Rapid Risk Minimization with Bayesian Models Through Deep Learning Approximation

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Abstract—We introduce a novel combination of Bayesian Models (BM) and Neural Networks (NN) for making predictions with a minimum expected risk. Our approach combines the best of both worlds, the data efficiency and interpretability of a BM with the speed of a NN. For a BM, making predictions with the lowest expected loss requires integrating over the posterior distribution. When exact inference of the posterior predictive distribution is intractable, approximation methods are typically applied, e.g., Monte Carlo (MC) simulation. For MC, the variance of the estimator decreases with the number of samples – but at the expense of increased computational cost. Our approach removes the need for iterative MC simulation on the CPU at prediction time. In brief, it works by fitting a NN to synthetic data generated using the BM. In a single feed-forward pass, the NN gives a set of point-wise approximations to the BM’s posterior predictive distribution for a given observation. We achieve risk minimized predictions significantly faster than standard methods with a negligible loss on the test dataset. We combine this approach with Active Learning (AL) to minimize the amount of data required for fitting the NN. This is done by iteratively labeling more data in regions with high predictive uncertainty of the NN.

Index Terms—Bayesian Models, Neural Networks, Active Learning, Bayes’ risk

I. INTRODUCTION

The toolbox of machine learning is ever-growing and contains a wide spectrum of tools. Each new tool has its advantages and drawbacks. Neural Networks (NNs), for instance, are model free, universal approximators capable of learning complex characteristics and generally allow for making fast predictions once fitted. Their drawbacks are, among others, the need for a vast amount of data, difficulty to debug, and lack of interpretability. At the other end of the spectrum, we have model based methods like Probabilistic Graphical Models (PGMs). PGMs are handcrafted models describing the process of how the observed data arose. To learn the parameters of these models, Bayesian inference can be applied through the use of Bayes’ theorem. Throughout this paper, we will refer to such constructs as Bayesian Models (BMs). BMs are generative, meaning it is possible to generate synthetic data through sampling \[ p \]. Unlike NNs, BMs are data-efficient and have integrated uncertainty handling. This is at the cost of computational complexity, this being one of their main drawbacks. There are two computational issues with BMs

1) obtaining the posterior distribution over the free parameters, and 2) making predictions using the posterior predictive distribution. With the rise of sophisticated techniques for posterior inference like Variational Inference (VI) and Markov Chain Monte Carlo (MCMC), BMs have gained an increasing level of popularity over the past decades. In contrast to the former computational issue, the latter has gained little attention in academic research.

The core idea of this paper is taking the best of NNs and BMs to combine them for solving this issue through approximation. The proposed method allows one to obtain a fast approximation of the posterior predictive. In brief, it works by fitting a NN to synthetic data in which each prediction gives a set of point-wise approximations of the BM’s mean posterior predictive distribution. The method is especially useful in situations where a large number of predictions are needed, e.g., when optimizing over the posterior predictive. It utilizes each tool’s respective strengths to counter the weaknesses of the other, in particular the fast predictions of a NN with the data-efficiency of the BM. We present an algorithm on how to perform the combination of the two methods, how the approximation is conducted, and how the NN can be used as a surrogate function to enable fast, accurate, predictions. As our focus is not on obtaining the posterior distribution, we will assume a well-performing BM with parameters \( \phi \) on some dataset \( D_{\text{BM}} \) and with a well-approximated posterior distribution, \( p(\phi | D_{\text{BM}}) \).

In the following, we will first introduce some concepts from basic decision theory to define how one makes the best possible prediction given some input, hence minimizing the expected risk. This will serve as a key to understanding why making risk minimized predictions with BMs can be computationally heavy. Then, we present existing work in the field of approximating NNs to BMs. This will be followed by an introduction of the general method proposed in this paper and how it differs from related work. We do a formal analysis of the computational complexity involved in making predictions using our proposed method versus standard approaches, and present empirical results.

A. Minimizing Risk

Assume we can obtain pairs of data samples, \( (x, y) \), from some unknown joint probability distribution, \( p(X, Y) \). Now, we are given an observation \( x \) and intend to predict the correct corresponding, \( y \). We will denote this prediction, \( \tilde{y} \). Basic...
decision theory establish how one makes the best prediction in such a case by minimizing the expected loss $\mathbb{E} [\mathcal{L} (y, y')]$ which is risk minimization \(^{(1)}\), \(^{(2)}\). Throughout this paper, we are interested in regression problems and will assume a Euclidean loss function, $\mathcal{L} (y, y') = (y - y')^2$. It can be shown that the prediction, $\hat{y}$, which minimizes this expected loss is $\mathbb{E} [Y \mid X] \[^{(3)}\]$. Hence, the optimal prediction is the conditional expectation of the underlying data distribution. For other choices on the form of $\mathcal{L}$, the optimal prediction would be different \[^{(3)}\]. An oracle predicting $\hat{y} = \mathbb{E} [Y \mid X]$, would still incur some error due to the stochasticity of the data generation process, this error is sometimes called Bayes risk or Bayes error \[^{(3)}\], \[^{(4)}\]. Without access to an oracle, the ground true data distribution for most interesting problems is unknown, and we cannot compute the conditional expectation directly. Instead, one can create a model of it. If we assume a BM with a posterior distribution $p (\phi \mid D_{BM}) \propto p (D_{BM} \mid \phi) p (\phi)$, we can use $\mathbb{E} [\hat{y} \mid X]$ as a surrogate for the ground true expected conditional, where $p (\hat{y} \mid X, D_{BM})$ is the posterior predictive and $D_{BM}$ denotes the dataset used for inferring the posterior of the BM.

As we are working with a BM, the posterior predictive distribution requires marginalizing over the posterior

$$
\int p (\hat{y} \mid X, \phi) p (\phi \mid D_{BM}) \, d\phi. \quad (1)
$$

As a result, doing risk minimization with a BM requires computing the double integral

$$
\mathbb{E} [\hat{y} \mid X] = \int \hat{y} \int p (\hat{y} \mid X, \phi) p (\phi \mid D_{BM}) \, d\phi \, d\hat{y}
\begin{align*}
&= \int \mathbb{E} [\hat{y} \mid X, \phi] p (\phi \mid D_{BM}) \, d\phi.
\end{align*}

(2)

Integrating out the posterior is in most cases computationally intractable. As an approximation, one could ignore the full distribution over the posterior, and simply use a point estimate of the posterior, this point being the one with the highest probability, $\phi_{MAP}$ \[^{(4)}\]. This would constitute a Maximum a Posteriori (MAP) estimate. With uninformative priors, this would even be the Maximum Likelihood Estimate (MLE) \[^{(6)}\]. This estimate will not reflect the model's uncertainty and is not a prediction that minimizes risk. Further, using $\phi_{MAP}$ instead of marginalizing over the posterior can lead to more extreme predictions \[^{(3)}\], \[^{(6)}\].

Luckily, one can do better than MLE and MAP. One can obtain an estimate of (2) through the simple Monte Carlo (MC) estimator \[^{(7)}\], \[^{(8)}\]:

$$
\phi = \left[ \phi_m \sim p (\phi \mid D_{BM}) \right]_{m=1, \ldots, M}^T,
\hat{y} \approx \frac{1}{M} \sum_{m=1}^{M} \mathbb{E} [\hat{y} \mid X, \phi_m], \quad (3)
$$

where $M$ is the number of MC samples. Equation \(^{(3)}\) can be calculated in parallel across CPU cores as each simulation runs independently of the other. Despite MC simulation being a simple, efficient, and fairly accurate, approximation, the degree of parallelism is limited to the number of CPU cores available, and consequently insufficient in time-sensitive domains with the need for a high level of accuracy, i.e. more posterior samples used for prediction. For the most simplistic BMs, this is not a computational burden and involves only a few matrix operations. However, as the complexity of the model increases, so does the cost of making predictions. This is particularly the case for BMs requiring some form of recursion.

In section III we present a method for training a NN to predict the expectation $\mathbb{E} [\hat{y} \mid X, \phi]$ for a set of pre-generated posterior samples. This allows for computing the expectation using the NN as a surrogate, and provides a point-wise for $\phi$ approximation of the mean posterior predictive distribution in a single feed-forward pass. The mean of this set of conditional expectations constitutes an MC estimate of \(^{(2)}\), and can be used for minimizing risk when predicting. The general concept is visualized in Figure 1 which shows the transition from observational data, to a fitted BM with distributions over some parameters $\phi$, to a prediction using a NN as as surrogate for the BM.

II. RELATED WORK

There are several (dis)advantages of using BMs over NNs. Generally, BMs allow one to 1) specify prior beliefs on the parameters to be inferred, 2) explicitly model interactions between features, and 3) make decisions on how these features should affect the predictive distribution \[^{(9)}\], \[^{(10)}\]. This requires a thorough understanding of the data and domain at hand, which can be difficult, if not impossible, in some cases. However, this construct results in data-efficient models, capable of fitting even on very sparse datasets \[^{(4)}\], \[^{(11)}\]. The use of prior, likelihood, and posterior distribution, results in a strong, consistent, way of handling uncertainty throughout all aspects of the model. This is a result of the extensive use of marginalization over these distributions. This marginalization is what distinguishes the method from other pure optimization methods like NNs \[^{(12)}\]. It is also what makes many interesting BMs computationally heavy, as doing exact inference for those is not possible due to the lack of a closed-form solution. Therefore, a variety of approximation tools have been explored to overcome the computational demand for the integrals involved in the marginalization procedure \[^{(2)}\], \[^{(3)}\], \[^{(9)}\].

The theoretical framework is inherently founded on probability theory. Therefore, the Machine Learning (ML) community has adopted and applied many concepts from Bayesian theory in their work to improve NNs \[^{(12)}\]–\[^{(21)}\]. Bishop \[^{(18)}\] performed a thorough walk-through of some of these adopted concepts, including model comparison, hyperparameter optimization, Active Learning (AL), ensemble methods, and $L_2$ regularization \[^{(2)}\], \[^{(18)}\], \[^{(22)}\].

It would seem that NNs have little to contribute to Bayesian methods. However, one of the main assets of NNs is their extreme flexibility as they are universal approximators \[^{(4)}\], \[^{(23)}\], \[^{(24)}\]. This is a benefit of the vast amount of free parameters in the NNs. The number of free parameters of a NN
is often several orders of magnitude higher than most BMs. Taking for instance GPT-3 which uses 175 billion parameters\cite{25}. The large number of free-parameters in NNs gives them a high model capacity. A model with a high capacity is flexible, but dependent on large quantities of training data to prevent overfitting. The Vapnik-Chervonenkis (VC) dimension can be used to obtain an upper bound on the generalization loss of a model given its effective capacity and the size of the training dataset\cite{26}. As the capacity of the model increases, the required size of the training dataset increases to maintain the same generalization performance\cite{2}, \cite{4}, \cite{27}. NNs with millions of free parameters are, as a result, depending on large training datasets. Finally, NNs generally suffer a lack of interpretability compared to a BM. The inferred MLE of the free parameters of a NN are simply far more difficult to reason about and interpret compared to a BM. Despite having far more free parameters, their extended use of matrix multiplication, execution on GPUs, and lack of marginalization, make them very fast compared to BMs.

Recent development in the field of ML applies the Bayesian probabilistic framework and one or more NNs in a compound for doing variational inference\cite{28} of complex distributions. Examples of such approaches are generative models like Variational Autoencoders\cite{29} and normalizing flows\cite{30}, \cite{31}. For instance, normalizing flows can be used for approximating the posterior distribution of a Bayesian NN\cite{32}.

For such generative models, the posterior distribution and NN are optimized jointly and thus tightly coupled. The composition leverage the flexibility of NNs and the principled probabilistic framework to infer distributions over data.

Another type of combining Bayesian methods and NNs is fitting a NN to the posterior distribution of a BM. In such setups the posterior distribution of the BM is first inferred, and only afterwards the NN is introduced. This is done with the purpose of leveraging the predictive speed of the NN, and such an approach is also presented in this paper.

A pre-existing example of this method is presented by Jia et al.\cite{33}. In which case, the NN predicts a discrete approximation to the conditional posterior distribution for each free parameter in the BM. This is fundamentally different from our approach, as our NN has no notion of the parameters of the BM, it is simply latent in the dataset.

In the work of Pavone et al.\cite{34}, another approach was taken to approximate a NN to a BM. In this work, they took the domain of particle physics and sampled a target $t \sim p(T)$ using a joint prior distribution over the target variables. Then, using the likelihood, $I$ samples of datapoints $x = [x_i \sim p(X \mid t)]_{i=1}^{I}$ served as $I$ input examples to the NN. The NN would then gain robustness and learn the uncertainty of the model through the data sampling process. The NN itself though, predicts a single MLE for $t$, and thus has no way to represent the posterior predictive distribution in its output. The results show how using a NN for predictions rather than a BM, can reduce the prediction time from over four hours to a matter of milliseconds. This demonstrates the potential benefits from using such setups\cite{34}.

### III. Method

In this section, we introduce the method and algorithms proposed for approximating a BM with a NN. The purpose of
the approximation is to have the ability to make predictions on new data based on an approximation of the full posterior distribution of the BM. These predictions should minimize the risk one takes when making that prediction – meaning it should be the best possible prediction one can make given a BM. In the result section, we show how our method allows for such predictions faster than standard methods for BMs with higher complexity. This happens due to the architecture for such predictions faster than standard methods for BMs. In the result section, we show how our method allows it should be the best possible prediction one can make given but also gain the speed improvement from the NN. NN has no notion of the actual posterior samples of the BM. Our approximation of the model (i.e. our NN). For fitting the NN to a BM for risk minimization. MC simulation for a single prediction. If each BM prediction with MC has complexity $O(m)$, with $m$ being the number of samples, then making $n$ predictions has complexity $O(nm)$. As the number of predictions increases, the processing time increases linearly. In contrast, generating a dataset $D^{NN}$ and doing $n$ predictions has complexity $O(kmn + n)$ with $k$ being the number of dataset samples required for training the NN. When $n \geq \frac{m}{k}$, our method has the lowest overall complexity. One might wonder if that is a real use-case, as $\kappa$, is usually in the order of thousands. Some optimization problems and domains, however, are depending on solving the conditional expectation, $E[Y | X]$, a vast amount of times for varying input. Moreover, for a real-time application, once trained, the NN will provide better response times and thus improve user experience.

Having a fitted NN and $m > 1$, using the NN allows for risk minimized predictions with a lower complexity for a single observation compared to the BM. This makes our method appealing in some time-sensitive domains. These are domains with surplus time when fitting the BM, but at some point later require accurate predictions quickly for new input. Examples of such domains could be stock market trading or autonomously driving vehicles: both needing rapid, correct, reactions to new observations, but have surplus time when the stock market is closed, or doing research. Further, our method is beneficial when the rate of new incoming data surpasses the time it takes to evaluate using the BM. Examples are particle physics and big data applications with a high data velocity.

Some software frameworks such as Jax [36], enable executing BMs on the GPU rather than the CPU. This provides some gain in speed. However, the computational complexity analysis remains the same as the same sequence of statements needs to be computed for the BM.

### A. Computational Complexity

Generating data and fitting a NN to a BM is a computationally more time-consuming task compared to doing a

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**Algorithm 1:** Algorithm for the data sampling process for fitting the NN to a BM for risk minimization.

```plaintext
Input : $I$, $p(X)$, $\tau$, $p(Y | X, \phi)$
Output: $D^{NN}$
1 $D^{NN} \leftarrow \emptyset$
2 for $i \leftarrow 0$ to $I$ by 1 do
3    $\rho \leftarrow [\rho_j \sim \text{Bern}(\tau)]_{j=1,\ldots,J}$
4    $x \sim p(X)$
5    $x \leftarrow x \odot \rho$ // Dropout
6    $y \leftarrow [y_m \leftarrow E[Y | x, \phi, m]]_{m=1,\ldots,M}$
7 $D^{NN} \leftarrow D^{NN} \cup \{(x, y)\}$
end
```

----

1 As the conditional expectation of the BM is now the ground true value to be predicted by the NN, the output of the BM is now denoted $y$ and the output of the NN as $\bar{y}$. 

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### B. Active Learning

As the computational complexity of using our method depends on $\kappa$ (the size of the training set), minimizing $\kappa$ increases the computational benefit of our proposed method. Thus, we apply AL as an extension to the regular training algorithm to maximize the computational benefit. The approach is
Algorithm 2: Active Learning algorithm.

Input : $\phi$, $\tau$, $p(Y \mid X, \phi)$, $p(\phi \mid D^{BM})$, patience
Output: $g$
1. stopper ← EarlyStopping(patlience)
2. $X \sim \mathcal{U}(0_1, 1_1)$
3. $g \leftarrow$ initialize NN
4. $\phi \leftarrow \left[ \phi_m \sim p(\phi \mid D^{BM}) \right]_T^m=1,...,M$
5. $D^{NN} \leftarrow$ algorithm $\left[ I^\text{Init}, \phi, p(X), \ldots \right]$
6. do
7. $D^{NN} \leftarrow D^{NN} \cup$ algorithm $\left[ I^\text{AL}, \phi, p(X), \ldots \right]$
8. $g \leftarrow$ (re)train $g$ on $D^{NN}$
9. $\sigma \leftarrow \text{MeasureUncertainty}(g)$
10. $\pi \leftarrow \text{Softmax}(\sigma)$
11. $X \sim \text{Cat}(\pi)$
12. while stopper.should continue($g$)

IV. EXPERIMENTS

For the experiments in this paper, we assume a Bayesian regression model, $f : x \in \mathbb{R}^J \rightarrow y \in \mathbb{R}$, where $x$ is a single example. The model is as follows

$$
\begin{align*}
\alpha & \sim \mathcal{N}(1.5, \mathbf{1}_J) ; \\
\beta & \sim \mathcal{N}(0.5, 0.25\mathbf{1}_J) \\
\sigma^2 & \sim \mathcal{N}(0, 1) ; \\
\gamma & \sim \mathcal{N}(0, 0.5) \\
\end{align*}
$$

(5)

With $\mathbf{1}_J$ being the identity matrix with rank $J$. The intuition behind this model is that the output is the sum of a linear transformation of each feature which is altered by some function, $\psi$. This function is domain-dependent, and could be $\sqrt{\cdot}$, sin, log, sigmoid, or the like. $\alpha$, $\beta$ and $\sigma$ are $J$-dimensional column vectors and represent the parameters of the BM which needs to be inferred. The BM outlined above does not directly resemble any real-world model. Nonetheless, one can easily imagine such a setup for modeling periodic data as the sum of sin functions with each feature having a different period. Another example could be a model for diagnosing the risk of having a particular disease, here, $x$ could be a patient’s blood test results, $\beta$ the impact of each examined property, $\psi$ the sigmoid function to saturate the influence of each property, and $\alpha$ a scaling factor.

Next, we are interested in using the model for predictions over the full posterior on new data. Further, we will assume no closed-form solution of the posterior predictive distribution, hence for doing predictions with the BM, we will apply MC-sampling as in [3], and assume a sufficient posterior fit to the observed data $D^{BM}$.

When conducting predictions using this model, each of the $m = \{1, \ldots, M\}$ posterior samples of $\alpha$, $\beta$, and $\gamma$ need to be used. The computational complexity of (5) is linearly dependent on $J$. Thus, doing predictions over the full posterior becomes increasingly computationally heavy as the number of features grows. One could imagine other terms that reflect more complex effects such as synergies across features to take place in the model. A synergy effect between all features would transform the linearly growing complexity into an exponential one.

In contrast to the complexity growth of the BM for increasingly complex tasks, the same growth is not necessarily present for NNs. Using the property of NNs being universal approximators, adding more complexity to the BM does not necessarily require a larger NN as long as its capacity is not fully utilized. Even using a single hidden layer in the NN, with enough width, it remains a universal approximator [38]. Consequently, in the extreme case, the NN approximation provides extremely fast predictions, as it will only involve two matrix multiplications, two addition terms, and an activation function.

To examine this, our experiments will focus on approximating the BM from (5) with a NN. We will vary the computational complexity of the model through $J$ and evaluate
the NN’s fit to the BM. The main motivational factor for introducing a NN as an approximation of a BM is the gain of speed when making multiple predictions. To quantify this, we measure the runtime for making predictions on the whole testing dataset using \( M \) posterior samples. We will refer to this runtime as prediction time. Our results will focus on the prediction time as a function of model complexity, and the required size of the training dataset.

Throughout all experiments, we use a simple, feed-forward NN with a single hidden, dense, layer with a width of 5,000. We use dropout [39] with a rate of 0.5, and batch normalization [40] after the hidden layer. We let \( I_{\text{init}} = 10,000 \), \( I_{\text{AL}} = 1,000 \), \( \tau = 0.8 \), and \( M = 2,000 \). We keep \( M \) fixed for all experiments and instead vary \( J \), but one could make similar experiments for an increasing number of posterior samples. For training the NN we use a learning rate of \( 3 \times 10^{-4} \), and set the patience to 10 and 20 for inter- and intra-ES, respectively. The validation and testing dataset each contain 50,000 examples. The experiments are executed on an Intel Core i7-6700K with 48GB ram and a NVIDIA GeForce RTX 2080TI GPU. We use PyMC3 [41] version 3.9.3 for Bayesian inference with the No-U-Turn Sampler [42] using 2,000 warmup steps and 2,000 samples. \( \mathcal{D}_{\text{BM}} = \{X_{\text{BM}}, Y_{\text{BM}}\} \) contains \( N = 5,000 \) examples with \( X_{\text{BM}} \) being sampled from a standard Gaussian distribution, and \( Y_{\text{BM}} = \left[ Y_{\text{BM}}^n = f \left( X_{\text{BM}}^n \right) \right]_{n=1,\ldots,N} \) from (5) with the ground-true values pre-sampled using \( \hat{\gamma} \sim \mathcal{U} (-0.5,0.5) \), \( \hat{\alpha} \sim \mathcal{U} (0.3 \cdot 1_J, 3.0 \cdot 1_J) \), and \( \hat{\beta} \sim \mathcal{U} (0.1 \cdot 1_J, 1_J) \).

V. Results

In Figure 2, one can see the prediction time on the testing set for increasing model complexities, the corresponding Mean Squared Error (MSE), and the size of the training dataset used for fitting the NN. When measuring the prediction time of the BMs, the operation is run in parallel using all cores of the CPU when iterating over the \( M \) posterior samples. This is done using a pool of threads. All calculations make use of the Numpy library with vectorized operations to obtain the best possible performance. The PyMC3 framework also provides a method for making predictions using vectorized computations. However, this does not make use of parallelization and therefore yields a worse prediction time than those we have reported here using both vectorized operations and concurrency.

Measuring runtimes on modern computers is generally an error-prone task, and we, therefore, repeated each experiment five times. From the figure the linear relationship between complexity and prediction time using the BM is clear, whilst it remains constant for the NN. As complexity increases, we see a small decreasing tendency in the MSE. The MSEs are for all experiments considered low, spanning from \( 4.3 \times 10^{-5} \) to \( 2.1 \times 10^{-4} \). The results indicate a negative correlation between the MSE and model complexity. We find this somewhat surprising, as it seems intuitive that more complex models would be harder for the NN to approximate. We attribute this phenomenon to be a result of the central limit theorem [43], as the normalized distribution over \( Y_{\text{NN}} \) shrinks to a normal, making it easier for the NN.

A. Active Learning and the Size of the Training Dataset

To examine the strength of the correlation between the NN’s uncertainty and the predictive error on the \( X_{\text{uncert}} \) dataset, a calibration plot is shown in Figure 3. This figure shows the NN’s uncertainty (calculated using (4)) as a function of the average Root Mean Squared Error (RMSE), \( \mu_{\text{RMSE}} \). This average is taken over the \( K \times M \) predictions. The figure shows the correlation for an experiment with complexity \( J = 5 \). Although the correlation is not equally strong for all examples, it shows a general tendency. If the correlation was not present, the newly added data to the training dataset would provide little to no improvement on the validation dataset. If that was the case, the ES algorithm would terminate the training process...
predictive distribution $E$ dictates a vector of point-wise estimations of the BM’s posterior for future research. Summary statistics for the use of AL is unsettled, and an area of uncertainty over all predicted values. Whether this is sufficient mean over $M$ the training data for the NN. The MC simulation involves step on the output of the NN rather than when generating We argue that one might as well do the MC simulation averaging step in (3) when computing $Y$ an alteration to the generation of $D$ instead. Such a change would mean simplify the method by making the NN predict $E$ complexity as $\tilde{\gamma} \subset y$ a correlation exists for a range of different problems for which predictions, and the actual ground true error. [44] showed such a correlation between the standard deviation over the $K$ training dataset increases with a smaller constant factor than the increased complexity of the BM. This advocates such effects and evaluate the NN’s ability to approximate such constructs, as these leave room for even larger speed-gains over the BM.

A drawback of our method is the assumption the BM is fixed. Changes to the BM’s construct or posterior distribution would require a refit of the NN. Depending on the magnitude of the change in the BM, one might achieve good results by using transfer learning [4], [45], by transferring the state of the original NN to fit the updated BM.

VI. DISCUSSION AND FUTURE WORK

The use of dropout as a measure of uncertainty assumes a correlation between the standard deviation over the $K$ predictions, and the actual ground true error. [14] showed such a correlation exists for a range of different problems for which $\tilde{y} \subset \mathbb{R}^1$. In our domain presented here, we have increased complexity as $\tilde{y} \subset \mathbb{R}^M$ with $M \gg 1$. In (4) we take the mean over $M$ to obtain a single scalar reflecting the NN’s joint uncertainty over all predicted values. Whether this is sufficient

summary statistics for the use of AL is unsettled, and an area for future research.

In this paper, we presented a method for which the NN predicts a vector of point-wise estimations of the BM’s posterior predictive distribution $E \left[ \tilde{Y} \mid X, \phi \right]$. One could potentially simplify the method by making the NN predict $E \left[ \tilde{Y} \mid X \right]$ instead. Such a change would mean $M = 1$, and only require an alteration to the generation of $D^{NN}$ by performing the averaging step in (5) when computing $Y^{NN}$ using the BM. We argue that one might as well do the MC simulation step on the output of the NN rather than when generating the training data for the NN. The MC simulation involves a summation operation, and thus information to the NN is lost. Therefore, we argue the training task of the NN simply becomes easier. Further, having a discrete approximation of the posterior predictive distribution, allows one to recover the uncertainty of the BM in a way the summation function would make irrecoverable.

The BM presented in (5) is relatively simplistic. More complex effects such as synergies across features or an autoregressive component can significantly increase the prediction time of a BM. Future research should extend the BM with such effects and evaluate the NN’s ability to approximate such constructs, as these leave room for even larger speed-gains over the BM.

VII. CONCLUSION

In this paper, we presented a method for training a NN as a function of $x$ to predict a point-wise approximation of the BM’s posterior predictive distribution conditioned on $x$. This is achieved in a single feed-forward pass of the NN. We applied this approach on a set of generalized BMs, and showed how the fitted NNs achieved good approximations. We further evaluated the runtime when making predictions for each of the BMs involved. These predictions were conducted on the testing dataset using $M$ posterior samples. Here, we found a linear relation between the complexity of the BM and the runtime, while the runtime for making predictions using the NN remained unchanged. Thus, we found our method to make predictions on the testing dataset $> 14 \times$ faster than the largest evaluated BM – this with an imperceptible MSE. In addition, we show our method to be only slightly slower for the most trivial BMs. Hence, the proposed method is applicable when the same, complex, BM is needed for making predictions in time-sensitive domains. We also demonstrated how the use of AL can help reduce the dataset required to train the NN in such a context. This method minimizes the cost of obtaining this training dataset. In this regard, our results indicate that the size of the training dataset increases with a smaller constant factor than the increased complexity of the BM. This advocates the use of this method, as doubling the complexity of the BM only requires slightly larger training datasets.

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