URSABench: Comprehensive Benchmarking of Approximate Bayesian Inference Methods for Deep Neural Networks

Meet P. Vadera*1 Adam D. Cobb*2 Brian Jalaian2 Benjamin M. Marlin1

Abstract

While deep learning methods continue to improve in predictive accuracy on a wide range of application domains, significant issues remain with other aspects of their performance including their ability to quantify uncertainty and their robustness. Recent advances in approximate Bayesian inference hold significant promise for addressing these concerns, but the computational scalability of these methods can be problematic when applied to large-scale models. In this paper, we describe initial work on the development of URSABench (the Uncertainty, Robustness, Scalability, and Accuracy Benchmark), an open-source suite of benchmarking tools for comprehensive assessment of approximate Bayesian inference methods with a focus on deep learning-based classification tasks.1

1. Introduction

As deep learning models continue to improve their predictive accuracy across many application domains, significant issues remain with respect to other highly important aspects of performance including their ability to robustly quantify uncertainty (Guo et al., 2017) and their ability to provide robust predictions in the presence of adversarial manipulations (Goodfellow et al., 2015) and out-of-distribution examples (Ovadia et al., 2019).

Approximate Bayesian inference methods (Neal, 1996; Jaakkola & Jordan, 2000) hold considerable promise for addressing such issues, and recent advances have significantly improved the feasibility of deploying approximate Bayesian inference methods to increasingly larger deep learning models (Welling & Teh, 2011; Zhang et al., 2020).

This paper describes initial work on URSABench, an open source suite of benchmarking tools for assessment of approximate Bayesian inference methods applied to deep neural network classification tasks. URSABench includes benchmark models, data sets, tasks and evaluation metrics focused on simultaneously assessing the uncertainty quantification performance, robustness, computational scalability and accuracy of learning and inference methods. We begin by briefly reviewing approximate Bayesian supervised learning. We then discuss principles for evaluation of such methods, followed by a description of the initial URSABench infrastructure and initial benchmarking results.

2. Bayesian Supervised Learning

In supervised learning, the data set \( D \) consists of a set of labeled instances \( \{(x_i, y_i)\}_{1 \leq i \leq N} \). \( x_i \in \mathbb{R}^D \) is the feature vector and \( y_i \in \mathcal{Y} \) is the prediction target. We let \( D^x \) be the set of feature vectors and \( D^y \) be the set of targets. A probabilistic supervised learning model provides a conditional probability model of the form \( p(y|x, \theta) \) where \( \theta \in \mathbb{R}^K \) are the model parameters. The conditional likelihood of the targets given the feature vectors and parameters is given by \( p(D^y|D^x, \theta) \). The standard assumption that the data cases are independent and identically distributed leads to \( p(D^y|D^x, \theta) = \prod_{i=1}^{N} p(y_i|x_i, \theta) \) (Neal, 1996). Bayesian inference also requires asserting a prior distribution over the model parameters \( p(\theta|\theta^0) \) that itself depends on prior parameters \( \theta^0 \) (Neal, 1996).

The two key problems in Bayesian inference applied to supervised learning are the computation of the posterior distribution over the unknown parameters given a training data set \( D_{tr} \) as shown in Equation (1), and the computation of the posterior predictive distribution over the target variable \( y \) given a feature vector \( x \) and a data set \( D_{tr} \) as shown in Equation (2) (Neal, 1996).

\[
p(\theta|D_{tr}, \theta^0) = \frac{p(D_{tr}^y|D_{tr}^x, \theta)p(\theta|\theta^0)}{\int p(D_{tr}^y|D_{tr}^x, \theta)p(\theta|\theta^0)d\theta} \quad (1)
\]

\[
p(y|x, D_{tr}, \theta^0) = E_{p(\theta|D_{tr}, \theta^0)}[p(y|x, \theta)] \quad (2)
\]
It is well known that for neural network models the integrals required in Equations (1) and (2) are intractable. Approximate Bayesian inference methods thus aim to approximate either the parameter posterior or expectations taken with respect to the parameter posterior such as Equation (2). Below, we briefly review three categories of Approximate Bayesian inference methods: Monte Carlo methods, surrogate density methods, and posterior distillation methods.

**Monte Carlo Methods:** Monte Carlo methods are a classical approach to Bayesian computation that approximate the intractable parameter posterior \( p(\theta|D, \theta^0) \) via a distribution constructed from a finite set of samples \( \theta_s \) drawn from the true posterior \( p(\theta|D, \theta^0) \) (Smith & Roberts, 1993). This leads to the following approximate posterior predictive distribution: \( p(y|x, D, \theta^0) \approx \frac{1}{S} \sum_{s=1}^{S} p(y|x, \theta_s) \).

Of course, for complex models the problem of drawing samples from the true parameter posterior is also often computationally intractable. Markov chain Monte Carlo (MCMC) methods solve this problem by constructing a Markov chain with the true posterior \( p(\theta|D, \theta^0) \) as its equilibrium distribution. While classical MCMC methods are typically too slow to apply to large models (Casella & George, 1992; Chib & Greenberg, 1995; Duane et al., 1987; Neal, 2003; Girolami & Calderhead, 2011), a number of recent approaches have addressed this problem either by enabling sampling based on mini-batches of data (Welling & Teh, 2011; Chen et al., 2014; Zhang et al., 2020), or by sampling in reduced-dimensional parameter spaces (Izmailov et al., 2019).

**Surrogate Density Methods:** Another major family of methods is approaches based on approximating the true posterior density via an analytically tractable surrogate distribution \( q(\theta|D, \theta^0, \phi) \) where \( \phi \) are auxiliary parameters of the surrogate distribution (Jordan et al., 1999; Jaakkola & Jordan, 2000; Ghosh et al., 2016; Minka, 2001). The most commonly used approaches in this family learn the parameters \( \phi \) by minimizing the Kullback-Leibler (KL) divergence \( \text{KL}(p||p') = E_p[ \log(p/p')] \) (MacKay, 2003). When the surrogate posterior is used as the first argument, the result is the variational inference (VI) framework (Jaakkola & Jordan, 2000). When it is used as the second argument, it yields the expectation propagation (EP) framework (Minka, 2001). Advances in the past decade have led to significantly more scalable methods in this family (Hoffman et al., 2013; Gal & Ghahramani, 2016; Dusenberry et al., 2020).

**Distillation-Based Methods:** The final class of methods that we review are posterior distillation-based methods including Bayesian Dark Knowledge (BDK) (Balan et al., 2015) and Generalized Posterior Expectation Distillation (GPED) (Vadera et al., 2020a). These methods directly approximate statistics of the posterior distribution by learning an auxiliary neural network model to mimic the output of corresponding Monte Carlo approximations. Importantly, their goal is not to improve over the Monte Carlo approximation, but rather to reduce the computation time required to compute the Monte Carlo average at deployment time.

### 3. URSABench Evaluation Principles

While advances in supervised deep learning methods have focused heavily on accuracy over the last decade, there are multiple aspects of models and inference algorithms that are of great interest. URSABench focuses on simultaneously assessing the uncertainty quantification performance, robustness, computational scalability and accuracy of learning and inference methods. In this section, we describe the evaluation principles that underlie URSABench. In the next section, we describe their current implementation.

**Accuracy:** Predictive performance is by far the most widely considered property of supervised machine learning models. In the classification setting, evaluation measures that only require that the true label \( y \) be correctly predicted provide the coarsest measures of the predictive performance. Accuracy is the most common such measure.

**Uncertainty Quantification:** A number of metrics are helpful for assessing the degree to which a method results in properly quantified predictive uncertainty. Predictive log likelihood can provide more insight into the predictive distribution than accuracy as it is sensitive to the predicted value of \( p(y|x, D_{te}, \theta^0) \). Both high-confidence errors and low-confidence correct predictions will result in lower log likelihood values.

Calibration is also an important property of predictive models and recent evaluations of deep learning methods have shown that their calibration properties can be quite poor (Guo et al., 2017). In the binary case, a classifier is said to be perfectly calibrated if exactly \( p \) percent of instances are predicted to be positive with \( p \) percent probability. The degree of calibration of a binary classifier can be quantified using the expected calibration error (ECE) (Guo et al., 2017). In the case of multi-class classification, a one-vs-all formulation of calibration error can be used. The Brier score provides an alternate measure of calibration (Brier, 1950) that can be interpreted as mixing together aspects of calibration and accuracy. Finally, misclassification detection performance (Hendrycks & Gimpel, 2017) is also helpful in assessing the utility of various uncertainty metrics.

**Robustness:** Another key property of models and inference methods is their robustness. Both predictive performance and uncertainty quantification metrics are typically computed on a test data set \( D_{te} \) that is assumed to be sampled from the same distribution as the training...
data set $D_{tr}$. Out-of-distribution (OOD) detection tasks instead assess the ability of methods to detect examples from a set $D_{ood}$ drawn from a different distribution than $D_{tr}$ (Ovadia et al., 2019). The ability of methods to resist adversarial input perturbations as measured by the success rate of different adversarial attacks is also an important property (Goodfellow et al., 2015; Madry et al., 2018; Carlini & Wagner, 2017). We note that in the Bayesian supervised learning context, these attack methods require access to the posterior predictive distribution function and in many cases its gradients (Vadera et al., 2020b).

**Scalability:** Of primary interest in this work are how the accuracy, uncertainty quantification and robustness properties of methods trade off against their computational scalability properties with the goal of better understanding which methods offer the best trade-offs in different computational contexts (e.g., cluster, embedded system, etc.). The storage cost can be estimated via the number of parameters and the size of stored models (if variable bit depth is considered). The run-time of methods can be assessed in different ways including wall clock time as well as more portable statistics such as the number of floating point operations (flops) or multiply-accumulate operations (MACs).

### 4. URSABench Implementation Framework

In this section, we describe the current URSABench implementation framework, which leverages multiple datasets, models and tasks to implement the evaluation principles described in the previous section. The current framework includes small-scale and medium-scale benchmarks.

**Models and Data Sets:** The small-scale benchmark uses a basic, fully connected MLP with two hidden layers containing 200 units each as the benchmark model, with MNIST providing the benchmark in-domain data set (LeCun, 1998). At the medium-scale, we use ResNet50 (He et al., 2016) and WideResNet as the benchmark models (Zagoruyko & Komodakis, 2016), with CIFAR10 and CIFAR100 as the benchmark in-domain data sets (Krizhevsky et al., 2009).

**Tasks and Metrics:** The approximate parameter posterior and posterior predictive distribution are produced using each benchmark in-domain training set. Accuracy is assessed using the corresponding in-domain test sets. To assess uncertainty quantification, we compute negative log likelihood, Brier score, and performance on a misclassification detection task, all using the in-domain test sets. We also consider a decision-making task that focuses on assessing the quality of the tail of the predictive distribution using imbalanced data sets and costs that strongly penalize errors on the rare classes (Cobb et al., 2018) (see Appendix A for details). We assess robustness using an out-of-distribution (OOD) classification task (Ovadia et al., 2019; Vadera et al., 2020a) leveraging knowledge uncertainty (see Appendix B for a review of uncertainty decomposition). The small-scale benchmark uses Fashion-MNIST (Xiao et al., 2017) and KMNIST (Clanuwat et al., 2018) as OOD test sets, while the medium-scale benchmark uses SVHN (Netzer et al., 2011) and STL10 (Coates et al., 2011) as OOD test sets. Performance on OOD tasks is assessed using AUROC. Finally, the current version of the benchmark focuses on computation time as the measure of computational scalability, measured in seconds/sample.

**Composite Scores:** The simultaneous assessment of mul-

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**Table 1. URSABench small-scale benchmark performance. Results presented as mean ± std. dev. across 5 trials.**

| Inference | Accuracy ↑ | NLL ↓ | Robustness ↑ | Uncertainty ↑ | Scalability ↓ |
|-----------|------------|------|--------------|---------------|---------------|
| HMC       | 0.9819 ± 0.0010 | 0.0593 ± 0.0016 | 0.9570 ± 0.0075 | 0.9734 ± 0.0012 | 0.72 ± 0.01 |
| SGLD      | 0.9839 ± 0.0004 | 0.0492 ± 0.0022 | 0.9065 ± 0.0377 | 0.9679 ± 0.0233 | 2.02 ± 0.02 |
| SGHMC     | 0.9862 ± 0.0003 | 0.0446 ± 0.0003 | 0.9426 ± 0.0048 | 0.9807 ± 0.0003 | 2.03 ± 0.02 |
| cSGLD     | 0.9857 ± 0.0003 | 0.0476 ± 0.0011 | 0.9521 ± 0.0022 | 0.9795 ± 0.0007 | 14.08 ± 0.05 |
| cSGHMC    | 0.9836 ± 0.0009 | 0.0533 ± 0.0016 | 0.9276 ± 0.0094 | 0.9759 ± 0.0015 | 14.77 ± 0.03 |
| PCA + ESS (SI) | 0.9840 ± 0.0007 | 0.0520 ± 0.0016 | 0.9360 ± 0.0038 | 0.9695 ± 0.0012 | 70.67 ± 0.20 |
| MC dropout | 0.9858 ± 0.0007 | 0.0501 ± 0.0031 | 0.9429 ± 0.0059 | 0.9769 ± 0.0019 | 2.02 ± 0.03 |
| SGD       | 0.9860 ± 0.0002 | 0.0452 ± 0.0012 | -             | -              | 2.03 ± 0.02 |

**Table 2. URSABench medium-scale benchmark performance.**

| Inference | Accuracy ↑ | NLL ↓ | Robustness ↑ | Uncertainty ↑ | Scalability ↓ |
|-----------|------------|------|--------------|---------------|---------------|
| SGLD      | 0.869      | 0.524 | 0.803        | 0.916         | 129.3         |
| SGHMC     | 0.868      | 0.539 | 0.808        | 0.916         | 129.3         |
| cSGLD     | 0.892      | 0.396 | 0.810        | 0.912         | 2103.3        |
| cSGHMC    | 0.886      | 0.443 | 0.798        | 0.898         | 2114.9        |
| PCA + ESS (SI) | 0.869 | 0.482 | 0.804 | 0.901 | 1940.0 |
| MC dropout | 0.872      | 0.554 | 0.775        | 0.914         | 127.6         |
| SGD       | 0.861      | 0.625 | -            | -             | 127.7         |
tiple aspects of performance is the focus of URSABench. However, this yields many individual results for each inference method. An important design choice in URSABench is thus to summarize performance in terms of key selected individual metrics along with composite scores that combine related individual metrics. For accuracy we include an average over all benchmark models and all in-domain test sets. For robustness, we use an average over all models and OOD data sets. For uncertainty quantification, we separately compute an average over models and data sets in terms of negative log likelihood (NLL) and misclassification task performance.

5. URSABench Benchmark Results

In this section we report the initial benchmark results obtained using URSABench.

Inference Methods: We focus on benchmarking Monte Carlo methods including HMC\(^2\), SGLD (Welling & Teh, 2011), SGHMC (Chen et al., 2014), cSGLD, cSGHMC (Zhang et al., 2020), SWAG (Maddox et al., 2019) and PCA-based subspace inference + elliptical slice sampling (PCA+ESS (SI)) (Izmailov et al., 2019). As baselines, we also provide MC dropout (Gal & Ghahramani, 2016) and an SGD-point estimated model. Implementation details for the inference schemes have been provided in Appendix D.

Small-Scale Benchmark Results: The small-scale results are displayed in Table 1. The detailed experimental results behind each composite score can be found in Appendix E. The small-scale results show how challenging it can be to distinguish between different approximate inference schemes using relatively simple models and data sets. SGD and SGHMC are both marginally ahead in accuracy and NLL; HMC appears to show the most robust performance in OOD and SGHMC does best for the uncertainty metric. However the minor relative difference between all the performance metrics points to focusing on the compute time which shows HMC to be significantly less time consuming. This is due to the ability to fit all the data and model parameters on the GPU.

Medium-Scale Benchmark Results: The medium-scale results are displayed in Table 2. The detailed experimental results behind each composite score can again be found in Appendix E. Overall, the medium-scale experiments indicate a slight improvement on the predictive performance and decision-making tasks from both cSGHMC, and cSGLD followed by PCA + ESS (SI). However, once again a user may prefer using MC dropout or SGLD/SGHMC as they provide respectable performance in significantly less time. This is due to the large proportion of time that the cyclic schemes spend exploring without sampling. Furthermore, if the goal is to compute uncertainty metrics and ultimately use them for misclassification detection or OOD detection, then SGHMC/SGLD provide better performance in a majority of the cases. Another important result that can be seen from the Tables 6, 9, 12 and 15 in Appendix E is the demonstrated utility of the decision-making task in its ability to highlight the top performing approximate inference schemes for each model and data set, via its correlation with low NLL and high accuracy.

6. Conclusion and Future Work

This paper describes initial work on URSABench, a framework for benchmarking the performance of approximate Bayesian inference methods for deep neural networks. We hope that the development of this benchmarking toolbox will help to accelerate research in the domain of approximate Bayesian inference by helping to expose the trade-offs achieved by methods in terms of uncertainty, robustness, scalability and accuracy. We believe the simultaneous assessment of these properties is critical to better understand which methods are most effective on different downstream tasks and in different deployment contexts.

A further clear challenge in the development of this toolbox is ensuring a fair comparison between approaches. However, this can be difficult for new model/method/data set combinations without established hyperparameters, requiring careful hyperparameter optimization. This requirement highlights the issue of how to benchmark the end-to-end process of hyperparameter optimization and inference in terms of computational resource use.

As a first line of future work, we plan to continue to implement tasks and metrics to fully reflect all of the evaluation principles described in this paper. Important tasks and metrics yet to be implemented include robustness to adversarial examples (Vadera et al., 2020b) and common corruptions (Hendrycks & Dietterich, 2019), and assessment of test-time computational scalability. We further plan to add a large-scale benchmark that current approximate inference schemes will find challenging. Finally, we aim to expand the scope of models and data sets to include architectures such as recurrent neural networks and graph convolutional networks to provide a broader assessment of approximate inference methods.

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A. Decision-making task

Bayesian decision theory takes Monte Carlo samples and averages them over a predetermined cost function, C(h, y) to result in an expected risk:

$$R(h|x) \approx \frac{1}{S} \sum_{s=1}^{S} p(y|x, \theta_s)C(h, y).$$

The expected risk is a function of the decision, h, whereby the Bayesian optimal decision, h∗ minimises the risk:

$$h^* = \arg\min_{h} R(h|x).$$

Once we have applied Bayesian decision theory to find an h∗ for every input x, for supervised classification, we can then determine the true cost of the decision taken by averaging over the test data (i.e. \( \frac{1}{N} \sum_{n=1}^{N} C(y_n^{True}, h_n^{opt}) \)), where the arguments have been reversed such that we compare the true label y_n^{True}, with the Bayesian optimal decision h_n^{opt} (i.e. what cost did we actually have to pay when we took decision h_n^{opt} for labelling y_n, when it was in fact y_n^{True}). A more detailed discussion can be seen in Ch. 4 of Cobb (2020).

The purpose of the decision-making task is to penalise inference schemes that provide poor calibrated uncertainty over the rarer (and hence more uncertain) classes. In particular, for MNIST, we retrain our models over a highly imbalanced data set, where 90% of the labels corresponding to classes 3 and 7 are removed. However, we then use the predictive distribution to with a predefined cost function to select the Bayes optimal decision for each predicted label. We then calculate the expected decision cost by averaging over the costs attributed to each decision compared to the true label. False negatives of the less frequent classes are penalised 1000 times more than false positives for the rest of the classes.

The small-scale setting for the decision-making task requires retraining over an imbalanced training set. However,
for the medium-scale task we limit ourselves to using the same materialised samples from the balanced data set (although we expect to extend this to imbalanced training data in future work). We define our cost matrix to penalise false negatives 10 times as much as false positives. In particular, the task for the CIFAR10 penalises planes, automobiles, ships and trucks with a cost of 1.0 for false negatives and 0.1 for false positives. All other errors are penalised with 0.1 and correct decisions accrue zero cost. The same cost structure applies to CIFAR100, where tanks, rockets and pick-up trucks are deemed the critical classes.

The decision costs in Tables 6, 9, 12 and 15 demonstrate the utility of this task as they show a correlation with the NLL and the accuracy across all models and data sets.

B. Uncertainty Decomposition for downstream tasks

The posterior predictive distribution is not the only statistic of the posterior distribution that is of interest. The decomposition of posterior uncertainty has also received recent attention in the literature. For example, Depeweg et al. (2017) and Malinin et al. (2020) describe the decomposition of the entropy of the posterior predictive distribution (the total uncertainty) into expected data uncertainty and knowledge uncertainty. These three forms of uncertainty are related by the equation shown below:

$$
I[y, \theta | x, D] = \mathcal{H}[\mathcal{E}_p(\theta | D)] \mathcal{P}(y | x, \theta)] - \mathbb{E}p(\theta | D)[\mathcal{H}\mathcal{P}(y | x, \theta)]
$$

Total uncertainty, as the name suggests, measures the total uncertainty in a prediction. Expected data uncertainty measures the uncertainty arising from class overlap. Knowledge uncertainty corresponds to the conditional mutual information between labels and model parameters and measures the disagreement between different models in the posterior. However, it can be efficiently computed as the difference between total uncertainty and expected data uncertainty, both of which are (functions) of posterior expectations. In recent work, Wang et al. (2018), Malinin et al. (2020) and Vadera et al. (2020a) have leveraged this decomposition to explore a range of down-stream tasks that rely on uncertainty quantification and decomposition.

C. Composite Score Breakdown

As alluded to in the main text, we build composite scores for robustness and uncertainty. The robustness relies on averaging both the total uncertainty AUROC and the model uncertainty AUROC over the OOD data sets. We then average once again over the mean total uncertainty and model uncertainty. The uncertainty composite score is built from the average misclassification AUROCs (e.g. the first three columns of Tables 5, 8, 11, 14, 17). For the medium-scale experiment the uncertainty score is then averaged across CIFAR10 and CIFAR100 as well as ResNet50 and WideResNet28x10.

D. Implementation Details

In this section, we describe the implementation details for the different inference methods used in our benchmark. It must be noted that for all inference methods using ResNet50 and WideResNet28x10 models, we use a pre-trained SGD solution to warm-start our samplers. This is a standard pretraining procedure followed to make the methods more competitive (Maddox et al., 2019).

Further, the ensemble size is set to 50 for CIFAR datasets, and 100 for MNIST dataset. The difference in ensemble size is due to the large amount of computational requirements for training ResNet50 and WideResNet28x10 on CIFAR datasets. While tuning hyperparameters for MNIST, we apply Bayesian optimization with a limit of 200 evaluations for each approach (Balandat et al., 2019). On the other hand, for CIFAR datasets, we refer to existing literature and use the same hyperparameters if directly applicable, or search around the hyperparameters obtained for similar models and datasets.

SGLD: For CIFAR datasets, we use a burn-in of 100 epochs and initial learning rates of 0.1 for WideResNet28x10 model and 0.05 for ResNet50. The prior std. dev. is set to 1 for both the cases. We decay the learning rate using cosine annealing schedule to its half value by the end of sampling. For MNIST, the optimal hyperparameter values obtained are: initial learning rate of 0.099, prior std. dev. of 0.16 and 50 burn in epochs.

SGHMC: We use the same hyperparameters and learning rate schedule as described for SGLD for the CIFAR datasets. Additionally, we set the friction term to 0.5 (Chen et al., 2014). This is equivalent to the $\alpha$ term shown in Zhang et al. (2020). For MNIST, the optimal hyperparameter values obtained are: initial learning rate of 0.03, prior std. dev. of 0.14, 50 burn in epochs, and friction term set to 0.1.

cSGHMC: We use the same hyperparameters given in Zhang et al. (2020) for CIFAR datasets. For MNIST, the optimal hyperparameter values obtained are: initial learning rate of 0.06, prior std. dev. of 0.33, cycle length of 22 epochs, of which 17 epochs are used for SGD-exploration phase, and samples are collected from the last 4 epochs,
and friction term set to 0.21.

**cSGLD:** We use the same hyperparameters given in Zhang et al. (2020) for CIFAR datasets. For MNIST, the optimal hyperparameter values obtained are: initial learning rate of 0.06, prior std. dev. of 0.33, cycle length of 22 epochs, of which 17 epochs are used for SGD-exploration phase, and samples are collected from the last 4 epochs, and friction term set to 0.21.

**SWAG:** We use the same hyperparameters given in Izmailov et al. (2019) for CIFAR models, except that we set the weight decay for ResNet models to $10^{-4}$ and borrow its remaining hyperparameters from WideResNet28x10. This means that we utilize last 20 SGD iterates to find parameters for the gaussian approximation to the mode. For MNIST, we start with an initial learning rate of 0.018 and decay it 0.0006 over 50 epochs. Further, we run SGD at the same learning rate for another 50 epochs and collect the final 20 iterates to construct our SWAG approximation. The momentum for our SGD optimizer is set to 0.7 through the entire run. Furthermore, the variant of SWAG used in our benchmark is SWAG-diagonal.

**PCA + ESS (SI):** We use the same hyperparameters given in Izmailov et al. (2019) for CIFAR models, except that we set the weight decay for ResNet models to $10^{-4}$ and borrow its remaining hyperparameters from WideResNet28x10. We construct a subspace of rank 20 for all models and datasets. For MNIST, we start with an initial learning rate of 0.04 and decay it 0.002 over 50 epochs. Further, we run SGD at the same learning rate for another 50 epochs and collect the iterates from each of the final 20 epochs to construct our PCA subspace. The momentum for our SGD optimizer is set to 0.54 through the entire run. For all the dataset and model combinations, we use elliptical slice sampling (Murray et al., 2010) on the low rank PCA subspace with a prior of 2. and a temperature of 5000.

**MC Dropout:** For all the models on CIFAR datasets, we use a dropout of 0.2 before the final linear layer while we use dropout after both hidden layers for MNIST-MLP200 with a dropout rate of 0.04.

### E. Additional Experimental Results

Additional experimental results are provided in Tables 3 - 17.
Table 3. Comparison of predictive performance and decision making cost while using an MLP [784, 200, 200, 10] on MNIST. Results presented as mean ± std. dev. across 5 trials.

| Inference     | Accuracy | NLL       | BS        | ECE        | Decision Cost | Samples/second |
|---------------|----------|-----------|-----------|------------|---------------|----------------|
| HMC           | 98.19 ± 0.10% | 0.0593 ± 0.0016 | 0.0280 ± 0.0008 | 0.0079 ± 0.0008 | 7101 ± 346 | 0.72 ± 0.01 |
| SGLD          | 98.39 ± 0.04% | 0.0492 ± 0.0022 | 0.0236 ± 0.0005 | 0.0041 ± 0.0024 | 5410 ± 778 | 2.02 ± 0.02 |
| SGHMC         | 98.62 ± 0.03% | 0.0446 ± 0.0003 | 0.0210 ± 0.0002 | 0.0073 ± 0.0004 | 5408 ± 240 | 2.03 ± 0.02 |
| cSGLD         | 98.57 ± 0.03% | 0.0476 ± 0.0011 | 0.0223 ± 0.0003 | 0.0056 ± 0.0003 | 6526 ± 2241 | 14.08 ± 0.05 |
| cSGHMC        | 98.36 ± 0.09% | 0.0533 ± 0.0016 | 0.0256 ± 0.0010 | 0.0033 ± 0.0003 | 4824 ± 1855 | 14.77 ± 0.03 |
| PCA + ESS (SI)| 98.40 ± 0.07% | 0.0520 ± 0.0016 | 0.0251 ± 0.0007 | 0.0036 ± 0.0005 | 3809 ± 1150 | 70.67 ± 0.20 |
| MC dropout    | 98.58 ± 0.07% | 0.0501 ± 0.0031 | 0.0218 ± 0.0008 | 0.0042 ± 0.0006 | 15236 ± 1184 | 2.02 ± 0.07 |
| SGD           | 98.60 ± 0.02% | 0.0452 ± 0.0012 | 0.0213 ± 0.0003 | 0.0032 ± 0.0005 | 8613 ± 1428 | 2.03 ± 0.02 |

Table 4. Comparison of OOD detection performance while using an MLP [784, 200, 200, 10] on MNIST. Results presented as mean ± std. dev. across 5 trials.

| Inference              | OOD Dataset       | AUROC- Model Uncertainty ↑ | AUROC - Total Uncertainty ↑ |
|------------------------|-------------------|-----------------------------|----------------------------|
| HMC                    | Fashion MNIST     | 0.966 ± 0.013               | 0.946 ± 0.017              |
|                        | KMNIST            | 0.968 ± 0.013               | 0.948 ± 0.017              |
| SGLD                   | Fashion MNIST     | 0.867 ± 0.110               | 0.944 ± 0.005              |
|                        | KMNIST            | 0.871 ± 0.103               | 0.944 ± 0.005              |
| SGHMC                  | Fashion MNIST     | 0.933 ± 0.009               | 0.953 ± 0.010              |
|                        | KMNIST            | 0.932 ± 0.009               | 0.952 ± 0.010              |
| cSGLD                  | Fashion MNIST     | 0.954 ± 0.004               | 0.950 ± 0.005              |
|                        | KMNIST            | 0.954 ± 0.004               | 0.950 ± 0.005              |
| cSGHMC                 | Fashion MNIST     | 0.923 ± 0.021               | 0.931 ± 0.017              |
|                        | KMNIST            | 0.923 ± 0.020               | 0.933 ± 0.017              |
| PCA + ESS (SI)         | Fashion MNIST     | 0.933 ± 0.006               | 0.938 ± 0.009              |
|                        | KMNIST            | 0.934 ± 0.006               | 0.940 ± 0.009              |
| MC dropout             | Fashion MNIST     | 0.942 ± 0.013               | 0.943 ± 0.010              |
|                        | KMNIST            | 0.943 ± 0.013               | 0.944 ± 0.010              |
| SGD                    | Fashion MNIST     | N/A                         | 0.945 ± 0.010              |
|                        | KMNIST            | N/A                         | 0.943 ± 0.010              |

Table 5. Comparison of misclassification detection while using an MLP [784, 200, 200, 10] on MNIST.

| Inference     | AUROC- Model Confidence ↑ | AUROC- Total Confidence ↑ | AUROC- Model Uncertainty ↑ | AUROC- Total Uncertainty ↑ | AUROCPR- Model Uncertainty ↑ | AUROCPR- Total Uncertainty ↑ | AUROCPR- Model Confidence ↑ |
|---------------|---------------------------|---------------------------|---------------------------|---------------------------|-----------------------------|-----------------------------|---------------------------|
| HMC           | 0.9706                    | 0.9734                    | 0.9743                    | 0.3429                    | 0.3888                      | 0.4145                      | 0.4145                    |
| SGLD          | 0.9739                    | 0.9800                    | 0.9800                    | 0.3530                    | 0.4502                      | 0.4632                      | 0.4632                    |
| SGHMC         | 0.9786                    | 0.9815                    | 0.9823                    | 0.3546                    | 0.3929                      | 0.4131                      | 0.4131                    |
| cSGLD         | 0.9769                    | 0.9801                    | 0.9798                    | 0.3695                    | 0.4477                      | 0.4478                      | 0.4478                    |
| cSGHMC        | 0.9730                    | 0.9786                    | 0.9786                    | 0.3260                    | 0.4255                      | 0.4404                      | 0.4404                    |
| PCA + ESS (SI)| 0.9539                    | 0.9774                    | 0.9772                    | 0.2059                    | 0.4298                      | 0.4248                      | 0.4248                    |
| MC dropout    | 0.9754                    | 0.9763                    | 0.976                     | 0.4085                    | 0.43                        | 0.4199                      | 0.4199                    |
| SGD           | N/A                       | 0.9795                    | 0.9794                    | N/A                       | 0.4273                      | 0.4389                      | 0.4389                    |
| Inference      | Accuracy ↑ | NLL ↓ | BS ↓ | ECE ↓ | Decision Cost ↓ |
|---------------|------------|------|------|-------|-----------------|
| SGLD          | 0.954      | 0.144 | 0.069 | 0.009 | 139.500         |
| SGHMC         | 0.954      | 0.144 | 0.068 | 0.011 | 138.100         |
| cSGLD         | 0.966      | 0.128 | 0.053 | 0.020 | 112.100         |
| cSGHMC        | 0.951      | 0.243 | 0.086 | 0.106 | 153.900         |
| SWAG          | 0.931      | 0.311 | 0.114 | 0.047 | 200.900         |
| PCA + ESS (SI)| 0.949      | 0.174 | 0.080 | 0.027 | 166.600         |
| MC dropout    | 0.948      | 0.208 | 0.083 | 0.032 | 159.500         |
| SGD           | 0.943      | 0.274 | 0.095 | 0.040 | 171.700         |

| Inference      | AUROC- Model Uncertainty ↑ | AUROC - Total Uncertainty ↑ |
|---------------|-----------------------------|-----------------------------|
| SGLD          | 0.677                       | 0.684                       |
| SVHN          | 0.948                       | 0.945                       |
| SGHMC         | STL10 0.682                 | 0.687                       |
| SVHN          | ST10 0.949                  | 0.955                       |
| cSGLD         | STL10 0.624                 | 0.641                       |
| SVHN          | STL10 0.966                 | 0.968                       |
| cSGHMC        | STL10 0.631                 | 0.657                       |
| SVHN          | STL10 0.920                 | 0.945                       |
| SWAG          | STL10 0.618                 | 0.671                       |
| SVHN          | STL10 0.878                 | 0.908                       |
| PCA + ESS (SI)| STL10 0.673                 | 0.677                       |
| SVHN          | STL10 0.949                 | 0.947                       |
| MC dropout    | STL10 0.665                 | 0.695                       |
| SVHN          | ST10 0.926                  | 0.938                       |
| SGD           | STL10 N/A                   | 0.682                       |
|               | SVHN N/A                    | 0.892                       |

| Inference      | AUROC- Model Confidence ↑  | AUROC - Total Confidence ↑ |
|---------------|-----------------------------|-----------------------------|
| SGLD          | 0.945                       | 0.949                       |
| SGHMC         | 0.943                       | 0.949                       |
| cSGLD         | 0.927                       | 0.943                       |
| cSGHMC        | 0.885                       | 0.935                       |
| SWAG          | 0.890                       | 0.927                       |
| PCA + ESS (SI)| 0.932                       | 0.934                       |
| MC dropout    | 0.946                       | 0.947                       |
| SGD           | N/A                         | 0.937                       |

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**Table 6.** Comparison of predictive performance and decision making cost while using ResNet50 on CIFAR10.

**Table 7.** Comparison of OOD detection performance while using ResNet50 on CIFAR10.

**Table 8.** Comparison of Misclassification detection while using ResNet50 on CIFAR10.
Table 9. Comparison of predictive performance and decision making cost while using ResNet50 on CIFAR100.

| Inference | Accuracy ↑ | NLL ↓ | BS ↓ | ECE ↓ | Decision Cost ↓ |
|-----------|------------|-------|------|-------|-----------------|
| SGLD      | 0.751      | 1.079 | 0.364| 0.107 | 277.500         |
| SGHMC     | 0.755      | 1.084 | 0.362| 0.103 | 272.500         |
| cSGLD     | 0.804      | 0.711 | 0.272| 0.019 | 211.900         |
| cSGHMC    | 0.814      | 0.667 | 0.261| 0.012 | 198.500         |
| SWAG      | 0.735      | 1.221 | 0.400| 0.135 | 295.200         |
| PCA + ESS (SI) | 0.761   | 0.920 | 0.335| 0.032 | 261.200         |
| MC dropout| 0.786      | 1.006 | 0.330| 0.115 | 233.100         |
| SGD       | 0.732      | 1.302 | 0.408| 0.148 | 303.700         |

Table 10. Comparison of OOD detection performance while using ResNet50 on CIFAR100.

| Inference | OOD Dataset | AUROC- Model Uncertainty ↑ | AUROC - Total Uncertainty ↑ | AUROC- Model Confidence ↑ | AUROC - Total Confidence ↑ |
|-----------|-------------|-----------------------------|-----------------------------|----------------------------|-----------------------------|
| SGLD      | STL10       | 0.769                       | 0.782                       |                            |                             |
|           | SVHN        | 0.772                       | 0.802                       |                            |                             |
| SGHMC     | STL10       | 0.773                       | 0.784                       |                            |                             |
|           | SVHN        | 0.809                       | 0.823                       |                            |                             |
| cSGLD     | STL10       | 0.806                       | 0.827                       |                            |                             |
|           | SVHN        | 0.809                       | 0.816                       |                            |                             |
| cSGHMC    | STL10       | 0.804                       | 0.832                       |                            |                             |
|           | SVHN        | 0.791                       | 0.823                       |                            |                             |
| SWAG      | STL10       | 0.748                       | 0.778                       |                            |                             |
|           | SVHN        | 0.732                       | 0.771                       |                            |                             |
| PCA + ESS (SI) | STL10 | 0.779                       | 0.797                       |                            |                             |
|           | SVHN        | 0.816                       | 0.807                       |                            |                             |
| MC dropout| STL10       | 0.785                       | 0.801                       |                            |                             |
|           | SVHN        | 0.755                       | 0.752                       |                            |                             |
| SGD       | STL10       | N/A                         | 0.765                       |                            |                             |
|           | SVHN        | N/A                         | 0.763                       |                            |                             |

Table 11. Comaparison of Misclassification detection while using ResNet50 on CIFAR100.

| Inference | AUROC- Model Uncertainty ↑ | AUROC - Total Uncertainty ↑ | AUROC- Model Confidence ↑ | AUROC - Total Confidence ↑ |
|-----------|-----------------------------|-----------------------------|----------------------------|-----------------------------|
| SGLD      | 0.870                       | 0.882                       | 0.897                       | 0.648                       | 0.683                       | 0.672                       |
| SGHMC     | 0.863                       | 0.873                       | 0.871                       | 0.635                       | 0.659                       | 0.651                       |
| cSGLD     | 0.872                       | 0.880                       | 0.891                       | 0.564                       | 0.623                       | 0.654                       |
| cSGHMC    | 0.873                       | 0.879                       | 0.890                       | 0.572                       | 0.593                       | 0.626                       |
| SWAG      | 0.855                       | 0.870                       | 0.869                       | 0.625                       | 0.671                       | 0.667                       |
| PCA + ESS (SI) | 0.858 | 0.863                       | 0.877                       | 0.618                       | 0.634                       | 0.667                       |
| MC dropout| 0.875                       | 0.880                       | 0.877                       | 0.613                       | 0.639                       | 0.624                       |
| SGD       | N/A                         | 0.873                       | 0.870                       | N/A                         | 0.687                       | 0.680                       |
### Table 12. Comparison of predictive performance and decision making cost while using WideResNet28x10 on CIFAR10.

| Inference  | Accuracy ↑ | NLL ↓ | BS ↓ | ECE ↓ | Decision Cost ↓ |
|------------|------------|-------|------|-------|-----------------|
| SGLD       | 0.965      | 0.113 | 0.054| 0.004 | 115.800         |
| SGHMC      | 0.965      | 0.114 | 0.053| 0.004 | 112.200         |
| cSGLD      | 0.967      | 0.104 | 0.050| 0.006 | 102.900         |
| cSGHMC     | 0.957      | 0.196 | 0.072| 0.079 | 140.800         |
| SWAG       | 0.919      | 0.260 | 0.121| 0.028 | 270.000         |
| PCA + ESS (SI) | 0.951  | 0.177 | 0.082| 0.054 | 163.100         |
| MC dropout | 0.957      | 0.158 | 0.067| 0.019 | 149.000         |
| SGD        | 0.963      | 0.138 | 0.060| 0.018 | 117.100         |

### Table 13. Comparison of OOD detection performance while using WideResNet28x10 on CIFAR10.

| Inference          | OOD Dataset | AUROC - Model Uncertainty ↑ | AUROC - Total Uncertainty ↑ |
|--------------------|-------------|-----------------------------|-----------------------------|
| SGLD               | STL10       | 0.680                       | 0.680                       |
|                    | SVHN        | 0.951                       | 0.963                       |
| SGHMC              | STL10       | 0.678                       | 0.683                       |
|                    | SVHN        | 0.956                       | 0.967                       |
| cSGLD              | STL10       | 0.685                       | 0.686                       |
|                    | SVHN        | 0.968                       | 0.974                       |
| cSGHMC             | STL10       | 0.614                       | 0.648                       |
|                    | SVHN        | 0.864                       | 0.952                       |
| SWAG               | STL10       | 0.649                       | 0.667                       |
|                    | SVHN        | 0.914                       | 0.943                       |
| PCA + ESS (SI)     | STL10       | 0.663                       | 0.673                       |
|                    | SVHN        | 0.897                       | 0.970                       |
| MC dropout         | STL10       | 0.672                       | 0.688                       |
|                    | SVHN        | 0.897                       | 0.922                       |
| SGD                | STL10       | N/A                         | 0.667                       |
|                    | SVHN        | N/A                         | 0.963                       |

### Table 14. Comparison of Misclassification detection while using WideResNet28x10 on CIFAR10.

| Inference          | AUROC- Model Uncertainty ↑ | AUROC - Total Uncertainty ↑ | AUROC- Model Confidence ↑ | AUCPR- Model Uncertainty ↑ | AUCPR - Total Uncertainty ↑ | AUCPR- Model Confidence ↑ |
|--------------------|-----------------------------|-----------------------------|---------------------------|---------------------------|-----------------------------|---------------------------|
| SGLD               | 0.952                       | 0.954                       | 0.955                     | 0.402                     | 0.414                       | 0.435                     |
| SGHMC              | 0.954                       | 0.956                       | 0.958                     | 0.380                     | 0.415                       | 0.439                     |
| cSGLD              | 0.949                       | 0.952                       | 0.953                     | 0.354                     | 0.383                       | 0.406                     |
| cSGHMC             | 0.889                       | 0.936                       | 0.945                     | 0.298                     | 0.382                       | 0.452                     |
| SWAG               | 0.900                       | 0.915                       | 0.916                     | 0.375                     | 0.468                       | 0.468                     |
| PCA + ESS (SI)     | 0.918                       | 0.931                       | 0.948                     | 0.337                     | 0.387                       | 0.478                     |
| MC dropout         | 0.946                       | 0.947                       | 0.947                     | 0.432                     | 0.467                       | 0.467                     |
| SGD                | N/A                         | 0.941                       | 0.942                     | N/A                       | 0.390                       | 0.387                     |
Table 15. Comparison of predictive performance and decision making cost while using WideResNet28x10 on CIFAR100.

| Inference     | Accuracy ↑ | NLL ↓  | BS ↓  | ECE ↓  | Decision Cost ↓ |
|---------------|------------|--------|-------|--------|-----------------|
| SGLD          | 0.809      | 0.760  | 0.278 | 0.066  | 204.300         |
| SGHMC         | 0.798      | 0.815  | 0.292 | 0.076  | 216.200         |
| cSGLD         | 0.832      | 0.640  | 0.242 | 0.033  | 179.300         |
| cSGHMC        | 0.821      | 0.666  | 0.258 | 0.059  | 191.800         |
| SWAG          | 0.710      | 1.149  | 0.414 | 0.110  | 316.900         |
| PCA + ESS (SI)| 0.817      | 0.656  | 0.263 | 0.038  | 196.600         |
| MC dropout    | 0.798      | 0.846  | 0.293 | 0.081  | 214.300         |
| SGD           | 0.806      | 0.785  | 0.280 | 0.046  | 205.100         |

Table 16. Comparison of OOD detection performance while using WideResNet28x10 on CIFAR100.

| Inference     | OOD Dataset | AUROC- Model Uncertainty ↑ | AUROC- Total Uncertainty ↑ |
|---------------|-------------|----------------------------|----------------------------|
| SGLD          | STL10       | 0.797                      | 0.822                      |
| SGHMC         | STL10       | 0.799                      | 0.814                      |
| cSGLD         | STL10       | 0.791                      | 0.846                      |
| cSGHMC        | STL10       | 0.816                      | 0.845                      |
| SWAG          | STL10       | 0.732                      | 0.753                      |
| PCA + ESS (SI)| STL10       | 0.813                      | 0.827                      |
| MC dropout    | STL10       | 0.798                      | 0.815                      |
| SGD           | SVHN        | N/A                        | 0.820                      |

Table 17. Comparison of Misclassification detection while using WideResNet28x10 on CIFAR100.

| Inference     | AUROC- Model Uncertainty ↑ | AUROC- Total Uncertainty ↑ | AUROC- Model Confidence ↑ | AUROC- Model Uncertainty ↑ | AUROC- Total Uncertainty ↑ | AUROC- Model Confidence ↑ |
|---------------|----------------------------|----------------------------|----------------------------|----------------------------|----------------------------|----------------------------|
| SGLD          | 0.881                      | 0.888                      | 0.892                      | 0.579                      | 0.616                      | 0.629                      |
| SGHMC         | 0.884                      | 0.893                      | 0.894                      | 0.625                      | 0.650                      | 0.654                      |
| cSGLD         | 0.870                      | 0.874                      | 0.892                      | 0.499                      | 0.543                      | 0.595                      |
| cSGHMC        | 0.854                      | 0.865                      | 0.888                      | 0.516                      | 0.553                      | 0.609                      |
| SWAG          | 0.837                      | 0.857                      | 0.860                      | 0.601                      | 0.675                      | 0.686                      |
| PCA + ESS (SI)| 0.853                      | 0.868                      | 0.888                      | 0.520                      | 0.559                      | 0.603                      |
| MC dropout    | 0.883                      | 0.887                      | 0.887                      | 0.617                      | 0.638                      | 0.637                      |
| SGD           | N/A                       | 0.869                      | 0.879                      | N/A                       | 0.586                      | 0.622                      |