Practical Bayesian Learning of Neural Networks via Adaptive Subgradient Methods

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Abstract

We introduce a novel framework for the estimation of the posterior distribution of the weights of a neural network, based on a new probabilistic interpretation of adaptive subgradient algorithms such as AdaGrad and Adam. Having a confidence measure of the weights allows several shortcomings of neural networks to be addressed. In particular, the robustness of the network can be improved by performing weight pruning based on signal-to-noise ratios from the weight posterior distribution. Using the MNIST dataset, we demonstrate that the empirical performance of BADAM, a particular instance of our framework based on Adam, is competitive in comparison to related Bayesian approaches such as Bayes By Backprop.

1 Introduction

For decades, many different approaches have been suggested to integrate Bayesian inference and neural networks. In such Bayesian neural networks (BNNs), we have, after training, not a single set of parameters, or weights, but an (approximate) posterior distribution over those parameters. The posterior distribution, for example, enables uncertainty estimates over the network output, selection of hyperparameters and models in a principled framework, as well as guided data collection (active learning).

In general, exact Bayesian inference over the weights of a neural network is intractable as the number of parameters is very large and the functional form of a neural network does not lend itself to exact integration. For this reason, much of the research in this area has been focused on approximation techniques. Most modern techniques stem from key works which used either a Laplace approximation MacKay (1992), variational methods (Hinton and van Camp, 1993), or Monte Carlo methods (Neal, 1995). Over the past few years, many methods for approximating the posterior distribution have been suggested, falling into one of these categories. These methods include assumed density filtering (Lobato and Adams, 2015; Soudry et al., 2014), approximate power Expectation Propagation (Lobato et al., 2016), Stochastic Langevin Gradient Descent (Balan et al., 2015; Ahn et al., 2012; Welling and Teh, 2011), incremental moment matching (Lee et al., 2017), and variational Bayes (Blundell et al., 2015; Graves, 2011).

The standard variational Bayes approach developed by Blundell et al. (2015), called Bayes By Backprop (BBB), has several shortcomings. The variational free energy minimized in BBB is a sum of a log-likelihood cost function and a complexity cost function. The complexity cost function acts as a regularizer, enforcing a solution that captures the complexity of the data while keeping the posterior close to the prior. Finding a good prior is usually a non-trivial task, and over-restricting priors could potentially cause underfitting. To alleviate these issues, Kingma et al. (2015) introduced variational dropout, which uses an improper prior to ensure that the complexity cost function becomes constant in the weight parameters. Later modifications of this approach (Khan et al., 2018; Molchanov et al., 2017; Achterhold et al., 2018) were shown to be useful for weight pruning (without re-training, similarly to BBB). However, Hron et al. (2017) recently pointed out that such variational dropout approaches are not Bayesian. To avoid these issues altogether, Zeno et al. (2018) proposed an online variational Bayes scheme using a new prior for...
each minibatch, instead of one prior for all the data.

In this paper, we develop a novel Bayesian approach to learning for neural networks, built upon adaptive subgradient methods such as ADAGRAD (Duchi et al. 2011), RMSProp (Tieleman and Hinton 2012) and ADAM (Kingma and Lei 2015). Unlike the aforementioned approaches, ours does not require the specification of a method for approximating the posterior distribution, as it relies on a new probabilistic interpretation of adaptive subgradient algorithms that effectively shows these can readily be utilized as approximate Bayesian posterior inference schemes. This has similar underpinnings as the work of Mandt et al. (2017), although the latter is based on a stochastic model for gradient variations that imposes a number of restrictions on the gradient noise covariance structure, which our framework is able to sidestep by utilizing ADAM as the underlying subgradient method. Our proposed algorithm is also similar in spirit to the work of Khan et al. (2018), but there are some important differences that we discuss in detail in Section 6.

2 Preliminaries

Notation. Vectors are denoted by lower case Roman letters such as $a$, and all vectors are assumed to be column vectors. Upper case roman letters, such as $M$, denote matrices, with the exception of the identity matrix which we denote by $I$ and whose dimension is implicit from the context. Finally, for any vector $g_t \in \mathbb{R}^d$, $g_{i,j}$ denotes its $j$th coordinate, where $j \in [d]$.

Problem setup. Let $f(\theta)$ be a noisy objective function: a stochastic scalar function that is differentiable w.r.t. the parameters $\theta \in \Theta$, where $\Theta$ denotes the parameter space. In general, $\Theta$ is a subset of $\mathbb{R}^d$, but for simplicity, we shall assume that $\Theta = \mathbb{R}^d$ throughout the remainder of this paper. We are interested in minimizing the expected value of this function, $E[f(\theta)]$, w.r.t. its parameters $\theta$. Let $f_1(\theta), \ldots, f_T(\theta)$ denote the realizations of the stochastic function at the subsequent time steps $t \in [T]$. The stochastic nature may arise from the evaluation of the function at random subsamples (minibatches) of datapoints, or from inherent function noise.

The simplest algorithm for this setting is the standard online gradient descent algorithm (Zinkevich 2003), which moves the current estimate $\theta_t$ of $\theta$ in the opposite direction of the last observed (sub)gradient value $g_t = \nabla f_t(\theta_t)$, i.e.,

$$
\theta_{t+1} = \theta_t - \eta_t g_t,
$$

where $\eta_t > 0$ is an adaptive learning rate that is typically set to $\eta_t = \eta / \sqrt{t}$, for some positive constant $\eta$. While the decreasing learning rate is required for convergence, such an aggressive decay typically translates into poor empirical performance.

Generic adaptive subgradient descent. We now present a framework that contains a wide range of popular adaptive subgradient methods as special cases, and highlights their flaws and differences. The presentation here follows closely that of Reddi et al. (2018). The update rule of this generic class of adaptive methods can be compactly written in the form

$$
\theta_{t+1} = \theta_t - \eta_t V_t^{-1/2} m_t,
$$

where $m_t$ and $V_t^{-1/2}$ are estimates of the (sub)gradient and inverse Hessian, respectively, of the functions $f_t(\cdot)$, based on observations up to and including iteration $t$. In other words, they are functions of the (sub)gradient history $g_{1:t} \equiv g_1, \ldots, g_t$, which we express as

$$
m_t = \hat{g}_t(g_{1:t}), \quad V_t^{-1/2} = \hat{H}_t(g_{1:t}),
$$

where $\hat{g}(\cdot)$ and $\hat{H}(\cdot)$ denote estimator functions for the (sub)gradient and Hessian of the loss function at iteration $t$, respectively. The corresponding procedure is outlined in Algorithm 1.

Algorithm 1: Generic Adaptive Subgradient Descent

**Input:** $\theta_1 \in \mathbb{R}^d$, learning-rate schedule $\{\eta_t\}_{t=1}^T$, sequence of (sub)gradient and Hessian estimators $\{\hat{g}_t(\cdot), \hat{H}_t(\cdot)\}_{t=1}^T$

**for** $t = 1 \text{ to } T - 1$ **do**

$$
g_t = \nabla f_t(\theta_t), \quad m_t = \hat{g}_t(g_{1:t}) \quad \text{and} \quad V_t^{-1/2} = \hat{H}_t(g_{1:t})
$$

$$\theta_{t+1} = \theta_t - \eta_t V_t^{-1/2} m_t,
$$

**end for**

**Output:** $\theta_T$

For computational performance many popular algorithms restrict themselves to diagonal variants of the general method encapsulated by Algorithm 1 such as $V_t = \text{diag}(v_t)$, where $v_t$ is the vector of diagonal elements. We first observe that the standard online gradient descent (OGD) algorithm arises as a special case of this framework if we use:

$$
m_t = g_t, \quad V_t = I. \quad \text{(OGD)}
$$

The key idea of adaptive methods is to choose estimator functions appropriately so as to entail good convergence. For instance, the first adaptive method ADA-GRAD (Duchi et al. 2011), which propelled research much further, uses the following estimator functions:

$$
m_t = g_t, \quad V_t = \frac{1}{t} \text{diag} \left( \sum_{i=1}^t g_i g_i^\top \right). \quad \text{(ADA-GRAD)}
$$
In contrast to the learning rate of $\eta/\sqrt{t}$ in OGD with learning-rate decay, such a setting effectively implies a modest learning-rate decay of $\eta/\sqrt{\sum_j g_{j,t}^2}$ for some $j \in [d]$. When the gradients are sparse, this can potentially lead to huge gains in terms of convergence (see Duch et al. (2011)). These gains have also been observed in practice even in some non-sparse settings.

Adaptive methods based on EWMA. Exponentially weighted moving average (EWMA) variants of ADAGRAD are popular in the deep learning community. AdaDELTA (Zeiler 2012), RMSProp (Tieleman and Hinton 2012), ADAM (Kingma and Lei 2015) and NADAM (Dozat 2016) are some prominent algorithms that fall in this category. The key difference between these and ADAGRAD is that they use an EWMA as the function $V_t$ instead of a simple average. ADAM, a particularly popular variant, is based on the following estimator functions:

$$m_t = \frac{1 - \beta_1}{1 - \beta_1^t} \sum_{i=1}^t \beta_1^{t-i} g_i$$
$$V_t = \frac{1 - \beta_2}{1 - \beta_2^t} \text{diag} \left( \sum_{i=1}^t \beta_2^{t-i} g_i g_i^\top \right),$$

(ADAM)

where $\beta_1, \beta_2 \in [0, 1)$ are exponential decay rates. This update can alternatively be stated in terms of the following simple recursions:

$$m_{t,i} = \frac{\beta_1 m_{t-1,i} + (1 - \beta_1) g_{t,i}}{1 - \beta_1^t},$$
$$v_{t,i} = \frac{\beta_2 v_{t-1,i} + (1 - \beta_2) g_{t,i}^2}{1 - \beta_2^t},$$

(AMSGrad)

for all $t \in [T]$, with $m_0,i = v_0,i = \dot{v}_0,i = 0$ for all $i \in [d]$. Note that the denominator represents a bias-correction term. A value of $\beta_1 = 0.9$ and $\beta_2 = 0.999$ is typically recommended in practice (Kingma and Lei 2015). RMSProp, which appeared in an earlier unpublished work (Tieleman and Hinton 2012), is essentially a variant of ADAM with $\beta_1 = 0$. In practice, especially in deep-learning applications, the momentum term arising due to non-zero $\beta_1$ appears to significantly boost performance.

More recently, Reddi et al. (2018) pointed out that the aforementioned methods fail to converge to an optimal solution (or a critical point in non-convex settings). They showed that one cause for such failures is the use of EWMAs and, as a result of this, proposed AMSGrad, a variant of ADAM which relies on a long-term memory of past gradients. Specifically, the AMSGrad update rule is characterized by the following system of recursive equations:

$$m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t$$
$$v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t g_t^\top$$
$$\dot{v}_{t,i} = \max(\dot{v}_{t-1,i}, v_{t,i})$$
$$V_t = \text{diag}(\dot{v}_{t,1}, \ldots, \dot{v}_{t,d}),$$

for all $t \in [T]$, with $m_0 = v_0 = \dot{v}_0 = 0$ for all $i \in [d]$, and where $\beta_{1,t} = 0$ is a sequence of exponential smoothing factors.

Bayesian neural networks. As the name suggests, a Bayesian neural network (BNN) is a neural network equipped with a prior distribution over its weights $\theta$. Consider an i.i.d. data set of $N$ feature vectors $x_1, \ldots, x_N \in \mathbb{R}^d$, with a corresponding set of outputs $D = \{y_1, \ldots, y_N\} \subset \mathbb{R}$. For illustration purposes, we shall suppose that the likelihood for each datapoint is Gaussian, with an $x$-dependent mean given by the output $\text{NN}(x, \theta)$ of a neural-network model and with variance $\sigma^2$:

$$p(y_n|x_n, \theta, \sigma^2) = \mathcal{N}(y_n|\text{NN}(x_n, \theta), \sigma^2).$$

Similarly, we shall choose a prior distribution over the weights $\theta$ that is Gaussian of the form

$$p(\theta|\alpha, \sigma^2) = \mathcal{N}(\theta|0, \alpha^{-1}\mathbb{I}).$$

Since the data set $D$ is i.i.d., the likelihood function is given by

$$p(D|\theta, \sigma^2) = \prod_{n=1}^N \mathcal{N}(y_n|\text{NN}(x_n, \theta), \sigma^2)$$

and so by virtue of Bayes’ theorem, the resulting posterior distribution is then

$$p(\theta|D, \alpha, \sigma^2) \propto p(\theta|\alpha)p(D|\theta, \sigma^2)$$

which, as a consequence of the nonlinear dependence of $\text{NN}(x, \theta)$ on $\theta$, will be non-Gaussian. However, we can find a Gaussian approximation by using the Laplace approximation (MacKay 1992). Alternative approximation methods have been briefly discussed in Section II.

3 Probabilistic Interpretation of Adaptive Subgradient Methods

Our probabilistic interpretation of adaptive subgradient methods represented by Algorithm II is based on a second-order Taylor expansion of the loss function $f(\theta)$ around the current iterate $\theta_t$:

$$f(\theta) \approx f(\theta_t) + \nabla f(\theta_t)^\top (\theta - \theta_t)$$
$$+ \frac{1}{2}(\theta - \theta_t)^\top [\nabla^2 f(\theta_t)] (\theta - \theta_t).$$
Since the gradient and Hessian are unknown, we replace them with the unbiased estimates
\[ \nabla f(\theta_t) \approx \eta_t m_t, \quad \nabla^2 f(\theta_t) \approx V_t^{1/2}, \quad (10) \]
which results in the following approximation:
\[ \hat{f}_t(\theta) \equiv f(\theta_t) + \eta_t m_t^\top (\theta - \theta_t) + \frac{1}{2} (\theta - \theta_t)^\top V_t^{1/2} (\theta - \theta_t). \]
(11)
The corresponding likelihood model is given by
\[ l_t(\theta) \propto \exp \left\{ -N \hat{f}_t(\theta) \right\} \]
\[ \propto \exp \left\{ -N \eta_t m_t^\top (\theta - \theta_t) - \frac{N}{2} (\theta - \theta_t)^\top V_t^{1/2} (\theta - \theta_t) \right\}, \quad (12) \]
where the number of samples \( N \) corrects the averaging over samples that is implicitly contained in the loss function \( f(\theta) \).

Under an improper prior over \( \theta \), i.e. \( p(\theta) = \text{const} \), Eq. (12) coincides with the unnormalized posterior over \( \theta \) given the gradient history \( g_{1:t} \). Completing the square with respect to \( \theta \) in the exponential yields
\[ - N \eta_t m_t^\top (\theta - \theta_t) - \frac{N}{2} (\theta - \theta_t)^\top V_t^{1/2} (\theta - \theta_t) \]
\[ = - \frac{N}{2} (\theta - \theta_{t+1})^\top V_t^{1/2} (\theta - \theta_{t+1}) + \text{const}, \quad (13) \]
where, as a reminder, \( \theta_{t+1} = \theta_t - \eta V_t^{-1/2} m_t \) and “const” denotes terms that are independent of \( \theta \). This leads to a Gaussian posterior of the form
\[ p(\theta | g_{1:t}, \eta_t, \omega) = \mathcal{N} \left( \theta | \theta_{t+1}, \frac{1}{N} V_t^{-1/2} \right), \quad (14) \]
where \( \omega \) is a vector of hyperparameters other than the learning rate, if any, that govern the underlying adaptive subgradient method. For example, \( \omega = \emptyset \) in the case of ADAGRAD, whereas \( \omega = (\beta_1, \beta_2) \) for ADAM.

A few comments are in order regarding Eq. (14). Even though it was easily derived, the final posterior distribution in Eq. (14) is closely related to those obtained via several other approaches. Firstly, note that the posterior mean of the weight distribution is merely the point estimator of the descent algorithm. This is also the case for most of the alternative approaches (e.g., Blundell et al. (2015), Mandt et al. (2017), Zenq et al. (2018)). The expression for the variance, and the nature of our approach in general, is closest in spirit to the work of Mandt et al. (2017). In fact, Eq. (12) is closely related to Assumption 4 in their paper. A notable difference between their paper and ours, however, is that the former relies on an Ornstein-Uhlenbeck process to describe the stochastic dynamics of the gradients. Specifically, Mandt et al. (2017) assume that the variability of the gradients can be reasonably captured by a constant covariance matrix, which is an unrealistic assumption given the fact that, in practice, this covariance matrix evolves as one explores different regions of the energy landscape. Instead, our approach, as we shall discuss in the next section, is to use ADAM’s EWMA estimates for \( m_t \) and \( V_t \). This enables us to filter out the noise arising from the stochastic nature of the gradients, while at the same time accounting for changes in these quantities over different areas of the energy landscape.

4 Practical Algorithms for Bayesian Learning of Neural Networks

Based on the insights from the previous section, we obtain the following generic algorithm for Bayesian learning of neural networks via adaptive subgradient methods.

Algorithm 2 Generic Bayesian Learning of Neural Networks via Adaptive Subgradient Methods

Input: \( \theta_1 \in \mathbb{R}^d \), learning-rate schedule \( \{\eta_t\}_{t=1}^T \), sequence of (sub)gradient and Hessian estimators \( \{g_t(\cdot), \hat{H}_t(\cdot)\}_{t=1}^T \)
for \( t = 1 \) to \( T - 1 \) do
\[ g_t = \nabla f_t(\theta_t) \]
\[ m_t = \hat{g}_t(g_{1:t}) \quad \text{and} \quad V_t^{1/2} = \hat{H}_t(g_{1:t}) \]
\[ \theta_{t+1} = \theta_t - \eta V_t^{-1/2} m_t \]
end for
Output: final weight distribution \( \mathcal{N}(\theta_T, N^{-1} V_T^{-1/2}) \)

Intuitively, we can understand Algorithm 2 as follows. Recall that \( V_t^{1/2} \) is an estimate of the Hessian of the loss function \( f_t(\cdot) \), and thereby captures the curvature of the energy landscape. Large curvature in a given direction will thus result in a small variance in that direction, while small curvature leads to large variance, which is intuitively clear.

Refining Algorithm 2 to OGD, we would get a covariance matrix proportional to the identity. To approximate the correct covariance of the weights, one needs a good estimate of the curvature. Furthermore, due to the stochastic nature of the energy surface, this curvature estimate should not be based on a single (the final) observation, but rather on a history of observations, so as to mitigate the noise in the resulting curvature estimate. Algorithms like ADAGRAD and ADAM do exactly that. Furthermore, since working with a full covariance matrix becomes computationally intractable for large networks, one can use approximations that diagonalize the covariance matrix.
This occurs when using Algorithm 2 with the values taken by the estimator functions $\hat{g}_t(g_{1:t})$ and $\hat{H}_t(g_{1:t})$ in ADAGRAD and ADAM. Note that the online variational Bayes algorithms in [Blundell et al., 2015] and (Zeno et al., 2018) also employ a diagonal approximation. Additionally, the model discussed in (Mandt et al. 2017) arguably bears certain similarities with Algorithm 2 when refining the latter to ADAGRAD. For this reason, we shall focus here on discussing how to instantiate Algorithm 2 with ADAM.

ADAM has many appealing features when used as an optimizer for neural networks. The reasons for this are twofold:

1. Given that the posterior mean of our algorithm is identical to the point estimate generated by ADAM, we expect it to perform well in practice, for the same reasons that ADAM excels and is widely used in practice.

2. There is a trade-off in estimating the curvature of the landscape, and thus the covariance matrix: if we just focus on the last observation, our estimate will be too noisy; however, if we base it on the entire history – like ADAGRAD does – we are implicitly assuming that it is constant throughout the landscape. Ideally, therefore, we should base our estimate on the most recent observations close to the final weight update. This is achieved by using EWMAs, as in ADAM\footnote{For the same reason, EWMAs are popular in finance where one encounters noisy observations from non-stationary distributions.}.

The specific approach whereby Algorithm 2 uses the update rules of ADAM is illustrated in Algorithm 3.

**Algorithm 3 BADAM:** Bayesian Learning of Neural Networks via ADAM

**Input:** $\theta_t \in \mathbb{R}^d$, global learning rate $\eta$, exponential decay rates $\beta_1, \beta_2$, regularizer $\epsilon$

Set $m_0 = v_0 = 0$

for $t = 1$ to $T$ do

\[ g_t = \nabla f_t(\theta_t) \]

\[ m_t = \frac{\beta_1 m_{t-1} + (1-\beta_1)g_t}{1-\beta_1^t} \quad \text{and} \quad v_t = \frac{\beta_2 v_{t-1} + (1-\beta_2)g_t^2}{1-\beta_2^t} \]

\[ \theta_{t+1} = \theta_t - \eta m_t/(v_t^{1/2} + \epsilon) \quad \text{(element-wise division)} \]

end for

**Output:** final weight distribution $\mathcal{N}(\theta|\theta_T, N^{-1}\text{diag}(1/(v_{T-1}^{1/2} + \epsilon)))$

Note that the denominators $(1 - \beta_1^t)$ and $(1 - \beta_2^t)$ in the updates for $m_t$ and $v_t$, respectively, correct the initialization bias. These factors quickly converge to 1 and any effect on the final posterior variance quickly deteriorates. Thus, in practice, we can absorb those factors into the learning rate by using $\eta_t = \eta\sqrt{(1-\beta_1^t)/(1-\beta_2^t)}$ in place of $\eta$, as is usually done in many implementations of ADAM, including that in TensorFlow.

### 5 Proof-of-concept experiments

In this section, we evaluate the empirical performance of our Bayesian adaptive subgradient framework using the Bayes by Backprop (BBB) algorithm of [Blundell et al., 2015] as the baseline. For brevity, we confine ourselves to a classification exercise on the MNIST data set. While we could have employed alternative approaches such as variational dropout (Kingma et al., 2015) or Bayesian gradient descent (Zeno et al., 2018), we did not consider the former because variational dropout cannot be used for weight pruning (the variances are simply proportional to the weight values), while the latter achieves similar performance on the MNIST classification task as the more widely used BBB, and for this reason we decided to omit it.

We remark that our goal here is not to establish the superiority of our family of algorithms over BBB. Rather, we want to establish a proof of concept that, compared to BBB, our methods are competitive, at least on the MNIST classification experiment. Our methods have the big advantage that posterior distributions, and thus uncertainties, can be extracted for “free” from the standard ADAM algorithm which is widely used in practice. It thus provides an out-of-the-box tool to measure the uncertainty in the weights of a neural network, and the fact that we are able to achieve empirical results that are comparable to those obtained by considerably more complex Bayesian modelling approaches, such as BBB, is very promising.
While the results reported in (Blundell et al., 2015) exhibit better performance, they rely on extensive hyperparameter tuning as well as on a large number of epochs. However, with a smaller number of epochs, the BBB algorithm performs worse than our framework, whose major strengths are the lesser reliance on hyperparameters and the fact that it works better out of the box.

5.1 Description of the data

MNIST is a database of handwritten digits comprising a training and test set of 60,000 and 10,000 pixelated images, respectively, each of size 28 by 28. Each image is labeled with its corresponding digit (between 0 and 9, inclusive).

5.2 Experimental setup

In order to make the results of our framework comparable to those obtained by the BBB algorithm, we replicate the experimental setup proposed in (Blundell et al., 2015), except for the few modifications below:

- we preprocess the pixels by dividing values by 255 instead of by 126 as in (Blundell et al., 2015);
- there are two dropout layers after each hidden layer; while Blundell et al. (2015) use implicit regularization at this level, we apply dropout combined with $L_2$-regularization on the weights and biases;
- while the authors of (Blundell et al., 2015) base their results on 600 epochs, we only experiment with 20 and 300 epochs, respectively.

Otherwise, our experimental configuration is identical to that used by the authors of (Blundell et al., 2015). Specifically, we use the same neural network architecture with 2 hidden layers made up of 1,200 units each, ReLUs as activation functions, and a softmax output layer with 10 units, one for each possible digit. The total number of parameters, i.e. weights and biases, is approximately 2.4 million. The biases were all initialized at 0, while the initial weights were randomly drawn from a zero-mean Gaussian distribution with a standard deviation of 0.1. As in (Blundell et al., 2015), we used a training set of 50,000 examples and a test set of 10,000 examples.

5.3 Results

We do not place much emphasis on the convergence properties of our algorithms, as these properties are directly inherited from the underlying subgradient method which, in the case of BADAM, is ADAM. As the convergence of ADAM is widely studied, and the algorithm is commonly used because of its good convergence properties among other things, the main goal of our experiments is to assess the quality of the confidence measure provided by BADAM, which represents its competitive edge.

Figure 2 shows the distribution of posterior means over the entire network for various algorithms. The values for OGD and BBB are taken from (Blundell et al., 2015). It is seen that when compared to OGD, BBB widens the range of weight values. The same holds for the weight values obtained from BADAM.

Figure 3: Test accuracy of different methods on MNIST as a function of the percentage of pruned weights.

Because the posterior means of BADAM have a similar distribution compared to those of BBB, we need to compare the respective variances, which quantify the uncertainties in weights. To assess the quality of the obtained uncertainties and to show that our poste-
Table 1: Classification errors after applying weight pruning to different algorithms on the MNIST dataset. The number in parentheses appended to the name of a given algorithm represents the underlying number of epochs. The smallest test error in each epoch category is highlighted in bold.

| Proportion removed | # weights | BBB (600) | BBB (300) | BADAM (300) | BADAGRAD (300) | BBB (20) | BADAM (20) |
|--------------------|-----------|-----------|-----------|-------------|----------------|----------|-----------|
| 0%                 | 2.4m      | 1.24%     | 1.49%     | 1.66%       | 1.60%          | 1.86%    | 1.96%     |
| 50%                | 1.2m      | 1.24%     | 1.53%     | 1.66%       | 1.70%          | 1.90%    | 1.95%     |
| 75%                | 600k      | 1.24%     | 1.77%     | 1.75%       | 2.19%          | 2.13%    | 1.96%     |
| 95%                | 120k      | 1.29%     | 4.53%     | 1.93%       | 27.91%         | 3.16%    | 2.20%     |
| 98%                | 48k       | 1.39%     | 11.7%     | 2.15%       | 71.12%         | 5.40%    | 2.38%     |

prior distributions are meaningful, we follow the weight-pruning experiment carried out in (Blundell et al. 2015). Given a posterior mean $\mu$ and a standard deviation $\sigma$, we compute the signal-to-noise ratio as $\mu/\sigma$. An illustration of the distribution of the signal-to-noise ratio across all weights in a network is depicted in Figure 2. To perform the pruning of weights, we sort the weights by their signal-to-noise ratio and discard the fraction $p$ of weights with the lowest values, by setting these weights equal to zero. As a baseline, we perform pruning on a model with constant variances, $\Sigma \sim I$. For this model, pruning via the signal-to-noise ratio is equivalent to pruning via the absolute value of the weights.

Figure 3 exhibits the test accuracy as a function of the pruning percentage $p$ for various models. The hyperparameter configurations we utilized to obtain these results are outlined in Table 3. It is worth noting that, when increasing the number of epochs in BADAM from 20 to 300, we considerably lower the learning rate while simultaneously altering $\beta_2$, which governs the horizon of the EWMA estimate of the curvature. Since we are using a much smaller learning rate, and are thus sampling from a smaller region, it is instructive to increase the horizon by changing $\beta_2$. Our implementations of BBB for 20 and 300 epochs, respectively, perform less well and are arguably noisier, as seen when comparing them against their BADAM counterparts. In our implementation of BBB, we used only one Monte-Carlo sample, while in (Blundell et al. 2015), the authors considered either 1, 2, 5 or 10 samples. Increasing the number of samples helps improve the estimate and makes it more robust, but it also increases the computational overhead, which is why we only chose one sample to have a fairer comparison against BADAM. This is arguably better for us as we do well out-of-the-box and BBB requires more sampling. The bottom line of Figure 3 is that the BADAM instances of our framework based on 20 and 300 epochs, respectively, beat the BBB algorithm with 20 epochs in terms of robustness to weight pruning. As detailed below, this suggests that, relative to BBB, BADAM provides a more accurate measure of the uncertainty about neural-network weights.

We end this section by emphasizing that the key underlying principle of the Bayesian treatment we propose in this paper is to provide a measure of uncertainty over a neural network’s weight parameters, and not just a better or faster (in convergence terms) point estimate thereof. The quality of this uncertainty metric can be assessed by pruning the weights: the more robust the classification error of a Bayesian algorithm for learning neural networks is to weight pruning, the better the quality of the uncertainty embedded in the corresponding (approximate) weight posterior distribution will be. This remark is especially valid for larger pruning proportions. Obtaining a better error without performing any pruning (i.e., for a pruning percentage equal to 0%) just means having done a better work at tuning the network architecture and hyperparameters. On the other hand, an algorithm achieving a smaller error at higher pruning rates – even if its corresponding error rate at 0% pruning is less attractive – comes with genuinely desirable uncertainty estimates. This is clearly illustrated in Table 1 for the BADAM variants of our algorithm with 20 and 300 epochs, respectively. We can clearly discern the robustness of BADAM to weight pruning, compared to BBB, which suffers from abrupt jumps in its error rate as we increase the pruning percentage.

6 Conclusion

In this paper, we introduced a novel approach to Bayesian learning for neural networks, derived from a new probabilistic interpretation of adaptive subgradient algorithms. In particular, we discussed how to refine this framework to ADAM and ADAGRAD, calling the resulting Bayesian neural networks BADAM and BADAGRAD, respectively. Finally, we demonstrated the competitive empirical performance of BADAM on MNIST classification, employing the variational Bayes approach of Blundell et al. (2015) as a benchmark.

While completing this work, we became aware of the VADAM algorithm (Khan et al. 2018). The latter ap-
Table 2: Hyperparameters used to generate the results in Figure 3. The number in parentheses appended to the name of a specific model represents the underlying number of epochs. The acronym “n/a” stands for “not applicable”.

| Hyperparameter          | BADAGRAD (300) | BADAM (300) | BADAM (20) | BBB (300) | BBB (20) |
|-------------------------|----------------|-------------|------------|-----------|----------|
| Learning rate           | 0.01           | 0.0001      | 0.001      | 0.001     | 0.01     |
| Regularization parameter| 0.002          | 0.001       | 0.001      | n/a       | n/a      |
| Dropout                 | 0.6            | 0.6         | 0.5        | n/a       | n/a      |
| $\beta_2$               | n/a            | 0.9999      | 0.999      | n/a       | n/a      |
| Minibatch size          | 128            | 128         | 128        | 128       | 128      |
| # samples               | n/a            | n/a         | n/a        | 0.25      | 0.25     |
| $\pi$                   | n/a            | n/a         | n/a        | n/a       | n/a      |
| $\sigma_p$              | n/a            | n/a         | n/a        | n/a       | n/a      |
| $\sigma_1$              | n/a            | n/a         | n/a        | 0.75      | 0.75     |
| $\sigma_2$              | n/a            | n/a         | n/a        | 0.1       | 0.1      |

It applies weight perturbations to the ADAM method in order to arrive at an approximate posterior distributions over a neural network’s weights. Although close in spirit, there are some important differences to our BADAM algorithm as outlined below:

1. **BADAM**, unlike **VADAM**, does not use weight perturbations. This is non-trivial as **VADAM** without weight perturbations boils down to the **deterministic ADAM** method without uncertainties. In fact, the underlying derivation is entirely different: while **VADAM** uses uncertainties from variational Bayes which results in weight perturbations, **BADAM** uses a geometrical derivation where uncertainties are related to the curvature of the loss function. This results in conceptually different and arguably more intuitive theoretical underpinnings.

2. **VADAM** relies on the inverse of the diagonal Fisher information matrix as an approximation to the inverse Hessian, whereas **BADAM** uses the square root of the inverse of the diagonal Fisher information matrix approximation, i.e., $V_t^{-1/2}$. As already pointed out in the context of **ADAM** [Kingma and Li, 2015], this preconditioner (which is also used in **ADAGrad**) adapts to the geometry of the data and is more conservative in its adaptation than the inverse of the diagonal Fisher information matrix. In fact, using $V_t$ in place of $V_t^{1/2}$ does not result in good uncertainties as is manifested when using them for weight pruning.

We hope that **BADAM** will find usage as a practical off-the-shelf Bayesian adaptive subgradient algorithm, providing posterior distributions with highly accurate confidence measures over neural-network parameters.

**References**

Jan Achterhold, Jan M. Kohler, Anke Schmeink, and Tim Genewein. Variational Network Quantization. In **6th International Conference on Learning Representations**, 2018.

Sungjin Ahn, Anoop Korattikara, and Max Welling. Bayesian Posterior Sampling via Stochastic Gradient Fisher Scoring. In **Proceedings of the 29th International Conference on Machine Learning**, 2012.

Anoop Korattikara Balan, Vivek Rathod, Kevin P. Murphy, and Max Welling. Bayesian Dark Knowledge. In **Advances in Neural Information Processing Systems 28**, 2015.

Charles Blundell, Julien Cornebise, Koray Kavukcuoglu, and Daan Wierstra. Weight Uncertainty in Neural Networks. In **Proceedings of the 32nd International Conference on Machine Learning**, 2015.

Timothy Dozat. Incorporating Nesterov Momentum into Adam. In **4th International Conference on Learning Representations – Workshop Track**, 2016.

John C. Duchi, Elad Hazan, and Yoram Singer. Adaptive Subgradient Methods for Online Learning and Stochastic Optimization. **Journal of Machine Learning Research**, 12:2121–2159, 2011.

Alex Graves. Practical Variational Inference for Neural Networks. In **Advances in Neural Information Processing Systems 24**, 2011.

Geoffrey E. Hinton and Drew van Camp. Keeping Neural Networks Simple by Minimizing the Description
Length of the Weights. In *Proceedings of the 6th Annual ACM Conference on Computational Learning Theory*, 1993.

Jiri Hron, Alexander G. de G. Matthews, and Zoubin Ghahramani. Variational Gaussian Dropout is not Bayesian. *arXiv:1711.02989 [stat.ML]*, 2017.

Mohammad Emtiyaz Khan, Didrik Nielsen, Voot Tangkaratt, Wu Lin, Yarin Gal, and Akash Srivastava. Fast and Scalable Bayesian Deep Learning by Weight-Perturbation in Adam. In *Proceedings of the 35th International Conference on Machine Learning*, 2018.

Diederik P. Kingma and Jimmy B. Lei. Adam: A method for stochastic optimization. In *Proceedings of the 3rd International Conference on Learning Representations*, 2015.

Diederik P. Kingma, Tim Salimans, and Max Welling. Variational Dropout and the Local Reparameterization Trick. *CoRR*, abs/1506.02557, 2015.

Sang-Woo Lee, Jin-Hwa Kim, Jaehyun Jun, Jung-Woo Ha, and Byoung-Tak Zhang. Overcoming Catastrophic Forgetting by Incremental Moment Matching. In *Advances in Neural Information Processing Systems 30*, 2017.

José Miguel Hernández Lobato and Ryan P. Adams. Probabilistic Backpropagation for Scalable Learning of Bayesian Neural Networks. In *Proceedings of the 32nd International Conference on Machine Learning*, pages 1861–1869, 2015.

José Miguel Hernández Lobato, Yingzhen Li, Mark Rowland, Thang Bui, Daniel Hernández-Lobato, and Richard Turner. Black-Box Alpha Divergence Minimization. In *Proceedings of the 33rd International Conference on Machine Learning*, pages 1511–1520, 2016.

David J. C. MacKay. A Practical Bayesian Framework for Backpropagation Networks. *Neural Computation*, 4:448–472, 1992.

Stephan Mandt, Matthew D. Hoffman, and David M. Blei. Stochastic Gradient Descent as Approximate Bayesian Inference. *Journal of Machine Learning Research*, 18:1–35, 2017.

Dmitry Molchanov, Arsenii Ashukha, and Dmitry Vetrov. Variational Dropout Sparsifies Deep Neural Networks. In *Proceedings of the 34th International Conference on Machine Learning*, 2017.

Radford M. Neal. *Bayesian Learning for Neural Networks*. PhD thesis, University of Toronto, 1995.

Sashank J. Reddi, Satyen Kale, and Sanjiv Kumar. On the Convergence of Adam and Beyond. In *6th International Conference on Learning Representations*, 2018.