lin et al., 2020) update. Our results imply that VIPS (Arenz et al., 2018; 2020) updates the whole GMM along the NG.
- We evaluate several design choices and propose a novel method that significantly outperforms both prior methods. In particular, we combine KL-constrained trust regions, which have been popularized in the gradient-free reinforcement learning setting (Peters et al., 2010; Schulman et al., 2015; Otto et al., 2021), with gradient-based estimates of the natural gradient (Lin et al., 2019b), use samples from each component and adapt the number of components. Our test suites includes problems from both prior works.
- We release an open-source implementation for our generalized framework for GMM-based VI. Our implementation is highly modular—allowing each design choice to be set independently—and outperforms the reference implementations of iBayes-GMM and VIPS when using their respective design choices. We also publish the scripts we used for starting each experiment, including hyperparameter optimization.

2 Variational Inference with GMMs

We will now review the typical optimization problem for variational inference, and prior works that are central to our contributions, namely VIPS (Arenz et al., 2018; 2020) and iBayes-GMM (Lin et al., 2020).

2.1 Problem Formulation

The problem of approximating a target distribution $p(\mathbf{x})$ with a model $q_{\boldsymbol{\theta}}(\mathbf{x})$ is typically framed as the problem of minimizing the reverse Kullback-Leibler (KL) divergence (Kullback and Leibler, 1951),

$$\mathrm{KL}(q_{\boldsymbol{\theta}}||p) = \int_{\mathbf{x}} q_{\boldsymbol{\theta}}(\mathbf{x}) \log \frac{q_{\boldsymbol{\theta}}(\mathbf{x})}{p(\mathbf{x})} d\mathbf{x} = \int_{\mathbf{x}} q_{\boldsymbol{\theta}}(\mathbf{x}) \log \frac{q_{\boldsymbol{\theta}}(\mathbf{x})}{\tilde{p}(\mathbf{x})} d\mathbf{x} + \log Z.$$

The reverse KL divergence is a principled choice for the optimization problem, as it directly corresponds to the average amount of information (measured in nats), that samples from the approximation $q_{\boldsymbol{\theta}}(\mathbf{x})$ contain for discriminating between the approximation and the target distribution. Furthermore, the optimization can be performed despite the intractability of the normalizing constant Z, which does not affect the optimal parameters $\boldsymbol{\theta}$. When ignoring the normalizing constant and reframing the problem as a maximization problem, we obtain the evidence lower bound objective (ELBO). When using a GMM $q_{\boldsymbol{\theta}}(\mathbf{x}) = \sum_o q_{\boldsymbol{\theta}}(o) q_{\boldsymbol{\theta}}(\mathbf{x}|o)$, with weights $q_{\boldsymbol{\theta}}(o)$ and Gaussian components $q_{\boldsymbol{\theta}}(\mathbf{x}|o)$ as variational distribution, the ELBO is given by

$$J(\boldsymbol{\theta}) = \sum_o q_{\boldsymbol{\theta}}(o) \int_{\mathbf{x}} q_{\boldsymbol{\theta}}(\mathbf{x}|o) \log \tilde{p}(\mathbf{x}) d\mathbf{x} + H(q_{\boldsymbol{\theta}}), \tag{1}$$

where $H(q_{\boldsymbol{\theta}}) = -\int_{\mathbf{x}} q_{\boldsymbol{\theta}}(\mathbf{x}) \log(q_{\boldsymbol{\theta}}(\mathbf{x})) d\mathbf{x}$ denotes the entropy of the GMM. Hence, our objective is to maximize Equation 1 with respect to the parameters $\boldsymbol{\theta}$, which correspond to the weights $q(o)$ and the mean and covariance matrix for each Gaussian component $q(\mathbf{x}|o)$. Different methods have been proposed on how to (i) decompose the objective into independent objectives for components and weights (ii) update each component using either zero-order or first-order information and (iii) update the component weights.

2.2 Obtaining Decomposed Updates

Maximizing the ELBO in Eq. 1 with respect to the whole mixture model can be reduced to individual updates of the components and the weight distribution (Arenz et al., 2018; Lin et al., 2019a). VIPS (Arenz et al., 2018) achieves this reduction using a lower-bound objective for an expectation-maximization procedure. In contrast, Lin et al. (2019a) investigated the natural gradient of Eq. 1 with respect to the GMM parameters and showed that it can be estimated independently for the parameters of the individual components and the parameters of the weight distribution. While both decompositions can be applied to larger classes of latent variable models, in the following we restrict our discussion to Gaussian mixture models.

2.2.1 Fisher Information Matrix Decomposition

The ELBO objective (Eq. 1) could be straightforwardly optimized using (vanilla) gradient descent, using the reparameterization trick (Kingma and Welling, 2014; Rezende et al., 2014) for obtaining the gradient with respect to the parameters of each component and the weights. However, compared to gradient descent, natural gradient descent (Amari, 1998) has been shown to be much more efficient for variational inference (Khan and Nielsen, 2018). Whereas gradient descent performs steepest descent subject to the constraint of (infinitesimal) small (in the Euclidean sense) changes to the parameters, natural gradient descent performs steepest descent subject to small changes to the underlying distribution (with respect to the Fisher information metric). The natural gradient can be obtained from the vanilla gradient by preconditioning it with the inverse Fisher information matrix (FIM), but explicitly computing the FIM is expensive. Instead, Khan and Nielsen (2018) have shown that the natural gradient with respect to the natural parameters of an exponential family distribution (such as a Gaussian) is given by the vanilla gradient with respect to the expectation parameters, which can be efficiently computed—as we will discuss in more detail in Section 3.1.2. However, GMMs do not belong to the exponential family and are, thus, not directly amenable to this procedure.

To derive efficient natural gradient updates for a broader class of models, Lin et al. (2019a) considered latent variable models, such as GMMs, where the marginal distribution of the latent variable $q(o)$ and the conditional distribution of the observed variable $q(x|o)$ are both minimal exponential family distributions. They showed that for such minimal conditionally exponential family (MCEF) distributions, the Fisher information matrix of the joint distribution $q(x, o)$ is block-diagonal, which in turn justifies computing the natural gradients of the individual components and the weight distribution independently.

2.2.2 Lower-Bound Decomposition

Whereas Lin et al. (2019a) showed that a single natural gradient update can be performed for every component independently and that such procedure also performs natural gradient descent on the whole mixture model, Arenz et al. (2018) proposed a method for GMM-based variational inference that is not derived for natural gradient descent and that allows for independent optimizations (going beyond single step updates).

For understanding how VIPS (Arenz et al., 2018) decomposed the ELBO objective (Eq. 1) into independent objectives, it is helpful to first understand which terms prevent independent optimization in the first place. In particular, note that the first term of the ELBO given in Equation 1 already decomposes into independent objectives for each component, and only the second term (the model entropy) prevents us from optimizing each component independently. More specifically, when using Bayes' theorem to write the probability density of the GMM in terms of the marginals and conditionals, the interdependence between the different components can be narrowed down to the (log-)responsibilities $q_{\boldsymbol{\theta}}(o|\mathbf{x})$ within the entropy,

$$H(q_{\boldsymbol{\theta}}) = -\sum_o q_{\boldsymbol{\theta}}(o) \int_{\mathbf{x}} q_{\boldsymbol{\theta}}(\mathbf{x}|o) \Big(\log \frac{q_{\boldsymbol{\theta}}(o) q_{\boldsymbol{\theta}}(\mathbf{x}|o)}{q_{\boldsymbol{\theta}}(o|\mathbf{x})} \Big),$$

which is the only term in Equation 1 that creates a mutual dependence between different components. Hence, Arenz et al. (2018) introduced an auxiliary distribution $\tilde{q}(o|\mathbf{x})$, to derive the lower bound

$$\begin{aligned} \tilde{J}(\tilde{q}, \boldsymbol{\theta}) =& \sum_o q_{\boldsymbol{\theta}}(o) \Big[\int_{\mathbf{x}} q_{\boldsymbol{\theta}}(\mathbf{x}|o) \Big(\log \tilde{p}(\mathbf{x}) + \log \tilde{q}(o|\mathbf{x}) \Big) d\mathbf{x} + H(q_{\boldsymbol{\theta}}(\mathbf{x}|o)) \Big] + H(q_{\boldsymbol{\theta}}(o)) \\ =& J(\boldsymbol{\theta}) - \int_{\mathbf{x}} q_{\boldsymbol{\theta}}(\mathbf{x}) \mathrm{KL}(q(o|\mathbf{x}) || \tilde{q}(o|\mathbf{x})) d\mathbf{x}. \end{aligned} \tag{2}$$

As an expected KL is non-negative for any two distributions and equals zero, if both distributions are equal, $\tilde{J}(\tilde{q}, \boldsymbol{\theta})$ is a lower bound of $J(\boldsymbol{\theta})$ that is tight when $\tilde{q}(o|\mathbf{x}) = q(o|\mathbf{x})$. Hence, VIPS uses a procedure similar to expectation maximization that alternates between recomputing the responsibilities based on the current model parameters (E-step) and optimizing the model parameters with respect to the lower bound $\tilde{J}(\tilde{q}, \boldsymbol{\theta})$. As the lower bound is tight, i.e, it matches the actual objective $J(\boldsymbol{\theta})$ before each M-step, the M-step always improves the original objective. As the auxiliary distribution $\tilde{q}(o|\mathbf{x})$ is independent of the model parameters (during the M-step), the optimization of the lower bound can be performed independently for the weights $q(o)$ and each component $q(\mathbf{x}|o)$, resulting in a component-wise loss function

$$\tilde{J}_o(\tilde{q}, \boldsymbol{\theta}) = \int_{\mathbf{x}} q_{\boldsymbol{\theta}}(\mathbf{x}|o) \Big(\log \tilde{p}(\mathbf{x}) + \log \tilde{q}(o|\mathbf{x}) - \log q(\mathbf{x}|o) \Big) d\mathbf{x}. \tag{3}$$

While these derivations would justify any procedure that improves the model with respect to the lower bound objective during the M-step, the method proposed by Arenz et al. (2018), VIPS, performs single natural gradient steps, closely connecting it to iBayes-GMM (Lin et al., 2020). Indeed, we will now show that the updates of both methods are equivalent, except for design choices that are not mandated by the derivations and can be interchanged arbitrarily.

2.2.3 Unifying the Decompositions

Both previously described methods iteratively improve the GMM by applying at each iteration a single natural gradient step independently to each component and the weight distribution. However, the natural gradient is computed with respect to different objective functions, since iBayes-GMM (Lin et al., 2020) uses

the original objective given by Eq. 1, whereas VIPS (Arenz et al., 2018) maximizes the lower bound given by Eq. 2. However, we will now show that the (natural) gradient of the lower bound objective, computed immediately after the E-Step, matches the gradient of the original objective. To do so, we first reformulate the lower bound in a form that was previously used by Becker et al. (2019)—which expresses the auxiliary distribution as $\tilde{q}(o|\mathbf{x}) = \frac{\tilde{q}(o)\tilde{q}(\mathbf{x}|o)}{\tilde{q}(\mathbf{x})}$—and contrast it with the objective $J(\boldsymbol{\theta})$ of iBayes-GMM (Lin et al., 2020),

$$\tilde{J}(\tilde{q}, \boldsymbol{\theta}) = \sum_o q_{\boldsymbol{\theta}}(o) \Big[\int_{\mathbf{x}} q_{\boldsymbol{\theta}}(\mathbf{x}|o) \Big(\log \frac{\tilde{p}(\mathbf{x})}{\tilde{q}(\mathbf{x})} \Big) d\mathbf{x} - \mathrm{KL}(q_{\boldsymbol{\theta}}(\mathbf{x}|o) || \tilde{q}(\mathbf{x}|o)) \Big] - \mathrm{KL}(q_{\boldsymbol{\theta}}(o)) || \tilde{q}(o), \tag{4}$$

$$\neq \sum_o q_{\boldsymbol{\theta}}(o) \int_{\mathbf{x}} q_{\boldsymbol{\theta}}(\mathbf{x}|o) \Big(\log \frac{\tilde{p}(\mathbf{x})}{q_{\boldsymbol{\theta}}(\mathbf{x})} \Big) d\mathbf{x} = J(\boldsymbol{\theta}). \tag{5}$$

We can see that the lower bound objective (Arenz et al., 2018; Becker et al., 2019) differs from the original ELBO objective by two additional KL divergences, and further, by computing the entropy based on the auxiliary distribution $\tilde{q}(\mathbf{x})$ rather than the model $q_{\boldsymbol{\theta}}(\mathbf{x})$. As the gradient of the KL divergence between two equal distribution is zero, these terms do not affect the gradient of the objective function directly after the E-step. Furthermore, the gradients of the entropy terms are equal, since

$$\frac{\partial}{\partial \boldsymbol{\theta}} \left[\int_{\mathbf{x}} q_{\boldsymbol{\theta}}(\mathbf{x}) \log q_{\boldsymbol{\theta}}(\mathbf{x}) d\mathbf{x} \right] = \int_{\mathbf{x}} \frac{\partial q_{\boldsymbol{\theta}}(\mathbf{x})}{\partial \boldsymbol{\theta}} \cdot \log q_{\boldsymbol{\theta}}(\mathbf{x}) d\mathbf{x} + \frac{\partial \left[\int_{\mathbf{x}} q_{\boldsymbol{\theta}}(\mathbf{x}) d\mathbf{x} \right]}{\partial \boldsymbol{\theta}} = \frac{\partial}{\partial \boldsymbol{\theta}} \left[\int_{\mathbf{x}} q_{\boldsymbol{\theta}}(\mathbf{x}) \log \tilde{q}(\mathbf{x}) d\mathbf{x} \right].$$

Pretending for a moment that we are optimizing both objectives using the reparameterization trick, it is inspiring to relate the lower bound, to the common practice of not backpropagating through the score function, yielding an unbiased, but often lower-variance estimate of the ELBO gradient (Roeder et al., 2017).

3 A Modular and General Framework

We have shown that both derivations suggest exactly the same updates (although the decision to perform single natural gradient steps is voluntary for the EM-based derivation). Yet, the reference implementations of the respective authors (Arenz et al., 2018; Lin et al., 2019a) differ quite significantly in terms of how the natural gradients are estimated based on samples, how the required samples are obtained, how the stepsizes are chosen, and whether the number of components is adapted throughout the optimization. To evaluate the effect of these design choices, we developed a modular framework that generalizes both algorithms by enabling us to select every design choice independently. Pseudo-Code for our framework is show in Algorithm 1. We make use of seven modules that can be implemented differently depending on the design choice: **(1)** The *SampleSelector* selects the samples that are used during the current iteration for estimating the natural gradients with respect to the parameters of the components and the weight distribution, **(2)** the *ComponentStepsizeAdaptation* module chooses the stepsizes for the next component updates, **(3)** the *NgEstimator* estimates the natural gradient for the component update based on the selected samples, **(4)** the *NgBasedUpdater* performs the component updates based on the estimated natural gradients and the stepsizes, **(5)** the *WeightStepsizeAdaptation* module chooses the stepsize for the next update of the weights, **(6)** the *WeightUpdater* updates the weight distribution along the natural gradient based on the chosen stepsize, and **(7)** the *ComponentAdaptation* module decides whether to add or delete components. The different design choices for each of the modules will be discussed in the following subsections.

3.1 Natural Gradient Estimation

For estimating the natural gradient for the individual component updates, VIPS only uses black-box evaluations of the unnormalized target distribution $\log \tilde{p}(\mathbf{x}_i)$ on samples $\mathbf{x}_i$. In contrast, the NG estimate used by iBayes-GMM (Lin et al., 2020), which is based on Stein's Lemma (Stein, 1981), uses first-order information $\nabla_{\mathbf{x}_i} \log \tilde{p}(\mathbf{x}_i)$ which is less general but typically more sample efficient.

3.1.1 Option 1: Zero-order NG Updates using Compatible Function Approximation

VIPS uses the policy search method MORE (Abdolmaleki et al., 2015), which is based on compatible function approximation (Pajarinen et al., 2019; Peters and Schaal, 2008; Sutton et al., 1999). Namely, as shown

Algorithm 1 Natural Gradient GMM Variational Inference

repeat
  samples, targetDensitiesAndGradients ← SampleSelector.selectSamples(GMM, SampleDatabase)
  compStepsizes ← ComponentStepsizeAdapation.updateStepsizes(numCompUpdates, compStepsizes)
  naturalGradients ← NGEstimator.getNGs(samples, targetDensitiesAndGradients, GMM)
  GMM ← NGBasedUpdater.applyNgUpdate(naturalGradients, stepsizes, GMM)
  weightStepsize ← WeightStepsizeAdaptation.updateStepsizes(numIterations, weightStepsize)
  GMM ← WeightUpdater.updateWeights(weightStepsize, samples, targetDensities, GMM)
  GMM ← ComponentAdaptation.adaptNumberOfComponents(numIterations, GMM, SampleDatabase)
until stoppingCriteria

by Peters and Schaal (2008), an unbiased estimate of the natural gradient for an objective of the form $\mathbb{E}_{\pi_{\boldsymbol{\theta}}}(\mathbf{x})[R(\mathbf{x})]$ for some distribution $\pi_{\boldsymbol{\theta}}$ is given by the weights $\boldsymbol{\omega}$ of a compatible function approximator (Sutton et al., 1999), $\tilde{R}(\mathbf{x}) = \boldsymbol{\omega}^\top \boldsymbol{\phi}(\mathbf{x})$, that is fitted using ordinary least squares to approximate R, based on a data set $\mathcal{X} = \{(\mathbf{x}, R(\mathbf{x}))_i\}$, with samples $\mathbf{x}_i$ that are obtained by sampling from the distribution $\pi_{\boldsymbol{\theta}}$. A function approximator is compatible to the distribution $\pi_{\boldsymbol{\theta}}$, if the basis functions $\boldsymbol{\phi}(\mathbf{x})$ are given by the gradient of the log distribution, $\boldsymbol{\phi}(\mathbf{x}) = \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(\mathbf{x})$. For updating a Gaussian component $q(\mathbf{x}|o)$ parameterized with its natural parameters, $\boldsymbol{\eta}_o = \left\{\boldsymbol{\Sigma}_o^{-1}\boldsymbol{\mu}_o, -\frac{1}{2}\boldsymbol{\Sigma}_o^{-1}\right\}$, the compatible function approximator can be written as

$$\tilde{R}(\mathbf{x}) = \mathbf{x}^\top \mathbf{R}\mathbf{x} + \mathbf{x}^\top \mathbf{r} + r,$$

where the matrix $\mathbf{R}$, the vector $\mathbf{r}$ and the scalar r, are the linear parameters that are learned using least squares. Here, the constant offset r can be discarded and $\mathbf{R}$ and $\mathbf{r}$ directly correspond to the natural gradients, that could be used to update the natural parameters,

$$-\frac{1}{2}\boldsymbol{\Sigma}_o^{-1} = -\frac{1}{2}\boldsymbol{\Sigma}_{\text{o,old}}^{-1} + \beta_o \mathbf{R}, \qquad \boldsymbol{\Sigma}_o^{-1}\boldsymbol{\mu}_{\boldsymbol{o}} = \boldsymbol{\Sigma}_{\text{o,old}}^{-1}\boldsymbol{\mu}_{\text{o,old}} + \beta_o \mathbf{r}. \tag{6}$$

The least squares targets $R(\mathbf{x}) = \log \frac{\tilde{p}(\mathbf{x})}{\tilde{q}(\mathbf{x})} = \log \frac{\tilde{p}(\mathbf{x})}{q_{\boldsymbol{\theta}}(\mathbf{x})}$ would be the same whether we use the formulation (Eq. 5) by Lin et al. (2019a) or by Becker et al. (2019) (Eq. 4). Please note that the original formulation of VIPS (Arenz et al., 2018) (Eq. 3) differs by a constant offset $\log q_{\boldsymbol{\theta}}(o)$ that would be consumed by the scalar r and not affect the NG estimates $\mathbf{R}$ and $\mathbf{r}$. For compatible function approximation, the data set $\mathcal{X}$ should be obtained by sampling the respective component. However, VIPS uses importance weighting to make use of samples from previous iterations and from different components, by performing weighted least squares, where the weight of each data point is given by its importance weight. The importance weights w_i can be computed as $\frac{q(\mathbf{x_i}|o)}{z(\mathbf{x_i})}$, where z is the actual distribution that was used for sampling the data set. However, VIPS uses the self-normalized importance weights $w_i^{\text{sn}} = (\sum_j w_j)^{-1} w_i$, which yield lower-variance, biased, but asymptotically (for large number of samples) unbiased estimates. Furthermore, VIPS applies ridge regularization during weighted least squares, which further introduces a bias.

3.1.2 Option 2: First-Order NG Updates using Stein's Lemma

Khan and Nielsen (2018) show that for exponential-family distributions, the natural gradient with respect to the natural parameters $\boldsymbol{\eta}$ (for Gaussians $\boldsymbol{\eta} = \{\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}, -\frac{1}{2}\boldsymbol{\Sigma}^{-1}\}$) corresponds to the vanilla gradient with respect to the expectation parameters $\mathbf{m}$ (for Gaussians $\mathbf{m} = \{\boldsymbol{\mu}, \boldsymbol{\Sigma} + \boldsymbol{\mu}\boldsymbol{\mu}^\top\}$). Using the chain rule, the gradient with respect to the expectation parameters can be expressed in terms of the gradient with respect to the covariance $\boldsymbol{\Sigma}$ and mean $\boldsymbol{\mu}$ (Khan and Lin, 2017, Appendix B.1). Combining these results, a natural gradient step for a Gaussian component $q(\mathbf{x}|o)$ with stepsize β_o and objective $J(\mathbf{x})$ can be computed as

$$-\frac{1}{2}\boldsymbol{\Sigma}_o^{-1} = -\frac{1}{2}\boldsymbol{\Sigma}_{\text{o,old}}^{-1} + \beta_o \nabla_{\boldsymbol{\Sigma}_o} J, \quad \boldsymbol{\Sigma}_o^{-1}\boldsymbol{\mu}_o = \boldsymbol{\Sigma}_{\text{o,old}}^{-1}\boldsymbol{\mu}_{\text{o,old}} + \beta_o \left(-2\left[\nabla_{\boldsymbol{\Sigma}} J\right]\boldsymbol{\mu}_{\text{o,old}} + \nabla_{\boldsymbol{\mu}} J\right), \tag{7}$$

as shown by Khan et al. (2018, Appendix C). As the objective J corresponds to an expected value, i.e., $J = \mathbb{E}_{q(\mathbf{x}|o)}\left[R(\mathbf{x})\right]$ with $R(\mathbf{x}) = \log \frac{\tilde{p}(\mathbf{x})}{\tilde{q}(\mathbf{x})}$, the gradient with respect to mean and covariance are given by the

expected gradient and Hessian (Opper and Archambeau, 2009),

$$\nabla_{\mathbf{\Sigma}} J = \frac{1}{2}\mathbb{E}_{q(\mathbf{x}|o)}\Big[\nabla_{\mathbf{xx}} R(\mathbf{x})\Big], \qquad \nabla_{\boldsymbol{\mu}} J = \mathbb{E}_{q(\mathbf{x}|o)}\Big[\nabla_{\mathbf{x}} R(\mathbf{x})\Big]. \tag{8}$$

Hence, using Monte-Carlo to estimate the gradients with respect to mean and covariance (Eq. 8), we can obtain unbiased estimates of the natural gradient (Eq. 7). However, evaluating the Hessian $\nabla_{\mathbf{xx}} R(\mathbf{x})$ is computationally expensive, and therefore, Lin et al. (2019b) proposed an unbiased first-order estimate of the expected Hessian based on Stein's Lemma (Stein, 1981) given by (Lin et al., 2019b, Lemma 11)

$$\mathbb{E}_{q(\mathbf{x}|o)}\Big[\nabla_{\mathbf{xx}} R(\mathbf{x})\Big] = \mathbb{E}_{q(\mathbf{x}|o)}\left[\mathbf{\Sigma}_o^{-1}(\mathbf{x}-\boldsymbol{\mu}_o)\left(\nabla_{\mathbf{x}} R(\mathbf{x})\right)^\top\right]. \tag{9}$$

Similar to VIPS, iBayes-GMM uses importance sampling to perform the Monte-Carlo estimates (Eq. 8 right, Eq. 9) based on samples from different components. However, in contrast to VIPS, iBayes-GMM uses standard (unbiased) importance weighting, rather than self-normalized importance weighting, which in our implementation, can be selected using a hyperparameter that is available for both options.

3.2 Natural Gradient based Component Updates

For performing the natural gradient update, we identified three different options in the related literature. Lin et al. (2019a) directly apply the natural gradient update (Eq. 6) based on the natural gradients $\mathbf{R}$, $\mathbf{r}$ and the stepsize β_o, which we assume given. However, this update may lead to indefinite covariance matrices, and therefore iBayes-GMM (Lin et al., 2020) uses the *improved Bayesian learning rule (iBLR)*, which modifies the update direction (no longer performing natural gradient descent) in a way that ensures that the updated covariance matrix is positive definite. Thirdly, VIPS indirectly control the stepsize by choosing an upper bound on the KL divergence between the updated and the old component, $\mathrm{KL}(q(\mathbf{x}|o)||q_{\mathrm{old}}(\mathbf{x}|o))$, and solves a convex optimization problem to find the largest β_o that satisfies the trust region constraint. As **Option 1** (directly performing the natural gradient step) is straightforward, we now only discuss the two latter options.

3.2.1 Option 2: The Improved Bayesian Learning Rule

Updating the parameters of the Gaussian along the natural gradient may in general lead to covariance matrices that are not positive definite which would make the optimization fail. Instead, the update direction can be replaced by the iBLR, which approximates Riemannian gradient descent (Lin et al., 2020),

$$-\frac{1}{2}\mathbf{\Sigma}_o^{-1} = -\frac{1}{2}\mathbf{\Sigma}_{\mathrm{o,old}}^{-1} + \beta_o(\mathbf{R} - \beta_o \mathbf{R}\mathbf{\Sigma}_{\mathrm{o,old}}\mathbf{R}), \qquad \mathbf{\Sigma}_o^{-1}\boldsymbol{\mu}_o = \mathbf{\Sigma}_o^{-1}\mathbf{\Sigma}_{\mathrm{o,old}}\left(\mathbf{\Sigma}_{\mathrm{o,old}}^{-1}\boldsymbol{\mu}_{\mathrm{o,old}} + \beta_o \mathbf{r}\right). \tag{10}$$

The iBLR update (Eq. 10) differs from the NG update (Eq. 6) due to the additional terms $-\beta_o \mathbf{R}\mathbf{\Sigma}_{\mathrm{o,old}}\mathbf{R}$ and $\mathbf{\Sigma}_o^{-1}\mathbf{\Sigma}_{\mathrm{o,old}}$. Using this update, the new precision matrix can be shown to be an average of a positive definite and a positive semidefinite term, $\mathbf{\Sigma}_o^{-1} = \frac{1}{2}\left(\mathbf{\Sigma}_{\mathrm{o,old}}^{-1} + \mathbf{U}^\top\mathbf{U}\right)$, where $\mathbf{U} = \mathbf{L} - 2\beta\mathbf{L}^{-\top}\mathbf{R}$ and $\mathbf{L}^\top\mathbf{L} = \mathbf{\Sigma}_{\mathrm{o,old}}^{-1}$.

3.2.2 Option 3: Trust Region Optimization

VIPS updates the components using natural gradient descent (Eq. 6). However, rather than controlling the change of the component using the stepsize β_o, it upper-bounds the KL divergence $\mathrm{KL}\left(q_{\boldsymbol{\theta}}(\mathbf{x}|o)||\tilde{q}(\mathbf{x}|o)\right) < \epsilon_o$ by solving for every component update an optimization problem that finds the largest stepsize β_o, such that the updated component will have a positive definite covariance matrix and a KL divergence to the original component that is smaller than a bound ϵ_o, which is assumed given instead of the stepsize β_o (Abdolmaleki et al., 2015). The additional optimization problems for finding the stepsize add little computational overhead since the KL divergence is convex in the stepsize and can be efficiently computed for Gaussian distributions.

3.3 Weight Update

The natural gradient update for the categorical distribution is performed by updating the log weights in the direction of the expected reward of the corresponding component, that is,

$$q(o) \propto q(o)_{\mathrm{old}} \exp\left(\beta \hat{R}(o)\right), \tag{11}$$

where $\hat{R}(o)$ is a Monte-Carlo estimate of $R(o) = \mathbb{E}_{q(\mathbf{x}|o)}\left[\log \frac{p(\mathbf{x})}{\tilde{q}(\mathbf{x})}\right]$. The NG update is presented differently by Lin et al. (2020), but we clarify in Appendix D that both updates are indeed equivalent[1]. However, we identified two different options to perform the weight update, namely, (**Option 1**) the stepsize β can be chosen directly, or (**Option 2**) it can be optimized with respect to a desired KL bound $\mathrm{KL}\left(q(o)||q_{\mathrm{old}}(o)\right) \leq \epsilon$, analogously to the component update described in Section 3.2.2. This trust-region update was proposed by Arenz et al. (2018), although they later found that a fixed stepsize $\beta = 1$, corresponding to a greedy step to the optimum of their lower bound objective, performs similarly well (Arenz et al., 2020).

3.4 Sample Selection

For estimating the natural gradients of the components and the weight distribution, the target distribution $\tilde{p}(\mathbf{x})$ needs to be evaluated on samples from the respective distribution. However, both iBayes-GMM and VIPS use importance sampling to use the same samples for updating all distributions at a given iteration. **Option 1** (Lin et al., 2020) is to obtain the samples for a given iteration by sampling from the current GMM, using importance sampling to share samples between different components. **Option 2** (Arenz et al., 2018) is to sample from the individual components, rather than the GMM. Arenz et al. (2018) also store previous samples (and their respective function evaluations) in a database. Furthermore, they use two hyperparameters, the number of reused samples n_{reused} and the number of desired samples per component, n_{des}, and start by obtaining the n_{reused} newest samples from the data base. Then, they compute the effective sample size $n_{\mathrm{eff}}(o) = \left(\sum_i w_i^{\mathrm{sn}}(o)^2\right)^{-1}$, and redraw $n_{\mathrm{des}} - n_{\mathrm{eff}}(o)$ from each component.

3.5 Stepsize Adaptation

Different approaches have been proposed for selecting the stepsizes (or trust-regions) for the component and weight update. Lin et al. (2020) used fixed stepsizes in their implementation but used different stepsizes for weights and for the components (**Option 1**). Khan and Lin (2017) discussed a backtracking method to adapt the stepsize while ensuring positive definiteness, but they found it slow in practice and did not test it in the GMM setting, and Khan et al. (2018) used a decaying stepsize (**Option 2**). While using a fixed stepsize $\beta = 1$ for updating the weights, VIPS uses adaptive trust regions for updating the components, where the bounds are chosen independently for each component, by increasing the bound if the reward of the corresponding component improved during the last update, and by decreasing it otherwise (**Option 3**).

3.6 Component Adaptation

iBayes-GMM (Lin et al., 2020) uses a fixed number of components K that is specified by a hyperparameter (**Option 1**). VIPS (Arenz et al., 2018; 2020) dynamically adapts the number of components by deleting components at poor local optima that do not contribute to the approximation, and by adding new components in promising regions (**Option 2**). The initial mean for the new component is chosen based on a single-sample estimate of the initial reward $\tilde{R}(o_{\mathrm{new}})$ for the new component, evaluated for samples from the database.

4 Experiments

To evaluate the effect of the individual design choices, we implemented all previously discussed options in a common framework, such that they can be chosen independently. Prior to the experiments we ensured that our implementation performs comparably to the MATLAB implementation of iBayes-GMM (Lin et al., 2020) and to the C++-implementation of VIPS (Arenz et al., 2020) when using the respective design choices. As shown in Appendix E, when comparing our implementation with the reference implementation on their target distributions, we always learn similar or better approximations. Additional details on the implementation are described in Appendix G. An overview of the available options is shown in Table 1. Available hyperparameters for each option are shown in Appendix F. Our framework allows for $2^4 \cdot 3^3 = 432$ different combinations of options. We assign a unique letter to each option (see Table 1), such that we can refer to each of the

[1]The respective implementations still differ slightly because VIPS uses self-normalized importance weighting, rather than standard importance-weighting, which we control in our implementation using a hyperparameter.

MODULE	OPTIONS					
NgEstimator	More	**Z**	Stein	**S**		
ComponentAdaptation	Fixed	**E**	Vips	**A**		
SampleSelector	Lin et al.	**P**	Vips	**M**		
NgBasedComponentUpdater	Direct	**I**	iBLR	**Y**	Trust-Region	**T**
ComponentStepsizeAdaptation	Fixed	**F**	Decaying	**D**	Adaptive	**R**
WeightUpdater	Direct	**U**	Trust-Region	**O**		
WeightStepsizeAdaptation	Fixed	**X**	Decaying	**G**	Adaptive	**N**

Table 1: We assign a unique letter to every option such that every combination of options can be specified with a 7-letter word (one letter per module).

Design Choice		BreastCancer	BreastCancerMB	Wine
Component NG Estimation	MORE (Z)	78.88	152.84	N/A
	Stein (S)	**78.46**	**68.22**	**1431.09**
Component Update	Direct (I)	78.95	70.96	2263.78
	iBLR (Y)	78.69	70.37	**1431.09**
	Trust-Region (T)	**78.46**	**68.22**	1443.40
Component Stepsize Adaptation	Fixed (F)	**78.46**	69.01	1450.11
	Decaying (D)	78.47	70.69	1468.50
	Adaptive (R)	**78.46**	**68.22**	**1431.09**

Table 2: We show optimistic estimates of the best performance (negated ELBO) that we can achieve with every option when optimizing a uniform GMM with a fixed number of components, by reporting the best performance achieved during Bayesian optimization among all runs that used the respective option.

combinations with a 7-letter codeword. For example, SEPYFUX refers to iBayes-GMM (Lin et al., 2020) and ZAMTRUX to VIPS (Arenz et al., 2020). However, evaluating each combination is computationally prohibitive. Instead, we designed the following sequence of experiments.

In the first group of experiments, we evaluate the stability of the component updates, using fixed weights, and without adapting the number of components. In the second group of experiments, we use the most promising design choices for the component update that we identified in the first group of experiments, and ablate over the design choices that affect the update of the weights and the adaptation of the number of components. Based on the results of the previous group of experiments, we then identify promising combinations and evaluate them on the full test suite. For comparison with prior work, we also evaluate the design choices used by iBayes-GMM (Lin et al., 2020) and VIPS (Arenz et al., 2020).

4.1 Experiment 1: Component Update Stability

For evaluating the effects of the design choices on the component update stability, we do not change the number of components (Option **E**) and do not update the (uniformly initialized) weights (**X** and **U**, with initial weight-stepsize $\beta = 0$). Furthermore, we always sample from the GMM (**P**), since the two options for the *SampleSelector* hardly differ for uniform GMMs. We evaluate the different options for the *NgEstimator*, *ComponentStepsizeAdaptation* and *NgBasedComponentUpdater* resulting in 18 different combinations.

We evaluate each candidate on three target distributions: In the *BreastCancer* experiment Arenz et al. (2018) we perform Bayesian logistic regression using the full "Breast Cancer" datatset (Lichman, 2013). Further, we introduce the variant *BreastCancerMB* which uses minibatches of size 64 to evaluate the effect of stochastic target distributions. Thirdly, we evaluate the candidates in a more challenging Bayesian neural network experiment on the "Wine" dataset (Lichman, 2013), where we use a batch size of 128. We use two hidden layer with width 8, such that the 177-dimensional posterior distribution is still amenable to GMMs with full covariance matrices. Please refer to Appendix H for details on the implementation for all experiments.

Candidate	BreastCancer		BreastCancerMB		Wine	
	-ELBO	MMD	-ELBO (full batch)	MMD	-ELBO	MSE
SEPYRUX	1042.28 ±2699.32	0.004 ±0.002	1130.81 ±799.66	0.033 ±0.014	1462.91 ±35.70	0.481 ±0.022
SEPTRUX	**78.53 ±0.02**	**0.002 ±0.000**	**81.21 ±1.13**	**0.002 ±0.000**	1444.01 ±30.78	0.478 ±0.021

Table 3: We evaluated the best hyperparameters for the most promising candidates of our experiments for Group 1 on 10 different seeds with respect to ELBO and a secondary metric (maximum mean discrepancy or mean squared error). SEPYRUX, which uses the iBLR update for the component updates did not achieve stable results on the breast cancer experiments. SEPTRUX which uses trust-region updates for the components outperformed SEPYRUX in all experiments, although in *WINE* the advantage is not statistically significant.

We tuned the hyperparameters of each of the 18 candidates separately for each test problem using Bayesian optimization. We granted each candidate exclusive access to a compute node with 96 cores with a time limit of two days for each experiment. The results of the hyperparameter search are summarized in Table 2, where we report the best ELBO achieved for every design choice (maximizing over all tested hyperparameters and all combinations of the remaining options). On *Wine*, which uses almost three times as many parameters as have been tested by Arenz et al. (2020), we could not obtain reasonable performance when using MORE, as the required number of samples is much larger when only using zero-order information to estimate the natural gradient, resulting in very slow optimization.

The values in Table 2 give an optimistic estimate of the best performance that we can expect for a given design choice, however, it is in general not guaranteed that this performance can be robustly achieved over different seeds. Hence, for the most promising candidates, SEPTRUX and SEPYRUX, we used the best hyperparameters from the Bayesian optimization and evaluated the performance over ten random seeds. The mean of the final performance and its 99.7% standard error are shown in Table 3. We also show for every experiment a second metric, where we use the maximum mean discrepancy (Gretton et al., 2012) (MMD) for *BreastCancer* and *BreastCancerMB* (comparing samples from the GMM with baseline samples (Arenz et al., 2020)), and the mean squared error of the Bayesian inference predictions for *Wine*. Unfortunately, the hyperparameters for SEPYRUX on *BreastCancer* and *BreastCancerMB* led to unstable optimization for some seeds, despite their good performance during hyperparameter optimization. We expect that using slightly more conservative hyperparameters, SEPYRUX could reliably achieve a performance that is only slightly worse than the optimistic value provided in Table 3 for *BreastCancer* (78.69). However, the performance of SEPTRUX is even in expectation over multiple seeds already better than this optimistic estimate of SEPYRUX. Furthermore, also on *WINE*, where SEPYRUX did not suffer from instabilities, the trust-region updates achieved better performance (albeit not statistically significant). Hence, we decided to use trust-region updates for the second group of experiments. We will further test the iBLR update in our main experiments (Experiment 3), to compare both options more thoroughly.

4.2 Experiment 2: Weight Update and Exploration

According to the first experiment, first-order estimates using Stein's Lemma, adaptive component stepsizes and trust-region updates are the most effective and stable options for the component updates, and therefore, we fix the corresponding design choices (**S**, **T**, **R**) for our second group of experiments. The modules that we did not evaluate in the first group of experiments (*ComponentAdaptation*, *SampleSelector*, *WeightUpdater* and *WeightStepsizeAdaptation*) are in particular relevant for discovering and approximating multiple modes of the target distribution. Hence, we focus on multi-modal target distributions for the second set of experiments. All test problems for these experiments were taken from prior work. Namely, we chose *GMM20* and *PlanarRobot4* from Arenz et al. (2020) and *STM20* from Lin et al. (2020). For *GMM20* and *STM20* the target distribution is given by an unknown mixture of 20-dimensional Gaussians and Student-Ts, respec-

Design Choice		GMM20	STM20	PlanarRobot4
Component Adaptation	Non-Adaptive (E)	**0.00**	0.08	12.33
	Adaptive (A)	**0.00**	**0.05**	**12.15**
Sample Selection	From Mixture (P)	0.11	1.52	12.77
	From Components (M)	**0.00**	**0.05**	**12.15**
Weight Update	Natural Gradient Descent (U)	**0.00**	0.06	12.30
	Trust-Region (O)	**0.00**	**0.05**	**12.15**
Weight Stepsize Adaptation	Fixed (X)	**0.00**	0.06	**12.15**
	Decaying (G)	**0.00**	**0.05**	12.33
	Improvement-Based (N)	**0.00**	0.06	12.22

Table 4: We show optimistic estimates of the best performance (negated ELBO) that we can achieve with every option (updating the components using the design choices identified in the first experiment). We report the best performance achieved during Bayesian optimization among all runs that used the respective option.

tively. In *PlanarRobot4* we want to approximate a distribution over joint configurations of a 10-link planar robot, such that it approximately reaches any of four possible goal positions. For Bayesian optimization of the hyperparameters, we grant each of the 24 candidates exclusive access to our compute node for one day per test problem. Optimistic estimates of the best performance for each design choices are shown in Table 4. Based on our experiments sampling according to the mixture weights (Option **P**) seems to be clearly inferior to sampling from the components (Option **M**), as it was the only option that was not able to solve the *GMM20* experiment. Furthermore, adapting the number of components (Option **A**) and using trust-region updates for the weight update (Option **O**) seem beneficial for multimodal target distributions. However, for *WeightStepsizeAdaptation*, also a fixed stepsize (when used as trust-region) achieved good performance.

4.3 Experiment 3: Evaluating the Promising Candidates

For our main experiment we focus on candidates that use first order NG estimates, adaptive number of components and adaptive component-stepsizes and sample from the individual components (Options **S**, **A**, **M**, **R**), and aim to better compare trust-region updates with the iBLR update (Option **T** vs. **Y**). For updating the weights, we evaluate fixed and adaptive trust-regions, and fixed direct NG updates (**OX** vs. **ON** vs. **UX**), resulting in six candidates: Samtrux, Samtrox, Samtron, Samyrux, Samyrox and Samyron. Furthermore, to compare with prior work, we also evaluate Zamtrux (Arenz et al., 2020) and Sepyfux (Lin et al., 2020) as well as the variant Sepyrux, combining iBLR updates with adaptive stepsizes.

We evaluate these candidates on the full test suite, which uses the following test problems on top of the previously discussed ones: *GermanCredit* (Arenz et al., 2020) and *GermanCreditMB* are similar to the *BreastCancer* experiment, but use the 25-dimensional *GermanCredit* dataset (Lichman, 2013); *GMM100* and *STM300* are higher-dimensional variants of the *GMM20* and *STM20* experiments; and, finally, *TALOS* is a new experiment that we introduced to evaluate the different options on a test problem that was not used during development. Somewhat related to the *PlanarRobot4* experiment, in the *TALOS* experiment we aim to learn a distribution over joint configurations to reach a goal position with the robot's endeffector. However, instead of a planar robot, the *TALOS* experiment uses the kinematics of an actual robot–the humanoid TALOS from PAL Robotics (Stasse et al., 2017). Furthermore, the target distribution is based on the work by Pignat et al. (2020) and is more complex by using a product of expert that penalize pose errors for each foot and hand as well as unstable configurations (that occur when the robot's center of mass projected on the ground is outside of the support polygon spanned by the feet), and that incorporate a prior distribution over the joint angles. The target distribution is 34 dimensional (7 joint configurations for each leg, 6 joint angles for each arm and 6 additional parameters that specify the position and orientation of the floating base (the torso) with respect to a fixed reference frame. On *TALOS*, prior to the experiments of this group, we only performed few experiments using SEPIFOX to optimize a single Gaussian component, to ensure that the target distribution is correctly implemented.

Candidate	BreastCancer	BreatCancerMB	GermanCredit	GermanCreditMB	PlanarRobot	GMM20	GMM100	STM20	STM300	WINE	TALOS
SAMTRON	**78.00** ±**0.02**	**78.41** ±**0.03**	**585.10** ±**0.00**	**585.12** ±**0.00**	**11.47** ±**0.04**	**−0.00** ±**0.00**	**0.01** ±**0.03**	**0.00** ±**0.00**	**14.96** ±**0.48**	**1423.12** ±**31.55**	**−24.43** ±**0.16**
SAMYRON	78.61 ±0.05	79.96 ±0.26	585.11 ±0.01	**585.12** ±**0.00**	12.93 ±0.13	**0.00** ±**0.00**	0.16 ±0.09	0.03 ±0.01	22.50 ±0.15	**1433.87** ±**30.49**	−24.00 ±0.23
iBayes-GMM (SEPYFUX)	79.78 ±0.40	80.13 ±0.69	585.12 ±0.01	**585.12** ±**0.00**	17.26 ±2.13	0.43 ±0.15	4.54 ±0.52	0.46 ±0.06	26.87 ±0.45	3279.32 ±1425.12	−16.64 ±5.26
VIPS (ZAMTRUX)	78.14 ±0.01	83.65 ±0.97	**585.10** ±**0.00**	585.35 ±0.03	**11.48** ±**0.04**	**−0.00** ±**0.00**	1.21 ±0.15	0.54 ±0.17	N/A	16 503.38 ±813.75	−23.69 ±0.16

Table 5: Along with the negated ELBO, we show the 3σ confidence intervals based on the standard error of its mean using ten different seeds. The proposed candidate clearly outperforms the prior methods VIPS (Arenz et al., 2020) and IBAYES-GMM (Lin et al., 2020). First-order natural gradient estimates with trust-region constraints (**T**) seem preferable over the iBLR update (**Y**). We observed instabilities for SEPYFUX on *PlanarRobot* and *TALOS* and, thus, removed bad outliers when computing the reported values.

For selecting the hyperparameters, we perform for each candidate and each experiment a small grid search, where we make use of the results from the previous experiments to select suitable ranges. Extensive hyperparameter search (e.g. using Bayesian optimization) would unfairly benefit options with more hyperparameters. Table 5 compares the final performance (negated ELBO) of the best-performing candidate (SAMTRON) with the prior methods VIPS (Arenz et al., 2020) and iBayes-GMM (Lin et al., 2020). We also show SAMYRON for comparing trust-region natural-gradient updates with the iBLR update. According to these experiments, we can clearly improve upon ZAMTRUX by using Stein's Lemma for estimating the natural gradient (in particular for higher-dimensional problems), and upon SEPIFUX, by sampling from the components and adapting their number during optimization. Interestingly, trust-region constraints seem to be beneficial also when using first-order estimates of the natural gradient, and showed a slight but consistent advantage compared to the iBLR update (Lin et al., 2020) in our experiments. Full results of our main experiments are shown in Appendix I, where we show the performance of all tested candidates, also with respect to secondary metrics.

5 Conclusion

Although VIPS and iBayes-GMM are derived from different perspectives—where the derivations for Bayes-GMM are less general (by requiring single NG steps for the component update) but enjoy stronger guarantees (by proving natural gradient descent on the whole mixture model)—, we showed that both algorithms only differ in design choices and could have been derived from the other perspective, respectively. This unification of both perspective shows that we can derive approximate natural gradient descent algorithms also for mixtures of non-Gaussian components—where the approximation errors of the natural gradient are potentially much larger—without having to give up on convergence guarantees. Furthermore, our results are of high relevance for the practitioner, both due to our extensive study on the effects of the individual design choices—which shows that both prior works can be improved by using a combination of first-order natural gradient estimates, adaptive number of components, KL-divergence constrained trust regions and sampling from the individual components—and by releasing our modular framework for natural gradient GMM-based variational inference, which is well-documented and easy to use and outperforms the reference implementations by Arenz et al. (2020) and Lin et al. (2020) when using the respective design choices. The limitations of this study and the potential for negative societal impact are discussed in Appendix A and B.

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A Limitations

The scope of this work is narrow, focusing on two specific approaches for natural-gradient GMM-based variational inference. There are of course many other models that can be applied for variational inference, and, depending on the problem setting, some of these models are highly preferable over GMMs, for example, normalizing flows should likely be preferred for high-dimensional problem settings, such as (deep) Bayesian neural networks. However, for this work we assume that we indeed want to optimize a Gaussian mixture model, for example, because we require an interpretable model with smooth gradients (Ewerton et al., 2020). Even in the field of GMM-based variational inference, alternative methods, based on boosting (Miller et al., 2017; Guo et al., 2016) or the reparameterization trick are possible. By not using natural gradients, these methods can be applied more straightforwardly to sparse covariance parameterizations which can be beneficial for higher-dimensional problems. However, in the considered problem setting where we can learn GMMs with full covariance matrices, these methods are not competitive (Arenz et al., 2020) to the natural gradient based methods described in this work. Please refer to Appendix C for a discussion of related work.

Regarding our empirical study, we want to point out several aspects that could lead to misinterpretations of the results. While we also report a secondary metric for each test problem in our main experiment (Table 8), please recall that the hyperparameter optimization was performed only with respect to the ELBO. We noticed on the *planar robot* experiment, that SAMTRUX could still achieve competitive ELBO when initializing the mixture model with fewer components than we used for our evaluation, while resulting in a significantly worse MMD. Hence, one should consider that for each method, the performance with respect to the secondary metric could potentially be better, if the hyperparameters were chosen correspondingly. Similarly, one should be careful when comparing the learning curves (which can be found in Appendix J), with respect to efficiency or stability, as the hyperparameters have only been chosen based on the final ELBO of each run. We used this simple and hard criterion for selecting the hyperparameters, to make the experimental study more transparent and objective by removing human influence.

Human influence, of course, could not be completely avoided: For our main experiment, we only allowed for a coarse hyperparameter search over carefully chosen parameters. In contrast to the first two groups of experiments, where we used extensive Bayesian optimization to identify the best performance that we can expect for each design choice, in the main experiment we took into account that the computational budget for hyperparameter search (also ours) is limited. As a consequence, the results of our main experiment, are to some extend affected by our ability to propose good hyperparameter ranges for the different design choices. However, we had good prior knowledge about suitable parameter ranges based on the previous groups of experiments and also based on the parameters reported by prior work, and furthermore the results of our main experiment are consistent with the performances we observed in the previous experiments (which used much less subjective Bayesian optimization), and, hence, we conclude that the effect of the human factor is rather small. To increase the transparency of our empirical study we release a separate reproducibility package, which contains scripts for running each experiment, thereby documenting the exact conditions under which all our experiments have been started (including hyperparameter search).

B Potential for Negative Societal Impact

Machine learning methods can have a significant impact on our daily lives. They can have a positive impact on society by taking work off our hands, addressing challenges like the climate crisis, or helping to develop better medical treatments. But they can also have a negative impact on society by reinforcing prejudices, discriminating against people, invading our privacy, wasting enormous amounts of energy, or exacerbating the imbalance of power and wealth. They can cause serious harm if we overestimate their capabilities, and they can be used maliciously, for example, to falsify data or carry out cyberattacks.

In terms of negative impact, this work is unlikely to contribute significantly to energy waste because we focus on structured representations with few parameters that can be learned efficiently. Furthermore, our work does not focus on processing or forgery of images, text, or speech, so it is unlikely to have a significant negative impact on society due to privacy violations or misinformation. We are confident that we can use

our findings to help people in their daily lives and have a net positive impact on society, although we of course can not foresee how our findings will be used by future work.

C Related Work

In addition to the aforementioned methods, several other methods have explored natural gradients and trust regions for variational inference. For mean-field approximations, Hoffman et al. (2013) propose an efficient method for estimating the natural gradient from mini-batches, and Theis and Hoffman (2015) proposed a related KL-constrained trust-region method. Regier et al. (2017) proposed a second-order method for Gaussian variational inference based on Euclidean trust regions. Khan et al. (2015) introduced a KL-based proximal point method for conjugate models and related it to natural gradient descent. For non-conjugate models, they proposed local linearizations. Khan et al. (2016) extended this approach to other divergences and stochastic gradients. Salimbeni et al. (2018) compute the natural gradient based on the Jacobian of the parameters of the Gaussian and its expectation parameters. The Jacobian can be computed using forward-mode differentiation, or by using reverse-mode differentiation twice. For GMM-based variational inference, Miller et al. (2017) and Guo et al. (2016) proposed boosting methods, which, however, can require unreasonably large mixture models, because components that have been added at previous iterations do not longer receive updates. Recently, Lin et al. (2021) investigated natural gradient GMM-based variational inference with a structured covariance matrix, which may be important for scaling these methods to higher dimensions.

D Equivalence of the Weight Updates

We will now compare the weight update used by Lin et al. (2019a; 2020), with the weight updated used by Arenz et al. (2018; 2020), and show their equivalence.

D.1 Weight Update of Lin et al. (2019a; 2020)

Lin et al. (2020) formulate the weight update in the natural parameter space,

$$\boldsymbol{\omega} = \boldsymbol{\omega}_{\text{old}} + \beta \boldsymbol{\delta} \tag{12}$$

where each dimension $\boldsymbol{\delta}_o$ of the natural gradient is given by

$$\begin{aligned}\boldsymbol{\delta}_o =& \mathbb{E}_q(\mathbf{x}|o) \left[\log \tilde{p}(\mathbf{x}) - \log q_{\boldsymbol{\theta}}(\mathbf{x})\right] \\ & - \mathbb{E}_q(\mathbf{x}|K) \left[\log \tilde{p}(\mathbf{x}) - \log q_{\boldsymbol{\theta}}(\mathbf{x})\right].\end{aligned}$$

Defining

$$\hat{R}(o) = \mathbb{E}_q(\mathbf{x}|o) \left[\log \tilde{p}(\mathbf{x}) - \log q_{\boldsymbol{\theta}}(\mathbf{x})\right],$$

the i-th index of the natural parameters is given by

$$\boldsymbol{\omega}_i = \boldsymbol{\omega}_{\text{old},i} + \beta \hat{R}(o) - \beta \hat{R}(K).$$

The new weight of component $o < K$ is given by

$$\begin{aligned}q(o;\boldsymbol{\omega}) =& \frac{\exp\left(\boldsymbol{\omega}_o\right)}{\left[\sum_{k=1}^{K-1} \exp \boldsymbol{\omega}_k\right] + 1} = \frac{\exp\left(\boldsymbol{\omega}_{\text{old},o} + \beta \hat{R}(o) - \beta \hat{R}(K)\right)}{\left[\sum_{k=1}^{K-1} \exp\left(\boldsymbol{\omega}_{\text{old},k} + \beta \hat{R}(k) - \beta \hat{R}(K)\right)\right] + 1} \\ =& \frac{\frac{q(o)_{\text{old}}}{q(K)_{\text{old}}} \exp\left(\beta \hat{R}(o)\right)}{\left[\sum_{k=1}^{K-1} \frac{q(k)_{\text{old}}}{q(K)_{\text{old}}} \exp\left(\beta \hat{R}(k)\right)\right] + \exp \beta \hat{R}(K)} = \frac{q(o)_{\text{old}} \exp\left(\beta \hat{R}(o)\right)}{\left[\sum_{k=1}^{K-1} q(k)_{\text{old}} \exp\left(\beta \hat{R}(k)\right)\right] + q(K)_{\text{old}} \exp\left(\beta \hat{R}(K)\right)}.\end{aligned}$$

Implementation	BreastCancer	GermanCredit	GMM20	PlanarRobot4
VIPS/ZAMTRUX (theirs)	78.20 ± 0.04	585.10 ± 0.00	0.01 ± 0.00	12.02 ± 0.13
VIPS/ZAMTRUX (ours)	$\mathbf{78.14 \pm 0.01}$	585.10 ± 0.00	$\mathbf{-0.00 \pm 0.00}$	$\mathbf{11.48 \pm 0.04}$

Table 6: We compare the final (negated) ELBO achieved by both implementations. When using the same design choices as VIPS (Arenz et al., 2020), our implementation and hyperparameters led to better approximations on their target distributions.

Hence, for all components (including K), we have

$$q(o) \propto q(o)_{\text{old}} \exp\Big(\beta \hat{R}(o)\Big). \tag{13}$$

D.2 Weight Update (VIPS)

We start be expressing the component's reward $R(o)$ in terms of $\hat{R}(o)$, namely,

$$\begin{aligned} R(o) &= \mathbb{E}_{q_{\boldsymbol{\theta}}(\mathbf{x}|o)}\Big[\log \tilde{p}(\mathbf{x}) + \log \tilde{q}(o|\mathbf{x})\Big] + \mathrm{H}(q(\mathbf{x}|o)) \\ &= \mathbb{E}_{q_{\boldsymbol{\theta}}(\mathbf{x}|o)}\Big[\log \tilde{p}(\mathbf{x}) + \log q(o|\mathbf{x}) - \log q(\mathbf{x}|o)\Big] \\ &= \mathbb{E}_{q_{\boldsymbol{\theta}}(\mathbf{x}|o)}\Big[\log \tilde{p}(\mathbf{x}) + \log q(o) - \log q(x)\Big] = \hat{R}(o) + \log q(o), \end{aligned}$$

where we exploited that the auxiliary distribution is chosen according to the true responsibilities, $\tilde{q}(o|x) = q(o|x)$.

Expressing the weight update of VIPS (Arenz et al., 2018, Eq.8) in terms of $\hat{R}(o)$,

$$\begin{aligned} q(o) \propto \Big[& q_{\text{old}}(o)^{\frac{\eta_w}{1+\eta_w}} \exp\left(R(o)\right)^{\frac{1}{1+\eta_w}} \\ &= q_{\text{old}}(o)^{\frac{\eta_w}{1+\eta_w}} \exp\Big(\hat{R}(o) + \log q_{\text{old}}(o)\Big)^{\frac{1}{1+\eta_w}} \\ &= q_{\text{old}}(o) \exp\left(\frac{1}{1+\eta_w}\hat{R}(o)\right)\Big], \end{aligned}$$

we can see that it exactly matches the update in Equation 13 for $\beta = \frac{1}{1+\eta_w}$. □

E Comparisons with Reference Implementations

The target distributions *BreastCancer*, *GermanCredit*, *GMM20* and *PlanarRobot4* were taken from VIPS (Arenz et al., 2020). The design choices of VIPS correspond to the codename ZAMTRUX in our implementation. Table 6 compares the final (negated) ELBO that we achieved in our main experiments (cf. Table 5) with the performance of VIPS reported by Arenz et al. (2020), that was obtained using their (C++) implementation. For all environments that have been tested in both works, the final ELBO performances published in this work are better than the results published in the original work, except for *GermanCredit* were, we could not measure any difference between both implementations.

We also compared our implementation with the Matlab implementation of Lin et al. (2020) on the target distributions that we took from their work (*STM20* and *STM300*). However, our problem setting slightly differs from the original setting, as Lin et al. (2020) use an expensive Hessian-based pre-training for initializing the GMM and compare the methods only with respect to their fine-tuning performance. We found that such pre-training is in general not necessary with our implementation and directly use the respective algorithms starting from the original initialization of Lin et al. (2020). Figure 1, which compares the learned model and the target distributions based on the marginals on the *STM20* experiment, demonstrates that even without pre-training, we can learn higher-quality approximations with our implementation (cf. Lin et al., 2020, Fig.3). Here, we used the SAMTRON design choices, which performed best in our experiments.

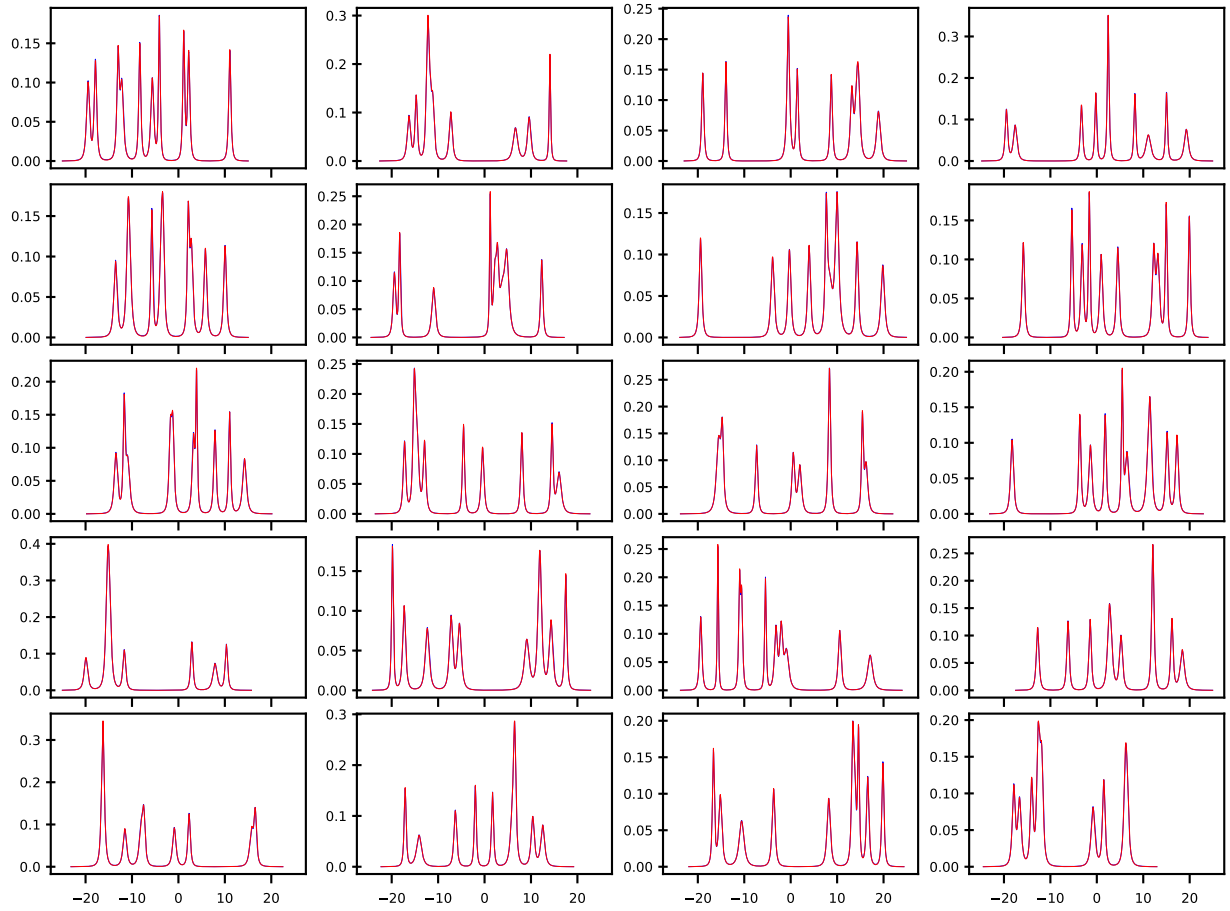
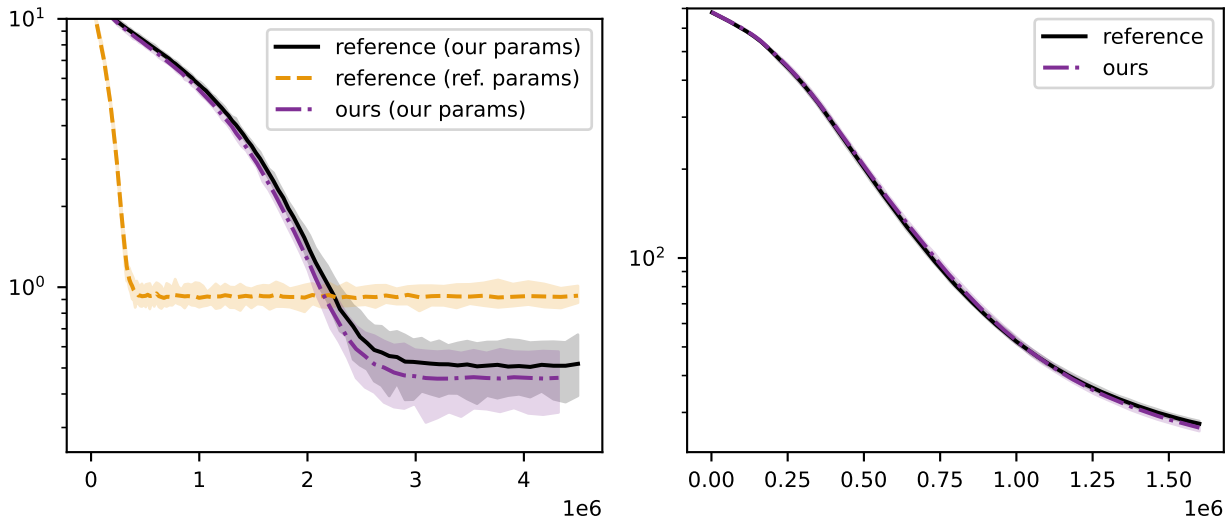


Figure 1: A representative plot of the 20 marginal distributions of the GMM learned with SAMTRON for the *STM20* experiment is shown in red. The marginals of the Mixture of Student-T target distribution are shown in blue and hardly distinguishable.

We ran the STM20 experiments on the reference implementation (with disabled pre-training) using our hyperparameters, and using the hyperparameters of Lin et al. (2020) and compare the learning curves with our SEPYFUX evaluation in Figure 2a. Our hyperparameters achieve better final ELBO even on the original implementation. Using the same hyperparameters, the learning curves of both implementations do not differ significantly, but our implementation performed slightly better. The *STM300* experiment was not evaluated by Lin et al. (2020) in the first-order setting, but only when using Hessian information (using Eq. 8 left), which is often computationally prohibitive. Hence, we can only compare both implementations using our hyperparameters. The respective learning curves are shown in Figure 2b and very similar for both implementations.

F Hyperparameters

We list the hyperparameters for each design choice in Table 7. Please refer to Appendix G for a description of the different hyperparameters. The tested and eventually chosen hyperparameters for each experiment can be found in the reproducibility package; please refer to its `README.rst` file for links to all relevant config files.



(a) STM20 (b) STM300

Figure 2: The learning curves plot the ELBO (in logarithmic scale) over the number of samples for our implementation and the reference implementation, where both use the SEPYFUX design choices. On *STM20* our hyperparameters lead to a better approximation than the hyperparameters used by Lin et al. (2020), and when using the same hyperparameters, our implementation performs slightly better. On *STM300* both implementations perform similarly using our hyperparameters. Reference hyperparameters are not available for *STM300*.

Module	Design Choice	Hyperparameters			
Component Adaptation	Fixed Adaptive	- adding iter.	- deletion iter.	- # prior samples	- # DB samples
Component Stepsize Adaptation	Fixed Decaying Adaptive	initial_stepsize initial stepsize initial stepsize	- annealing exponent min stepsize	- - max stepsize	- - -
NgBased Component Updater	Direct iBLR Trust-Region	- - -	- - -	- - -	- - -
NgEstimator	Stein MORE	self-normalized IW self-normalized IW	use own samples use own samples	- ℓ_2-coefficient	- -
Sample Selector	Comp.-Based Mixture-Based	desired samples desired samples	reused samples reused samples	- -	- -
Weight Stepsize Adaptation	Fixed Decaying Adaptive	initial_stepsize initial stepsize initial stepsize	- annealing exponent min stepsize	- - max stepsize	- - -
Weight Updater	Direct Trust-Region	self-normalized IW self-normalized IW	- -	- -	- -

Table 7: The table lists each hyperparameter that was tuned at any of the experiments.

G Notes On Our Implementations

We implemented two different options for estimating the natural gradients for the component update in two separate classes. The *MoreNgEstimator* uses weighted least squares to estimate the natural gradient as discussed in Section 3.1.1; the *SteinNgEstimator* makes use of gradient information, using Stein's Lemma to estimate the natural gradient as discussed in Section 3.1.2. For both options, a boolean hyperparameter is available to select whether self-normalized importance weighting, or standard importance weighting should be used to make use of samples from different distributions. Furthermore, a boolean hyperparameter can be used to disable importance sampling, only using samples from the respective component during the component update, which we enabled for all methods on *WINE* to reduce memory footprint. When using MORE, an additional hyperparameter can be used to select the initial ℓ_2-regularization for linear least-squares; the regularizer is automatically adapted as described by Arenz et al. (2020).

We implemented three options for performing the natural gradient update of the components based on the estimated natural gradients and given stepsizes (or trust regions). The *DirectNgBasedComponentUpdater* directly applies the natural gradient update given by Equation 6. If an updated component is no longer positive definite, the update is undone, hoping that the update would succeed in the next iteration (potentially with a smaller stepsize). The *NgBasedComponentUpdaterIblr* updates the components according to the improved Bayesian learning rule (Eq. 10). We noticed that the update may still result in non-invertible covariance matrices (albeit much less frequently compared to the natural gradient update) due to numerical errors, in which case we also undo the respective updates. The *KLConstrainedNgBasedComponentUpdater* solves an optimization problem to find stepsizes that result in positive definite covariance matrices and updated distributions that respect the desired bound on the KL divergence, as discussed in Section 3.2.2. For solving the convex optimization problem, Arenz et al. (2018) used an L-BFGS-B (Byrd et al., 1995) optimizer. However, it was difficult to efficiently integrate such optimizer into our Tensorflow (Abadi et al., 2015) implementation, and furthermore, the optimizer would sometimes fail for numerical reasons. Instead, we implemented a simple bracketing search, by iteratively refining an initially sufficiently large bracket on $\log \beta_o$ by evaluating the center of the bracket and using it as new upper value when the corresponding KL divergence is too small or the covariance matrix not positive definite, or, otherwise, as new lower value. Although naive, this approach is numerically robust by not requiring the gradient of the KL divergence, converges due to the convexity of the problem and can be efficiently compiled into a compute graph.

For the *SampleSelector* module, we implemented two options. Both options can make use of samples from previous iterations (as discussed by Arenz et al. (2020)), by setting the hyperparameter n_{reused} larger than zero. The *LinSampleSelector* computes the effective sample size n_{eff} on the GMM and draws $\max(0, N \cdot n_{\text{des}} - n_{\text{eff}})$ new samples from the GMM. For $n_{\text{reused}} = 0$ this approach corresponds to the procedure used by iBayes-GMM (Lin et al., 2020). The *VipsSampleSelector* computes $n_{\text{eff}}(o)$ for each component and draws $\max(0, n_{\text{des}} - n_{\text{eff}}(o))$ new samples from each component, matching the procedure used by VIPS (Arenz et al., 2020).

We implemented two options for performing the weight update. The *DirectWeightUpdater* directly updates the categorical distribution using Eq. 11, whereas the *TrustRegionBasedWeightUpdater* uses our bracketing search to stay within a given trust region. Whether standard importance sampling or self-normalized importance sampling should be used for estimating the component rewards $R(o)$ can be chosen with a hyperparameter, that is available for both options and can be chosen independently to the respective hyperparameter of the *NgEstimator*.

For stepsize adaptation, we implemented three options for both, the *ComponentStepsizeAdaptation* module and the *WeightStepsizeAdaptation* module. The *FixedComponentStepsizeAdaptation* and *FixedWeightStepsizeAdaptation* simply return a fixed stepsize, chosen as a hyperparameter. The *DecayingComponentStepsizeAdaptation* and *DecayingWeightStepsizeAdaptation* return an exponentially decaying stepsize based on the number of times the respective distribution has been updated, as described by Khan et al. (2018). The *ImprovementBasedComponentStepsizeAdaptation* and *ImprovementBasedWeightStepsizeAdaptation* increase the stepsize if the last update of the respective distribution improved its reward, and decrease it otherwise, as proposed by Arenz et al. (2020).

For the *ComponentAdaptation* module, we implemented two options. The *FixedComponentAdaptation* does nothing, keeping the number of components fixed throughout optimization; the *VipsComponentAdaptation* uses the procedure of VIPS (Arenz et al., 2020) to delete bad components, and to add new components in promising regions. Arenz et al. (2020) only considered samples from the sample database for initializing the mean of the new component, however, we had to disable the sample database for the high-dimensional problems *STM300* and *WINE* to reduce memory footprint. Hence, we introduced an additional hyperparameter to specify additional samples from the prior distribution (the same distribution that was used for drawing the means of the initial GMM), that should be drawn specifically for *ComponentAdaptation*.

H Test Problems

We performed several experiments on target distributions taken from related work. For additional details, please refer to the corresponding work. The *BreastCancer*, *GermanCredit*, *PlanarRobot* and *GMM* experiments were used by Arenz et al. (2020) and the Student-T experiments were used by Lin et al. (2020). For the most detailed (and fully accurate) specification of all target distributions, please refer to our code supplements.

- In the *BreastCancer* and *GermanCredit* experiments, we aim to approximate the posterior distribution of a logistic regression problem. The dimensions are 25 and 31, respectively. The data sets can be obtained from the UCI Machine Learning Repository (Lichman, 2013) and contain 1000 and 569 data points. Mimicking the setup of Arenz et al. (2020), the ELBO is computed on the full data set during training and evaluation. For the minibatch variants *GermanCreditMB* and *BreastCancerMB* we also use batches from the full data set, such that the respective ELBOs are comparable with the original experiments. However, we report the full-batch ELBOs to remove unnecessary noise in the evaluation.
- In the *WINE* experiment we want to approximate the posterior distribution over the weights of a neural network that predics the scalar wine quality based on eleven features using the WINE data set Lichman (2013). The network has two hidden layers of width 8, resulting in 177 parameters. The likelihood is given by the root mean squared error over a minibatch of size 128. We split the data set into a training and test set, and make sure that the training and test sets are deterministic given the seed. As we are primarily interested in the ability of the different methods to approximate a given target distribution (rather than testing how the approximations perform on the downstream task), we report the training set ELBOs. However, Table 8 reports as secondary metric the mean squared error of the prediction using approximate Bayesian inference on the test set.
- In the planar robot experiment, we aim to sample joint configurations of a 10-link *planar robot* (all links have the same length) and aim to reach one of four goal positions. The target distribution is Gaussian in the endeffector configuration space (but non-Gaussian in the joint configuration space). A zero-mean Gaussian prior on the joint angles is additionally used to prevent non-smooth configuration.
- In the *GMM* experiment we aim to approximate an unknown Gaussian mixture model with 10 components and a varying number of dimensions. Arenz et al. (2020) only considered 60 dimensions, but we increased the dimensionality to up to 100. The mean is sampled uniformly in the range $[-50, 50]$ and the covariance matrices $\mathbf{\Sigma} = \mathbf{A}^\top \mathbf{A} + I$ are created by randomly sampling the elements of the square matrix $\mathbf{A}$.
- The mixture of Student-T experiment (*STM*) is similar to the *GMM* experiment but uses Student-T components instead of Gaussians. We exactly follow Lin et al. (2020) by considering a 20-dimensional mixture with 10 components with mean uniformly sampled in $[-20, 20]$, and a 300-dimensional mixture with 20 components sampled in $[-25, 25]$. We follow Lin et al. (2020) by initializing the components of the GMM by sampling the mean from a zero-mean Gaussian distribution with diagonal covariance with standard deviation 100, and by initializing the diagonal covariance matrices with $\mathbf{\Sigma}_{\text{init}} = 300\mathbf{I}$. However, instead of pre-training with a second-order method, we directly start training from the initial GMM.

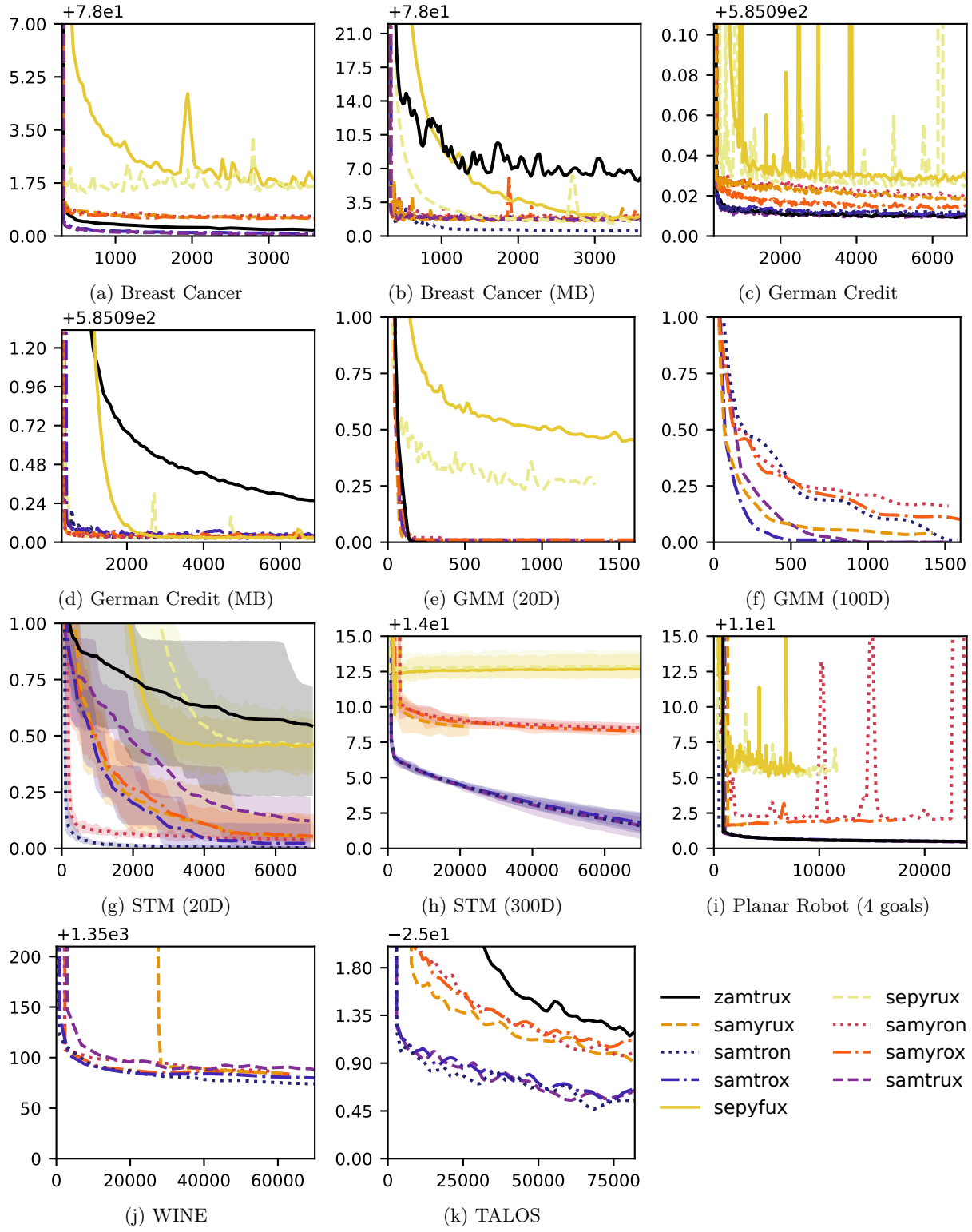
- The *TALOS* experiment is based on the implementation by Pignat et al. (2020). The poses of both feet, as well as the positions of the left end-effector and the center-of-mass are computed for the given joint positions based on a kinematic model of the robot. The target positions of the feet are given by $[-0.02, 0.09, -0.]$ and $[-0.02, -0.09, -0.]$ and their target orientation are given by identity rotation matrices $\mathbf{R} = \mathbf{I}_3$. The likelihood for each foot, is given by a 12-dimensional Gaussian distribution that penalizes deviations from these goal-parameters using a standard deviation of 0.2 for the Cartesian positions and a standard deviation of 0.1 for each entry of the rotation matrix. The likelihood of the left endeffector position is given by a Gaussian with mean $[0.1, 0.5, 1.]$ and diagonal standard deviations of 0.02. Violations of the inequality constraints that the joint angles should be within their limits, and the center-of-mass within the convex polygon spanned by the feet are penalized using the log-density of a Gaussian distribution placed on the violated bound (Pignat et al., 2020) using a standard deviation of 0.01 for the center-of-mass and 0.05 for the joint limits.

I Full Table for Experiment 3

The complete table for Experiment 3, showing all tested candidates, can be found in Table 8

J Learning Curves

The learning curves (ELBO over time) for our main experiments are shown in Figure 3.



(a) Breast Cancer (b) Breast Cancer (MB) (c) German Credit

(d) German Credit (MB) (e) GMM (20D) (f) GMM (100D)

(g) STM (20D) (h) STM (300D) (i) Planar Robot (4 goals)

(j) WINE (k) TALOS

Figure 3: The learning curves for our main experiment (Experiment 3) show the negated ELBO over time (in seconds). Shaded areas show best and worst performance. Note that hyperparameters were selected with respect to final ELBO.

Experiment	Metric	SAMTRUX	SAMTROX	SAMTRON	SAMYRUX	SAMYROX	SAMYRON	SEPYFUX	SEPYRUX	ZAMTRUX
BreastCancer	-ELBO	**78.01 ±0.02**	78.05 ±0.02	**78.00 ±0.02**	78.57 ±0.07	78.63 ±0.07	78.61 ±0.05	79.78 ±0.40	79.91 ±0.93	78.14 ±0.01
	MMD	**1.1e − 3 ±1e − 4**	**1.1e − 3 ±1e − 4**	**9.9e − 4 ±8e − 5**	1.2e − 3 ±1e − 4	**1.1e − 3 ±2e − 4**	1.3e − 3 ±1e − 4	2.3e − 3 ±3e − 4	2.8e − 3 ±3e − 4	**1.1e − 3 ±1e − 4**
BreastCancer (minibatches)	-ELBO	79.66 ±0.32	79.71 ±0.43	**78.41 ±0.03**	79.68 ±0.19	79.94 ±0.23	79.96 ±0.26	80.13 ±0.69	79.38 ±0.25	83.65 ±0.97
	MMD	**2.9e − 3 ±1e − 3**	**2.6e − 3 ±8e − 4**	**1.7e − 3 ±2e − 4**	**2.2e − 3 ±8e − 4**	2.8e − 3 ±9e − 4	2.9e − 3 ±8e − 4	2.5e − 3 ±4e − 4	**1.9e − 3 ±2e − 4**	8.3e − 3 ±2e − 3
GermanCredit	-ELBO	**585.10 ±0.00**	**585.10 ±0.00**	**585.10 ±0.00**	585.11 ±0.00	585.10 ±0.00	585.11 ±0.01	585.12 ±0.01	585.11 ±0.01	**585.10 ±0.00**
	MMD	**5.5e − 4 ±4e − 5**	**5.9e − 4 ±6e − 5**	**5.5e − 4 ±5e − 5**	**5.7e − 4 ±3e − 5**	**5.5e − 4 ±4e − 5**	**5.7e − 4 ±3e − 5**	**5.6e − 4 ±5e − 5**	**5.6e − 4 ±5e − 5**	**6.0e − 4 ±7e − 5**
GermanCredit (minibatches)	-ELBO	**585.12 ±0.01**	585.13 ±0.01	**585.12 ±0.00**	585.13 ±0.00	585.13 ±0.01	**585.12 ±0.00**	**585.12 ±0.00**	**585.12 ±0.00**	585.35 ±0.03
	MMD	**6.5e − 4 ±1e − 4**	8.1e − 4 ±2e − 4	**5.9e − 4 ±4e − 5**	**6.0e − 4 ±5e − 5**	**6.2e − 4 ±7e − 5**	**5.4e − 4 ±5e − 5**	**5.8e − 4 ±1e − 4**	**5.7e − 4 ±6e − 5**	1.9e − 3 ±6e − 4
Planar Robot	-ELBO	**11.47 ±0.05**	**11.47 ±0.04**	**11.47 ±0.04**	13.16 ±0.20	12.98 ±0.09	12.93 ±0.13	17.26 ±2.13	16.35 ±0.65	**11.48 ±0.04**
	MMD	**1.6e − 2 ±8e − 4**	**1.6e − 2 ±2e − 3**	**1.6e − 2 ±1e − 3**	3.7e − 2 ±7e − 3	2.6e − 2 ±2e − 3	2.4e − 2 ±2e − 3	4.5e − 1 ±6e − 2	4.4e − 1 ±7e − 2	**1.6e − 2 ±9e − 4**
GMM20	-ELBO	**−0.00 ±0.00**	**0.00 ±0.00**	**−0.00 ±0.00**	**0.00 ±0.00**	**0.01 ±0.03**	**0.00 ±0.00**	0.43 ±0.15	0.28 ±0.15	**−0.00 ±0.00**
	Modes	**10.00 ±0.00**	**10.00 ±0.00**	**10.00 ±0.00**	**10.00 ±0.00**	**9.90 ±0.28**	**10.00 ±0.00**	7.90 ±1.16	8.80 ±1.11	**10.00 ±0.00**
GMM100	-ELBO	**0.00 ±0.00**	**0.00 ±0.00**	**0.01 ±0.03**	0.05 ±0.03	0.09 ±0.07	0.16 ±0.09	4.54 ±0.52	0.96 ±0.36	1.21 ±0.15
	Modes	**10.00 ±0.00**	**10.00 ±0.00**	**9.90 ±0.28**	**10.00 ±0.00**	**9.70 ±0.43**	9.40 ±0.46	0.00 ±0.00	7.00 ±1.85	3.00 ±0.42
STM20	-ELBO	0.12 ±0.07	**0.02 ±0.04**	**0.00 ±0.00**	0.04 ±0.02	0.05 ±0.03	0.03 ±0.01	0.46 ±0.06	0.46 ±0.07	0.54 ±0.17
	Modes	8.90 ±0.66	**9.80 ±0.38**	**10.00 ±0.00**	**10.00 ±0.00**	**9.90 ±0.28**	**10.00 ±0.00**	**9.20 ±0.83**	9.20 ±0.71	6.10 ±0.99
STM300	-ELBO	**15.00 ±0.38**	**15.24 ±0.36**	**14.96 ±0.48**	22.41 ±0.23	22.28 ±0.13	22.50 ±0.15	26.69 ±0.39	26.87 ±0.45	N/A
	Modes	**13.70 ±1.80**	**14.10 ±1.50**	**14.30 ±1.53**	9.57 ±1.73	9.80 ±1.58	9.10 ±0.99	0.90 ±0.89	0.30 ±0.43	N/A
WINE	-ELBO	**1435.65 ±34.06**	**1429.02 ±30.93**	**1423.12 ±31.55**	**1432.72 ±30.49**	**1430.80 ±30.66**	**1433.87 ±30.49**	3279.32 ±1425.12	4100.92 ±1295.57	16 503.38 ±813.75
	MSE	**0.48 ±0.02**	**0.48 ±0.02**	**0.47 ±0.02**	**0.48 ±0.02**	**0.47 ±0.02**	**0.48 ±0.02**	0.67 ±0.14	0.76 ±0.17	0.80 ±0.13
TALOS	-ELBO	**−24.32 ±0.22**	**−24.30 ±0.10**	**−24.43 ±0.16**	**−24.13 ±0.14**	−23.91 ±0.13	−24.00 ±0.23	−16.64 ±5.26	−19.00 ±1.07	−23.69 ±0.16
	$H(q)$	**−16.81 ±0.07**	**−16.88 ±0.09**	**−16.82 ±0.07**	−17.26 ±0.10	−17.32 ±0.16	−17.25 ±0.16	−25.03 ±5.46	−22.34 ±1.11	**−16.91 ±0.07**

Table 8: The full table for our main experiment shows all tested candidates, as well as the secondary metrics.