# A Review of and Best Practices for Comparing Machine Learning Models

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**Abstract**

Comparing the performance of two or more different models is very common in machine learning. Despite this, it is often poorly done. The goal of this paper is to review the issues involved, and to provide guidance on best practices for comparing machine learning models. We cover: clarifying the question to be answered; factors of variation and experimental design; and frequentist and Bayesian statistical tests, especially highlighting paired testing. Because of well-known issues with null hypothesis significance testing, we follow Benavoli et al. (2017) in recommending Bayesian approaches. We provide two worked examples of such analyses, and a checklist for best practice.

In machine learning we often wish to compare two or more different models. For example, consider a problem like detecting malaria parasites in red blood cells, where the task is to classify each red blood cell as infected or not.[1] We may wish to compare a new method for this task with some standard models. This is a very common type of task in machine learning, but despite this very few textbooks in the field give advice on how to do this, and in my experience (as a reviewer of papers) this comparison is often badly done, despite the fact that there is a good literature on the topic. For example, of five papers I reviewed for a recent top-tier conference, only one had a satisfactory treatment of model comparison. The goal of this paper is to review the issues involved, and to provide guidance on best practices for comparing machine learning models.

## 1 What is the question we wish to answer?

Dietterich (1998) provides a nice taxonomy of questions that we may seek to answer. Firstly, is the focus on a single task, or on multiple tasks? In much applied research, a single task is of interest (like red blood cell classification mentioned above). But in more core machine learning research, the goal is to find learning algorithms that work well across a range of tasks.

Within a single task, the next question is if we are interested in comparing *predictors* or *learning algorithms*? In supervised learning we have input-output pairs $(x, y)$. A predictor takes

[1] This task is studied, for example, in Quinn et al. (2016).

in an input $x$, and makes a prediction for its associated output; this may be a classification label, a real-valued prediction, or some other kind of output. In contrast, a learning algorithm takes in a dataset of input-output pairs, and constructs a predictor. For the red blood cell classifier it may make sense to develop models that are used universally—in this case we wish to compare predictors. But these predictors will have been trained using learning algorithms on a particular dataset, and it is of interest to know how the performance of the predictors will change as the training datasets vary; this is the comparison of learning algorithms.

Benchmark problems like the PASCAL VOC contest (Everingham et al., 2010) and ImageNet (Deng et al., 2009) are usually concerned with comparing predictors which have been trained using a development set. This is used for model training and selection,[2] and the resulting predictor is then applied to the previously-unused test set to assess its performance.

Multiple tasks can arise from a set of related problems drawn from a distribution over tasks; this is termed a *context* by Lacoste et al. (2012). Examples of contexts are the 20 (binary) object class prediction problems in the PASCAL VOC contest, or the more diverse collection of 54 datsets selected from the UCI collection for Table 1 in Benavoli et al. (2017).

If there are multiple predictors or learning algorithms, it is also necessary to consider exactly what comparisons are being made. If we are running a contest such as the PASCAL VOC competition, we may care about establishing if the best performing method is significantly different to others. If we are proposing a new method, we may wish to establish if its performance is better, similar or worse than each of the other competitor methods. (This is a very common situation in machine learning papers where a new method is introduced.) Or we may wish to compare the performance of all algorithms against each other, and assess if there are significant differences.

We summarize the different questions as:

Q1: Comparison of predictors on a single task;

Q2: Comparison of learning algorithms on a single task;

Q3: Comparison of learning algorithms across multiple tasks.

# 2 Assessing predictions: Loss

When making comparisons, it is important to consider what is an appropriate measure of the loss of a predictor, based on the difference between the prediction made for an input value $x$ and the observed value $y$. For example in binary classification problems, one can obtain a "hard" prediction for each test example (e.g., by thresholding a probabilistic output at some value), and use the 0/1 loss, i.e. having zero loss if the labels agree, and 1 otherwise. But it may be important to consider the relative importance of false positives and false negatives, ascribing different losses to these situations, and setting the threshold to minimize the expected loss (a.k.a. risk). Another alternative is to use the log loss, $-\log p_{\text{model}}(y|x)$. Or one could summarize the probabilistic results on a test set using a receiver-operating-characteristic (ROC) curve, and assess the quality of the results using the area under the ROC curve (AUROC); note that this implicitly uses all possible thresholds.

For regression problems one commonly considers mean squared error (MSE), root mean squared error (RMSE), mean absolute error (MAE) or log loss. See, e.g., Rainio et al. (2024)

[2]The development set may be split into training and validation parts in order to carry out model selection.

for further measures for evaluating predictors on a variety of problems. In natural language processing one might use measures like BLEU or ROUGE scores (see, e.g., Dror et al. 2020) to define the loss. In all cases it is important to consider which metric best fits with the practical application of the predictor.

# 3 Factors of variation and experimental design

The problem we seek to address here is to compare two or more predictors or learning algorithms. It is important to note that this kind of question is ubiquitous in science; for example we may wish to compare the efficacy of a new drug treatment for a particular condition against a standard treatment (or placebo), or the yield a new crop variety against an older one. In all cases we seek to *design an experiment* to answer the question. See, for example, Montgomery (2013) for a discussion of experimental design.

In experimental design it is important to distinguish *fixed* and *random* factors of variation. Fixed factors are those of interest to the experimenter, and the experiment assesses specific values of these factors. In contrast, random factors have values that are chosen at random from a large set of possible values, and the aim is to *generalize* to new values of these factors.

If we apply these ideas to Q1, the comparison of predictors, then clearly a fixed factor is the predictor used, and a random factor is the test set consisting of $N$ $(x, y)$ pairs sampled from the distribution $p(x, y)$ that we wish to generalize over. But with methods such as neural networks, there are many other factors that give rise to variation; model architecture, random initialization of the weights, the order of the training examples (if using mini-batch training), weight decay parameters, and so on. For random factors such as weight initialization, we assume (following Rasmussen 1996b, sec. 2.1) that the loss should be defined by *averaging* over such factors. However, for method hyperparameters (such as the architecture or weight decay parameters) we will assume that these have been *optimized*, e.g., by using a validation set within the development dataset.

Another example of fixed and random effects occurs in Q2, the comparison of learning algorithms. Here as well as the fixed effect of the choice of learning algorithm, there is a random effect coming from the different training sets. The choice of test set is also a random factor (as above), but for simplicity we might assume that the common test set has large size, so we can ignore the variability that arises from this source. When comparing learning algorithms, the ideal situation statistically is to have multiple *independent* training sets (of size $n$) available, all drawn from the same distribution $p(x, y)$. This can be hard to achieve if there is limited real-world data without making the training sets very small, but it can be achieved for synthetic data. For real-world data it is tempting to use some form of resampling such as cross-validation or the bootstrap, but this gives rise to complications in the statistical analysis of the results, as the training sets are no longer independent. One example of how to handle this is (frequentist or Bayesian versions of) the correlated $t$-test described in Benavoli et al. (2017).

For Q3, we will take as fixed effects the different learning algorithms used, but we now consider the set of tasks used as *random effects*, drawn from some distribution over tasks. We then wish to compare the performance of different learning algorithms, generalizing over the choice of specific tasks, to make inferences for the distribution over tasks. We may still have to worry about additional variability arising from training and test sets.

One advantage in machine learning experiments is that we often have what are termed

*repeated measures*.[3] For example, we can use the same training and test datasets for all algorithms. This is in contrast to some other research areas, where, for example, when testing the efficacy of drug A vs drug B for treating a disease, we can only usefully give either drug A or drug B to a particular experimental subject (or test case). An advantage of a repeated measures design is that we can compare the *difference* in losses between two predictors on the same test case; generally such *paired testing* is more powerful, as it removes random variation due to differences in hardness between test cases. See Appendices A and B for an illustration of this for MSE loss.

A standard linear model that can take into account the fixed and random factors is the 2-way analysis of variance (ANOVA) model:

$$z_{ij} = \mu + \alpha_i + \beta_j + \epsilon_{ij}, \tag{1}$$

see e.g., Montgomery (2013, ch. 13). Here there are two discrete factors, indexed by $i$ and $j$. $z_{ij}$ denotes the loss incurred under the combination $(i, j)$, $\mu$ is the overall mean, $\alpha_i$ denotes the effect of factor $i$ (for $i = 1, \ldots, a$) and $\beta_j$ denotes the effect of factor $j$ (for $j = 1, \ldots, b$), and $\epsilon_{ij}$ is a random error term. It is assumed that $z_{ij}|\mu + \alpha_i + \beta_j \sim N(0, \sigma^2_\epsilon)$. We can consider the case where $i$ indexes a fixed factor, and $j$ a random factor. To ensure identifiability of the parameters, it is imposed that $\sum_i \alpha_i = 0$. The random effects, the $\beta_j$'s, are assumed to be independent and distributed as $N(0, \sigma^2_\beta)$. In general ANOVA is not limited to two factors (it can have one, or more than two) and each one can be fixed or random, but for simplicity we describe the two-factor mixed effects model here. One can also consider not only the "main effects" due to the individual factors, but also interaction terms; for example a term $\gamma_{ij}$ taking on $ab$ values could be included in eq. 1.

One can carry out frequentist or Bayesian inference for the ANOVA model. For example, Montgomery (2013, sec. 13.3) describes describes the estimation of the parameters ($\mu$, the $\alpha_i$'s, $\sigma^2_\epsilon$ and $\sigma^2_\beta$) for the 2-factor mixed effects model. One can also give a Bayesian treatment of this hierarchical linear model, as described, for example, in Gelman et al. (2013, sec. 15.6).

For Q1 (comparison of a number of different predictors for a given task on the basis of a common test set), $z_{ij}$ is the loss of predictor $i$ on test case $j$,[4] $\alpha_i$ ($i = 1, \ldots, a$) is the fixed effect of predictor $i$ and $\beta_j$ ($j = 1, \ldots, b$) is the random effect of test case $j$. $\epsilon_{ij}$ is the residual variation in losses unexplained by the model.

The above 2-way ANOVA model can also be used for Q2, the comparison of machine learning algorithms, taking into account the fixed factor of different algorithms, and the random factor being the choice of independent training sets. Here we have assumed that the test set is large, so that one can use the average loss over the test as $z_{ij}$. Alternatively we could consider a three-factor ANOVA model, with the third (random) factor indexing the test case.

We could also apply the 2-way ANOVA model to Q3. Here the fixed effects are the choice of learning algorithm, but in this case the random effects come from the different tasks (which we wish to generalize over). This choice would ignore variability arising from the training and test sets, but the model could be extended to address this variability.

Note that when considering the comparison of only two algorithms, the 2-way ANOVA model can be simplified somewhat by considering *paired differences*. For example, for Q1 consider the

[3]Also referred to as a within-subjects design; for human subjects this means that the same subjects are exposed to different experimental conditions.

[4]This loss is usually denoted by $y_{ij}$, but to avoid overloading notation from the $(x, y)$ input-output pairs, $z_{ij}$ is used here.

paired difference $d_j^{ii'}$ between predictors $i$ and $i'$ on test example $j$. We then have

$$z_{ij} = \mu + \alpha_i + \beta_j + \epsilon_{ij}, \tag{2}$$
$$z_{i'j} = \mu + \alpha_{i'} + \beta_j + \epsilon_{i'j}, \tag{3}$$

so that

$$d_j^{ii'} \stackrel{def}{=} z_{ij} - z_{i'j} = \alpha_i - \alpha_{i'} + (\epsilon_{ij} - \epsilon_{i'j}). \tag{4}$$

Note that the last term, which is the difference of two errors that are assumed to be normally distributed, is again normally distributed, but with twice the variance of the individual $\epsilon$'s. One could then use, e.g., a paired $t$-test on these differences to assess if the difference between predictors $i$ and $i'$ is statistically significant.

**The key issue for determining if a predictor or a learning algorithm is outperforming its competitors is to assess the variability coming from random factors and noise, in comparison to the differences that arise from the fixed effects (such as the identity of the predictor or algorithm).**

# 4 Literature review

An early paper on the evaluation of machine learning experiments is the technical report from the DELVE development group in Toronto (Rasmussen et al., 1996), where DELVE is an acronym for Data for Evaluating Learning in Valid Experiments. They considered frequentist and Bayesian analyses of ANOVA models to assess various effects, and also made available datasets and software to carry out testing. Example results are available in Rasmussen (1996b). The website `http://www.cs.utoronto.ca/~delve/` still exists, although it appears not to have been updated for many years.

The book *Empirical Methods for Artificial Intelligence* by Cohen (1995) covers issues of experimental design, hypothesis testing, ANOVA etc in relation to AI systems. But it appears not to have have had much impact on the literature for comparing machine learning methods, perhaps because it does not address *learning* problems very much.

Dietterich (1998) has a nice taxonomy of the questions we wish to answer, as described above in sec. 1. He also includes a question as to whether there is a large or small dataset available. If it is large then some data can be held out as a test set; if not some form of resampling such as cross-validation or the bootstrap must be used. Dietterich's main focus is on choosing between learning algorithms when a small amount of data is available (his question 8), with particular attention to type I errors (detecting a difference when no difference actually exists). For algorithms that can only be run once, he recommends McNemar's test (see sec. 5.1 below), while for algorithms that can be executed ten times he recommends the 5x2cv test (5 iterations of 2-fold cross validation). The latter was subsequently improved by Alpaydın (1999), who developed the combined 5x2cv F test that combines multiple statistics to get a more robust test.

Salzberg (1997) also discusses pitfalls to avoid when comparing algorithms, and finally recommends a $k$-fold cross-validation approach, followed by the binomial (sign) test or McNemar's test to assess statistical significance.

Demšar (2006) focuses on the the statistical comparison of classifiers over multiple data sets. He discusses repeated-measures ANOVA, but recommends instead the Friedman test, due to the strong assumptions necessary for ANOVA. This test is described further in sec. 5.1 under Q3.

Hansen et al. (2011) introduce the concept of the model confidence set (MCS), which is a set of models constructed such that it will contain the best model with a given level of confidence. The algorithm is initialized with all the possible models in the candidate set, and then statistical hypothesis tests are used to compare these models. If the null hypothesis that all models are equivalent in performance is rejected, an elimination rule is used to remove a model from the candidate set, and the hypothesis tests are applied again on the reduced set. This continues until the null hypothesis is not rejected.

The book by Dror et al. (2020) is entitled *Statistical Significance Testing for Natural Language Processing*, and covers parametric and non-parametric frequentist tests. Their Table 4.1 recommends appropriate tests for different evaluation measures. The book is motivated by Natural Language Processing (NLP), although most of the discussion is more general, with only the tasks and evaluation measures being NLP-specific.

The recent paper by Rainio et al. (2024) is concerned with evaluation metrics and statistical tests for machine learning. On the latter topic, the authors present a flow chart (their Figure 3) recommending different statistical tests for different questions and tasks. For example McNemar's test is recommended for comparing binary classifiers, and Friedman's test for comparing models over several test sets. Note that these are for the comparison of predictors rather than learning algorithms.

The tests referred to above are in the frequentist null hypothesis significance testing (NHST) framework. In contrast, one can apply Bayesian methods; this issue is discussed further in sec. 5.2. Lacoste et al. (2012) consider Bayesian methods for the comparison of classifiers (using 0/1 loss) on one or multiple tasks. Benavoli et al. (2017) give some Bayesian analyses of experimental results, including a Bayesian correlated t-test, a Bayesian signed-rank test, and a Bayesian hierarchical correlated t-test. These can also be used to compare predictors on one or multiple tasks.

# 5 Statistical testing

In sec. 5.1 we first discuss standard frequentist tests for addressing questions Q1, Q2 and Q3 for the comparison of two algorithms. These include the paired $t$-test, McNemar's test, and Friedman's test (for multiple tasks). We also discuss the effect size and its quantification. In sec. 5.2 we compare Bayesian and frequentist analyses for comparing predictors, and argue for using a Bayesian estimation approach. We follow this with a discussion of the Bayesian $t$-test (sec. 5.3), a Bayesian McNemar's test (sec. 5.4) and Bayesian hierarchical models to handle multiple tasks (sec. 5.5). In sec. 5.6 we discuss the issue of multiple comparisons when comparing multiple predictors. In sec. 5.7 software for carrying out the various tests is described.

## 5.1 Frequentist tests

**Q1:** For the comparison of predictors, the test to use will depend on the loss function. For a real-valued loss, a standard choice would be a paired $t$-test. We compute the difference of the losses of methods A and B on each test case, to obtain a vector of differences $\mathbf{d} = (d_1, d_2, \ldots, d_N)$. Under the null hypothesis $H_0$ the mean loss of methods A and B are equal, so that the mean difference will be zero. Under the alternative hypothesis $H_1$ the mean difference is non-zero. The paired $t$-test proceeds by computing a test statistic $t = \frac{m}{s/\sqrt{N}}$, where $m$ is the mean and $s$ the standard deviation of $\mathbf{d}$. A $p$-value for the test statistic can then be computed under the

null hypothesis, using a two-tailed test (to reflect that under $H_1$ the mean difference can be greater or less than zero). A small $p$-value will provide evidence to reject the null hypothesis.

In the case of 0/1 losses, we can use McNemar's test (see, e.g., Dietterich 1998). We have predictors A and B, and consider the four different outcomes that can occur on a test case: (00) the example is misclassified by both; (01) the example is misclassified by A but not by B; (10) the reverse of the previous case; and (11) the example is correctly classified by both. Let the counts associated with these four outcomes be $n_{00}$, $n_{01}$, $n_{10}$, and $n_{11}$ respectively, with their sum being $N$, the number of test cases. Under the null hypothesis the predictors should have the same error rate, so $n_{01} = n_{10}$. The statistic

$$\frac{(|n_{01} - n_{10}| - 1)^2}{n_{01} + n_{10}} \tag{5}$$

approximately follows the $\chi^2$ distribution with one degree of freedom, where the $-1$ term in the numerator is a "continuity correction". Again a $p$-value can be obtained under the null hypothesis.

In some cases the whole test set is used to produce one number, like the area under an ROC curve (AUROC), or the average precision score (AP) for a precision-recall curve. The DeLong test (DeLong et al., 1988) is a nonparametric test that can be used to compare differences between two AUROC scores, based on the theory of generalized $U$-statistics. It is also possible to use bootstrap replicates of the data to make this comparison, as available in the R function `roc.test`. Everingham et al. (2015) made use of the bootstrap to compare AP scores.

**Q2:** This situation seems to be considered much more rarely in machine learning, but notably the DELVE team did address this question, when using multiple independent training sets and a common test set. Rasmussen (1996a, sec. 2.5) used a 2-way ANOVA model for comparing the difference in losses between methods A and B, with random effects for both the choice of training set and the choice of test example. The goal was to assess if the mean difference is significantly different from zero. This was carried out using a quasi-F test.

If we ignore that test-set variability (by assuming it is of large size) then the question can be simplified, and a paired $t$-test used on the differences in losses over the different training sets. Benavoli et al. (2017) propose a correlated $t$-test when a resampling procedure such as cross-validation is used, so that the training sets are no longer independent.

**Q3:** Demšar (2006) focuses on the the statistical comparison of classifiers over multiple tasks. He discusses a repeated-measures ANOVA analysis, but recommends instead the Friedman test, due to the strong assumptions necessary for ANOVA. The Friedman test assesses the ranked performance of each algorithm on each task, and uses a $\chi^2$ test to compare the observed ranks to the null hypothesis that all algorithms are equivalent.

If the null hypothesis is rejected with the Friedman test, then a post-hoc test (e.g., the Nemenyi test, Nemenyi 1963) can be used to compare pairs of predictors to assesses if the difference in their average ranks is statistically significant. This is similar to the standard ANOVA analysis, where if the null hypothesis that the predictor effect is zero is rejected, "post-hoc" tests are carried out pairwise—see, e.g., Montgomery (2013, sec. 3.5) for further details.

**Effect sizes:** One of the criticisms of NHST is that having enough data can often reject the null hypothesis for arbitrarily small effects (see discussion in sec. 5.2). This can be seen, for

example, in the the $t$-test statistic $t = \frac{m}{s/\sqrt{N}}$, when increasing $N$ makes the statistic larger. To guard against this, it is often recommended that not only a $p$-value but also an effect size be reported, see, e.g., Appelbaum et al. (2018). Cohen (1988, p. 9) defines the effect size as "the degree to which the phenomenon is present in a population". The effect size can be based on properties such as group differences, risk estimates, and indices of association. Below we discuss two examples, Cohen's $d$ and Cohen's $g$, which are used in the worked examples in sec. 6.

Cohen's $d$ is defined as the difference between two means divided by a standard deviation for the data, $d = m/s$ in the notation used above. Note that, in comparison with the $t$-statistic, there is no $\sqrt{N}$ present. For calibration Cohen (1988, p. 40) terms a value of $d = 0.2$ as "small", 0.5 as "medium" and 0.8 as "large".

For 0/1 losses, one can compute $\hat{\phi} = n_{01}/(n_{01} + n_{10})$, the maximum likelihood estimator of the fraction of (01) cases relative to the total of (01) and (10) cases. Under the null hypothesis this fraction would be 1/2, so the difference is $g = \hat{\phi} - 1/2$, which is known as Cohen's $g$ (Cohen, 1988, pp. 147-149). Values of $|g| < 0.05$ are regarded as "negligible", in the interval $(0.05, 0.15)$ as "small", $(0.15, 0.25)$ as medium and $|g| > 0.25$ as "large".

## 5.2 Bayesian and frequentist analyses for comparing predictors

Suppose that we are interested in comparing two predictors A and B. We can evaluate the loss on each test case, and consider paired differences, as in the paired $t$-test discussed in sec. 5.1. We are interested in the parameter $\Delta$, the difference between the expected loss for model A and the expected loss for model B. $\Delta$ is defined as a population quantity, with the average over the distribution $p(x, y)$. However, we only have access to $N$ test samples from this distribution. Below we describe Bayesian and frequentist analyses for this situation.

**Bayesian analysis:** For a Bayesian analysis we combine a prior $p(\Delta)$ with a likelihood model $p(\mathbf{d}|\Delta)$ to obtain a posterior distribution $p(\Delta|\mathbf{d})$ . (This may require dealing with some additional parameters—see, for example, the noise variance $\sigma^2$ in the Bayesian $t$-test described in sec. 5.3.)

In addition to the standard Bayesian analysis, one can add the notion of the *region of practical equivalence* (ROPE), as discussed in Kruschke (2015a), Kruschke and Liddell (2018) and Benavoli et al. (2017). The ROPE indicates "a small range of parameter values that are considered to be practically equivalent to the null value for purposes of the particular application" (Kruschke, 2015a). (The ROPE is somewhat analogous to the frequentist notion of equivalence testing.) If the parameter is interpretable, for example being the difference in classification accuracies, we may be able to set the ROPE based on our knowledge of the problem; for example we may believe that a difference of 1% in classification accuracies is practically equivalent.[5] If the parameter is less interpretable, a standard choice is to set the ROPE to $[-0.1s, 0.1s]$ where $s$ denotes the standard deviation of the difference vector (Kruschke, 2015b; Makowski et al., 2025). This is based on the notion of the "effect size", defined as Cohen's $d$ (see sec. 5.1), with $d = 0.2$ taken to be a small effect.

To use the ROPE in practice, we consider three regions in $\Delta$-space: (i) the ROPE, where the performance of A and B is regarded as practically equivalent; (ii) the region outside of the ROPE

[5]This choice may depend on the level of performance of the classifiers. For example if the accuracy is 95%, so that the error rate is 5%, an improvement of 1% would make a 20% reduction in the error rate to 4%. But if the error rate was 25%, a 1% change would be of much less importance.

where A practically outperforms B; and (iii) the region outside of the ROPE where B practically outperforms A. Let us denote these regions as $(A = B)$, $(A > B)$ and $(A < B)$. Making use of the posterior over $\Delta$ we can compute the probability masses $p(A = B)$, $p(A > B)$, $p(A < B)$.[6] To draw inferences, suppose we define a threshold $\theta$ such as 0.95 (although other values like 0.90 or 0.99 could also be used). Then the decision rule is that if a fraction $\theta$ or more of the probability mass lies within the ROPE, we decide that A and B are practically equivalent; if a fraction $\theta$ or more of the probability mass lies within either of the regions $A > B$ or $A < B$ we make that decision; otherwise we cannot decide if the methods are practically equivalent or practically different.

**Frequentist analysis:** Here we define the null hypothesis $H_0 : \Delta = 0$, and an alternative hypothesis (e.g. $\Delta \neq 0$). For null hypothesis significance testing (NHST) we then select a statistical test and compute the relevant test statistic (e.g., the $t$ statistic given in sec. 5.1 for the paired $t$-test). To assess the significance of the observed test statistic, we derive its distribution under $H_0$. One then sets a significance level $\alpha$ (e.g., 5% or 1%) corresponding to the maximum acceptable false positive rate for the test, and derives the rejection region of the test, i.e. values of the statistic for which $H_0$ will be rejected. Depending on the observed value of the statistic and the chosen $\alpha$, the decision is either to reject the null hypothesis, or to not reject it. Alternatively one can calculate the value of $\alpha$ which would just lead to rejection of $H_0$, and report it as the $p$-value for the test. See, e.g., Wasserman (2004, ch. 12) for more discussion of hypothesis testing and $p$-values.

Note that unlike the Bayesian analysis, the frequentist analysis does not carry out probabilistic inference for $\Delta$. Instead it makes use of the sampling distribution of the test statistic under $H_0$ to define a decision rule. There has been much criticism of $p$-values in recent years, see e.g., the statement by the American Statistical Association (ASA) (Wasserstein and Lazar, 2016). See also sec. 5.5.4 in Murphy (2022) entitled "p-values considered harmful". Below we reproduce three of the six principles from the ASA Statement, along with some comments.

Principle 2: **The p-value is not the probability that the null hypothesis is true.** *Researchers often wish to turn a p-value into a statement about the truth of a null hypothesis, or about the probability that random chance produced the observed data. The p-value is neither. It is a statement about data in relation to a specified hypothetical explanation, and is not a statement about the explanation itself.*
Comment: In the Bayesian framework one can write quantities like $p(H_0|data)$, given one or more alternative hypotheses. Note that frequentist statistics does not consider probabilities of hypotheses.

Principle 3: **Scientific conclusions and business or policy decisions should not be based only on whether a p-value passes a specific threshold.**
Comment: For example the use of the 0.05 significance level is just a conventional value.

Principle 5: **A p-value, or statistical significance, does not indicate the size an observed effect, or the importance of a result.**
Comment: The $p$-value does not separate between the effect size and the sample size—having enough data can often reject the null hypothesis for arbitrarily small effects.

For these reasons we adopt a Bayesian estimation approach to the comparison of predictors below.

[6] Here we have used the "ROPE (full)" as recommended in Makowski et al. (2019), rather than 'ROPE ('95%)" method suggested in Kruschke (2015a).

## 5.3 Bayesian $t$-test for difference in means

Consider first Q1, the comparison of two different predictors A and B for a given task on the basis of a common test set. Let $z_{ij}$ be the loss of predictor $i$ on test case $j$. Now consider the *paired difference* $d_j = z_{Aj} - z_{Bj}$, and let $\mathbf{d} = (d_1, \ldots, d_N)$. As discussed around eq. 4, it makes sense to consider the *paired* difference, as a random effect that makes a given example hard to predict (e.g., larger variability in the ground-truth $p(y|x)$) will be common across both predictors. See Appendix A for more on this point.

We assume that $d_j \sim N(\Delta, \sigma^2)$, where $\Delta$ is the mean difference in losses, and $\sigma^2$ is the variance of the distribution. We also assume that the $d_j$'s are sampled independently. We are interested in the posterior $p(\Delta|\mathbf{d})$. Using an non-informative prior over the parameters $(\Delta, \sigma^2)$, Murphy (2012, sec. 4.6) shows that

$$p(\Delta|\mathbf{d}) = t_{N-1}(\Delta|m, s^2/N), \tag{6}$$

where $m = \frac{1}{N}\sum_{j=1}^{N} d_j$, the sample mean, $s^2 = \frac{1}{N-1}\sum_{j=1}^{N}(d_j - m)^2$ is an unbiased estimate of the variance, and $t_{N-1}$ is the Student-$t$ distribution with $N-1$ degrees of freedom. Benavoli et al. (2017) consider a more complicated case where there are correlations between test cases, e.g. due to cross-validation; they term this the correlated Bayesian $t$-test.

This paired testing model can also be used for Q2, the comparison of two machine learning algorithms, taking into account the fixed factor of different algorithms, and the random factor being the choice of independent training sets. Here we have assumed that the test set is large, so that one can use the average loss over the test set as $z_{ij}$.

The above model makes strong assumptions, e.g. about the normality of the differences. The standard model checking approach to assess this is to make a quantile-quantile (QQ) plot of the differences data. One way to handle violations of normality would be to robustify the model for $p(d_i|\Delta)$; for example following Kruschke (2015a, sec. 16.2) one might use a Student-$t$ distribution rather than a normal distribution. This is less amenable to an analytical treatment, but is easy to handle with MCMC methods, such as the `brms` library in R.

A non-parametric frequentist alternative to the $t$-test is the Wilcoxon signed-rank test, which assumes that the observations are drawn from a symmetric distribution and are i.i.d. Note that Benavoli et al. (2017, sec. 4.2.1) developed a Bayesian signed-rank test, based on a Dirichlet process prior.

## 5.4 Bayesian McNemar's test

The paired $t$-test cannot be applied to the comparison of two binary classifiers that make "hard" 0/1 predictions—in this case there are only three possible values of the difference (1, 0 and -1), and it is not a credible assumption that these are drawn from a normal distribution.

We have seen in sec. 5.1 that the (frequentist) McNemar's test can be used in this situation. Chechile (2020, sec. 4) discusses a "Bayesian McNemar's test" that can be used for the analysis of paired categorical responses. Recall that the counts associated with the four different outcomes are denoted $n_{00}$, $n_{01}$, $n_{10}$, and $n_{11}$ respectively, with their sum being $N$, the number of test cases. Let the probabilities of the four outcomes be $\theta_{00}, \theta_{01}, \theta_{10}, \theta_{11}$. Under the null hypothesis that the error rates are equal, we have that $\theta_{00} + \theta_{01} = \theta_{00} + \theta_{10}$, or that $\theta_{01} = \theta_{10}$.

An appropriate Bayesian model for this 4-outcome case is the Dirichlet distribution. Given prior parameters $\alpha_{00}, \alpha_{01}, \alpha_{10}, \alpha_{11}$ for the four cells, the posterior after observing the counts is again Dirichlet with parameters $\alpha_{ij} + n_{ij}$ for $i,\ j \in \{0, 1\}$. A common non-informative

choice for the prior parameters is to set $\alpha_{ij} = 1$ for $i,\ j \in \{0, 1\}$. However, we wish to focus attention on the (01) and (10) cells. To draw a sample from the Dirichlet distribution one can make use of a "stick breaking" construction that samples from marginal and conditional Beta distributions, see e.g. Chechile (2020, Theorem 3.5). This can be used to show that the fraction $\phi = \theta_{01}/(\theta_{10} + \theta_{01})$ after observing the data is distributed as $\text{Beta}(\alpha_{01} + n_{01}, \alpha_{10} + n_{10})$, see Chechile (2020, sec. 4.3.2). Note that as the (01) event denotes *misclassifications* by algorithm A, values of $\phi$ which are less than 0.5 indicate that A outperforms B. Lacoste et al. (2012, sec. 4) provide a similar argument to Chechile (2020) by direct integration of the Dirichlet distribution. They effectively compute $p(\text{left}) = \int_0^{0.5} p(\phi|n_{01}, n_{10}, \alpha_{01}, \alpha_{10})d\phi$ and declare algorithm A to be superior if $p(\text{left}) > 1/2$, and algorithm B otherwise.

To define a ROPE for this case, consider the variance of a 0/1 Bernoulli random variable $W$ drawn with probability $\phi$. We have that the mean of $\phi$ is $\bar{\phi} = \alpha_{01} + n_{01}/(\alpha_{10} + n_{10} + \alpha_{01} + n_{01})$. Then

$$\text{var}(W) = \mathbb{E}[(W - \bar{\phi})^2] = p(W = 1)(1 - \bar{\phi})^2 + p(W = 0)\bar{\phi}^2 = \bar{\phi}(1 - \bar{\phi})^2 + (1 - \bar{\phi})\bar{\phi}^2 = \bar{\phi}(1 - \bar{\phi}). \tag{7}$$

Then the standard deviation $s = \sqrt{\bar{\phi}(1 - \bar{\phi})}$, and one can use the usual ROPE construction of $[0.5 - 0.1s, 0.5 + 0.1s]$. Note that if $\bar{\phi} = 0.5$, then the variance is maximized as 0.25, and the ROPE is $[0.45, 0.55]$.

## 5.5 Multiple tasks: Bayesian hierarchical models

The above analyses apply basically to Q1, the comparison of two predictors on a single task.[7] In this section we consider Q3, the comparison of two predictors across multiple tasks. The approach we shall follow is to use a Bayesian *hierarchical* model. These are discussed, for example, in chapter 5 of Gelman et al. (2013). The use of such hierarchical models assumes that the losses across the different tasks are commensurate.

**Bayesian hierarchical $t$-test:** Let $\mathbf{d}_i$ be the vector of loss differences for task $i$ over the test cases for that task. For a given task we consider a model as in sec. 5.3, so that for test case $j$ of task $i$, we have $d_{ij} \sim N(\Delta_i, \sigma_i^2)$. Following Benavoli et al. (2017, sec. 4.3.1) (henceforth BCDZ) we now consider a *hierarchical* model so that for $q$ tasks we have

$$\Delta_1, \ldots, \Delta_q \sim t_\nu(\Delta_0, \sigma_0^2), \tag{8}$$

$$\sigma_1, \ldots, \sigma_q \sim U(0, \bar{\sigma}). \tag{9}$$

Here the $\Delta_i$'s are drawn from a $t$-distribution with $\nu$ degrees of freedom, with mean $\Delta_0$ and scale parameter $\sigma_0$; the $\sigma_i$s are drawn from a Uniform distribution on $[0, \bar{\sigma}]$. BCDZ set $\bar{\sigma}$ to be a large multiple of $\bar{s}$, the average of the empirical standard deviations of the $\mathbf{d}_i$ vectors across the $q$ tasks. They argue that the inferences are insensitive to $\bar{\sigma}$ as long as it is set large enough. The model is completed with uniform priors for $\Delta_0$ and $\sigma_0$ and a prior on $\nu$. Obviously one might choose a somewhat different parameterization for various parts of the hierarchical model, but our description here follows BCDZ. (As for the Bayesian $t$-test, the BCDZ model actually allows for correlations between test cases, induced, e.g., by cross-validation.)

[7] The Bayesian $t$-test could also be used to address Q2, when ignoring variability in the test set.

The most important parameter in the hierarchical model is $\Delta_0$, which is the average difference in loss across the datasets. We therefore wish to explore $p(\Delta_0|\mathbf{d}_1, \ldots, \mathbf{d}_q, \psi)$ where $\psi$ denotes the various parameters in the prior distributions. Computations for the hierarchical model can be obtained via Markov chain Monte Carlo (MCMC) sampling.

A simpler alternative to the hierarchical model would be to compute the mean difference on each dataset, and then do a (Bayesian) $t$-test on this vector of these differences. But this ignores the variability within the different datasets, which might differ across datasets—this is modelled explicitly in the hierarchical model.

**Bayesian hierarchical McNemar test:** The Bayesian McNemar test (see sec. 5.4) can also be extended to a hierarchical model if there are multiple tasks, each with 0/1 loss data. In this case there would be $q$ parameters $\phi_1, \ldots, \phi_q$, being the true proportion for cell (01) against cells (10) and (01) in each task. A hierarchical model would assume that these parameters are drawn from a common prior. One possibility is to make this a Beta$(a, b)$ distribution, with $a$ and $b$ drawn from a suitable hyperprior. For example Gelman et al. (2013, sec. 5.3) discuss reparameterizing this in terms of priors on $\rho_1 = \log(a/b) = \text{logit}(a/a+b)$ and $\rho_2 = \log(a+b)$. Choosing a diffuse hyperprior which is uniform on $(\frac{a}{a+b}, (a+b)^{-1/2})$ results in a hyperprior in $(a, b)$ space of $p(a, b) \propto (a+b)^{-5/2}$.

Given the count data for each of the $q$ tasks, samples from the posterior distribution for $a$ and $b$ can be obtained, In our experiments below we have used the `hef` function in the `bang` (Bayesian Analysis, No Gibbs) library in R by Northrop and Hall (2025) to carry out this sampling using the generalized ratio-of-uniforms method.

The aim of the hierarchical model is to predict $\phi_{next}$, the $\phi$ parameter for the next dataset drawn from the same underlying distribution as the $q$ datasets. We have that

$$p(\phi_{next}|D) = \int p(\phi_{next}|a, b)p(a, b|D)\, da\, db \tag{10}$$

$$\simeq \frac{1}{S}\sum_{s=1}^{S} p(\phi_{next}|a_s, b_s) \tag{11}$$

where the samples $\{a_s, b_s\}_{s=1}^S$ are drawn from the posterior $p(a, b|D)$. We have that

$$\mathbb{E}[\phi_{next}|D] \stackrel{def}{=} \bar{\phi} \simeq \frac{1}{S}\sum_{s=1}^{S} \frac{a_s}{a_s + b_s}, \tag{12}$$

where we have used that the mean of a beta distribution with parameters $a_s, b_s$ is $a_s/(a_s + b_s)$. We can also approximate the distribution $p(\phi_{next}|D)$ as per eq. 11.

**Comparison of incommensurate datasets:** To build a hierarchical model it is necessary to assume that the parameters $\Delta_1, \ldots, \Delta_q$ or $\phi_1, \ldots, \phi_q$ are drawn from a common prior. If the losses are *incommensurate*, this is not reasonable. In this case Lacoste et al. (2012) pose the question "Does algorithm A have a higher chance of producing a better classifier than algorithm B in the given context?". This question is refined for a context $\mathcal{W}$ by defining

$$\bar{q}_{AB|\mathcal{W}} \stackrel{def}{=} \mathbb{E}_{(\mathcal{D},n)\sim\mathcal{W}}\, \mathbb{E}_{S\sim\mathcal{D}^n}\, I[A(S) \stackrel{\mathcal{D}}{\succ} B(S)], \tag{13}$$

and declaring that algorithm A outperforms algorithm B in context $\mathcal{W}$ (denoted $A \overset{\mathcal{W}}{\succ} B$) if $\bar{q}_{AB|\mathcal{W}} > 1/2$. In eq. 13 the outer expectation is over tasks denoted by $\mathcal{D}$ drawn from the context $\mathcal{W}$, and the inner one is over training sets $S$ of size $n$ drawn from task $\mathcal{D}$. The notation $A(S) \overset{\mathcal{D}}{\succ} B(S)$ means that algorithm A using training set $S$ outperforms algorithm B on the same training set, i.e., that the expected loss (or risk) of algorithm A is less than algorithm B. $I[a]$ denotes the indicator function, with $I[a] = 1$ if $a$ is true, and 0 otherwise. Lacoste et al. (2012, sec. 5) develop a Poisson Binomial test to estimate $\bar{q}_{AB|\mathcal{W}}$ in the case of 0/1 losses.

## 5.6 Comparing multiple predictors

Above we have argued that it usually makes sense to choose a reference predictor, and to compare the other predictors to it. In the NHST framework one has to handle such *multiple comparisons* with care. One common approach is the Bonferroni correction, see e.g., Wasserman (2004, sec. 10.7). Consider a single test with type I error $\alpha^*$, i.e. the probability of erroneously rejecting a true null hypothesis is $\alpha^*$. Then if we conduct a family of $m$ such tests independently, the family-wise error rate (FWER, the probability of making at least one type I error in the family) is $1 - (1 - \alpha^*)^m$. We seek to have FWER $\leq \alpha$. The Bonferroni correction achieves this by setting $\alpha^* = \alpha/m$.[8] So if we were, for example, conducting $m$ paired $t$-tests, the FWER can be controlled by using a significance level of $\alpha/m$ for each one.

The above discussion relates to the issue of multiple comparisons with NHST, and controlling type I errors. But how is this issue addressed under a Bayesian analysis? In their paper entitled *Why We (Usually) Don't Have to Worry About Multiple Comparisons*, Gelman et al. (2012) state that "we are typically not terribly concerned with Type 1 error because we rarely believe that it is possible for the null hypothesis to be strictly true." I.e., by better modelling of the situation with a posterior on $\Delta$, and the use of the ROPE, the issue of multiple comparisons is mitigated.

We have recommended making comparisons between a reference algorithm and each of the alternative algorithms in a pairwise fashion. It would be possible to consider a hierarchical model over algorithms (as opposed to tasks, as in sec. 5.5), with a prior on the "algorithm effects" (the $\alpha_i$'s in the ANOVA model of eq. 1). This would lead to joint inferences for these effects, which could then be used to consider the differences, e.g. $\alpha_i - \alpha_{i'}$. Although this approach has merits, we believe it is rather simpler to focus on the difference vector for comparing two algorithms, and leave exploration of this issue to future work.

## 5.7 Software

The code made available by Benavoli et al. (2017) in Python and R at `https://github.com/BayesianTestsML/tutorial` can be used for the Bayesian $t$-test and for the hierarchical model discussed in sec. 5.5. This repository also contains code for several other Bayesian nonparametric tests.

R code for the Bayesian McNemar test and for the hierarchical extension is available from our repository `https://github.com/ckiwgithub/compareMLModels`. The latter makes use of the hierarchical exponential family (`hef`) function from Northrop and Hall (2025). Our repository also contains code for the worked examples in sec. 6.

[8] The validity of the Bonferroni correction does not in fact require independence of the tests; it can be proved simply by using Boole's inequality, see e.g., Goeman and Solari (2014).

There are many software resources for Bayesian modelling in general, including various packages for R, and libraries in Python (such as PyMC[9]) Also Stan[10] enables sophisticated Bayesian statistical modelling, and has interfaces for Python, R and Julia.

# 6 Worked examples

We provide two worked examples, the first for a single task, and the second for multiple, related tasks.

## 6.1 Comparing four classifiers on one task

We illustrate the above methods on a binary classification task taken from (Camilleri et al., 2024). Their general investigation concerns the analysis of patterns of behaviour of three mice in their homecage based on video data. As part of this study they need to detect whether each of three mice are observable at a given time. A given mouse is identified by an RFID tag, and it may not be visible due to occlusion, either by the other animals, or by materials in the cage (e.g., a tube).

The data was obtained from 200 two-minute snippets of video, with 100 snippets used for training, 40 for validation and 60 for testing. The original task was to classify if a given mouse was observable for each second of video. There are 20,343 examples in the test set. Note that this is an *imbalanced* task, as only 7% of the data were labelled "not observable". The features extracted for this task were the position of the mouse (based on RFID data), the fraction of frames within the one second interval in which a bounding box (BBox) for the mouse appears in the processed video data, the average area of such BBoxes, and the first 30 principal components from a feature-vector obtained by applying the Long-term Feature Bank (LFB) model (Wu et al., 2019) to the video.

We consider here four classifiers: logistic regression (LgR), Naïve Bayes using a multinomial encoding (NB), a multilayer perceptron (MLP) and a support vector machine (SVM) using the RBF kernel. The threshold was chosen to set the fraction of true observable examples misclassified as not observable for each to 8%, see Camilleri et al. (2024, sec. 5.1.2) for further details.

We are addressing Q1 here, i.e., the comparison of predictors on a single task. On the basis of results on the validation set, the LgR classifier was selected by Camilleri et al. (2024) for use in the full system. We thus compare the LgR model with the other three (generically denoted as X), and assess if the differences in results are significantly different. This is assessed by applying a Bayesian t-test to the differences in log probability[11] of the correct label under the LgR and X models,

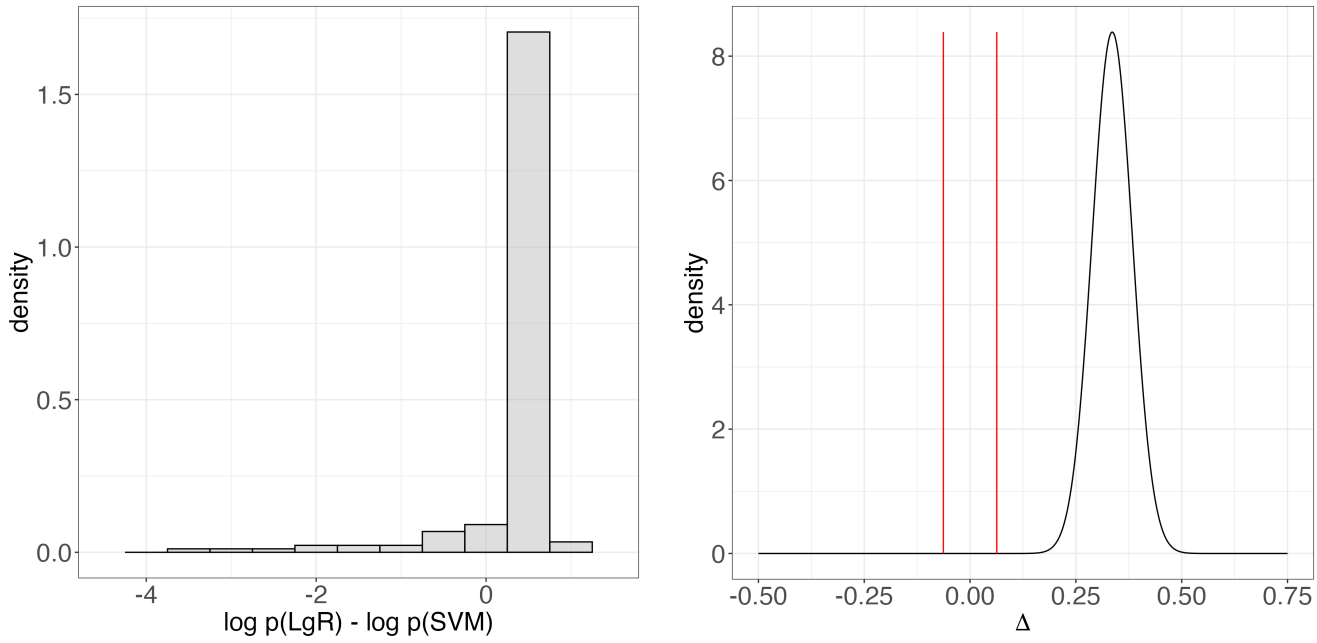
Although there are 20,343 examples in the test set, these are derived from only 176 snippet-mouse combinations. The observations of a given mouse in a snippet are heavily autocorrelated, and are thus not independent. To handle this, we averaged the log probability scores for a given mouse in each snippet, and treated this as one observation.[12] Hence we set $N = 176$ in eq. 6.

[9]PyMC: `https://www.pymc.io`.

[10]Stan: `https://mc-stan.org`.

[11]For the SVM, the numerical output lying in $(0, 1)$ was treated as a probability.

[12]I thank Antoni Sieminski, Nicole Augustin and Torben Sell for helpful discussions on this point. Averaging is a "conservative" solution, it might otherwise be possible to assess the autocorrelation of the observations, and thus estimate the effective sample size of a mouse-snippet combination.




(a) (b)

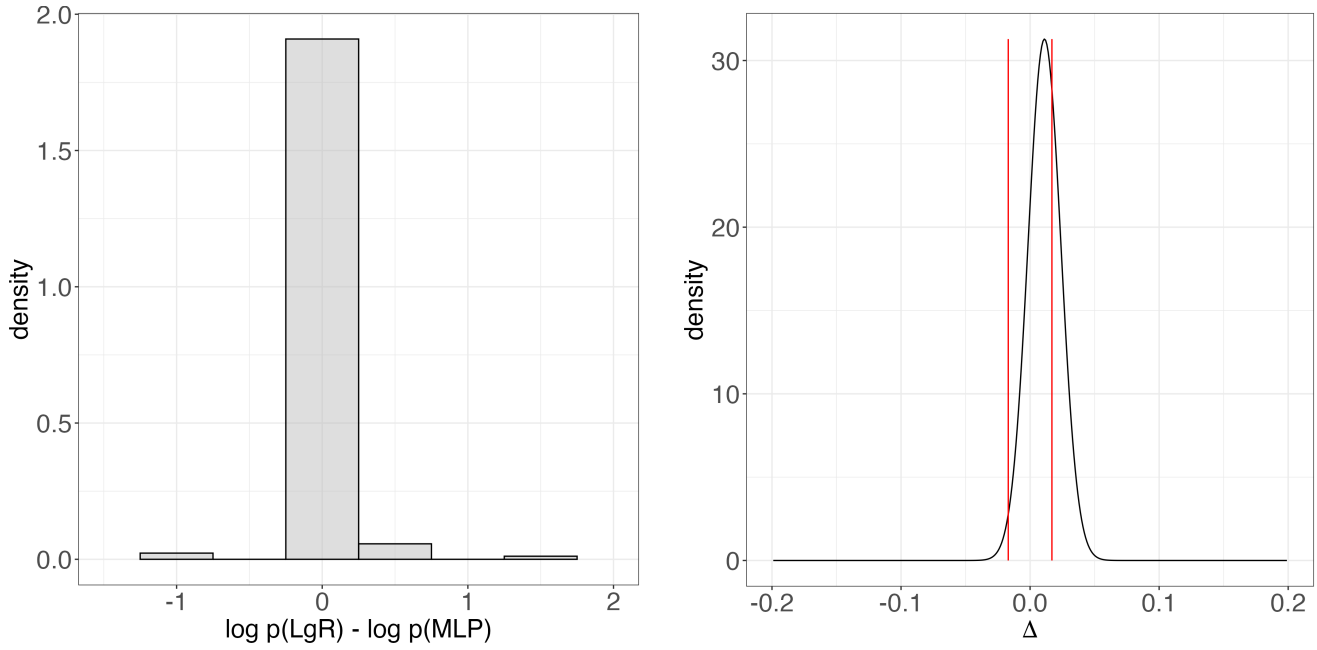
Figure 1: (a) Histogram of the differences $\log p(LgR) - \log p(SVM)$. (b) The posterior distribution for $\Delta$ (black line), and the ROPE boundaries (shown in red).

**Bayesian t-test:** We set the ROPE to $[-0.1s, 0.1s]$ where $s$ denotes the standard deviation of the difference vector. This follows the advice given in Kruschke (2015b) and Makowski et al. (2025). Note that $s$ is the standard deviation of the data, not the standard error of the mean, so that it does not scale as $\sqrt{1/N}$.

As an example, consider the difference in the log scores of the LgR and SVM models. A histogram of these differences is shown in Fig. 1(a). Notice that the differences are generally greater than zero, reflecting that the log scores are generally higher for LgR than SVM. In fact the median difference is 0.51; the mean is 0.34, pulled down by the left-hand tail of the distribution, where there are a few examples where the SVM scores much better. Applying the Bayesian $t$-test[13] we obtain Fig. 1(b). The posterior is quite tightly concentrated around the mean because of the $1/N$ scaling of the variance in eq. 6) with $N = 176$. The plot clearly shows that the probabilities associated with the three alternatives are $p(LgR < SVM) = 0.0, p(LgR = SVM) = 0.0, p(LgR > SVM) = 1.0$. Thus with a threshold of $\theta = 0.95$ we can conclude that practically LgR outperforms SVM on the basis of the log scores. For comparison, the standard (frequentist) $t$-test rejects the null hypothesis with a $p$-value of $3.7 \times 10^{-11}$ ($t = 7.06$, $df = 175$). The effect size is given by Cohen's $d = 0.53$, which is termed a medium strength effect.

The Bayesian $t$-test, as described in sec. 5.3, makes an assumption of normality for the $d_i$'s around $\Delta$. The histogram in Fig. 1(a) shows that the distribution is skewed around its mean, and a Q-Q plot (not shown) suggests heavy tails. These features can be traced back to the fact that log probability scores of the LgR model for the disaggregated data show very different behaviour for class 0 (negative examples) and class 1 (positives); for class 0 the mean score is -2.69 with std. dev. of 1.50; for class 1 the mean is -0.07 and std. dev. is 0.14. In contrast for the SVM, the distributions of log probability scores are very similar for classes 0 and 1.

[13]The function `correlatedBayesianTtest.R` from `https://github.com/BayesianTestsML/tutorial` was used.




(a) (b)

Figure 2: (a) Histogram of the differences $\log p(LgR) - \log p(MLP)$. (b) The posterior distribution for $\Delta$ (black line), and the ROPE boundaries (shown in red).

The skewness of the histogram in Fig. 1(a) derives from these differences. One way to handle this would be to robustify the model for $p(d_i|\Delta)$ as discussed in sec. 5.3, by using a Student-$t$ distribution rather than the normal distribution.

For a contrasting example, consider the differences between the LgR and MLP classifiers, as shown in Fig. 2. Panel (a) shows the histogram of the differences in log scores. In this case the distribution appears to be symmetric about zero, and the mean and median are both very close to 0. The posterior for $\Delta$ (panel (b)) shows that the posterior mass spans all three regions, with $p(LgR < MLP) = 0.014, p(LgR = MLP) = 0.660, p(LgR > MLP) = 0.326$. Thus with a threshold of $\theta = 0.95$ we cannot conclude that the two classifiers are practically equivalent or practically different. For comparison, the standard (frequentist) $t$-test fails to reject the null hypothesis with a $p$-value of 0.38 ($t = 0.87$, $df = 175$), and the effect size is $d = 0.066$, which is regarded as "negligible".

See the comments above with respect to the robustness of the Bayesian $t$-test, but noting that the distribution shown in Fig. 2(a) is much less skewed than Fig. 1(a).

The above analysis illustrates significant differences between the LgR and SVM classifiers, but is in fact a bit misleading. It is well known that the outputs of a SVM are not well calibrated as probabilities. Platt (2000) showed that this can be mitigated by transforming the SVM scores with a sigmoid function, with adjustable offset and scaling parameters. Applying this "Platt scaling" to all of the classifiers, we find that for all three comparisons (MLP, NB and SVM against LgR), we cannot conclude that the two classifiers are practically equivalent or practically different.

| count | de-en | da-en | es-en | fr-en | it-en | id-en | nl-en | sv-en | tr-en | tr-de | zh-en |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $n_{00}$ | 18 | 54 | 58 | 79 | 36 | 52 | 68 | 48 | 19 | 39 | 19 |
| $n_{01}$ | 63 | 159 | 175 | 180 | 202 | 185 | 195 | 156 | 64 | 113 | 44 |
| $n_{10}$ | 66 | 198 | 149 | 167 | 167 | 193 | 176 | 133 | 30 | 103 | 46 |
| $n_{11}$ | 183 | 589 | 478 | 574 | 595 | 570 | 561 | 423 | 103 | 298 | 92 |

Table 1: Counts for outcomes $n_{00}$, $n_{01}$, $n_{10}$, and $n_{11}$ for the 11 language pairs. The language labels are Chinese (zh), Danish (da), Dutch (nl), English (en), French (fr), German (de), Indonesian (id), Italian (it), Spanish (es), Swedish (sv) and Turkish (tr).

## 6.2 Comparing two classifiers on multiple tasks

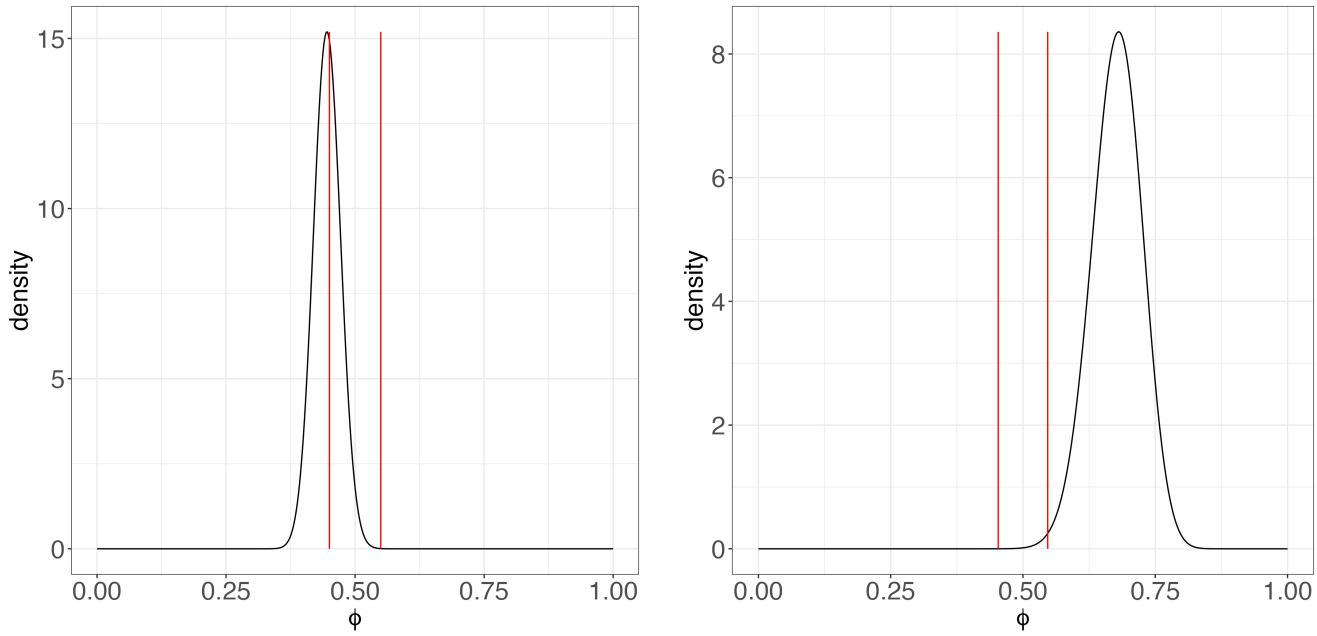
We illustrate model comparison across multiple tasks (Q3) using data from an experiment on linguistic code-switching. (Code-switching occurs when multilingual speakers use more than one language in an utterance.) Sterner and Teufel (2025b) developed a benchmark containing up to 1,000 minimal pairs of code-switching (CS) sentences for 11 language pairs. Each pair consists of one naturally occurring CS sentence and one minimally manipulated variant, where the variant has the code-switch at an altered location. The classification task for each sentence pair is to identify the naturally occurring CS sentence. In a subsequent paper (Sterner and Teufel, 2025a) the authors compared the performance of a graph neural network (GNN) against a large language model (LLM) for this task.

The results of the experiments are summarized in Table 1.[14] For each language pair there are four counts labelled $n_{00}$, $n_{01}$, $n_{10}$, and $n_{11}$. For example $n_{10}$ indicates the number of test examples where the GNN was correct and the LLM incorrect. As per sec. 5.4 it is only the $n_{01}$ and $n_{10}$ counts that are used in the Bayesian McNemar's test (BMcT). A naïve comparison of these numbers shows that the GNN is more accurate than the LLM on 4 of the 11 language pairs.

We first consider carrying out the BMcT for each language pair individually. For example Fig. 3(a) shows the posterior for $\phi$ for language pair 2 (da-en). The posterior mean is around 0.45 indicating that the GNN is outperforming the LLM, but the posterior probabilities are for the three regions are $p(GNN > LLM) : 0.571$, $p(GNN = LLM) : 0.429$, $p(GNN < LLM) : 0.00004$. Hence we cannot conclude that the two classifiers are practically equivalent or practically different for this pair. Fig. 3(b) shows the posterior for language pair 9 (tr-en). In this case the posterior mean is around 0.68, and the posterior region probabilities are $p(GNN > LLM) : 0.000005$, $p(GNN = LLM) : 0.004$, $p(GNN < LLM) : 0.996$. So for this pair we can conclude that the LLM practically outperforms the GNN. In fact tr-en is the only pair where such a conclusion can be made, in all other cases we cannot conclude that the two classifiers are practically equivalent or practically different. Notice that the lower $n_{01}$ and $n_{10}$ counts for the tr-en example relative to the da-en example mean that the posterior variance is greater in Fig. 3(b) than in Fig. 3(a).

In contrast, the standard McNemar's test (`mcnemar.test` in R) gives a $p$-value of 0.045 for language pair 2, and 0.00067 for language pair 9. The $p$-values for all other language pairs are greater than 0.05. So the performance difference on language pair 2 (da-en) would be judged just significant at the $\alpha = 0.05$ level by the standard McNemar's test, but not using the Bayesian McNemar's test (with ROPE). The performance difference for language pair 9 (tr-en) is significantly different at the 0.05 level for both the standard and Bayesian McNemar's tests.

[14] Thanks to Igor Sterner for providing this data.




(a) (b)

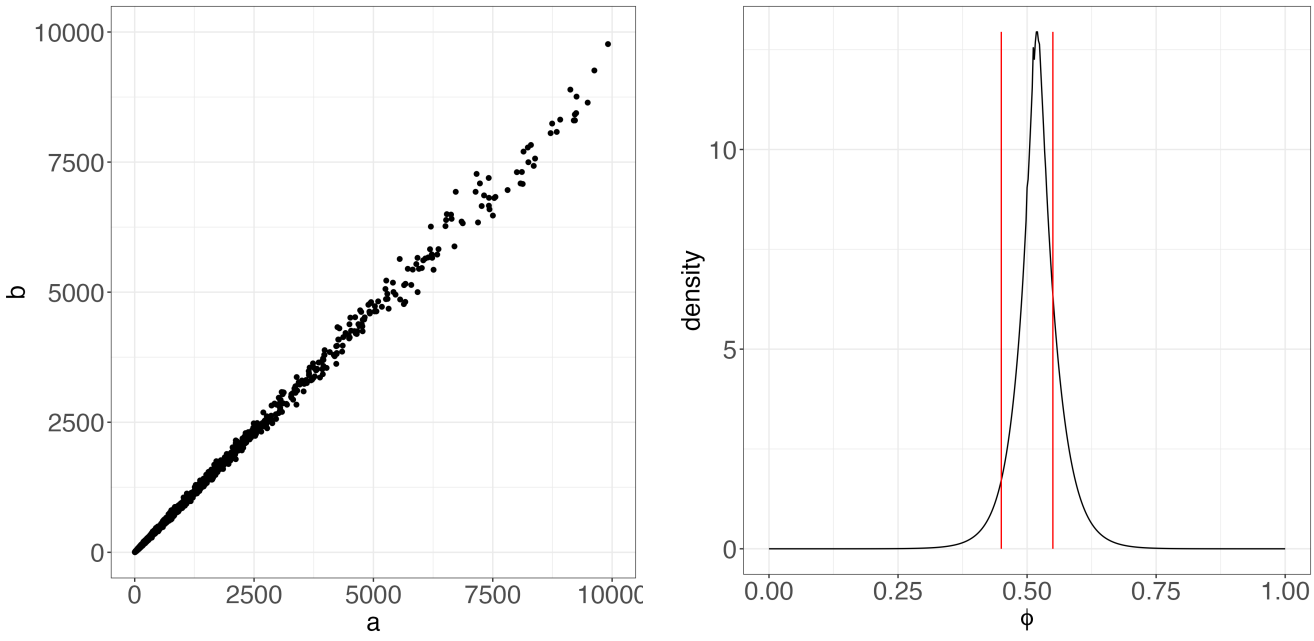
Figure 3: (a) Posterior distribution for $\phi$ (black line), and the ROPE boundaries (shown in red) for the da-en language pair. (b) Same for the tr-en language pair.

To estimate the effect size for a given language pair, we first compute $\hat{\phi} = n_{01}/(n_{01} + n_{10})$, and then Cohen's $g = \hat{\phi} - 1/2$. For language pair 9 we have a medium effect of $|g| = 0.18$, and for pair 2 we have $|g| = 0.055$ which just qualifies for the term small. For all all other pairs the effect size would be described as negligible.

We can also illustrate model comparison across multiple tasks with this dataset, using the hierarchical beta-binomial model discussed in sec. 5.5. This model has hyperparameters $a$ and $b$. One can obtain posterior samples for $a$ and $b$; here we have used the `bang` (Bayesian Analysis, No Gibbs) library in R to do so. Samples from the posterior for $a$ and $b$ are shown in Fig. 4(a). (Note that 221 out of 10,000 generated samples are omitted from this plot, these have values lying beyond the top right corner.) From the plot, notice that $a$ and $b$ are very nearly equal, but that there is a large amount of variability in $a + b$. $\log(a + b)$ shows significant variability between values of 3 and 8 around its modal value of 5.28 (data not shown). The posterior mean $\bar{\phi}$ (as defined in eq. 12) is equal to 0.521, very close to 0.5. This is not very surprising given the balance between tasks where the GNN wins and cases where the LLM wins, as noted above.

The aim of the hierarchical model is to predict $\phi_{next}$, the $\phi$ parameter for the next dataset drawn from the same underlying distribution as the 11 language-pair samples. Fig. 4(b) shows the resulting posterior distribution, and also the ROPE limits (derived from the standard deviation $s = \sqrt{\bar{\phi}(1-\bar{\phi})}$ and the ROPE $[0.5 - 0.1s, 0.5 + 0.1s]$). The probabilities for the three regions are $p(GNN > LLM) : 0.053$, $p(GNN = LLM) : 0.737$, $p(GNN < LLM) : 0.210$.[15] Thus from the predictive distribution for $\phi_{next}$ based on the 11 observed tasks, we cannot

[15]Note that the analysis in Benavoli et al. (2017, sec. 4.3.2) is slightly different than that given here. For each posterior sample they compute the ROPE probabilities, and then threshold these according to the maximum probability to assign each sample to one of the three regions. These counts are then divided by $S$ to obtain the probabilities shown in their Table 12. In contrast, our results are obtained by averaging the ROPE probabilities over the samples.




(a) (b)

Figure 4: (a) Posterior samples for $(a, b)$ given the data for the 11 tasks. (b) The predictive distribution for $\phi$ (black line), and the ROPE boundaries (shown in red).

conclude that the two classifiers are expected to be practically equivalent or practically different. For comparison, Friedman's test applied to the 11 pairs of counts gives a $p$-value of 0.366 (Friedman chi-squared $= 0.818$, $df = 1$), and would thus not reject the null hypothesis at the $\alpha = 0.05$ level. But note that this test depends only on the observation that the GNN is more accurate than the LLM on 4 of the 11 language pairs, and does not take into account the closeness of some of the $n_{01}$ and $n_{10}$ counts in Table 1, and possible sampling variation. This aspect is modelled explicitly in the Bayesian hierarchical McNemar test.

# 7 Checklist for best practice

Based on the discussion above, we recommend to:

- Clarify which question (Q1-Q3) you seek to answer.
- Identify a suitable loss function that fits well with the practical application.
- Clearly identify the relevant fixed and random factors of variation that enter into your experiments, and an appropriate experimental design.
- Identify and carry out an appropriate statistical test. We have recommended Bayesian tests such as the Bayesian $t$-test, Bayesian McNemar's test, and (for comparisons across multiple tasks) Bayesian hierarchical models. Check the assumptions underlying the selected test, including independence assumptions.
- Report the inferences drawn from the test.

- THINK! It is easy to blindly apply tests, but it is important to maintain a sceptical/critical mindset.

# 8 Discussion

As observed, the current practice on the comparison of machine learning algorithms is often poor. In this paper we have reviewed the issues involved, highlighting the existing body of work on the design and analysis of experiments, including fixed and random effects. There are standard frequentist tests, such as paired $t$-tests, McNemar's test, the Friedman test. However, because of criticisms of NHST as discussed in sec. 5.2, we recommend Bayesian approaches, including the notion of the region of practical equivalence (ROPE) (Benavoli et al., 2017; Kruschke, 2015a). In sec. 6 we have provided worked examples of the comparison of machine learning models for both a single task, and over multiple tasks.

What will it take to change current practice? In certain fields, such as medicine and psychology, there are reporting guidelines that must be followed when papers are submitted, see, e.g., the Equator network (Enhancing the QUAlity and Transparency Of health Research)[16] and Appelbaum et al. (2018). We are seeing some moves towards this in the field of machine learning, like the NeurIPS Paper Checklist Guidelines,[17] where item 7 addresses Experiment Statistical Significance. This item mainly covers the reporting of error bars for each algorithm. These are important, but, as highlighted (for example) by Loftus and Masson (1994), they do not take into account the use of paired comparisons. Doing so allows a more powerful comparison of models, which (we argue) is often what is desired. This paper should be seen as contributing towards the creation of such reporting guidelines for work in machine learning and related fields.

As per the final bullet in sec. 7, it is important that authors do not blindly apply tests, but maintain a critical attitude. Thus there should be scope for novel analyses, but in this case the authors will need to justify why standard guidance has not been followed.

# A The advantages of paired differences

Consider, for concreteness, the squared error for the prediction $f_A$ of a deterministic predictor $A$ for some test case $(x, y)$. Assume also that the true distribution $p(y|x)$ has mean $\mu_y$ and variance $\sigma_y^2$.[18] We wish to study the squared error $SE_A = (f_A - y)^2$. It is useful to decompose this with respect to the true mean $\mu$, i.e.

$$(f_A - y)^2 = (f_A - \mu_y + \mu_y - y)^2, \tag{14}$$

$$= (f_A - \mu_y)^2 - 2(f_A - \mu_y)(y - \mu_y) + (y - \mu_y)^2. \tag{15}$$

The first *deterministic* term arises from the derivation of $f_A$ from the optimal MSE predictor $\mu_y$. The second and third are stochastic terms depending on $y$. We can compute the expectation of this squared error (or MSE) as

$$MSE_A = \mathbb{E}_y[(f_A - y)^2] = (f_A - \mu)^2 + \mathbb{E}_y[(y - \mu)^2] = (f_A - \mu)^2 + \sigma_y^2. \tag{16}$$

[16] `https://www.equator-network.org/`.

[17] `https://neurips.cc/public/guides/PaperChecklist`.

[18] We do not require this to be Gaussian, only to have the given mean and variance.

Note that this MSE has an irreducible component due to the variance of $y$. This may vary as a function of $x$, meaning that the scale of the squared error can be different in different locations.

Now consider the paired difference $MSE_A - MSE_B$ between predictors $A$ and $B$ for this same test case. We have that

$$MSE_A - MSE_B = (f_A - \mu)^2 - (f_B - \mu)^2, \tag{17}$$

i.e. the $\sigma_y^2$ term cancels out. Even if we consider the unaveraged difference $SE_A - SE_B$ we have that

$$SE_A - SE_B = (f_A - \mu)^2 - (f_B - \mu)^2 + 2(f_B - f_A)(y - \mu_y). \tag{18}$$

The last term has zero mean, so the difference $SE_A - SE_B$ does not have an additive offset, unlike $SE_A$ (or $SE_B$).

The above analysis was carried out for MSE, but similar (although more complicated) analyses can also be carried out, e.g. for log loss.

We can also understand the advantages of paired differences if the losses follow the 2-way ANOVA model of eq. 1. In this case we have that the difference in the losses of methods $A$ and $B$ on test case $j$ is

$$d_j^{AB} = z_{Aj} - z_{Bj} = \alpha_A - \alpha_B + (\epsilon_{Aj} - \epsilon_{Bj}); \tag{19}$$

observe that the $\beta_j$ terms in the ANOVA cancel out. Note that the last term, which is the difference of two errors that are assumed to be normally distributed, is again normally distributed, but with variance $2\sigma_\epsilon^2$.

# B ANOVA for MSE loss

Eq. 1 describes the repeated measures 2-way ANOVA model, with a fixed effect indexed by $i$, and a random effect indexed by $j$. Consider the (idealized) mean squared error loss, as discussed above in sec. A. This means that for predictor $i$ on example $j$ we have that

$$z_{ij} = (f_{ij} - \mu_j)^2 + \sigma_j^2 \stackrel{def}{=} \delta_{ij}^2 + \sigma_j^2, \tag{20}$$

where $f_{ij}$ is the prediction from method $i$ at test case $j$, and $\mu_j$ and $\sigma_j^2$ are the mean of variance of $p(y_j|x_j)$.

The ANOVA model can be fitted by least squares, making use of the quantities

$$\bar{z}_{i.} = \frac{1}{b}\sum_{j=1}^{b} z_{ij}, \qquad \bar{z}_{.j} = \frac{1}{a}\sum_{i=1}^{a} z_{ij}, \qquad \bar{z}_{..} = \frac{1}{ab}\sum_{i=1}^{a}\sum_{j=1}^{b} z_{ij}. \tag{21}$$

One then obtains the parameter estimates

$$\hat{\mu} = \bar{z}_{..}, \qquad \hat{\alpha}_i = \bar{z}_{i.} - \bar{z}_{..}, \tag{22}$$

see, e.g. Montgomery 2013, sec. 13.3. Plugging in eq. 20 we first obtain

$$\bar{z}_{..} = \langle \delta_{ij}^2 \rangle_{ij} + \langle \sigma_j^2 \rangle_j, \qquad \bar{z}_{i.} = \langle \delta_{ij}^2 \rangle_j + \langle \sigma_j^2 \rangle_j, \qquad \bar{z}_{.j} = \langle \delta_{ij}^2 \rangle_i + \sigma_j^2, \tag{23}$$

where, e.g., the notation $\langle \cdot \rangle_{ij}$ denotes averaging over both $i$ and $j$. Hence we obtain

$$\hat{\alpha}_i = \langle \delta_{ij}^2 \rangle_j - \langle \delta_{kj}^2 \rangle_{kj}. \tag{24}$$

Notice that in the expression for $\hat{\alpha}_i$ the noise variance terms have cancelled. An estimate of the random effect variance $\hat{\sigma}^2_\beta$ can be obtained as $(MS_B - MS_E)/a$, see Montgomery (2013, eq. 13.11), where $MS_B$ is the mean square value of the random factor, and $MS_E$ the mean square value of the noise. These are obtained by normalizing the sum-of-squares terms in the standard decomposition $SS_T = SS_A + SS_B + SS_E$ by the appropriate degrees of freedom, where, e.g., the total sum of squares is given by $SS_T = \sum_i \sum_j (z_{ij} - z_{..})^2$.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