

# **Model Correlation in Random Forests**

Master Thesis

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# Abstract

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# 1. Introduction

## 1.1. Overview

## 1.2. Contributions

## 1.3. Statistics

We want to reason in a general manner about algorithms which act on data. We use statistical language for this. Consider a data point  $X$  that is provided as input to an algorithm. Our intention is to say that  $X$  could be essentially *any* data point from some kind of data source. In other words, we can consider  $X$  to be *random*, that is,  $X$  is a random variable (a symbol) that can take different values. Which values exactly it can take depends on the data source – the *distribution* of the data. If our data source is a fair 6-sided die,  $X$  can take values in  $\Omega = \{1, \dots, 6\}$  and the distribution of values is constant where each outcome has probability  $\frac{1}{6}$ , i.e.  $\mathbb{P}[1] = \dots = \mathbb{P}[6] = \frac{1}{6}$ .

A  $\sigma$ -algebra over  $\Omega$  can be thought of a set of subsets of  $\Omega$ , containing  $\Sigma$ , such that it is closed under complement and countable union and intersection.

**Definition 1.3.1** A probability space is a triple  $(\Omega, \Sigma, \mathbb{P})$  where

- ▶  $\Omega$  is an arbitrary set modelling the sample space i.e. the set of all possible outcomes.
- ▶  $\Sigma$  is a  $\sigma$ -algebra over  $\Omega$ , modelling the set of events.
- ▶  $\mathbb{P}$  is a function  $\Sigma \rightarrow [0, 1]$  such that  $\mathbb{P}(\Omega) = 1$  and  $\mathbb{P}(\bigcup_{i=1}^{\infty} A_i) = \sum_{i=1}^{\infty} \mathbb{P}(A_i)$  for a countable collection of (pairwise disjoint) sets in  $\Sigma$ , and models the probability measure.

In the following, we assume an underlying probability space implicitly.

**Definition 1.3.2** A random variable is a quantity that depends on a random event, i.e. a function  $\Omega \rightarrow M$  (commonly, we have  $M = \mathbb{R}$ ).

Further, we not only want to reason about the behaviour of an algorithm with respect to one point  $X$  but many such points. A basic notion is the *expected value* of  $X$ . Further, since  $X$  is considered random,  $f(X)$  is also a random variable and we can talk about the expected value of functions of random variables.

**Definition 1.3.3** The probability density function  $f_X$  of a random variable  $X$  is a nonnegative function such that

$$\mathbb{P}(a < X < b) = \int_a^b f_X(x) dx$$

**Definition 1.3.4** The expected value (expectation) of random variable  $X$  is defined as

$$\mathbb{E}[X] := \int x \cdot f_X(x) dx$$

where the integral is over the support of  $X$ .

A function  $g(X)$  of a random variable  $X$  is a random variable itself and  $\mathbb{E}[g(X)] = \int g(x)f_X(x) dx$ . To emphasize the random variable the function is dependent on, we sometimes mention it in the subscript and write  $\mathbb{E}_X[g(X)]$ .

**Lemma 1.3.1** (*Linearity of Expectations*) A basic property of expected values is that they are linear: For any two random variables  $X, Y$  and a constant  $\alpha$  it holds that  $\mathbb{E}[X + Y] = \mathbb{E}[X] + \mathbb{E}[Y]$  and  $\mathbb{E}[\alpha X] = \alpha \mathbb{E}[X]$ .

**Lemma 1.3.2** (*Law of total expectation*) For a function  $g$ :

$$\mathbb{E}_{(X,Y)}[g(X,Y)] = \mathbb{E}_X[\mathbb{E}_Y[g(X,Y) | X]]$$

As a special case of this, it holds that

$$X, Y \text{ independent} \rightarrow \mathbb{E}_X[\mathbb{E}_Y[g(X,Y)]] = \mathbb{E}_Y[\mathbb{E}_X[g(X,Y)]]$$

and we write  $\mathbb{E}_{X,Y}[g(X,Y)] =_{\text{def}} \mathbb{E}_X[\mathbb{E}_Y[g(X,Y)]]$

A random variable is *discrete* if its set of outcomes is a countable set  $\{x_1, \dots, x_n\}$  with probabilities  $\{p_1, \dots, p_n\}$ . The probability density function then is  $f_X(x_i) = \mathbb{P}(X = x_i) = p_i$ . The expected value of a discrete random variable is given by a sum.

$$\mathbb{E}[X] = \sum p_i x_i$$

The expected value is a statement depending on the entire distribution. Usually, we do not know the distribution itself, but only have a limited set of samples of it. For instance, we may have a certain number of data points or run an algorithm a certain number of times and observe its output. We can use this set of samples to approximate the value of the expectation. Given that the samples are independent and identically distributed, the arithmetic mean of samples approximates the expected value.

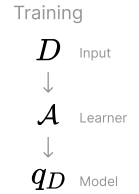
$$\frac{1}{n} \sum_{i=1}^n x_i \rightarrow \mathbb{E}[X] \quad \text{as } n \rightarrow \infty$$

## 1.4. Supervised Learning

Our goal is to find an algorithm that is able to map objects from  $\mathcal{X}$  to outcomes in  $\mathcal{Y}$ . Objects are described by their *features*. These are commonly numerical, so  $\mathcal{X}$  can be thought of as  $\mathbb{R}^d$  where  $d$  is the number of features. We will call such a representation of an object an *example*.

In *classification* problems, the outcomes are discrete among  $k$  possible outcomes and we refer to them as *labels* or *classes*. For sake of simplicity, we identify these with integers, i.e.  $\mathcal{Y}$  can be thought of as the set  $\{1, \dots, k\}$ . In *binary* classification, there are only two possible outcomes. Depending on what is more convenient in the mathematical context, we assume either  $\mathcal{Y} = \{0, 1\}$  or  $\mathcal{Y} = \{-1, 1\}$ . In *regression* problems, the outcomes are continuous. We can think of  $\mathcal{Y}$  as  $\mathbb{R}$ .

The desired mapping  $q : \mathcal{X} \rightarrow \mathcal{Y}$  may be nontrivial such that it is not feasible to come up with explicit rules of how to map examples to outcomes. However, we may try to algorithmically infer such a mapping from a given set of examples and their known outcomes. More specifically, we want to find a deterministic *learning algorithm*, also called *learner*, that, given a random input  $D$ , produces a mapping  $q_D$ <sup>1</sup>. We call  $q_D$



Testing

$$(\mathbf{X}, \mathbf{Y}) \sim P(\mathcal{X}, \mathcal{Y})$$

$$q_D(\mathbf{X}) = \mathbf{Y}'$$

$$\ell(\mathbf{Y}, \mathbf{Y}')$$

**Figure 1.1.:** Illustration of the main components of supervised learning. A learning algorithm  $\mathcal{A}$  produces a model  $q_D$  given some input  $D$ . The model is then evaluated on example-outcome pairs of the original data distribution.

1: For the statistical analysis it is essential that the learning algorithm is regarded as deterministic. However, any kind of randomness can be introduced by providing it with random input.

a *model* and note that it is dependent on  $D$ . The task of choosing and configuring a learning algorithm is known as *supervised learning*.

To be useful, a model should not only accurately estimate outcomes for the given training examples, but also provide reasonable predictions for examples that were not part of the input to the learning algorithm. To express this formally in a general setting, we use statistical language.

Consider a probability distribution  $P(\mathcal{X}, \mathcal{Y})$  from which realisations of example-training pairs are drawn. We write this as  $(X, Y) \sim P(\mathcal{X}, \mathcal{Y})$  where  $(X, Y)$  are random variables from a joint distribution. This distribution is unknown – else the problem is trivially solved already. In order for our solution to be widely applicable, we strive to make as few assumptions about the distribution  $P$  as possible.

The training dataset  $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$  is considered a random vector  $D$  drawn from  $P(\mathcal{X}, \mathcal{Y})^n$  where  $n$  is the number of data points. If there are other sources of randomness in model construction such as, for instance, weight initialisation or neural networks, these can also be considered components of  $D$ .

**Definition 1.4.1** A model is a function  $q : \mathcal{X} \rightarrow \mathcal{Y}$ . In supervised learning the model depends on the training input  $D$ . Its output (prediction) when queried with a random variable  $X$  taking values in  $\mathcal{X}$  is written as

$$q_D(X)$$

To shorten notation, we sometimes omit explicitly specifying either random variable and write  $q$  for  $q_D(X)$ . A dependency on both  $D$  and  $X$  is always to be understood.

The quality of a single model prediction is measured by means of a *loss function*  $\ell : \mathcal{Y} \rightarrow \mathcal{Y}$  whose value should be low if the predicted outcome is close to the true outcome. To describe the expected loss across the entire distribution, we consider a pair of random variables  $(X, Y) \sim P(\mathcal{X}, \mathcal{Y})$ .

**Definition 1.4.2** (Risk and Generalisation Error) The risk of a model is the expected loss over all example-outcome pairs.

$$\text{Risk}(q_D) =_{\text{def}} \mathbb{E}_{(X,Y) \sim P} [\ell(Y, q_D(X))]$$

The quality of a given learning algorithm  $\mathcal{A}$  is the expected risk over all possible inputs. We refer to this as the *generalisation error*.

$$GE(\mathcal{A}) =_{\text{def}} \mathbb{E}_D [\text{Risk}(q_D)] = \mathbb{E}_{(X,Y), D} [\ell(Y, q_D(X))]$$

Note that the choice of the loss function  $\ell$  is fundamental to the evaluation of a learning algorithm.

## 1.5. Bias, Variance and their Effects

Since we are ultimately interested in the generalisation error of a learning algorithm, the question arises what forces influence it. To this end, one can strive to mathematically express the generalisation error in terms of specific meaningful quantities. A classical decomposition is the *bias-variance-decomposition*. It is an essential tool to understand learning algorithms in general and ensembles such as Random Forests in particular. For the purpose of this thesis, it is important to understand the decomposition and its

motivation in detail. We will begin by considering the widely known bias-variance-decomposition for regression using the squared-error loss  $\ell(y, y') =_{\text{def}} (y - y')^2$ . We will then proceed to generalise the decomposition to arbitrary loss functions.

The variance of a random variable with respect to the squared-error loss is defined as the expected distance in terms of loss to the expected value.

$$\text{Var}_X(X) =_{\text{def}} \mathbb{E}_X [(X - \mathbb{E}_X[X])^2]$$

As such,  $\mathbb{E}_X[X]$  is a centroid to the different realisations of  $X$  with respect to the loss function  $\ell(Y, Y') = (Y - Y')^2$ .

$$\mathbb{E}_X[X] = \arg \min_z \mathbb{E}_X [(X - z)^2]$$

Recall that a model is a function dependent on the training input  $D$ . The variance is a measure of how different the models produced by the learning algorithm will be in terms of outputs if supplied with different realisations of training input  $D$ .

$$\text{Var}_D(q_D(X)) = \mathbb{E}_D [(q_D(X) - \mathbb{E}_D[q_D(X)])^2]$$

$q^*(X) =_{\text{def}} \mathbb{E}_D[q_D(X)]$  is the *central model* and does not depend on  $D$ .

Further, recall that we are considering a joint distribution of example-output pairs  $(X, Y)$ . We can not assume that the outcomes are not ambiguous. Let  $y(X)$  be the outcome associated with  $X$ . We measure the variance of actual outcomes  $y(X)$  for a given example  $X$  around the expected outcome.

$$\text{Var}_Y(y(X)) = \mathbb{E}_Y [(Y - \mathbb{E}_Y[y(X)])^2]$$

$y^*(X) =_{\text{def}} \mathbb{E}_Y[y(X)]$  is the *central label* and does not depend on  $Y$ .

Using this notation, the bias-variance decomposition for the squared-error loss is given as follows. Note that each variance term is the expected distance in terms of loss to a certain centroid.

$$\mathbb{E}_{(X,Y),D} [(Y - q_D(X))^2] = \underbrace{\mathbb{E}_{(X,Y)} [(Y - y^*(X))^2]}_{\text{Var}(Y) \text{ ("noise")}} \quad (1.1)$$

$$+ \underbrace{\mathbb{E}_X [(y^*(X) - q^*(X))^2]}_{\text{Bias}(Y,q) \text{ ("learner bias")}} \quad (1.2)$$

$$+ \underbrace{\mathbb{E}_{X,D} [(q^*(X) - q_D(X))^2]}_{\text{Var}(q) \text{ ("learner variance")}} \quad (1.3)$$

The first term,  $\text{Var}(Y)$  is independent of  $D$  and  $q_D$ . This means we have no means of influencing it with our choice of  $q_D$ .  $\text{Var}(Y)$  is also referred to as *noise*, *bayes error* or *irreducible error*. The second term,  $\text{Var}(q)$  measures the variance of our model around its non-random centroid with respect to different realisations of the random training dataset  $D$ . This can be understood as a measure of spread of the learning algorithm with respect to different realisations of  $D$ . The third term,  $\text{Bias}(q_D, Y)$  is the distance in terms of loss between the expected classifier and the expected label. This can be thought of as a measure of precision of the learning algorithm.

Note that we developed two things: On the one hand, we derived quantities that measure the notions of bias and variance. On the other hand, by virtue of these

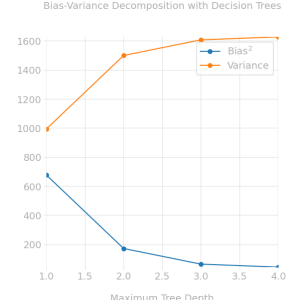


Figure 1.2.: foo!

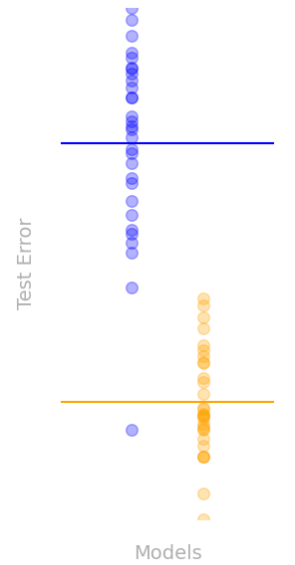


Figure 1.3.: Visualising the variance of decision tree and Random Forest models. Each glyph corresponds to the test error of one model trained on a random subset of the full available data. The variation of the test error around the mean test error across many dataset samples is exactly the variance. Not only do Random Forests show lower test errors on average, they seem to also have lower variance.

This decomposition is usually derived by expanding the square [todo]. The cross-terms then vanish due to that  $q^* = \mathbb{E}_D[q_D]$  and  $y^* = \mathbb{E}_Y[y(X)]$ . This is but a special case of a more general structure applying to a certain class of losses. We will provide a more general proof in lemmas 4.3.1 and 4.3.2.

quantities appearing in the error decomposition, we have expressed the *effect* these quantities have on the generalisation error.

While the bias-variance decomposition for the squared-error loss is widely accepted, there are many competing decompositions for a range other loss functions [pfau\_GeneralizedBiasVarianceDecomposition\_, 1–5]. For instance, we are particularly interested in the 0/1-loss for classification. A decomposition of it where the model variance is independent of the outcome variable as in term ?? is been proven to not exist [7]. We will now argue that approaching the matter from the perspective of such *loss-effects* allows us to state a general bias-variance decomposition that holds for any loss function. The decomposition for the squared-error loss is a special case of it.

**Definition 1.5.1** (*Loss-Effect*) For a loss function  $\ell$ , and random variables  $Y, Z, Z'$ , we define the change in loss between  $Z$  and  $Z'$  in relation to  $Y$  as:

$$LE(Z, Z') =_{\text{def}} \ell(Y, Z') - \ell(Y, Z)$$

**Definition 1.5.2** (*Central model*) Given a model  $q$ , it's central model is the centroid with respect to  $D$ :

$$q^\star =_{\text{def}} \arg \min_z \mathbb{E}_D [\ell(z, q_D)]$$

**Definition 1.5.3** (*Central label*) The central label is

$$y^\star =_{\text{def}} \mathbb{E}_{Y|X} [Y]$$

The *variance-effect* is the expected change in loss caused by using  $q_D$  instead of the non-random centroid  $q^\star(X)$ . Likewise, the *bias-effect* is the expected change in loss caused by using the expected model instead of the expected label. In the following, to lighten notation, we will omit explicitly stating the dependence on  $X$ .<sup>2</sup> Formally:

$$\begin{aligned} \text{Bias-Effect} &=_{\text{def}} \mathbb{E}_{D,Y} [\ell(Y, q^\star) - \ell(Y, y^\star)] \\ \text{Variance-Effect} &=_{\text{def}} \mathbb{E}_{D,Y} [\ell(Y, q_D) - \ell(Y, q^\star)] \end{aligned}$$

This allows us to state a decomposition of the generalisation error simply in terms of loss-effects.

$$\mathbb{E} [\ell(Y, q)] = \mathbb{E} \left[ \underbrace{\ell(Y, y^\star)}_{\text{"noise"}} + \underbrace{\ell(Y, q^\star) - \ell(Y, y^\star)}_{\text{"bias-effect"}} + \underbrace{\ell(Y, q) - \ell(Y, q^\star)}_{\text{"variance-effect"}} \right]$$

Note that the individual terms on the right-hand side simply cancel out and reduce to  $\ell(Y, q)$ . As illustrated in figure 1.4, this decomposition divides the the interval from  $\ell(Y, Y) = 0$  to  $\ell(Y, q)$  into meaningful sections. Note that this decomposition depends solely on the linearity of expectation and is independent of the loss function  $\ell$  or the definitions of  $y^\star$  and  $q^\star$ .

For the squared-error loss  $\ell(Z, Z') = (Z - Z')^2$ , bias-effect equals bias and variance-effect equals variance.

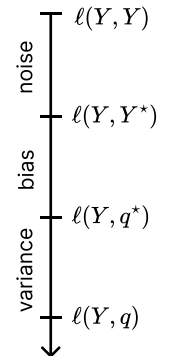
$$\mathbb{E} [\ell(Y, q^\star) - \ell(Y, y^\star)] = \mathbb{E} [\ell(y^\star, q^\star)]$$

$$\mathbb{E} [\ell(Y, q) - \ell(Y, q^\star)] = \mathbb{E} [\ell(q^\star, q)]$$

Note that the arguments of loss-effect appear in inverse order in the difference. This is to give the expression a suggestive shape since in section 4.3, we will show that, for a Bregman divergence  $B_\phi$ , it holds that

$$\mathbb{E} [LE(Z', Z)] = B_\phi(Z', Z)$$

2: In the original publication [8], bias-effect is called the *systematic effect*, i.e. the effect of the systematic components. However, it is clearer to call this *bias-effect*, particularly when we begin to introduce notions of diversity in 4.1.



**Figure 1.4.:** Illustration how the bias-variance-effect decomposition decomposes the loss  $\ell(Y, q)$  into meaningful segments.



Thus, the bias-variance decomposition for the squared-error loss is a special case of this.

**Theorem 1.5.1** (*Bias-Variance-Effect-Decomposition [8]*) For any loss function  $L$ , it holds that

$$\mathbb{E}_{(X,Y),D} [\ell(Y, q_D)] = \underbrace{\mathbb{E}_{(X,Y)} [\ell(Y, y^*)]}_{\text{noise}} + \underbrace{\mathbb{E}_X [LE(q^*, y^*)]}_{\text{bias-effect}} + \underbrace{\mathbb{E}_{X,D} [LE(q_D, q^*)]}_{\text{variance-effect}}$$

This decomposition holds for *any* loss function since, by linearity of expectation, the individual terms on the right-hand-side simply cancel out. Further, this decomposition is independent of the definitions of  $y^*$  and  $q^*$ .

Note that while for the squared error the variance compares *model predictions*, the variance-effect is based solely on the *change in loss*. In section 4.3, we will see that the former is in fact only a special property of a specific family of loss functions.

## 1.6. Bregman Divergences and Centroids

To measure the difference between predicted and ground-truth outcomes, we use a loss function  $\ell$ . The choice of loss function depends on the data domain, the learning task and computational considerations.

Often, learners are analysed with respect to a specific loss function, such as the squared-error loss [9] for regression or the 0/1-loss [10] or the KL-divergence [11] for classification. The well-known bias-variance decomposition for the squared-error loss is usually shown directly in teaching materials [12, 13]. The question then arises which properties are specific to the loss function and which are part of a more general structure.

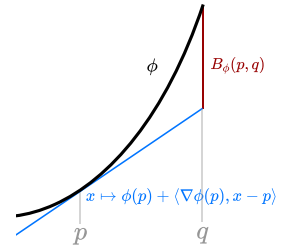
We will now define a family of loss functions, called *Bregman divergences*, that encompasses many widely used loss functions in supervised learning (see table 1.1).

**Definition 1.6.1** (*Bregman Divergence [pfau, adlam22]*) The Bregman divergence  $B_\phi(p, q) : \mathcal{S} \times \mathcal{S} \rightarrow \mathbb{R}$  is defined based on a generator function  $\phi$  as follows:

$$B_\phi(p, q) =_{\text{def}} \phi(\mathbf{p}) - \phi(\mathbf{q}) - \langle \nabla \phi(\mathbf{q}), (\mathbf{p} - \mathbf{q}) \rangle$$

where  $\langle \cdot, \cdot \rangle$  is the inner product,  $\nabla \phi(\mathbf{q})$  is the gradient vector of  $\phi$  at  $\mathbf{q}$  and  $\phi : \mathcal{S} \rightarrow \mathbb{R}$  is a strictly convex function on a convex set  $\mathcal{S} \subseteq \mathbb{R}^k$  such that it is differentiable on the relative interior of  $\mathcal{S}$ .

In order to talk about variances with respect to Bregman divergences, we need a notion of a centroid with respect to a Bregman divergence. Bregman divergences are in general not symmetric and hence there is a *left* and *right* centroid.



**Figure 1.5.:** Given a strictly convex generator  $\phi$ , the Bregman divergence for points  $p, q$  is the difference between the linear approximation around  $p$  and  $\phi$  at the point  $q$ .

**Lemma 1.6.1** (Left and right Bregman centroids, [6]) Let  $B_\phi$  be a Bregman divergence of generator  $\phi : \mathcal{S} \rightarrow \mathbb{R}$ . For a random variable  $Y$  taking values in  $\mathcal{S}$ , it holds that

- the right Bregman centroid is

$$\arg \min_z \mathbb{E}_X [B_\phi(X, z)] = \mathbb{E}[X]$$

- the left Bregman centroid is

$$\arg \min_z \mathbb{E}_X [B_\phi(z, X)] = (\nabla \phi)^{-1} \mathbb{E} [\nabla \phi(X)] =_{\text{def}} \mathfrak{E}[X]$$

If  $B_\phi$  is symmetric, i.e.  $B_\phi(Y, Y') = B_\phi(Y', Y)$  then  $\mathbb{E}[X] = \mathfrak{E}[X]$ .

**Definition 1.6.2** (Dual expectation [6]) The left Bregman centroid is the expected value in the dual space implied by  $\nabla \phi$ . Due to this, we define the dual expectation as

$$\mathfrak{E}[X] =_{\text{def}} (\nabla \phi)^{-1} \mathbb{E} [\nabla \phi(X)]$$

A generalised measure of variance is then the expected divergence around a Bregman centroid.

**Definition 1.6.3** The variance around the right Bregman centroid is known as the Bregman information  $I_\phi(X)$  [14].

$$I_\phi(X) =_{\text{def}} \mathbb{E}_X [B_\phi(X, \mathbb{E}_X[X])]$$

In other words, the choice of loss function implies a measure of variance. Various well-known variance measures can now be seen to actually be implied by a Bregman divergence. For example, let  $X = \{X_1, \dots, X_n\} \subset \mathbb{R}^d$ . Then the squared Euclidean distance corresponds to the *sample variance* [14].

$$B_\phi(p, q) = \|p - q\|^2 \rightarrow I_\phi(X) = \frac{1}{n} \sum_{i=1}^n (X_i - \mathbb{E}[X])^2$$

For the KL-divergence, the Bregman information is the *mutual information*. Consider a

**Table 1.1.:** Examples of commonly used loss functions that are Bregman divergences [7, 14]

Divergence $B_\phi(p, q)$	Generator $\phi(q)$	Domain $\mathcal{S}$	Loss function
$(p - q)^2$	$q^2$	$\mathbb{R}$	Squared Error
$x \log\left(\frac{x}{y}\right) + (1 - x) \log\left(\frac{1-x}{1-y}\right)$	$x \log x + (1 - x) \log(1 - x)$	$[0, 1]$	Logistic loss
$\frac{x}{y} - \log\left(\frac{x}{y}\right) - 1$	$-\log x$	$\mathbb{R}_{>0}$	Ikura-Saito distance
$\ x - y\ ^2$	$\ x\ ^2$	$\mathbb{R}^d$	Squared Euclidean distance
$(x - y)^\top A(x - y)$	$x^\top A y$	$\mathbb{R}^d$	Mahalanobis distance
$\sum_{j=1}^d x_j \log_2\left(\frac{x_j}{y_j}\right)$	$\sum_{j=1}^d x_j \log_2 x_j$	$d$ -simplex	KL-divergence
$\sum_{j=1}^d x_j \log\left(\frac{x_j}{y_j}\right) - \sum_{j=1}^d (x_j - y_j)$	$\sum_{j=1}^d x_j \log x_j$	$\mathbb{R}_{\geq 0}^d$	Generalized I-divergence
$\sum_{j=1}^d x_j \log x_j$	$\sum_{j=1}^d x_j \log x_j$	$\mathbb{R}_{\geq 0}$	Poisson loss

random variable  $X$  over probability distributions with probability measure  $p$  [14].

$$B_{\phi}(u, v) = \sum_{j=1}^d u_j \log \left( \frac{u_j}{v_j} \right) \rightarrow I_{\phi}(X) = \sum_{i=1}^n \sum_{j=1}^m p(u_i, v_j) \log \frac{p(u_i, v_j)}{p(u_i) p(v_j)}$$

## 2. Ensemble Learning

*Ensemble Learning* is the method of training  $M$  individual models  $q_1, \dots, q_M$  for a given task and aggregating their output via an *ensemble combiner*  $\bar{q}$  to form an ensemble prediction [15]. The individual models  $q_1, \dots, q_M$  are referred to as *members*. When all members are constructed using the same learning algorithm, we call it a *homogeneous* ensemble. The learning algorithm is then referred to as the *base learner*. Otherwise the ensemble is *heterogeneous*.

### 2.1. Methods

There are three main variants of ensemble learning [16]:

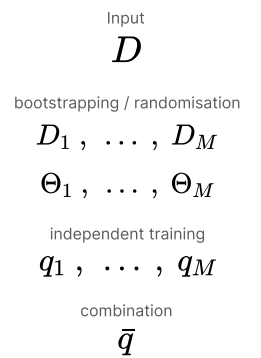
- *Parallel*: All members are trained independently. The outputs of all members are then aggregated to form the ensemble prediction.
- *Stacking or Meta-Learning*: All members are trained independently. The member outputs serve as input data for another learning algorithm, which then provides the ensemble prediction.
- *Sequential*: Members are trained in sequence. The output of the previous ensemble member informs the construction of the next member.

Random Forests [17] are an example of parallel ensemble construction.  $M$  decision trees are constructed independently and the tree's predictions are aggregated by a kind of mean (see section 3.1). A classical example for sequential ensemble construction is *Boosting* [18]. In boosting algorithms, the ensemble combiner  $\bar{q}$  is not a mean but a (weighted) sum  $\bar{q} = \sum_{i=1}^M \alpha_i q_i$ . The first member  $q_1$  provides a base prediction. Successive members are then trained to predict not an output value but *increments* (*pseudo-targets*) to the base prediction such that the sum  $\alpha_1 q_1 + \alpha_2 q_2 + \dots$  moves towards a more precise prediction. In this thesis, we will focus on the Random Forest learner and variations of it.

### 2.2. Notation

In the supervised learning setting with a single model, we have defined the model as a function  $q_D(X)$ . In ensemble learning,  $M$  individual models are constructed and their outputs are aggregated via an ensemble combiner  $\bar{q}$  to form an ensemble output. The individual models are referred to as *members*.

Analysing ensembles means analysing differences between the members. There are two dimensions in which ensemble members can differ. First, in terms of provided training data.<sup>1</sup> Second, in terms of other randomness used in model construction.<sup>2</sup> To distinguish these two sources, we sometimes denote the training data as a random vector  $D = (D_1, \dots, D_M)$  and other parameters as  $\Theta = (\Theta_1, \dots, \Theta_M)$ .



**Figure 2.1:** Illustration of parallel ensemble learning.

1: For instance, each learner may be trained on a random subset of the available training data (see section 3.2)

2: For instance, random numbers used in decision tree construction (see section 3.1).

**Definition 2.2.1** (Ensemble member model) The  $i$ -th ensemble member model  $q_i : \mathcal{X} \rightarrow \mathcal{Y}$  is a function depending on training input  $D_i$  and additional parameters  $\Theta_i$ .

$$q_{D_i, \Theta_i}(X)$$

To shorten notation, we also write  $q_i =_{\text{def}} q_{D_i, \Theta_i}(X)$ .

Due to that the  $i$ -th member then depends only on  $D_i$  and  $\Theta_i$  and is independent of  $D_j$  and  $\Theta_j$  for  $j \neq i$ , using the law of total expectation (see lemma 1.3.2), we can write

$$\mathbb{E}_D [q_i] = \mathbb{E}_{D_{j \neq i}} [\mathbb{E}_{D_i} [q_i]] = \mathbb{E}_{D_i} [q_i]$$

and likewise for  $\Theta$ .

The output of an ensemble is produced by aggregating the outputs of the member models using a combiner function.

**Definition 2.2.2** (Ensemble combiner) The ensemble combiner  $\bar{q} : \mathcal{X} \rightarrow \mathcal{Y}$  for a given loss function  $\ell$  is the centroid with respect to model parameters  $\Theta$ :

$$\bar{q} =_{\text{def}} \arg \min_z \mathbb{E}_{\Theta} [\ell(z, q_{\Theta})]$$

Note that this is the central model with respect to  $\Theta$  (compare definition 1.5.2). For Bregman divergences, this shows to be the dual expectation (def. 1.6.2). This definition agrees with combiners commonly used in practise (plurality vote, arithmetic mean). It links combiners to loss functions. Further, it suggests combiners for other loss functions. In each case, using a combiner as defined here enables a very general and expressive theory of ensemble diversity and a decomposition of the ensemble generalisation error exactly measuring ensemble improvement due to diversity.

An ensemble is homogeneous iff  $\Theta_1, \dots, \Theta_M$  are identically and independently distributed. This is the case if the member models are constructed according to the same base learner and do not influence each other.

**Lemma 2.2.1** ★ In homogeneous ensembles, the central models of any two members and the combiner are the same. That is, for any  $i, j \in \{1, \dots, M\}$  it holds that

$$q_i^{\star} = q_j^{\star} = \bar{q}^{\star}$$

*Proof.* If  $D_1, \dots, D_M$  and  $\Theta_1, \dots, \Theta_M$  are identically distributed and independent, it holds that

$$q_i^{\star} = \mathbb{E}_D [q_{D_i, \Theta_i}] = \mathbb{E}_{D_i} [q_{D_i, \Theta_i}] = \mathbb{E}_{D_j} [q_{D_j, \Theta_j}] = q_j^{\star}$$

For the ensemble combiner, it holds that

$$\begin{aligned} \bar{q}^{\star} &= \mathcal{E}_{\Theta} [q_{D, \Theta}]^{\star} = \mathcal{E}_D [\mathcal{E}_{\Theta} [q_{D, \Theta}]] \\ &= (\nabla \phi)^{-1} \mathbb{E}_D [(\nabla \phi)(\nabla \phi)^{-1} \mathbb{E}_{\Theta} [q_{D, \Theta}]] \\ &= \mathcal{E}_{\Theta} [\mathcal{E}_D [q_{D, \Theta}]] = \mathcal{E}_{\Theta} [q_{\Theta}^{\star}] \end{aligned}$$

Due to the result above,  $q_{\Theta}^{\star}$  is constant over  $\Theta$  and thus  $\mathcal{E}_{\Theta} [q_{\Theta}^{\star}] = q_{\Theta}^{\star}$ .

Both properties also hold for dual expectations for Bregman divergences defined in definition 1.6.1.  $\square$

For the 0/1-loss for a  $k$ -class classification problem, the implied combiner is the plurality vote:

$$\bar{q} = \arg \min_{z \in [k]} \mathbb{E}_{\Theta} [\ell_{0/1}(z, q_{\Theta})]$$

For Bregman divergences, i.e.  $\ell = B_{\phi}$ , the combiner implied by  $\ell$  is the dual expectation:

$$\begin{aligned} \bar{q} &= \mathcal{E}_{\Theta} [q_{\Theta, D}] \\ &= (\nabla \phi)^{-1} \mathbb{E}_{\Theta} [\nabla \phi(q_{\Theta})] \end{aligned}$$

The squared-error loss is a symmetric Bregman divergence and hence the ensemble combiner is the arithmetic mean:

$$\bar{q} = \mathcal{E}_{\Theta} [X] = \mathbb{E}_{\Theta} [X] \approx \frac{1}{M} \sum_{i=1}^M q_i$$

A basic measure for classification ensembles under the 0/1-loss is the winning margin of the majority vote.

**Definition 2.2.3** (Ensemble margins for majority voting [17]) The margin for class  $y$  of an example  $x$  is the difference between the number of member votes for class  $Y$  and the number of votes for the next-best class.

$$mr(x, y) =_{\text{def}} \frac{1}{M} \sum_{i=1}^M \mathbb{1}[q_i = y] - \max_{j \neq y} \frac{1}{M} \sum_{i=1}^M \mathbb{1}[q_i = j] \in [-1, 1]$$

## 2.3. Motivation

We will now review some classical arguments that motivate ensemble learning. We do this to provide context to the results in chapter 4, which also show when and how ensemble learning is beneficial.

**Ensemble improvement is non-negative** The arithmetic mean combiner can be seen as approximating an expectation over member models, i.e.  $\bar{q} = \mathbb{E}_{\Theta} [q_{\Theta}] \approx \frac{1}{M} \sum_{i=1}^M q_i$ . This motivated [19] to invoke Jensen's inequality. For a loss function  $\ell$  that is convex in its first argument, it holds that

$$\underbrace{\ell(Y, \mathbb{E}_{\Theta} [q_{\Theta}(X)])}_{\text{"ensemble loss"}} \leq \mathbb{E}_{\Theta} \left[ \underbrace{\ell(q_{\Theta}(X), Y)}_{\text{"member loss"}} \right]$$

and thus

$$\mathbb{E}_{\Theta} [\ell(q_{\Theta}(X), Y)] - \ell(\mathbb{E}_{\Theta} [q_{\Theta}(X)], Y) \geq 0$$

Jensen's inequality, in a probabilistic setting, states that, for a function  $\phi : \mathbb{R} \rightarrow \mathbb{R}$  and a random variable  $X$

$$\phi \text{ convex} \rightarrow \phi(\mathbb{E}[X]) \leq \mathbb{E}[\phi(X)]$$

**Corollary 2.3.1** For convex loss functions and using the arithmetic mean combiner, ensembling can never hurt performance: The ensemble loss is always smaller-equal than the average member error.

Abe et al. [19] interpret the difference between these quantities, as a measure of ensemble improvement.

**Ensemble bias equals average member bias** It can be shown that the bias of a homogeneous ensemble is equal to the average bias of the ensemble members. We will give an illustrative argument for the arithmetic mean combiner here. We will show this in detail in a more general and intuitive way in chapter 4.

**Lemma 2.3.2** (Ensemble bias equals average member bias under arithmetic mean combiner [20])

$$\mathbb{E}_X [\ell(y^*(X), \bar{q}^*(X))] = \mathbb{E}_X [\ell(y^*(X), q^*(X))]$$

*Proof.* Consider individual learner inputs  $D = (D_1, \dots, D_M)$ . Each member depends on some  $D_i$  and the combiner  $\bar{q}$  depends only on  $D$ . Assuming that  $D_1, \dots, D_M$  are

independent and identically distributed, we can write

$$\mathbb{E}_{D,\Theta} [\bar{q}] = \mathbb{E}_D \left[ \frac{1}{M} \sum_{i=1}^M q_{D_i} \right] = \frac{1}{M} \sum_{i=1}^M \mathbb{E}_{D_i} [q_{D_i}] = \mathbb{E}_{D'} [q_{D'}]$$

where  $D'$  is distributed as any  $D_i$ . We can conclude  $\mathbb{E}_D [\bar{q}] = \mathbb{E}_D [q_D]$  (see section 2.2). This implies

$$\bar{q}^* = \mathbb{E}_D [\bar{q}] = \mathbb{E}_D [q_D] = q^*$$

and thus the bias of the ensemble is the same as the bias of a member model  $q$ .  $\square$

This argument depends on the linearity of expectations, the arithmetic mean combiner and the fact that the ensemble is homogeneous. We will later show this more directly for any loss function and any combiner (see 4.2).

**Corollary 2.3.3** *For homogeneous ensembles under the arithmetic mean combiner, ensemble improvement is solely due to variance reduction.*

**Variance reduction for squared-error regression** Consider the regression setting under the squared-error loss and the arithmetic mean combiner. Assume  $q_1, \dots, q_M$  are identically and independently distributed with equal variance  $\sigma^2$ .

$$\text{Var}(\bar{q}) = \text{Var} \left( \frac{1}{M} \sum_{i=1}^M q_i \right) = \frac{1}{M^2} \sum_{i=1}^M \text{Var}(q_i) = \frac{1}{M} \sigma^2$$

As the number of members  $M$  increases, the ensemble variance is reduced. Further, one can also see that the interactions between members determine the variance reduction. Assume ensemble members have equal pairwise covariance  $\rho$ . Then

$$\rho =_{\text{def}} \frac{\text{Cov}(q_i, q_j)}{\sigma^2} \leftrightarrow \text{Cov}(q_i, q_j) = \rho \sigma^2$$

Further,

$$\text{Var}(\bar{q}) = \text{Var} \left( \frac{1}{M} \sum_{i=1}^M q_i \right) = \frac{1}{M^2} \left( \underbrace{\sum_{i=1}^M \text{Var}(q_i)}_{M\sigma^2} + 2 \underbrace{\sum_{i<j}^M \text{Cov}(q_i, q_j)}_{M(M-1)\rho\sigma^2} \right) = \frac{\sigma^2}{M} + \frac{M-1}{M} \rho \sigma^2$$

One can show that  $\rho \geq 0$  [20].

**Corollary 2.3.4** *Under the squared-error loss, ensemble variance is minimised if member outputs are uncorrelated.*

**Variance reduction for classification margins** For classification, a classical analysis is the bound given by Breiman [17], in which Random Forests are first introduced. The basic idea is to consider variances with respect to the ensemble margin (see definition 2.2.3). We open with Chebychev's inequality to bound the generalisation error in terms

of the variance of the ensemble margin.

$$\mathbb{E}[\ell(Y, \bar{q}(X))] = \mathbb{P}[\text{mr}(X, Y; D) < 0] \leq \frac{\text{Var}(\text{mr}(X, Y; D))}{\mathbb{E}_{X,Y}[\text{mr}(X, Y; D)]^2}$$

We can already see that we have an interaction between the performance of the individual members, as reflected in the ensemble margin  $\mathbb{E}_{X,Y}[\text{mr}(X, Y; D)]$  and the variance of the margin. The generalisation error is in part determined by the ratio of these two quantities.

Note that

$$\text{mr}(X, Y; D) = \mathbb{E}_{\Theta} \left[ \underbrace{\mathbb{1}[q_i = Y] - \mathbb{1}[q_i = K]}_{=\text{def } \text{rmg}(X, Y, \Theta)} \mid (X, Y), D \right]$$

where  $K$  is the next-best class and we define the *raw margin function*  $\text{rmg}(X, Y, \Theta)$  to be the inner part of that expectation. So,  $\text{mr}(X, Y; D) = \mathbb{E}_{\Theta}[\text{rmg}(X, Y, \Theta) \mid (X, Y), D]$ .

$s =_{\text{def}} \mathbb{E}_{X,Y}[\text{mr}(X, Y; D)]$  is also called the *strength* of the ensemble.  $s$  is assumed to be non-negative. For binary classification, this is equivalent to the weak-learner assumption (see 4.4.4).

**Theorem 2.3.5 ([17])** *The variance of the ensemble margin can be expressed in terms of the covariance between the raw member margins of two members parameterised by i.i.d  $\Theta, \Theta'$ .*

$$\text{Var}_{X,Y}(\text{mr}(X, Y; D)) = \mathbb{E}_{\Theta, \Theta'}[\text{Cov}_{(X,Y)}(\text{rmg}(\Theta), \text{rmg}(\Theta'))]$$

*Proof.* For brevity, we write  $Z =_{\text{def}} (X, Y)$ ,  $\text{mr}(Z) =_{\text{def}} \text{mr}(X, Y; D)$  and  $\text{rmg}(\Theta) =_{\text{def}} \text{rmg}(X, Y; \Theta)$ . By the definition of variance, have

$$\begin{aligned} \text{Var}_Z(\text{mr}(Z)) &= \mathbb{E}_Z[(\text{mr}(Z) - \mathbb{E}_Z[\text{mr}(Z)])^2] \\ &= \mathbb{E}_Z[\text{mr}(Z)^2] - \mathbb{E}_Z[\text{mr}(Z)]^2 \end{aligned}$$

For the left term, by the rule of iterated expectation and the fact that  $Z$  and  $\Theta$  are independent (see lemma 1.3.2), it holds that

$$\mathbb{E}_Z[\text{mr}(Z)^2] = \mathbb{E}_Z[\mathbb{E}_{\Theta}[\text{rmg}(\Theta) \mid Z]^2] = \mathbb{E}_{Z, \Theta}[\text{rmg}(\Theta)^2] = \mathbb{E}_{\Theta}[\mathbb{E}_Z[\text{rmg}(\Theta)^2]]$$

For the right-hand-side term, we can make use of the fact that, for some function  $f$ , it holds that  $\mathbb{E}_{\Theta}[f(\Theta)^2] = \mathbb{E}_{\Theta, \Theta'}[f(\Theta)f(\Theta')]$  where  $\Theta$  and  $\Theta'$  are independent and identically distributed. We apply the rule of iterated expectation and exploit that  $Z$  and  $\Theta$  are independent.

$$\begin{aligned} \mathbb{E}_Z[\text{mr}(Z)^2] &= \mathbb{E}_Z[\mathbb{E}_{\Theta}[\text{rmg}(\Theta) \mid Z] \cdot \mathbb{E}_{\Theta'}[\text{rmg}(\Theta') \mid Z]] \\ &= \mathbb{E}_Z[\mathbb{E}_{\Theta}[\text{rmg}(\Theta)] \mathbb{E}_{\Theta'}[\text{rmg}(\Theta')]] \\ &= \mathbb{E}_{\Theta, \Theta'}[\mathbb{E}_Z[\text{rmg}(\Theta)] \mathbb{E}_Z[\text{rmg}(\Theta')]] \\ &= \mathbb{E}_{\Theta}[\mathbb{E}_Z[\text{rmg}(\Theta)]^2] \end{aligned}$$

In summary, we can conclude that the variance of the ensemble margin is equal to the expected variance of the raw classifier margin. This variance can then also be expressed as the covariance between two independent, identically distributed random



variables  $\Theta$  and  $\Theta'$ .

$$\begin{aligned}
 \text{Var}_Z(\text{mr}(Z)) &= \mathbb{E}_\Theta [\mathbb{E}_Z [\text{rmg}(\Theta)^2]] - \mathbb{E}_\Theta [\mathbb{E}_Z [\text{rmg}(\Theta)]^2] \\
 &= \mathbb{E}_\Theta [\mathbb{E}_Z [\text{rmg}(\Theta)^2] - \mathbb{E}_Z [\text{rmg}(\Theta)]^2] \\
 &= \mathbb{E}_\Theta [\text{Var}_Z(\text{rmg}(\Theta))] \\
 &= \mathbb{E}_{\Theta, \Theta'} [\text{Cov}_Z(\text{rmg}(\Theta), \text{rmg}(\Theta'))]
 \end{aligned}$$

□

**Corollary 2.3.6** *Under the 0/1-loss in classification ensembles, the ensemble error can be bounded from above by a pointwise covariance between ensemble margins. The ensemble error is lower if individual members are uncorrelated.*

Unfortunately, due to the initial application of Chebychev's inequality, this is only an upper bound.

## 3. Random Forests

In this chapter, we describe the Random Forest learning algorithm. We first motivate and describe decision trees, which are the basic components of a Random Forest. We then proceed to describe a particular property of decision trees: they are likely to exhibit high variance. While this is undesirable for a learning algorithm, we will see that combining several randomized decision trees into a Random Forest ensemble turns exactly that property into a crucial advantage (see section 4.2).

A Random Forest is a collection of randomized decision trees. A decision tree is a data-driven recursive partitioning scheme, combined with a means to produce a prediction based on the training points in a partition cell. The Random Forest prediction then is an aggregate of the predictions of all individual trees.

### 3.1. Decision Trees

We are interested in learning algorithms that, given some training data, produce a model that is able to predict a reasonable outcome when queried with a previously unseen example (see section 1.4). One intuitive approach is to consider the examples in the training data that are "close" to the query point. Then, one might claim that the outcome for the query point must surely be similar to the outcomes of the close points – which we already know. Indeed, finding a proper notion of "closeness" is at the heart of many machine learning algorithms such as  $k$ -Nearest-Neighbours,  $k$ -Means, and others.

Constructing a decision tree means recursively partitioning the input space  $\mathcal{X}$ , guided by the training data  $D$ . Then, given a query  $X$ , we check the partition cell that  $X$  belongs to and all the training examples that are in it. These are the examples we consider "close" to  $X$ . The tree's prediction will be an aggregation of the outcomes of all training points in that cell.

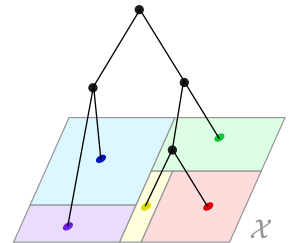
Because we are recursively partitioning the input space, we have at hand a tree structure of decision rules. The cells of the resulting partition are the leaves of the tree. The non-leaf nodes are also referred to as *decision nodes*, but there is no inherent difference between leaf and non-leaf nodes. We will use either of the terms *leaf* and *cell*, depending which aspect we want to emphasize.

There are the following main components to the implementation of a decision tree:

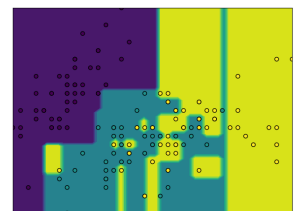
- ▶ The *splitting criterion* to apply recursively to subsets of the training data.
- ▶ The *stopping criterion* that determines whether a node should be split further. This will determine the depth of the decision tree.
- ▶ The *leaf aggregation function* that produces a prediction for a specific cell. When using the constructed tree for prediction, this will be the leaf node that the query point is assigned in.

#### 3.1.1. Centroids as leaf combiners

We will consider the leaf aggregation function first. Consider a parent node  $P$  that, due to some split, was partitioned into the disjoint union  $L \dot{\cup} R$ . Let  $y_P$ ,  $y_L$  and  $y_R$  be the output values of the parent and the two new leaf nodes, produced by the leaf



**Figure 3.1.:** Rendering of a decision tree structure. Each inner node corresponds to a partitioning of the parent edge. In standard decision trees, this is a binary partition. In other words, the examples are *split* at a certain value threshold in a certain feature dimension.



**Figure 3.2.:** Decision boundaries of a tree in two (arbitrary) features constructed on the *iris* dataset. Visualisation based on [21].

aggregation function. Since the leaf output is constant over a single cell, the gain in loss due to a split is the difference between the loss of the parent node and the sum of losses of the two individual child nodes. For brevity, we write  $\ell_P(y) =_{\text{def}} \sum_{i \in P} \ell(y, y_i)$ .

$$\begin{aligned} \text{Loss Gain: } & \sum_{i \in P} \ell(y_P, y_i) - \left( \sum_{i \in L} \ell(y_L, y_i) + \sum_{i \in R} \ell(y_R, y_i) \right) \\ &= \ell_P(y_P) - (\ell_L(y_L) + \ell_R(y_R)) \end{aligned}$$

In order for a split to yield positive loss gain, the leaf aggregation function needs to be such that the loss does not increase as constraints are removed, i.e. the set of considered examples is reduced. Recall that  $\bar{z}$  is a centroid with respect to a loss function  $\ell$  and a set of outcomes  $P$  if and only if  $\bar{z} = \arg \min_z \sum_{i \in P} \ell(z, y_i) = \arg \min_z \ell_P(z)$  (??).

**Lemma 3.1.1** *For a loss function  $\ell$ , if the leaf aggregator of a node  $P$  is  $y_P =_{\text{def}} \arg \min_z \sum_{i \in P} \ell(z, y_i)$ , i.e. the centroid with respect to  $\ell$ , the loss gain is nonnegative.*

*Proof.* Let  $\ell_P(y) =_{\text{def}} \sum_{i \in P} \ell(y, y_i)$ . Since  $P = L \dot{\cup} R$ , we need to show that  $\ell_P(y_P) = \ell_L(y_P) + \ell_R(y_P) \geq \ell_L(y_L) + \ell_R(y_R)$ . Assume  $\ell_L(y_P) < \ell_L(y_L)$ . This contradicts the definition of  $y_L$  as the minimizer, and as such  $\ell_L(y_P) \geq \ell_L(y_L)$ . Likewise, we can conclude that  $\ell_R(y_P) \geq \ell_R(y_R)$ . Combining the two inequalities yields the statement.  $\square$

This rigorously motivates the specific choice of leaf aggregation function. The majority vote is a centroid with respect to the 0/1-loss for classification, while the arithmetic mean is the centroid with respect to the squared error loss for regression.

### 3.1.2. Splitting criteria greedily minimise loss functions

In the best possible case, all training examples in a given cell correspond to the same (classification) or very similar (regression) outcomes. If a query point then falls within that cell, i.e. it has similar features, one can say with high confidence that the query point should have the same (similar) outcome. In the spirit of greedy optimisation, we aim to split cells such that the resulting child cells are more *pure* with respect to their outcomes.

Consider a split, parameterised by  $\Theta$ , that partitions a parent node  $P$  into the disjoint union  $L_\Theta \dot{\cup} R_\Theta$ . Let  $n, n_L, n_R$  be the cardinalities of the parent and the two child nodes. Let  $H$  be an impurity measure. We will select the split that yields the lowest impurity.

$$\arg \min_{\Theta} \frac{n_L}{n} H(L_\Theta) + \frac{n_R}{n} H(R_\Theta)$$

The gain in purity is then the difference between impurities before and after the split.

$$\text{Purity Gain: } H(P) - \left( \frac{n_L}{n} H(L_\Theta) + \frac{n_R}{n} H(R_\Theta) \right) \quad (3.1)$$

Note that this is different from the gain in *loss* achieved due to a split.

We now proceed to define two commonly used splitting criteria. These are the Gini impurity for classification and Variance Reduction (also known as CART) for regression [12]. For a splitting function criterion to produce useful decision trees, a reasonable impurity measure should also imply a positive loss gain. Often, this is intuitively clear

The notion of local purity is linked to the training error: If a leaf cell is perfectly pure, all training examples in that cell correspond to the same outcome. Hence, the leaf aggregation function, which is usually implemented as some kind of mean, will produce exactly that outcome for any query point that belongs to this cell, in particular any training points. Consequently, for a suitable definition of "error", perfectly pure cells have zero training error.

but particularly for the case of Gini impurity, a comprehensive explanation appears to be hard to find in the literature. We clarify this in the following.

### Variance Reduction for regression estimates

A commonly used impurity measure for regression is the squared-error variance.

$$H_{\text{var}}(P) =_{\text{def}} \frac{1}{n_P} \sum_{i \in P} (y_i - y_P)^2 \quad \text{for} \quad y_P =_{\text{def}} \frac{1}{n_P} \sum_{i \in P} y_i$$

To motivate this impurity measure, it remains to be shown that a split guided by this impurity measure actually reduces the value of a specific loss function and which one that is. Luckily, it is easy to see that this holds for the squared error loss. Plugging the definition into the purity gain (eq. (3.1)) yields

$$H(P) = \frac{1}{n_P} \sum_{i \in P} (y_i - y_P)^2 = \frac{1}{n_P} \underbrace{\sum_{i \in L} (y_i - y_P)^2}_{\ell_L(y_P)} + \frac{1}{n_P} \underbrace{\sum_{i \in R} (y_i - y_P)^2}_{\ell_R(y_P)}$$

and

$$\frac{n_L}{n_P} H(L) + \frac{n_R}{n_P} H(R) = \frac{n_L}{n_P} \frac{1}{n_L} \underbrace{\sum_{i \in L} (y_i - y_L)^2}_{\ell_L(y_L)} + \frac{n_R}{n_P} \frac{1}{n_R} \underbrace{\sum_{i \in R} (y_i - y_R)^2}_{\ell_R(y_R)}$$

By lemma 3.1.1, we can directly conclude that the loss gain is positive for any split if the arithmetic mean is used as a leaf combiner.

### Gini Impurity for class labels

To measure the purity of class labels in a cell, one may consider the probability of drawing two different outcomes from the examples in the current cell. Let  $p_k$  be the probability of drawing an example of class  $k$  from node  $P$ . The probability of drawing one example of class  $k$  and one of a different class is  $p_k(1 - p_k)$ . The probability of drawing two examples of *any* two different classes then is the *Gini impurity*

$$H_{\text{Gini}}(P) =_{\text{def}} \sum_k p_k(1 - p_k) = 1 - \sum_k p_k^2$$

We will now argue that a reduction in the Gini impurity in fact pushes values  $p_k$  to the extremes of the probability simplex. We perform a slight shift in perspective and consider the classification *margin* (see 3.1.1) instead of the estimated probabilities. The margin can be thought to represent the classifier's confidence in its prediction.  $\mathbb{P}[k|x]$  describes the probability estimated by the classifier that  $X$  is of class  $k$ .

**Definition 3.1.1** (Classifier margins [12]) *The margin for class  $k$  of an example  $X$  is the difference between the model's confidence that  $X$  is of class  $k$  and the next-best class:*

$$m(x, y) =_{\text{def}} \mathbb{P}[y|x] - \max_{j \neq y} \mathbb{P}[j|x]$$

- The vector  $m(x) = [m_1(x), \dots, m_K(x)]^\top$ , where  $K$  is the total number of classes, is called a *margin vector* iff its components sum to zero.
- For a pair  $(X, y)$  of example and true outcome, the model's prediction is correct iff  $m_y(x) > 0$

In binary classification, i.e. if outcomes are in  $\{0, 1\}$ , the squared error reduces to the 0/1-loss. As such, the mean 0/1-loss, i.e. the error rate, trivially also is a measure of variance.

*Recap:*  $P$  is the parent node before the split with combiner  $y_P$ .  $L$  and  $R$  are the two child nodes after a split with combiners  $y_L$  and  $y_R$ .

We will argue that the Gini impurity split criterion, which finds a split such that the Gini impurity is reduced, maximises the classification margins.

**Proposition 3.1.2 ★** Let  $p$  be a probability distribution and  $u$  an arbitrary vector. Let  $G = \sum_k p_k(1 - p_k)$  be the Gini impurity. Then  $-G$  is the generator for the Bregman divergence

$$B_{-G}(p, u) = \sum_k (p_k - u_k)^2$$

*Proof.* Let  $\phi(q) =_{\text{def}} (-1) \sum_k p_k(1 - p_k)$  as assumed.

$$\begin{aligned} B_{-G}(p, u) &= \underbrace{(-1) \sum_k p_k(1 - p_k)}_{\phi(p)} - \underbrace{(-1) \sum_k u_k(1 - u_k)}_{\phi(u)} - \underbrace{\sum_k (2u_k - 1)(p_k - u_k)}_{\langle \nabla \phi(u), p - u \rangle} \\ &= \sum_k (p_k - u_k)^2 \end{aligned}$$

the first equality follows by definition of a Bregman divergence (see 1.6.1) and the second equality by arithmetic.  $\square$

Note further that maximising the value of the generator function  $\phi$  with respect to  $p$  while leaving the other parameter  $u$  fixed also maximises the divergence  $B_{\phi}(p, u)$ .

<sup>1</sup> The sign of the generator value and the sign of the divergence are related in that  $B_{-\phi}(p, u) = -B_{\phi}(p, u)$ . This means that minimising the Gini impurity during splitting maximises component-wise sum of squared errors between  $p$  and  $u$ .

1: TODO explain, at least with intuition. Convexity of generator etc.

$$\min G \rightarrow \min B_G(p, u) \rightarrow \max B_{-G}(p, u) = \sum_k (p_k - u_k)^2$$

If  $p$  is a class probability distribution and  $u =_{\text{def}} [1/k, \dots, 1/k]^T$  a uniform distribution, then  $p - u$  is a margin vector and the optimisation corresponds to maximising the classification margins as measured by the squared error.

A common approach in training classification models is *margin maximisation* [18] in which we aim to maximise the margin of the true label  $m_y(X)$ . A margin loss function  $\ell : \mathbb{R} \rightarrow \mathbb{R}$  is a *margin-maximising* loss if  $\ell'(m_y(X)) \leq 0$  for all values of  $m_y$  [22]. A decision tree can also be evaluated based on a margin loss. The empirical error of a decision tree node  $P$  with respect to a margin loss  $\ell$  can be written as  $L(P) = \frac{1}{|P|} \sum_{i \in P} \ell(m_y(x_i))$  where  $m_y(x_i)$  is the value of the true margin. Then the following holds [22].

$$\begin{aligned} L(P) &= \frac{1}{|P|} \sum_{i \in P} \sum_k \mathbb{1}[y_i = k] \cdot \ell(m_y(x_i)) \\ &= \sum_k \frac{1}{|P|} \sum_{i \in P} \mathbb{1}[y_i = k] \cdot \ell(m_y(x_i)) \\ &= \sum_k p_k(x_i) \ell(m_y(x_i)) \end{aligned}$$

An example for a margin-maximising loss function is the *hinge loss* defined as  $\ell(m_y(x)) =_{\text{def}} \max\{0, 1 - p\}$ . Its subderivative is

$$\frac{\partial \ell}{\partial p} = \begin{cases} -1 & p \leq 1 \\ 0 & \text{else} \end{cases}$$

and hence it is a margin-maximising loss.

In summary, the Gini impurity splitting criterion greedily optimises classification margins and thus margin-maximising losses.

### Information Gain for class probabilities

Another common impurity measure is the *Shannon entropy*. Let  $p_k$  be the probability of drawing an example of class  $k$  from node  $P$ .

$$H_{\text{entr}}(P) =_{\text{def}} - \sum_k p_k \log p_k$$

The purity gain with respect to the entropy is referred to as *information gain*. Seeing that the negative entropy is the Bregman generator of the KL-divergence (see table 1.1), one can apply similar arguments to see that constructing a tree using the entropy impurity measure corresponds to greedily optimising for a KL-divergence whose second argument is a uniform distribution – which is also known as *relative entropy* or *cross-entropy*.

$$-\frac{1}{n} \sum_i^n \sum_k \mathbf{1}[y_i = k] \log(p_k(x_i))$$

### Relationship to 2-means clustering

As established in section 3.1.2, splitting criteria aim to find a binary partition of the examples in the parent node. The quality of a partition is evaluated according to the purity of the labels. Note that the example features are not considered at all here. If indeed a centroid is chosen as leaf combiner, the notion of impurity is very similar to the objective function of  $k$ -means clustering on the class labels.

Let  $I_\phi$  be the Bregman information as defined in definition 1.6.3. Let  $X$  be a random variable representing data points. Let  $M$  be a random variable taking values in  $\mathcal{M}$  representing the set of cluster centroids. Then the objective for generalised  $k$ -means hard clustering [14] is to minimise the loss in Bregman information due to the quantisation induced by  $M$ :

$$\ell_\phi(M) =_{\text{def}} I_\phi(X) - I_\phi(M)$$

One can show [14] that

$$\ell_\phi(M) = \mathbb{E}_\pi [I_\phi(X_k)] \approx \sum_{h=1}^K \sum_{x_i \in \mathcal{X}_h} v_i B_\phi(x_i, \mu_h)$$

where  $K$  is the number of clusters,  $\mathcal{X}_k$  are the cells of the clustering,  $v_i$  is the distribution of the  $x_i$  and  $\mu_k$  is the right Bregman centroid of  $\mathcal{X}_k$ .

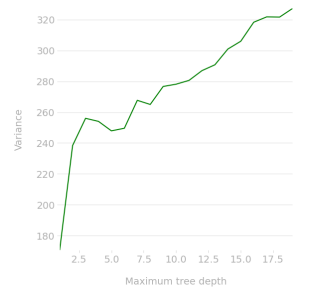
Classical  $k$ -means is a special case of this for the squared-error divergence. The KL-divergence implies the mutual information as a variance and yields *information-theoretic clustering* [todo]. The Ikura-Saito divergence yields the *LBG algorithm* [todo].

Particularly relevant for decision trees is the following insight: The choice of Bregman divergence implies a measure of variance (see 1.6.3 for examples). Optimising for this measure of variance implies the splitting criterion<sup>2</sup>. This gives a theoretical rationale for choosing splitting function and leaf combiner in decision trees.

## 3.2. The Random Forest scheme

The deeper a decision tree is grown, the closer the resultig partition cells will fit the training data. This approximation is in fact guided *only* by the training data. In the extreme case, if the tree is fully grown, each partition cell will correspond to a single

2: The leaf combiner, which corresponds to the right Bregman centroid is independent on the chosen divergence, see ??.



**Figure 3.3.:** Variances of decision trees of increasing depths. Evaluated for squared-error regression on a synthetic dataset.

example and the outcome for that cell will be the outcome of that example. The tree essentially turns into a 1-nearest-neighbour scheme with respect to the training dataset. This means that trees constructed with different samples  $D$  of training datasets from the original distribution  $P(X, Y)$  potentially predict quite different outcomes for testing examples. This is captured in the concept of learner variance as defined in 1.5. In ??, one can indeed observe that trees of greater depth have greater variance. At the same time, their fit to the training data improves, which is captured by lower bias. Mitigating this strong dependence on the training data is one of the main motivations of Random Forests. The basic idea is as follows: If we produce several uncorrelated decision trees and average their predictions, then the predictions should exhibit lower variance. In standard forests, this is achieved by introducing randomness into the decision tree construction algorithm by two mechanisms:

- *Bootstrapping*: Each tree is constructed not on the entire training dataset but a random subset of it. Usually, this *bootstrap sample* is produced by drawing the same amount of points with replacement.
- *Random feature selection*: When determining where to split a node, not all features are considered but only a random subset of a certain size.

Thus, a random forest additionally requires the following parameters:

- number of trees...

### 3.2.1. Bagging

A vital ingredient to Random Forests is the *Bagging* procedure, which stands for *bootstrapping and aggregating*. Bagging is an ensemble learning technique not specific to Random Forests. In Bagging, each member is constructed not on the full training dataset but a *bootstrap sample* of it. The bootstrap sample is usually determined by drawing  $n$  out of  $n$  examples uniformly with replacement [breiman, others]. We will refer to this as *uniform bootstrapping*. One can also determine the bootstrap sample by drawing  $n$  out of  $n$  points with replacement according to a probability distribution  $\{p_1, \dots, p_n\}$ , which we call *weighted bootstrapping*. Bootstrapping means that each member will be trained on a different dataset.

### 3.2.2. Feature & Split selection

### 3.2.3. Number of trees

### 3.2.4. Depth of trees

### 3.2.5. Random Forests converge

As the number of trees increases, for almost surely all sequences  $(\Theta_1, \dots)$ , the generalisation error  $PE^*$  converges:

$$\mathbb{E}_{(X,Y),D} [\ell(Y, q_D(X))] \rightarrow \mathbb{P}_{X,Y} [\text{mr}(X, Y) < 0]$$

In uniform bootstrapping, if we draw  $n$  samples from  $n$  available points, the probability of an example being selected in a single draw is  $\frac{1}{n}$ . Conversely, the probability of an example not being selected in a single draw is  $1 - \frac{1}{n}$ . We draw  $n$  times. Hence, the probability of an observation not being selected in any of the draws is  $(1 - \frac{1}{n})^n$ . The probability of an example indeed being selected in at least one of the draws then is  $1 - (1 - \frac{1}{n})^n$ . For large  $n$ , one can approximate  $\lim_{n \rightarrow \infty} 1 - (1 - \frac{1}{n})^n = 1 - e^{-1} \approx 0.632$  [23].



### 3.2.6. Random Forests do not overfit

### 3.2.7. Random Forests are consistent

### 3.2.8. Tree and Forest Partitions

The generalisation error, and consequently individual terms of any decomposition of it have been defined point-wise. That is, they are measured by an expectation over possible realisations of example-outcome pairs  $(X, Y)$ . They further depend on a random variable  $D$  representing the training input to the learner. In order to estimate such an expectation for a given model (a realisation of  $D$ ), one has to sample realisations of  $(X, Y)$ . In practise, these example-outcome pairs typically come from a validation dataset that was withheld from training. We have seen in ?? that for some losses, diversity can be expressed independently of the outcome variable  $Y$ . To approximate an actual value, we would still need to sample realisations of  $X$ .

Decision Trees, particularly if grown deeply, can be considered to *approximate* the training data, i.e. they are a lossy representation of the training data. A grown decision tree model contains two kinds of parameters, both derived from the training data  $D$ .

- The tree structure, i.e. the decision boundaries. These are used for determining the leaf node for a query example.
- The output value of a leaf node. This is the predicted value for a query example falling into that leaf. The leaf predictions depend on the decision boundaries but are not solely determined by them.

This leads to the question whether characteristics of a Random Forest model could be expressed solely in terms of its tree parameters, and not in terms of predictions on query points.

Each level of a decision tree induces a partition of the space of examples  $\mathcal{X}$ . Because each example is associated with an outcome, we can also think of it as a partition of  $(\mathcal{X}, \mathcal{Y})$ . We call such a partition a *tree partition* and a cell a *tree cell*. Decision trees produce predictions via an aggregate of the queried leaf node's outcomes. Thus, the predictions of a decision tree over a single cell are constant. An ensemble of trees also induces a partition: the partition obtained by intersecting all tree partitions. We call these *forest cells*. Formally, if  $T_1, \dots, T_M$  are tree partitions, the forest partition is given as

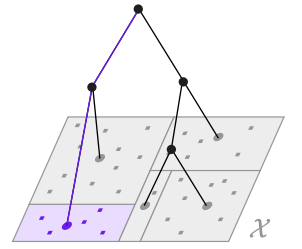
$$\{c_1 \cap \dots \cap c_M \mid c_1 \in T_1, \dots, c_M \in T_M\}$$

Each forest cell is associated with  $M$  tree cells whose intersection constitutes it. For any query point that falls within a certain tree cell, the forest prediction is given by an aggregate over the associated tree cells. Thus, the predictions of a random forest are constant over a single forest cell. This means that also a loss, as well as any decomposition constituents of the loss are constant over forest cells.

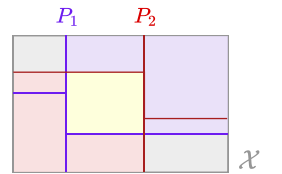
However, exploiting that partitions are cell-wise constant, we can apply a special case of the law of total expectation to express it in terms of cells.<sup>3</sup> Consider a forest partition  $Z = Z_1 \dot{\cup} \dots \dot{\cup} Z_P$  of  $Z = (X, Y)$ . Using the linearity of expectations and the law of total expectation, we can write the generalisation error of the forest as follows.

**Proposition 3.2.1 ★**

$$\mathbb{E}_{Z,D} [\ell(y, \bar{q})] = \mathbb{E}_D \left[ \sum_{p=1}^P \mathbb{P}[Z_p] \cdot \mathbb{E}_Z [\ell(y, \bar{q}) \mid Z_p] \right]$$



**Figure 3.4.:** A decision tree partitioning the data space. For a query example, the corresponding leaf node is determined by traversing the tree downwards from the root node and applying the learned decision criteria.



**Figure 3.5.:** The data space  $\mathcal{X}$  (gray) and partitions  $P_1$  (purple) and  $P_2$  (red) of it induced by two decision trees. The intersections of any cell of  $P_1$  and any cell of  $P_2$  form the *forest partition*. One such intersection is highlighted in yellow.

3: Let  $X_1 \dot{\cup} \dots \dot{\cup} X_M$  be a disjoint, countable partition of the sample space of  $X$ . Then

$$\mathbb{E}_X [X] = \sum_{i=1}^M \mathbb{E}_X [X \mid X_i] \cdot \mathbb{P}[X_i]$$



While we have eliminated the dependence on a query point  $X$ , the quantity  $\mathbb{E}_Z [\ell(y, \bar{q}) \mid Z_p]$  still depends on a realisation of an outcome  $Y$ . In section ?? we will see that we can decompose this term further into components that are dependent and independent of  $Y$ , respectively.

## 4. Diversity

It is evident that the interactions between members are a driving force behind member performance (see, for example, section 2.3). Understanding ensembles means understanding how individual member models can be related to each other and how these relationships affect the ensemble performance. In this section, we will give an overview over some of the measures proposed to quantify ensemble diversity. We focus on the classification task.

### 4.1. Measures of Diversity

For a suitable diversity measure, the following properties are desirable.

- ▶ The measure captures the differences between member models.
- ▶ There is a relationship between the diversity measure and the ensemble generalisation error.
- ▶ The diversity measure is independent of the outcome variable.

Naturally, many diversity measures are based on some notion of spread of the member models. This can, for instance, be a measure of disagreement, variance, impurity, entropy, or covariance.

#### 4.1.1. Disagreement

We will begin with two simple measures based on the contingency table [15]. To shorten notation, we will refer to its entries as given in table 4.1. The *Disagreement Measure* is the proportion of examples on which two members make different predictions.

$$\frac{1}{n}(n_{(+,-)} + n_{(-,+)})$$

The *Q-Statistic* is given as

$$Q_{ij} =_{\text{def}} \frac{n_{(+,+)}n_{(-,-)} - n_{(-,+)}n_{(+,-)}}{n_{(+,+)}n_{(-,-)} + n_{(-,+)}n_{(+,-)}}$$

$Q_{ij} = 0$  if  $q_i$  and  $q_j$  are independent, positive if the members make similar predictions and negative if the members make different predictions.

#### 4.1.2. Ambiguity

[24] propose a decomposition of the ensemble generalisation error into two terms: One describing the average error of ensemble members and a so-called *ambiguity* term.

$$\mathbb{E}[\ell(y, \bar{q})] = \frac{1}{M} \sum_{i=1}^M \ell(y, q_i) - \frac{1}{M} \sum_{i=1}^M \ell(\bar{q}, q_i)$$

This perfectly divides the ensemble error into error due to characteristics of the individual member models and error due to interactions between member predictions. Note that the contribution of the ambiguity term here is negative, that is, ambiguity is

	$q_i = +1$	$q_i = -1$
$q_j = +1$	$n_{(+,+)}$	$n_{(+,-)}$
$q_j = -1$	$n_{(-,+)}$	$n_{(-,-)}$

**Table 4.1.:** Notation for entries of the contingency table.

a beneficial influence. This decomposition was originally given for the squared-error loss [24] and the KL-divergence [todo]. We will treat this quantity in detail in the rest of this chapter. Right now, note that the ambiguity term can be interpreted as a measure of *variance* where individual distances are measured by the loss  $\ell$ . For the squared-error loss and the arithmetic mean combiner, this is exactly the "statistical" variance over the members  $\frac{1}{M} \sum_{i=1}^M (q_i - \frac{1}{M} \sum_{i=1}^M q_i)^2$ . For other loss functions, this yields other well-known quantities (see definition 1.6.3).

### 4.1.3. Impurity

**KohaviWolpert** give a bias-variance decomposition of the 0/1-loss as follows.

$$\begin{aligned} \mathbb{E} [\ell_{0/1}(Y, q(X))] &= \mathbb{E} [1/2 (\sigma_x^2 + \text{bias}(q) + \text{var}(q))] \\ \text{for } \text{bias}(q) &= \sum_y (\mathbb{P}[y^* = y | x] - \mathbb{P}[q = y | x])^2 \\ \text{var}(q) &= 1 - \sum_y \mathbb{P}[q = y | x]^2 \\ \sigma^2 &= 1 - \sum_y \mathbb{P}[y^* = y | x] \end{aligned}$$

Note that the variance and noise terms are of the form of the Gini impurity (see 3.1.2) and can be interpreted as measures of impurity. Kuncheva take inspiration from this variance term and proceed as follows. Instead of considering the impurity over positive or negative labels, they instead consider the impurity over labels for which the ensemble is correct ( $\tilde{y} = +1$ ) or incorrect ( $\tilde{y} = -1$ ), respectively. As such, the probability is not with respect to the distribution of labels but the distribution  $\Theta$  of members in the ensemble. Let the number of correct classifiers on an example be  $m_+(x) =_{\text{def}} \sum_j^M \mathbb{1}[q_j(x) = y(x)]$  where  $y(x)$  is the true label of  $x$ . This yields

$$\text{var}'_x =_{\text{def}} 1 - \sum_{\tilde{y}} \mathbb{P}_{\Theta}[q = \tilde{y} | x]^2$$

Averaging this over the entire training dataset, this can be understood as a measure of diversity. More precisely, it is the impurity as measured by the Gini impurity of the predictions of the ensemble members.

### 4.1.4. Entropy

Cunningham and Carney propose the entropy between member predictions as a diversity measure. For a single point, it is given as

$$\sum_{y \in \{-1, +1\}} -\mathbb{P}_{\Theta}[y | x] \log \mathbb{P}_{\Theta}[y | x]$$

where, for an ensemble,  $\mathbb{P}_{\Theta}[y | x] \approx \frac{1}{M} \sum_{i=1}^M \mathbb{1}[q_i(x) = y]$ . Shipp and Kuncheva propose a target-dependent measure that is reminiscent of the entropy. With  $m_+(x) = \sum_{j=1}^M \mathbb{1}[q_j(x) = y(x)]$ :

$$\frac{1}{M - \lceil \frac{M}{2} \rceil} \min\{m_+(x), M - m_+(x)\}$$

### 4.1.5. Covariance

**Covariance of members** In section 2.3, we have already seen evidence that the covariance between members is an essential factor to ensemble performance. Indeed, the notion of covariance and uncorrelatedness has been a guiding thought in the literature [4, 28, 29]. We will now introduce an exact decomposition of the ensemble error for the squared-error loss that includes the average covariance between member predictions.

**Theorem 4.1.1** (*Bias-Variance-Covariance decomposition ??*) It holds that

$$\mathbb{E}_{(X,Y),D} [(y - \bar{q})^2] = \overline{bias}^2 + \frac{1}{M} \overline{var} + \left(1 - \frac{1}{M}\right) \overline{covar}$$

$$\text{for } \overline{bias} =_{\text{def}} \frac{1}{M} \sum_{i=1}^M (\mathbb{E}_D [q_i] - y)$$

$$\overline{var} =_{\text{def}} \frac{1}{M} \sum_{i=1}^M \mathbb{E}_D [(q_i - \mathbb{E}_D [q_i])^2]$$

$$\overline{covar} =_{\text{def}} \frac{1}{M(M-1)} \sum_{i \neq j} \mathbb{E}_D [(q_i - \mathbb{E}_D [q_i])(q_j - \mathbb{E}_D [q_j])]$$

*Proof.* We begin by applying the bias-variance decomposition (theorem 1.5.1) to the ensemble model  $\bar{q}$ .

$$\mathbb{E} [\ell(y, \bar{q})] = \mathbb{E} [\ell(Y, y^*)] + \mathbb{E} [\ell(\bar{q}^*, y^*)] + \mathbb{E} [\ell(\bar{q}^*, \bar{q})]$$

For the bias term, it holds that

$$\begin{aligned} \text{bias}(\bar{q}) &= \ell(\bar{q}^*, y^*) = (\mathbb{E}_D [\bar{q}] - y^*) \\ &= \mathbb{E}_D \left[ \left( \left( \frac{1}{M} \sum_{i=1}^M q_i \right) - y^* \right)^2 \right] \\ &= \left( \frac{1}{M} \sum_{i=1}^M \mathbb{E}_D [q_i - y^*] \right)^2 \\ &= \overline{bias}^2 \end{aligned}$$

The variance of the ensemble can be decomposed into terms describing variances of individual members and covariances between members.<sup>1</sup>

$$\begin{aligned} \text{Var}(\bar{q}) &= \mathbb{E}_D [\ell(\bar{q}, \bar{q}^*)] \\ &= \mathbb{E}_D [(\bar{q} - \mathbb{E}_D [\bar{q}])^2] \\ &= \mathbb{E}_D \left[ \left( \frac{1}{M} \sum_{i=1}^M q_i - \mathbb{E}_D \left[ \frac{1}{M} \sum_{i=1}^M q_i \right] \right)^2 \right] \\ &= \frac{1}{M^2} \sum_{i=1}^M \mathbb{E}_D [(q_i - \mathbb{E}_D [q_i])^2] + \frac{1}{M^2} \sum_{j \neq i} \mathbb{E}_D [(q_i - \mathbb{E}_D [q_i])(q_j - \mathbb{E}_D [q_j])] \end{aligned}$$

1: Using that

$$\left( \sum_{i=1}^n a_i \right)^2 = \sum_{i=1}^n a_i^2 + \sum_{j \neq i} 2a_i a_j$$

Rearranging the coefficients yields the form of the theorem.<sup>2</sup>

□

2: The coefficients are rearranged using

$$\frac{1}{M^2} = \left(1 - \frac{1}{M}\right) \frac{1}{M(M-1)}$$

The Bias-Variance-Covariance decomposition can be interpreted as a decomposition into characteristics of individual learners (mean bias and variance), plus a quantity describing the interactions between different learners. Again, one can see that ensemble performance profits if members are uncorrelated. However, this decomposition is only given for the squared error and the arithmetic mean combiner.

#### 4.1.6. Relationship between Ambiguity and Covariance

Ambiguity as a generalised notion of variance, and the well-known covariance decomposition. Can see that strictly speaking, these belong to the "variance" section.

We have now seen two approaches to expressing the ensemble generalisation error:

- In terms of *covariance* as in the bias-variance-covariance decomposition of theorem 4.1.1. A very similar notion also appears in when considering ensemble margins as in 2.3.5
- In terms of variation around a centroid with respect to some loss function as in the diversity decomposition of theorems 4.2.2. For the squared-error loss, this is exactly the variance. The generalisations to Bregman divergences and arbitrary loss functions can be understood as generalised measures of variance.<sup>3</sup>

Inspecting the proofs of theorems 4.1.1 and 2.3.5, one can observe that in both cases, one begins with a measure of variance. Based on this, a covariance expression is then extracted, enabled by the definition of variance involving a square, producing cross-terms. In other words, *the covariance term is an artifact of the squared-error loss*. The notion of variance is more general.

For the case of squared-error loss, Brown et al. [28] relate the ambiguity decomposition (4.2.1) and the bias-variance-covariance decomposition (theorem 4.1.1) directly.

$$\mathbb{E} \left[ \frac{1}{M} \sum_{i=1}^M (y - q_i)^2 - \frac{1}{M} \sum_{i=1}^M (\bar{q} - q_i)^2 \right] = \overline{\text{bias}} + \frac{1}{M} \overline{\text{var}} + \left(1 - \frac{1}{M}\right) \overline{\text{covar}}$$

which yields

$$\begin{aligned} \mathbb{E} \left[ \frac{1}{M} \sum_{i=1}^M (y - q_i)^2 \right] &= \overline{\text{bias}} + \Omega \\ &= \Omega - \left( \frac{1}{M} \overline{\text{var}} + \left(1 - \frac{1}{M}\right) \overline{\text{covar}} \right) \\ \text{for } \Omega &=_{\text{def}} \overline{\text{var}} + \frac{1}{M} \sum_{i=1}^M (\mathbb{E}[q_i] - \mathbb{E}[\bar{q}])^2 \end{aligned}$$

The first quantity describes the average member error, the second the diversity of the ensemble. The appearance of  $\Omega$  in both terms illustrates that there is a trade-off between individual member error and diversity. In other words, one cannot maximise diversity without also affecting other parts of the ensemble error. Vice versa, optimising for other components of the error will also affect diversity.

3: For any loss function:

$$\mathbb{E}_D [\ell(q^\star, q)]$$

For the squared-error loss:

$$\mathbb{E}_D [(q - \mathbb{E}_D[q])^2] = \mathbb{E}_D [\ell(q^\star, q)]$$

For Bregman divergences, this is analogous to the *Bregman information*, see definition 1.6.3:

$$\mathbb{E}_D [B_\phi(q^\star, q)]$$

## 4.2. The Diversity-Effect Decomposition

**Generalising Ambiguity** In section 1.5, we have derived a generalised bias-variance decomposition by considering the effect on the loss of using a random variable instead of its non-random centroid. For the variance, this would be the expected difference in loss between using a model dependent on the training input  $D$  and the expected model, where the expectation is over  $D$ . Consider now an ensemble of learners, in which each learner is constructed according to a random parameter  $\Theta$ . Similar to bias and variance, we may consider the distribution of models over  $\Theta$  around a central model  $\bar{q}$  that is non-random with respect to  $\Theta$ . The expected *effect* of using the central model instead of some single member is expressed as follows.

$$\mathbb{E}_{\Theta} [\ell(Y, q_{\Theta}) - \ell(Y, \bar{q})] \approx \frac{1}{M} \sum_{i=1}^M \ell(Y, q_i) - \ell(Y, \bar{q})$$

Using the same strategy as for the bias-variance-effect decomposition of theorem 1.5.1, we can use this to formulate a decomposition of the generalisation error with respect to the central model.

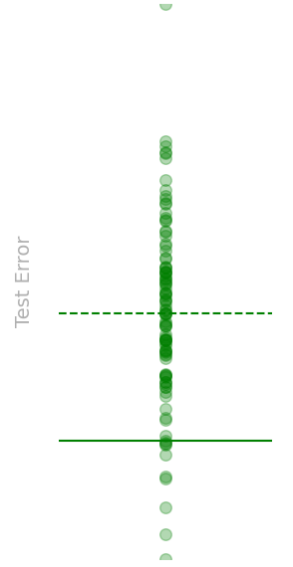
**Theorem 4.2.1** (*Ambiguity-Effect decomposition [todo]*) For any loss function  $L$ , target label  $Y$ , ensemble members  $q_1, \dots, q_M$  with combiner  $\bar{q}$

$$\begin{aligned} \ell(Y, \bar{q}) &= \frac{1}{M} \sum_{i=1}^M \ell(Y, q_i) - \underbrace{\left( \frac{1}{M} \sum_{i=1}^M \ell(Y, q_i) - \ell(Y, \bar{q}) \right)}_{\text{Ambiguity-Effect / Ensemble Improvement}} \\ &= \frac{1}{M} \sum_{i=1}^M \ell(Y, q_i) - \frac{1}{M} \sum_{i=1}^M LE(\bar{q}, q_i) \end{aligned}$$

If the ensemble combiner  $\bar{q}$  is chosen to be the central model (as defined in def. 2.2.2), this is a decomposition of the ensemble generalisation error and a generalisation of the ambiguity decomposition described in section 4.2.

We can then also find an intuitive interpretation of ambiguity-effect: It is the effect of ensembling on the error. If we consider the members to be constructed according to a parameter  $\Theta$ , a reasonable measure of the member performance is its loss in expectation over the parameter distribution:  $\mathbb{E}_{\Theta} [L(Y, q(X; \Theta))] \approx \frac{1}{M} \sum_{i=1}^M L(Y, q(X; \Theta_i))$ . What we gain or lose from using an ensemble  $\bar{q}$  over just a single member model is exactly measured by ambiguity-effect. Due to this, this quantity is also known as *ensemble improvement* [theisen, and others?].

**Diversity-Effect** The ambiguity decomposition divides the ensemble error into the average member error and the variance among members. How does this relate to the well-known bias-variance decomposition? Indeed, nothing prevents us from applying the bias-variance decomposition of theorem 1.5.1 to the error of an individual member, resulting in a decomposition into *average* bias, *average* variance and expected ambiguity, which is also referred to as *diversity* [7]. In summary, the decomposition is given in the following theorem. Note that it holds for *any* loss function.



**Figure 4.1:** The spread of individual tree predictions in a random forest ensemble. Glyphs correspond to test errors of individual trees. The dashed line is the average test error of individual trees  $\frac{1}{M} \sum_{i=1}^M L(y, q_i)$ . The solid line is the test error of the ensemble  $L(y, \bar{q})$ . The difference between these values is the *ensemble improvement* or *ambiguity-effect*. (TODO resolve double terms)

Similar to variance, ambiguity and ambiguity-effect are measures of spread. Variance measures the spread of training error across models trained with different draws of the training dataset  $D$  around a model that is a centroid with respect to the distribution of  $D$ . Similarly, ambiguity measures the spread of individual member model errors around a model that is centroid with respect to the distribution of  $\Theta$ , namely the combiner  $\bar{q}$ . In case of squared loss, this is indeed the statistical variance around the arithmetic mean. For other losses, this is a different quantity.

**Figure 4.2:** Components of the diversity-effect decomposition by number of trees in a standard Random Forest ensemble trained on *mnist-subset*. Average bias and average variance stay (almost) constant with increasing number of trees, while diversity increases. The ensemble error is the difference between the average member error (which is the sum of average bias and average variance) and diversity.

**Theorem 4.2.2** (*Bias-Variance-Diversity-Effect decomposition [7]*)

$$\begin{aligned}
 \mathbb{E} [\ell(y, \bar{q})] &= \underbrace{\mathbb{E} \left[ \frac{1}{M} \sum_{i=1}^M \ell(y, q_i) \right]}_{\text{avg. member error}} - \underbrace{\mathbb{E} \left[ \frac{1}{M} \sum_{i=1}^M LE(\bar{q}, q_i) \right]}_{\text{ambiguity-effect}} \\
 &= \underbrace{\mathbb{E} \left[ \frac{1}{M} \sum_{i=1}^M LE(q_i^*, y^*) \right]}_{\text{avg. bias-effect}} + \underbrace{\mathbb{E} \left[ \frac{1}{M} \sum_{i=1}^M LE(q_i^*, q_i) \right]}_{\text{avg. variance-effect}} - \underbrace{\mathbb{E} \left[ \frac{1}{M} \sum_{i=1}^M LE(\bar{q}, q_i) \right]}_{\text{diversity-effect}}
 \end{aligned}$$

**Unchanged bias and reduction in variance** In section 2.3 we gave arguments for how in specific cases, the ensemble bias equals the bias of any member. We now have the tools to show this in a more general manner [7].

For the ensemble bias, application of the ambiguity-effect decomposition (4.2.1) to a set of centroid models  $q_i^*$  yields:

$$\underbrace{LE(y, \bar{q}^*)}_{\text{ens. bias}} = \underbrace{\frac{1}{M} \sum_{i=1}^M LE(y, q_i^*)}_{\text{avg. bias}} - \underbrace{\frac{1}{M} \sum_{i=1}^M LE(\bar{q}^*, q_i^*)}_{\Delta}$$

For the ensemble variance, application of the diversity-effect decomposition (4.2.2) while substituting  $y \leftarrow \bar{q}^*$ :

$$\underbrace{\mathbb{E}_D [LE(\bar{q}^*, \bar{q})]}_{\text{ens. var.}} = \underbrace{\frac{1}{M} \sum_{i=1}^M LE(\bar{q}^*, q_i^*)}_{\Delta} + \underbrace{\frac{1}{M} \sum_{i=1}^M \mathbb{E}_D [LE(q_i^*, q_i)]}_{\text{avg. var.}} - \underbrace{\mathbb{E}_D \left[ \frac{1}{M} \sum_{i=1}^M LE(\bar{q}, q_i) \right]}_{\text{diversity}}$$

Due to lemma 2.2.1 which states that in homogeneous ensembles  $q_i^* = q_j^* = \bar{q}^*$ , we can conclude that  $\Delta = 0$ .

**Corollary 4.2.3** *For homogeneous ensembles, we can conclude the following:*

- *The ensemble bias is equal to the average member bias:*

$$\Delta = 0 \rightarrow LE(y, \bar{q}^*) = \frac{1}{M} \sum_{i=1}^M LE(y, q_i^*)$$

- *Diversity is a component of ensemble variance. The other component is the average member variance. In other words, ensemble variance reduction is measured exactly by diversity.*
- *Diversity is bounded from above by the average member variance.*

### 4.3. Diversity for Bregman Divergences

Note that bias-effect, variance-effect and ambiguity-effect are all of the form  $\mathbb{E} [LE(\circ, \square)]$  and depend directly on the target label  $Y$ . With variance-effect, we have captured the *effect* of variations between different training datasets) on the prediction error.

With ambiguity-effect, we have captured the effect of variations between the different member models on the prediction error. We have already seen that for the squared error, the variance-effect coincides with familiar notion of "statistical" variance between the predictions. We will now argue that for Bregman divergences as defined in definition 1.6.1, the loss-effect terms reduce to the loss between the two objects. The class of Bregman divergences covers many widely used loss functions and thus allows us to formulate a unified bias-variance-decomposition.

**Lemma 4.3.1** ([6], Theorem 0.1b) *Let  $q$  be a function of a random variable  $Z$  and independent of  $Y$ . For  $y^\star = \mathbb{E}_Y[Y]$ , i.e. the right Bregman centroid w.r.t.  $Y$ , it holds that*

$$\mathbb{E}_Z [B_\phi(y^\star, q)] = \mathbb{E}_{Z,Y} [B_\phi(Y, q) - B_\phi(Y, y^\star)]$$

Using  $q \leftarrow q^\star$  shows that bias-effect collapses to bias for Bregman divergences:

$$B_\phi(y^\star, q^\star) = \mathbb{E} [B_\phi(Y, q^\star) - B_\phi(Y, y^\star)]$$

**Lemma 4.3.2** ( $\star$ , Generalised from [7]) *Let  $q$  be a function of random variable  $Z$  and independent of  $Y$ . For  $q^\star = \mathcal{E}_Z[q]$ , i.e. the left Bregman centroid w.r.t.  $Z$ , it holds that*

$$\mathbb{E}_Z [B_\phi(q^\star, q)] = \mathbb{E}_{Z,Y} [B_\phi(Y, q) - B_\phi(Y, q^\star)]$$

*Proof.* The proof is given in section A.3.1. □

This shows that variance- and ambiguity-effect collapse to variance and ambiguity. The variance (in the bias-variance sense) is the variance of the estimates  $q_D$  dependent on  $D$  with respect to different realisations of  $D$  around its  $D$ -centroid.

$$\text{For } q^\star = \mathcal{E}_D[q_D]: B_\phi(q^\star, q) = \mathbb{E} [B_\phi(Y, q^\star) - B_\phi(Y, q)]$$

Ambiguity/Diversity is the variance of the estimates  $q_\Theta$  dependent on  $\Theta$  with respect to different realisations of  $\Theta$  around its centroid.

$$\text{For } \bar{q} = \mathcal{E}_\Theta[q_\Theta]: B_\phi(\bar{q}, q) = \mathbb{E} [B_\phi(Y, \bar{q}) - B_\phi(Y, q)]$$

This yields a generalised bias-variance-diversity decomposition for bregman divergences as a special case of the corresponding effect decomposition.



**Theorem 4.3.3** (*Bias-Variance-Diversity decomposition for Bregman divergences*)

$$\begin{aligned}
 \mathbb{E}_{(X,Y),D} [B_\phi(Y, q)] &= \underbrace{\mathbb{E}_{Y|X} [B_\phi(Y, y^*)]}_{\text{noise}} \\
 &\quad + \underbrace{\frac{1}{M} \sum_{i=1}^M B_\phi(\bar{Y}, \mathbf{q}_i^*)}_{\text{bias}} \\
 &\quad + \underbrace{\frac{1}{M} \sum_{i=1}^M \mathbb{E}_D [B_\phi(\mathbf{q}_i^*, \mathbf{q}_i)]}_{\text{variance}} \\
 &\quad - \underbrace{\mathbb{E}_D \left[ \frac{1}{M} \sum_{i=1}^M B_\phi(\bar{\mathbf{q}}, \mathbf{q}_i) \right]}_{\text{diversity}}
 \end{aligned}$$

**Ensemble improvement for Bregman Divergences** In section 2.3, we have used Jensen's inequality to show that the ensemble improvement is non-negative for some cases.

$$\mathbb{E}_\Theta [\ell(q_\Theta(X), Y)] - \ell(\mathbb{E}_\Theta [q_\Theta(X)], Y) \geq 0$$

It is evident, that the Jensen gap is but a special case of ambiguity-effect (4.2.1) for  $\bar{q} =_{\text{def}} \frac{1}{M} \sum_{i=1}^M q_i$  and convex loss functions. This shows that the ensemble loss is always smaller-equal than the expected member loss, but *only* if the ensemble output is actually produced by an arithmetic mean.

However, it can not be assumed from the outset that the arithmetic mean is the best ensemble combiner. Indeed, for the cross-entropy loss, **abe** proceed to note that the Jensen gap corresponds to a form that is "not immediately recognizable". Although they do find an interpretation of it, it is still necessarily dependent on the outcome  $Y$ . As illustrated in 4.3 on Bregman divergences, it seems reasonable to define the ensemble combiner in accordance to the Bregman divergence, i.e. to be the *dual* expectation  $\mathcal{E}_\Theta [q_\Theta]$ . Non-negativity is then easily shown since in that case ambiguity-effect reduces to ambiguity.

In fact, for the case of cross-entropy, [7] show that the ambiguity term is still nonnegative, i.e. that the arithmetic mean combiner does not hurt performance.

$$B_\phi(\bar{q}, q) = \mathbb{E} [B_\phi(Y, \bar{q}) - B_\phi(Y, q)] \quad \text{for } \bar{q} = \mathcal{E}_\Theta [q_\Theta]$$

and the value of any Bregman divergence is always non-negative. Further, ambiguity is now independent of the outcome  $Y$ .

#### Corollary 4.3.4

- ▶ For any Bregman divergence, ensembling using the combiner implied by the divergence can not hurt performance.
- ▶ The diversity is an intuitive measure of ensemble improvement.
- ▶ This ensemble improvement appears in an exact decomposition of the ensemble generalisation error.

## 4.4. Diversity for the 0/1-Loss

**Definition 4.4.1** The 0/1-loss between two outcomes is

$$\ell_{0/1}(Y, Y') =_{\text{def}} \mathbb{1}[Y \neq Y']$$

The ensemble combiner implied by the 0/1-loss is the plurality vote.

**Definition 4.4.2** (Majority/Plurality vote combiner) For a  $k$ -class classification problem, the majority vote combiner is defined as

$$\bar{q}(X) = \arg \min_{z \in [k]} \mathbb{E}_{\Theta} [\ell_{0/1}(z, q_{\Theta})]$$

This assumes that each member model predicts a single class, although this does not imply that member models must necessarily be trained based on the 0/1-loss, too. If a member predicts a class, we also say that the member *votes* for that class.

In the remainder of this section, we will analyse classification ensembles as measured by the 0/1-loss. A basic quantity for this will be the ratio of members that are incorrect for a given example-outcome pair.

**Definition 4.4.3** For a distribution of members constructed according to input data  $D = (D_1, \dots, D_M)$  and parameters  $\Theta = (\Theta_1, \dots, \Theta_M)$ , the ratio of incorrect ("wrong") members is

$$W(X, Y) =_{\text{def}} \mathbb{E}_{D, \Theta} [\ell_{0/1}(Y, q_{D, \Theta}(X))] \approx \frac{1}{M} \sum_{i=1}^M \ell_{0/1}(Y, q_i(X))$$

As with other variables, we sometimes omit explicitly stating the dependence on  $(X, Y)$ . Further, we write  $W_{\Theta} =_{\text{def}} \mathbb{E}_{\Theta} [\ell_{0/1}(Y, q_{D, \Theta})]$ . For the complement, we write  $\bar{W} =_{\text{def}} 1 - W$

**A simple bound** Using Markov's inequality, we can readily upper-bound the error of the ensemble in terms of expected errors of the members [10]<sup>4</sup>.

$$0 \leq \mathbb{E} [\ell_{0/1}(Y, \bar{q})] = \mathbb{P}[W \geq \kappa] \leq \mathbb{P}[W \geq 1/2] \leq 2\mathbb{E}[W]$$

While there exist examples for which this upper bound is tight [10], it is reasonable to suspect that the ensemble being worse by a factor of two is only a pathological case and not relevant for practise.

#### 4.4.1. Diversity in binary classification problems

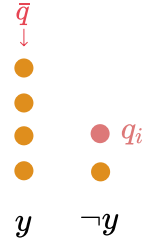
We begin by considering binary classification problems which have  $k = 2$  two possible outcomes. The special property of binary classification problems is that any vote which is not correct is automatically a vote for the single other class. In other words, diversity can be measured in terms of disagreement between members. This is not given for problems with  $k > 2$  where an incorrect vote might correspond to any other class. We will see that, in this case, diversity will be measured in terms of differences in *correctness* of members.

The dichotomy of binary classification problems allows us to succinctly express the diversity-effect.

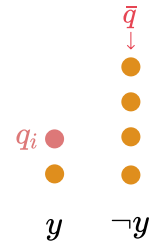
The proper term here would actually be *plurality* vote since, for a class to win the vote, it is required to have more than  $1/k$  votes. Strictly speaking, a *majority* vote win requires the majority of all votes, i.e. more than  $1/2$ . For  $k = 2$ , majority and plurality voting is equivalent.

4: Markov's inequality states that for a nonnegative random variable  $X$  and  $a > 0$

$$\mathbb{P}[X \geq a] \leq \frac{\mathbb{E}[X]}{a}.$$



**Figure 4.3:** Example of the effect of a member's vote  $q_i$  on the diversity on a point for which the ensemble majority vote is correct. Example where  $q_i$  has positive contribution to the diversity effect term, i.e.  $\ell_{0/1}(y, q_i) - \ell_{0/1}(y, \bar{q}) = 1$ . The member  $q_i$  is incorrect but due to the discreteness of the majority vote combiner, the ensemble performance does not suffer – unless the majority vote is tipped. Any correct vote while the ensemble already is correct is effectively "wasted" and incorrect votes correspond to diversity.



**Figure 4.4:** Example where  $q_i$  has negative contribution to the diversity effect term, i.e.  $\ell_{0/1}(y, q_i) - \ell_{0/1}(y, \bar{q}) = -1$ . Any further incorrect vote while the ensemble is already incorrect would be wasted. The negative effect here eventually results in the 0/1-loss of 1.

**Lemma 4.4.1** ([30]) For a classification problem with  $k = 2$  classes, let  $y, \bar{q} \in \{-1, 1\}$ . It then holds that

$$\frac{1}{M} \sum_{i=1}^M [\ell_{0/1}(y, q_i) - \ell_{0/1}(y, \bar{q})] = (y \cdot \bar{q}) \frac{1}{M} \sum_{i=1}^M \ell_{0/1}(\bar{q}, q_i) \in \{-1, 0, 1\}$$

*Proof.* Let  $y, \bar{q} \in \{-1, 1\}$ .

- Assume the ensemble is correct, i.e.  $y = \bar{q}$ . Then  $\ell_{0/1}(y, \bar{q}) = 0$  and the left-hand-side equals  $\frac{1}{M} \sum_{i=1}^M \ell_{0/1}(y, q_i) = \frac{1}{M} \sum_{i=1}^M \ell_{0/1}(\bar{q}, q_i)$ . Further,  $y \cdot \bar{q} = 1$ .
- Assume the ensemble is incorrect, i.e.  $y \neq \bar{q}$ . Then  $y \cdot \bar{q} = -1$  and, for the left-hand-side, we can write

$$\frac{1}{M} \sum_{i=1}^M [\ell_{0/1}(y, q_i)] - 1 = - \left( 1 - \frac{1}{M} \sum_{i=1}^M \ell_{0/1}(y, q_i) \right) = - \left( \frac{1}{M} \sum_{i=1}^M \ell_{0/1}(\bar{q}, q_i) \right)$$

using that, since  $y \neq \bar{q}$ ,  $(1 - \frac{1}{M} \sum_{i=1}^M \ell_{0/1}(y, q_i)) = \frac{1}{M} \sum_{i=1}^M \ell_{0/1}(\bar{q}, q_i)$ .

□

We can divide the range of  $X$  into two disjoint subsets. Let  $X_+$  be the examples on which the ensemble is correct. Ambiguity on these points has a decreasing effect on the overall ensemble error. Let  $X_-$  be the examples on which the ensemble is incorrect. Ambiguity on these points has an increasing effect on the overall ensemble error. This yields a decomposition into *good* and *bad* diversity.

**Corollary 4.4.2** ([30]) For a classification problem with  $k = 2$  classes, let  $y, \bar{q} \in \{-1, 1\}$ . It then holds that

$$\begin{aligned} \mathbb{E}_X [L(Y, \bar{q})] &= \mathbb{E}_X \left[ \frac{1}{M} \sum_{i=1}^M \ell_{0/1}(Y, q_i) \right] \\ &\quad - \underbrace{\mathbb{E}_{X_+} \left[ \frac{1}{M} \sum_{i=1}^M \ell_{0/1}(\bar{q}, q_i) \right]}_{\text{"good" diversity}} \\ &\quad + \underbrace{\mathbb{E}_{X_-} \left[ \frac{1}{M} \sum_{i=1}^M \ell_{0/1}(\bar{q}, q_i) \right]}_{\text{"bad" diversity}} \end{aligned}$$

Note that this is a special case of the ambiguity-effect decomposition of theorem 4.2.1. There is a tradeoff between average member error and diversity. Here, however, diversity is not always beneficial. On points where the ensemble is incorrect, disagreements have a negative effect on the overall ensemble error. In other words, for majority vote ensembles, diversity is only beneficial *on points at which the ensemble can actually afford to be diverse*.

Further, from corollary 4.4.2, one can already see that the ensemble improvement (i.e. diversity-effect) in binary classification problems is only non-negative if good diversity outweighs bad diversity.

Good and bad diversity can be expressed solely in terms of the ratio of incorrect members.

An intuition of this is also that of "wasted votes": Under the majority vote combiner, for the ensemble to be correct, we require only at least half of the members to be correct. Any higher ratio of correct ensemble members does not improve the ensemble performance on this point and these can be seen as "wasted". Likewise, the ensemble is incorrect if not more than half of the members are correct. Any positive votes do not influence the ensemble improvement and can be considered "wasted".

**Lemma 4.4.3** ★ Let  $y$  be the true outcome for a given example. Let  $\neg y$  be an outcome that is not  $y$ . Write  $\ell_{0/1}(q_i, \neg y) \stackrel{\text{def}}{=} \sum_{k \neq y} \ell_{0/1}(q_i, k)$  for the indication whether  $q_i$  is incorrect. Then the following identities hold.

$$\begin{aligned} \mathbb{E}_{X_+} \left[ \frac{1}{M} \sum_{i=1}^M \ell_{0/1}(q_i, \bar{q}) \right] &= \mathbb{E}_{X_+} [W_1^M] \\ \mathbb{E}_{X_-} \left[ \frac{1}{M} \sum_{i=1}^M \ell_{0/1}(q_i, \bar{q}) \right] &= \mathbb{E}_{X_-} \left[ \frac{1}{M} \sum_{i=1}^M \ell_{0/1}(q_i, \neg y) \right] \\ &= \mathbb{E}_{X_-} [1 - W_1^M] \end{aligned}$$

Analogous equalities hold in expectation over member parameter  $\Theta$ .

#### 4.4.2. Weak Learners

A common idea is that, in order for ensembling to be effective, the performance of individual members must not be too bad. In the remainder of this section, we will review some assumptions that imply ensemble effectivity and show that they are in fact tightly related.

**Definition 4.4.4** (Weak learner) need to check / reformulate this

**Theorem 4.4.4** ([7]) In an ensemble of weak learners, diversity-effect is non-negative:

$$\mathbb{E}_D \left[ \mathbb{E}_Y \left[ \frac{1}{M} \sum_{i=1}^M \ell_{0/1}(Y, q_i) - \ell_{0/1}(Y, \bar{q}) \right] \right] \geq 0$$

*Proof.* ... essentially using jury theorem

□

However, this is not a sufficient

#### 4.4.3. Competence in binary classification problems

Theisen et al. consider the question of ensemble improvement under the 0/1-loss. They define an assumption on the ratio of incorrect members.

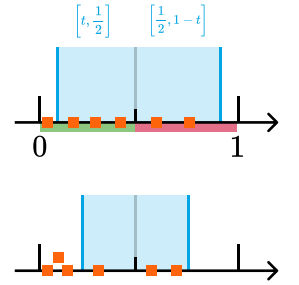
**Definition 4.4.5** (2-competence, [10]) An ensemble is 2-competent iff

$$\forall t \in [0, 1/2] : \mathbb{P}_{(X,Y)} [W(X,Y) \in [t, 1/2]] \geq \mathbb{P}_{(X,Y)} [W(X,Y) \in [1/2, 1-t]]$$

The condition is illustrated in figure 4.5. It is used to show two results:

- In 2-competent ensembles, diversity-effect is non-negative.<sup>5</sup>
- bounds on the generalisation error

One can see that competence is essentially determined by the distribution of examples  $(X, Y)$  over the range of  $W(X, Y)$  which is divided by the majority vote threshold  $1/2$ . We have already seen that, similarly, diversity-effect in its apparent form of good and bad diversity is determined by just the same characteristics. How are these two related? In this section, we will argue that non-negative diversity-effect is in fact equivalent



**Figure 4.5.:** Illustration for the competence condition 4.4.5 for binary classification. Red squares correspond to pairs  $(X, Y)$  from the joint distribution of examples and outcomes. For each of these pairs, the average/expected member error  $W_\Theta(X, Y) \approx \frac{1}{M} \sum_{i=1}^M \ell_{0/1}((\cdot, y), q_i)$  is the ratio of incorrect members. The center  $1/2$  is the majority vote threshold. Informally, an ensemble is competent, if, for any two intervals defined by  $t$  left and right of the threshold, more examples are in the left part. For the upper example, this holds. For the lower example, even though many examples are classified correctly by many members, the ensemble is not competent.

5: Although not acknowledging the role of diversity-effect as a component of the ensemble generalisation error and thus referring to it only as "ensemble improvement", one of the main results of [10] is that, in competent ensembles, ensemble improvement (i.e. diversity-effect) is non-negative.

to a notion of competence generalised to  $k > 2$  classes. Unless otherwise noted, all expectations and probabilities are over the distribution of  $(X, Y)$ .

While proving that 2-competence implies non-negative diversity-effect, Theisen et al. establish the following fact.

$$\text{ens. 2-competent} \leftrightarrow \mathbb{E}[W \mathbb{1}[W < 1/2]] \geq \mathbb{E}[\overline{W} \mathbb{1}[\overline{W} \leq 1/2]] \quad (4.1)$$

We can rearrange this into a more suggestive form. Recall that  $W = \mathbb{E}_{D,\Theta}[\ell_{0/1}(Y, q_{D,\Theta}(X))]$ . We now split off the expectation over  $D$  and instead consider  $W_\Theta = \mathbb{E}_\Theta[\ell_{0/1}(Y, q_{D,\Theta}(X))]$ . Rearranging the above and exploiting the linearity of expectation, we obtain

$$d =_{\text{def}} \mathbb{E}_{(X,Y),D}[W_\Theta \mathbb{1}[W_\Theta < 1/2]] - \mathbb{E}_{(X,Y),D}[\overline{W}_\Theta \mathbb{1}[\overline{W}_\Theta \leq 1/2]] \geq 0$$

The indicator functions are mutually exclusive and can thus be understood as a case distinction. With slight abuse of notation, where the expectations are only over the subset of the distribution for which the case condition holds, we can write

$$d = \begin{cases} \mathbb{E}[W_\Theta] & \leftrightarrow W_\Theta < 1/2 \\ \mathbb{E}[\overline{W}_\Theta] = \mathbb{E}[1 - W_\Theta] & \leftrightarrow \overline{W}_\Theta \leq 1/2 \end{cases}$$

For  $k = 2$ , the majority vote threshold is  $1/2$  and thus the conditions correspond exactly to the ensemble being either correct or incorrect.

$$k = 2 \rightarrow \begin{cases} W_\Theta < 1/2 \leftrightarrow \bar{q}(X) = Y \\ \overline{W}_\Theta \leq 1/2 \leftrightarrow \bar{q}(X) \neq Y \end{cases} \quad (4.2)$$

Recalling the characterisation of good and bad diversity of lemma 4.4.3, we can see that  $d$  is nothing else but the diversity-effect. This means that non-negative effect is exactly equivalent to 2-competence for a classification problem with  $k = 2$  classes. Moreover, it is important to note that the gap of equation 4.1 and consequently the gap in the definition of 2-competence (4.4.5) is exactly the diversity-effect and hence exactly measures the ensemble improvement. In other words, one can now speak about the degree of competence of an ensemble.

#### 4.4.4. Competence and Diversity in non-binary classification problems

However, for  $k > 2$ , the equivalence in equation 4.2 is not given. While it is sufficient (a class with more than  $1/2M$  votes will win any plurality vote), it is not necessary: a plurality vote can be won with less than  $1/2M$  votes. Thus, there are ensembles which have non-negative diversity-effect (ensemble improvement) that are not 2-competent.

The key difference is that for  $k > 2$ , the voting threshold for a pair  $(X, Y)$  is no longer the same value for all examples. Since a class wins if and only if it has more votes than any other class, the voting threshold depends on the distribution of class votes, which is potentially different for any pair  $(X, Y)$ . Nevertheless, there is still a classification threshold, namely the ratio of votes for the next-best class. Because we

will be considering the ratio of incorrect votes as a basic quantity, we will now define it from the reciprocal perspective:

$$\kappa(X, Y) = 1 - \max_{Z \neq Y} \mathbb{E}_{\Theta} [\mathbb{1}[q_{\Theta} = Z]]$$

and it holds that

$$\begin{aligned} W_{\Theta} < \kappa &\leftrightarrow \bar{q}(X) = Y \\ \overline{W_{\Theta}} \leq 1 - \kappa &\leftrightarrow \bar{q}(X) \neq Y \end{aligned}$$

**Definition 4.4.6** ★ (*k*-competence) An ensemble is *k*-competent iff

$$\forall t \in [0, 1] : \mathbb{P}_{(X, Y)} [W \in [t, \kappa]] \geq \mathbb{P}_{(X, Y)} [W \in [1 - \kappa, 1 - t]]$$

for  $\kappa =_{\text{def}} 1 - \max_{Z \neq Y} \mathbb{E}_{\Theta} [\mathbb{1}[q_{\Theta} = Z]]$ .

Theisen et al. showed that 2-competence implies non-negative diversity-effect. We now show that a very similar line of argument using *k*-competence actually holds in both directions.

**Theorem 4.4.5** ★ Consider an ensemble for a *k*-class classification problem. Then

$$k\text{-competence} \leftrightarrow \text{diversity-effect} \geq 0$$

The main work lies in establishing the following lemma, which is a generalised form of equation 4.1.

**Lemma 4.4.6** ★ (Generalised from [10]) For an increasing function *f* with *f*(0) = 0, it holds that

$$k\text{-competence} \leftrightarrow \mathbb{E} [f(W) \mathbb{1}[W < \kappa]] \geq \mathbb{E} [f(\overline{W}) \mathbb{1}[\overline{W} \leq \kappa]]$$

where  $\kappa =_{\text{def}} 1 - \max_{Z \neq Y} \mathbb{E}_{\Theta} [\mathbb{1}[q_{\Theta} = Z]]$ .

*Proof.* We begin by observing that, for all  $x \in [0, 1]$

$$\begin{aligned} \mathbb{P} [W \in [x, \kappa]] \cdot \mathbb{1}[x \leq \kappa] &= \mathbb{P} [W \mathbb{1}[W < \kappa] \geq x] \\ \mathbb{P} [W \in [1 - \kappa, 1 - x]] \cdot \mathbb{1}[x \leq \kappa] &= \mathbb{P} [\overline{W} \mathbb{1}[\overline{W} \leq \kappa] \geq x] \end{aligned}$$

where the first factors on the left-hand-side appear in the definition of *k*-competence. Since *W* is nonnegative, using that  $\mathbb{E} [X] = \int \mathbb{P} [X \geq x] dx$ , we can conclude that, for any  $x \in [0, 1]$

$$\begin{aligned} (k\text{-comp.}) &\leftrightarrow \mathbb{P} [W \mathbb{1}[W < \kappa] \geq x] \geq \mathbb{P} [\overline{W} \mathbb{1}[\overline{W} \leq \kappa] \geq x] \\ &\leftrightarrow \mathbb{E} [W \mathbb{1}[W < \kappa]] \geq \mathbb{E} [\overline{W} \mathbb{1}[\overline{W} \leq \kappa]] \end{aligned}$$

□

Using this, we can now directly prove theorem 4.4.5.

Let

$$t =_{\text{def}} \max_{Z \neq Y} \mathbb{E}_{\Theta} [\mathbb{1}[q_{\Theta} = Z]]$$

. Then

$$\begin{aligned} \bar{q} = y &\leftrightarrow \overline{W} \geq t \\ &\leftrightarrow W = 1 - \overline{W} < 1 - t = \kappa \end{aligned}$$

and

$$\begin{aligned} \bar{q} \neq y &\leftrightarrow \overline{W} < t \\ &\leftrightarrow 1 - \overline{W} \geq 1 - t = \kappa \\ &\leftrightarrow 1 - (1 - \overline{W}) \leq 1 - \kappa \\ &\leftrightarrow \overline{W} \leq 1 - \kappa \end{aligned}$$

*Proof.* (Theorem 4.4.5, generalised from [10])

$$\begin{aligned}
0 &= \mathbb{E}[(W - 1) \mathbb{1}[W \geq \kappa]] - \mathbb{E}[(W - 1) \mathbb{1}[W \geq \kappa]] \\
&= \mathbb{E}[(W - 1) \mathbb{1}[W \geq \kappa]] + \mathbb{E}[(1 - W) \mathbb{1}[W \geq \kappa]] \\
&= \mathbb{E}[(W - 1) \mathbb{1}[W \geq \kappa]] + \mathbb{E}\left[\overline{W} \mathbb{1}\left[\overline{W} < \kappa\right]\right]
\end{aligned}$$

Applying lemma 4.4.6 for  $f = \text{id}$  to the second term yields

$$\begin{aligned}
&\mathbb{E}[(W - 1) \mathbb{1}[W \geq \kappa]] + \mathbb{E}\left[\overline{W} \mathbb{1}\left[\overline{W} < \kappa\right]\right] \\
&\leq \mathbb{E}[(W - 1) \mathbb{1}[W \geq \kappa]] + \mathbb{E}[W \mathbb{1}[W < \kappa]]
\end{aligned}$$

The above already is nothing but the diversity-effect:

$$\begin{aligned}
0 &\leq \mathbb{E}[(W - 1) \mathbb{1}[W \geq \kappa]] + \mathbb{E}[W \mathbb{1}[W < \kappa]] \\
&= \mathbb{E}[W] - \mathbb{E}[\mathbb{1}[W \geq \kappa]] \\
&= \mathbb{E}[W] - \mathbb{P}[W \geq \kappa]
\end{aligned}$$

The first term is the ratio of incorrect members in expectation over all examples and is equal to the error rate of an average member.

$$\mathbb{E}_{(X,Y)}[W] = \mathbb{E}_{(X,Y)}\left[\mathbb{E}_{D,\Theta}\left[\ell_{0/1}(Y, q_{D,\Theta}(X))\right]\right] = \mathbb{E}_{D,\Theta}\left[\mathbb{E}_{(X,Y)}\left[\ell_{0/1}(Y, q_{D,\Theta}(X))\right]\right]$$

The second term is the ensemble error.  $\square$

#### 4.4.5. Bounds for competent ensembles

2-competence was used to show upper and lower bounds for the diversity-effect [10]. Now we show that, with minor adjustments, the same bounds can be derived from  $k$ -competence. Besides giving performance guarantees, these bounds are interesting due to that they are expressed in terms of disagreements between members, which until now we have only seen for Bregman divergences.

**Theorem 4.4.7** (*Upper bound*) In  $k$ -competent ensembles,

$$\mathbb{E}[W] - \mathbb{P}[W \geq \kappa] \leq \mathbb{E}_{\rho,\rho'}[D(q_\rho, q_{\rho'})]$$

$$\text{for } D(q_\rho, q_{\rho'}) = \mathbb{E}_X[\mathbb{1}[q_\rho \neq q_{\rho'}]]$$

*Proof.* The proof can be found in [10]. It does not make use of competence and therefore still holds for  $k$ -competent ensembles.  $\square$

**Theorem 4.4.8** (*Lower bound*) In  $k$ -competent ensembles,

$$\frac{2(k-1)}{k} \mathbb{E}[D(q_\rho, q_{\rho'})] - \frac{3k-4}{k} \mathbb{E}[W] \leq \mathbb{E}[W] - \mathbb{P}[W \geq \kappa]$$

$$\text{for } D(q_\rho, q_{\rho'}) = \mathbb{E}_X[\mathbb{1}[q_\rho \neq q_{\rho'}]]$$

*Proof.* Lemmas 3 and 4 hold without adjustments for  $k$ -competence and are shown in [cited-by-theisen] and [10], respectively.

$$\begin{aligned}
\mathbb{P}[W \geq \kappa] & \leq 2\mathbb{E}[W^2] && \text{(Lemma 4.4.9)} \\
& = 2\mathbb{E}_{\rho, \rho'}[L(q_\rho, q_\rho)] && \text{(Lemma 3 in [10])} \\
& = \frac{4(k-1)}{k} (\mathbb{E}[W] - \frac{1}{2}\mathbb{E}_{\rho, \rho'}[D(q_\rho, q_{\rho'})]) && \text{(Lemma 4 in [10])}
\end{aligned}$$

Rearranging the terms yields the statement.  $\square$

We conclude by checking the inequality in the proof of theorem 4.4.8.

**Lemma 4.4.9** ★ (Generalised from [10]) In  $k$ -competent ensembles it holds that

$$\mathbb{P}[W \geq \kappa] \leq 2\mathbb{E}[W^2]$$

*Proof.* The proof is given in A.3.2.  $\square$

## 4.5. Dependency of diversity on outcomes

In the general case, diversity cannot be expressed independently of the outcome variable  $Y$ . If  $\ell$  satisfies the triangle inequality, then diversity-effect can be bounded from above by a target-independent term that is reminiscent of the diversity term for Bregman divergences introduced in theorem 4.3.3.

**Lemma 4.5.1** ★ Under a symmetric loss satisfying the triangle inequality, diversity-effect is bounded from above by diversity.

$$\ell \text{ metric} \rightarrow \mathbb{E}_{(X,Y),D} \left[ \frac{1}{M} \sum_{i=1}^M \ell(Y, q_i) - \ell(Y, \bar{q}) \right] \leq \mathbb{E}_{(X,Y),D} \left[ \frac{1}{M} \sum_{i=1}^M \ell(\bar{q}, q_i) \right]$$

*Proof.* For a  $a, b, c \in X$ , due to the triangle inequality and symmetry of  $d$ , it holds that

$$\begin{aligned}
d(a, b) - d(b, c) & \leq d(a, c) + d(c, b) - d(b, c) \\
& = d(a, c)
\end{aligned}$$

$\square$

In particular, the 0/1-loss is symmetric and satisfies the triangle inequality.

## 4.6. Diversity in Random Forests and in Neural Networks

**Interpolating and non-interpolating models** In the majority of this section, we have considered general ensembles without assumptions on the actual member learners. It appears much of the work on ensemble diversity has been done in the context of neural



networks [diversity-nns], potentially due to the early publishing of Negative Correlation Learning [31] in 1999 and the ease of encouraging diversity simply via a regularisation term. However, it has been observed that encouraging diversity is not always beneficial for neural networks [adnan\_ComplementRandomForest\_2015 liu\_EnsembleLearningNegative\_1999, li\_NeuralNetworkEnsembles\_2021]. We will now provide a brief explanation on when and why diversity in neural network ensembles is beneficial. Further, we will argue that diversity is an essential component of Random Forests, even more so than for neural network ensembles.

Recall the lower and upper bounds for diversity-effect in theorems [thm:theisen-lower, thm:theisen-upper]. In simplified form for  $k = 2$  classes, these are

$$D(q_\rho, q_{\rho'}) \geq \underbrace{\mathbb{E}[W] - \mathbb{P}[W \geq \kappa]}_{\text{diversity-effect / ensemble improvement}} \geq D(q_\rho, q_{\rho'}) - 1$$

where  $D(q_\rho, q_{\rho'}) = \mathbb{E}_X [\mathbb{1}[q_\rho \neq q_{\rho'}]]$  is the *disagreement rate*. If  $D < 1$ , then the lower bound is less than zero and the ensemble improvement can potentially be negative, i.e. ensembling may hurt performance. If  $D \geq 1$ , the power bound is greater than zero and ensembling can not hurt performance. theisen analyse the behaviour of  $D$  with varying model complexity. Of particular interest is the behaviour around the *interpolation threshold*, which is the minimum model complexity that allows a zero training error. They show that, in neural networks and bagged logistic regression ensembles, disagreement rate and ensemble improvement are maximised at the interpolation threshold and decrease beyond. In other words, higher-capacity models benefit less from diversity, or diversity may even hurt performance. The same conclusion was reached after empirical investigation in neural network ensembles by abe [abe]. In Random Forests, on the other hand, the model complexity is inherently bounded by the data [buschj]. A decision tree can only be grown until each leaf is perfectly pure, which corresponds to zero training error. In other words, Random Forests naturally can not go *into* the interpolation regime.

Further, decision trees could be understood to be of much lower capacity than deep neural networks. This likely reflects in the average member error, although a quantitative comparison has to be left for future work. Ensemble improvement can only be high if the average member error is high to begin with. In other words, ensembling can be expected to be much more beneficial for low-capacity models. This was also observed by abe [abe] for the case of neural networks.

**Expressing diversity and average member error in terms of tree structure** As we have seen in section 3.2.8, the generalisation error can be expressed as a weighted sum over forest cells. We can also express the ambiguity decomposition (see 4.2.1) in terms of forest cells. For sake of clarity we omit the expectation over  $D$  and write  $Z =_{\text{def}} (X, Y)$ .

**Proposition 4.6.1** ★ Let  $Z = Z_1 \dot{\cup} \dots \dot{\cup} Z_P$  be a forest partition of  $Z = (X, Y)$ .

$$\begin{aligned} \mathbb{E}_Z [\ell(y, \bar{q})] &= \sum_{p=1}^P \mathbb{P}[Z_p] \underbrace{\frac{1}{M} \sum_{i=1}^M \mathbb{E}_Z [\ell(y, q_i)]}_{\text{err}(Z_p)} - \underbrace{\frac{1}{M} \sum_{i=1}^M \mathbb{E}_Z [LE(\bar{q}, q_i)]}_{\text{div}(Z_p)} \\ &= \sum_{p=1}^P \mathbb{P}[Z_p] \frac{1}{M} \sum_{i=1}^M \mathbb{E}_Z [\ell(y, q_i) - LE(\bar{q}, q_i) \mid Z_p] \end{aligned}$$

$\mathbb{P}[Z_p]$  corresponds to the area of the forest cell  $p$  and can be determined based solely on the decision boundaries of the corresponding tree cells.  $\text{div}(Z_p)$  depends solely on the outputs of the tree cells that constitute  $Z_p$ . It is simply the generalised variance (see 1.6.3) of these leaf outputs. If leaf outputs are saved with the tree model after construction, these can be directly read off the model. However, these values still depend directly on the training data. Instead, we would like to infer the value based on the decision boundaries alone. In Random Forests, trees are grown *deeply*, that is, until each leaf contains only a single point. Consequently, if the number of data points  $n$  is large, leaf cells will become small. Provided that the regression function  $m(x) = \mathbb{E}[Y | X = x]$  is uniformly continuous, small leaf cells imply that the variation of  $m$  throughout a leaf is bounded. In fact Scornet, Biau, and Vert show that, as  $n$  grows, the variation in a leaf becomes arbitrarily small. This motivates that, instead of the data-dependent leaf output  $q_i(x)$ , one could instead use the center of the cell  $\tilde{q}_i(x)$ , depending only on the decision boundaries. If the variation inside a cell vanishes, then also the error of using  $\tilde{q}_i(x)$  over  $q_i(x)$  vanishes.

## 5. Growth Strategies

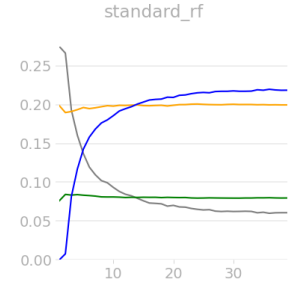
In the previous chapters, we have developed an understanding of how diversity affects the ensemble generalisation error. We have seen that the ensemble error is determined by a tradeoff between the average member error and the diversity, a measure of variance between member predictions. We will now consider how to influence this tradeoff during ensemble construction. The basic idea is to guide the construction of an ensemble member with respect to its interactions with the ensemble constructed so far.

We begin by considering the question what it means for an ensemble to be diverse. The theory around ensemble diversity allows us to explain previously published approaches and inform new ones.

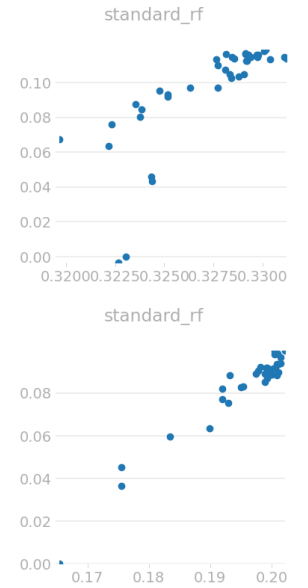
### 5.1. Diversity is a measure of model fit

There has been a line of ongoing research about capturing the notion of diversity in general ensembles [melville\_CreatingDiversityEnsembles\_2005, 25, 33] in Random Forests [adnan\_ComplementRandomForest\_2015, 35, 36] or in neural networks [li\_NeuralNetworkEnsembles\_2021, 31, 37] in particular (see also the review in section 4.1). One of the early insights was that many *ad-hoc* diversity measures are not clearly correlated to the ensemble performance [25]. We claim that the search for a diversity measure that is directly correlated with ensemble performance is misguided. As can be seen from the diversity decomposition, there is a trade-off between average member error (in turn decomposed into average member bias and variance) and diversity. As such, diversity is a measure of model fit, just like bias and variance. This was already observed empirically by Buschjäger and Morik [23] for the case of Negative Correlation Learning with neural network ensembles (as introduced in section 5.3). They showed that by varying the regularisation strength parameter  $\lambda$ , one can obtain ensembles with varying diversity but equal ensemble performance. We can also observe this in Random Forests for 0/1-classification problems. Figure 5.1 often shows a linear trend between average member error and diversity.

The ambiguity-effect decomposition holds for both the 0/1-loss and Bregman divergences. The key difference is that Bregman divergences are non-negative and thus there are no points with "bad" diversity which contribute negatively to the ambiguity-effect term. In other words, any kind of ambiguity is "beneficial" under Bregman divergences – as previously observed empirically for the squared-error loss in [19]. However, there is still the tradeoff between average member error and ambiguity. Since  $\frac{1}{M} \sum_{i=1}^M B_\phi(y, q_i) - B_\phi(\bar{q}, q_i) = B_\phi(y, \bar{q}) \geq 0$ , ambiguity is upper-bounded by the average member error. This means that any improvement due to diversity can only happen by reducing the amount of error introduced by the individual member error. If there is little average member error to begin with, encouraging diversity will not necessarily improve ensemble performance.



**Figure 5.1.:** Development of the ensemble error of a standard Random Forest ensemble as an increasing number of trees are added (evaluated on *mnist* under 0/1-loss). One can see that average member bias and average member variance stay roughly equal while diversity increases, causing the ensemble error to decrease.



**Figure 5.2.:** Random Forests with varying number of trees plotted across average member error (vertical axis) and diversity (horizontal axis).

The ambiguity-effect decomposition states that

...

For Bregman divergences, this becomes

$$B_\phi(y, \bar{q}) = \frac{1}{M} \sum_{i=1}^M B_\phi(y, q_i) - B_\phi(\bar{q}, q_i)$$

(see theorem 4.2.1)

**Observation 5.1.1**

- ▶ *A more diverse ensemble is not necessarily better. The ensemble performance depends on the trade-off between member performance and diversity.*
- ▶ *Diversity behaves fundamentally differently when measured in terms of a Bregman divergence or the 0/1-loss. For Bregman divergences, diversity in predictions on a single example is always beneficial (section 4.3). For the 0/1-loss, additional assumption on the member performance have to be required (section 4.4).*

## 5.2. Guided sequential training of member models

The statistical analysis in chapter 4 has always considered a given ensemble of fixed size. We consider the question on how to make use of the diversity theory to guide ensemble construction.

**Can we encourage diversity in Random Forests?** In previous chapters, we have seen that diversity is *the* essential force that makes Random Forests work. In the standard Random Forest scheme as introduced by Breiman, individual trees are diverse due to random choices made during tree construction. Can we instead guide tree construction such that the Random Forest ensemble is more diverse? Encouraging diversity informed by the ambiguity decomposition has already been investigated for neural networks under the Negative Correlation Learning framework. For Random Forests, there are many proposed variations that are thought to influence an intuitive notion of diversity but to the best of our knowledge none so far have considered the theory based on the ambiguity decomposition we introduced here.

**Can we produce Random Forests with better generalisation error?** Early experiments have shown that diversity-informed training strategies can indeed produce forests with better generalisation error as compared to training trees independently [29, 38, 39]. However, the approaches were based on intuition or disconnected theory. Informed by the diversity theory presented herein, can we guide tree construction such that the ensemble performance is better?

**Can we produce smaller ensembles?** In standard Random Forests, the ensemble becomes increasingly diverse as more random trees are grown. Can we make more informed choices during tree construction such that fewer trees are needed to achieve the same diversity, without affecting other components of the error?

We focus on classification problems evaluated by the 0/1-loss. Due to the inherently different nature of binary and non-binary classification problems ( $\leadsto$  4.4.4 on competence), we first focus on binary classification problems and then later consider non-binary problems later.

Arguably one of the simplest ways to influence a learning algorithm is by assigning *weights*  $w : X \rightarrow [0, 1]$  to examples. During any computations that involve a term corresponding to an example, for instance the impurity for a tree node ( $\leadsto$  3.1), the term is multiplied by the example weight. For random forests, example weights can possibly come into effect via two mechanisms. We perform experiments for both approaches.

- *Weighted bootstrapping*: Instead of drawing the bootstrap samples uniformly, draw a sample with probability according to its weight. If the bootstrap sample is large, examples with higher weight are more likely to be oversampled and thus appear multiple times in the bootstrap sample.
- *Weighted tree construction*: We have seen in 3.1 that tree construction according to some impurity measure greedily optimises a loss function. Likewise, weighting examples during computation of the impurity measure optimises a weighted loss.

Note that if a next member is constructed based on the performance of a previous members, the member models are no longer statistically independent and the ensemble is no longer homogeneous. This does not prevent us from considering their bias-variance-diversity decomposition (it holds just as well for heterogeneous ensembles).

### 5.2.1. A simple weighting function for binary classification

We begin by considering a simple weighting function that is already given in the literature without theoretical motivation. We explain this weighting function from the perspective of diversity and argue that, while its application can be beneficial, it is in contradiction to theory. This motivates further weighting functions which show equal or better performance. We further close some gaps in the original publication.

**Definition 5.2.1** (DRF weighting scheme [38]) Let  $\bar{q}$  be the ensemble constructed so far. For a pair  $(X, Y) \in D$ , define the Dynamic Random Forest weighting scheme as

$$w_{\text{DRF}}(X) =_{\text{def}} W(X) \quad \text{for } W(X) =_{\text{def}} \frac{1}{M} \sum_{i=1}^M \ell_{0/1}(Y, q_i(X))$$

This will have the effect that correctly classified examples are assigned lower weight and incorrectly classified examples are assigned higher weight.

Xu and Chen [40] re-iterate on the DRF weighting scheme and propose an alternative scheme.

$$w_{\text{XuChen}}(X) =_{\text{def}} \begin{cases} W(X)^2 & \text{if } W(X) \leq 1/2 \\ \sqrt{W(X)} & \text{if } W(X) > 1/2 \end{cases}$$

Again, the authors provide only a heuristic motivation, which is that, compared to  $w_{\text{DRF}}$ , their method has a more drastic effect of up- and downweighting.

Assuming the weights are used effectively,  $w_{\text{DRF}}$  and  $w_{\text{XuChen}}$ , will have the effect of moving example-outcome pairs towards  $1/2$  on the distribution of  $W(X, Y)$ .

We perform experiments using  $w_{\text{DRF}}$  (both weighted bootstrapping and weighted tree construction) and  $w_{\text{XuChen}}$  (weighted bootstrapping only). The full results for all benchmark datasets are given in A. An illustrative comparison for a single dataset is given in figures 5.5 and 5.4.

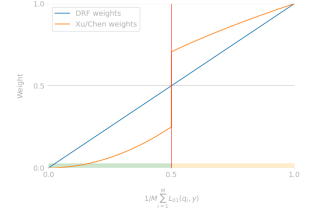


Figure 5.3.: Illustration of  $w_{\text{DRF}}$  and  $w_{\text{XuChen}}$ .

Using diversity-effect, we can give a more informed interpretation of  $w_{\text{XuChen}}$ . Inspecting  $w_{\text{DRF}}$ , which is continuous around the majority vote threshold, one can see that very similar weights are assigned to examples which are classified just barely correctly (resulting in a 0/1-loss of 0) and examples which are classified just barely incorrectly (resulting in a 0/1-loss of 1). This may mean suboptimal guidance in ensemble construction since both cases have very similar weights, but their effect on the ensemble loss is actually dramatically different. One disadvantage is that we take a heuristic step away from theory.

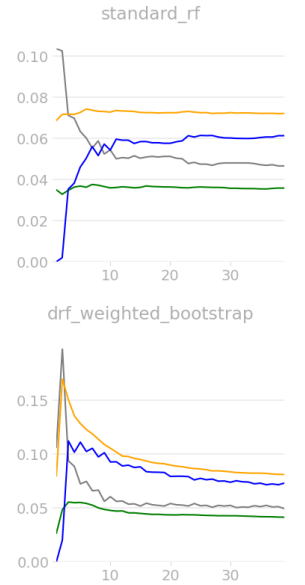


Figure 5.4.: Standard Random Forest and an ensemble constructed with the DRF weighting scheme (def. 5.2.1, weighted bootstrapping). For the DRF scheme, neither average bias nor average variance are lower, hence the average member error is not lower. However, diversity is much larger.

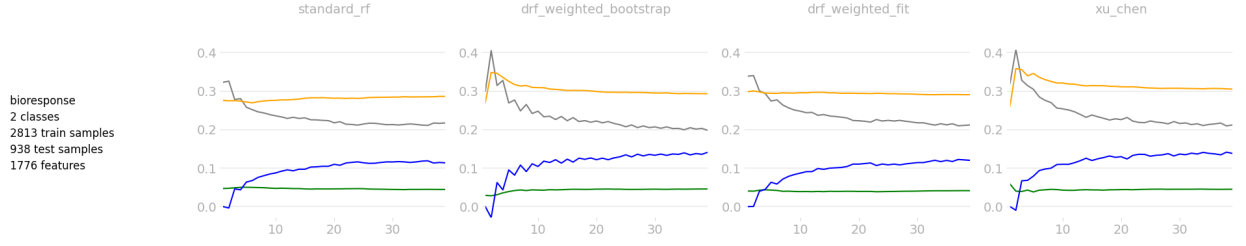


Figure 5.5.: ... The full results for all benchmark datasets can be found in figure A.1

#### Observation 5.2.1

- ▶  $w_{DRF}$  and  $w_{XuChen}$  with weighted bootstrapping indeed lead to more diverse ensembles. For weighted tree construction, diversity is very similar to standard Random Forests.
- ▶ For weighted bootstrapping, there is an initial sharp increase in diversity and average member error. Later, diversity decreases. We will come back to this effect in later experiments.

**Comparing weighted bootstrapping and weighted tree construction** In practise, any bootstrap sample is finite. The bootstrap sample is drawn with replacement, thus a bootstrap sample does not necessarily include all examples from the training dataset. Under uniform bootstrapping, each example has equal chance to be included in the bootstrap sample ( $\leadsto$  3.2.1). It is then considered during tree construction according to its weight. On the other hand, under weighted bootstrapping, examples with high weight are more likely and examples with low weight are less likely to appear in the bootstrap sample. In particular, this means that examples with low weight are more likely to not be included at all in the bootstrap sample and consequently not be considered at all during tree construction. This might be an intuitive explanation why weighted bootstrapping shows a stronger effect than weighted tree construction in our experiments. A thorough discussion has to be left for future work.

### 5.2.2. A weighting function informed by diversity for binary classification

Informed by the theory on diversity, we make the following two claims.

1. Incorrectly classified examples should not receive a particularly higher weight. If anything, examples for which the majority of members is incorrect should receive *lower* weight since any subsequent correct vote will only increase bad diversity (unless the majority vote is tipped).
2. Weights should not be related linearly to the ratio of incorrect members  $W$ . For diversity in 0/1-classification tasks, it does not matter how many members are correct, as long as the ensemble prediction is correct. Thus, any correctly classified point should receive the same low weight. In the extreme case, the weighting function could be a step function. Interpolating between a step function and a linear function could be expected to provide some sort of smoothing.

We introduce a weighting function in the form of a parameterised sigmoid function. This is mostly a pragmatic choice as it easily allows to configure the shape of the function by varying its parameters. We make no claims of the superiority of this function as compared to, for example, a piecewise linear function with varying slope.

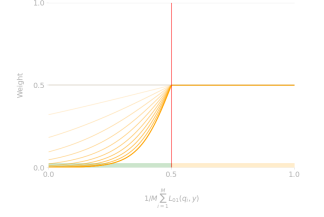
For  $a = 0$  and  $k = 1$ , this function ranges in  $[0, 1]$  with its inflection point at  $(0, 1/2)$  and its lower half in the range  $[0, 1/2]$ . The parameter  $b$  controls the "steepness". For low  $b$ , sigmoid becomes similar to  $x \mapsto 1/2$ . For high  $b$ , sigmoid becomes similar to the step function with threshold 0.

$$\text{sigmoid}(x; a, b, k) =_{\text{def}} 1/k(1 + \exp(a - bx))$$

**Definition 5.2.2** (*Clipped sigmoid weighting function*)

$$\begin{aligned} w_{\text{sigm}}(X) &=_{\text{def}} \min\{s, 1/2\} \\ \text{for } s &=_{\text{def}} \text{sigmoid}(W(X) - t; 0, b, 1) \\ t &=_{\text{def}} 1/2 \\ b &=_{\text{def}} b_{\text{max}} \end{aligned}$$

where the minimum clips the function values to a maximum of  $1/2$ ,  $t = 1/2$  is the voting threshold.



**Figure 5.6.:** Illustration of  $w_{\text{sigm}}$  for  $t = 1/2$  and varying  $b$ .

The value  $b_{\text{max}} =_{\text{def}} 15$  was chosen based on intuition to provide a smoothed version of a step function (compare Figure 5.6). The clipping using  $t$  has the effect of clipping the function exactly at the classification threshold, meaning that incorrectly classified points will be assigned uniform weights.

Additionally,  $W \approx \frac{1}{M} \sum_{i=1}^M \ell_{0/1}(Y, q_i)$  can not be expected to be a good approximation for low  $M$ . For the first couple of trees, the distribution will in fact be very discrete. We have already observed that This may cause an overshooting where for the first few trees, weights are very extreme. We have already seen that in weighted bootstrapping, there is an initial sharp increase in member error and diversity ( $\leadsto$  5.2.1)

This motivates, we will aim to downregulate the influence of the weighting function for the first couple of trees in the ensemble. After this initial period, the function should have the same shape for all  $M > M_{\text{max}}$ .

**Definition 5.2.3** (*Lerped clipped sigmoid weighting function*)  $w_{\text{lerp}}(X)$  is defined analogously to  $w_{\text{sigm}}$  ( $\leadsto$  5.2.2) but  $b$  is linearly interpolated ("lerp"-ed) between 0 and  $b_{\text{max}}$  according to  $M$ .

$$b \leftarrow \frac{\min\{M, M_{\text{max}}\}}{M_{\text{max}}} b_{\text{max}}$$

**Observation 5.2.2** ( $\leadsto$  Figure 5.7 and ??)

- Clipping (not assigning higher weights to incorrectly classified examples) already mitigates the spike in member error and diversity. Interpolating the steepness of the weighting function  $b$  is not required for this. However, for diversity is lower and the ensemble error higher.
- Surprisingly, interpolating leads to higher diversity (sometimes even higher than  $w_{\text{DRF}}$ ) and lower or similar ensemble generalisation error.

### 5.2.3. Weighting functions for non-binary classification

The weighting schemes of the previous section are all based on influencing the ratio of incorrect members for a given example. Due to the diversity decomposition, for examples that are still classified correctly by the ensemble, the improvement due to diversity is greater if the ratio of incorrect members is closer to the classification threshold. For binary classification problems, one can always assume a voting threshold



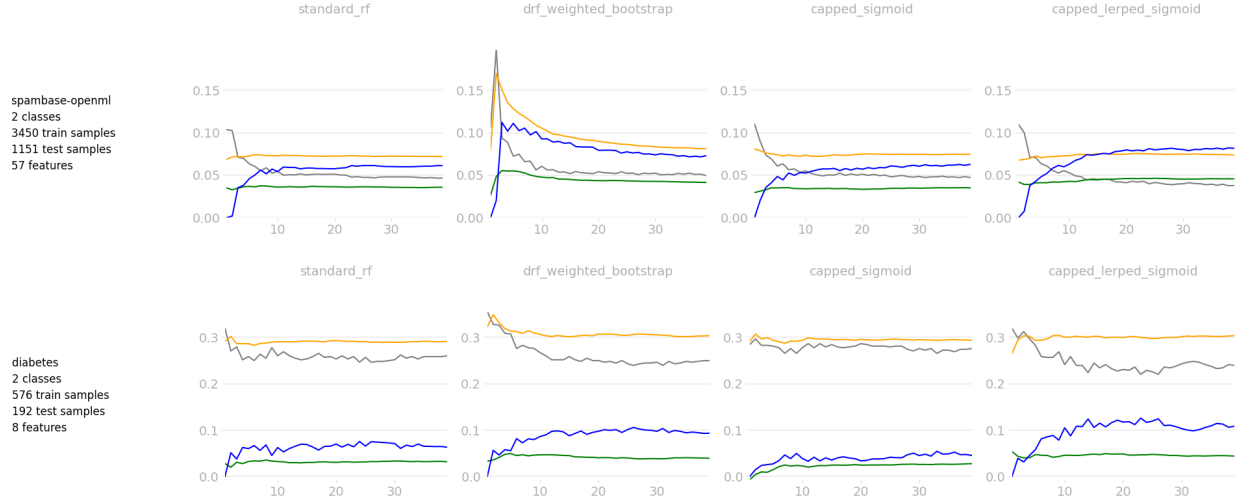


Figure 5.7.: The full results for all benchmark datasets can be found in figure ??

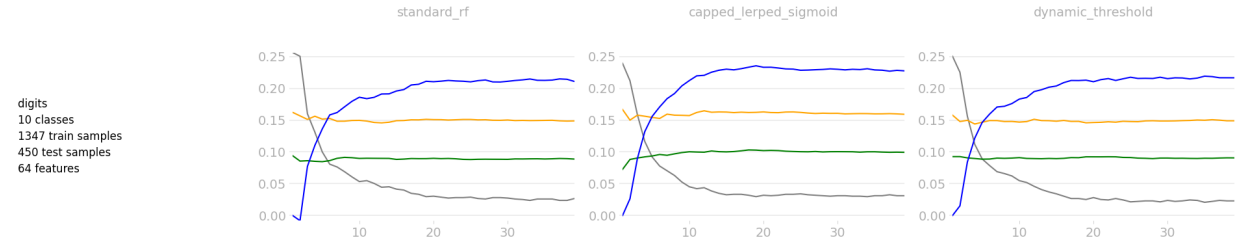


Figure 5.8.: ...

of  $1/2$ .

$$k = 2 \rightarrow \begin{cases} W_{\Theta} < 1/2 \leftrightarrow \bar{q}(X) = Y \\ \overline{W_{\Theta}} \leq 1/2 \leftrightarrow \bar{q}(X) \neq Y \end{cases} \quad (5.1)$$

In section 4.4.4, we have observed that for non-binary classification problems, the voting threshold is exactly the ratio of votes for the next-best class. This is a quantity that depends on the ensemble and the given example and the equivalences above no longer hold. Because of this, we hypothesize that it is inadequate to use a weighting function centered around a threshold of  $1/2$  and it should rather be centered around the actual, dynamic threshold  $\kappa$ .

**Definition 5.2.4** (Sigmoid weighting function with dynamic threshold)  $w_{\text{dyn}}$  is defined analogously to  $w_{\text{lerp}}$ , but  $t$  is given as

$$t =_{\text{def}} \kappa(X, Y) = 1 - \max_{Z \neq Y} \mathbb{E}_{\Theta} [1[q_{\Theta} = Z]]$$

We evaluate this approach on multiple non-binary classification problems.

**Observation 5.2.3** ... dont seem to gain anything

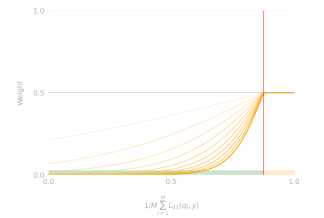


Figure 5.9.:  $t = 1 - \frac{1}{8}$



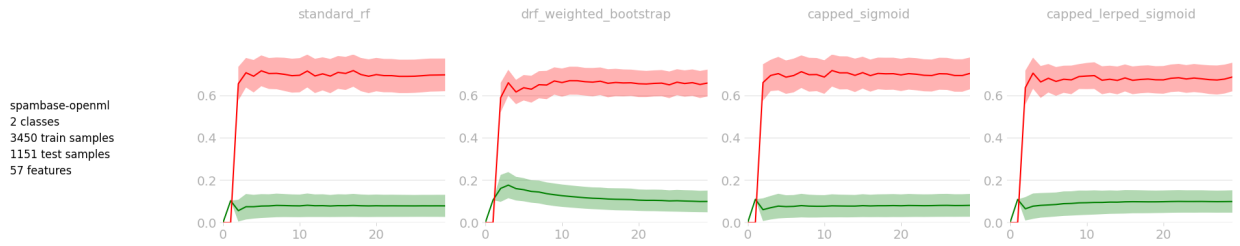


Figure 5.11.: ...

### 5.2.4. Ensemble margins

Recall that the ensemble margin for an example-outcome pair  $(X, Y)$  is the difference between the ratio of members voting for the correct class and the ratio of members voting for the next-best class. In binary classification problems, this corresponds to the average member error. The main motivation behind the voting schemes introduced in this section is that they supposedly encourage diversity. We have argued that diversity should be encouraged on examples while the ensemble prediction is still correct. In other words, on correctly classified examples, the average member error should *increase*. This corresponds to the notion of "good" diversity in binary classification. Weighting schemes like  $w_{\text{DRF}}$  and  $w_{\text{XuChen}}$  further encourage diversity on incorrectly classified examples. The expected member error should *decrease*. We can measure and visualise these two components separately as they develop as the size of the ensemble grows.

Likewise, for a given ensemble, we look at the distribution of ensemble margin per example. We plot a histogram of examples with respect to the number of trees incorrectly classifying that example. In binary classification, more than  $1/2M$  trees being incorrect leads to an incorrect ensemble prediction.

**Observation 5.2.4** ▶ (margin plots) For DRF do have increased green, decreased red.  
For lerped sigmoid, slightly increased green, very similar red (nice).  
▶ (margin hists) seemingly shifted a little

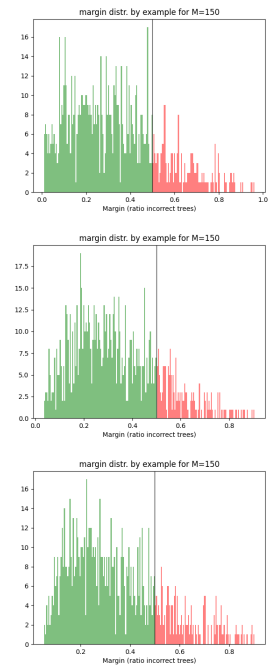


Figure 5.10.: ...

### 5.2.5. Ensemble size and generalisation error

We evaluate the overall ensemble generalisation error of ensembles produced by different weighting strategies. We emphasize that we make no claims about the applicability of a specific learner to a specific dataset. We specifically picked the benchmark datasets to provide diverse classification problems. The datasets have different properties: some are higher-dimensional and some have a high best achievable error rate, implying that the data may be noisy. Likewise, we make no claims about the adequacy of hyperparameter choices for a given dataset. We merely compare different strategies on the same benchmark datasets and for the same hyperparameter choices.

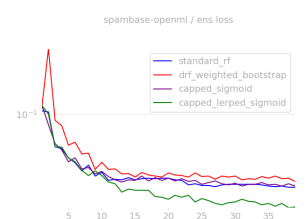


Figure 5.12.: ...

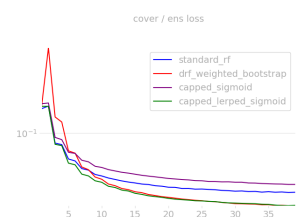


Figure 5.13.: ...

	RF	$w_{\text{DRF}}$	$w_{\text{sigm}}$	$w_{\text{lerp}}$
qsar-biodeg	<b>0.101</b>	0.144	0.130	0.133
diabetes	0.247	0.240	0.266	<b>0.220</b>
bioresponse	0.211	<b>0.198</b>	0.217	0.209
spambase-openml	0.047	0.050	0.047	<b>0.038</b>
digits	<b>0.024</b>	0.033	0.029	0.030
mnist-subset	<b>0.060</b>	0.066	0.064	0.062
cover	0.049	<b>0.042</b>	0.054	0.042

**Table 5.1.:** minimum ensemble test error achieved over all  $M$

### Observation 5.2.5

- There is no evident relationship between diversity and ensemble generalisation error. This is not surprising, as we have already argued that ensemble performance is determined by a trade-off of member performance and diversity.
- It is indeed possible to obtain better ensembles using diversity-encouraging weighting strategies, as compared to the standard Random Forest procedure. However, none of the evaluated strategies yielded consistently better ensembles across all benchmark datasets.
- It is possible to obtain smaller ensembles with similar generalisation error. However, here too no strategy yields a consistent improvement.

It is interesting that  $w_{\text{sigm}}$  consistently performs worse than  $w_{\text{lerp}}$ . This suggests that the interpolation of the steepness of the weighting function indeed has a beneficial effect.

We further note that even though we have argued that  $w_{\text{DRF}}$  is counterproductive in theory in that it also increases bad diversity, we observe that nevertheless, we often obtain competitive models with this strategy. This strategy has a very characteristic growth behaviour, as described in Section 5.2.

### 5.2.6. "Boosting" rationale for example weighting in classifier ensembles

re. spike: not super surprising, if there are only 1, 2, 3 trees, weights as ratio of incorrect trees are super extreme – motivation to dampen – okay yeah actually is surprising since simply capping is also enough!!

would be good to put here to explain "spike". Can such a spike be observed in boosting methods?

initial increase in bias also observed for classical boosting models? (wood23 p26)



**Figure 5.14.:** ...

### 5.3. Guided parallel training of member models

Consider the bias-variance-covariance decomposition for the squared error loss given in theorem 4.1.1. The covariance term contributes positively to the ensemble error if the outputs of the members are positively correlated. This suggests the idea that it might be beneficial to train ensemble members in coordination such that their outputs are uncorrelated. [31] provide an implementation of this idea for neural network ensembles called *Negative Correlation Learning* (NCL). Neural network training involves a *forward* and a *backward* pass. In the forward pass, the neural network in its current state is queried with training data. Its prediction is evaluated according to a loss function. Then, the model parameters are updated according to the gradient of the loss function with respect to the parameters. A common practise is to add a *regularisation term* to this loss function in order to bias the model towards e.g. sparse predictions [todo]. In Negative Correlation Learning, forward and backward pass are performed synchronously for all members. This enables using loss functions that depend not only on an individual member but the entire ensemble.

The  $i$ -th member network is trained using a loss function  $\ell_i$  that contains a regularisation term  $p_i$ , which is intended to influence the training of the  $i$ -th member such that its predictions are uncorrelated with the other members. The hyperparameter  $\lambda \in \mathbb{R}$  determines how much weight is put on either of the two components. The training objective for the  $i$ -th network is be written as

$$e_i =_{\text{def}} (y - q_i)^2 + \lambda p_i$$

where the first term is the individual error of the  $i$ -th member and  $p_i$  is the regularisation term. [31] defined  $p_i$  as

$$p_i =_{\text{def}} \left( (\bar{q} - q_i) \sum_{i \neq j}^M (\bar{q} - q_j) \right) = -(\bar{q} - q_i)^2$$

This is reminiscent in shape of the contribution of the  $i$ -th member to the covariance term in the bias-variance-covariance decomposition — however, the expectation over  $D$  is replaced with the ensemble combiner  $\bar{q}$ ! Seeing that here the ensemble combiner is the arithmetic mean of member outputs, this means that instead of a variance under variations in  $D$ , this considers the variance between member model outputs.

Note that the penalty term corresponds to the contribution of the  $i$ -th member to the ambiguity (??). Indeed, as [28] noted, the NCL approach can be motivated more soundly via the ambiguity decomposition.

**Definition 5.3.1** (NCL neural network objective for squared error [28]) The loss function of the  $i$ -th neural network ensemble member is defined as

$$e_i(y, x) =_{\text{def}} (y - q_i)^2 - \lambda (\bar{q} - q_i)^2$$

The penalty coefficient  $\lambda$  smoothly interpolates between training  $q_i$  to either maximise its individual performance or the ensemble performance. For sake of simplicity, let us assume a factor of  $1/2$  on the objective. This yields an equivalent optimisation problem, but allows us to express the gradients in a simple form.

$$\frac{\partial e_i}{\partial q_i} = \frac{1}{M} ((q_i - y) - \lambda(q_i - \bar{q}))$$

Note that the name is misleading here. The goal is not that members are negatively correlated, but *uncorrelated*.

$\bar{q}$  is the arithmetic mean:

$$\bar{q} = \frac{1}{M} \sum_{i=1}^M q_i$$

The sum of deviations around the mean is zero:

$$\sum_{i=1}^M (\bar{q} - q_i) = 0$$

Omitting one member from the sum implies

$$\sum_{i \neq j} (\bar{q} - q_i) = -(\bar{q} - q_j)$$

and

$$\begin{aligned}\lambda = 0 &\rightarrow \frac{\partial e_i}{\partial q_i} = \frac{1}{M}(q_i - y) = \frac{1}{M} \frac{\partial e_i}{\partial q_i} \\ \lambda = 1 &\rightarrow \frac{\partial e_i}{\partial q_i} = \frac{1}{M}(\bar{q} - y) = \frac{\partial e_{\text{ens}}}{\partial q_i}\end{aligned}$$

Several authors have attempted to generalise Negative Correlation Learning or transfer it to other loss functions. For instance, [webb21] directly prove an ambiguity decomposition for the KL-divergence  $K$  and propose the objective

$$e_i(x, y) =_{\text{def}} \frac{1}{M} \sum_{i=1}^M K(y \parallel q_i) - \lambda \frac{1}{M} \sum_{i=1}^M K(\bar{q} \parallel q_i)$$

where  $\bar{q}$  is the geometric mean combiner (see ??). The proof is not trivial and does not give insight into whether such a decomposition and learning strategy might also exist for other loss functions.

Buschjäger, Pfahler, and Morik [29] approached the problem by attempting to derive a generalised decomposition of the ensemble error that incorporates diversity. The basic idea is to consider a Taylor approximation around the ensemble combiner, which is assumed to be the arithmetic mean combiner.  $\bar{q} =_{\text{def}} \mathbb{E}_{\Theta} [q_{\Theta}] \approx \frac{1}{M} \sum_{i=1}^M q_i$ .

$$\begin{aligned}\mathbb{E} [\ell(y, q)] &= \mathbb{E} [\ell(\bar{q})] + \mathbb{E} [(q - \bar{q})^T \nabla_{q^*}(\ell(\bar{q}))] \\ &\quad + \mathbb{E}_{\Theta} \left[ \frac{1}{2}(q - \bar{q})^T \nabla_{\bar{q}}^2(\ell(q^*)) (q - \bar{q}) \right] \\ &\quad + \mathbb{E} [R_3]\end{aligned}$$

$R_3$  is the remainder of the Taylor approximation, which vanishes if the third derivative of  $\ell$  is zero. By definition of  $\bar{q}$ ,  $\mathbb{E}_{\Theta} [\nabla_{\bar{q}}(\ell(\bar{q}))] = \nabla_{\bar{q}}(\ell(\bar{q}))$  and  $\mathbb{E}_{\Theta} [q - \bar{q}] = 0$  and thus the second term vanishes. Note that here they *assume* the expected model  $\bar{q}$  to also be the ensemble combiner, i.e.  $\bar{q} \approx \frac{1}{M} \sum_{i=1}^M q_i$ . Based on this, they propose the following generalised training objective.

**Definition 5.3.2** (Generalised NCL objective as proposed by [29])

$$e_i =_{\text{def}} \frac{1}{M} \sum_{i=1}^M \ell(y, q_i) - \frac{1}{2} \frac{1}{M} \sum_{i=1}^M d_i^T D d_i$$

where  $D =_{\text{def}} \nabla_{\bar{q}}^2(\ell(y, \bar{q}))$  and  $d_i =_{\text{def}} (q_i - \bar{q})$

This is based on the assumption that the remainder to the Taylor approximation  $R_3$  is negligibly small. Further, it does not apply to all loss functions. Let us consider some examples of commonly used loss functions.

- For the squared error, the third derivative vanishes and thus the decomposition is exact.
- For the negative log-likelihood, the third derivate is not bounded and thus this decomposition can not be used.
- For the cross-entropy loss, the third derivative is bounded and while the decomposition is not exact, it can be used for approximation.
- For any other loss function, this would have to be checked.

It is evident however, that we already have a fully general ambiguity decomposition at hand, namely the ambiguity-effect decomposition (?). This decomposition is exact and holds for *any* loss function (including the 0/1-loss). For Bregman divergences, this

The expectations can be approximated as follows:

$$\bar{q} = \mathbb{E}_{\Theta} [q_{\Theta}] \approx \frac{1}{M} \sum_{i=1}^M q_i$$

$$\begin{aligned}\mathbb{E}_{\Theta} \left[ \frac{1}{2}(q - \bar{q})^T \nabla_{\bar{q}}^2(\ell(\bar{q})) (q - \bar{q}) \right] &\approx \frac{1}{2} \frac{1}{M} \sum_{i=1}^M \\ &\text{for } D =_{\text{def}} \nabla_{\bar{q}}^2(\ell(\bar{q}), y) \text{ and } d_i =_{\text{def}}\end{aligned}$$

$$\mathbb{E}_{\Theta} [R_3(x)] \approx \tilde{R}$$

Squared error loss:

$$\ell(y, x) =_{\text{def}} (y - x)^2$$

Negative log-likelihood:

$$\ell(z, y) =_{\text{def}} - \sum_i^k y_i \log(z_i)$$

Cross-entropy loss:

$$\ell(z, y) =_{\text{def}} - \sum_i^k y_i \log \frac{e^{z_i}}{\sum_j e^{z_j}}$$

reduces to the ambiguity decomposition ???. We claim that the adequate generalisation of the NCL objective follows this structure.

**Proposition 5.3.1** ★ *We propose the following generalisation of the NCL neural network objective. For general loss functions  $\ell$ :*

$$e_i =_{\text{def}} \ell(y, q_i) - \lambda (\ell(y, q_i) - L(y, \bar{q}))$$

*And for Bregman divergences:*

$$e_i =_{\text{def}} B_\phi(y, q_i) - \lambda B_\phi(\bar{q}, q_i)$$

NCL for the squared error loss as introduced by [31] and [28], as well as for the KL-divergence as given by [11] are special cases of this.

This provides a general framework for Negative Correlation Learning with arbitrary loss functions. Because it is founded on the exact and intuitive bias-variance-diversity decomposition, this also yields a natural and intuitive means for understanding and analysing Negative Correlation Learning and its effects.

Note that the Dynamic Random Forest approach ??? implicitly optimises a very similar objective. The construction procedure of individual decision trees greedily optimises its own performance (???), which corresponds to the first term in the NCL neural network objective. The introduction of example weights based on the ensemble diversity influences the decision tree construction to improve the ambiguity, which corresponds to the regularisation term. Note also that Negative Correlation learning already is "dynamic" in the sense that the ambiguity term is evaluated per point.

Although the term *Negative Correlation Learning* in the literature refers specifically to neural networks, we can now see that it is rather a style of training ensemble members with respect to the ambiguity decomposition. To the best of our knowledge, only one other algorithm has been published that realises this: **[negative-correlation-forests]** proposes to refine the leaf predictions in a given Random Forest using using gradient descent according to the objective defined in definition 5.3.2.

While an experimental evaluation has to be left for future work, we note that the case of KL-divergence was already investigated empirically in detail in [11].

## 6. Conclusion

...

# APPENDIX

# A. Full experiment results

## A.1. DRF weighting function

### A.1.1. Comparison to [38]

Bernard, Adam, and Heutte evaluated only the following combined approach: They would perform both weighted bootstrapping and weighted tree construction. Further, weights would be determined only on out-of-bag-trees (see section ??). Additionally, unrelated to the question at hand, they also employed a different way to determine candidate split features. Unlike in standard random forests, where a fixed number of candidate split features is sampled from all available features, the number of sampled candidate features was left fully random here. It was left unanswered which of these components actually affect the ensemble to what extent. Further, they did not provide any explanation or empirical analysis in terms of diversity. Looking at our results, the following points seem likely:

- ▶ An improvement in generalisation error is still obtained with standard candidate split feature sampling.
- ▶ The improvement can be explained using the notions of diversity.
- ▶ Weighted tree construction alone appears to have only very little effect as compared to a standard Random Forest.
- ▶ Weighted bootstrapping seems to provide the main effect.
- ▶ Determination of weights using out-of-bag-trees only does not improve performance for weighted tree construction.

Weighted tree construction with out-of-bag weights does not appear to bring any advantage.

It may seem reasonable to expect that this [DRF] improves the average member error since the member to be trained puts more emphasis on "hard" examples and disregards "easy" examples, an idea very similar to boosting. This is also the motivation given in [38, 40]. However, across all experiments, we can observe that this is *not* the case, as can be seen e.g. in figures 5.4 and 5.5. This tradeoff is exactly reflected in the ambiguity decomposition.



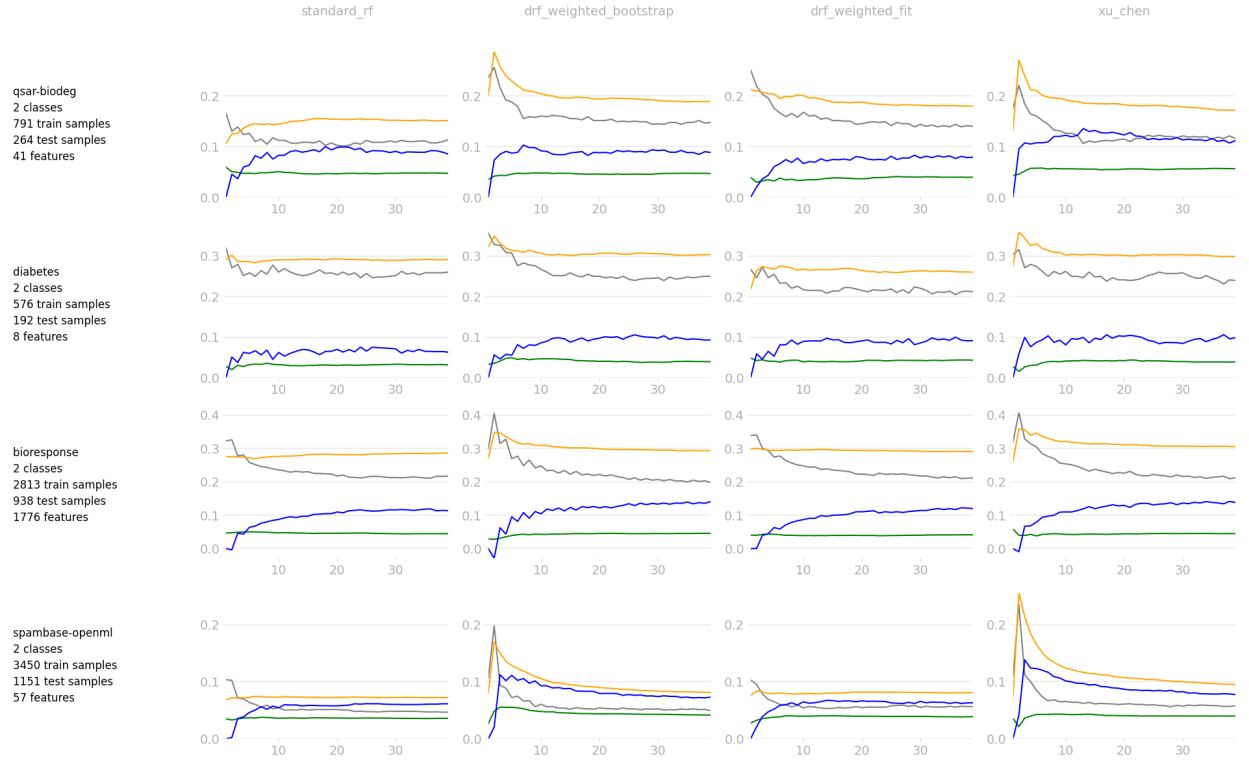


Figure A.1.: ...

## A.2. Sigmoid weighting functions

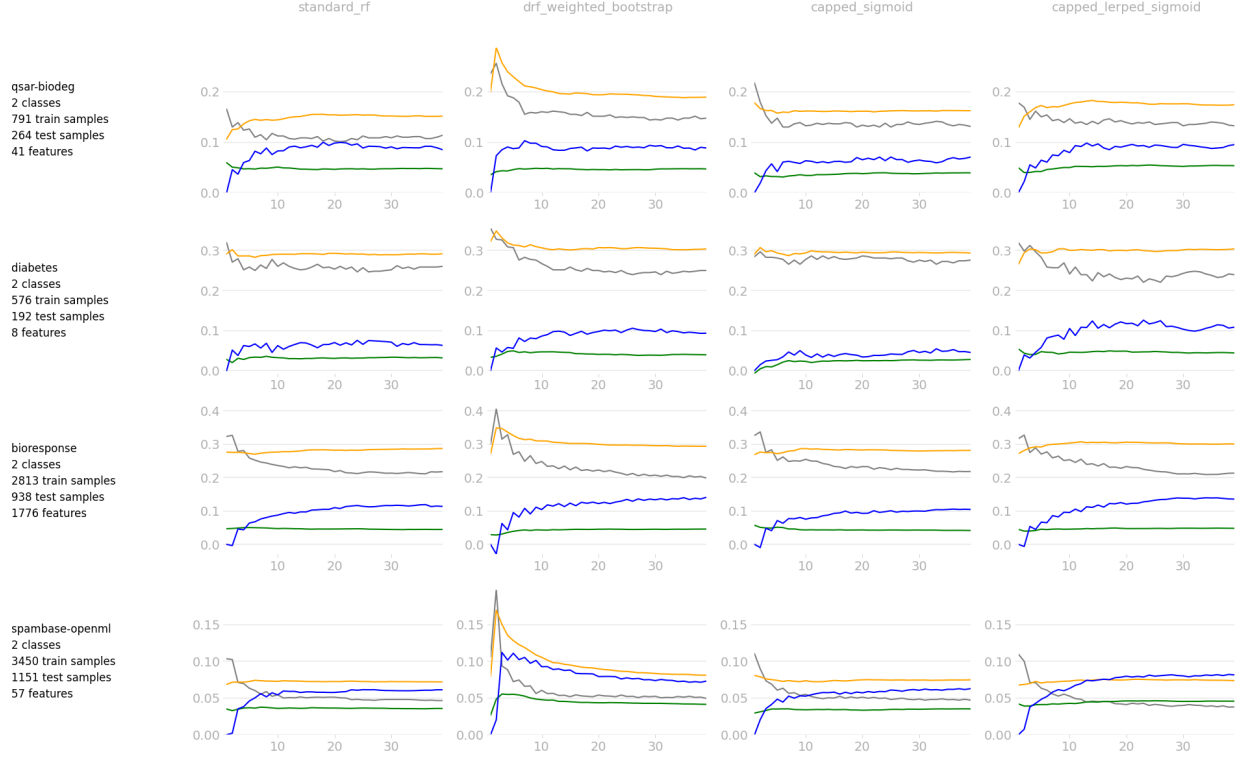


Figure A.2.: backref ??

## A.3. Proofs

### A.3.1. Proof of lemma 4.3.2

**Lemma A.3.1** (★, Generalised from [7]) Let  $q$  be a function of random variable  $Z$  and independent of  $Y$ . For  $q^\star = \mathcal{E}_Z[q]$ , i.e. the left Bregman centroid w.r.t.  $Z$ , it holds that

$$\mathbb{E}_Z [B_\phi(q^\star, q)] = \mathbb{E}_{Z,Y} [B_\phi(Y, q) - B_\phi(Y, q^\star)]$$

*Proof.*

$$\begin{aligned} \mathbb{E}_{Z,Y} [B_\phi(Y, q) - B_\phi(Y, q^\star)] &= \mathbb{E}_{Z,Y} [(\phi(Y) - \phi(q) - \langle \nabla \phi(q), Y - q \rangle) - (\phi(Y) - \phi(q^\star) - \langle \nabla \phi(q^\star), Y - q^\star \rangle)] \\ &= \mathbb{E}_{Z,Y} [\phi(q^\star) - \phi(q) - \langle \nabla \phi(q), Y - q \rangle + \langle \nabla \phi(q^\star), Y - q^\star \rangle] \quad q^\star, q \text{ indep. of } Y \\ &= \mathbb{E}_Z [\phi(q^\star) - \phi(q)] \\ &\quad - \mathbb{E}_{Z,Y} [\langle \nabla \phi(q), Y \rangle] + \mathbb{E}_Y [\langle \nabla \phi(q^\star), Y \rangle] \\ &\quad + \mathbb{E}_Z [\langle \nabla \phi(q), q \rangle - \langle \nabla \phi(q^\star), q^\star \rangle] \end{aligned}$$

By definition of  $q^\star$ ,  $\mathbb{E}_Z [\nabla \phi(q^\star)] = \mathbb{E}_Z [\nabla \phi(\nabla \phi)^{-1} \mathbb{E}_Z [\nabla \phi(q)]] = \mathbb{E}_Z [\nabla \phi(q)]$ . This allows us to apply the linearity of  $\langle \cdot, \cdot \rangle$  twice to obtain

$$\begin{aligned} \dots &= \mathbb{E}_Z [\phi(q^\star) - \phi(q)] - 0 + \mathbb{E}_Z [\langle \nabla \phi(q), q - q^\star \rangle] \\ &= \mathbb{E}_Z [\phi(q^\star) - \phi(q) - \langle \nabla \phi(q), q^\star - q \rangle] \\ &= \mathbb{E}_Z [B_\phi(q^\star, q)] \end{aligned}$$

□

### A.3.2. Proof for lemma 4.4.9

**Lemma A.3.2** ★ (Generalised from [10]) In  $k$ -competent ensembles it holds that

$$\mathbb{P}[W \geq \kappa] \leq 2\mathbb{E}[W^2]$$

*Proof.* Note that

$$\mathbb{P}[W \geq \kappa] \leq 2\mathbb{E}[W^2] \leftrightarrow \mathbb{P}[W \geq \kappa] - 2\mathbb{E}[W^2] \geq 0$$

$$2\mathbb{E}[W^2] - \mathbb{P}[W \geq \kappa] = \mathbb{E}[(2W^2 - 1) \mathbb{1}[W \geq \kappa]]$$

We will aim to show that this above expression is nonnegative. The final inequality is due to applying lemma 4.4.6 to the second term.

$$\begin{aligned} & \mathbb{E}[2W^2] - \mathbb{P}[W \geq \kappa] \\ &= \mathbb{E}[2W^2] - \mathbb{E}[\mathbb{1}[W \geq \kappa]] \\ &= \mathbb{E}[(2W^2 - 1) \mathbb{1}[W \geq \kappa]] + \mathbb{E}[2W^2 \mathbb{1}[W < \kappa]] \\ &\geq \mathbb{E}[(2W^2 - 1) \mathbb{1}[W \geq \kappa]] + \mathbb{E}[2\bar{W}^2 \mathbb{1}[\bar{W} < \kappa]] \end{aligned}$$

$$\begin{aligned} W \geq \kappa & \leftrightarrow 1 - W < 1 - \kappa \\ & \leftrightarrow \bar{W} \leq 1 - \kappa \end{aligned}$$

Note that for  $k \geq 2$ ,  $\kappa > 1 - \kappa$  and thus  $\mathbb{E}[\mathbb{1}[\bar{W} \leq \kappa]] \geq \mathbb{E}[\mathbb{1}[\bar{W} \leq 1 - \kappa]]$ , allowing us to continue

$$\begin{aligned} & \dots \geq \mathbb{E}[(2W^2 - 1) \mathbb{1}[W \geq \kappa]] + \mathbb{E}[2\bar{W}^2 \mathbb{1}[\bar{W} < 1 - \kappa]] \\ &= \mathbb{E}[1 - 4\bar{W} + 2\bar{W}^2 \mathbb{1}[\bar{W} < 1 - \kappa]] \\ &\geq 0 \end{aligned}$$

□

## A.4. Implementation

Ensemble error decompositions were computed using the *decompose* library\*. Learners were implemented using *scikit-learn*<sup>†</sup> and *numpy*<sup>‡</sup>. Experiments were managed using DVC<sup>§</sup>. The full source code and configuration can be obtained from the [GitHub repository](#).

**Compared datasets** We give a brief motivation for the classification datasets we have selected for evaluation. *cover* is a dataset with a relatively high number of examples and low feature dimensionality. *mnist-subset* is a dataset with a moderate number of examples and high dimensionality. *diabetes* is a dataset with relatively high error rates. *bioresponse* is a small dataset with a very high number of features ( $d \approx 1/2n$ ). *qsar-biodeg* is a small dataset used for quick testing. Further, [bernard, xuChen] evaluated on *mnist* (although not just a subset of it), *spambase*, *digits* and *diabetes*.

\* <https://github.com/EchoStatements/Decompose/> and [3]

† <https://scikit-learn.org/>

‡ <https://numpy.org/>

§ <https://dvc.org>

**Approximating statistical quantities** For a dataset with  $n$  examples,  $n_{\text{train}} =_{\text{def}} \frac{3}{4}n$  examples were assigned to be part of the *training split*, the other  $n_{\text{test}}$  for the *testing split*. Examples in the testing split are used for evaluation only and were never used in training a model. If  $X$  is a random variable taking values in the space of examples  $\mathcal{X}$ , expectations over  $X$  are approximated as the arithmetic mean over given examples in the testing split, i.e. for a function  $g$ :

$$\mathbb{E}_X [g(X)] \approx \sum_{i=1}^{n_{\text{test}}} g(x_i)$$

If  $D$  is a random variable corresponding to the input to a learner, for instance the training dataset or randomness in the learning algorithm, an expectation over  $D$  is approximated by an arithmetic mean over results of a fixed number of trials. In our case, we performed 3 trials.

## B. Outlook

**The role of diversity in learning problems** We have seen that diversity is a central aspect of ensembles and determines the ensemble error in great part. However, it has become clear that a more diverse ensemble is not necessarily better on all tasks. In Section 4.6, we have considered this question under the light of the capacity of the base models. However, the characteristics of the underlying data are another variable that have not been considered at all. Two approaches seem interesting:

1. **Noise:** We have already seen that combining decision trees to a Random Forest can be understood to mitigate the tight fit of a tree to the training dataset. For instance, it has been observed that limiting the maximum depth has a regularisation effect and helps dealing with noisy data [41]. What is the effect of diversity in relationship to the signal-to-noise ratio?
2. **Adversarial Robustness:** It has already been observed that diverse neural network ensembles are more robust against adversarial attacks [42, 43]. However, these approaches do not consider a diversity decomposition and their measures of diversity are *ad-hoc* and disconnected from the ensemble error.

**Generalised impurity measures** Variance-effect is a natural generalisation of variance. We have seen that commonly used impurity measures are in fact variances implied by different Bregman divergences, i.e. special cases of variance-effect. This motivates (a) using other corresponding Bregman divergences if another loss is used, and (b) considering the variance-effect as an impurity measure if no specialisation is available (as is the case for the 0/1-loss).

**A diversity-aware splitting criterion** Imagine growing  $M$  trees simultaneously as follows: In each iteration, one split is determined for each tree. Which node is being split is left to the choice of the splitting criterion. One could then attempt to derive a splitting criterion that optimises not only for a split that is pure (improves the prediction performance of the tree), but also one that implies predictions different to those of other trees (improves diversity). Each split of a tree node yields a new forest partition  $Z_1, \dots, Z_P$ . We have already seen that splitting criteria in standard Random Forests optimise a loss function. Hence, the objective function for a general splitting criterion for the  $i$ -th member could be written as  $\ell(y, q_i)$ , which is simply the member error. However, informed by the above discussion, one could define the splitting criterion in coordination to other ensemble members, i.e.

$$\ell(y, q_i) - \lambda \ell(\bar{q}, q_i)$$

Note that this is directly analog to the NCL objective. In the NCL objective, however, this criterion is evaluated per point. In our case, it is evaluated per split, and (under some assumptions), only depends on previous splits in the forest and no extra sampling to determine the values.

**Connection to boosting methods** The guided sequential training of member models as introduced in Section 5.2 can be viewed as gradient descent in function space. That is, by training the next member, we are searching for a function  $f_{i+1}$  such that the ensemble output  $\bar{q} = \sum \alpha_i q_i + \alpha_{i+1} q_{i+1}$  is improved. This is the case exactly when  $q_{i+1}$

Here,  $\alpha_i$  are weights. These can be chosen such that  $\bar{q}$  is a mean; then this corresponds to the combination methods of Random Forests. Otherwise, particularly with decreasing weights  $\alpha_i$  this is exactly the formulation of boosting ([anyboost, ...]).

corresponds to a step in the direction of the (negative) gradient of the loss ensemble loss, i.e.

$$\max_q \langle -\nabla \bar{q}, q \rangle$$

In boosting methods for classification,  $q$  is obtained by setting adequate example weights. Likewise, the weights in the growth schemes presented herein correspond to a gradient step with respect to a loss function that resembles the NCL objective.

**Functional derivatives** The basic subject of analysis has been the function  $q : X \rightarrow Y$  that corresponds to a member model. However, we have seen with the effect decomposition that it only ever appears in it's effect of the loss, i.e. as an argument to the loss function  $\ell$ . In supervised learning, we are always concerned with finding a function  $q$  that minimises a loss or cost function  $\ell$ . The Framing boosting (or any ensemble construction procedure) as gradient descent in function space means that we are considering the gradient of  $\ell(q(X))$  with respect to argument  $X$ . This means that a gradient descent step amounts to modifying the training data (weights in classification or pseudo-targets in boosting). However, what we really are looking for is a better *model*. One can understand  $\ell$  as a functional, i.e. a function that maps a given function (the model) to a scalar value (the model's error). One could then use *functional derivatives* [44] to analyse questions such as "What function  $q$  will minimise  $\ell(q)$ ?". Based on this idea, one can define *functional Bregman Divergences* [45] which considers Bregman divergences between *functionals*. It would be interesting to see whether the learning objectives can be expressed in these terms and whether this can provide new insight.

**Diverse Bregman ensembles** In this thesis, we have only considered growth strategies for classification ensembles under the 0/1-loss. The theory laid out in Section 4.3 on Bregman divergences and ?? on Negative Correlation Learning suggests that similar methods can be developed for regression tasks (this includes tasks where class probabilities are to be estimated). We have already seen hints that diversity behaves fundamentally different in this regime since the ensemble improvement can never be non-negative. We hypothesize that obtaining higher diversity and possibly also achieving lower ensemble error is easier in the regression regime due to the continuous nature of the outcome space.

**Generalised  $k$ -means** We have seen that the purity gain objective corresponds to the  $k$ -means objective for  $k = 2$ . This raises the question whether one may consider  $k$ -way splits instead of binary splits when constructing a tree.

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