Variational Variance: Simple and Reliable Noise Variance Parameterization

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Abstract

Models employing heteroscedastic Gaussian likelihoods parameterized by amortized mean and variance networks are both probabilistically interpretable and highly flexible, but unfortunately can be brittle to optimize. Maximizing log likelihood encourages local Dirac densities for sufficiently flexible mean and variance networks. Data lacking nearby neighbors can provide this flexibility. Gradients near these unbounded optima explode, prohibiting convergence of the mean and thus requiring high noise variance to explain the dependent variable. We propose posterior predictive checks to identify such failures, which we observe can surreptitiously occur alongside high model likelihoods. We find existing approaches that bolster optimization of mean and variance networks to improve likelihoods still exhibit poor predictive mean and variance calibrations. Our notably simpler solution, to treat heteroscedastic variance variationally in an Empirical Bayes regime, regularizes variance away from zero and stabilizes optimization, allowing us to preserve or outperform existing likelihoods while improving predictive mean and variance calibrations and thereby sample quality. We empirically demonstrate these findings on a variety of regression and variational autoencoding tasks.

1 Introduction

Deep learning coupled with ever improving computing power has revolutionized machine learning. Using neural networks to map conditioning variables onto the parameter space of dependent variables is now ubiquitous as it leverages the expressive power of deep learning and preserves probabilistic interpretability. While reliable uncertainty estimation has long been important to machine learning in the forms of *active learning* (Cohn et al., 1996) and *reinforcement learning* (Ghavamzadeh et al., 2016), improving predictive uncertainty estimation in deep learning has largely been an afterthought (Valdenegro-Toro, 2021) as state-of-the-art predictive mean and mode estimation wars rage on. Fortunately, the last few years have seen progress towards better predictive uncertainty estimation.

Bayesian uncertainty is comprised of *epistemic* (model) and *aleatoric* (data) uncertainties (Der Kiureghian & Ditlevsen, 2009; Kendall & Gal, 2017), both of which a model's predictive distribution ideally captures (Detlefsen et al., 2019). Sicking et al. (2021) broadly categorize predictive uncertainty estimation into Bayesian approximations (e.g. Monte Carlo dropout (Gal & Ghahramani, 2016; Kendall & Gal, 2017)), ensemble approaches (Lakshminarayanan et al., 2016), and parametric models that output heteroscedastic variance or covariance estimates (Nix & Weigend, 1994; Heskes et al., 1997). This article focuses on the latter: modeling conditional $Y|X = x$ as a heteroscedastic Gaussian $\mathcal{N}(Y|\mu(x), \sigma^2(x))$ parameterized by mean network $\mu(\cdot)$ and variance network $\sigma^2(\cdot)$. Optimizing $\mu(\cdot)$ and $\sigma^2(\cdot)$ simultaneously using maximum likelihood estimation (MLE), however, can be unstable (Takahashi et al., 2018). They identify the mean network's sensitivity to errors when the variance network approaches zero as the culprit. For sufficiently flexible networks, maximizing the local log likelihood simultaneously encourages $\mu(x_i) \to y_i$ and $\sigma^2(x_i) \to 0$. The fact that $\sigma^{-2}(x_i)$ appears as a multiplicative factor in the mean's gradient underlies why jointly optimizing $\mu(\cdot)$ and $\sigma^2(\cdot)$ can be brittle: minuscule errors by $\mu(x_i)$ produce inappropriately large parameter updates. In essence, the variance network increases the learning rate of the mean network as it improves, directly opposing stochastic gradient descent convergence criteria (Robbins & Monro, 1951).

We make several expansions to the study of Takahashi et al. (2018). First, we propose mean network flexibility predicates MLE optimization instability. If x_i has nearby neighbor x_j and the mean network is not sufficiently flexible to become arbitrarily close to both y_i and y_j simultaneously, then placing unbounded impulse densities on both $Y = y_i | X = x_i$ and $Y = y_j | X = x_j$ is no longer an option. Thus, data with meaningful neighbors in covariate and/or response spaces can eliminate local conditions for instability and allow the model to produce sensible local mean and variance estimates that capture underlying aleatoric uncertainty. Second, we suspect a model that attempts placing a Dirac density on $Y = y_i | X = x_i$ will experience exploding gradients that prohibit $\mu(x_i)$ from converging to y_i, thus forcing the model to use high variance. Together, these observations suggest that $\mu(x_i)$ failing to converge can hide behind high model likelihoods. Indeed, this problem should only occur for isolated (rare) data and can be explained away with noise variance, possibly worsening predictive mean and variance estimates for under represented groups (e.g. algorithmic fairness and racial bias). Lastly, we propose lacking stabilizing neighbors is severely exacerbated in higher dimensions. Increasing dimensionality even moderately (10-15) can make Euclidean distances between a point and its nearest and furthest neighbors indistinguishable (Beyer et al., 1999).

Our work makes several novel contributions towards improving optimization of heteroscedastic Gaussian likelihoods that use neural network parameter maps. First, we propose several posterior predictive checks (PPCs) (Gelman et al., 2013) to critique predictive mean and variance, allowing us to detect MLE optimization failures, which we indeed find alongside high model likelihoods. PPCs posit a well-fit model should, with high probability, produce new data that looks similar to the observed data since any discrepancy could be the result of model misfit or chance. A common PPC is to evaluate the log predictive likelihood on held-out test data. Alternatively, one can sample values from the predictive distribution and look for systematic discrepancies with the original data that may indicate model failure. Our second contribution is a previously unrecognized, attractively simple, and probabilistically principled solution to stabilize gradient-based optimization of heteroscedastic Gaussian densities. We treat heteroscedastic noise variance variationally and allow appropriately selected priors to counteract variance's tendency towards zero when mean errors are small. We advance this solution by adopting an Empirical Bayes perspective, allowing prior parameters to be optimized. Section 2 formalizes our variational treatment of noise variance and introduces our proposed priors, some of which are novel. Sections 3 and 4 respectively apply our proposals to regression and variational autoencoders (VAEs) (Kingma & Welling, 2013; Rezende et al., 2014). We emphasize our proposals are broadly applicable, yet, for regression and VAEs, we notably outperform methods specific to each context.

2 Variational Empirical Bayes for Noise Variance

We propose reparameterizing local heteroscedastic Gaussian likelihoods from $\mathcal{N}(Y_i|\mu(x_i), \sigma^2(x_i))$ to $\mathcal{N}(Y_i|\mu(x_i), \lambda_i)$ using local latent precision λ_i rather than variance for computational convenience. We then place a prior over local precisions and perform variational inference (VI) (Blei et al., 2017). In our setting, VI posits local variational family $q(\lambda_i|\alpha(x_i), \beta(x_i))$ to approximate the true posterior $p(\lambda|\mathcal{D}) \approx \prod_i q(\lambda_i|\alpha(x_i), \beta(x_i))$, where $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$. Using neural networks $\alpha(\cdot)$ and $\beta(\cdot)$ to parameterize a variational distribution is known as *amortized variational inference* (Kingma & Welling, 2013). Amortized VI minimizes the variational posterior's Kullback–Leibler (KL) divergence from the true posterior by maximizing the evidence lower bound (ELBO or $\mathcal{L}$ for short),

$$\sum_{i=1}^{N} \mathop{\mathbb{E}}_{q}\left[\log \mathcal{N}(Y_i = y_i|\mu(x_i), \lambda_i)\right] - D_{KL}\big(q(\lambda_i|\alpha(x_i), \beta(x_i)) \;||\; p(\lambda_i)\big). \tag{1}$$

The expected log likelihood evaluates analytically (supplement eq. (5)). The KL divergence in the ELBO provides a probabilistically principled way to regularize variance away from pathological zeros. Because precision is local, we maintain a 1:1 ratio of local log likelihoods to KL divergences. Thus, our proposed ELBO's stabilizing effect is independent of dataset size–the data cannot overwhelm the prior as it would for a global (homoscedastic) variance parameter. After optimization, we turn our attention to making predictions on some newly observed covariate $x_* \notin \mathcal{D}$, for which we define the *variational posterior predictive*

$$p(Y_*|X_* = x_*, \mathcal{D}) = \int \mathcal{N}(Y_*|\mu(x_*), \lambda) q(\lambda|\alpha(x_*), \beta(x_*)) d\lambda = \mathrm{T}(Y_*|\mu(x_*), \nu(x_*), \lambda(x_*)), \tag{2}$$

the expectation of the reparameterized likelihood w.r.t. our variational posterior. Integration analytically admits a Student's t with degrees-of-freedom $\nu(x_*) \equiv 2\alpha(x_*)$ and precision $\lambda(x_*) \equiv \frac{\alpha(x_*)}{\beta(x_*)}$. If the variational posterior reasonably approximates the true posterior, integration over λ accounts for epistemic uncertainty. Conditioning on $\mathcal{D}$ is absent in the integrand; it is implicit since the network parameters for $\mu(\cdot)$, $\alpha(\cdot)$, and $\beta(\cdot)$ were fit using $\mathcal{D}$. We therefore abbreviate the *variational posterior predictive* as $p(Y_*|X_*)$. In contrast to eq. (2), the predictive distribution resulting from MLE of the original parameterization is simply the likelihood evaluated at these new data $p(Y_*|X_* = x_*) = \mathcal{N}(Y_*|\mu(x_*), \sigma^2(x_*))$.

We consider the homoscedastic $p(\lambda_i)$ and heteroscedastic $p(\lambda_i|x_i)$ priors in table 1, but use $p(\lambda_i)$ to generally refer to both throughout this article (e.g. eq. (1)). Because of our chosen variational family, $q(\lambda|\alpha(x), \beta(x))$, our variational posterior predictive is always heteroscedastic. Thus, we really only care about which prior(s) offer optimal PPC performance. That said, having heteroscedasticity exist both in the generative process and in inference may be philosophically preferable.

Table 1: Precision priors. Amortized parameters are those of shared parameter maps. We use '(*)' to mark priors for which we tested Empirical Bayes. When '*' appears next to a prior's name, the Empirical Bayes parameters are optimized; when absent, we fix Empirical Bayes parameters a priori.

		Prior Parameters		
Name	Prior Form	Amortized	Empirical Bayes	Fixed
Gamma	$p(\lambda_i) = \Gamma(\lambda_i; a, b)$	None	None	$a, b \in \mathbb{R}_{>0}$
VAP	$p(\lambda_i|x_i) = q(\lambda_i|\alpha(x_i), \beta(x_i))$	$\alpha(\cdot), \beta(\cdot)$	None	None
VAMP(*)	$p(\lambda_i) = K^{-1}\sum_{j=1}^{K} q(\lambda_i|\alpha(u_j), \beta(u_j))$	$\alpha(\cdot), \beta(\cdot)$	$u_j \in \mathbb{R}^{\dim(X)}$	$K \in \mathbb{N}_+$
xVAMP(*)	$p(\lambda_i|x_i) = \sum_{j=1}^{K} \pi_j(x_i) q(\lambda_i|\alpha(u_j), \beta(u_j))$	$\alpha(\cdot), \beta(\cdot), \pi(\cdot)$	$u_j \in \mathbb{R}^{\dim(X)}$	$K \in \mathbb{N}_+$
VBEM(*)	$p(\lambda_i|x_i) = \sum_{j=1}^{K} \pi_j(x_i)\Gamma(\lambda_i|a_j, b_j)$	$\pi(\cdot)$	$a_j, b_j \in \mathbb{R}_{>0}$	$K \in \mathbb{N}_+$

We test the standard conjugate **Gamma** prior as a baseline, which can saturate in a single-sided (lower bounding variance) or double-sided (upper and lower bounding variance) manner depending on its parameters; this allows us to avoid optimization instabilities while also regularizing variance to pass our PPCs. The **Variational Posterior (VAP)** prior independently sets every local prior to its corresponding variational posterior such that the KL divergence penalty in eq. (1) vanishes. This 'prior' serves as an ablation test for the KL divergence's regularization effect. The Empirical Bayes **VAMP** prior (Tomczak & Welling, 2017) is the prior that maximizes the ELBO: the aggregate posterior $p^*(\lambda) = N^{-1}\sum_{j=1}^{N} q(\lambda|\alpha(x_j), \beta(x_j))$, taken over the N training points. For computational efficiency, Tomczak & Welling (2017) propose using $K < N$ randomly selected (without replacement) training points (pseudo-inputs) instead of all N. They denote the j'th pseudo-input as u_j and consider optimizing pseudo-inputs $\{u_1, \ldots, u_K\}$ as trainable parameters, which we denote as **VAMP***. It is worth noting both VAMP priors are homoscedastic. For heteroscedastic priors, we first consider a novel modification to the VAMP prior, **xVAMP**, which preserves heteroscedasticity by using $\pi(\cdot)$, a neural network that maps x_i onto the simplex to determine the mixture proportions. Intuitively, $\pi(x_i)$ should up weight the most relevant mixture component, whereas VAMP treats all weights uniformly. The KL divergence for xVAMP decomposes into

$$\mathop{\mathbb{E}}_{q(\lambda_i|x_i)}[\log q(\lambda_i|x_i)] - \mathop{\mathbb{E}}_{q(\lambda_i|x_i)}\left[\log \sum_{j=1}^{K} \pi_j(x_i) q(\lambda_i|u_j)\right], \tag{3}$$

where we evaluate the first term analytically as the Gamma distribution's negative entropy and Monte-Carlo (MC) estimate the second. We derive eq. (3) in our supplement. We too consider trainable pseudo-inputs for our xVAMP prior, which we denote as **xVAMP***. Our second heteroscedastic prior, **VBEM**, is a mixture of Gamma distributions where a trainable simplex mapping similarly determines the mixture proportions. VBEM stands for *Variational Bayes Expectation Maximization*, since optimizing the prior parameters during VI is analogous to performing M steps. VBEM's KL divergence replaces $q(\lambda|\alpha(u_j), \beta(u_j))$ with $p(\lambda|a_j, b_j)$ in eq. (3). The non-trainable set of scalar parameters $\{a_j, b_j\}_{j=1}^{K}$ is the Cartesian square of a set of scalars in

$[0.05, 4.0]$ (see supplement). **VBEM*** is the Empirical Bayes version, which randomly initializes parameters $\{\hat{a}_1, \hat{b}_1, \ldots, \hat{a}_K, \hat{b}_K\}$ from a Uniform($[-3, 3]$) and applies a softplus to ensure valid Gamma parameters (e.g. $a_j = \text{softplus}(\hat{a}_j)$). It is worth considering how variational variance might avoid zero while optimizing prior parameters: maximizing the ELBO's negative KL divergence (eq. (1)) involves maximizing the variational posterior's entropy thereby ensuring non-zero variances are integrated over in eq. (2).

3 Heteroscedastic Regression Experiments

Parameterizing local Gaussian likelihoods with amortized mean and variance networks (Nix & Weigend, 1994), $p(y_i|x_i) \triangleq \mathcal{N}(y_i|\mu(x_i), \sigma^2(x_i))$, leverages deep learning to model heteroscedasticity thereby quantifying predictive uncertainty. Regression assumes y_i and x_i are both observed and MLE simply maximizes the sum of local log likelihoods. However, we previously hypothesized that local optimization instabilities occurring for data lacking neighbors will produce poorly calibrated local predictive mean and variance estimates. We refer to this MLE baseline as the **Normal** model and depict its generative process in supplement fig. 3 (left) for which the predictive distribution is simply the likelihood since there are no priors (section 2). Note $\sigma^2(\cdot)$ applies a softplus to ensure positive variances and $\dim(y_i) = \dim(\sigma^2(x_i))$ (i.e. diagonal covariance).

Detlefsen et al. (2019) make four proposals to improve predictive variance estimates, which our supplement discusses in detail. We use **Detlefsen** to refer to their top method, which employs all four of their proposals and generally outperforms their chosen baselines: Gaussian process regression (Williams & Rasmussen, 2006; Snelson & Ghahramani, 2006; Damianou & Lawrence, 2013), unmodified neural-network parameterizations of mean and variance (Nix & Weigend, 1994; Bishop, 1994; Kingma & Welling, 2013; Rezende et al., 2014), Bayesian neural networks (MacKay, 1992; Hernández-Lobato & Adams, 2015), and MC Drop Out (Gal & Ghahramani, 2016). One proposal replaces the Normal likelihood with a Gamma-Normal parameterized Student's t, $\mathrm{T}(y_i|x_i) \equiv \int_0^\infty \mathcal{N}(y_i|\mu(x_i), \lambda_i)\,\mathrm{Gamma}(\lambda_i|\alpha(x_i), \beta(x_i))d\lambda_i$, which they MC integrate, inspiring us to implement our own **Student** baseline, where we analytically integrate precision as in eq. (2). Using local Student likelihoods without a prior (supplement fig. 3, middle) is MLE, for which the predictive distribution is simply the local likelihood. Our variational objective (eq. (1)) with a VAP prior lower bounds the log predictive likelihood of the Student's t regression via Jensen's inequality.

In contrast to Detlefsen et al. (2019), we propose a single, simple modification: treat precision variationally (supplement fig. 3, right) using the priors from table 1 and optimizing eq. (1). Variational variance in regression is not novel by itself. Menictas & Wand (2015) propose CAVI (coordinate ascent variational inference) to speed up inference over MCMC methods in a fully Bayesian treatment of heteroscedastic spline regression. CAVI employs closed-form updates that provably increase the ELBO monotonically (i.e. no optimization instabilities), rather than (stochastic) gradient steps. Thus, we feel well distinguished from Menictas & Wand (2015)–we are solving a separate problem with a different (arguably more general) type of variational inference. Employing amortized VI may seem superfluous, however, since the exact posterior, $p(\lambda|x, y)$, is available (see supplement). However, the resulting predictive distribution's variance lacks dependence on x_* rendering it homoscedastic. Thus, we forego posterior exactness for heteroscedasticity and the ability to probabilistically regularize variance. Amortized VI preserves the modeling capacity of the Student's t regression as it requires the same number of neural parameterizations and too yields a Student's t posterior predictive (eq. (2)).

3.1 Toy Data

We modify the toy data process of Detlefsen et al. (2019) to simulate heteroscedastic data with a rogue data point. We sample covariates $x_i \sim$Uniform$(0, 5)$ and add $x = 7.5$ as an isolated covariate. We then generate $y \triangleq x \cdot \sin(x) + \epsilon$ where $\epsilon|x \sim \mathcal{N}(0, [0.3 \cdot (1 + x)]^2)$. Detlefsen et al. (2019)'s log likelihood code had a bug that only affected this particular experiment. Fixing it significantly improves their predictive variance on $[0, 8]$ (bottom left subplot, fig. 1). Our methods mimic their remaining implementation details (see supplement). The predictive mean is well calibrated for all methods on the $[0, 5]$ interval where data is abundant (top two rows of subplots, fig. 1). As we hypothesized, the baseline Normal model is unable to converge on the isolated covariate at $x = 7.5$. The Student model also cannot converge here suggesting neurally parameterized MLE Student regression suffers similar complications. Detlefsen does well in this one-dimensional setting, likely

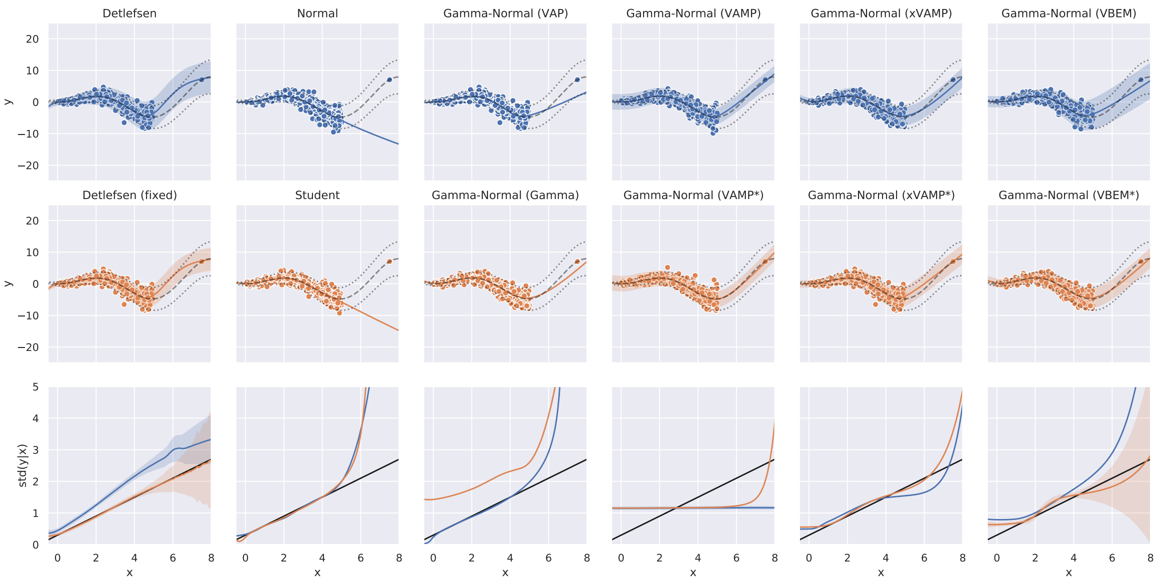

Figure 1: Toy regression results. Top two rows: dots are training data, black dashed/dotted lines and colored lines/areas are the true and predictive $\mathbb{E}[y|x] \pm 2 \cdot \sqrt{\text{var}(y|x)}$, respectively. Third row: the true (black) and average predictive (colors correspond to methods above) $\sqrt{\text{var}(y|x)}$ for 20 trials (area is one deviation).

because $x = 7.5$ still has meaningful nearby neighbors at $x \approx 5$, which they leverage in their proposals. The VAP model's inability to converge on $x = 7.5$ coupled with the fact that *all* our other priors enjoy convergence confirm the beneficial regulatory effect of our variational treatment of precision. The VAMP and VAMP* priors are poor at capturing heteroscedastic variance because $D_{KL}(q(\lambda|x)||K^{-1}\sum_{j=1}^{K} q(\lambda|u_j))$ is minimized when the variational distributions are uniform. Indeed, they predict homoscedasticity with a nearly constant standard deviation that is approximately equal to the expected value of the true standard deviation over the training interval. Our xVAMP(*) and VBEM(*) exhibit well calibrated predictive uncertainty across the test interval $[-0.5, 8]$.

3.2 UCI Data

We consider many of the same UCI datasets as Detlefsen et al. (2019). We independently normalize covariates and targets to zero mean and unit variance, but report metrics for the original target scalings. Remaining implementation specifics match Detlefsen et al. (2019) (see supplement). We perform PPCs on randomly held-out validation sets that each constitute 10% of the data across 20 trials. We report $|\mathcal{D}_{\text{test}}|^{-1} \sum_{(x_*, y_*) \in \mathcal{D}_{\text{test}}} \log p(Y_* = y_*|X_* = x_*)$, the average log predictive likelihood over validation data. Recall $p(Y_*|X_*)$ is a Student's t for all methods except the Normal model. The remaining PPCs require residuals for the predictive mean: $\mathbb{E}[y_*|x_*] - y_*$, variance: $\text{var}[y_*|x_*] - \big(\mathbb{E}[y_*|x_*] - y_*\big)^2$, and sampling: $\big(y_* \sim p(Y_*|X_* = x_*)\big) - y_*$. All expectations and variances are w.r.t. $p(Y_*|X_* = x_*)$, which has mean $\mu(x_*)$. The Normal model's predictive variance is $\sigma^2(x_*)$. For the remaining models, predictive variance is $\forall \alpha(x_*) > 1 : \frac{\beta(x_*)}{\alpha(x_*) - 1}$ (i.e. the expectation of an Inverse-Gamma), which is always available since we offset $\alpha(\cdot)$'s softplus output by 1. We emphasize this adjustment still allows variances arbitrarily close to zero and infinity. For the mean and sample residuals we compute root mean square error (RMSE). A mean network that always outputs zero (for centered data) trivially achieves zero mean and sampling bias. For variance, we compute bias to understand when predictive uncertainty is over/under estimated.

We jointly report log predictive likelihood and predictive variance bias in table 2. We include independent tables for each of our four proposed PPCs in our supplement alongside recent log likelihoods and mean RMSEs (Sun et al., 2019; Sicking et al., 2021), which we generally match. We tally the number of datasets for which a method was the top PPC performer or was statistically indistinguishable from the winner according

Table 2: UCI log predictive likelihood and predictive variance bias (mean±std.). Tuples appearing below dataset are $(N_{\text{observations}}, \dim(x), \dim(y))$. Winners are in bold, statistical ties are not.

Algorithm	Prior	boston (506, 13, 1)	carbon (10721, 5, 3)	concrete (1030, 8, 1)	energy (768, 8, 2)	naval (11934, 16, 2)
		Log Predictive Likelihood				
Detlefsen	N/A	-2.98±0.09	8.77±0.24	-3.66±0.08	-4.90±0.27	9.67±0.19
Normal	N/A	-2.42±0.23	13.20±1.35	-3.06±0.17	-0.48±0.69	14.15±0.17
Student	N/A	-2.37±0.19	**17.19±0.21**	-3.10±0.17	0.22±0.31	13.60±0.39
Gamma-Normal	VAP	-2.36±0.17	15.52±0.24	-3.12±0.17	0.17±0.44	13.36±0.41
	Gamma	-2.48±0.29	11.28±0.02	-3.20±0.16	-1.05±0.18	12.33±0.16
	VAMP	-2.39±0.17	14.37±0.17	-3.09±0.16	-0.18±0.21	14.16±0.78
	VAMP*	-2.39±0.16	14.38±0.12	-3.09±0.16	-0.16±0.20	13.96±0.88
	xVAMP	**-2.33±0.17**	15.38±0.24	-3.01±0.14	0.05±0.28	13.50±0.59
	xVAMP*	-2.33±0.17	15.41±0.18	-3.01±0.13	0.11±0.39	13.34±0.47
	VBEM	-2.46±0.11	4.57±1.00	-3.11±0.07	-4.52±0.26	9.02±0.61
	VBEM*	-2.36±0.14	14.64±0.16	**-2.99±0.13**	**0.49±0.28**	**14.42±0.15**
		Predictive Variance Bias				
Detlefsen	N/A	1.0e+02±79.11	9.8e-05±1.6e-04	2.2e+02±91.85	18.60±8.88	nan±nan
Normal	N/A	31.63±1.5e+02	3.5e+23±1.6e+24	-2.01±8.67	-0.16±0.24	3.1e-07±2.0e-06
Student	N/A	18.08±63.79	0.12±0.23	-2.20±9.28	24.00±85.42	4.9e-06±2.2e-05
Gamma-Normal	VAP	3.3e+02±1.3e+03	0.25±1.11	-2.13±7.85	0.04±0.31	3.1e-07±6.8e-07
	Gamma	3.18±20.09	1.5e-04±5.8e-05	0.76±11.35	0.31±0.40	3.7e-06±2.9e-06
	VAMP	-2.96±7.96	-6.6e-06±6.0e-05	-6.15±5.18	-0.15±0.39	1.7e-07±2.9e-07
	VAMP*	-3.00±7.84	**-6.0e-06±6.0e-05**	-6.16±5.18	-0.13±0.40	**1.3e-07±3.3e-07**
	xVAMP	0.65±16.20	2.7e-05±9.7e-05	-4.82±4.63	**6.0e-03±0.36**	3.1e-07±7.4e-07
	xVAMP*	0.51±20.17	5.0e-04±2.2e-03	-4.66±5.07	-8.5e-03±0.36	2.7e-07±6.3e-07
	VBEM	6.74±8.48	0.01±4.5e-03	25.86±8.94	22.06±5.58	3.6e-05±1.4e-05
	VBEM*	**-0.11±8.62**	-7.2e-06±6.1e-05	**-0.58±5.05**	0.02±0.28	3.9e-07±4.9e-07

Algorithm	Prior	power plant (9568, 4, 1)	superconductivity (21263, 81, 1)	wine-red (1599, 11, 1)	wine-white (4898, 11, 1)	yacht (308, 6, 1)
		Log Predictive Likelihood				
Detlefsen	N/A	-3.26±9.1e-03	-5.21±0.02	-1.04±0.06	-1.12±0.04	-3.15±0.10
Normal	N/A	-2.82±0.05	-3.51±0.10	-0.92±0.05	-1.05±0.04	-1.55±0.65
Student	N/A	**-2.78±0.03**	-3.41±0.05	**-0.80±0.10**	-1.05±0.04	-1.73±0.59
Gamma-Normal	VAP	-2.81±0.04	-3.45±0.06	-0.87±0.06	-1.04±0.04	-1.79±0.50
	Gamma	-2.88±0.03	-3.45±0.04	-0.98±0.07	-1.13±0.05	-1.73±0.38
	VAMP	-2.83±0.03	-3.94±0.02	-0.94±0.05	-1.05±0.04	-2.83±0.70
	VAMP*	-2.83±0.03	-3.94±0.03	-0.94±0.05	-1.05±0.04	-2.77±0.77
	xVAMP	-2.81±0.04	-3.40±0.04	-0.90±0.05	-1.03±0.04	-1.68±0.38
	xVAMP*	-2.81±0.04	**-3.39±0.05**	-0.89±0.06	-1.03±0.04	-1.71±0.47
	VBEM	-2.89±0.05	-3.77±0.09	-0.91±0.05	-1.03±0.03	-2.64±0.23
	VBEM*	-2.81±0.03	-3.41±0.04	-0.89±0.06	**-1.03±0.04**	**-1.11±0.57**
		Predictive Variance Bias				
Detlefsen	N/A	69.25±2.40	5.5e+04±6.2e+03	2.16±1.57	0.83±0.36	96.62±54.08
Normal	N/A	**0.05±1.53**	2.3e+13±1.0e+14	-3.8e-03±0.04	-0.02±0.06	20.68±54.95
Student	N/A	-0.27±1.47	1.6e+05±3.3e+05	12.52±30.71	-5.6e-03±0.05	1.7e+03±2.3e+03
Gamma-Normal	VAP	0.52±1.29	9.0e+05±2.6e+06	0.03±0.05	0.13±0.64	1.3e+03±1.5e+03
	Gamma	2.34±1.43	1.1e+02±81.21	0.04±0.11	**-2.3e-03±0.05**	**-7.28±40.88**
	VAMP	0.89±1.04	**-9.83±7.97**	0.05±0.06	-8.8e-03±0.04	38.05±83.39
	VAMP*	0.89±1.04	-9.89±7.98	0.05±0.06	-8.9e-03±0.04	38.07±83.29
	xVAMP	0.46±1.25	14.40±42.90	3.5e-03±0.05	-0.03±0.03	4.8e+02±1.7e+03
	xVAMP*	0.44±1.24	1.3e+02±4.7e+02	**2.1e-03±0.05**	-0.03±0.03	1.7e+02±1.5e+02
	VBEM	16.53±9.32	91.44±25.39	0.08±0.04	0.07±0.04	20.70±25.23
	VBEM*	1.86±1.44	9.87±16.22	0.05±0.06	0.01±0.04	26.48±26.88

to a two-sided Kolmogorov–Smirnov test with $p \leq 0.05$ (supplement table 4). VBEM* offers the best log predictive likelihood and is the overall top performer. Detlefsen has the lowest predictive likelihoods (table 2), even against our implementation of the Normal baseline. Their code did not support multivariate y–we modified it to do so and remain unsure how they generated their results for UCI data with multidimensional targets. Perhaps, they labeled covariates and targets differently and/or performed additional preprocessing (their code loads unprovided numpy files as its data source). For naval, rescaling their algorithm's MC-sampled variances to the original target scalings produces very small values that introduce NaNs when estimating the variance of their predictive Student via a mixture of Gaussians parameterized by these small variances. The Normal, Student, and VAP baselines exhibit severely biased and wildly varying predictive variance on about half the datasets compared to our other methods, reaffirming the benefit of our probabilistic regularization of variance. The Student baseline achieves top likelihood on both carbon and power plant, for which its predictive variance calibration ranges from horrendous to excellent; this paradox highlights the need for looking beyond just likelihood. The VAMP(*) and VBEM* *never* exhibit wildly varying predictive variance and generally produce top-performing estimates. xVAMP(*) exhibits poor variance calibration only on yacht. We repeat Detlefsen et al. (2019)'s active learning experiments (see supplement) and find VBEM* is most frequently the top performer for these same UCI datasets.

4 Variational Autoencoder Experiments

The VAE (Kingma & Welling, 2013; Rezende et al., 2014) is a deep latent variable model that provides computationally efficient VI for a generative process from a low-dimensional latent local Gaussian variable Z to high-dimensional data X. Any (decoder) distribution can be placed over X, but we specifically focus on Gaussian likelihoods $p(X|Z=z) \triangleq \mathcal{N}(X|\mu_x(z), \sigma_x^2(z))$. As is common, we use $p(Z) \triangleq \mathcal{N}(0, I)$ as the prior, posit $q(Z|X=x) \triangleq \mathcal{N}(Z|\mu_z(x), \sigma_z^2(x))$ as the variational family (encoding distribution), and perform black-box VI (Ranganath et al., 2014) with reparameterization gradients (Salimans et al., 2013; Figurnov et al., 2018) to maximize the ELBO,

$$\sum_{x \in \mathcal{D}} \mathop{\mathbb{E}}_{q(z|x)} \Big[\log \mathcal{N}(x|\mu_x(z), \sigma_x^2(z)) \Big] - D_{KL}\big(q(z|x) \mid\mid p(z)\big). \tag{4}$$

Encoder maps, $\mu_z(x)$ and $\sigma_z^2(x)$, are bifurcated outputs of the same neural network as is common practice. We explore decoder parameter maps $\mu_x(z)$ and $\sigma_x^2(z)$ as being either bifurcated outputs of the same neural network (**VAE**) or separate neural networks (**VAE-Split**). Additionally, we evaluate batch normalization's effect (**+ BN**). Softplus activations ensure positive variance.

Alemi et al. (2018) refer to $p(X_*) = \mathbb{E}_{\hat{p}(X)} \mathbb{E}_{q(Z|X)}[p(X_*|Z)]$ as the *empirical data reconstruction distribution*, where $\hat{p}(X)$ approximates the true data generating distribution by uniformly sampling from a sufficiently large dataset. Computing $p(X_*)$'s outer expectation for N data points and approximating the inner expectation with M Monte-Carlo samples requires evaluating MN mixture components. Conditioning just the inner expectation on a specific x yields what we call the *local reconstruction distribution*, $p(X_*|X=x) = \mathbb{E}_{q(Z|X=x)}[p(X_*|Z)]$, a more manageable M-component mixture. This distribution also implicitly conditions on $\mathcal{D}$, $p(X_*|X=x, \mathcal{D})$, since parameters maps for $p(X_*|Z)$ and $q(Z|X)$ were fit using $\mathcal{D}$. Calling $p(X_*|X=x)$ the *variational posterior predictive* distribution is a slight abuse of Bayesian lexicon, yet we do so to maintain harmony with our regression methods. For VAEs, there is a subtle distinction between the *expected log likelihood* $\mathbb{E}_{q(Z|X=x)}[\log p(X_*=x|Z)]$ from the variational objective and the *log reconstruction likelihood* $\log \mathbb{E}_{q(Z|X=x)}[p(X_*=x|Z)]$. The former lower bounds the latter via Jensen's inequality. Similarly, $\mathbb{E}_{x\sim\mathcal{D}}[-\log p(X_*=x|X=x)]$, average negative log reconstruction likelihood, upper bounds *distortion* $\mathbb{E}_{x\sim\mathcal{D}} \mathbb{E}_{q(Z|X=x)}[-\log p(X_*=x|Z)]$ (Alemi et al., 2018); thus minimizing the former minimizes the latter (i.e. reconstruction error).

VAE papers using Gaussian likelihoods that claim improvements to sample quality (van den Oord et al., 2017; Razavi et al., 2019) and imputation (Nazabal et al., 2018; Mattei & Frellsen, 2018b) *never* sample the predictive distribution despite sometimes fitting a global (homoscedastic) scalar noise variance to improve mean calibration (Dai & Wipf, 2019). These methods ancestrally resample latent variables from the variational posterior (or prior) and report the expected value of the decoder density. This procedure is actually a Monte-Carlo estimate of the reconstruction mean $\mathbb{E}[X_*|X=x]$ (or prior predictive mean $\mathbb{E}[X_*]$). Reporting the expectation as a sample obfuscates predictive uncertainty. More recently, Vahdat & Kautz (2020) employ per-pixel heteroscedastic scale parameters but with a discretized logistic mixture likelihood (Salimans et al., 2017) to achieve state-of-the-art VAE image sampling. Their code employs a clamp that prevents their scale parameter from approaching zero suggesting brittle optimization may still exist. Adapting our proposals to this alternative likelihood is compelling, but beyond the scope of this work.

Detlefsen et al. (2019) apply their regression proposals to VAEs. Takahashi et al. (2018) propose using a Student's t likelihood and demonstrate improved optimization stability and predictive likelihood. Their method, **VAE-Student**, has an ELBO similar to eq. (4) but with a Student's t likelihood $\mathrm{T}(X|\mu_x(z), \lambda_x(z), \nu_x(z))$ parameterized by three separate neural networks, $\mu_x(z)$, $\lambda_x(z)$ and $\nu_x(z)$ for mean, precision, and degrees-of-freedom, respectively. Since the Student's t variance is undefined for $\nu_x(z) \in (0, 1]$, infinite for $\nu_x(z) \in (1, 2]$, and arbitrarily close to ∞ for $\nu_x(z) \approx 2$, we restrict $\nu_x(z) > 3$ using a shifted softplus. We found that allowing the posterior predictive to attain these high variances worsens its PPC performance beyond what we report. Takahashi et al. (2018) also propose **MAP-VAE**, where precision is absorbed into the likelihood: $p(\lambda|z) \triangleq \text{Gamma}(\lambda_x(z); a, b)$ for pre-defined constants a and b. Our method, **V3AE** (variational variance VAE) treats precision variationally with $q(\lambda|z) \triangleq \text{Gamma}(\lambda|\alpha(z), \beta(z))$. We use the priors discussed in section 2, except we now condition on latent codes z_i. The resulting ELBO for V3AE,

$$\sum_{x \in \mathcal{D}} \mathop{\mathbb{E}}_{q(z|x)} \left[\mathop{\mathbb{E}}_{q(\lambda|z)} \Big[\log \mathcal{N}(x|\mu_x(z), \lambda) \Big] - D_{KL}\big(q(\lambda|\alpha(z), \beta(z)) \mid\mid p(\lambda)\big) \right] - D_{KL}\big(q(z|x) \mid\mid p(z)\big),$$

introduces a KL divergence that regularizes the predictive variance. This proposal with an appropriate prior addresses the theoretical preference of an optimal decoder for zero variance (Dai & Wipf, 2019) and the theoretical concern that continuous VAEs are ill-posed with unbounded likelihood functions (Mattei & Frellsen, 2018a). See supplement for additional details (e.g. network architectures).

We use local reconstruction distribution $p(X_*|X = x)$ as the posterior predictive distribution for our PPCs. For VAE (+ BN), VAE-Split (+ BN), and MAP-VAE, we Monte-Carlo estimate predictive $p(X_*|X = x) = \mathbb{E}_{q(z|x)}[\mathcal{N}(X_*|\mu_x(z), \sigma_x^2(z))]$ with 20 samples, which yields a uniform mixture of 20 Gaussians. Similarly, the predictive distribution of VAE-Student is a uniform mixture of 20 Student's t. Our V3AE has two variational distributions, $q(z|x)$ and $q(\lambda|z)$, such that $p(X_*|X = x) = \mathbb{E}_{q(z|x)q(\lambda|z)}[\mathcal{N}(X_*|\mu_x(z), \lambda)]$. We integrate V3AE's normal likelihood w.r.t. $q(\lambda|z)$ analytically, yielding a Student's t (as in eq. (2)). Thereafter, MC integration w.r.t. $q(z|x)$ yields a uniform mixture of 20 Student's t. As with regression, we consider the normalized log predictive likelihood, $\mathbb{E}_{x\sim\mathcal{D}_{\text{test}}}[\log p(X_* = x|X = x)]$, the RMSE of the predictive mean residuals $\mathbb{E}[X_*|x] - x$, the bias of predictive variance residuals $\text{var}[X_*|x] - (\mathbb{E}[X_*|x] - x)^2$, and the RMSE of predictive sampling errors $x_* - x$, where $x_* \sim p(X_*|X = x)$. Comparing ELBOs (including tighter importance weighted ELBOs (Burda et al., 2015)) across these methods is problematic. The marginal likelihood $p(x)$ is $\mathbb{E}_{p(z)}[\mathcal{N}(x|\mu_x(z), \sigma_x^2(z))]$ for VAE(-Split)(+BN), $\mathbb{E}_{p(z)}[\text{T}(x|\mu_x(z), \lambda_x(z), \nu_x(z))]$ for VAE-Student, and $\mathbb{E}_{p(z)p(\lambda)}[\mathcal{N}(x|\mu_x(z), \lambda)]$ for V3AE. Hence, each parameterizations has a different $p(x)$. Comparing lower bounds for different $p(x)$ is meaningless, unfortunately.

Table 3: VAE PPCs for Fashion MNIST (mean±std.)

Method	ELBO	LL	Mean RMSE	Var Bias	Sample RMSE
Fixed-Var. VAE (1.0)	-735.71±9.3e-02	-730.05±0.11	0.15±1.8e-03	0.98±5.7e-04	1.01±3.7e-04
Fixed-Var. VAE (0.001)	-1577.55±3.74	-1452.44±3.65	**9.4e-02±4.6e-05**	-7.8e-03±8.6e-06	**9.9e-02±4.7e-05**
VAE	1993.91±41.37	2154.31±42.11	0.25±1.4e-03	3.3e-02±1.5e-03	0.39±3.1e-03
VAE + BN	1557.71±17.49	1639.39±15.33	0.20±1.8e-03	2.1e-02±3.0e-03	0.31±5.6e-03
VAE-Split	1881.85±34.43	2099.28±39.97	0.27±2.9e-03	4.7e-02±1.6e-03	0.45±4.8e-03
VAE-Split + BN	1831.40±21.77	1948.30±25.87	0.26±6.2e-03	3.1e-02±3.6e-03	0.41±1.1e-02
Detlefsen (0.001)	-7219.37±55.49	-7214.05±55.55	0.15±4.7e-04	-2.1e-02±1.1e-03	0.16±4.1e-03
Detlefsen (0.25)	-218.91±0.99	-213.89±0.12	0.15±2.6e-04	0.23±7.9e-05	0.52±1.1e-04
Detlefsen (10.0)	-1630.04±1.12	-1623.98±5.1e-03	0.15±6.2e-04	9.98±2.5e-04	3.17±5.3e-04
MAP-VAE	-5631.89±71.86	1003.51±32.75	0.11±4.1e-03	-9.1e-03±6.2e-04	0.13±4.8e-03
Student-VAE	**2957.27±17.40**	**3134.52±18.60**	0.29±3.3e-03	7.4e-02±1.6e-02	0.49±2.2e-02
V3AE-VAP	1783.45±27.40	2146.46±67.83	0.28±3.5e-03	**9.9e-04±3.0e-03**	0.40±8.2e-03
V3AE-Gamma	-186.31±74.94	1201.95±25.25	0.11±2.8e-03	-8.0e-03±4.1e-04	0.12±3.4e-03
V3AE-VAMP	1390.37±13.47	1632.22±12.89	0.17±1.3e-03	1.5e-03±2.7e-04	0.25±2.4e-03
V3AE-VAMP*	1391.86±19.58	1630.10±17.87	0.18±2.6e-03	1.3e-03±2.5e-04	0.25±3.4e-03
V3AE-xVAMP	1372.45±16.77	1601.60±21.49	0.18±2.5e-03	1.3e-03±4.1e-04	0.25±3.8e-03
V3AE-xVAMP*	1388.48±26.46	1619.97±25.95	0.18±3.3e-03	1.5e-03±4.6e-04	0.25±5.0e-03
V3AE-VBEM	230.11±0.89	306.46±1.04	0.10±6.8e-04	6.4e-02±9.7e-05	0.29±3.3e-04
V3AE-VBEM*	869.41±2.56	1153.11±4.20	0.10±5.5e-04	**4.4e-04±3.9e-05**	0.15±8.0e-04

In fig. 2, we curate a subset of the VAE methods to qualitatively visualize our PPCs for MNIST and a downsampled Celeb-a. We include additional PPC visualizations for all methods in our supplement. Table 3 bolds top performers and statistical ties (using the same test from section 3.2) for all four of our PPCs on Fashion MNIST. We include tabular results for MNIST and Celeb-a in our supplement. We include baselines with a fixed global scalar variance to confirm variance impacts mean quality (Dai & Wipf, 2019).

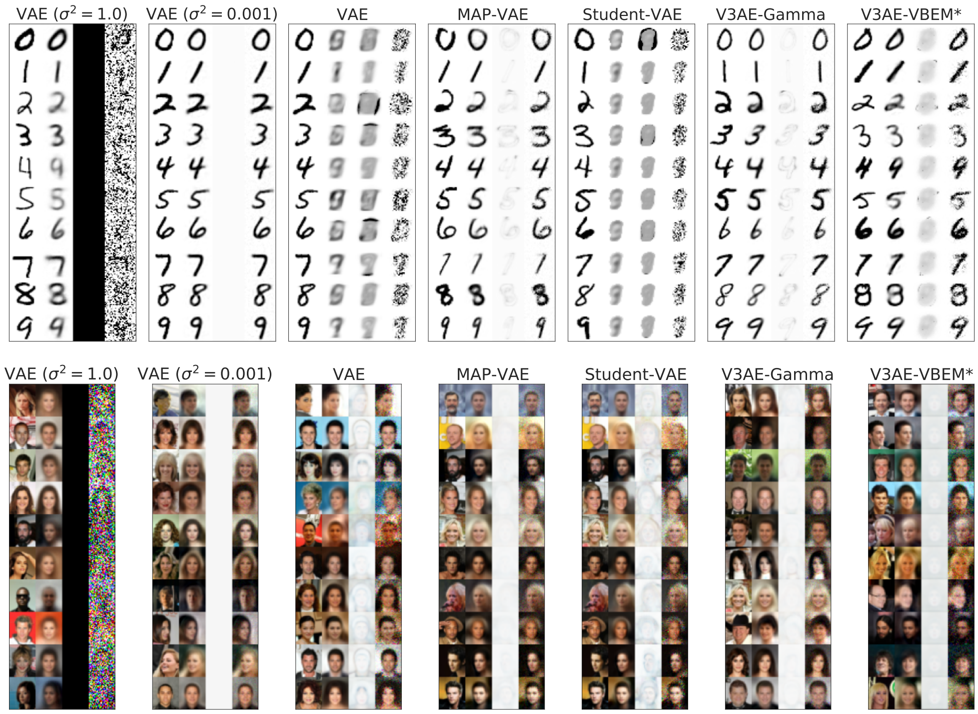

Figure 2: VAE PPCs for MNIST and downsampled Celeb-a: Columns of a subplot, left to right, are randomly selected test data followed by the predictive mean and variance and a sample from the predictive distribution. We clamp pixel values to $[0, 1]$ and invert RGB variances.

For MNIST and Fashion MNIST, the predictive mean estimates are better calibrated when fixing variance to 0.001 than to 1.0; this confirms the mean network has the flexibility to produce well-calibrated predictive mean estimates. However, we see no such difference for Celeb-a; this occurs since the predictive task has grown in complexity as we move from greyscale to RGB and consider non-homogeneous backgrounds. Here, the added data complexity prohibits the same-sized network from collapsing to Dirac densities and thus all methods produce similar quality predictive mean estimates that represent the flexibility limit of the network. Returning to the problematic MNIST and Fashion MNIST data, the Normal and Student models, like their regression counterparts, exhibit poor predictive mean and variance estimates, which hide behind high model likelihoods (table 3). Figure 2 captures these models using high variance to explain MNIST data. The Detlefsen VAE employs nearest neighbors to estimate heteroscedastic variance and then extrapolates between this estimate and some fixed value, which we varied (see parentheses in table 3). For each value, we observed this mechanism latching onto the fixed value for most data points suggesting their methods do not generalize to high-dimensional data. The MAP-VAE and our V3AE-Gamma make up much of likelihood lost when fixing variance to 0.001 and exhibit well calibrated predictive mean and variance enabling predictive samples that resemble the data. Again, VBEM* generally does well in all PPC categories. Perhaps intuitively, the methods with well-calibrated predictive variances indicate the model struggles most at edge localization. Conversely, the baseline methods' predictive uncertainty is largely uninterpretable.

5 Conclusion

This article addresses poor predictive mean and variance calibrations resulting from MLE optimization of heteroscedastic Gaussian likelihoods that employ amortized neural-network parameter maps. We posit necessary local conditions for poorly calibrated predictive distributions. Namely, the mean network operating on covariates must possess sufficient flexibility to place Dirac densities on the targets; data lacking meaningful nearby neighbors in either covariate or response spaces provide this flexibility. We demonstrate that affected models will use high noise variance to explain away poor mean estimates. Because rare data enable necessary conditions and can be explained away with noise variance, we caution against selecting models on the basis of log likelihood alone. We propose PPCs to measure predictive mean and variance calibration and find that our claims are empirically supported. Our attractively simple solution, to treat noise variance variationally with an amortized variational family, preserves heteroscedasticity in the predictive distribution and provides a probabilistically principled method to regularize optimization away from destabilizing Dirac densities. Our variational Empirical Bayes methods coupled with our novel priors, particularly VBEM*, provide substantial and tangible improvements to predictive mean and variance calibration on a variety of tasks.

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A Appendix

Hereafter, we include supplementary material for our manuscript. Our code is available as part of this submission. We organize this supplement using the same (major) section names as the main article. Any reference to the supplement from the main article will appear in the corresponding (major) section. Figure and table numbers continue from the main article.

B Variational Empirical Bayes for Noise Variance

B.1 Analytic Integration of ELBO's Expected Log Likelihood

The first expectation of eq. (1) (main article) evaluates analytically as

$$\frac{1}{2}\Big(\psi(\alpha(x)) - \log\beta(x) - \log(2\pi) - \frac{\alpha(x)}{\beta(x)}(y-\mu(x))^2\Big) \tag{5}$$

($\psi(\cdot)$ is the Digamma function) for univariate y and, with a diagonal covariance assumption, for multivariate y.

B.2 Derivation of xVAMP ELBO

We derive the xVAMP ELBO and decompose its KL divergence. The xVAMP generative process is

$$\begin{aligned} u_1,\ldots,u_K &\sim \text{UniformWithoutReplacement}(\{x_1,\ldots,x_N\}) \\ \lambda_i|x_i &\sim p(\lambda_i|x_i,u_1,\ldots,u_K) \triangleq \sum_{j=1}^{K}\pi_j(x_i)\cdot q(\lambda_i|u_j) \\ y_i|x_i,\lambda_i &\sim p(y_i|x_i,\lambda_i) \triangleq \mathcal{N}(y_i|\mu(x_i),\lambda_i). \end{aligned}$$

We treat $\{u_j\}_{j=1}^K$ as prior parameters (not random variables). The resulting local (per-point) ELBO is

$$\begin{aligned} \log p(y_i|x_i) &= \mathop{\mathbb{E}}_{q(\lambda_i|x_i)}\left[\log p(y_i|x_i,\lambda_i) - \log\frac{q(\lambda_i|x_i)}{p(\lambda_i|x_i)} + \log\frac{q(\lambda_i|x_i)}{p(\lambda_i|x_i,y_i)}\right] \\ &= \mathop{\mathbb{E}}_{q(\lambda_i|x_i)}\big[\log p(y_i|x_i,\lambda_i)\big] - D_{KL}\big(q(\lambda_i|x_i)||p(\lambda_i|x_i)\big) + D_{KL}\big(q(\lambda_i|x_i)||p(\lambda_i|x_i,y_i)\big) \\ &\geq \mathop{\mathbb{E}}_{q(\lambda_i|x_i)}\big[\log p(y_i|x_i,\lambda_i)\big] - D_{KL}\big(q(\lambda_i|x_i)||p(\lambda_i|x_i)\big) \\ &= \mathop{\mathbb{E}}_{q(\lambda_i|x_i)}\left[\log p(y_i|x_i,\lambda_i) - \log q(\lambda_i|x_i) + \log\sum_{j=1}^{K}\pi_j(x_i)q(\lambda_i|u_j)\right]. \end{aligned}$$

From the ELBO, we determine

$$\begin{aligned} D_{KL}\big(q(\lambda_i|x_i)||p(\lambda_i|x_i)\big) &= \mathop{\mathbb{E}}_{q(\lambda_i|x_i)}\left[\log q(\lambda_i|x_i) - \log\sum_{j=1}^{K}\pi_j(x_i)q(\lambda_i|u_j)\right] \\ &= -\mathbb{H}\big[q(\lambda_i|x_i)\big] - \mathop{\mathbb{E}}_{q(\lambda_i|x_i)}\left[\log\sum_{j=1}^{K}\pi_j(x_i)q(\lambda_i|u_j)\right]. \end{aligned} \tag{6}$$

B.3 VBEM Parameter Set

For VBEM's prior parameters we use the Cartesian square of a set of scalars ranging from 0.05 to 4.0. That set of integers is

$$\{0.05, 0.1, 0.25, 0.5, 0.75, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0\}.$$

C Heteroscedastic Regression Experiments

Figure 3 contains the graphical models we refer to from the main report. In the rightmost model, where we treat local precision variationally, one can draw an arrow from x_i to λ_i without introducing a cycle in the generative process, confirming the validity of our heteroscedastic priors $p(\lambda_i|x_i)$. As depicted, the model uses a homoscedastic prior $p(\lambda_i)$. We are not generative w.r.t. x, but one could model x and maintain validity so long as no generative cycles exist.

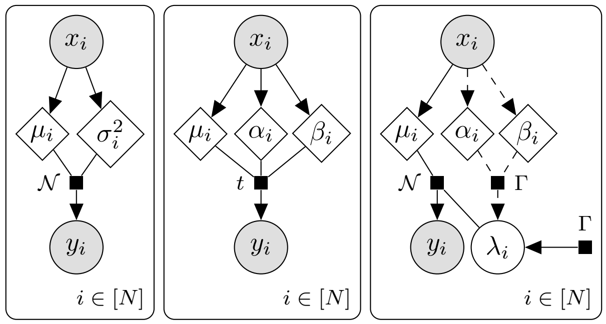

Figure 3: Graphical models for regression: Normal, Student's t, and Variational Variance (left to right). Diamonds are deterministic neural network parameter maps. Solid arrows denote the generative process. Dashed arrows define the variational family.

C.1 Discussion of Detlefsen et al. (2019)

Detlefsen et al. (2019) argue a batch containing x_i, but lacking other nearby data, while sufficient for updating the mean, is insufficient for updating the variance. Accordingly, they propose a 'locality sampler' that ensures any batch sample (x_i, y_i) is accompanied by its K nearest neighbors (w.r.t. x_i). Unfortunately, nearest-neighbor distance can produce meaningless relationships in high dimensions. Second, they optimize the mean and variance networks in isolation. The first half of training fits only the mean network (using a fixed variance) to ensure that, during the latter half of training where coordinate ascent alternates every few batches, variance estimation is feasible since the mean network is presumably now reasonable. Gradient-based coordinate ascent complicates optimization and may introduce interplay between the two separate adaptive gradient optimizers. Third, they replace the Normal likelihood with a Gamma-Normal parameterized Student's t, $\mathrm{T}(y_i|x_i) \equiv \int_0^\infty \mathcal{N}(y_i|\mu(x_i), \lambda_i)\,\mathrm{Gamma}(\lambda_i|\alpha(x_i), \beta(x_i))d\lambda_i$, which they Monte-Carlo integrate. Student's t variance can be undefined and arbitrarily close to ∞, which makes it famously robust against outliers, but unfortunately can hamstring its ability to generate sensible data under our PPC framework. Lastly, they extrapolate variance as a learnable convex combination between the estimated heteroscedastic variance (inverted samples from the parameterized Gamma) and some pre-defined, larger, non-trainable variance. They perform ablation and find that their methods are complementary on three UCI regression tasks with the locality sampler and Student's t distribution individually providing the most benefit.

C.2 Precision's Exact Posterior

The following derivation shows that precision's true posterior for regression results in a distribution that depends both on the covariates x_i and responses y_i. This dual dependence implies the true posterior falls outside the scope of heteroscedasticity due to the additional dependence on y_i and limits predictive utility when y_* is unobservable.

$$\begin{aligned} p(\lambda|y,x) &= \frac{p(y,\lambda|x)}{p(y|x)} = \frac{p(y,\lambda|x)}{\int p(y,\lambda|x)d\lambda} = \frac{p(y|x,\lambda)p(\lambda)}{\int p(y,\lambda|x)d\lambda} = \frac{\prod_{i=1}^n \mathcal{N}(y_i|\mu(x_i),\lambda_i)p(\lambda_i)}{\int \prod_{i=1}^n \mathcal{N}(y_i|\mu(x_i),\lambda_i)p(\lambda_i)d\lambda_i} \\ &= \frac{\prod_{i=1}^n \mathcal{N}(y_i|\mu(x_i),\lambda_i)p(\lambda_i)}{\prod_{i=1}^n \int \mathcal{N}(y_i|\mu(x_i),\lambda_i)p(\lambda_i)d\lambda_i} = \prod_{i=1}^n p(\lambda_i|y_i,x_i) \end{aligned}$$

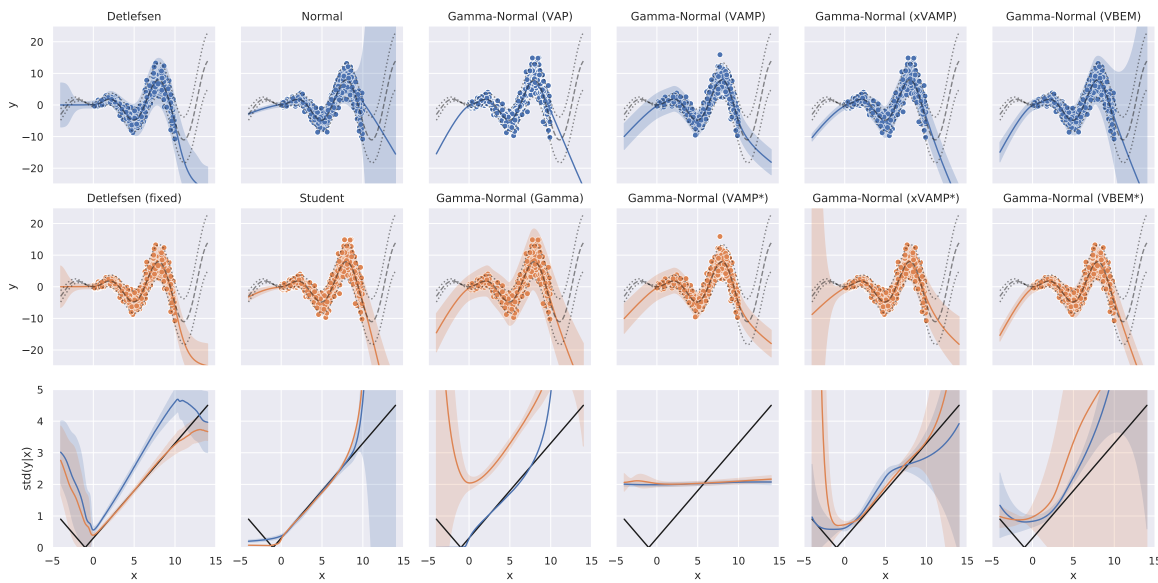

Figure 4: Toy regression results for the unmodified toy process (e.g. no isolated data point) from Detlefsen et al. (2019). The subplot descriptors are identical to fig. 1

Above, we use $p(\lambda_i|y_i, x_i) \triangleq \frac{\mathcal{N}(y_i|\mu(x_i),\lambda_i)p(\lambda_i)}{\int \mathcal{N}(y_i|\mu(x_i),\lambda_i)p(\lambda_i)d\lambda_i}$ to symbolically capture the local factorization.

C.3 Toy Data

For the toy regression task, Detlefsen et al. (2019) use single-layer neural networks with 50 sigmoid activations. We use the same size network but with ELU activations. We use ELU activations for all experiments, whereas Detlefsen et al. (2019) change activations for the UCI and VAE tasks. For the standard Gamma prior's parameters, we fit a MLE Gamma to the true precisions of the training data. For our VAMP(*), xVAMP(*), and VBEM* priors, we set $K = 20$. For VAMP(*) and xVAMP(*), we sample pseudo-inputs $u_i \overset{iid}{\sim} \text{Uniform}([-4, 14])$. Like Detlefsen et al. (2019), we use ADAM (Kingma & Ba, 2014) for optimization. While Detlefsen et al. (2019) employ separate optimizers for the mean and variance networks that respectively use 1e-2 and 1e-3 as learning rates, we employ a single ADAM instance with a learning rate of 5e-3. We run all algorithms for 6e3 epochs without batching (the single batch contains all 500 training points). We ran the toy experiments on a NVIDIA RTX2070.

In **??**, we modify the toy process from Detlefsen et al. (2019) to introduce an isolated data point in order to demonstrate the inability of the Normal, Student, and VAP baselines to converge on the target. There, these models employ high noise variance to explain the rogue point. Figure 4 contains results for the unmodified toy process where covariates are sampled from $\text{Uniform}([0, 10])$. Now, the under performing baseline models do well since there are no rogue data points for which the mean network would experience exploding gradients; this further confirms our claims.

C.4 UCI Data

For the UCI regression tasks, Detlefsen et al. (2019) employ single-layer neural networks with 50 ReLU activations. We use the same network architecture but with ELU activations, which we found to be more robust during our Monte-Carlo estimation of the right-most term of eq. (6)'s RHS. Detlefsen et al. (2019) allow training to run for some number of batch iterations, whereas our code uses the notion of an epoch, which encompasses the number of batches required to see each example in the training set exactly once. To keep things equal, we allow each algorithm to run for a dataset-specific number of batch iterations with a batch size of 256, which we convert to epochs ($\lceil \frac{\text{iterations}}{\text{batch size}} \rceil$) for our methods. All UCI datasets use 2e4 batch iterations except for those with larger ($N > 9000$) sample sizes (e.g. carbon, naval, power plant, and superconductivity), which use 1e5 batch iterations. Here, Detlefsen et al. (2019) use 1e-2 and 1e-4 as learning rates for the mean and variance networks' ADAM optimizers, respectively. We use 1e-3 as the learning rate for our single ADAM instance. We use $a = 1$ and $b = 0.001$ as the standard Gamma prior's parameters. For VAMP(*) and xVAMP(*) we sample $K = 100$ pseudo-inputs uniformly from the training set without replacement. We also use $K = 100$ for our VBEM* prior. We employ early stopping on the validation set's log (posterior) predictive likelihood with a patience of 50 epochs. We implemented an equivalent early stopping mechanism in the baseline code of Detlefsen et al. (2019), in which we also introduced support for multivariate response variables. We ran the UCI experiments on a NVIDIA RTX2070 and were able to parallelize up to five trials (i.e. five concurrent training sessions for any of the tested models)–our system ram (16GB) was the limiting factor.

Tables 5 to 8 each contain one of our four proposed PPCs. When available, we italicize any cited (i.e. reported) results. In these tables, we bold just the top performer, but never bold cited results since we did not validate these methods under our experimental conditions (e.g. some reported results use wider and/or deeper neural networks). Table 4 tallies the number of top PPC performances as well as statistical ties for top PPC performance across UCI datasets. We exclude cited results from table 4, but compare performances in the following paragraphs.

Sun et al. (2019) introduce functional variational Bayesian neural networks, which they test on some of the same UCI regression tasks that we consider. For power plant, they employ single hidden layer networks with 100 neurons, but otherwise use 50 neurons like we do. They report energy and naval metrics as well, but we suspect they only regressed one dimension of the two-dimensional targets. Unfortunately, their code loads *.data files for these two sets making it difficult for us to confirm our suspicion and identify the regressed dimension. As such, we exclude any multi-dimensional sets. Sun et al. (2019) provide mean, standard deviation, and the number of trials (10) for their metrics; this allows us to conduct a two-sided Welch's T-test against our Gamma-Normal VBEM* model. For log likelihood p-values, we obtain 0.088, 0.001, 0.012, and 0.539 respectively for boston, concrete, power plant, and yacht. Using a $p \leq 0.05$ threshold, VBEM* statistically beats and ties Sun et al. (2019) twice each. For mean RMSE p-values, we obtain 0.005, 0.033, 0.663, and 1.19 e-7 suggesting Sun et al. (2019) statistically outperforms VBEM*'s mean RMSE for three of these data sets.

Sicking et al. (2021) introduce a second-moment loss term to improve uncertainty estimation. They report negative log likelihood and mean RMSE for normalized target scalings (i.e. zero mean and unit variance). We multiplied their reported RMSEs by the target's standard deviation to attain RMSEs for the original target scalings, which we report. These rescaled RMSEs seemed reasonable compared to other results. However, adjusting their reported log likelihoods to the original target scalings produces nonsensible results that were too good to be true when compared to their RMSEs. Without access to their code, we cannot confirm that our adjustment by $\frac{1}{2}\log\sigma^2_{\text{target}}$ is appropriate. Furthermore, we exclude any results they report for multi-dimensional targets since rescaling likelihood is no longer straight forward. Recognizing Sicking et al. (2021) employ neural networks with two hidden layers, each with 50 ReLU activations, we implemented our VBEM* prior with these network sizes and denote it 'Gamma-Normal (2x)' in tables 5 to 8. Because this additional model uses larger networks and because we only tested it on the univariate UCI sets that overlap with Sicking et al. (2021), we never bold it in tables 5 to 8 and also exclude it from table 4. Examining table 6, we find that the single reported mean RMSE value from Sicking et al. (2021) is within two standard deviations of (similar to) Gamma-Normal (2x) VBEM* for four data sets, above two standard deviations (worse than) once (yacht), and below two standard deviations (better than) once (superconductivity).

Table 4: UCI regression summary: We tally the number of datasets for which a method was the top PPC performer or was statistically indistinguishable from the winner according to a two-sided Kolmogorov–Smirnov test with $p \leq 0.05$. Tallied statistical ties appear in parentheses.

Algorithm	Prior	LL	Mean RMSE	Var Bias	Sample RMSE	Total
Detlefsen	N/A	0 (0)	1 (1)	0 (0)	0 (0)	1 (1)
Normal	N/A	0 (3)	2 (7)	1 (6)	**3** (6)	6 (22)
Student	N/A	3 (**7**)	0 (6)	0 (5)	2 (5)	5 (23)
Gamma-Normal	VAP	0 (4)	0 (6)	0 (7)	0 (5)	0 (22)
	Gamma	0 (0)	0 (6)	**2** (6)	0 (5)	2 (17)
	VAMP	0 (3)	0 (8)	1 (7)	1 (**9**)	2 (**27**)
	VAMP*	0 (3)	1 (8)	**2** (7)	2 (**9**)	5 (**27**)
	xVAMP	1 (4)	0 (7)	1 (6)	2 (6)	4 (23)
	xVAMP*	1 (4)	0 (7)	1 (**8**)	0 (6)	2 (25)
	VBEM	0 (1)	**5** (**10**)	0 (0)	0 (0)	5 (11)
	VBEM*	**5** (**7**)	1 (7)	**2** (5)	0 (5)	**8** (24)

Table 5: UCI predictive log likelihood reported as mean±std. Tuples appearing below dataset are $(N_{\text{observations}}, \dim(x), \dim(y))$.

Algorithm	Prior	boston (506, 13, 1)	carbon (10721, 5, 3)	concrete (1030, 8, 1)	energy (768, 8, 2)	naval (11934, 16, 2)
Sun et al. (2019)	N/A	*-2.30±0.04*	–	*-3.10±0.02*	–	–
Detlefsen	N/A	-2.98±0.09	8.77±0.24	-3.66±0.08	-4.90±0.27	9.67±0.19
Normal	N/A	-2.42±0.23	13.20±1.35	-3.06±0.17	-0.48±0.69	14.15±0.17
Student	N/A	-2.37±0.19	**17.19±0.21**	-3.10±0.17	0.22±0.31	13.60±0.39
Gamma-Normal	VAP	-2.36±0.17	15.52±0.24	-3.12±0.17	0.17±0.44	13.36±0.41
	Gamma	-2.48±0.29	11.28±0.02	-3.20±0.16	-1.05±0.18	12.33±0.16
	VAMP	-2.39±0.17	14.37±0.17	-3.09±0.16	-0.18±0.21	14.16±0.78
	VAMP*	-2.39±0.16	14.38±0.12	-3.09±0.16	-0.16±0.20	13.96±0.88
	xVAMP	**-2.33±0.17**	15.38±0.24	-3.01±0.14	0.05±0.28	13.50±0.59
	xVAMP*	-2.33±0.17	15.41±0.18	-3.01±0.13	0.11±0.39	13.34±0.47
	VBEM	-2.46±0.11	4.57±1.00	-3.11±0.07	-4.52±0.26	9.02±0.61
	VBEM*	-2.36±0.14	14.64±0.16	**-2.99±0.13**	**0.49±0.28**	**14.42±0.15**
Gamma-Normal (2x)	VBEM*	-2.31±0.17	–	-2.88±0.14	–	–

Algorithm	Prior	power plant (9568, 4, 1)	superconductivity (21263, 81, 1)	wine-red (1599, 11, 1)	wine-white (4898, 11, 1)	yacht (308, 6, 1)
Sun et al. (2019)	N/A	*-2.83±0.01*	–	–	–	*-1.03±0.03*
Detlefsen	N/A	-3.26±9.1e-03	-5.21±0.02	-1.04±0.06	-1.12±0.04	-3.15±0.10
Normal	N/A	-2.82±0.05	-3.51±0.10	-0.92±0.05	-1.05±0.04	-1.55±0.65
Student	N/A	**-2.78±0.03**	-3.41±0.05	**-0.80±0.10**	-1.05±0.04	-1.73±0.59
Gamma-Normal	VAP	-2.81±0.04	-3.45±0.06	-0.87±0.06	-1.04±0.04	-1.79±0.50
	Gamma	-2.88±0.03	-3.45±0.04	-0.98±0.07	-1.13±0.05	-1.73±0.38
	VAMP	-2.83±0.03	-3.94±0.02	-0.94±0.05	-1.05±0.04	-2.83±0.70
	VAMP*	-2.83±0.03	-3.94±0.03	-0.94±0.05	-1.05±0.04	-2.77±0.77
	xVAMP	-2.81±0.04	-3.40±0.04	-0.90±0.05	-1.03±0.04	-1.68±0.38
	xVAMP*	-2.81±0.04	**-3.39±0.05**	-0.89±0.06	-1.03±0.04	-1.71±0.47
	VBEM	-2.89±0.05	-3.77±0.09	-0.91±0.05	-1.03±0.03	-2.64±0.23
	VBEM*	-2.81±0.03	-3.41±0.04	-0.89±0.06	**-1.03±0.04**	**-1.11±0.57**
Gamma-Normal (2x)	VBEM*	-2.76±0.03	-3.31±0.03	-0.89±0.06	–	-0.91±0.29

Table 6: UCI predictive mean RMSE reported as mean±std. Tuples appearing below dataset are $(N_{\text{observations}}, \dim(x), \dim(y))$.

Algorithm	Prior	boston (506, 13, 1)	carbon (10721, 5, 3)	concrete (1030, 8, 1)	energy (768, 8, 2)	naval (11934, 16, 2)
Sun et al. (2019)	N/A	*2.38±0.10*	–	*4.94±0.18*	–	–
Sicking et al. (2021)	N/A	*3.03*	–	*4.17*	–	–
Detlefsen	N/A	4.48±1.06	0.02±4.6e-03	8.13±1.65	2.05±0.49	4.2e-03±6.3e-04
Normal	N/A	3.36±1.29	**7.5e-03±3.3e-03**	6.05±0.66	1.30±0.14	3.5e-03±3.1e-04
Student	N/A	3.62±1.42	7.6e-03±3.3e-03	6.71±0.81	1.42±0.17	3.4e-03±5.0e-04
Gamma-Normal	VAP	3.44±1.21	7.7e-03±3.3e-03	6.61±0.84	1.38±0.15	3.2e-03±5.3e-04
	Gamma	3.82±1.72	7.6e-03±3.3e-03	6.63±0.70	1.31±0.14	3.2e-03±5.1e-04
	VAMP	3.15±1.06	7.8e-03±3.2e-03	5.47±1.00	1.36±0.13	1.2e-03±1.0e-03
	VAMP*	3.15±1.05	7.8e-03±3.2e-03	5.47±1.00	1.36±0.13	1.6e-03±1.3e-03
	xVAMP	3.25±1.16	7.6e-03±3.3e-03	5.61±0.67	1.36±0.14	3.2e-03±5.2e-04
	xVAMP*	3.28±1.17	7.6e-03±3.3e-03	5.72±0.59	1.36±0.14	3.2e-03±4.9e-04
	VBEM	**3.14±1.07**	8.7e-03±3.3e-03	**5.26±0.58**	1.36±0.14	**5.6e-04±1.6e-04**
	VBEM*	3.18±1.12	7.6e-03±3.3e-03	5.59±0.70	**1.30±0.13**	2.4e-03±2.8e-04
Gamma-Normal (2x)	VBEM*	3.04±1.14	–	5.00±0.59	–	–

Algorithm	Prior	power plant (9568, 4, 1)	superconductivity (21263, 81, 1)	wine-red (1599, 11, 1)	wine-white (4898, 11, 1)	yacht (308, 6, 1)
Sun et al. (2019)	N/A	*4.10±0.05*	–	–	–	*0.61±0.07*
Sicking et al. (2021)	N/A	*3.75*	*10.96*	*0.65*	–	*1.21*
Detlefsen	N/A	4.33±0.27	17.72±1.29	0.71±0.06	0.76±0.04	**2.42±1.06**
Normal	N/A	**4.12±0.20**	14.53±0.44	0.62±0.03	0.70±0.04	3.42±2.30
Student	N/A	4.12±0.19	14.85±0.42	0.63±0.03	0.71±0.03	15.03±3.30
Gamma-Normal	VAP	4.14±0.21	14.83±0.48	0.62±0.03	0.70±0.03	14.70±3.31
	Gamma	4.18±0.18	14.44±0.43	0.63±0.03	0.72±0.03	12.17±2.38
	VAMP	4.16±0.20	12.81±0.33	0.62±0.03	0.70±0.04	5.42±3.54
	VAMP*	4.16±0.20	**12.80±0.35**	0.62±0.03	0.70±0.04	5.30±3.65
	xVAMP	4.14±0.20	14.13±0.39	0.62±0.03	0.70±0.04	12.30±3.09
	xVAMP*	4.13±0.21	14.25±0.42	0.62±0.03	0.70±0.03	12.51±3.20
	VBEM	4.16±0.19	13.13±0.37	**0.62±0.03**	**0.69±0.03**	3.51±1.46
	VBEM*	4.12±0.19	14.08±0.42	0.62±0.03	0.69±0.03	5.33±2.58
Gamma-Normal (2x)	VBEM*	3.92±0.20	12.71±0.34	0.62±0.03	–	0.47±0.18

Table 7: UCI predictive variance bias reported as mean±std. Tuples appearing below dataset are $(N_{\text{observations}}, \dim(x), \dim(y))$.

Algorithm	Prior	boston (506, 13, 1)	carbon (10721, 5, 3)	concrete (1030, 8, 1)	energy (768, 8, 2)	naval (11934, 16, 2)
Detlefsen	N/A	1.0e+02±79.11	9.8e-05±1.6e-04	2.2e+02±91.85	18.60±8.88	nan±nan
Normal	N/A	31.63±1.5e+02	3.5e+23±1.6e+24	-2.01±8.67	-0.16±0.24	3.1e-07±2.0e-06
Student	N/A	18.08±63.79	0.12±0.23	-2.20±9.28	24.00±85.42	4.9e-06±2.2e-05
Gamma-Normal	VAP	3.3e+02±1.3e+03	0.25±1.11	-2.13±7.85	0.04±0.31	3.1e-07±6.8e-07
	Gamma	3.18±20.09	1.5e-04±5.8e-05	0.76±11.35	0.31±0.40	3.7e-06±2.9e-06
	VAMP	-2.96±7.96	-6.6e-06±6.0e-05	-6.15±5.18	-0.15±0.39	1.7e-07±2.9e-07
	VAMP*	-3.00±7.84	**-6.0e-06±6.0e-05**	-6.16±5.18	-0.13±0.40	**1.3e-07±3.3e-07**
	xVAMP	0.65±16.20	2.7e-05±9.7e-05	-4.82±4.63	**6.0e-03±0.36**	3.1e-07±7.4e-07
	xVAMP*	0.51±20.17	5.0e-04±2.2e-03	-4.66±5.07	-8.5e-03±0.36	2.7e-07±6.3e-07
	VBEM	6.74±8.48	0.01±4.5e-03	25.86±8.94	22.06±5.58	3.6e-05±1.4e-05
	VBEM*	**-0.11±8.62**	-7.2e-06±6.1e-05	**-0.58±5.05**	0.02±0.28	3.9e-07±4.9e-07
Gamma-Normal (2x)	VBEM*	-1.60±6.98	–	-2.69±4.29	–	–

Algorithm	Prior	power plant (9568, 4, 1)	superconductivity (21263, 81, 1)	wine-red (1599, 11, 1)	wine-white (4898, 11, 1)	yacht (308, 6, 1)
Detlefsen	N/A	69.25±2.40	5.5e+04±6.2e+03	2.16±1.57	0.83±0.36	96.62±54.08
Normal	N/A	**0.05±1.53**	2.3e+13±1.0e+14	-3.8e-03±0.04	-0.02±0.06	20.68±54.95
Student	N/A	-0.27±1.47	1.6e+05±3.3e+05	12.52±30.71	-5.6e-03±0.05	1.7e+03±2.3e+03
Gamma-Normal	VAP	0.52±1.29	9.0e+05±2.6e+06	0.03±0.05	0.13±0.64	1.3e+03±1.5e+03
	Gamma	2.34±1.43	1.1e+02±81.21	0.04±0.11	**-2.3e-03±0.05**	**-7.28±40.88**
	VAMP	0.89±1.04	**-9.83±7.97**	0.05±0.06	-8.8e-03±0.04	38.05±83.39
	VAMP*	0.89±1.04	-9.89±7.98	0.05±0.06	-8.9e-03±0.04	38.07±83.29
	xVAMP	0.46±1.25	14.40±42.90	3.5e-03±0.05	-0.03±0.03	4.8e+02±1.7e+03
	xVAMP*	0.44±1.24	1.3e+02±4.7e+02	**2.1e-03±0.05**	-0.03±0.03	1.7e+02±1.5e+02
	VBEM	16.53±9.32	91.44±25.39	0.08±0.04	0.07±0.04	20.70±25.23
	VBEM*	1.86±1.44	9.87±16.22	0.05±0.06	0.01±0.04	26.48±26.88
Gamma-Normal (2x)	VBEM*	1.33±1.34	59.40±1.3e+02	0.04±0.05	–	0.86±0.55

Table 8: UCI predictive sample RMSE reported as mean±std. Tuples appearing below dataset are $(N_{\text{observations}}, \dim(x), \dim(y))$.

Algorithm	Prior	boston (506, 13, 1)	carbon (10721, 5, 3)	concrete (1030, 8, 1)	energy (768, 8, 2)	naval (11934, 16, 2)
Detlefsen	N/A	12.02±3.89	0.03±3.6e-03	17.93±2.55	5.07±0.98	6.2e-03±5.7e-04
Normal	N/A	4.92±3.57	2.6e+11±1.2e+12	8.23±1.08	**1.85±0.21**	5.0e-03±5.4e-04
Student	N/A	4.64±1.10	**8.1e-03±3.1e-03**	9.18±1.36	2.07±0.37	5.0e-03±1.7e-03
Gamma-Normal	VAP	4.69±0.86	0.01±2.2e-03	9.42±1.82	2.02±0.35	4.5e-03±7.2e-04
	Gamma	4.92±2.18	0.02±1.8e-03	8.67±1.20	1.88±0.38	4.6e-03±9.1e-04
	VAMP	4.27±0.87	0.01±1.9e-03	7.27±1.05	1.93±0.19	**1.8e-03±1.4e-03**
	VAMP*	4.26±0.86	0.01±2.0e-03	**7.27±1.05**	1.93±0.20	2.2e-03±1.8e-03
	xVAMP	**4.23±1.15**	0.01±2.0e-03	7.84±1.05	1.88±0.29	4.5e-03±7.5e-04
	xVAMP*	4.23±1.14	0.01±2.5e-03	8.00±1.01	1.87±0.30	4.5e-03±7.1e-04
	VBEM	5.03±0.92	0.11±0.03	9.21±0.98	5.13±0.83	5.9e-03±1.5e-03
	VBEM*	4.41±1.07	0.01±1.9e-03	7.90±1.10	1.85±0.30	3.5e-03±3.7e-04
Gamma-Normal (2x)	VBEM*	4.03±0.88	–	6.96±0.83	–	–
Algorithm	**Prior**	**power plant (9568, 4, 1)**	**superconductivity (21263, 81, 1)**	**wine-red (1599, 11, 1)**	**wine-white (4898, 11, 1)**	**yacht (308, 6, 1)**
Detlefsen	N/A	10.36±0.28	2.4e+02±15.98	1.43±0.34	1.27±0.10	10.71±2.19
Normal	N/A	5.85±0.20	1.7e+06±7.4e+06	**0.86±0.07**	0.98±0.03	**4.73±3.68**
Student	N/A	**5.79±0.28**	21.25±1.46	0.88±0.06	0.99±0.04	20.24±7.84
Gamma-Normal	VAP	5.90±0.26	21.05±0.81	0.89±0.06	0.99±0.04	20.00±7.47
	Gamma	6.01±0.51	23.75±13.27	0.90±0.13	0.98±0.06	14.20±4.40
	VAMP	5.97±0.28	17.86±0.41	0.90±0.07	0.99±0.06	8.67±6.43
	VAMP*	5.97±0.28	**17.85±0.42**	0.90±0.07	0.99±0.06	8.50±6.57
	xVAMP	5.92±0.20	19.98±0.49	0.89±0.05	**0.97±0.06**	15.57±5.76
	xVAMP*	5.91±0.20	20.19±0.77	0.89±0.05	0.97±0.06	15.81±5.05
	VBEM	7.17±0.65	20.92±0.70	0.93±0.06	1.02±0.05	6.66±2.53
	VBEM*	6.00±0.20	19.78±0.48	0.89±0.07	0.97±0.03	6.84±4.58
Gamma-Normal (2x)	VBEM*	5.67±0.23	18.09±0.49	0.89±0.07	–	1.08±0.31

Comparing Gamma-Normal (2x) VBEM* PPC performance in tables 5 to 8 to Gamma-Normal VBEM*, which uses shallower neural networks, is evidence our methods improve as parameter map flexibility increases. This observation suggests variance is still well regularized away from zero even as model flexibility increases.

Active Learning We consider the same active learning regime from Detlefsen et al. (2019). We split each data set into 20% train, 60% reserve, and 20% test. The first active learning step utilizes the 20% training split. Thereafter, we move the n points from the reserve pool with highest predicted variance to the training set. We define n to be 5% of the original size of the reserve pool. We repeat this process ten times for each experiment and repeat each experiment ten times per data set. We preserve the remaining implementation details from the fully-supervised regression experiments, with two exceptions. First, we grow K, the number of mixture components available to the (x)VAMP(*) and VBEM(*) priors, proportionally to the ratio of utilized training data to total available. Specifically, we multiply $K = 100$ by this ratio at each active learning step to set the number of mixture components. Second, we identically scale the maximum allowed mini-batch iterations at each active learning step.

We plot the log predictive likelihoods and predictive mean RMSE on the held out test set across active learning steps in figs. 5 and 6. For clarity, we integrate these curves to reduce performance to a scalar for each dataset-method pair (tables 9 and 10). We find that VBEM* generally reigns supreme, which makes sense given its previous top performances on these data sets. Interestingly, we find cases for all methods, but on differing data sets, where additional training data does not improve test-set performance.

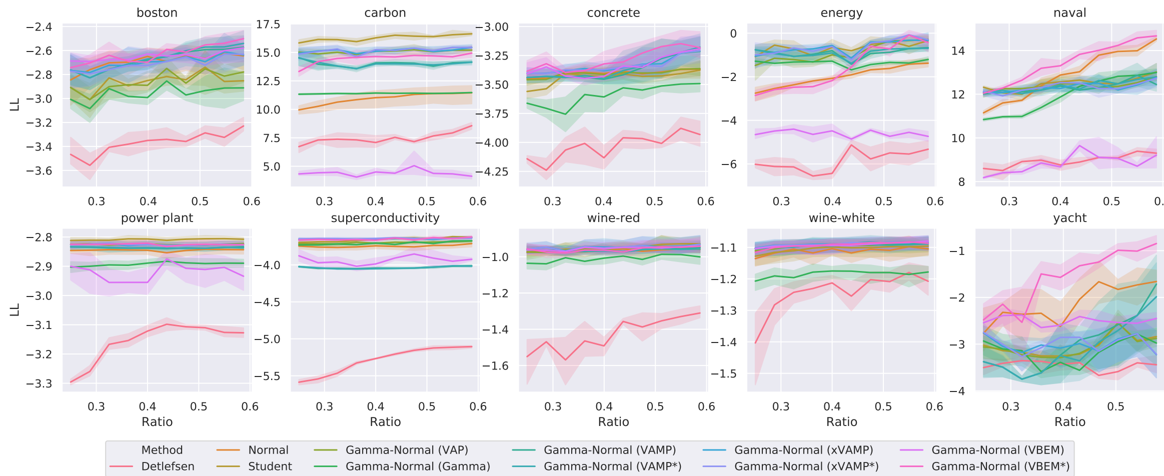

Figure 5: Log predictive likelihood across active learning steps for UCI data sets. The x axis is the ratio of utilized training data to the available. Darker lines are mean performance across trials. Shaded areas denote 95% confidence intervals.

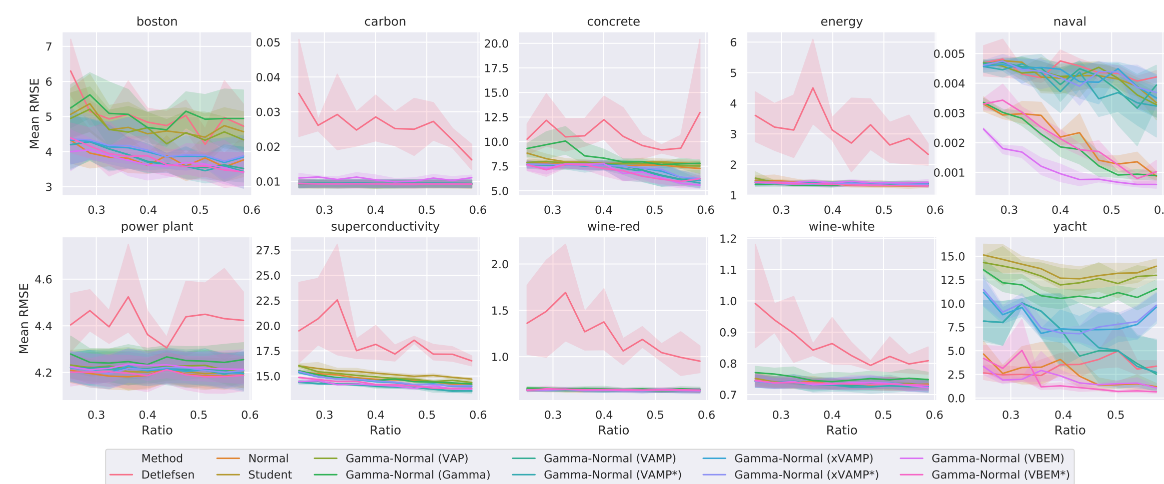

Figure 6: RMSE (of the predictive mean) across active learning steps for UCI data sets. The x axis is the ratio of utilized training data to the available. Darker lines are mean performance across trials. Shaded areas denote 95% confidence intervals.

Table 9: UCI cumulative sum of log predictive likelihood across active learning steps reported as mean±std. We bold only the top performer. Tuples appearing below dataset are $(N_{\text{observations}}, \dim(x), \dim(y))$.

Algorithm	Prior	boston (506, 13, 1)	carbon (10721, 5, 3)	concrete (1030, 8, 1)	energy (768, 8, 2)	naval (11934, 16, 2)
Detlefsen	N/A	-33.70±0.56	74.68±1.54	-40.33±0.27	-58.53±1.33	89.54±0.64
Normal	N/A	-26.92±1.30	1.1e+02±8.71	-34.03±0.75	-19.93±1.82	1.3e+02±1.03
Student	N/A	-28.60±0.77	**1.6e+02±0.91**	-34.41±0.47	-6.67±2.24	1.2e+02±0.98
Gamma-Normal	VAP	-28.56±0.95	1.5e+02±2.78	-34.06±0.31	-8.90±2.16	1.2e+02±0.73
	Gamma	-29.57±0.75	1.1e+02±0.32	-35.90±0.81	-13.62±1.34	1.2e+02±1.36
	VAMP	-26.76±0.70	1.4e+02±2.50	-33.69±1.06	-9.10±1.35	1.2e+02±1.70
	VAMP*	-26.66±0.76	1.4e+02±2.46	-33.57±1.08	-9.02±1.10	1.2e+02±0.94
	xVAMP	-26.98±1.20	1.5e+02±4.01	-33.36±0.89	-6.59±1.70	1.2e+02±0.70
	xVAMP*	-27.10±1.19	1.5e+02±3.29	-33.39±0.89	**-6.43±1.29**	1.2e+02±0.76
	VBEM	-26.48±0.53	44.05±2.86	-33.43±0.54	-46.01±0.83	88.31±2.09
	VBEM*	**-26.27±0.66**	1.4e+02±3.85	**-32.84±1.09**	-15.95±1.04	**1.3e+02±1.53**
Algorithm	Prior	power plant (9568, 4, 1)	superconductivity (21263, 81, 1)	wine-red (1599, 11, 1)	wine-white (4898, 11, 1)	yacht (308, 6, 1)
Detlefsen	N/A	-31.57±0.06	-52.89±0.20	-14.28±0.48	-12.43±0.28	-34.55±1.28
Normal	N/A	-28.45±0.19	-37.46±0.52	-9.66±0.30	-11.12±0.30	-21.33±2.80
Student	N/A	**-28.08±0.12**	-36.57±0.07	-9.49±0.31	-11.05±0.33	-30.38±1.15
Gamma-Normal	VAP	-28.25±0.13	-36.99±0.07	-9.56±0.39	-10.95±0.29	-30.52±0.91
	Gamma	-28.93±0.19	-37.08±0.10	-10.10±0.41	-11.85±0.33	-31.59±1.64
	VAMP	-28.37±0.12	-40.36±0.10	-9.61±0.30	-10.95±0.27	-29.86±4.92
	VAMP*	-28.36±0.12	-40.37±0.06	-9.64±0.29	-10.92±0.27	-30.87±4.02
	xVAMP	-28.26±0.13	-36.48±0.05	**-9.46±0.43**	**-10.89±0.27**	-30.11±2.68
	xVAMP*	-28.26±0.13	**-36.42±0.04**	-9.48±0.42	-10.89±0.28	-29.85±1.34
	VBEM	-29.21±0.10	-39.35±0.37	-9.53±0.35	-10.92±0.25	-24.99±0.77
	VBEM*	-28.26±0.14	-36.50±0.07	-9.59±0.36	-10.93±0.26	**-15.64±1.91**

Table 10: UCI cumulative sum of RMSE (of predictive mean) across active learning steps reported as mean±std. We bold only the top performer. Tuples appearing below dataset are $(N_{\text{observations}}, \dim(x), \dim(y))$.

Algorithm	Prior	boston (506, 13, 1)	carbon (10721, 5, 3)	concrete (1030, 8, 1)	energy (768, 8, 2)	naval (11934, 16, 2)
Detlefsen	N/A	49.96±3.89	0.26±0.04	1.1e+02±13.71	31.41±4.79	0.04±1.4e-03
Normal	N/A	38.17±6.22	0.09±0.01	75.95±5.43	13.68±0.99	0.02±1.2e-03
Student	N/A	47.08±7.00	**0.09±0.01**	80.01±2.80	14.14±0.85	0.04±1.3e-03
Gamma-Normal	VAP	46.02±6.50	0.09±0.01	77.75±3.04	13.98±0.78	0.04±1.7e-03
	Gamma	50.29±6.97	0.09±0.01	85.00±5.72	**13.41±0.64**	0.02±7.9e-04
	VAMP	38.11±5.99	0.09±0.01	71.79±7.33	13.95±0.63	0.04±3.3e-03
	VAMP*	37.88±6.21	0.09±0.01	70.86±7.23	13.99±0.62	0.04±2.5e-03
	xVAMP	39.99±7.30	0.09±0.01	72.43±5.52	13.74±0.82	0.04±1.2e-03
	xVAMP*	40.36±7.08	0.09±0.01	72.82±5.74	13.67±0.78	0.04±1.6e-03
	VBEM	**37.17±5.66**	0.11±0.01	69.39±5.31	14.20±0.63	**0.01±1.1e-03**
	VBEM*	37.93±5.86	0.09±0.01	**69.25±6.34**	13.50±0.63	0.02±1.3e-03
Algorithm	Prior	power plant (9568, 4, 1)	superconductivity (21263, 81, 1)	wine-red (1599, 11, 1)	wine-white (4898, 11, 1)	yacht (308, 6, 1)
Detlefsen	N/A	44.20±0.76	1.8e+02±8.63	12.42±1.50	8.58±0.39	32.56±6.07
Normal	N/A	**41.93±0.81**	1.5e+02±1.62	6.36±0.19	7.37±0.22	25.62±9.98
Student	N/A	42.09±0.86	1.5e+02±1.73	6.41±0.17	7.37±0.20	1.4e+02±11.74
Gamma-Normal	VAP	42.21±0.85	1.5e+02±0.96	6.38±0.20	7.35±0.20	1.3e+02±10.75
	Gamma	42.51±0.76	1.5e+02±0.69	6.52±0.22	7.53±0.30	1.1e+02±5.96
	VAMP	42.14±0.92	1.4e+02±1.32	6.39±0.23	7.35±0.24	63.26±22.50
	VAMP*	42.11±0.93	**1.4e+02±0.72**	6.40±0.22	**7.32±0.23**	66.27±19.49
	xVAMP	42.09±0.92	1.4e+02±0.59	**6.36±0.22**	7.35±0.22	82.86±9.68
	xVAMP*	42.11±0.89	1.5e+02±0.52	6.37±0.22	7.36±0.22	84.89±7.17
	VBEM	42.22±0.79	1.4e+02±0.58	6.39±0.22	7.35±0.23	19.66±2.97
	VBEM*	41.94±0.88	1.4e+02±0.91	6.44±0.24	7.36±0.21	**18.97±4.82**

D Variational Variance for VAEs

Figure 7 depicts the graphical models for the various VAE methods. For V3VAE, one can draw a solid arrow from z_i to λ_i without introducing a generative cycle, thus confirming the validity of $p(\lambda_i|z_i)$ as a

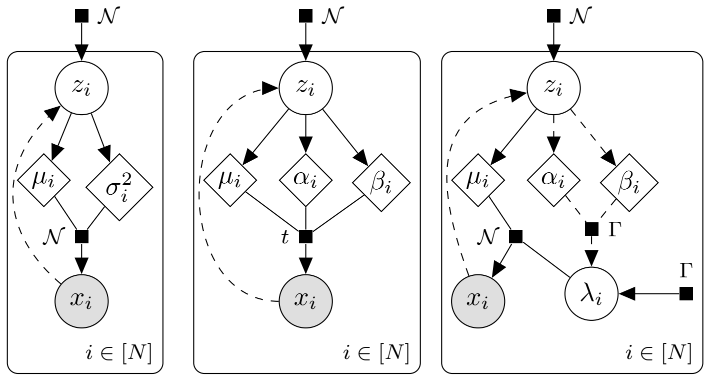

Figure 7: Graphical models for VAEs: Normal, Student's t, and Variational Variance VAE (left to right). Diamonds are deterministic neural network parameter maps. Solid arrows denote the generative process. Dashed arrows define the variational family.

heteroscedastic prior. For these experiments, we use ADAM with a 5e-5 learning rate. All Monte-Carlo (MC) approximations use 20 samples. We found additional samples did not improve log local reconstruction likelihood approximations. Since our VAMP(*), xVAMP(*), and VBEM* priors require twice as many MC samples ($q(\lambda|x)$ in addition to $q(z|x)$), their memory footprint is higher, requiring a batch size of 125 on a NVIDIA RTX2070. The remaining models use a batch size of 256. Because the lower batch size has twice as many batch updates per epoch, those models train for half (500) the number of epochs used by the other models (1000). For Celeb a, we further reduce the number of training epochs by half given the larger number of training examples (i.e. more batch iterations per epoch). We employ early stopping on the validation set's log posterior predictive probability with a patience of 25 for the 500 epoch models and 50 for the 1000 epoch models. We use an encoder architecture with hidden layers of sizes 512, 256, and 128, each of which applies an ELU activation. The decoder architecture is the transpose of the encoder. Because we only consider dense architectures, we had to resize Celeb-a images to 32×26 pixels in order to fit the weight matrices in our NVIDIA RTX2070's available VRAM. The dimensions of the latent variable, $\dim(z)$, are 10 for MNIST, 25 for Fashion MNIST, and 50 for Celeb-a. We include PPC metrics for MNIST and Celeb-a in tables 11 and 12, which we could not fit in the main report. Additionally, we include figs. 8 to 10, which are similar to fig. 7 (main article) but have additional samples for *all* tested methods.

Table 11: VAE PPCs for MNIST (mean±std.)

Method	ELBO	LL	Mean RMSE	Var Bias	Sample RMSE
Fixed-Var. VAE (1.0)	-739.38±4.1e-02	-732.10±0.11	0.17±1.1e-03	0.98±4.2e-04	1.02±2.5e-04
Fixed-Var. VAE (0.001)	-3004.40±29.78	-2902.66±29.23	**0.11±3.3e-04**	-1.2e-02±7.4e-05	**0.12±3.1e-04**
VAE	2498.68±264.48	2593.51±267.72	0.25±2.7e-03	4.3e-02±2.6e-02	0.41±3.5e-02
VAE + BN	2308.01±20.36	2386.70±23.17	0.25±1.8e-03	0.13±2.6e-02	0.50±2.6e-02
VAE-Split	2149.52±70.20	2282.32±65.63	0.25±2.7e-03	7.4e-02±2.6e-02	0.44±3.2e-02
VAE-Split + BN	2321.77±63.06	2482.36±75.34	0.28±4.4e-03	6.2e-02±1.1e-02	0.47±1.5e-02
Detlefsen (0.001)	-1070.91±82.37	-1063.51±83.32	0.17±3.9e-04	15.03±3.39	3.86±0.51
Detlefsen (0.25)	-173.56±2.83	-168.23±2.39	0.17±4.6e-04	0.20±1.2e-03	0.51±9.6e-04
Detlefsen (10.0)	-1563.84±1.79	-1556.55±1.72	0.17±5.4e-04	9.09±2.2e-02	3.02±4.0e-03
MAP-VAE	-5287.96±19.46	1291.42±6.94	0.13±1.9e-03	-1.3e-02±4.1e-04	0.15±2.0e-03
Student-VAE	**4758.25±537.13**	**4826.82±530.95**	0.27±1.7e-02	0.38±0.45	0.68±0.28
V3AE-VAP	2024.03±170.14	3243.11±445.47	0.24±3.5e-03	**8.1e-04±9.7e-04**	0.34±5.5e-03
V3AE-Gamma	180.78±9.29	1495.01±2.75	0.13±7.0e-04	-1.2e-02±1.9e-04	0.15±9.2e-04
V3AE-VAMP	2094.64±47.29	2355.12±13.40	0.20±6.7e-04	**6.2e-04±1.1e-03**	0.28±1.7e-03
V3AE-VAMP*	1991.74±73.17	2270.76±41.89	0.20±7.9e-04	**1.2e-03±1.1e-03**	0.29±2.2e-03
V3AE-xVAMP	2064.18±81.72	2323.38±94.35	0.20±2.6e-03	**1.9e-03±6.8e-04**	0.29±3.2e-03
V3AE-xVAMP*	2041.25±47.12	2280.13±48.29	0.20±2.0e-03	**6.5e-04±7.2e-04**	0.29±3.7e-03
V3AE-VBEM	223.04±0.76	296.95±0.92	0.12±8.1e-04	6.1e-02±2.7e-04	0.30±2.7e-04
V3AE-VBEM*	1528.76±8.29	2107.63±5.44	0.14±1.2e-03	**1.6e-03±1.1e-04**	0.20±1.6e-03

Table 12: VAE PPCs for Celeb-a (mean±std.)

Method	ELBO	LL	Mean RMSE	Var Bias	Sample RMSE
Fixed-Var. VAE (1.0)	-739.38±4.1e-02	-732.10±0.11	0.17±1.1e-03	0.98±4.2e-04	1.02±2.5e-04
Fixed-Var. VAE (0.001)	-3004.40±29.78	-2902.66±29.23	**0.11±3.3e-04**	-1.2e-02±7.4e-05	**0.12±3.1e-04**
VAE	2498.68±264.48	2593.51±267.72	0.25±2.7e-03	4.3e-02±2.6e-02	0.41±3.5e-02
VAE + BN	2308.01±20.36	2386.70±23.17	0.25±1.8e-03	0.13±2.6e-02	0.50±2.6e-02
VAE-Split	2149.52±70.20	2282.32±65.63	0.25±2.7e-03	7.4e-02±2.6e-02	0.44±3.2e-02
VAE-Split + BN	2321.77±63.06	2482.36±75.34	0.28±4.4e-03	6.2e-02±1.1e-02	0.47±1.5e-02
Detlefsen (0.001)	-1070.91±82.37	-1063.51±83.32	0.17±3.9e-04	15.03±3.39	3.86±0.51
Detlefsen (0.25)	-173.56±2.83	-168.23±2.39	0.17±4.6e-04	0.20±1.2e-03	0.51±9.6e-04
Detlefsen (10.0)	-1563.84±1.79	-1556.55±1.72	0.17±5.4e-04	9.09±2.2e-02	3.02±4.0e-03
MAP-VAE	-5287.96±19.46	1291.42±6.94	0.13±1.9e-03	-1.3e-02±4.1e-04	0.15±2.0e-03
Student-VAE	**4758.25±537.13**	**4826.82±530.95**	0.27±1.7e-02	0.38±0.45	0.68±0.28
V3AE-VAP	2024.03±170.14	3243.11±445.47	0.24±3.5e-03	**8.1e-04±9.7e-04**	0.34±5.5e-03
V3AE-Gamma	180.78±9.29	1495.01±2.75	0.13±7.0e-04	-1.2e-02±1.9e-04	0.15±9.2e-04
V3AE-VAMP	2094.64±47.29	2355.12±13.40	0.20±6.7e-04	**6.2e-04±1.1e-03**	0.28±1.7e-03
V3AE-VAMP*	1991.74±73.17	2270.76±41.89	0.20±7.9e-04	**1.2e-03±1.1e-03**	0.29±2.2e-03
V3AE-xVAMP	2064.18±81.72	2323.38±94.35	0.20±2.6e-03	**1.9e-03±6.8e-04**	0.29±3.2e-03
V3AE-xVAMP*	2041.25±47.12	2280.13±48.29	0.20±2.0e-03	**6.5e-04±7.2e-04**	0.29±3.7e-03
V3AE-VBEM	223.04±0.76	296.95±0.92	0.12±8.1e-04	6.1e-02±2.7e-04	0.30±2.7e-04
V3AE-VBEM*	1528.76±8.29	2107.63±5.44	0.14±1.2e-03	**1.6e-03±1.1e-04**	0.20±1.6e-03

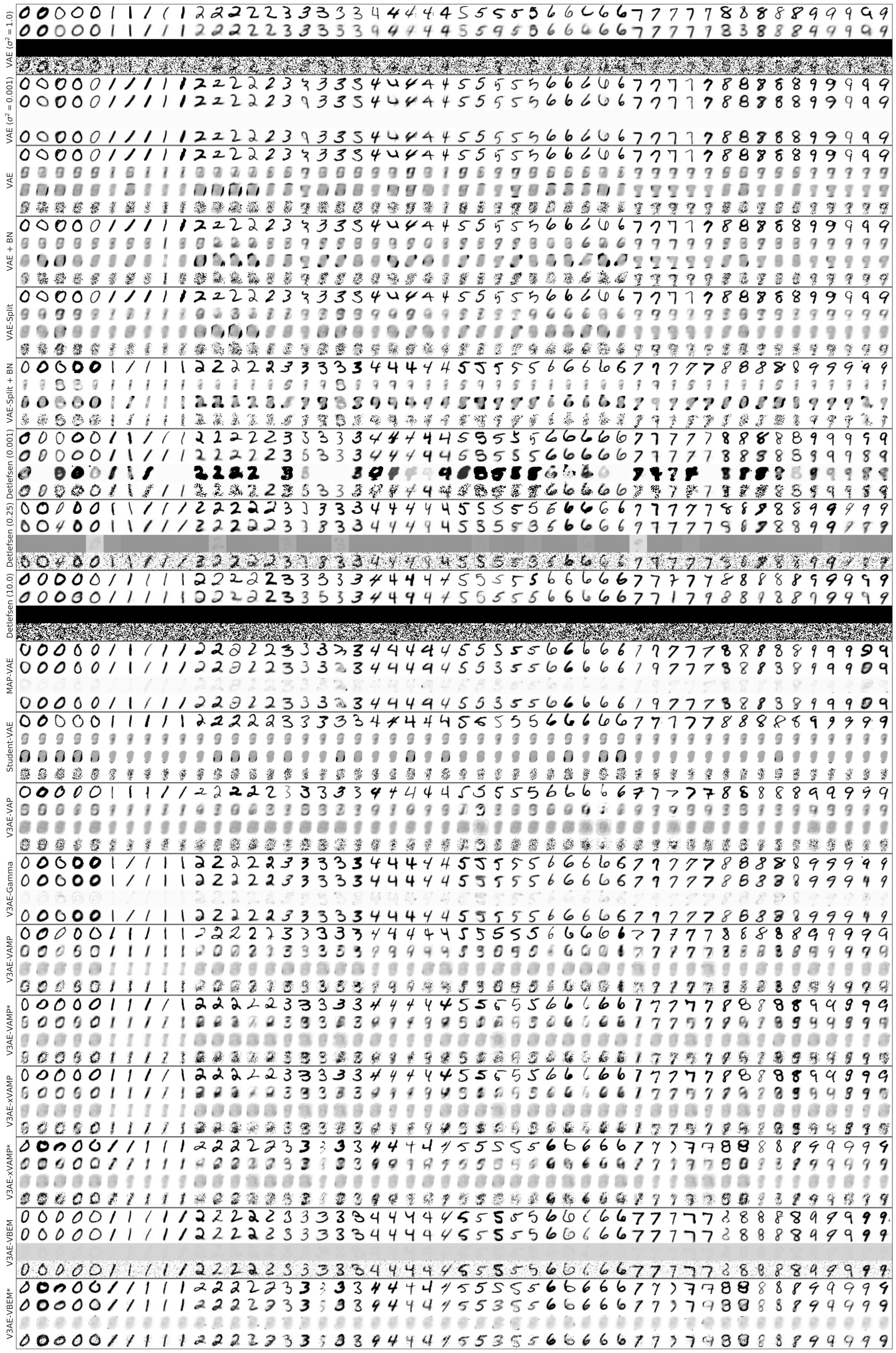

Figure 8: VAE PPC visualization for MNIST: The rows within a subplot from top to bottom are randomly selected test data followed by the local reconstruction distribution's mean and variance and a sample from it. Pixel values are clamped to $[0, 1]$, when PPC values exit this interval. Darker regions of variance images denote areas of higher predictive variance.

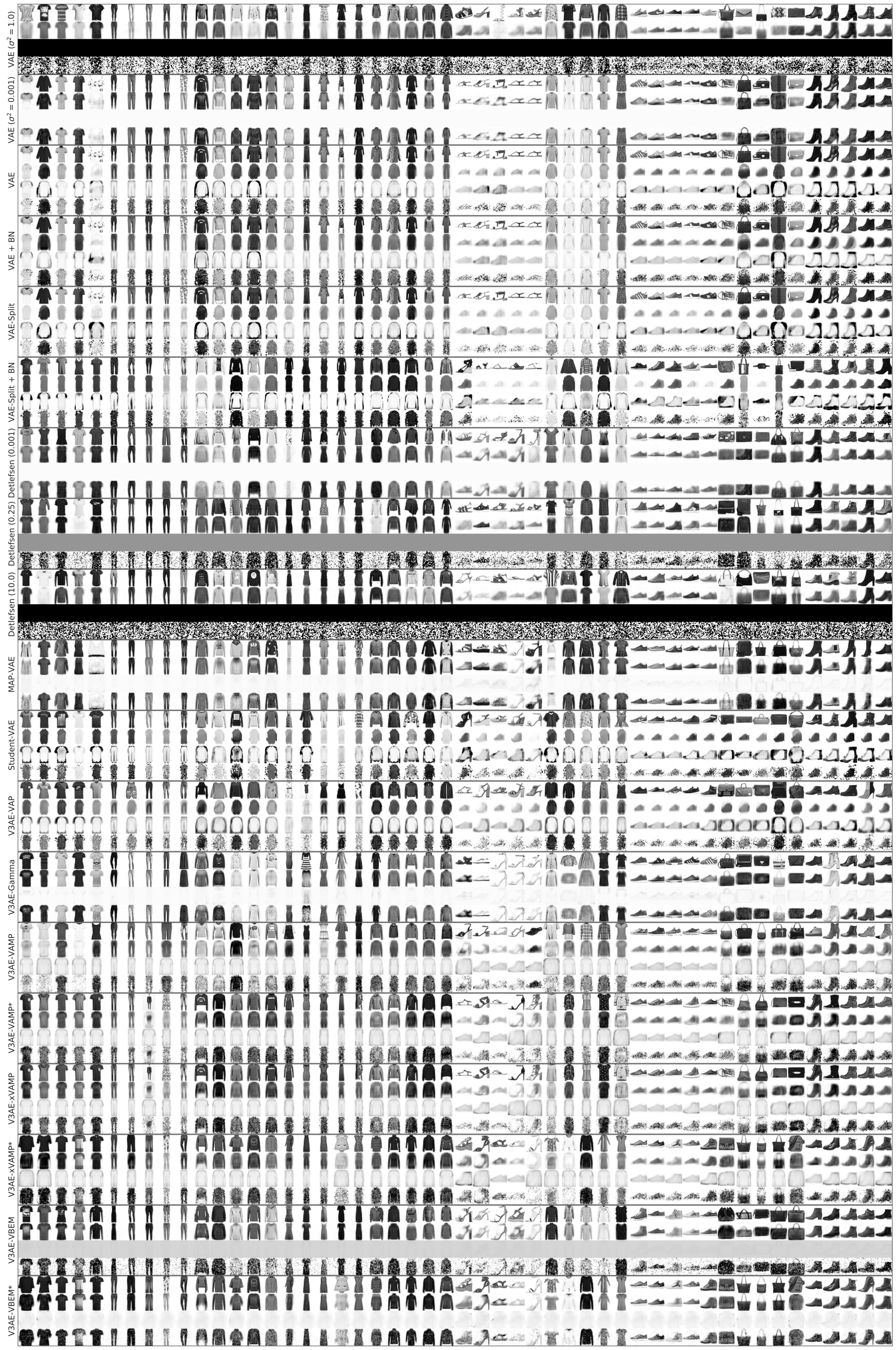

Figure 9: VAE PPC visualization for Fashion MNIST: The rows within a subplot from top to bottom are randomly selected test data followed by the local reconstruction distribution's mean and variance and a sample from it. Pixel values are clamped to $[0, 1]$, when PPC values exit this interval. Darker regions of variance images denote areas of higher predictive variance.

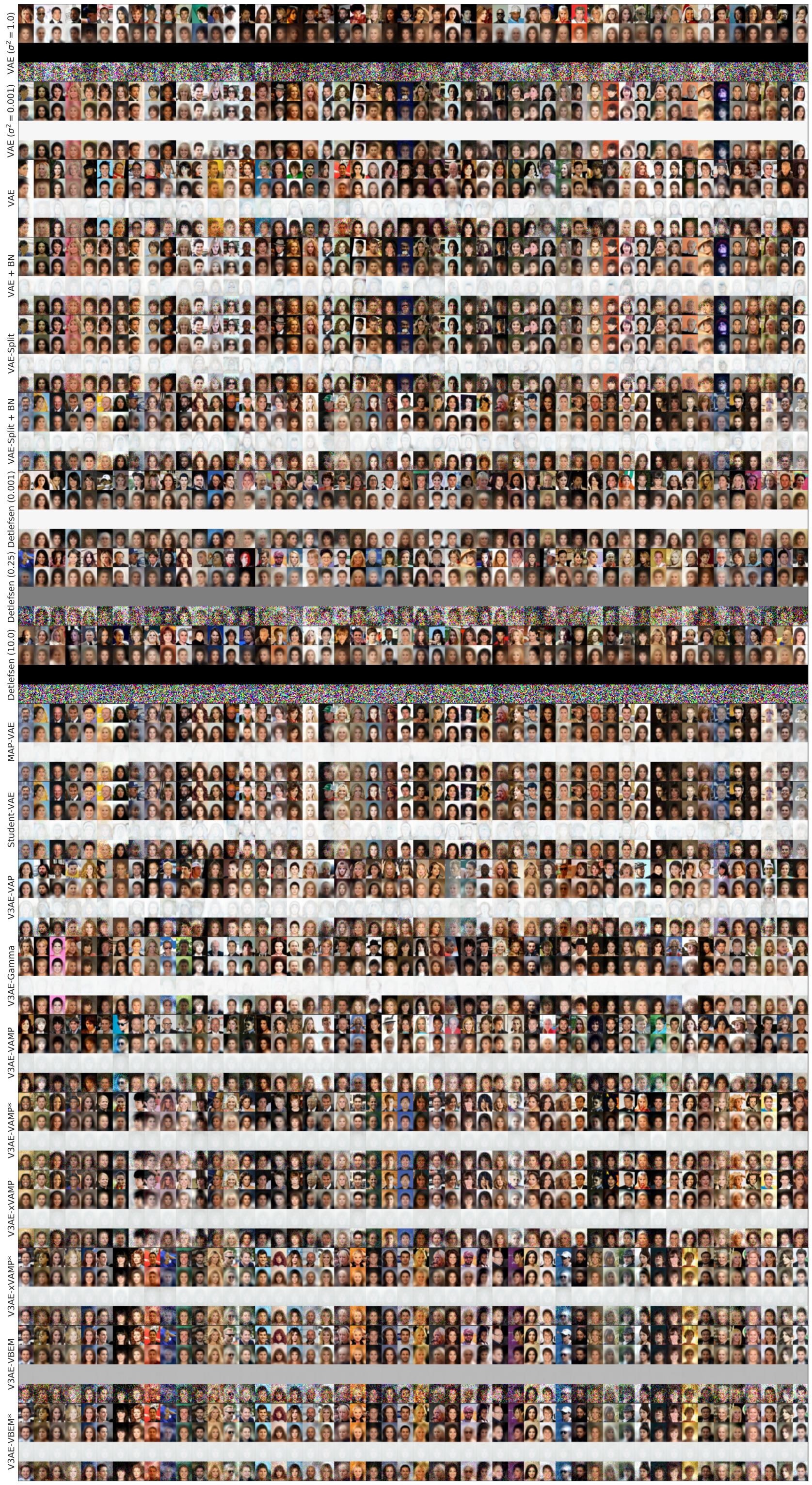

Figure 10: VAE PPC visualization for Celeb-a: The rows within a subplot from top to bottom are randomly selected test data followed by the local reconstruction distribution's mean and variance and a sample from it. Pixel values are clamped to $[0, 1]$, when PPC values exit this interval. Variance images are inverted such that lighter regions have lower predictive variance.