Ensembling over Classifiers: a Bias-Variance Perspective

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Abstract

Ensembles are a straightforward, remarkably effective method for improving the accuracy, calibration, and robustness of models on classification tasks; yet, the reasons that underlie their success remain an active area of research. We build upon the extension to the bias-variance decomposition by Pfau (2013) in order to gain crucial insights into the behavior of ensembles of classifiers. Introducing a dual reparameterization of the bias-variance tradeoff, we first derive generalized laws of total expectation and variance for nonsymmetric losses typical of classification tasks. Comparing conditional and bootstrap bias/variance estimates, we then show that conditional estimates necessarily incur an irreducible error. Next, we show that ensembling in dual space reduces the variance and leaves the bias unchanged, whereas standard ensembling can arbitrarily affect the bias. Empirically, standard ensembling reduces the bias, leading us to hypothesize that ensembles of classifiers may perform well in part because of this unexpected reduction. We conclude by an empirical analysis of recent deep learning methods that ensemble over hyperparameters, revealing that these techniques indeed favor bias reduction. This suggests that, contrary to classical wisdom, targeting bias reduction may be a promising direction for classifier ensembles.

1 Introduction

The success of deep learning has catalyzed many extensions of classical learning theory to modern models and algorithms. In particular, the double-descent phenomenon (Belkin et al., 2019) has inspired a wide breadth of research, in which the classical bias-variance (BV) decomposition has been key (Neal et al., 2019; Adlam & Pennington, 2020). Such analyses have been instrumental to understanding the performance of various strategies that improve deep learning methods, including ensembles of deep networks (Hansen & Salamon, 1990; Lakshminarayanan et al., 2017) — a simple method with state-of-the-art robustness and uncertainty results (Ovadia et al., 2019; Gustafsson et al., 2020).

Most bias-variance analyses are specific to the mean-squared error (MSE) loss. Although it is possible to analyze classifiers from an MSE perspective (Yang et al., 2020), such a restriction inevitably reduces the power of our analysis. However, generalizing bias-variance decompositions to non-MSE losses is challenging. Although the MSE allows a decomposition based on the performance of the mean predictor, this is a peculiarity of the MSE rather than the rule. In the general case, bias-variance decompositions require manipulating a “central prediction” which is much less amenable to analysis. And although bias-variance decompositions can be derived for losses that take the form of a Bregman divergence (Pfau, 2013), such decompositions are difficult to interpret, and appear to break away from standard intuitions.

We begin by bridging the gap between the classical bias-variance decomposition and its generalization to losses such as the KL divergence. Analyzing the properties of the bias and variance for non-symmetric...
losses, we characterize their departure from standard intuition, and show that alternate ensembling techniques recover the standard behavior of ensembles under the MSE. Crucially, our analysis suggests that ensembles of classifiers may be particularly effective due to their ability to reduce the bias as well as the variance.

Based on this theoretical analysis, we investigate recent promising techniques that ensemble over the hyperparameters of deep learning algorithms (Wenzel et al., 2020; Zaidi et al., 2021). We will see that, by augmenting the hypothesis space, these methods achieve higher bias reduction but comparable or worse variance reduction than deep ensembles.

Contributions. Using a dual reparameterization of the central prediction in the bias-variance decomposition of Pfau (2013), we tease apart which behaviors of the bias and variance are specific to the mean squared error,¹ and which behaviors are common to all Bregman divergences. Our key contributions are the following.

- The central prediction for arbitrary Bregman divergences can be viewed as the primal projection of the mean prediction in a dual space defined by the loss itself.
- The variance for any arbitrary Bregman divergence satisfies a generalized law of total variance.
- Conditional estimates of the bias and variance are biased by an irreducible quantity; iterative bootstrapping can improve these estimates.
- Ensembling predictions in dual space recovers the behavior of ensembles under the squared Euclidean loss.
- Vanilla ensembling can increase or decrease the bias; empirically, vanilla ensembling reduces the bias.
- Recent ensemble methods show lower bias and higher variance than ensembling over random seeds.

2 Related work

Bias-variance decompositions. The bias-variance tradeoff has been an important tool in understanding the behavior of machine learning models (Geman et al., 1992; Kong & Dietterich, 1995; Breiman, 1996; Adlam & Pennington, 2020; Yang et al., 2020; d’Ascoli et al., 2020; Neal et al., 2019). Key to the decomposition are the notions of a “central label” (if label noise exists) — and of a “central prediction”. Most analyses focus on the bias-variance decomposition for the Euclidean square loss; in this case, the central label and prediction correspond respectively to the mean label and prediction. James (2003) proposed a more general decomposition for symmetric losses, Domingos (2000) focussed on the 0-1 loss, and Pfau (2013) proposed a generalization to the space of all Bregman divergences. Hansen & Heskes (2000) identify which loss functions admit bias-variance decompositions with specific properties (but do not analyze the decompositions themselves). Jiang et al. (2017); Buschjäger et al. (2020) decompose twice differentiable losses via second order Taylor expansion. In the general case — including for the KL divergence — the resulting decompositions are approximate. Additionally, the variance term may depend on target labels, in a significant departure from any standard definition of a variance.

Bregman divergences. Bregman divergences are a generalization of the notion of distance, similar to but less restrictive than metrics. Bregman divergences and operations in their associated dual space are instrumental to optimization techniques such as mirror descent and dual averaging (Nemirovski & Yudin, 1983; Nesterov, 2009; Juditsky et al., 2021). Closer to our work, the Bregman representative defined in Banerjee et al. (2005) is closely related to the central label defined in (Pfau, 2013).

Ensembles of deep networks. Ensembling combines the predictions of multiple models to improve upon the performance of a single model; see, e.g., (Zhou, 2019; Dietterich, 2000). Recently, ensembling over neural networks which only differ in their random seed (“deep ensembles”) has been shown to be a particularly strong baseline for a variety of benchmarks (Lakshminarayanan et al., 2017). This result, in turn, prompted

¹Or, more accurately, to symmetric losses.
further research into alternative ensemble methods, including ensembling over hyper-parameters (Wenzel et al., 2020), architectures (Zaidi et al., 2021), and joint ensemble training (Webb et al., 2020). In parallel, several hypotheses have been proposed to explain the performance of deep ensembles. Fort et al. (2019) showed empirically that deep ensembles explore diverse modes in the loss landscape. Allen-Zhu & Li (2020) argued that the effectiveness of deep ensembles hinges on the assumption that inputs to the model have multiple correct features, which will be learned by the different ensemble members. Wilson & Izmailov (2020); Hoffmann & Elster (2021) focus on understanding the relationship between the generalization of neural networks and the diversity for deep ensembles, both from theoretical and empirical perspectives. Lobacheva et al. (2020); Kobayashi et al. (2021) considered the interplay between model and ensemble size.

Results specific to the KL divergence. Due to its importance in machine learning, the KL divergence (and thus, the cross-entropy loss) is one of the few non-MSE losses for which the bias-variance tradeoff has been specifically analyzed (Heskes, 1998; Yang et al., 2020). For the KL divergence, the “central predictor” corresponds to an average in log-probability space, which has been studied in many works, including (Brofos & Shu, 2019; Webb et al., 2020). The fact that the bias remains unchanged when averaging predictions in log-probability space has been mentioned briefly in (Dietterich, 2005).

3 Bias-Variance decomposition

We begin with some background material regarding Bregman divergences, which also serves to set our notation. We refer the interested reader to Cesa-Bianchi & Lugosi (2006) for more background on Bregman divergences and proofs.

Our theoretical results are presented for arbitrary Bregman divergences; proofs not provided in the main text can be found in Appendix A. Our experimental results use the KL divergence (which corresponds to the cross-entropy loss for one-hot labels), which is standard for classification models.

3.1 Preliminaries

Let $\mathcal{X}$ be a closed, convex subset of $\mathbb{R}^d$, and let $F : \mathcal{X} \to \mathbb{R}$ be a strictly convex, differentiable function over $\mathcal{X}$. The Bregman divergence associated with $F$ is the function $D_F : \mathcal{X} \times \mathcal{X} \to \mathbb{R}^+$, such that

$$D_F[y||x] := F(y) - F(x) - \nabla F(x)^T (y - x). \quad (1)$$

It follows directly from the convexity of $F$ that $D_F$ is convex in its first argument, although not necessarily in its second argument (Bauschke & Borwein, 2001).

The Bregman divergence of the convex conjugate $F^*$ of $F$ will also be of particular importance. We recall that the convex conjugate of a convex function $F$ is defined as

$$F^*(z) = \sup_x \langle z, x \rangle - F(x).$$

As $F$ is differentiable, we denote by $x^* = \nabla F(x)$ the dual of $x \in \mathcal{X}$; in particular, $x = (x^*)^* = \nabla F^*(\nabla F(x))$.

A Bregman divergence $D_F$ and its conjugate equivalent $D_{F^*}$ are related by the following equality:

**Proposition 3.1** (Cesa-Bianchi & Lugosi (2006)). $\forall x, y \in \mathcal{X}, D_F[x || y] = D_{F^*}[y^* || x^*].$

3.2 General statement

A bias-variance analysis decomposes the average divergence between two independent random variables, $\mathbb{E}D[Y||X]$, into a bias and two separate variance terms. The bias measures the divergence between the
average label and the average prediction; the variances measure the amount of fluctuation in the labels (Bayes error) and predictions (model variance).

These variances measure fluctuations around an “average”, or “central” variable. Under the mean squared error, these central variables are the expected label and expected prediction. For Bregman divergences more generally, these “average” labels and predictions are the minimizers of the expected Bregman divergence.

**Definition 3.2** (Central label). Let $Y$ be a random variable over $X$ (intuitively, the label). We call **central label** the unique minimizer $\arg\min_{z \in X} E D[Y \| z]$.

**Definition 3.3** (Central prediction). Let $X$ be a random variable over $X$ (intuitively, the prediction). We call **central prediction** the unique minimizer $\arg\min_{z \in X} E D[z \| X]$.

**Proposition 3.4** (Banerjee et al. (2005)). The central label satisfies $\arg\min_{z \in X} E D[Y \| z] = E Y$.

By analogy to Proposition 3.4, and for reasons that will appear clear momentarily, we will refer to the minimizer $z = \arg\min_{z \in X} E D[z \| X]$ as the **dual mean**, and write it $E X$.

We can now write out the bias-variance decomposition for any Bregman divergence $D$ (Pfau, 2013):

$$
ED[Y \| X] = ED[Y \| EY] + D[EY \| EX] + ED[EX \| X].
$$

(2)

Because Bregman divergences are not guaranteed to be symmetric, Equation (2) takes a more complicated form than the mean squared error decomposition: central label and central prediction are computed differently, and the ordering of terms within the bias and variances is now important.

The main obstacle in bias-variance decompositions for Bregman divergences lies in the form of the central prediction, $\arg\min_{z \in X} E D[z \| X]$; the central label remains easily interpretable as $\arg\min_{z \in X} E D[Y \| z] = E Y$.

Our first contribution resolves this difficulty via a simple observation: the central prediction $E X$ has a straightforward interpretation when we leverage the dual space defined by the convex conjugate of $F$.

**Proposition 3.5** (Dual mean). The dual mean $E X$ is the primal projection of the mean of $X$ in dual space:

$$
E X = (E X^*)^*.
$$

**Proof.** By simple application of Proposition 3.1.

$$
\arg\min_{z \in X} ED_F[z \| X] = \arg\min_{z \in X} ED_{F^*}[X^* \| z^*] = \left( \arg\min_{z^* \in X^*} D_{F^*}[X^* \| z^*] \right)^* = (E X^*)^*.
$$

This reformulation is crucial to our analysis, and, to the extent of our knowledge, novel.$^2$

**Remark 3.6.** For $F(x) = \|x\|_2^2$, $D_F$ is the MSE, and $E X = E Y$. More generally, $E X = E X$ if $D_F$ is symmetric.

**Remark 3.7.** When $F$ is the negative entropy over the probability simplex, $D_F$ is the KL divergence, and $E X = \text{softmax}(E \log X)$.

**Remark 3.8.** Reordering Equation (2) for the KL divergence, we can write the loss of an ensemble of models averaged in log-probability space as the average loss of each model minus the variance term, thus recovering the ensemble diversity regularizer from (Webb et al., 2020).

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$^2$Pfau (2013) showed the characterization $z = \arg\min_{z} ED[z \| X]$ satisfies $\nabla F(z) = E[\nabla F(X)]$, which also entails Prop. 3.5.
3.3 Laws of total expectations and variance

Despite its more general form, the model variance $\forall X = D[\mathcal{E}X || X]$ in Equation (2) satisfies fundamental properties associated with the standard variance $\mathbb{E}(X - \mathbb{E}X)^2$. In particular, one can easily verify that $\forall X \geq 0$, and that $\forall X = 0$ if and only if $X$ is almost surely constant.

We next show that $\forall X$ also follows a generalization of the law of total variance. This law disentangles the effect of different sources of randomness, and is thus a fundamental tool in model analysis. Given two variables $X$ and $Z$, the law of total variance decomposes the standard (Euclidean) variance as $\forall X = \mathbb{E}[\forall (X | Z)] + \forall[\mathbb{E}(X | Z)]$: the variance of $X$ is the sum of the variances respectively unexplained and explained by $Z$.

We begin by showing that the dual mean satisfies its own form of the law of total expectation; proving this is straightforward with the reparameterization of Proposition 3.5.

Lemma 3.9. Let $X, Z$ be random variables on $\mathcal{X}$. Then $\mathcal{E}X = \mathcal{E}_Z[\mathcal{E}[X|Z]]$, where $\mathcal{E}[X | Z] := (\mathbb{E}_{X|Z}[X^*])^*$.

Proof. The proof follows directly from the (standard) law of total expectation and Proposition 3.5.

$\mathcal{E}_Z(\mathcal{E}_X|Z)X = \mathcal{E}_Z \left[ (\mathbb{E}_{X|Z} X^*)^* \right] = (\mathbb{E}_Z \mathbb{E}_{X|Z} X^*)^* = (\mathbb{E}X^*)^* = \mathcal{E}X$.

With Lemma 3.9 in hand, we can easily show a generalized form of the law of total variance, which simply accounts for the definition of dual mean and generalized variance.

Lemma 3.10. Let $X, Z$ be random variables over $\mathcal{X}$. The variance $\forall X := \mathbb{E}D[\mathcal{E}X || X]$ satisfies a generalized law of total variance.

\[ \forall X = \mathbb{E}[\forall (X | Z)] + \forall[\mathbb{E}(X | Z)]. \]

We cannot overstate the importance of Lemma 3.10, which is key to disentangling sources of randomness in ML algorithms (Neal et al., 2019; Adlam & Pennington, 2020).

4 Conditional and bootstrapped estimates

The bias-variance tradeoff of Equation (2) applies to any source of randomness. This includes the dependency on the random seed chosen to train the model, as well as the randomness in the training data $T$. However, although we can easily draw a new random seed and retrain any model, sampling a true new training set is often more difficult, if not completely impossible. As deep models are notoriously data hungry, it is often optimal to train on all the training points available: we only get one draw of the training set.

When there is randomness that cannot be controlled for, the empirical estimates of the bias and variance in Equation (2) will necessarily be only approximate. If we only get one draw of the training set, for example, our estimates will be conditioned on the available training data. The following proposition quantifies to which extent these conditional estimates depart from their unconditional equivalents.

Proposition 4.1. Let $X, Z$ be two random variables. Applying Equation (2) to $X|Z$ then taking the expectation over $Z$ yields an alternate decomposition of the expected Bregman divergence:

\[ \mathbb{E}D[y||X] = \mathbb{E}_Z \mathbb{E}_X[D[y||\mathcal{E}(X|Z)] + \mathbb{E}_Z \mathbb{E}_X \mathbb{E}_Z [D[\mathcal{E}(X|Z)||X]|Z]. \]

The conditional bias (resp. variance) overestimates (resp. underestimates) their respective total values by the fixed quantity $\mathbb{E}_Z D[\mathcal{E}X || \mathcal{E}(X|Z)]$:

\[ \text{Bias}_Z = \text{total bias} + \mathbb{E}_Z D[\mathcal{E}X || \mathcal{E}(X|Z)] \quad \quad \quad \text{Var}_Z = \text{total variance} - \mathbb{E}_Z D[\mathcal{E}X || \mathcal{E}(X|Z)]. \]
Figure 1: Conditional and bootstrapped estimates of the bias and variance on variations of the CIFAR-10 dataset. The approximations of the CIFAR-10 dataset in figures (a) and (b) allow us to compute the true bias and variance; in both cases, the bootstrap estimates are more accurate than the conditional estimates. Figure (c) shows the bootstrap and conditional estimates on the true CIFAR-10 dataset, for which the true estimate cannot be computed.

**Remark 4.2.** The quantity $E_Z D[\mathcal{E} X \| \mathcal{E}(X|Z)]$ is non-negative, and equal to 0 if $X$ and $Z$ are independent.

A alternative to the conditional estimates instead partitions the entire training set into disjoint subsets. Models are trained on these smaller subsets, which act as different draws of the training distribution; this approach yields an unbiased estimator that is consistent as the number of partitions goes to infinity. However, partitioning raises the difficult question of how (and if) the model itself should be also modified: should the width or number of layers be reduced to accommodate the smaller training set? Furthermore, this approach is by construction incapable of estimating the bias and variance of the models on the full training set.

A second option lies in classical bootstrapping (Efron & Tibshirani, 1994; Hall, 1992): we create new datasets by sampling with replacement from the original dataset, and use these samples to estimate the bias and variance. Repeating this procedure by resampling from the bootstrap samples in turn estimates the quantity required to correct (Hall, 1992) the bootstrapped estimate (Algorithm 1 and Figure 2). This approach does not require reducing the size of the training set, but bootstrapped samples will contain duplicate points.

To compare the conditional and bootstrapped estimates, we trained wide WRNs with the cross-entropy loss on different partitionings of the CIFAR-10 dataset. Figure 1a uses 50 partitions of 1k training points, and Figure 1b uses 20 partitions of 2.5k training points. These partitions allow us to also compute the true bias and variance of the algorithm. 

In both cases, we see that the bootstrapped estimates are significantly more accurate than the conditional samples, but both estimation methods systematically underestimate the variance and overestimate the bias. Additionally, the bootstrap bias is more accurate than the bootstrap variance; for this reason, practitioners may prefer to estimate the variance as the total error minus the bootstrapped bias.

Finally, Figure 1c shows the bootstrap and conditional estimates on the full dataset, for which we cannot compute the actual bias and variance. Since as we decrease the number of partitions, the gap between bias and variance widens, it is likely that the true bias dominates the variance in the non-partitioned regime (Figure 1c and Appendix C).

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3See Figure 7 in App. C for an empirical analysis of how many partitions are necessary for estimates to converge.

4We insist here that these are the bias and variance of the algorithm trained on respectively 1k and 2.5k points, rather than the bias and variance of the algorithm trained on the entire dataset.
Figure 2: Generating bootstrap samples from a dataset \( D \). The child of every node is sampled with replacement from its parent so that all datasets have the same size.

Often, however, we care directly about the conditional estimates. This can be because bootstrapped estimates are computationally intensive, requiring training \( O(B^2) \) models where each model itself may be an ensemble.

Alternatively, we simply might care about a training algorithm’s performance on a specific training set; This is the case for standard benchmarking suites and many real-world applications where the training set cannot be modified, even when the test distribution itself shifts over time.

## 5 Ensembles and the BV decomposition

We conclude our theoretical analysis by considering ensembles within the context of the bias-variance decomposition for non-symmetric losses.

### 5.1 Primal ensembling

Most often in deep learning, ensembling simply averages the outputs of \( n \) models that differ in their initialization (Lakshminarayanan et al., 2017). This ensembling is commonly motivated by the desire to reduce the variance of the predictive model. Indeed, for the MSE, we know that ensembling by averaging the outputs of models drawn in \( i.i.d. \) fashion (a) reduces the variance, and (b) conserves the bias.

We begin by recovering (a) under some additional weak convexity assumptions on the Bregman divergence, but (b) will prove impossible in the general case.

**Proposition 5.1.** Let \( D \) be a Bregman divergence that is jointly convex in both variables. Let \( X_1, \ldots, X_n \) be \( n \) \( i.i.d. \) random variables drawn from some unknown distribution, and define \( \hat{X} = \frac{1}{n} \sum_i X_i \). Then,

\[
\mathbb{E}D[\mathcal{E} \hat{X} \| \hat{X}] \leq \mathbb{E}D[\mathcal{E} X \| X].
\]

Both KL divergence and mean squared error are jointly convex, and are special cases of Proposition 5.1.

However, conserving the bias under ensembling requires that the Bregman divergence be symmetric — ensuring that \( \mathcal{E} \) and \( \mathcal{E}' \) are equivalent. In general, ensembling can either decrease or increase the bias.

**Proposition 5.2.** Let \( D \) be the KL divergence. There exists a distribution \( \mathcal{D} \) over predictions \( X \in \mathbb{R}^2 \) and a label \( y \in \{0, 1\} \) such that the divergence bias \( D[y \| \mathcal{E}[\cdot]] \) satisfies

\[
D[y \| \mathcal{E} \hat{X}] < D[y \| \mathcal{E} X] \quad \text{and} \quad D[1 - y \| \mathcal{E} \hat{X}] > D[1 - y \| \mathcal{E} X],
\]

```
Algorithm 1 Bootstrap estimate of bias (or variance)

Input: Training set \( T \), number of bootstrap samples \( B \)
for \( i \in \{1, \ldots, B\} \) do
    \( T_i \leftarrow \text{uniform sample}(T) \) ⊳ Of size \( |T| \)
for \( j \in \{1, \ldots, B\} \) do
    \( T_{ij} \leftarrow \text{uniform sample}(T_i) \) ⊳ Of size \( |T| \)
\( b^{(2)}_i \leftarrow \text{bias}(\{T_{ij}\}_j) \) ⊳ Bootstrap estimate for \( T_i \)
\( b^{(1)} \leftarrow \text{bias}(\{T_i\}_i) \) ⊳ Bootstrap estimate for \( T \)
\( b^{(2)} \leftarrow \frac{1}{B} \sum_i b^{(2)}_i \) ⊳ Corrective term
\( t \leftarrow b^{(1)}/b^{(2)} \)
\( b^{(0)} \leftarrow tb^{(1)} \)
return Bias estimate \( b^{(0)} \).
```
where as above we define the random variable for ensemble predictions $\hat{X} = \frac{1}{n} \sum_i X_i$, and by abuse of notation we conflate $y \in \{0, 1\}$ with its one-hot representation.

**Remark 5.3.** Despite Proposition 5.2, ensembling reduces the total cross-entropy loss due to Jensen’s inequality.

That vanilla ensembling does not preserve the bias (and can, in fact, increase it!) is a strong departure from what one might naively expect. Given this, it is natural to seek an ensembling method that would maintain the following two behaviors: the variance decreases, and the bias is conserved.

### 5.2 Dual ensembling

Once again, our path forward is guided by the dual expectation $E$. To keep the bias unchanged by ensembling, it suffices to ensemble in such a way that the ensemble predictor $\hat{X}$ satisfies the equality $E\hat{X} = EX$.

**Proposition 5.4.** Let $D$ be any Bregman divergence. Let $X_1, \ldots, X_n$ be $n$ i.i.d. random variables drawn from some unknown distribution, and define

$$\hat{X} = \left(\frac{1}{n} \sum_i X_i^*\right)^*.$$

This operation reduces the variance and conserves the bias: for any label $y \in \mathcal{X}$, we have

$$D[y \| E\hat{X}] = D[y \| EX],$$

$$\mathbb{E}D[E\hat{X} \| \hat{X}] \leq \mathbb{E}D[EX \| X].$$

In contrast to the reduction in variance that occurs for vanilla ensembles, we no longer require that $D$ be jointly convex; the natural convexity of $D$ in its first argument is sufficient. We refer to the operation in Proposition 5.4 as dual ensembling, and to that of Proposition 5.1 as primal ensembling.

**Remark 5.5.** Under the KL divergence, dual ensembling amounts to averaging in log-probability space (sometimes referred to as geometric averaging):

$$\hat{X} = \text{softmax}\left(\frac{1}{n} \sum_i \log(X_i)\right).$$

Figure 3 shows the evolution of the total loss, bias and variance when training ensembles of wide residual networks (WRN) (Zagoruyko & Komodakis, 2016) with the cross-entropy loss on CIFAR-10 and CIFAR-100. As expected, the bias is overall unaffected by the size of the ensemble when dual ensembling, whereas the bias decreases under primal ensembling. For both ensembling methods, the variance reductions are comparable, and so primal ensembling achieves a lower NLL than dual ensembling. Furthermore, under primal ensembling, the decrease in variance is significantly higher than the decrease in bias.

These results suggest the following hypotheses. Firstly, the empirical bias dominates the variance in both experiments. As these are conditional estimates subject to the estimation error described in Proposition 4.1, we cannot affirm with certainty that the true bias dominates the true variance, although this is a plausible scenario based on the conclusions of Figure 1.

Secondly, primal ensembling may be successful in classification in part because it affects the bias. Although theory does not guarantee that primal ensembling will reduce the bias, this appears to be the case in practice, thus providing a significant advantage to primal ensembling over dual ensembling.

The following section analyzes under which conditions primal ensembling is favorable to dual ensembling.
Figure 3: Conditional bias, variance, and NLL of primal and dual WRN-28–10 ensembles. As expected, the dual bias remains essentially constant as a function of the number of ensemble members, while the primal bias changes over time. As both primal and dual variance are reduced similarly by ensembling, the reduction in primal bias lets primal ensembling achieves better overall negative log likelihood on both datasets. The bias, variance and NLL are estimated by drawing 20 different draws of each ensemble size.

6 Empirical analysis of modern ensembles

Different forms of networks ensembles have been shown to achieve state-of-the-art results (Dietterich, 2000; Lakshminarayanan et al., 2017; Ruiz et al., 2021; Ovadia et al., 2019; Gustafsson et al., 2020). These ensembling techniques range from deep ensembles (Lakshminarayanan et al., 2017), which ensemble over the uniform distribution over random seeds, to ensembling over larger hypothesis spaces, architectures, and hyperparameters (Zaidi et al., 2021; Simonyan & Zisserman, 2015; He et al., 2016; Antoran et al., 2020; Wenzel et al., 2020).

Our previous analysis covers deep ensembles (which sample ensemble members in \( i.i.d. \) fashion over random seeds, as required by Props. 5.1, 5.2 and 5.4). To test whether improving the bias over the variance is a viable path to improving classification performance, we now focus on three ensembling techniques over hyperparameters: the width, depth, or regularization hyperparameters of the model. These techniques have been shown to be successful for several classification tasks (Zaidi et al., 2021; Wenzel et al., 2020).

As we are interested in the effects of ensembling over bias and variance rather than improving state-of-the-art results, we reuse standard hyperparameters for a single WRN 28-10. When ensembling over learning hyperparameters (Wenzel et al., 2020), we reuse the hyperparameters of the original paper. Bias and variance are estimated using 5 draws of an ensemble, over 3 total runs for depth and width ensembles, and over 2 runs for hyperdeep ensembles due to computational costs. Additional details are provided in Appendix B.

**Ensembling over depths.** Zaidi et al. (2021) showed that ensembling over different model architectures can yield a larger gain in accuracy compared to deep ensembles. We begin by ensembling over different depths, training 100 WRNs of depths of 28, 40, and 52 following the prescribed pattern depth = 6\(d\) + 4, and set the width multiplier to 10.

As expected, Figure 4 shows that ensembling over different depths, \(d \sim \text{Unif}(\{4, 6, 8\})\), decreases the bias significantly more than just increasing the depth for standard ensembles (Figure 4a).
Depth $= 6d + 4$ 

$d = 4$  
$d = 6$  
$d = 8$  

$d \sim \text{Unif}\{4, 6, 8\}$

Unif\{4, 6, 8\}

(a) Bias  
(b) Variance  
(c) NLL

Figure 4: Bias, variance, error and NLL on CIFAR-100. Networks are trained with different initial random seeds and different depths and then ensembled in probability space (\textit{primal ensembling}), either for a fixed depth ($d = 4, 6, 8$), or with depths sampled uniformly ($d \sim \text{Unif}\{4, 6, 8\}$). We average over three estimates of the bias and variance, each estimate using 5 draws of an ensemble. Ensembling over depths dramatically reduces the bias, but in turn increases the variance. However, the increase in variance is much smaller than the decrease in bias, and ensembles over multiple depths outperform ensembles of fixed depth – even when the expected number of parameters is higher for fixed-depth ensembles.

(a) Bias  
(b) Variance  
(c) Cross entropy loss

Figure 5: Bias, variance and NLL on CIFAR-100. Networks are trained with different initial random seeds and different widths and then ensembled together in probability space (\textit{primal ensembling}), either for a fixed width (width = 10, 20, 30) or with widths sampled uniformly (width $\sim \text{Unif}\{10, 20, 30\}$). We average over three estimates of the bias and variance, each estimate using 5 draws of an ensemble. As when varying the depth, ensembling over the width improves the bias at the cost of the variance. However, the bias improvements for ensembles of models with random widths are too low to improve over the overall performance of standard deep ensembles: the random width ensemble and the ensemble of width=20 have roughly the same number of parameters and similar NLLs.

Ensembling over depths also unsurprisingly increases the variance of the models (Figure 4b). Overall, though, the bias decrease is sufficient to improve the overall performance (Figure 4c), and ensembles of random depths outperform ensembles of fixed depth $= 40$ ($d = 6$), which have roughly the same number of parameters.

**Ensembling over widths.** We repeat the above process, fixing the depth to $6d + 4 = 28$ and letting the width multiplier take values in \{10, 20, 30\}. We see in Figure 5 that ensembling across multiple widths is less successful than ensembling over depths: the bias reduction (Figure 5a) is not sufficient to compensate for the gain in variance (Figure 5b).
Thus, ensembles of random widths perform on par with ensembles of fixed width $= 20$ that have roughly the same number of parameters (Figure 5c).

**Hyperdeep ensembles.** Wenzel et al. (2020) showed that ensembling over networks trained with multiple hyperparameters lead to additional gain in accuracy. As previously, we see in Figure 6 that ensembling over hyperparameters reduces the bias, at the cost of increasing the variance.

Overall, we see across all three experiments that ensembling over hyperparameters of the model yields lower biases and higher variances than ensembling over random seeds. These results are in line with previous literature (Yang et al., 2020) as well as our intuition: increasing the hypothesis space of a model should reduce the bias but increase the variance.

### 7 Conclusion and Future Work

Ensembles of deep classifiers achieve state-of-the-art performance across a variety of benchmark tasks. Where ensembling has previously been analyzed for regression models through the lens of the bias-variance decomposition, applying this decomposition proves more complicated for non-symmetric losses.

We begin by reformulating the bias-variance decomposition for Bregman divergences by Pfau (2013), showing that for any loss function that is a Bregman divergence, the key quantity required to define the bias and variance is the dual mean $\mathcal{E}X = (\mathbb{E}X^*)^*$ of the prediction random variable $X$. When the loss is the mean-squared error, we recover $\mathcal{E}X = \mathbb{E}X$, but this equality does not hold as soon as the loss is non-symmetric.

Using this reparameterization in dual space of the central prediction, we show that the model variance satisfies a generalized law of total variance, allowing us to disentangle the contributions of different sources of randomness on model performance. Unfortunately, it is impossible to estimate the bias and variance directly, as certain sources of randomness cannot typically be controlled. We show that the resulting conditional estimates are guaranteed to overestimate the bias and underestimate the variance by a fixed quantity; however, these estimates can be improved by iterated bootstrapping.

The dual perspective on the bias-variance tradeoff also allows to introduce a theoretical framework for ensembling under which standard (regression) ensembling behavior is recovered in the classification setting. We show theoretically and empirically that ensembling in dual space will always reduce the variance and leave the bias unchanged. In primal space, however, ensembling will reduce the variance under gentle assumptions, but can have arbitrary effects on the bias. This leads us to hypothesise that, contrary to models trained with the Euclidean squared loss, there may be further room to improve ensembles of classification models by focusing on bias reduction over variance reduction.

We test these hypotheses by evaluating recent ensembling techniques that ensemble over different hyperparameters rather than simply ensembling over the training algorithm’s random seed. As expected, we see that these methods reduce the bias significantly more than vanilla ensembles, albeit at the cost of a comparatively lesser increase in variance.

Finally, we note that the bias-variance perspective may be helpful to further understand how diversity affects the behavior of an ensemble, as suggested by Remark 3.8.
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A  Proofs

Proposition A.1 (Generalized triangle inequality for Bregman divergences). For any \( x, y, z \) in the domain of \( F \), we have \( D(x, z) = D(x, y) + D(y, z) + (\nabla F(y) - F(z), x - y) \).

A.1  Bias-variance decomposition

Proposition A.2. Let \( X, Z \) be two random variables. Applying Equation (2) to \( X \| Z \) then taking the expectation over \( Z \) yields an alternate decomposition of the expected Bregman divergence:

\[
\mathbb{E} [D[y \| X]] = \mathbb{E}_Z D[y \| \mathbb{E}(X \| Z)] + \mathbb{E}_Z \mathbb{E}_X \left[ D[\mathbb{E}(X \| Z) \| X] \right].
\]

The conditional bias (resp. variance) overestimates (resp. underestimates) their respective total values by the fixed quantity \( \mathbb{E}_Z D[\mathbb{E}(X \| Z)] \):

\[
\text{Bias}_Z = \text{total bias} + \mathbb{E}_Z D[\mathbb{E}X \| \mathbb{E}(X \| Z)] \quad \text{Var}_Z = \text{total variance} - \mathbb{E}_Z D[\mathbb{E}X \| \mathbb{E}(X \| Z)].
\]

Proof. Applying equation 2 to the conditional bias \( \mathbb{E}_Z D[y \| \mathbb{E}(X \| Z)] \), we have

\[
\mathbb{E}_Z D[y \| \mathbb{E}(X \| Z)] = D[y \| \mathbb{E}[\mathbb{E}(X \| Z)] + \mathbb{E}_Z D[\mathbb{E}(X \| Z)] \| \mathbb{E}(X \| Z)]
\]

where the last equality stems from the law of iterated expectations for \( \mathbb{E} \), showing the equality for the bias terms. The result for the variance terms follows immediately, as conditional bias and variance have the same sum as the full bias and variance.

A.2  Ensembling

Proposition A.3. Let \( D \) be a Bregman divergence that is jointly convex in both variables. Let \( X_1, \ldots, X_n \) be \( n \) i.i.d. random variables drawn from some unknown distribution, and define \( \hat{X} = \frac{1}{n} \sum_i X_i \). Then,

\[
\mathbb{E} D[\mathbb{E} \hat{X} \| \hat{X}] \leq \mathbb{E} D[\mathbb{E} X \| X].
\]

Proof. Let \( D : S \times S \rightarrow \mathbb{R}^+ \) be a Bregman divergence jointly convex in both variables. Let \( \hat{X} = \frac{1}{n} \sum_i X_i \), where the \( X_i \) are i.i.d.. By convexity, for any \( z \in X \),

\[
D[z \| \hat{X}] \leq \frac{1}{n} \sum_i D[z \| X_i]
\]

\[
\mathbb{E} D[z \| \hat{X}] \leq \frac{1}{n} \sum_i \mathbb{E} D[z \| X_i] = \mathbb{E} D[z \| X]
\]

\[
\min_z \mathbb{E} D[z \| \hat{X}] \leq \min_z \mathbb{E} D[z \| X].
\]

As \( \mathbb{E} X = \arg \min_z \mathbb{E} D[z \| X] \), it follows that \( \mathbb{E} D[\mathbb{E} X \| X] = \min_z \mathbb{E} D[z \| X] \), concluding the proof.

A.4  Ensembling

Proposition A.4. Let \( D \) be the KL divergence. There exists a distribution \( \mathcal{D} \) over predictions \( X \in \mathbb{R}^2 \) and a label \( y \in \{0, 1\} \) such that the divergence bias \( D[y \| \mathbb{E} \hat{X}] \) satisfies

\[
D[y \| \mathbb{E} \hat{X}] < D[y \| \mathbb{E} X] \quad D[1 - y \| \mathbb{E} \hat{X}] > D[1 - y \| \mathbb{E} X],
\]
where as above we define the random variable for ensemble predictions \( \hat{X} = \frac{1}{n} \sum_i X_i \), and by abuse of notation we conflate \( y \in \{0, 1\} \) with its one-hot representation.

**Proof.** For any one-hot label \( y \in \{0, 1\} \) and probability vector \( x \), we have \( \text{KL}(y \| x) = \log x_y \) and \( \text{KL}(1 - y \| x) = \log(1 - x_y) \). As \( x \to \log 1 - x \) is decreasing, it suffices to prove that there exists a distribution \( \mathcal{D} \) such that \( \text{KL}(y \| \mathcal{E} \hat{X}) \neq \text{KL}(y \| \mathcal{E} X) \). In fact, it suffices to prove the existence of a distribution \( \mathcal{D} \) such that \( \mathcal{E} X \neq \mathcal{E} \hat{X} \).

For the cross-entropy loss, we know\(^3\) that \( \mathcal{E} X = \text{softmax}(e^{\mathcal{E} \log X}) \). Let \( \mathcal{D} \) be the distribution that assigns equal probability to \( x = (0.8, 0.2) \) and \( x = (0.6, 0.4) \), and is zero elsewhere. The equivalent ensemble distribution assigns 1/4 probability to \( (0.8, 0.2) \) and \( (0.6, 0.4) \), and 1/2 probability to \( (0.7, 0.3) \). A simple numerical computation then shows that \( \mathcal{E} X \neq \mathcal{E} \hat{X} \), concluding our proof.

**Proposition A.5.** Let \( \mathcal{D} \) be any Bregman divergence. Let \( X_1, \ldots, X_n \) be \( n \) i.i.d. random variables drawn from some unknown distribution, and define \( \hat{X} = \left( \frac{1}{n} \sum_i X_i \right)^* \).

This operation reduces the variance and conserves the bias: for any label \( y \in \mathcal{X} \), we have
\[
\mathcal{D}[y \| \mathcal{E} \hat{X}] = \mathcal{D}[y \| \mathcal{E} X] \\
\mathbb{E} \mathcal{D}[\mathcal{E} \hat{X} \| \hat{X}] \leq \mathbb{E} \mathcal{D}[\mathcal{E} X \| X].
\]

**Proof.** To preserve bias, it suffices to have \( \mathcal{E} \hat{X} = \mathcal{E} X \). By definition of \( \hat{X} \), we have
\[
\mathcal{E} \hat{X} = \left( \mathbb{E} \hat{X}^* \right)^* = \left( \mathbb{E} \left[ \frac{1}{n} \sum_i X_i^* \right] \right)^* = (\mathbb{E} X^*)^* = \mathcal{E} X.
\]

We now focus on the variance. Using the fact that \( D_F[p||q] = D_{F^*}[q^*||p^*] \) (Cesa-Bianchi & Lugosi, 2006, Chapter 11), we have
\[
\mathbb{E} D_F(\mathcal{E} \hat{X} \| \hat{X}) = \mathbb{E} D_F[\mathcal{E} X \| \hat{X}] \\
= \mathbb{E} D_{F^*}[\hat{X}^* \| (\mathcal{E} X)^*] \\
= \mathbb{E} D_{F^*}\left[ \frac{1}{n} \sum_i X_i^* \| (\mathcal{E} X)^* \right] \\
\leq \frac{1}{n} \sum_i \mathbb{E} D_{F^*}[X_i^* \| (\mathcal{E} X)^*] \\
\leq \frac{1}{n} \sum_i \mathbb{E} D_F[\mathcal{E} X \| X_i] \\
\leq D_F[\mathcal{E} X \| X].
\]

where (a) follows from the convexity of \( D_{F^*} \) in its first argument.

**B Experimental Details**

The models used in this work are wide residual networks (WRN-28-10) (Zagoruyko & Komodakis, 2016) with the cross-entropy loss unless specified otherwise. We train models with SGD + momentum to optimize

\(^3\)See, e.g., (Yang et al., 2020).
the cross-entropy loss. We use the learning rate schedule, batch size, and data augmentations specified in the deterministic baseline provided by Nado et al. (2021).

As hyperdeep ensembles require the use of a validation set to form the ensemble, we nonetheless set aside 10% of the training data for validation purposes across all methods.

For hyperdeep ensembles, we exactly replicated the experimental setup from Wenzel et al. (2020). The only difference is we used 0.9 fraction of the CIFAR dataset as training data and 0.1 as validation. For each dataset, we train multiple (1000) neural networks where first multiple hyperparameters are chosen randomly from each neural network and then 10 random seeds are chosen for each setting of the hyperparameter. The hyperparameters that are varied are the same as in Wenzel et al. (2020) and include $\ell_2$ regularization for various layers and label smoothing.

As in Wenzel et al. (2020), we used the greedy selection strategy to form the ensemble where each ensemble member is chosen greedily based on which member reduces the validation cross entropy loss the most. We trained a total of 1000 models and then divided randomly into groups of 10 where 10 ensemble models were formed where each model was formed by the greedy selection strategy on one group of 100 models. These 10 ensemble models were used to do the bias variance decomposition where each decomposition used 5 models and the bias variance values were averaged over 2 runs.

C Partitioned estimates of the bias and variance

Figure 7: Bias and variance of a smaller WRN-16-5 over the CIFAR-100 dataset. We create 20 partitions of the CIFAR-100 dataset, and estimate the bias either by conditioning on a partition (partition fixed), or by including the partition into the expectations that define the bias and variance (partition multiple). We see that it takes $\geq 10$ partitions for the estimates of bias and variance to begin converging, and that the converged values appear to still show the bias dominating the variance.
D Depth and width experiments on CIFAR-10

Depth = 6d + 4  \quad \begin{align*}
\text{d = 2} & \quad \text{d = 4} & \quad \text{d = 6} & \quad \text{d \sim Unif \{2, 4, 6\}}
\end{align*}

(a) Cross entropy loss  \quad (b) Bias  \quad (c) Variance

Figure 8: Plots for bias, variance, error and accuracy with increasing ensemble size for CIFAR-10 when multiple networks are trained with different initial random seeds and different depths and then ensembled together in probability space. The line with d=d denotes the setting where different models with depth as 6d + 4 are ensembled together. The line with d = Unif[2, 4, 6] denotes the setting where we first randomly sample a depth from [16, 28, 40] and then randomly sample a model with that depth.

width = 10  \quad \begin{align*}
\text{width = 20} & \quad \text{width = 30} & \quad \text{width \sim Unif\{10, 20, 30\}}
\end{align*}

(a) Cross entropy loss  \quad (b) Bias  \quad (c) Variance

Figure 9: Plots for bias, variance, error and accuracy with increasing ensemble size for CIFAR-10 when multiple networks are trained with different initial random seeds and different widths and then ensembled together in probability space. The line with width=w denotes the setting where different models with width as w are ensembled together. The line with width=Unif[10, 20, 30] denotes the setting where we first randomly sample a width from [10, 20, 30] and then randomly sample a model with that width.