Mitigating Confirmation Bias in Semi-supervised Learning via Efficient Bayesian Model Averaging

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Abstract

State-of-the-art (SOTA) semi-supervised learning (SSL) methods have been highly successful in leveraging a mix of labeled and unlabeled data, often via self-training or pseudo-labeling. During pseudo-labeling, the model's predictions on unlabeled data are used for training and may result in confirmation bias where the model reinforces its own mistakes. In this work, we show that SOTA SSL methods often suffer from confirmation bias and demonstrate that this is often a result of using a poorly calibrated classifier for pseudo labeling. We introduce BaM-SSL, an efficient Bayesian Model averaging technique that improves uncertainty quantification in SSL methods with limited computational or memory overhead. We demonstrate that BaM-SSL mitigates confirmation bias in SOTA SSL methods across standard vision benchmarks of CIFAR-10, CIFAR-100 and ImageNet, giving up to 16% improvement in test accuracy on the CIFAR-100 with 400 labels benchmark. Furthermore, we also demonstrate their effectiveness in additional realistic and challenging problems, such as class-imbalanced datasets and in photonics science.

1 Introduction

While deep learning has achieved unprecedented success in recent years, its reliance on vast amounts of labeled data remains a long standing challenge. Semi-supervised learning (SSL) aims to mitigate this by leveraging unlabeled samples in combination with a limited set of annotated data. In computer vision, two powerful techniques that have emerged are consistency regularization (Bachman et al., 2014; Sajjadi et al., 2016) and pseudo-labeling (also known as self-training) (Rosenberg et al., 2005; Xie et al., 2019b). Broadly, consistency regularization enforces that random perturbations of the unlabeled inputs produce similar predictions, while pseudo-labeling assigns artificial labels to unlabeled samples, which are then used to train the model. These two techniques are typically combined by minimizing the cross-entropy between pseudo-labels and predictions that are derived from differently augmented inputs, and have led to strong performances on vision benchmarks (Sohn et al., 2020; Assran et al., 2021).

In many SOTA SSL methods, a selection metric (Lee, 2013; Sohn et al., 2020) based on the model's confidence is often used in conjunction with pseudo-labeling, where only confident pseudo-labels are selected to update the model. As such, there is a need for proper confidence estimates; in other words, the calibration of the model should be of paramount importance. Model calibration (Guo et al., 2017) can be understood as a measure of how a model's output truthfully quantifies its predictive uncertainty, i.e. it denotes the alignment between its prediction confidence and its ground-truth accuracy. Apart from the importance of calibration arising from the selection metric, the use of cross-entropy minimization objectives common in SSL implies that models will naturally be driven to output high-confidence predictions (Grandvalet & Bengio, 2004). Having high-confidence predictions is highly desirable in SSL since we want the decision boundary to lie in low-density regions of the data manifold, i.e. away from labeled data points (Murphy, 2022). However, without proper calibration, a model would easily become over-confident. This is highly detrimental as the model would be encouraged to reinforce its mistakes, resulting in the phenomenon commonly known as *confirmation bias* (Arazo et al., 2019).

In this work, we propose to mitigate confirmation bias in semi-supervised learning by incorporating approximate Bayesian techniques, which have been widely known to improve uncertainty estimates (Wilson & Izmailov,

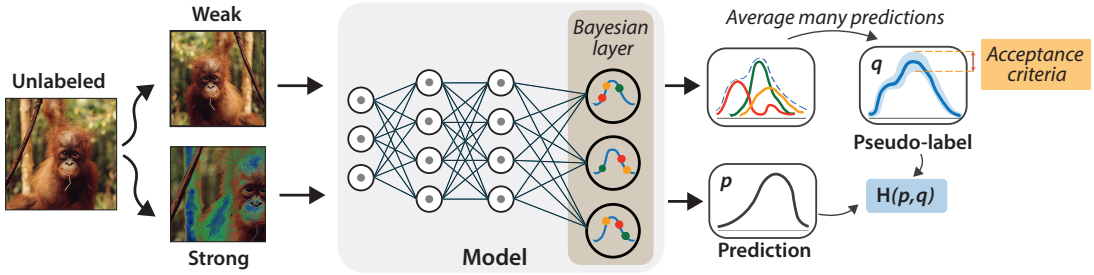

Figure 1: **Illustration of our Bayesian Model averaging (BaM) approach.** The last layer of the model has weights that are represented by probability distributions rather than the typical single fixed value. BaM- incorporates two main modifications to a traditional semi-supervised learning approach: 1) During pseudo-labeling of each unlabeled data point, multiple weights are sampled and averaged to derive the prediction; and 2) the selection criteria is based upon the variance over predictions.

Table 1: **Comparison of techniques used in BaM- with techniques used in prior art of SSL.**

SSL method	Augmentation	Pseudo-label	Selection metric
Temporal ensemble (Laine & Aila, 2016)	Weak	Model from earlier step	-
Mean teacher (Tarvainen & Valpola, 2017)	Weak	EMA	-
UDA (Xie et al., 2019a)	Weak & strong	Sharpen	Logit thresholding
MixMatch (Berthelot et al., 2019)	Weak	Averaging aug + sharpen	-
FixMatch (Sohn et al., 2020)	Weak & strong	Hard labels	Logit thresholding
FlexMatch (Zhang et al., 2021)	Weak & strong	Hard labels	Class-wise logit threshold
Our main method BaM-	Weak & strong	**Posterior sampling** + sharpen	**Variance thresholding**

2020). Our main approach, BaM-, performs Bayesian Model averaging during pseudo-labeling by incorporating a Bayesian last layer to the model and is illustrated in Fig. 1. Broadly, BaM- can be described as follows; instead of single-fixed-value weights, the last layer are parameterized as Gaussian random variables and two main modifications are made during pseudo-labeling: 1) multiple weight samples are drawn from the layer and averaged to derive the predictions and 2) the selection criterion is based on their posterior variances (further details follow in Section 4.1). We further contextualize the novelty of BaM- against prior art in the SSL literature in Table 1. In contrast to prior methods, BaM- is designed to specifically target improving model calibration in order to mitigate confirmation bias.

Our contributions are summarized as follows:

1. We introduce BaM-, which is designed to mitigate confirmation bias via Bayesian model averaging in SOTA SSL methods based upon a selection metric. BaM- incorporates two new features to improve uncertainty estimation: 1) bayesian averaging over multiple weight samples and 2) a selection metric based on the variance of the predictions

2. We empirically demonstrate that BaM- effectively improves model calibration, resulting in better performances on standard benchmarks like CIFAR-10 and CIFAR-100, notably giving up to 16% gains in test accuracy.

3. We also demonstrate the efficacy of BaM- in more challenging and realistic scenarios, such as class-imbalanced datasets and a real-world application in photonic science.

2 Related Work

Semi-supervised learning (SSL) and confirmation bias. A fundamental problem in SSL methods based on pseudo-labeling (Rosenberg et al., 2005) is that of confirmation bias (Tarvainen & Valpola, 2017;

Murphy, 2022), i.e. the phenomenon where a model overfits to incorrect pseudo-labels. Several strategies have emerged to tackle this problem; Guo et al. (2020) and Ren et al. (2020) looked into weighting unlabeled samples, Thulasidasan et al. (2019) and Arazo et al. (2019) proposes to use augmentation strategies like MixUp (Zhang et al., 2017), while Cascante-Bonilla et al. (2020) proposes to re-initialize the model before every iteration to overcome confirmation bias. Another popular technique is to impose a selection metric (Yarowsky, 1995) to retain only the highest quality pseudo-labels, commonly realized via a fixed threshold on the maximum class probability (Xie et al., 2019a; Sohn et al., 2020). Recent works have further extended such selection metrics to be based on dynamic thresholds, either in time (Xu et al., 2021) or class-wise (Zou et al., 2018; Zhang et al., 2021). Different from the above approaches, our work proposes to overcome confirmation bias in SSL by directly improving the calibration of the model through approximate Bayesian techniques.

Model calibration and uncertainty quantification. Proper estimation of a network's prediction uncertainty is of practical importance (Amodei et al., 2016) and has been widely studied. A common approach to improve uncertainty estimates is via Bayesian marginalization (Wilson & Izmailov, 2020), i.e. by weighting solutions by their posterior probabilities. Since exact Bayesian inference is computationally intractable for neural networks, a series of approximate Bayesian methods have emerged, such as variational methods (Graves, 2011; Blundell et al., 2015; Kingma et al., 2015), Hamiltonian methods (Springenberg et al., 2016) and Langevin diffusion methods (Welling & Teh, 2011). Other methods to achieve Bayesian marginalization also exist, such as deep ensembles (Lakshminarayanan et al., 2016) and efficient versions of them (Wen et al., 2020; Gal & Ghahramani, 2015), which have been empirically shown to improve uncertainty quantification. The concept of uncertainty and calibration are inherently related, where calibration is commonly interpreted as the frequentist notion of uncertainty. It is known that a well specified Bayesian model (i.e. one where the prior captures the model uncertainty) has a well-calibrated posterior (Gelman et al., 2021). Motivated by this, in our work we adopt some approximate bayesian techniques specifically for the context of semi-supervised learning in order to improve model calibration during pseudo-labeling and empirically validate their effectiveness. While other methods for improving model calibration exists (Platt, 1999; Zadrozny & Elkan, 2002; Guo et al., 2017), these are most commonly achieved in a post-hoc manner using a held-out validation set; instead, we seek to improve calibration during training and with a scarce set of labels. In the intersection of SSL and calibration, Rizve et al. (2021) proposes to leverage uncertainty to select a better calibrated subset of pseudo-labels. Our work builds on a similar motivation, however, in addition to improving the selection metric with uncertainty estimates, we show that directly incorporating approximate Bayesian techniques into SSL methods can indeed improve calibration via its better-calibrated approximate posterior. Finally, our work also bears some close resemblance to acquistion functions used in Bayesian active learning. There, we seek data points for which the parameters under the posterior disagree about the outcome the most (Houlsby et al., 2011; Kirsch et al., 2019). In contrast, in semi-supervised learning where the goal is to reduce confirmation bias by selecting samples where the network is most certain about predicting, we instead seek data points for which the parameters under the posterior agree the most.

3 Notation and Background

Given a small amount of labeled data $\mathcal{L} = \{(x_l, y_l)\}_{l=1}^{N_l}$ (here, $y_l \in \{0,1\}^K$, are one-hot labels) and a large amount of unlabeled data $\mathcal{U} = \{x_u\}_{u=1}^{N_u}$, i.e. $N_u \gg N_l$, in SSL, we seek to perform a K-class classification task. Let $f(\cdot, \theta_f)$ be a backbone encoder (e.g. ResNet or WideResNet) with trainable parameters θ_f, likewise let $h(\cdot, \theta_h)$ be a linear classification head, and H denote the standard cross-entropy loss.

SSL methods based on a selection metric. Many SSL methods such as Pseudo-Labels (Lee, 2013), UDA (Xie et al., 2019a) and FixMatch (Sohn et al., 2020) use a selection metric in conjunction with pseudo-labeling to achieve SOTA performance. These methods minimizes a cross-entropy loss on augmented copies of unlabeled samples whose confidence exceeds a pre-defined threshold. Let α_1 and α_2 denote two augmentation transformations and their corresponding network predictions for sample x to be $q_1 = h \circ f(\alpha_1(x))$ and $q_2 = h \circ f(\alpha_2(x))$, the total loss on a batch of unlabeled data has the following form:

$$L_u = \frac{1}{\mu B} \sum_{u=1}^{\mu B} \mathbb{1}(\max(q_{1,u}) \geq \tau) H(\rho_t(q_{1,u}), q_{2,u}) \tag{1}$$

where B denotes the batch-size of labeled examples, μ a scaling hyperparameter for the unlabeled batch-size, $\tau \in [0, 1]$ is a threshold parameter often set close to 1. ρ_t is either a sharpening operation on the pseudo-labels, i.e. $[\rho_t(q)]_k := [q]_k^{1/t} / \sum_{c=1}^{K} [q]_c^{1/t}$ when soft-pseudo-labels are used, or a one-hot operation (i.e. $t \to 0$) when hard pseudo-labels are used. In the latter, we only care about the class where the maximum logit occurs. ρ_t also implicitly includes a "stop-gradient" operation, i.e. gradients are not back-propagated from predictions of pseudo-labels. L_u is combined with the expected cross-entropy loss on labeled examples, $L_l = \frac{1}{B} \sum_{l=1}^{B} H(y_l, q_{1,l})$ to form the combined loss $L_l + \lambda L_u$, with a scaling hyperparameter λ. Differences between Pseudo-Labels, UDA and FixMatch are detailed in Appendix D.1.

Calibration metrics. A popular empirical metric to measure a model's calibration is via the *Expected Calibration Error (*ECE*)*. Following (Guo et al., 2017; Minderer et al., 2021), we focus on a slightly weaker condition and consider only the model's most likely class-prediction, which can be computed as follows. Let $q_{\max}$ denote the model's confidence, or the prediction at the most likely class (i.e. the maximum logit value after the softmax), the model's confidence on a batch of N samples are grouped into M equal-interval bins, i.e. $\mathcal{B}_m$ contains the set of samples with $q_{\max} \in (\frac{m-1}{M}, \frac{m}{M}]$. ECE is then computed as the expected difference between the accuracy and confidence of each bin over all N samples:

$$\text{ECE} = \sum_{m=1}^{M} \frac{|\mathcal{B}_m|}{N} |\text{acc}(\mathcal{B}_m) - \text{conf}(\mathcal{B}_m)| \tag{2}$$

where $\text{acc}(\mathcal{B}_m) = (1/|\mathcal{B}_m|) \sum_{i \in \mathcal{B}_m} \mathbb{1}(\text{argmax}(q_i) = y_i)$ and $\text{conf}(\mathcal{B}_m) = (1/|\mathcal{B}_m|) \sum_{i \in \mathcal{B}_m} q_{\max,i}$ with y_i the true label of sample i. In this work, we estimate ECE using $M = 10$ bins. We also caveat here that while ECE is not free from biases (Minderer et al., 2021), we chose ECE over alternatives (Brier, 1950; DeGroot & Fienberg, 1983) due to its simplicity and widespread adoption.

4 Mitigating Confirmation Bias in Semi-supervised learning

As we see from Eq. (1), the model's confidence (the maximum softmaxed logit value) is used to determine if the pseudo-label of a particular unlabeled data point is used to update the model; as such it is important for the model to have proper confidence estimates, i.e. to be well-calibrated. More recently, temperature scaling (Guo et al., 2017) or other similar methods (Platt, 1999; Zadrozny & Elkan, 2002) have been highly effective towards model calibration. However, such methods pose several challenges in the semi-supervised setting; 1) they operate post-hoc, i.e. *after* training is completed, while in SSL the model needs to be calibrated constantly *during* training to reduce confirmation bias of pseudo-labels; 2) these methods use a held-out labeled set (typically around 10% of the total dataset size (Guo et al., 2017)) to perform calibration, while common benchmarks of SSL typically have label percentages less than that (up to as little as <1%), making it challenging to create a held-out set with so little data to begin with.

4.1 Mitigating Confirmation Bias with Bayesian Model Averaging

Given the above limitations of post-hoc calibration methods, in this work we propose to incorporate approxmate Bayesian methods such as Bayesian Neural Networks (BNN) into existing SSL methods. Bayesian models, when well-specified (i.e. where the prior captures the model's uncertainty), are known to produce well-calibrated posteriors (Gelman et al., 2021) and approximate Bayesian techniques have been widely empirically shown to produce well-calibrated uncertainty estimates in deep neural networks (Wilson & Izmailov, 2020; Lakshminarayanan et al., 2016; Blundell et al., 2015).

Implementing a last-layer BNN. In order to minimize the computational overhead and reduce the risk of overall poorer model accuracy arising from a full Bayesian approach Wenzel et al. (2020), we propose to only replace the **final layer** of the network, i.e. the linear classification head h, with a BNN layer. While there may be several options towards the implementation of the BNN layer, we propose to use a BNN with a variational posterior trained via stochastic variational inference (SVI) for computational efficiency. This would allow one to optimize both the non-bayesian backbone and the BNN layer simulataneously in a single

backward pass, as opposed to other Bayesian approaches such as Hamiltonian Monte Carlo (Neal, 2012) which may require separate optimization loops.

Stochastic variational inference in BaM-. For notation convenience, we denote the input embedding to the BNN layer to be v in this section. In SVI, we first assume a prior distribution on weights $p(\theta_h)$. Given some training data $\mathcal{D}_\mathcal{X} := (X, Y)$, we seek to calculate the posterior distribution of weights, $p(\theta_h|\mathcal{D}_\mathcal{X})$, which can then be used to derive the posterior predictive $p(y|v, \mathcal{D}_\mathcal{X}) = \int p(y|v, \theta_h)p(\theta_h|\mathcal{D}_\mathcal{X})d\theta_h$. This process is also known as "Bayesian model averaging" or "Bayesian marginalization" (Wilson & Izmailov, 2020). Since exact Bayesian inference is computationally intractable for neural networks, we adopt a variational approach following Blundell et al. (2015), where we learn a Gaussian variational approximation to the posterior $q_\phi(\theta_h|\phi)$, parameterized by ϕ, by maximizing the evidence lower-bound (ELBO) (see Appendix C.1 for details). The ELBO $= \mathbb{E}_q \log p(Y|X; \theta) - KL(q(\theta|\phi)\|p(\theta))$ consists of a log-likelihood (data-dependent) term and a KL (prior-dependent) term. We provide some preliminary theoretical connections to generalization bounds via Corollary 1 in Appendix A. Corollary 1 shows that the generalization error is upper bounded by the negative ELBO, i.e. by maximizing the ELBO we may improve generalization. Apart from the last layer, the rest of the network is non-bayesian and are point values which are trained via regular Maximum Likelihood Estimation (MLE).

Pseudo-labeling via BaM-. As depicted in Fig. 1, pseudo-labeling in BaM- proceeds in two-stages: 1) M weights from the BNN layer are sampled and predictions are derived from the Monte Carlo estimated posterior predictive, i.e. $\hat{q} = (1/M)\sum_m^M h(v, \theta_h^{(m)})$, and 2) the selection criteria is based upon their variance, $\sigma_c^2 = (1/M)\sum_m^M (h(v, \theta_h^{(m)}) - \hat{q})^2$, at the predicted class $c = \text{argmax}_{c'}\,[\hat{q}]_{c'}$. This constitutes a more intuitive measure of model uncertainty compared to the maximum logit value commonly used in prior SSL methods which **does not have an uncertainty interpretation**. In section 7, we verify through ablations that the variance of predictions is indeed more effective than the maximum logit value for mitigating confirmation bias. The variance is also highly intuitive — if the model's prediction has a large variance, it is highly uncertain and the pseudo-label should not be accepted. We later show that better uncertainty estimates from BaM- effectively mitigates confirmation bias. In practice, as σ_c^2 decreases across training, we use a simple quantile Q over the batch to define the threshold where pseudo-labels of samples with $\sigma_c^2 < Q$ are accepted, with Q as a hyperparameter. Algorithm 1 shows a snippet of pseudo-code to highlight the main modifications introduced by BaM- during pseudo-labeling (a more complete version of the pseudo-code can be found in Appendix C.1).

We explore the effectiveness of BaM- by modifying upon SOTA SSL methods and denote them with the BaM- suffix, i.e. "BaM-X" incorporates approximate Bayesian Model averaging (BaM) during pseudo-labeling for SSL method X.

Algorithm 1 Snippet of PyTorch-style pseudocode showing pseudo-labeling in BaM-UDA.

```
# Q: quantile parameter
# num_samples: number of weight samples

q_list = []
for x_weak, x_strong in unlabeled_loader:
    z_weak, z_strong = encoder(x_weak), encoder(x_strong) # get representations
    mean_weak, std_weak = bayes_predict(bayes_classifier, z_weak) # get mean and std of predictions
    q_list.pop(0) if len(q_list) > 50 # keep 50 most recent quantiles
    q_list.append(quantile(std_weak, Q))
    accept_mask = std_weak.le(q_list.mean()) # determine acceptance for samples with small std

    # compute unlabeled loss using soft pseudo-labels on accepted samples
    loss_unlab = cross_entropy_loss(bayes_classifier(z_strong), sharpen(mean_weak)) * accept_mask
    loss_kl = KL_loss(bayes_classifier) # prior-dependent (data-independent) loss
    loss = loss_unlab + loss_kl

def bayes_predict(h, z):
    outputs = stack([h(z).softmax(-1) for _ in range(num_samples)] # sample weights
    return outputs.mean(), outputs.std() # mean and std of predictions
```

Table 2: **BaM- in SSL** showing "Test accuracy (%) / ECE". BaM- improves calibration and result in better test accuracies, consistently across all benchmarks and across two SSL methods, FixMatch (FM) (Sohn et al., 2020) and UDA (Xie et al., 2019a). For each benchmark, results are averaged over 3 random dataset splits.

	CIFAR-10		CIFAR-100		
	250 labels	2500 labels	400 labels	4000 labels	10000 labels
FM (repro)	95.0±0.19 / 0.046±0.002	95.7±0.03 / 0.039±0.0	56.4±1.6 / 0.366±0.017	74.2±0.2 / 0.183±0.003	78.1±0.2 / 0.147±0.001
BaM-FM (ours)	95.1±0.07 / 0.044±0.000	95.7±0.1 / 0.039±0.0	59.0±1.4 (↑2.6) / 0.331±0.015	74.8±0.09 (↑0.6) / 0.171±0.002	78.1±0.2 / 0.139±0.002
UDA (repro)	94.1±0.6 / 0.053±0.006	95.7±0.05 / 0.039	44.1±0.7 / 0.473±0.013	72.9±0.01 / 0.189±0.003	77.2±0.3 / 0.154±0.002
BaM-UDA (ours)	**95.2**±0.04 (↑1.1) / **0.042**±0.00	**95.9**±0.08 (↑0.2) / **0.038**	**60.3**±0.6 (↑16.2) / **0.314**±0.005	**75.2**±0.1 (↑2.3) / **0.165**±0.002	**78.3**±0.2 (↑1.1) / **0.138**±0.003

5 Experimental Setup

In all our experiments, we begin with and modify upon the original implementations of the baseline SSL methods. The backbone encoder f is a Wide ResNet-28-2 and Wide ResNet-28-8 for the CIFAR-10 and CIFAR-100 benchmarks respectively. We use the default hyperparameters and dataset-specific settings (learning rates, batch size, optimizers and schedulers) recommended by the original authors for both the baselines and in BaM-. We set the weight priors in BaM- as unit Gaussians and use a separate Adam optimizer for the BNN layer with learning rate 0.01, no weight decay and impose the same cosine learning rate scheduler as the backbone. We set $Q = 0.75$ for the CIFAR-100 benchmark and $Q = 0.95$ for the CIFAR-10 benchmark; which are both linearly warmed-up from 0.1 in the first 10 epochs. As Q is computed across batches, we improve stability by using a moving average of the last 50 quantiles.

ECE and test accuracy evaluation. In our experiments, we found that the test accuracy exhibits a considerable amount of noise across training, especially in label-scarce settings. Sohn et al. (2020) proposes to take the median accuracy of the last 20 checkpoints, while Zhang et al. (2021) argues that this fixed training budget approach is not suitable when convergence speeds of the algorithms are different (as the faster converging algorithm would over-fit more severely at the end) and thus report also the overall best accuracy. In our experiments, we adopt a balance between the two aforementioned approaches: we consider the median of 20 checkpoints around the best accuracy checkpoint as the *convergence criteria*, and report this value as the test accuracy. The ECE is reported when the model reaches this convergence criteria (one could also also aggregate the ECEs up till convergence — we found this gave similar trends and thus report the simpler metric).

6 Results

6.1 BaM- improves model calibration and consistently leads to better SSL performances

Results on the CIFAR-10 and CIFAR-100 benchmarks for various number of labels are depicted in Table 2. Table 2 demonstrates that BaM- successfully reduces the ECE over the baselines across all the benchmarks and as a result, we also attained significant improvements in test accuracies, notably up to 16.2% (for UDA on CIFAR-100-400 labels). Interestingly, while the baseline FixMatch outperforms UDA across all the benchmarks, improving calibration in UDA (i.e. BaM-UDA) allows it to outperfom both FixMatch and BaM-FixMatch. A key difference between FixMatch and UDA is the use of hard pseudo-labels in FixMatch (i.e. $t \to 0$ in ρ_t defined in Section 3) versus soft pseudo-labels in UDA (with $t = 0.4$); this suggests that a Bayesian classifier is more effective in conjunction with soft pseudo-labels. Leveraging on this insight, we set $t = 0.9$ in BaM-UDA (also see Section 7.2 for ablations on t), resulting in consistently better performances over the two SSL baselines across all CIFAR benchmarks.

Overall, we found that the improvements in both calibration and test accuracy are more significant for label-scarce settings, as expected, since the problem of confirmation bias is more acute there and BaM- can provide greater benefits by mitigating this. The additional computation overhead incurred from BaM- is minimal, adding approximately only 2-5% in wall-clock time (see Appendix H). While previous works (Sohn et al., 2020) also include extreme low label settings such as CIFAR-10-40 labels, we found this benchmark to be highly sensitive to the random initialization and different splits of the data, giving up to 2% variance with the exact same SSL method and thus we exclude them in our study.

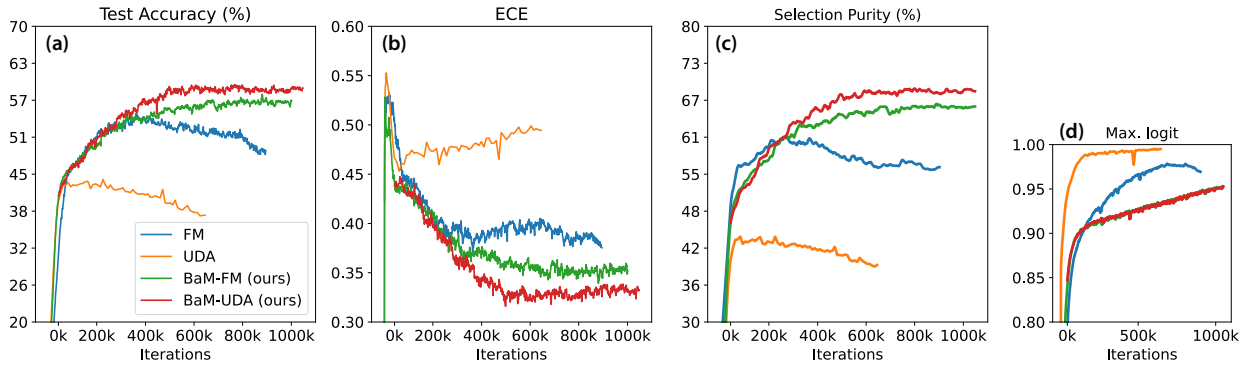

Figure 2: **FixMatch, UDA, BaM-FM and BaM-UDA across training** on CIFAR-100 with 400 labels (a) Test accuracies and (b) ECE as a function of training time. (c) Selection purity shows the accuracy of unlabeled samples that are accepted by the selection metric and (d) Max. logit shows the model's confidence, i.e. the average maximum class probability of all unlabeled samples.

Table 3: **Long-tailed CIFAR-10 & CIFAR-100** showing "Test accuracy (%) / ECE". We use 10% of labels from each class. For better interpretation, we also show the supervised (100% labels) accuracy reported in Cao et al. (2019), which use a different architecture, ResNet-32, and an algorithm targeted for long-tailed problems.

	CIFAR-10-LT		CIFAR-100-LT	
	$\alpha = 10$	$\alpha = 100$	$\alpha = 10$	$\alpha = 100$
FixMatch	91.3 / 0.073	70.0 / 0.26	48.8 / 0.38	28.6 / 0.55
BaM-UDA (ours)	**91.6** (↑0.3) / **0.067**	**71.2** (↑1.2) / **0.24**	**53.6** (↑4.8) / **0.32**	**31.9** (↑3.3) / **0.50**
Supervised (reported)	88.2	77.0	58.7	42.0

6.2 BaM- improves performances by reducing confirmation bias

To further understand how BaM- mitigates confirmation bias, we track the test accuracy, ECE, model confidence and ground-truth accuracy of *accepted* pseudo-labels (i.e. the "selection purity") over the course of training for the baselines and BaM-, as shown in Fig. 2. While the baselines learn effectively for the initial stages of training, learning is eventually hindered. Due to the entropy minization objective, the model is encouraged to output increasingly confident predictions (as evident from the growing model confidence in Fig. 2d). Thus, in the absence of explicit calibration, the baselines quickly become *over-confident*, resulting in confirmation bias where the model reinforces its mistakes. Confirmation bias in the baselines is particularly evident from the selection purity (i.e. the ground truth accuracy of accepted pseudo-labels) in Fig. 2c — after a short amount of training, the selection purity starts to drop suggesting that the model begins to accept pseudo-labels that it makes mistakes on. In contrast, BaM- successfully mitigates confirmation bias as evident from the constantly improving selection purity, thus promoting learning for longer periods to result in better final performances. Further ablation studies are discussed in Section 7.2 and Appendix G.

6.3 BaM- is more effective in class-imbalanced settings

Long-tailed image datasets. Datasets in the real world are often long-tailed or class-imbalanced, where some classes are more commonly observed while others are rare. We curate long-tailed versions from the CIFAR datasets following Cao et al. (2019), where α indicates the imbalance ratio (i.e. ratio between the sample sizes of the most frequent and least frequent classes). We randomly select 10% of the samples in each class to form the labeled set; see further details in Appendix E. We use the best performing baseline method from Table 2, i.e. FixMatch (FM), as our baseline and compare against BaM-UDA. Results are shown in Table 3, where BaM-UDA achieves consistent improvements over FM in both calibration and accuracy across all benchmarks. Notably, gains from BaM- are more significant than those in the class-balanced settings (for e.g. BaM-UDA improves upon FM by a smaller margin of 1.5% on the CIFAR-100-4000 labels

benchmark which is also approximately 10%). Further analysis are provided in Appendix E.2, where test samples were separated into three groups depending on the number of samples per class and test accuracies are plotted for each group.

Table 4: **Photonic crystals (PhC) band gap prediction** showing "Test accuracy (%) / ECE". The fully-supervised (100% labels) accuracy is 88.5%.

	PhC-10%	PhC-1%
FixMatch	78.8 / 0.098	55.0 / 0.385
BaM-UDA	**81.0** (↑2.2) / **0.052**	**56.9** (↑1.9) / **0.356**

Photonics science. A practical example of a real-world domain where long-tailed datasets are prevalent is that of science – samples with the desired properties are often much rarer than trivial samples. Further, SSL is highly important in scientific domains since labeled data is particularly scarce (owing to the high resource cost needed for data collection). To demonstrate the effectiveness of BaM-, we adopt a problem in photonics (Loh et al., 2022), where the task is a 5-way classification of photonic crystals (PhCs) based on their band gap sizes. A brief summary and visualization of this dataset are available in Appendix F. We explored an approach similar to FixMatch for the baseline and similar to BaM-UDA for ours (some modifications were needed in the augmentation strategies to respect the correct physics of this problem; see Appendix F). Results are shown in Table 4, where we demonstrate the consistency of BaM-UDA's effectiveness in improving calibration and accuracies in this real-world problem.

7 Ablation studies on BaM

7.1 Ablating the key components of BaM

BaM- consists of two main features; 1) several weight samples are taken from the BNN layer and averaged to derive the predictions, and 2) the selection criteria is modified to be based upon the variance of the samples. To further investigate the effect of each feature, we perform ablation studies on BaM-UDA to isolate the contribution of averaging predictions from the contribution of replacing the selection metric. Results are shown in Table 5, rows indicated with "BNN no σ^2" show experiments using a BNN layer in BaM-UDA *only for averaging predictions* while maintaining the original selection metric, i.e. pseudo-labels are accepted if the maximum prediction class probability is greater than $\tau = 0.95$. Comparing the first two rows, indeed we see that by not using the uncertainty estimates from the BNN, we already get some improvements (minor improvements in cases where labels are not so scarce). The difference between the last two rows show the effect of replacing the selection metric and indeed we observe larger and consistent gains across the benchmarks from doing so.

Table 5: **Uncertainty estimate by BNN.** Ablating the importance of uncertainty estimate provided by the variance of BNN predictions. "BNN no σ^2" indicates that the BNN layer is only used for bayesian model averaging, i.e. predictions are replaced by the posterior predictive but selection metric still follows the baseline, i.e. pseudolabels are accepted if maximum logit value after the softmax > 0.95. Cyan indicates the default configuration.

	CIFAR-100	
	400	4000
UDA (t=0.4)	44.0 / 0.491	72.9 / 0.185
BaM-UDA, BNN no σ^2 (t=0.4, τ=0.95)	48.3 / 0.418	73.0 / 0.184
BaM-UDA, BNN no σ^2 (t=0.9, τ=0.95)	54.2 / 0.368	74.5 / 0.170
BaM-UDA (t=0.9)	59.7 / 0.327	75.3 / 0.167

7.2 Importance of sharpening temperature

From our results in Section 6, we found that BaM was more effective in conjunction with soft pseudo-labels. In Table 6, we show ablation experiments on the temperature of the sharpening operation on the CIFAR-100-400 labels benchmark. Overall, we observe a trend that softer pseudo-labels (i.e. reducing the sharpening of pseudo-labels) led to better calibration and improved test performance. As such, in our experiments we modify upon the original sharpening parameter of UDA and set $t = 0.9$ for BaM-UDA in all our benchmarks.

Table 6: Ablation of sharpening temperature in BaM-UDA. Dataset is CIFAR-100 with 400 labels. Highlighted in cyan is the main configuration used.

t	Test Accuracy	ECE
0.4	57.9	0.344
0.8	58.1	0.340
0.9	59.7	0.327
1.0	59.2	0.334

8 Conclusion and Broader Impact

Since confirmation bias is a fundamental problem in SSL, in this work we showed that it is imperative for the model to have proper uncertainty estimates, or be well-calibrated, to mitigate this problem. In particular, we empirically demonstrated that approximate Bayesian techniques such as a last Bayesian layer or weight averaging approaches can be used to improve a model's uncertainty estimates which can result in better model performance across a variety of SSL methods. We further underscore their importance in more challenging real-world datasets. We hope that our findings can motivate future research directions to incorporate techniques targeted for optimizing calibration during the development of new SSL methods. Furthermore, while the primary goal of improving calibration is to mitigate confirmation bias during pseudo-labeling, an auxiliary benefit brought about by our approach is a better calibrated network, i.e. one that can better quantify its uncertainty, which is highly important for real-world applications. A potential limitation in our work lies in the use of ECE as a metric to measure calibration which, while commonly used across literature, are not free from flaws (Nixon et al., 2019). However, in our work, we empirically demonstrate that despite their flaws, the ECE metric still provides good correlations to measuring confirmation bias and test accuracy. We provide further discussion of the societal impact and ethical considerations of our work in Appendix I.

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