A Bayesian Bradley-Terry model to compare multiple ML algorithms on multiple data sets

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Abstract

This paper presents a Bayesian model, called the Bayesian Bradley Terry (BBT) model, for comparing multiple algorithms on multiple data sets based on any metric. The model is an extension of the Bradley Terry model, which tracks the number of wins each algorithm has on different data sets. Unlike frequentist methods such as Demsar tests on mean rank or multiple pairwise Wilcoxon tests, the Bayesian approach provides a more nuanced understanding of the algorithms' performance and allows for the definition of the "region of practical equivalence" (ROPE) for two algorithms. Additionally, the paper introduces the concept of "local ROPE," which assesses the significance of the difference in mean measure between two algorithms using effect sizes, and can be applied in frequentist approaches as well. Both an R package and a Python program implementing the BBT are available for use.

Keywords: Bayesian, Bradley-Terry model, Comparison of classifiers, Comparison of regressors, Multiple data sets, Multiple algorithms

1. Introduction

In the field of Machine Learning, new models or algorithms are often compared to existing ones using a variety of data sets. These comparisons usually result in a table similar to Table 1, where each line indicates a data set, and each column the algorithms being compared.

| | Alg A | Alg B | Alg L |
|------|-------|-------|-----------|
| DB 1 | a_1 | b_1 | l_1 |
| DB 2 | a_2 | b_2 | l_2 |
| DB 3 | a_3 | _ | l_3 |
| | | | |
| DB K | a_k | b_k | l_k |

Table 1: The table of measures of comparing algorithms A, B, ..., L on data sets DB1, DB 2, ..., DB K.

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In the example above a_2 is the measure of algorithm A on the data set DB 2. Usually, this measure is the average of a set of measures of algorithm A on different cross validations of the data set DB 2.

The different results will be compared using a **comparison procedure**. The goals of a comparison procedure are in order of importance:

- 1. The procedure should tell which algorithm is better, which is second place, which one is third place, and so on when measured on a particular set of data sets. We will call this the **aggregated ranking** of the algorithms for that set of data sets. In particular, for the example above, the aggregated ranking would result in a total order such as $C \succ B \succ E \dots A$ stating that C is better than B which is better than E, and so on, and that A is the worse algorithm in the set. We will indicate that algorithm C is better than algorithm B as $C \succ B$. Of course, the meaning of better depends on the metric being used; higher numbers are better for metrics such as accuracy, F1, AUC, and lower numbers are better for metrics such as error, execution time, energy consumption and so on.
- 2. The procedure should compute how confident or how hopeful one should be that the ordering will remain true when one tests the same algorithms on a new data set. That is, the procedure should indicate the confidence in each of the comparisons $C \succ B$, $C \succ E$, $C \succ A$, $B \succ E$, and so on.
- 3. The procedure should state how much one algorithm is better than another or at least when one algorithm is not much better than another one, that is, when both algorithms are equivalent. Ideally one would like a measure dist(C,B) which indicates how much better C is from B. Or at least one would like such a distance measure that would indicate when C is not really much better than B and that, for practical purposes, they are equivalent.
- 4. The procedure should not require that all algorithms must be evaluated in all data sets. In the example above, algorithm B did not run for data set B, as indicated by the "-" entry in the table.

There are numerous methods for aggregating rankings in machine learning. The obvious method of computing the mean of the measures of each algorithm and ordering them based on that mean is not considered appropriate for machine learning comparisons. There are two reasons for that. The first is that there are some metrics used in Machine Learning, and especially in regression tasks which are **non-comparable**. Two of such metrics are RMSE (root mean square error) and MAE (mean absolute error). Let us assume an algorithm that has an RMSE of \$30'000,00 in predicting housing values of Boston suburbs (DB 1) and an RMSE of 3.3 on predicting the quality of red wine (DB 2). How can one add those two numbers to obtain an average? In fact, we cannot even compare those two numbers; which one is higher? But even for comparable metrics, such as accuracy, AUC, and so on for classification, or MAPE (mean absolute percentage error) for regression, which are dimensionless quantities, there is a subtle problem in averaging those measures. For example, an improvement in accuracy from 76% to 78% is less "significant" than an improvement from 96% to 98%, even though both represent a 2% increase. Two algorithms that have a mean

accuracy of 0.86, but one with 78% and 96% accuracy on two data sets, and the other with 76% and 98% accuracy, would have the same mean accuracy, but the second algorithm would be considered "better" as its 2% increase on the second data set is more "significant." Thus, computing the aggregated ranking based on the mean of the measures, even for comparable metrics, is not considered a "correct" procedure in Machine Learning.

Another alternative (Benavoli et al., 2016; Stapor et al., 2021) is to compute the median measure for each algorithm, provided the metric used is comparable. The aggregated ranking is then determined by ranking the medians. One common method (Demsar, 2006) is to compute the rank of each algorithm within each data set, assigning 1 to the best, 2 to the second, and taking the average rank in case of ties. The mean rank of each algorithm is then calculated, and the ranking of these mean ranks determines the final aggregated rank.

Additionally, there are numerous ranking aggregation methods discussed in other disciplines (Langville and Meyer, 2012), such as social choice theory where rankings are referred to as preferences and a wide range of voting procedures are used to aggregate them (List, 2022). However, it is important to note that these aggregation procedures in other disciplines are not usually associated with a measure of confidence in determining which item is "better" than another in the aggregated rank.

The second goal of evaluating the confidence of the aggregated ranking is only necessary when a sample of the relevant population is used for comparison. In the case of determining the winner of an election or a sports championship, the entire population is considered, and there is no need for a statistical evaluation of the victory. In these cases, the purpose of the comparison procedure is simply to calculate the aggregated ranking.

However, when comparing machine learning algorithms, the aggregated ranking obtained from a particular set of data sets is not the ultimate goal. The objective is to make claims about the ranking of algorithms on future, yet-to-be-seen data sets. To assess the confidence in the aggregated ranking, statistical tests are often used to determine the trustworthiness of paired comparisons between algorithms. Historically, the most common approach has been the **frequentist** approach, where a null hypothesis significance test is used to make a binary decision on the significance of the difference between algorithms.

In recent times, there has been a shift towards **Bayesian** approaches to statistical testing. Bayesian approaches do not provide a binary decision on the significance of paired comparisons, but instead provide a probability of one algorithm being better than the other.

Regarding the third goal, there is a clear need to state that two algorithms are similar for practical purposes. However, frequentist methods are not well-suited to make this claim¹. Some researchers mistakenly assume that if there is no statistical difference between two algorithms, they are similar or equivalent. However, a non-significant result from a frequentist test only indicates that the sample size was not large enough to detect a significant difference, not that the algorithms are equivalent. With a large enough sample size, all p-values will go to 0.0 (Shalizi, 2015; Kruschke and Liddell, 2015) and all differences will become significant. In contrast, Bayesian methods do allow for the claim of practical equivalence, as we will see in a later section (Section 2).

^{1.} There are frequentist tests that determine when two alternatives do not have practical difference. These are known as equivalence tests (Wellek, 2010) but are not of common use in Machine Learning or other areas of Computing.

Finally, regarding the fourth goal, it is desirable to have the comparison procedure handle missing measures gracefully, as algorithms may not converge on some data sets, may require more memory than is available, or may exceed the allotted computational time. This is particularly relevant in the case of frequentist approaches, as there is no universally agreedupon way of handling missing measures.

This paper presents a new comparison procedure that is based on the number of times an algorithm outperforms another on various data sets. The proposed procedure is as follows:

- The statistical framework used is the Bradley-Terry model for ranks, which assumes that each algorithm has a latent "merit number" or "ability" that determines the probability of it outperforming another algorithm.
- The aggregated ranking of algorithms is determined by the ordering of these merit numbers.
- The proposed procedure utilizes a Bayesian implementation of the Bradley-Terry model, which allows for the computation of the probability of one algorithm being better than another, and serves as a measure of confidence in the ordering.
- The Bayesian model also enables the definition of when two algorithms are considered equivalent for practical purposes through the concept of the region of practical equivalence (ROPE).
- The ROPE is defined in the probability space, allowing for a generic notion of equivalence that can be understood and modified by researchers, regardless of their experience with the particular metric being used.
- A concept of local ROPE is also introduced, which is a decision criterion for comparing two algorithms on a specific data set. The decision is based not only on the difference between the two mean measures but also takes into consideration the "noise level" or effect size of the differences.

This paper is laid out as follows: Section 2 is a short tutorial on Bayesian tests. Section 3 discusses the previous frequentist and Bayesian approaches to comparing multiple algorithms on multiple data sets. Section 4 discusses this proposal, the use of a Bayesian Bradley Terry model. Section 5 shows some first results of using the BBT model. Section 6 discusses our proposal of considering more than the mean across different cross-validations when determining if one algorithm is better than the other. Section 7 discusses the quality of the BBT model as a predictive estimation of the future behavior of the algorithms on new data sets. Section 8 discusses some of the advantages and shortcomings of the BBT model, and section 9 summarizes the main conclusions.

2. A short review of Bayesian tests

Bayesian tests (also known as **Bayesian estimation procedures**) compute the posterior joint distribution of some parameters of the model that are important for the analysis. The simpler case to discuss herein is a Bayesian version of the two samples (non-paired) t-test for the means. A simple Bayesian test will model each set of data (X and Y) as samples from two Gaussian distributions with mean μ_X and μ_Y and with standard deviation σ_X and σ_Y respectively. Additionally, the model assumes that μ_X and μ_Y are themselves sampled from another Gaussian with mean μ and standard deviation σ , while σ_X and σ_Y are sampled from a uniform distribution between L and H^2 . This is expressed by the following notation:

$$x_{i} \sim \operatorname{Normal}(\mu_{X}, \sigma_{X})$$

$$y_{i} \sim \operatorname{Normal}(\mu_{Y}, \sigma_{Y})$$

$$\mu_{X} \sim \operatorname{Normal}(\mu, \sigma)$$

$$\mu_{Y} \sim \operatorname{Normal}(\mu, \sigma) \qquad (1)$$

$$\sigma_{X} \sim \operatorname{Unif}(L, H)$$

$$\sigma_{Y} \sim \operatorname{Unif}(L, H)$$

The variables of interest are called **parameters** and in this case, are μ_X and μ_Y (and maybe σ_X and σ_Y).

The distributions Normal(μ, σ) and Unif(L, H) are called **hyper-priors**. The **hyperparameters** μ, σ, L , and H are set externally so that the distributions for the true data X and Y are likely. For example, if the measured average of the data in X is 5 and the measured average of the data in Y is 5.2, then the random variables μ_X and μ_Y should be around 5, and thus the mean of the Gaussian from which both μ_X and μ_Y are sampled should have mean (the μ hyper-parameter) of 5.

The choice of hyper-priors and the hyper-parameters σ , L, and H, can significantly impact the results of a Bayesian estimation procedure. Narrow hyper-priors may result in limited range of values for the parameters, and the results may be driven more by these constraints than the actual data. On the other hand, overly wide hyper-priors may have little to no constraints on the parameters, leading to potential convergence issues in the MCMC algorithm (as discussed in section~2.2). The debate on the appropriate width of hyper-priors is known as the non-informative vs weakly informative vs strongly informative prior debate (Lemoine, 2019; Gelman et al., 2017).

In general terms, a Bayesian test will compute (or sample, as we will see below) the posterior distribution of the parameters of interests, in this case μ_X and μ_Y given the data. That is, we want to compute:

$$P(\mu_X, \mu_Y|M, X, Y) = K P(X, Y|M, \mu_X, \mu_y) P(\mu_X, \mu_Y|M)$$

where X and Y are the data, and M is the model itself (Equations 1), and K is a constant that normalizes the distribution $P(\mu_X, \mu_Y|...)$.

Once the posterior distribution $P(\mu_X, \mu_Y|M, X, Y)$ is computed, one can use it to make probabilistic statements about the parameters of interest. For example, $P(\mu_X > \mu_Y|M, X, Y)$ represents the probability that the mean of the distribution that generated the data X is greater than the mean of the distribution that generated the data Y. If this probability is 0.8, then the researcher is 80% confident that X comes from a population whose

^{2.} A more complex model for this problem was proposed by Kruschke (2013).

mean is greater than the population from which Y comes from. This type of probabilistic statement is different from the claims made using frequentist methods.

2.1 ROPE

Another useful statement to derive from the posterior distribution is the probability that the difference between μ_X and μ_Y is of no practical consequence. If δ is the value below which the difference is considered as insignificant, then the value of $P(|\mu_X - \mu_Y| < \delta | M, X, Y)$ represents the probability that there is no important difference between μ_X and μ_Y . In Bayesian analysis, the value δ is referred to as the **region of practical equivalence (ROPE)**. Differences smaller than the ROPE are considered to be of no practical significance.

2.2 MCMC and convergence

Typically, Bayesian tests do not calculate the probability distribution $P(\mu_X, \mu_Y | M, X, Y)$ analytically, but instead use a method from the Markov Chain Monte Carlo (MCMC) family of algorithms to sample pairs $\langle \mu_{X_s}, \mu_{Y_s} \rangle$ from that distribution, denoted as $\langle \mu_{X_s}, \mu_{Y_s} \rangle \sim$ $P(\mu_X, \mu_Y | M, X, Y)$. In this paper, s will be used as the index for samples generated from the MCMC algorithm. From the sample set $\langle \mu_{X_s}, \mu_{Y_s} \rangle$, determining the probability that $\mu_X > \mu_Y$ simply involves counting the proportion of samples for which $\mu_{X_s} > \mu_{Y_s}$.

MCMC algorithms eventually converge to the target distribution, but in practice, the algorithm will run for a pre-determined number of steps, and **convergence diagnostics** are used to assess whether the samples generated are representative of the target distribution. A comprehensive discussion of convergence diagnostics can be found in Roy (2019).

It is important to run convergence diagnostics every time a Bayesian model is run, as they provide information on whether the samples generated by the algorithm are representative of the posterior distribution of the parameters, or if more steps of the MCMC algorithm need to be run.

2.3 Posterior Predictive Check

Posterior predictive diagnostics aim to assess the accuracy of the Bayesian model (i.e., the model given by Equations 1) in representing the data. Even if the MCMC algorithm converges and returns samples from the posterior distributions of the parameters, the model may still not correctly describe the data. The posterior predictive check (PPC) verifies that the data generated by the model, using the posterior values of the parameters, is similar to the observed data.

In essence, when the parameters assume the "correct values" (as determined by the posterior distribution of the parameters), the model can be "run forward" to generate new values of x_{is} .³ The distribution of the generated data for the first observation x_{1s} should be compared to the "real data" x_1 . If the model fits the data well, the real data should be very similar to the set of generated data.

^{3.} This is a simplification to provide an intuitive understanding. In reality, the MCMC algorithm also samples from $P(X_{rep}, Y_{rep} | M, X, Y)$, where X_{rep} is the data generated from the model (M) given the real data (X and Y).

Other methods for evaluating the fit of a model to the data, such as leave-one-out crossvalidation approximations (e.g., WAIC (Watanabe-Akaike information criteria) (Watanabe and Opper, 2010) and loo (Vehtari et al., 2017)), are also available. However, we will not go into detail about these approaches here but we will use them later when discussing alternative modeling options.

2.4 Bayesian tests for multiple comparisons

The example above involves a Bayesian test on two sets of data (X and Y). If one wants to compare multiple sets of data, can one repeat the Bayesian test for all pairs? For frequentist tests, repeating the test for all pairs of comparisons would require some p-value adjustment procedure. However, the issue of performing multiple Bayesian comparisons is still unclear. It has been suggested that if the Bayesian model is hierarchical or multilevel, there would be no problem with performing multiple comparisons (Gelman et al., 2012). A hierarchical model contains a model step similar to the line 1 in the Bayesian model described above where the two parameters are sampled from a single distribution.

To perform multiple comparisons, a hierarchical Bayesian model is needed where each of the parameters of interest $\mu_X, \mu_Y, \mu_W, \dots, \mu_Z$ are sampled from a common distribution. This process is known as partial pooling or shrinkage and it helps to pool the different estimates of the parameters towards each other. An example of such a hierarchical model is the Bayesian ANOVA (Kruschke, 2014, ch. 19).

2.5 Frequentist versus Bayesian approaches

There are many differences between frequentist and Bayesian approaches. We will not discuss them in this paper, but we point the reader to Benavoli et al. (2017) discussion on the limitations of the frequentist approach.

3. Previous Frequentist and Bayesian approaches

In this section, we will discuss the previous approaches to comparing multiple algorithms on multiple data sets.

3.1 Demsar's procedure (mean rank plus Nemenyi test) and extensions

The standard frequentist procedure for comparing multiple algorithms on multiple data sets was introduced by Demsar (2006). The main steps of this comparison procedure are:

- Convert each data set's results into ranks, with 1 being the best result and 2 being the second best, etc.
- Treat ties as the average rank. For example, if two algorithms have the same measure on a data set and they are the fourth best ranked algorithms, then they both receive a rank of 4.5, which is the average of 4 and 5.
- Determine the final order by decreasing the mean rank across all data sets. In other words, an algorithm with a lower mean rank is considered to be better than an algorithm with a higher mean rank.

- The confidence in this order is indicated by a pairwise binary statement on whether one algorithm is better than another, using the phrase "the difference is statistically significant."
- The significance of the pair comparisons is calculated using the Friedman test, followed by the Nemenyi test. If the difference in mean rank between two algorithms is smaller than the critical difference computed by the test, the difference is **not** statistically significant.

Frequentist tests usually loose power, or in other words, find "less differences than it should" as the number of comparisons increase. Comparing against a control (or 1xN or many-to-one comparisons) reflects the situation where the researcher is interested in comparing a new algorithm, called the **control**, against a set of other algorithms viewed as competitors, but is not interested in ranking the competitors amongst each other. This will reduce the number of comparisons and may increase the power of the comparisons, finding more significant differences than a *all-pairs* or NxN comparisons would. Demsar (2006) also discusses a different comparison procedure when comparing against a control. In this paper we will limit ourselves to all-pairs comparisons.

Garcia and Herrera (2008) proposed and tested different extensions to Demšar's procedure, including Shaffer's static and Bergmann-Hommel's procedures, which they claimed were stronger than the Nemenyi test. Garcia et al. (2010) proposed new omnibus tests, such as the Friedman aligned ranks and Quade tests, and tested other post-hoc procedures for p-value adjustments. The authors concluded that procedures such as Holm, Hochberg, Hommel, Holland and Rom produce equivalent results.

In summary, Demsar (2006) and its extensions are a family of non-parametric and paired multiple comparison procedures that are based on the rank of the algorithms within each data set. The omnibus procedure can be the Friedman test or other tests proposed by Garcia et al. (2010), and the post-hoc procedures can be critical difference on the ranks (Demsar, 2006; Garcia and Herrera, 2008) or Wilcoxon pairwise procedures on the rank data, followed by various p-value adjustment procedures (Garcia et al., 2010).

3.2 Pairwise Wilcoxon plus p-value adjustment procedures

Benavoli et al. (2016) highlights a problem with comparison procedures based on mean ranks, that the results of the comparison between two algorithms can be dependent on the other algorithms being compared. To address this issue, they suggest using a pairwise Wilcoxon signed rank test between the measures obtained by each algorithm for all data sets, followed by an appropriate multiple comparisons adjustment procedure. This approach is also suggested by Stapor et al. (2021).

This procedure computes the aggregated ranking based on the median measure of each algorithm across the data sets. Of course, such a procedure requires comparable metrics.

Before we proceed, let's address the issues regarding missing data in frequentist approaches — the cases where an algorithm did not execute for a particular data set. The problem lies in the lack of a universally accepted method for handling missing data. For mean rank approaches, such as Demsar's procedure, one option is to exclude the rank of the algorithm that did not run for a specific data set from the calculation of the mean rank. However, this suggests that not running an algorithm on a data set indirectly attributes to it its mean rank. While this is a possibility, it is not a standard practice. For instance, Fernandez-Delgado et al. (2014) adopted a similar approach, but this method was criticized by Wainberg et al. (2016) for introducing a positive bias to the algorithm that did not run on the data set. The same could be done for pairwise Wilcoxon tests, but this would imply that an algorithm that did not execute on a data set would be assigned its median measure for that data set. We do not hold a firm opinion on whether this is the right approach, or if one should assign the worst rank to the algorithm. The main issue remains that there is no universally agreed-upon method for handling missing data in frequentist tests.

3.3 Bayesian pairwise signed-rank test

Benavoli et al. (2017) developed two forms of a Bayesian version of the Wilcoxon signed rank test (BSR), and argued for their use within the Machine Learning practice. The first, simpler form uses a single measure per algorithm and data set, usually the mean of various measures obtained through cross-validation. The second form is more complex, it is referred to as the Bayesian hierarchical correlated t-test, and it uses the measures from each crossvalidation fold in the computation. However, the authors suggest that practitioners use the simpler form.

The model's parameter is the mean of the pairwise difference between of the accuracy of the algorithms on the different data sets, and the model computes a probability distribution for this parameter. The authors state that if this parameter is between -0.01 and 0.01 (or a ROPE of 1%) there is no practical difference between the two algorithms being compared. The justification for the 1% ROPE for accuracy is not presented in the paper, but that number is not too different from the ROPE threshold proposed by Wainer (2016) and twice as large than the one proposed by Wainer and Cawley (2021), based on different sets of empirical evidence.

For each data set a 1% of difference may or may not be important, depending on the accuracy itself. A 1% change for a 79% accuracy is likely insignificant but a 1% change for an accuracy of 98% is impressive. Given the range of accuracy values that appear in practical cases of comparing two classifiers (some high, some low) the authors are claiming that changes on the *mean value* of less than 1% are irrelevant from a practical point of view.

Even if one accepts the 0.01 ROPE for accuracy, there is no agreed upon, or even proposed (as far as this author is aware) ROPEs for other classification metrics such as AUC, F1, MCC, and for other comparable regression metrics. Additionally, there is no ROPE for incomparable metrics, nor will the Bayesian signed rank method be applicable to incomparable metrics, given that the mean of the pairwise differences is not well defined.

The Bayesian signed rank test was defined for comparing *two* algorithms on multiple data sets, and there may be issues when applying it to multiple comparisons. Benavoli et al. (2017) do not perform any multiple comparison in the paper. They do perform many signed-rank procedures with different algorithms but not with the goal of ranking those algorithms. The paper acknowledge that the Bayesian signed rank model lacks a hierarchical component and therefore its use in multiple comparisons is problematic. However, they argue that using ROPE would mitigate the false alarm rate (the rate of false positive claims), but this argument is not widely accepted and would require the use of ROPEs for all comparisons.

Since the authors only propose a ROPE for accuracy, it would be imprudent to use the Bayesian signed rank test for other metrics without further proposals for ROPEs for those metrics.

4. Bradley-Terry model

The Bradley-Terry (BT) model (Bradley and Terry, 1952) is a method for ranking "players" in "tournaments" where the payers compete pairwise in matches, such as soccer teams or chess payers. The model assigns to each player X_i an *intrinsic value* or *ability* $w_i \ge 0$. The intrinsic value relates to the probability that player *i* will win player *j* in a match by:

$$P(X_i \text{ wins } X_j) = P(X_i \succ X_j) = \frac{w_i}{w_i + w_j}$$

The final ranking of the players is defined by the rank of their intrinsic values w_i .

The intrinsic values are invariant to a multiplicative constant, that is, if the set $\{w_i\}$ correctly models all the probabilities $P(a \succ b)$, so will $\{\alpha w_i\}$. Therefore, to specify a single set of intrinsic values, one also requires that $\sum w_i = 1$.

An alternative to w_i is to use their natural logarithms $\beta_i = \log w_i$. The useful formula regarding β is:

$$\operatorname{logit}(i \succ j) = \log \frac{P(i \succ j)}{1 - P(i \succ j)} = \log \frac{P(i \succ j)}{P(j \succ i)} = \beta_i - \beta_j$$

The β values are invariant to additive constant, since the w_i were invariant to multiplicative constants. To specify a single set of solutions, a common practice is to require that $\sum \beta_i = 0.$

The standard BT model does not deal with ties, meaning that $1 - P(i \succ j) = P(j \succ i)$. However, there have been extensions to the model that incorporate ties (Rao and Kupper, 1967; Davidson, 1970; Baker and Scarf, 2021). The model proposed by Davidson (1970) will be discussed in Section 6.2.

In the case of ties, a common approach is to change the data used for estimation so that a tie between players i and j is counted as both a victory for i and for j or sometimes as half a victory for each. This will be further explained in Section 6.2.

4.1 Bayesian estimation of the w or β

Let us assume that players i and j play $N_{ij} = N_{ji}$ matches against each other, and W_{ij} is the number of matches that i wins and W_{ji} is the number of matches j wins (and thus $N_{ij} = W_{ij} + W_{ji}$ given that there are no ties). Let us also assume that $W_{ii} = 0$, and that there are t players.

The Bayesian model for BT is based on the beta coefficients:

$$W_{ij} \sim \text{Binomial}(N_{ij}, \frac{e^{\beta_i}}{e^{\beta_i} + e^{\beta_j}})$$

$$\beta_i \sim \text{Normal}(0, \sigma)$$

$$\sigma \sim \text{LogNormal}(0, 0.5)$$
(2)

The binomial expression captures the fact that the number of times i wins from j is a binomial distribution given the total number of matches between i and j (N_{ij}) and the probability that i will win each match $(P(i \succ j) = \frac{w_i}{w_i + w_j})$.

The β parameters can have positive and negative values and thus it is reasonable to sample them from a normal distribution with mean 0, and variance σ (a hyper-parameter). This is the hierarchical component of the Bayesian BT model (BBT): all β_i are sampled from the same distribution and thus the model can be used to compare multiple algorithms, since there will be partial pooling. The hyper-prior for σ is a log-normal distribution, as proposed by Carpenter (2018), but there is no difference on using other hyper-priors such as half-normal or Cauchy, as reported in the longer version of this paper (Wainer, 2022).

5. Exploration of the BBT

This section presents an analysis of the BBT model applied to a specific set of algorithms and data sets (detailed in Section 5.1). The outputs of the model are be discussed in Section 5.2. Additionally, two forms of diagnostic checks are examined in Sections 5.3 and 5.4, as well as the concept of ROPE appropriate for the model in Section 5.5. The section concludes with a discussion of the two interpretations of the parameters of the model in Section 5.6.

5.1 Data

We will explore the use of the BBT model on four use-cases regarding the comparison of machine learning algorithms on multiple data sets. The four use cases are called small-small, small-large, medium-medium, and large-large.

The large-large $(\ell \ell)$ use-case involves the evaluation of 16 out-of-the-box classifiers on 132 data sets. These classifiers were trained without any tuning of their hyper-parameters and the data sets are the first 132 smallest data sets from the PMLB data set curated by Olson et al. (2017). The accuracy metric was used for comparison with the BSR procedure. Details of the algorithms used are discussed in the longer version of this paper (Wainer, 2022).

The large-large results reflect the scenario where a large number of algorithms are compared on a large number of data sets. Most curated sets of data sets, such as PMLB (Olson et al., 2017), KEEL imbalanced data sets (Alcala-Fdez et al., 2011), and the OpenML-CC18 Curated Classification benchmark (Bischl et al., 2019), include around 100 data sets. In this scenario, a researcher might typically compare around 20 algorithms, although there are some studies that test up to 50 (Wainer and Fonseca, 2021) or 100 (Fernandez-Delgado et al., 2014; Wang et al., 2021). However, these studies do not perform statistical tests to confirm the statistical significance of their results within the frequentist framework or make any other probabilistic claims within a Bayesian framework. The $\ell\ell$ -results are part of the R package developed for this research (Section 8.1).

The other use cases are:

• the small-small (ss) use-case, which represents the comparison of a small number of algorithms (5) on a small number of data sets (20).

| db | dt | lda | lgbm | \mathbf{xgb} | svm |
|------------------------|-------|-------|-------|----------------|-------|
| biomed | 0.837 | 0.842 | 0.876 | 0.890 | 0.886 |
| breast | 0.931 | 0.951 | 0.964 | 0.961 | 0.957 |
| breast_w | 0.940 | 0.950 | 0.961 | 0.961 | 0.961 |
| buggyCrx | 0.790 | 0.861 | 0.867 | 0.867 | 0.861 |
| clean1 | 1.000 | 1.000 | 1.000 | 1.000 | 0.968 |
| cmc | 0.455 | 0.513 | 0.525 | 0.524 | 0.544 |
| colic | 0.761 | 0.837 | 0.815 | 0.815 | 0.641 |
| corral | 1.000 | 0.900 | 1.000 | 1.000 | 1.000 |
| credit_g | 0.668 | 0.718 | 0.766 | 0.769 | 0.724 |
| diabetes | 0.714 | 0.772 | 0.747 | 0.742 | 0.758 |
| ionosphere | 0.869 | 0.866 | 0.940 | 0.932 | 0.934 |
| irish | 1.000 | 0.740 | 1.000 | 1.000 | 0.988 |
| molecular_by_promoters | 0.727 | 0.689 | 0.896 | 0.887 | 0.802 |
| monk3 | 0.975 | 0.792 | 0.980 | 0.986 | 0.964 |
| prnn_crabs | 0.880 | 1.000 | 0.950 | 0.935 | 0.960 |
| prnn_synth | 0.800 | 0.852 | 0.824 | 0.828 | 0.856 |
| saheart | 0.626 | 0.723 | 0.660 | 0.671 | 0.712 |
| threeOf9 | 0.996 | 0.809 | 1.000 | 0.998 | 0.992 |
| tokyo1 | 0.902 | 0.920 | 0.928 | 0.926 | 0.931 |
| vote | 0.929 | 0.956 | 0.945 | 0.959 | 0.956 |

| Table 2: T | 'he base | results. |
|------------|----------|----------|
|------------|----------|----------|

- the small-large (sl) use-case which represents the comparison of 5 algorithms on 100 data sets.
- the medium-medium (mm) use case which represents the comparison of 10 algorithms on 50 data sets.

In this paper, the ss, the sl, and the mm cases will be used in *repeated experiments* to test some general claim regarding the BBT procedure, by sampling from the $\ell\ell$ -results 10 random ss and mm results, and 5 random sl results.

A fixed ss result will be used to illustrate the BBT procedure throughout this paper. This result is called the *base* results. For the base results we selected *lgbm* (LightGBM), xgb (XGBoost), svm (SVM with RBF kernel), *lda* (Linear discriminant analysis), and *dt* (CART decision trees) as the classification algorithms, and selected 20 arbitrary data sets from the 132 in the $\ell\ell$ -results.

The table of values for the base results is displayed in Table 2. The table represents the *mean* accuracy on the *same* 4-fold evaluation of the algorithms on each data-set.

5.2 Basic outputs of the model

A win/loss table is the representation of the number of wins and losses for each pair of algorithms. This data is the input for the Bayesian model.

| alg1 | alg2 | win1 | win2 | ties | | alg1 | alg2 | win1 | win2 |
|----------------------|----------------------|------|------|------|---|----------------------|----------------------|------|------|
| dt | lda | 6 | 13 | 1 | - | dt | lda | 7 | 14 |
| dt | lgbm | 0 | 17 | 3 | | dt | lgbm | 2 | 19 |
| dt | xgb | 0 | 17 | 3 | | dt | xgb | 2 | 19 |
| dt | svm | 5 | 14 | 1 | | dt | svm | 6 | 15 |
| lda | lgbm | 6 | 13 | 1 | | lda | lgbm | 7 | 14 |
| lda | xgb | 5 | 14 | 1 | | lda | xgb | 6 | 15 |
| lda | svm | 5 | 15 | 0 | | lda | svm | 5 | 15 |
| lgbm | xgb | 9 | 8 | 3 | | lgbm | xgb | 11 | 10 |
| lgbm | svm | 10 | 9 | 1 | | lgbm | svm | 11 | 10 |
| xgb | svm | 11 | 8 | 1 | | xgb | svm | 12 | 9 |

(a) The win/loss table for the base results. The win/loss table lists all win, ties, and losses for each pair of algorithms. (b) The final win/loss table for the base results once the ties have been added as half-victories (rounded up in the final) to both algorithms.

Table 3: The win/loss tables pre as post processing of the ties.

Table 3a displays some ties between algorithms, such as dt and lda both having accuracy of 1.0 in the **clean1** data set. The BBT model does not handle ties. To address this, we implement the "spread" policy, which considers half (rounded up) of the ties as partial victories for both algorithms. Alternatives to the spread policy are discussed in Section 6.2. The resulting win/loss table is presented in Table 3b.

The MCMC solution to the BBT model in Equations 1 for the data in Table 3b is a set of tuples for the parameters β_i , and for σ . In our case, we are interested in using, for example, each β_{as} and β_{bs} to compute $P_s(a \succ b)$. This computation is performed for all pairs of algorithms, and the results can be visualized and summarized in a plot or table.

The Bayesian approach to the BT model presents a challenge in determining the aggregated ranking of the algorithms. One commonly used solution is to calculate the ranking for each sample generated by the MCMC algorithm by ordering the algorithms based on their decreasing values of β_{is} (Carpenter, 2018, Issa Mattos and Martins Silva Ramos (2021)). However, this approach results in a distribution of rankings, making it unclear how to arrive at a single, final ordering. One can choose the most frequent ranking among the samples, or compute the rank of each algorithm in each ranking and order them based on the mean rank.

We believe that determining the order of the algorithms is a crucial part of the comparison process, so we propose a different solution. We order the algorithms based on their mean β across all samples, resulting in a single, aggregated ranking for the BBT comparison procedure.

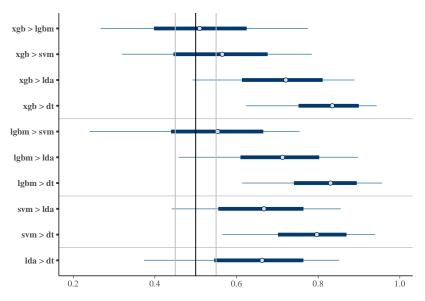


Figure 1: The graphical representation of the distribution of P(a > b). The pair of algorithms are ordered best > worse. The central dot represents the median of the distribution of P (a > b), and the wider line represents the 89% highest density interval (HDI) of the distribution. The thin line represents the full range of the distribution. The two vertical gray lines represent the ROPE region from [0.45, 0.55] (discussed in section 5.5 below).

Figure 1 presents the distributions of $P_s(a \succ b)$. The algorithms are ordered from the best to the worst, where the best algorithm is compared with all others, the second best with the remaining worse, and so on. The central dot represents the mean of the distribution of $P_s(a \succ b)$, and the wider line represents the 89% highest density interval (HDI) of the distribution. The thin line represents the full range of the distribution. The figure also includes the ROPE region, the two vertical lines, as discussed in Section 5.5

Some Bayesian estimation researchers use 89% (instead of 95%) to distinguish a credible interval, which is an interval that contains a specified amount of the mass of a distribution (in this case 89%), from the "95% confidence interval" concept in frequentist statistics, which has a slightly different meaning (Makowski et al., 2019). There are infinitely many intervals that contain 89% of the mass of a distribution, and the HDI is the smallest of these intervals for unimodal distributions (Kruschke, 2014).

Some of the information presented in Figure 1 can be condensed into Table 4, which includes the mean, as well as the low and high limits of the 89% HDI. The column *above.50* is the mass of probability above the 0.50 threshold, the column *in.rope* is the mass of probability within the ROPE region (discussed in Section 5.5). *above.50* is further discussed in Section 5.6.

5.3 Convergence Diagnostics and execution times

As previously mentioned, it is important to assess the convergence of an MCMC algorithm with every run. In this study, we utilized Stan (Stan Development Team, 2022) as the tool to implement the BBT model (2) and to perform the MCMC. Stan provides various

| pair | mean | low | high | delta | above.50 | in.rope |
|--------------------------------|------|------|------|-------|----------|---------|
| $\mathrm{xgb} > \mathrm{lgbm}$ | 0.51 | 0.40 | 0.63 | 0.23 | 0.55 | 0.52 |
| $\mathrm{xgb} > \mathrm{svm}$ | 0.56 | 0.45 | 0.68 | 0.23 | 0.80 | 0.36 |
| xgb > lda | 0.72 | 0.62 | 0.82 | 0.20 | 1.00 | 0.00 |
| xgb > dt | 0.83 | 0.76 | 0.91 | 0.14 | 1.00 | 0.00 |
| $\mathrm{lgbm} > \mathrm{svm}$ | 0.55 | 0.45 | 0.67 | 0.22 | 0.77 | 0.40 |
| lgbm > lda | 0.71 | 0.62 | 0.81 | 0.19 | 1.00 | 0.01 |
| $\mathrm{lgbm} > \mathrm{dt}$ | 0.83 | 0.75 | 0.90 | 0.15 | 1.00 | 0.00 |
| $\mathrm{svm} > \mathrm{lda}$ | 0.66 | 0.57 | 0.77 | 0.21 | 0.99 | 0.05 |
| $\mathrm{svm}>\mathrm{dt}$ | 0.79 | 0.71 | 0.88 | 0.16 | 1.00 | 0.00 |
| lda > dt | 0.66 | 0.55 | 0.77 | 0.22 | 0.98 | 0.06 |

Table 4: The table representation of the distributions of probabilities P(a > b). Pair is the pair of better/worse algorithms, mean is the mean probability; low and high are the lower and higher limits of the 89% HDI of the distribution; delta is the difference between high and low. above 50 is the proportion of probabilities samples > 0.50; and in.rope is the proportion of probabilities samples > 0.55] (discussed in section 5.5 below).

convergence diagnostics data, which are analyzed to determine whether the convergence is acceptable or not. The results of the simplified Stan check are presented below.

```
## Checking sampler transitions treedepth.
## Treedepth satisfactory for all transitions.
##
## Checking sampler transitions for divergences.
## No divergent transitions found.
##
## Checking E-BFMI - sampler transitions HMC potential energy.
##
## Effective sample size satisfactory.
##
## Effective sample size satisfactory all parameters.
##
## Processing complete, no problems detected.
```

The MCMC sampling of the model is unproblematic – in all the examples presented in this paper, including those in later sections, we used 1000 steps of warm-up and 1000 steps of sampling, across 4 chains. The execution time on a modern laptop, such as an Intel i5 running at 1.4 GHz, took no more than 0.5 seconds per chain, with all four chains running simultaneously on the different cores.

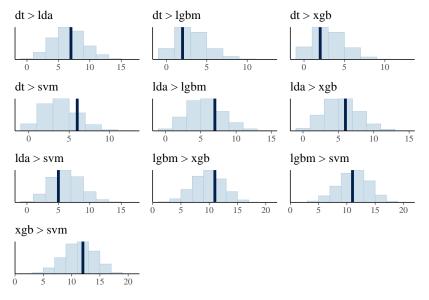


Figure 2: Graphical representation of the PPC. For each observered variable (number of wins of first algorithm over the second), the histogram represents the distribution of the generated data, and the wider bar represents the observed number of wins.

| hdi | proportion |
|------|------------|
| 0.50 | 0.8 |
| 0.90 | 1.0 |
| 0.95 | 1.0 |
| 1.00 | 1.0 |

Table 5: The table representation of the PPC. Hdi indicates a HDI interval (50%, 90%, 95% and 100%), and proportion is the proportion of the observed data that falls within the corresponding HDI.

5.4 Posterior Predictive Check and WAIC

Figure 2 illustrates the results of the posterior predictive check (PCC). The histogram represents the data generated by the Bayesian model, while the vertical bar shows the actual value of the win1 variable from the win/loss table, associated with each pair of algorithms. If the Bayesian model accurately generates the data, the actual values should be centered in the histogram of possible values for that variable.

We also present a non-graphical representation of the PPC by computing the 50%, 90%, 95%, and 100% HDI (highest density interval) of the generated values for each variable. We then calculate the proportion of the true data that falls within each HDI. Ideally, the proportion of data values that fall within the 90% HDI should be at least 0.9. Table 5 provides this alternative representation of the PPC.

5.5 ROPE

As discussed above, the Bayesian approach offers the advantage of defining a difference between parameters that may not be meaningful in practical terms, and allows one make statements regarding the likelihood of these parameters being equivalent in a practical sense.

The BBT model provides a simple way to adopt the concept of practical equivalence. The ultimate measure from the BBT model is the probability that a particular algorithm outperforms another. A universal ROPE can be defined for making probability statements, regardless of the metric used to determine superiority between algorithms. We propose that if the probability that one algorithm is better than another falls within the range of 0.45 to 0.55, it can be concluded that the two algorithms are practically equivalent.

This claim is not based on an established community understanding or the author's personal experience with comparing multiple algorithms, but rather on a universal ROPE for probability statements. The choice of the ROPE limits, [0.45, 0.55], is somewhat arbitrary, reflecting the author's belief that an algorithm whose probability of being better than another is below 55% (and above 45%) is not significantly better than the other. Other researchers may have different intuitions and are free to adjust the ROPE to suit their specific applications.

Figure 1 and Table 4, shown above, also include information regarding the ROPE.

5.6 Strong and weak interpretations of the probability estimates

We believe that the four important columns to report are: mean, delta (the difference between the high and low values of the HDI) in.rope, and above.50. In particular, the mean and the above.50 measures measures play a crucial role in what we refer to as the **strong** and the **weak interpretations** of the probability estimates. The BBT model generates a set of numbers $P_s(A \succ B)$ which we interpreted as probabilities that algorithm A is better than algorithm B. And in fact, these numbers are used in the BBT model as the parameters of the binomial distribution that are interpreted as probabilities of the event happening.

Under the strong interpretation, we understand each of $P_s(A \succ B)$ as a probability estimate that A is better than B in the sense that in the long run, for a large number of data sets, the proportion of times A wins from B should approach that number. In the strong interpretation, the *mean* column is the best estimation of how much better algorithm A is compared to algorithm B. The *delta* column or both *low* and *high* are estimates of the uncertainty surrounding that probability.

The weak interpretation views each $P_s(A \succ B)$ as a measure of the superiority of A over B, expressed as a number ranging from 0.0 to 1.0. A value less than 0.5 indicates that B is better than A. Under this interpretation, $P_s(A \succ B)$ represents evidence in favor of A's superiority over B, rather than a guarantee of future outcomes. The value of *above.50* reflects the degree of confidence one can have in the superiority of A over B. For example, if 90% of the evidence $(P_k(A \succ B))$ is above 0.5, one can have 90% confidence that A is better than B."

The *in.rope* measure combines elements of both interpretations. While it calculates the proportion of evidence that falls within a specific interval (from 0.45 to 0.55), this range was determined based on the strong interpretation's perspective.

5.7 Further results: missing data and too many comparisons

Regarding missing values, the cases where an algorithm cannot run on one or more data sets, the BBT model simply does not count it as a win or a loss for that algorithm in comparison to the others.

For example, let us assume that the algorithm xgb does not run on the first two data sets in Table 2 (data sets **biomed** and **breast**). The resulting win/loss table is displayed in Table 6a, which should be contrasted with the win/loss table in Table 3b, and the summary results are displayed in Table 6b, which should be contrasted with the results in Table 4.

| alg1 | alg2 | win1 | win2 | pair | mean | delta | above.50 | in.rope |
|------|----------------------|------|------|-------------------------------|------|-------|----------|---------|
| dt | lda | 7 | 14 | lgbm > xgb | 0.51 | 0.23 | 0.55 | 0.50 |
| dt | lgbm | 2 | 19 | lgbm > svm | 0.54 | 0.23 | 0.74 | 0.42 |
| dt | xgb | 2 | 17 | lgbm > lda | 0.70 | 0.20 | 1.00 | 0.01 |
| dt | svm | 6 | 15 | lgbm > dt | 0.82 | 0.15 | 1.00 | 0.00 |
| lda | lgbm | 7 | 14 | xgb > svm | 0.53 | 0.23 | 0.68 | 0.47 |
| lda | xgb | 6 | 13 | xgb > lda | 0.69 | 0.20 | 1.00 | 0.02 |
| lda | svm | 5 | 15 | xgb > dt | 0.81 | 0.16 | 1.00 | 0.00 |
| lgbm | xgb | 10 | 9 | $\mathrm{svm} > \mathrm{lda}$ | 0.66 | 0.21 | 0.99 | 0.05 |
| lgbm | svm | 11 | 10 | $\mathrm{svm} > \mathrm{dt}$ | 0.79 | 0.17 | 1.00 | 0.00 |
| xgb | svm | 10 | 9 | lda > dt | 0.66 | 0.22 | 0.99 | 0.06 |

(a) The win/loss table

(b) Results for the corresponding BBT model

Table 6: Results when *xrg* does not run on the first two data sets.

In all-pairs comparisons, when dealing with a very large number of algorithms, one either avoids statistical tests altogether (as discussed above), or performs a two step procedure. If the algorithms can be naturally grouped into (few) families, one compares the algorithms within a single family, to select the best of that family, and then compare the "best representatives" of each family among each other (using the full frequentist tests). This was done, for example within the context of comparing imbalanced data algorithms by López et al. (2013).

For BBT, under the strong interpretation, there is no need to perform the two steps procedure; there is no large and biased difference between the probability estimates when comparing a large number of algorithms and a small one. Figure 3 displays the results of comparing the mean probability $P_s(A \succ B)$ of a random sample of three algorithms when all the 16 algorithms' results are fed to the BBT procedure, contrasted to the mean when only the results from those 3 algorithms are fed to BBT. In these test we randomly selected 20 data sets for each experiment and 40 experiments were run. The difference between the two mean estimates has mean 0.006, median 0.010, 1st quartile -0.020, and 3th quartile 0.030. That is, although the new mean probability is not necessarily the same as when tested for all algorithms, the difference in magnitude is small, and there is no bias - the difference is as likely to be positive as it is to be negative.

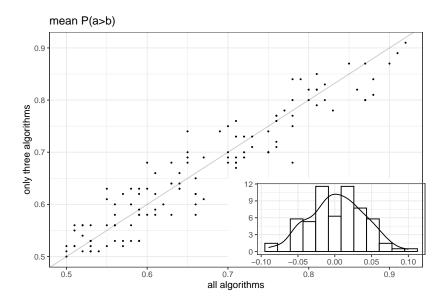


Figure 3: The results for mean P(a>b) of comparing 3 algorithms when all 16 algorithms' results are fed to BBT (on a random sample of 20 data sets) and when only the results for the three algorithms are fed to the BBT procedure. The inset is the distribution of the differences between the two average probability of winning.

Unfortunately, the insensibility to large number of comparisons is not true for the weak interpretation. Figure 4 compare the *above.50* results for the full 16 algorithms comparison and for a limited 3 algorithm comparison. There is a clear bias in the limited number of comparisons but the direction of the bias is surprising. The *above.50* numbers when only comparing 3 algorithms are *smaller* than the corresponding numbers when the full set of algorithms, which indicates that with more algorithms being compared, the procedure will be *more* sure of the difference between them. That is in the opposite direction one would expect from the frequentist tests: many more algorithms will decrease the power of the test and reduce the number of pairs which will be classified as statistically significant.

6. What counts as a win? Folds and local rope

Typically, the final performance measure for a particular algorithm for a particular data set is obtained by averaging the results from some form of repeated cross-validation, where the algorithm is trained on different subsets of the data set and its performance is measured on the corresponding test subsets. Standard forms of repeated cross-validations are k-fold, repeated k-folds, repeated train/test split, and bootstrapped samples of the data set. In each case, the data set is divided into k pairs of subsets, TR_i (train) and TE_i (test) such that $TR_i \cup TE_i = DS$ and $TR_i \cap TE_i = \emptyset$ (DS is the whole data set). The term **fold** will be used to refer to each TE_i , although we do not assume that k-fold cross-validation is being used – almost all cross-validation procedures can be used.

For the data in this research, the mean of a 4-fold cross-validation was calculated for each algorithm on each data set. Additionally, the folds were fixed and identical for all

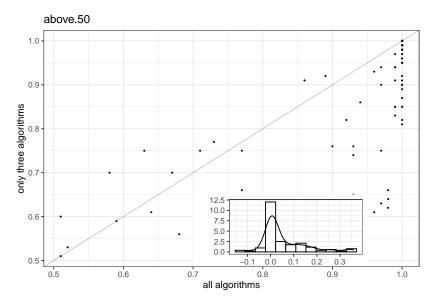


Figure 4: The results for above.50 of comparing 3 algorithms when all 16 algorithms' results are fed to BBT (on a random sample of 20 data sets) and when only the results for the three algorithms are fed to the BBT procedure. The inset is the distribution of the differences between the two average probability of winning.

| db | \mathbf{dt} | lda | lgbm | \mathbf{xgb} | \mathbf{svm} |
|-----|---------------|-------|-------|----------------|----------------|
| cmc | 0.455 | 0.513 | 0.525 | 0.524 | 0.544 |

Table 7: Detail of the base results for the cmc data set

algorithms, meaning that for the first fold, all algorithms were trained on TR_1 and tested on TE_1 , and so on.

Let us consider the entries for the "cmc" data set from Table 2, repeated in Table 7. The entries for the lgbm and xgb algorithms are 0.525 and 0.524, respectively. Although the difference between these two values is small, it still counts as a win for lgbm, just as the much larger difference in accuracy between dt and lgbm also counts as a win.

If we examine the performance of the algorithms on each fold separately, as displayed in Table 8 for the "cmc" data set, the small difference in accuracy between lgbm and xgb becomes even less convincing as a win for lgbm. In this case, since we used the same fold 1, fold 2, etc. for all algorithms, it is reasonable to compare the performance of each algorithm on each fold. In this scenario, lgbm wins on two of the four folds, but loses on the other two. As a result, if we use the individual folds as evidence instead of the mean of their results, lgbm would receive two wins and xgb would receive two wins, rather than a single win for lgbm based on the mean accuracy.

From another perspective, if we take into account the standard deviations of the measures on the folds for each algorithm, as shown in Table 8, the difference in the means of both algorithms (0.001) is much smaller compared to the standard deviations (0.02 and 0.03). In some intuitive sense, the difference in the averages that led to the win for lgbm is much

| db | fold | lgbm | \mathbf{xgb} | diff |
|----------------------|------|-------|----------------|-----------------------|
| cmc | 1 | 0.547 | 0.531 | 0.016 |
| cmc | 2 | 0.522 | 0.538 | -0.016 |
| cmc | 3 | 0.503 | 0.481 | 0.022 |
| cmc | 4 | 0.527 | 0.546 | -0.019 |
| sd | | 0.018 | 0.029 | 0.001 |

Table 8: Detail of the base results for the cmc data set

smaller than the "noise level" of the evaluation procedure itself, given the variability of the measures within each classifier in the folds.

There are two ways of interpreting the results: one that takes into account each fold as individual sources of evidence to determine the wins and losses of the algorithms, and another that considers the difference between the means across all folds while also taking into account the "noise level" derived from the variability among the folds. Both methods aim to reduce the strength of evidence that lgbm won over xgb, resulting in a tie between the two algorithms.

In this research, we will adopt the latter approach, the one that considers the "noise level." We argue that a difference of 0.001 in the means, given that the variability of the measures in the folds for each classifier is at least 10 times higher, should not be considered a win, but rather a tie between the two algorithms. We refer to this approach as the **local ROPE**, which is a threshold below which differences between two classifiers are considered unimportant and would not count as a victory to one of the algorithms. However, as we will see, the local ROPE is not a fixed value but it depends on the results of the two algorithms on the different folds.

In regards to the first line of reasoning, where the folds are used as the source of evidence for wins and losses, we believe that issues such as the dependence of the fold results on each other would make the analysis too complex. This conclusion was also reached by Benavoli et al. (2017) in their analysis, and as such, we will leave this approach for exploration in future research.

6.1 Local ROPE threshold

In almost all statistical tests, one has two sets of measures and the goal is to determine whether there is enough evidence that the difference of the means (or some other summary measure) of the two sets is "real" or not. This is exactly the problem in hand: should one consider the difference of the means of the folds as "real" – and thus that one algorithm wins over the other – or not?

Cohen's D is a measure of effect size between two sets of data. If the two sets have the same number of data, as it is our case, the Cohen's D is computed as the difference between the means, divided by an "average" standard deviation of the two sets, where the "average" standard deviation is actually the square root of the average variance of the two sets. This is displayed in Equation 3 where μ_1 and σ_1 are the mean and standard deviation of the fold measures for the first algorithm, and similarly μ_2 and σ_2 for the second algorithm.

Cohen's D is the measure of the separation between the the means of two sets of measures as a proportion of the standard deviation, and can be seen as a signal-to-noise ratio measure: the difference in means is the signal, and the "average" standard deviation is the noise.

$$d = \frac{\mu_1 - \mu_2}{\sqrt{\frac{\sigma_1^2 + \sigma_2^2}{2}}} \tag{3}$$

We can compute the Cohen's D of two sets of fold measures, and consider that there is no important difference, and thus, a tie between the two algorithms, if the D is below a threshold d_{\min} which we will call the **local ROPE threshold**. Therefore, if:

$$|\mu_1 - \mu_2| \le d_{\min} \sqrt{\frac{\sigma_1^2 + \sigma_2^2}{2}} \tag{4}$$

we should consider that there was a tie between algorithms 1 and 2 for that data set.

We will argue that the threshold can be safely set to the value of 0.4 using the theory of power analysis for t-tests. Type 1 and type 2 errors in statistical test are a false positive (claiming that there is a difference when there is no difference) and a false negative error (claiming that there is no difference when there is one), and their probabilities are indicated by α and β . The power analysis relates α , β , the effect size of the measure, and the number of samples in each set. Unfortunately, the relation between these variables is almost never displayed as an equation, but as tables (Cohen, 1988, ch. 2) or embedded into programs, such as G*power (Faul et al., 2007) or the pwr R package (Champely, 2020). We will show the results of running the pwr package.

For our present goals, there is no conceptual difference between false positive and false negative errors. We want to find out whether the two sets of fold measures indicate that the difference between the means is "real" or "not real", and erring to one side is not worse than erring to the other. Thus, let us assume a 30% probability of making a mistake, both false positive or false negative, that is, $\alpha = 0.3$ and $\beta = 0.3$. Assuming a Cohen's D of 0.4, the necessary number of data in each set is given by running the pwr function. In that function sig.level is α , poweris $1 - \beta$, and d is Cohen's D.

That is, one would need at least 30 measures in each set to be able to find a true difference or a true non-difference with 70% probability. But the traditional cross-validations in machine learning are from 3 to 10 folds. That is, using the usual cross-validation in machine learning, a minimum effect size of 0.4 is very safe - one would not be able to detect differences whose effect sizes are 0.4 or below, if one requires a 70% of sensitivity

and specificity. If one is using 10 repetitions of 10-folds as cross-validation, one can use $d_{\min} = 0.2$.

The discussion above assumes that the two samples of fold measures are not paired, that is, that possibly different folds were used in the evaluation of the different algorithms. But if researchers have control over it, they can use the same folds for all algorithms. For the paired case, the definition of Cohen's D is somewhat different than the one presented in Equation 3. Instead of dealing with the mean and standard deviations of the two sets, one should compute the mean and standard deviation of the differences between the corresponding paired data in the two sets. In Equation 5, $\mu X_1 - X_2$ is the mean and $\sigma_{X_1-X_2}$ the standard deviation of the pairwise differences of the corresponding folds for algorithm 1 and 2,

$$d_z = \frac{\mu_{X_1 - X_2}}{\sigma_{X_1 - X_2}} = \frac{\mu_1 - \mu_2}{\sigma_{X_1 - X_2}} \tag{5}$$

The power analysis for paired samples is also somewhat different, and with the same numbers as before ($\alpha = 0.3$ and $\beta = 0.3$), and using Equation 5 for the effect size calculation, the resulting lower bound for the number of samples is 15, lower than the case for unrelated samples, but still well above the usual number of folds used in machine learning evaluations.

The same decision process as described in 4 can be followed, using the same d_{min} threshold of 0.4, but using the paired definition for the effect size.

$$\mu_1 - \mu_2 \le d_{\min} \sigma_{X_1 - X_2} \tag{6}$$

6.2 How to deal with ties?

The local ROPE concept introduces new ties to the win/loss table, as it is designed to do. The standard ways of dealing with ties in the Bradley-Terry model are:

- add: add the ties as victories to both players involved.
- spread: add the ties as half a victory to each player involved
- forget: do not add ties as victories to any of the players.

Another alternative is to use an extension of the Bradley-Terry model that includes ties, for example, the one proposed by Davidson (1970). The Davidson model is displayed in Equation 7 and it includes a new parameter ν , similar to the β_i . ν controls how likely are

ties "in that sport", despite the differences between the players. If $\nu \to -\infty$, the probability of a tie between player *i* and player *j* will be 0, meaning there are no ties; if $\nu \to \infty$, P(i ties j) will be 1, regardless of the players' different β . Finally, for $\nu = 0$, and if $\beta_i = \beta_j$ then the probability of a tie is 1/3.

$$P(i \succ j \mid \text{no tie}) = \frac{\exp \beta_i}{\exp \beta_i + \exp \beta_j + \exp(\nu + (\beta_i + \beta_j)/2)}$$
(7)
$$P(i \text{ ties } j) = \frac{\exp(\nu + (\beta_i + \beta_j)/2)}{\exp \beta_i + \exp \beta_j + \exp(\nu + (\beta_i + \beta_j)/2)}$$

We will compare the various policies for dealing with ties, using a repeated experiment as described above. To evaluate how well each policy fits the actual data, we will use the posterior predictive check and the WAIC. With respect to the WAIC, while the numerical value itself can be difficult to interpret, when comparing two models, a lower WAIC value indicates a better fit.

Table 9 presents the average results of the WAIC and PPC for the repeated experiments comparing various methods for handling ties. These results are based on averaging across the ss, mm, sl use cases, and the $\ell\ell$ -results, taking into account whether the local ROPE or the paired local ROPE was used. The results clearly demonstrate that the Davidson model is significantly inferior to the others in terms of both WAIC and PPC. The add, forget, and spread policies are all equivalent, and for the purpose of this paper, we have arbitrarily chosen to use the spread policy.

The poor performance of the Davidson model is unexpected, given that it was specifically designed to handle ties, while the other policies are *ad hoc* in nature. Table 10 further illustrates this point, as the PPC summary shows that the wins and ties are not well-calibrated according to their corresponding HDI.

7. BBT as a prediction

Frequentist methods can be seen as decision procedures: given the data available, which algorithms can be said to be better than others. However, they do not make predictions about future data. The result of a frequentist test, such as a non-significant difference between two algorithms does not necessarily indicate that future data from new data sets will also not be significantly different. Given new data, the previously non-significant difference may become significant.

On the other hand, Bayesian methods can make predictions. For example, the output of the BBT model as shown in Table 4 can be considered as probabilities of one algorithm being better than the others for future data sets. There are two different predictions in the BBT model, as discussed in Section 5.6. In the strong interpretation, the *mean* measure predicts the proportion of wins for the better algorithm compared to the worse for future data sets. In the weak interpretation, the *above.50* measure predicts the proportion of wins for the better algorithm compared to the worse. In this section, we will test both of these predictions.

We conducted a series of experiments with the aim of determining the accuracy of predictions on future data sets. For each sample of a training ss table, we sampled 10 additional

| policy | waic | h50 | h90 | h95 | h100 |
|---------------|---------|------|------|------|------|
| SS | | | | | |
| add | 42.41 | 0.87 | 1.00 | 1.00 | 1.00 |
| davidson | 118.59 | 0.40 | 0.78 | 0.86 | 1.00 |
| forget | 40.27 | 0.78 | 0.99 | 1.00 | 1.00 |
| spread | 41.41 | 0.82 | 1.00 | 1.00 | 1.00 |
| mm | | | | | |
| add | 225.51 | 0.73 | 1.00 | 1.00 | 1.00 |
| davidson | 873.01 | 0.29 | 0.58 | 0.66 | 0.88 |
| forget | 227.61 | 0.61 | 0.96 | 0.99 | 1.00 |
| spread | 223.76 | 0.68 | 0.99 | 1.00 | 1.00 |
| \mathbf{sl} | | | | | |
| add | 61.62 | 0.81 | 0.97 | 0.99 | 1.00 |
| davidson | 325.65 | 0.21 | 0.51 | 0.56 | 0.78 |
| forget | 65.46 | 0.67 | 0.95 | 0.97 | 0.99 |
| spread | 62.25 | 0.75 | 0.97 | 0.99 | 1.00 |
| 11 | | | | | |
| add | 760.49 | 0.57 | 0.95 | 0.97 | 1.00 |
| davidson | 4730.36 | 0.17 | 0.38 | 0.43 | 0.70 |
| forget | 823.52 | 0.39 | 0.85 | 0.91 | 0.99 |
| spread | 773.98 | 0.47 | 0.92 | 0.95 | 1.00 |

Table 9: The PPC for the different policies. WAIC is the mean WAIC result; h50 is the proportion of observed values that fall in the 50% HDI; h90, h95, and h100 are the proportions for the 90%, 95% and 100% HDIs.

| hdi | proportion | ties |
|------|------------|------|
| 0.50 | 0.23 | 0.23 |
| 0.90 | 0.48 | 0.45 |
| 0.95 | 0.52 | 0.48 |
| 1.00 | 0.89 | 0.81 |

Table 10: The Davidson model on the large-large results. Ties is the proportion of ties that fall within the corresponding HDI for the ties generated data.

data sets not used in the training sample, and evaluated the performance of each pair of algorithms on these test data sets. We counted the number of times one algorithm outperformed the other and referred to this count as "win1" for algorithm A1 and "win2" for algorithm A2. We did not apply local ROPE to the test data. The ratio win1/(win1+win2) is the *empirical estimate* of the probability that algorithm A1 is better than algorithm A2 on future test data sets.

For the strong interpretation, we examine the fit between the distribution of probability estimates $P_s(1 \geq 2)$ and the empirical probability win1/(win1+win2). Similar to the PPC summary table, we calculate the 50%, 70%, and 90% highest density intervals (HDIs) of each distribution (for each pair of algorithms) and compare the proportion of empirical probabilities that fall within these intervals. In a well-calibrated distribution, 50% of the empirical probabilities should fall within the 50% HDI and so on. We also determine the proportion of empirical probabilities that fall outside of the 90% HDI, both above its maximum value and below its minimum value. Finally, we calculate the mean error and the median absolute difference (MAD) between the mean prediction and the empirical probability.

For the weak interpretation, we do not have a distribution and therefore cannot use the same evaluation procedure as previously described. The *above.50* measure provides a probability statement, and we want to assess its accuracy. We will use the calibration plot procedure commonly used for classifiers. We divide the range of *above.50* values into three bins and compare the actual and expected number of cases where win1 > win2. The actual number of cases is determined from the test data where *above.50* falls within the limits of the bin. The expected number of cases is the sum of *above.50* values in that bin. Typically, calibration plots divide probability estimates into 10 bins, but for this analysis, we have divided *above.50* into three bins: from 0.5 to 0.7, from 0.7 to 0.9, and from 0.9 to 1.0. This division represents low confidence (0.5 to 0.7), middle confidence (0.7 to 0.9), and high confidence (0.9 to 1.0) in the superiority of algorithm A over B.

Table 11 shows the results of the strong interpretation evaluation. The predictions made by the BBT are not well-calibrated, as a much smaller proportion of empirical probabilities falls within the different HDIs than expected. In all cases, less than 50% of the empirical probabilities fall within the 90% HDI, which should contain 90% of them. The values of *above90* and *below90* are somewhat similar, indicating that the BBT model is not systematically overestimating or underestimating the probability that one algorithm is better than another. The miss-calibration of the strong interpretation of the parameter is a problem of variance (incorrectly predicting the range of possible values) rather than a problem of bias (incorrectly predicting the most probable value). The mean prediction errors are low, ranging from 0.02 to 0.01, suggesting low bias. Therefore, we conclude that the BBT is calibrated for its mean prediction, but too overconfident in the range of possible values, its credal interval.

The inclusion of the local ROPE was intended to serve both aesthetic and practical purposes. On one hand, it was included to address the issue of small differences that occur when computing average of cross-validations still counted as wins for one algorithm. On the other hand, local ROPE also aimed to reduce the model's overconfidence in its certainty regarding the estimates. The local ROPE reduces the number of wins for one algorithm over another, which should result in a decrease in the BBT's confidence in the probability that one algorithm is better than the other, thereby widening the credal interval. However,

| lrope | paired | within.90 | within.70 | within.50 | above90 | below90 | err | mad |
|------------------------|--------------|-----------|-----------|-----------|---------|---------|-------|------|
| ss | | | | | | | | |
| F | F | 0.39 | 0.25 | 0.15 | 0.33 | 0.28 | 0.00 | 0.13 |
| Т | F | 0.44 | 0.25 | 0.14 | 0.33 | 0.23 | -0.01 | 0.12 |
| Т | Т | 0.42 | 0.23 | 0.13 | 0.33 | 0.25 | -0.01 | 0.13 |
| $\mathbf{m}\mathbf{m}$ | | | | | | | | |
| F | F | 0.33 | 0.22 | 0.16 | 0.37 | 0.31 | 0.00 | 0.08 |
| Т | F | 0.34 | 0.22 | 0.14 | 0.39 | 0.27 | -0.01 | 0.08 |
| Т | Т | 0.32 | 0.22 | 0.16 | 0.41 | 0.27 | -0.01 | 0.08 |
| \mathbf{sl} | | | | | | | | |
| F | \mathbf{F} | 0.40 | 0.22 | 0.14 | 0.48 | 0.12 | -0.06 | 0.07 |
| Т | F | 0.38 | 0.26 | 0.14 | 0.50 | 0.12 | -0.07 | 0.07 |
| Т | Т | 0.34 | 0.20 | 0.12 | 0.54 | 0.12 | -0.06 | 0.06 |

Table 11: Prediction results - strong interpretation. Lrope and paired indicate whether local rope and the paired version of local rope was used. Within90 indicates the proportion of empirical win probability that falls within the 90% HDI. Similarly for within70 and within50. Above90 is the proportion of empirical win probability that falls above the higher limit for the 90% HDI; err is the mean error between the mean and the empirical win probability; and mad is the mean absolute error.

as Table 11 indicates, the introduction of the local ROPE has limited impact in widening the credal interval, although it did have a small impact in reducing the error.

Table 12 presents the results of the weak interpretation calibration. The results indicate better calibration compared to the strong interpretation. The predictions for the range of 0.5 to 0.7 are few and align closely with the empirical results for all three use cases. Similarly, the predictions for the range of 0.7 to 0.9 are accurate. However, for the high confidence range of 0.9 to 1.0, the predictions appear to be slightly overconfident, slightly higher than the empirical value. The BBT model seems to have an over-confidence in its predictions, and the introduction of the local ROPE and paired local ROPE had no effect on reducing this over-confidence.

8. Discussion

The Bradley-Terry formalism seems simple but sufficiently complex to model a comparison of machine learning algorithms on multiple data. The predictive posterior check shows that the Bayesian model is indeed a good model of the data that was given, and it showed that a more complex model such as Davidson's is not needed and it worsens the fitness between the model and the data. The model is not sensitive to different reasonable hyper priors (Wainer, 2022), and the test on different policies to deal with ties (Section 6.2), besides using the Davidson model, are basically equivalent. All this should point to the conclusion that the model is stable to different decisions, and it is generally a good fit to the data.

| WAI | NER |
|-----|-----|
|-----|-----|

| lrope | paired | pred50-70 | real50-70 | pred70-90 | real70-90 | pred90-100 | real90-100 |
|------------------------|--------------|-----------|-----------|-----------|-----------|------------|------------|
| ss | | | | | | | |
| F | \mathbf{F} | 4.3 | 3 | 13.8 | 11 | 75.3 | 64 |
| Т | F | 8.1 | 7 | 10.7 | 7 | 73.3 | 63 |
| Т | Т | 6.1 | 4 | 11.1 | 8 | 75.2 | 65 |
| $\mathbf{m}\mathbf{m}$ | | | | | | | |
| F | \mathbf{F} | 11.5 | 7 | 27.4 | 25 | 394.8 | 361 |
| Т | \mathbf{F} | 9.9 | 8 | 25.2 | 20 | 398.4 | 370 |
| Т | Т | 9.0 | 12 | 33.1 | 25 | 392.0 | 363 |
| \mathbf{sl} | | | | | | | |
| \mathbf{F} | \mathbf{F} | 1.9 | 2 | 0.0 | 0 | 46.6 | 45 |
| Т | F | 2.0 | 3 | 0.0 | 0 | 46.5 | 45 |
| Т | Т | 2.0 | 3 | 0.0 | 0 | 46.5 | 45 |

Table 12: Prediction results - weak interpretation. Lrope and paired indicate whether local rope and the paired version of local rope was used. Pred50-70 is the expected number of examples whose empirical win probability should fall within the [0.50,0.70] probability range; real50-70 is the observed number of empirical wins in that range. Similarly for the other pairs of columns.

As we already mentioned, the model is simple, the MCMC converges well with few samples, and our implementation (thanks to Stan's MCMC) runs in less than a second in a modern laptop.

Regarding the "predictive" part of the model it is yet unclear whether the apparent overconfidence of the model, specially under the strong interpretation is a problem. Since no frequentist test can make predictions, and the BSR did not test its predictive fitness, we do not have an alternative to compare against.

8.1 Code and data availability

An R package (bbtcomp) that implements the BBT model is available at https://github. com/jwainer/bbtcomp. To install it use remotes::install_github("jwainer/bbtcomp"). The R package uses the cmdstanr package to interface with Stan, which implements the MCMC sampler. At the time of the writing, cmdstanr is not available in CRAN, and should be installed following the instructions in https://mc-stan.org/cmdstanr/.

A Python program that implements all functionalities of the R package implementation the BBT model with the exception of the graphic generating functions, is available in the github directory above, in the folder python. The program also uses the cmdstanpy interface to Stan. The Rmarkdown version of this paper is available in the github directory above, in the folder paper.

8.2 How to use the BBT model - weak interpretation and 0.95 probabilities

We believe that there are two main approaches to utilizing the BBT model in research. For researchers or audiences who are more familiar with the frequentist approach, we recommend using the summary values related to the weak interpretation of the parameters (the *above.50* and *in.rope* values) and a 0.95 probability threshold. This approach utilizes familiar threshold numbers such as 0.95 or 95%.

The guidelines for this approach are as follows:

- If the *in.rope* value is 0.95 or above, the researchers can claim that the two algorithms are equivalent (according to the definition of ROPE).
- If *above.50* is 0.95 or above, the researchers can claim that one algorithm is better than the other. If both *in.rope* and *above.50* are above 0.95, the first rule applies, and researchers should claim that the algorithms are equivalent.
- For all other cases, researchers should not make any claim.

The BBT model also allows one to make claims of equivalence (when $in.rope \ge 0.95$) that are not possible in the frequentist case.

As we will see in Section 8.4 below, the weak interpretation will find more examples of significant differences that both frequentist and the BSR approaches.

Finally, the BBT model is reasonably well-calibrated although slightly overconfident regarding high values of *above.50*, so for the pairs with "significant" differences the researcher can make the claim that, *likely* with 90% probability or better, the best algorithm should perform better than the worse for *future data sets*. The claim for future data sets can be made even for comparisons that are not "significantly" different. If algorithm A has an *above.50* of 0.8 in relation to B, then it is not "significantly" different than B, but one still can make the claim that A will perform better than B with 80% probability (or a bit lower) on future data sets.

8.3 How to use the BBT model - strong interpretation and 0.70 probabilities

If researchers and their audiences are more comfortable with Bayesian results, we recommend following the strong interpretation (and the *mean* summary of the probabilities) and choosing a threshold of 0.70. The procedure is as follows:

- If *mean* is below 0.55, one can claim that both algorithms are equivalent.
- If *mean* is above 0.70, one can claim that one algorithm is "significantly" better than the other.

As we will see in Section 8.4, the strong interpretation will find the same number of significant differences that the other methods for a low number of algorithms and data sets. For cases of a high number of algorithms or a high number of data sets, the strong interpretation may find less significant differences.

For *future data sets*, the researcher can make the claim that the *most likely* value for the probability that A is better than B is 70% or better. The low predictive bias allows for such

| SS | | mm | | sl | | 11 | | |
|----------|------|--------------------------|-----|--------------------------|-----|--------------------------|-----|--------------------------|
| Method | sig | not sig | sig | not sig | sig | not sig | sig | not sig |
| strong | 49 | 51 | 180 | 270 | 23 | 27 | 54 | 66 |
| weak | 70 | 30 | 380 | 70 | 45 | 5 | 112 | 8 |
| Demsar | 31 | 69 | 177 | 273 | 34 | 16 | 70 | 50 |
| Wilcoxor | n 45 | 55 | 226 | 224 | 40 | 10 | 92 | 28 |
| BST | 65 | 35 | 313 | 137 | 41 | 9 | 92 | 28 |

Table 13: The comparisons of BBT and the previous comparison procedures. sig is the number of pairs of comparisions found significant by each method.

a claim, but the high variance does not allow for a credal interval to be defined for these estimates. Again, the claim of probabilities of performing better for future data sets can be made also for differences that are not "significant" according to the 0.70 threshold.

Finally, as discussed in section 5.7, the strong interpretation is somewhat independent of the number of algorithms being compared, and thus can be used in these situations.

8.4 Comparison with previous procedures

Table 13 compares the number of significant pairs found using the different comparison procedures: BBT under the strong and weak interpretations, Demsar, pairwise Wilcoxon, and BSR. We should remind the reader that it is unclear whether the BSR should be used in multiple comparisons. Also Benavoli et al. (2017) suggest that is a decision procedure similar to BBT's weak interpretation if the probability that the difference between the means falls above the 0.01 ROPE is above 0.95, one can declare the difference as "significant".

Table 13 shows that BBT under the weak interpretation find more significantly different pairs of comparisons than the other methods. BBT under the strong interpretation, is comparable to the other method for a small number of algorithms and datasets, but as each of those to sized increase, BBT under the stong interpretation will find less significantly different pairs.

9. Conclusion

The BBT model is a comparison procedure based on the Bradley-Terry model that assigns a merit value to each of the competing algorithms. The merit values determine the probability of an algorithm performing better than another on a data set. The BBT model is a Bayesian implementation of the Bradley-Terry model and offers several advantages over traditional frequentist approaches:

• It allows for a more nuanced description of the relationships between each pair of algorithms in the aggregated ranking, beyond simply determining whether the difference is significant or not.

- It enables the definition of a threshold below which two algorithms are considered equivalent for practical purposes and allow researchers to make claims about whether two algorithms are equivalent or not.
- It provides an understanding of the uncertainties associated with the claims.

In addition to the advantages of Bayesian estimation, the BBT model also:

- Works with any metric of interest, regardless of whether it is comparable or not.
- The main parameters are probabilities, making it easier to understand the definition of ROPEs, uncertainties, and so on.
- Accommodates missing data for algorithms that did not run on certain data sets.

Finally, we also introduced the idea of local ROPE, which is a method for determining when one algorithm can be considered truly better than another for a specific data set, based on their average performance across different folds. We believe that local ROPE can also be a useful addition to frequentist tests, particularly rank-based tests.

This paper did not dedicate extensive space to the defense of Bayesian testing methods. For a more in-depth examination of the advantages of Bayesian testing, we refer the reader to the work of Benavoli et al. (2017), which not only presents the BSR model but also makes compelling arguments for the machine learning community to transition away from frequentist tests and towards Bayesian tests. The author of this paper agrees with these arguments and recommendations.

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