A statistical theory of cold posteriors in deep neural networks

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Abstract

To get Bayesian neural networks to perform comparably to standard neural networks it is usually necessary to artificially reduce uncertainty using a “tempered” or “cold” posterior. This is extremely concerning: if the prior is accurate, Bayes inference/decision theory is optimal, and any artificial changes to the posterior should harm performance. While this suggests that the prior may be at fault, here we argue that in fact, BNNs for image classification use the wrong likelihood. In particular, standard image benchmark datasets such as CIFAR-10 are carefully curated. We develop a generative model describing curation which gives a principled Bayesian account of cold posteriors, because the likelihood under this new generative model closely matches the tempered likelihoods used in past work.

1 Introduction

Recent work has highlighted that Bayesian neural networks (BNNs) typically have better predictive performance when we “sharpen” the posterior (Wenzel et al., 2020). In stochastic gradient Langevin dynamics (SGLD) (Welling & Teh, 2011), this can be achieved by multiplying the log-posterior by $1/T$, where the “temperature”, $T$ is smaller than 1 (Wenzel et al., 2020). Broadly the same effect can be achieved in variational inference by “tempering”, i.e. downweighting the KL term. This approach has been used in many recent papers to obtain good performance, albeit without always emphasising the importance of this factor (Zhang et al., 2017; Bae et al., 2018; Osawa et al., 2019; Ashukha et al., 2020).

These results are puzzling if we take the usual Bayesian viewpoint, which says that the Bayesian posterior, used with the right prior, and in combination with Bayes decision theory should give optimal performance. Thus, these results may suggest we are using the wrong prior. While several new priors have been suggested (Farquhar et al., 2019; Ober & Aitchison, 2020), they give only minor improvements in performance — certainly nothing like enough to close the gap to carefully trained finite networks. In contrast, tempering directly gives performance comparable to a carefully trained finite network.

The failure to develop an effective prior suggests that we should consider alternative explanations for the effectiveness of tempering. Here, we consider the possibility that it is predominantly the likelihood, and not the prior that is at fault. In particular, we note that standard image benchmark datasets such as ImageNet and CIFAR-10 are carefully curated, and that it is important to consider this curation as part of our generative model. We develop a simplified generative model describing dataset curation, and find that it naturally multiplies the effect of each datapoint, and hence gives posteriors that closely match tempered or cold posteriors. Our approach suggests that carefully curated datasets should see considerable performance improvement with tempering, whereas uncurated datasets should see smaller improvements.
2 Background: cold and tempered posteriors

Tempered and cold posteriors differ slightly in how they apply the temperature parameter. For cold posteriors, we scale the whole posterior, whereas tempering is a method typically applied in variational inference, and corresponds to scaling the likelihood but not the prior,

\[
\log P_{\text{cold}}(\theta | X, Y) = \frac{1}{T} \log P(X, Y | \theta) + \frac{1}{T} \log P(\theta) + \text{const} \quad (1)
\]

\[
\log P_{\text{tempered}}(\theta | X, Y) = \frac{1}{\lambda} \log P(X, Y | \theta) + \log P(\theta) + \text{const} \quad (2)
\]

While cold posteriors are typically used in SGLD, tempered posteriors are usually targeted by variational methods. In particular, variational methods apply temperature scaling to the KL-divergence between the approximate posterior, \(Q(\theta)\) and prior,

\[
\mathcal{L} = \mathbb{E}_{Q(\theta)} [\log P(X, Y | \theta)] - \lambda D_{KL}(Q(\theta) \parallel P(\theta)) \quad (3)
\]

Our work justifies the use of tempered posteriors, but in practice we do believe that the main effect here comes from reducing the uncertainty, so scaling the prior should not have too strong an effect.

3 Methods: a generative model for curated datasets

Standard image datasets such as CIFAR-10 and ImageNet are carefully curated to include only unambiguous examples of each class. For instance, in CIFAR-10, student labelers were paid per hour (rather than per image), were instructed that “It’s worse to include one that shouldn’t be included than to exclude one.”, and then Krizhevsky et al. (2009) “personally verified every label submitted by the labelers”. For ImageNet, Deng et al. (2009) required the consensus of a number of Amazon Mechanical Turk labelers before including an image in the dataset.

Thus, these datasets have two odd properties:

1. Consensus labels exist only for a subset of images, e.g. for a white-noise image, consensus cannot be reached and the image cannot be labeled.

2. The inclusion of an image in a dataset like CIFAR-10 is informative in and of itself, as it indicates that the image shows an unambiguous example of one of the ten classes.

To understand the odd properties that result from creating consensus labels, we consider a highly simplified formal model of consensus-formation. In particular, we draw a random image \(Z\) from some underlying distribution over images and ask \(S\) humans to assign a label, \(\{Y_s\}_{s=1}^S\) (e.g. using Mechanical Turk). We force every labeler to label every image and if the image is ambiguous they are instructed to give a random label. If all the labelers agree, \(C = 1\), then we take consensus to be reached, and we include the datapoint in the dataset, and if any of them disagree (\(C = 0\)), we exclude the datapoint,

\[
C = \begin{cases} 
1 & \text{if } Y_1 = Y_2 = \cdots = Y_S \\
0 & \text{otherwise} 
\end{cases} \quad (4)
\]

Formally, the observed random variables, \(X\) and \(Y\), are taken to be the usual image-label pair if consensus can be reached and \(\text{None}\) if consensus cannot be reached,

\[
X | Z, C = \begin{cases} 
\text{None} & \text{if } C = 0 \\
Z & \text{if } C = 1 \text{ i.e. } Y_1 = Y_2 = \cdots = Y_S 
\end{cases} \quad (5)
\]

\[
Y | \{Y_s\}_{s=1}^S = \begin{cases} 
\text{None} & \text{if } C = 0 \\
Y_1 & \text{if } C = 1 \text{ i.e. } Y_1 = Y_2 = \cdots = Y_S 
\end{cases} \quad (6)
\]

Thus, taking the human labels, \(Y_s\), to come from the set \(\mathcal{Y}\), so \(Y_s \in \mathcal{Y}\), the consensus label, \(Y\), could be any of the underlying labels in \(\mathcal{Y}\), or will be \(\text{None}\) if no consensus is reached, so \(Y \in \mathcal{Y} \cup \{\text{None}\}\). Likewise, if \(Z\) lives in the space of all images, \(Z \in \mathcal{Z}\), then the observation could be any image, or, if no consensus is reached, it would be \(\text{None}\), so \(X \in \mathcal{Z} \cup \{\text{None}\}\).

In standard supervised learning, the posterior over parameters is given by,

\[
P(\theta | Y, X) \propto P(Y, X | \theta) P(\theta) = P(Y | X, \theta) P(X) P(\theta) \propto P(Y | X, \theta) P(\theta) , \quad (7)
\]
where the first proportionality is an application of Bayes theorem, and the second proportionality arises because we are interested in posterior parameter dependence, so we can drop $P(X)$ as it is independent of the parameters. Thus, for the purposes of inferring $\theta$, we can ignore the generative process for the inputs. However, in our case, the observed value of $X$, in particular whether it is None, depends on the classifications, $Y$, and hence on the model parameters. To begin, the likelihood if no consensus is reached is

$$P(Y = \text{None}, X = \text{None} | \theta) = \int dz P(Z = z) P(C = 0 | Z = z, \theta). \quad (8)$$

This term is difficult to compute as it requires us to know or integrate over the images, $Z$, for which consensus could not be reached, and these images are not typically included in the dataset. As such, we hypothesise that while this term can be dropped, estimating it accurately would improve performance.

When consensus was reached, i.e. for $X, Y$ not None, and for labelled data we have,

$$P(Y = y, X = z | \theta) = P(\{Y_s = y\}_{s=1}^S | Z = z, \theta) P(Z = z), \quad (9)$$

As we are ultimately interested in the parameter dependence of this term, and as $P(Z = z)$ is taken to be independent of the parameters, we can instead work with,

$$P(Y = y, X = z | \theta) \propto P(\{Y_s = y\}_{s=1}^S | Z = z, \theta) = \prod_s P(Y_s = y | Z = z, \theta) \quad (10)$$

This likelihood is equivalent to labelling each datapoint $S$ times with the same label, and therefore has the effect of setting $\lambda = S$ in a tempered posterior.

4 Agreement with past results

This theory already has support from published work in the literature. In particular, Wenzel et al. (2020) (e.g. their Fig. 5) found considerable cold posterior effects in CIFAR-10, as we would expect based on the above discussion. These cold-posterior effects were strong: there was a big performance increase from $T = 1$ to smaller temperatures, which were robust to increasing batch size, and performance degraded only slightly as the temperature was further lowered.

While they found some cold-posterior effects in the IMDB sentiment classification dataset Maas et al. (2011) (their Fig. 6), these effects were considerably weaker. First, the performance improvement from $T = 1$ to smaller temperatures depended strongly on batch size. This is important, because SGLD with small batches introduces additional noise, and reducing the temperature may help to compensate for that additional noise. Indeed, SGLD converges on Langevin sampling as the batch size increases, so the larger batches with smaller cold-posterior effects will be more representative of the true posterior. With the highest batch size, performance improvements for lower temperatures were much less marked than in CIFAR-10. Second, performance degraded far more dramatically as temperature was lowered beyond its optimal point. Note however that the way this dataset was collated suggest that we do expect to see some cold posterior effects, albeit likely weaker than for CIFAR-10. In particular, “A negative review has a score $\leq 4$ out of 10, and a positive review has a score $\geq 7$ out of 10. Neutral reviews are not included in the dataset” Maas et al. (2011).

In contrast, almost trivially, tempering will not be helpful if we consider datasets of arbitrary complexity generated from a known model, where we have performed exact Bayesian inference.

5 Related work

Concurrent work Adlam et al. (2020) has raised the possibility that BNNs overestimate aleatoric uncertainty, in part because of data curation, and argued that tempering is a mechanism for preventing this. However, they argued that tempering was a mechanism for better capturing our priors, and did not connect tempering to a new likelihood, motivated by a principled Bayesian generative model of the data curation process.
6 Conclusions

We showed that modelling the process of data-curation can explain the improved performance of tempering or cold posteriors in Bayesian neural networks. We hope that our work will prompt more careful dataset and study of data curation. Finally, the same likelihood has much broader applicability, as it also provides an explanation for the effectiveness of common semi-supervised learning methods. [Aitchison 2020]

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