

Paired t -test

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You want to show that algorithm A is better than algorithm B. You have a dataset $D = (x_1, y_1), \dots, (x_n, y_n)$ to prove it.

1 Do not Use These Methods

Here are some “natural” ideas which, unfortunately, will not support the claim due to the stochastic fluctuation in the dataset D :

- Training set accuracy. Train A on D , test A on D again to get the training set accuracy a_A . Repeat for B to get a_B . Show $a_A > a_B$. Problems: overfitting, stochastic fluctuation.
- Test set accuracy. Split D into D_{train} and D_{test} . Train A, B on D_{train} , get their accuracies on D_{test} . Show $a_A > a_B$. Problem: stochastic fluctuation.
- CV accuracy. Perform k -fold cross validation on D with A. Use exactly the same folds on B too. Show the CV accuracy $a_A > a_B$. Problem: stochastic fluctuation. (OK, people actually use this quite often. But it is better to assess the statistical significance. Read on...)
- Dataset selection. Select and only report experiments on certain datasets D that “worked”. Problem: Hmm...

2 Statistical Tests

An accepted method is to perform a statistical significance test. The idea is simple. Let us assume that A and B indeed have the same generalization accuracy. Their CV accuracies a_A and a_B will still exhibit all kinds of fluctuations (i.e., be different). If we were to be certain that we do not call A and B different, we will need to tolerate all possible differences in a_A and a_B , including very large ones. This is useless, because if A and another algorithm C is truly different we will not be able to detect that.

However, we expect most of the time a_A and a_B are “fairly close”. Only rarely do they differ a lot. In fact, we can find a threshold such that a_A and a_B differ by that much in only 5% of the times we do the test. We will call two algorithms different if their CV accuracies differ more than the threshold.

More formally, we entertain two hypotheses:

- H_0 : The null hypothesis that A and B have the same generalization performance.
- H_a : The alternative hypothesis that A and B have different generalization performance.

If the empirical results a_A and a_B differ more than the threshold, we reject H_0 and adopt H_a . Otherwise, we *retain* H_0 : this does not mean that we believe in H_0 , but simply that we do not have enough evidence to say otherwise. Some immediate observations:

- Statistical test does not really test whether H_a is true, i.e., two algorithms have different performance. It is only concerned with how often (5% in the above) we will call two algorithms with the same underlying performance different.

- Being able to say two algorithms are different is a *by-product*.
- We will make mistakes 5% of the time by calling A and B different, when they in fact have the same performance. This is known as Type I error.
- We do not know how often we call A and C the same because they fall within the threshold, when they are truly different. This is Type II error and is not addressed by statistical test (but is important in practice!).
- One can adjust the 5% figure by changing the threshold. When the threshold is close to zero, it is easier to say that A and C are different. But A and B will be called different more often too – the 5% figure will increase to, say, 10%. This is *less significant* (for the difference in A and C). When the threshold is far from zero, it is very hard for A and C to be called different (therefore harder to publish...). A and B will be called different much less frequently, say 1%. This is *significant* (for A and C). We of course prefer significant results. The default is 5%.

3 Paired t -Test

There are many different tests. In this case, we use a specific test called a paired t -test. Let $X_1, \dots, X_k \sim N(\mu, \sigma^2)$ where both μ and σ^2 are unknown, and k is relatively small. We want to test $H_0 : \mu = \mu_0$. Let the sample mean be

$$\bar{X}_k = 1/k \sum_{i=1}^k X_i, \quad (1)$$

and the sample variance be

$$S_k^2 = 1/(k-1) \sum_{i=1}^k (X_i - \bar{X}_k)^2. \quad (2)$$

The random variable

$$T = \frac{\sqrt{k}(\bar{X}_k - \mu_0)}{S_k} \quad (3)$$

follows a t -distribution with $k-1$ degree of freedom under H_0 . When k is somewhat large, $T \rightarrow N(0, 1)$.

How is this related to our goal? Recall we perform k -fold CV. Let the accuracy in each fold be a_{A1}, \dots, a_{Ak} for algorithm A, and a_{B1}, \dots, a_{Bk} for algorithm B. We assume that the pairwise differences $x_i = a_{Ai} - a_{Bi}$, $i = 1 \dots k$ follow $N(0, \sigma^2)$ under H_0 . Therefore T has a t -distribution with $k-1$ degree of freedom. We can look up the 5% threshold (2-sided) from a table. When T is outside the threshold we reject H_0 , and claim that A and B are truly different.

Keep in mind that this procedure has 5% Type I error. That roughly translates to “every 1 in 20 papers claims an advance that is really not there!”