Statistical hypothesis testing

Why hypothesis testing?

Q: If Accuracy(A) > Accuracy(B), can we conclude that classifier A is better than B?

A: No, not necessarily. Only if the difference between Accuracy(A) and Accuracy(B) is unlikely to arise by chance.

Hypothesis testing

We have a hypothesis H that we wish to show is true.
(H = "There is a difference between A and B")

We have a statistic *M* that measures the difference between A and B, and we have measured a value *m* of *M* in our data.

But *m* itself doesn't tell us whether H is true or false.

Instead, we estimate how likely *m* were to arise if the opposite of H (= the 'null hypothesis', H_o) was true.
(H_o = "There is no difference between A and B").

If $P(M \geq m \mid H_o) < p$, we can *reject* H_o with p-value p

Rejecting H_0

- H_0 defines a distribution $P(M \mid H_0)$ over some statistic M
  (e.g. M = the difference in accuracy between A and B)
- Select a significance value S (e.g. 0.05, 0.01, etc.)
  You can only reject H_0 if $P(M=m \mid H_0) \leq S$
- Compute the test statistic m from your data
  e.g. the average difference in accuracy over N folds
- Compute $P(M \geq m \mid H_0)$
- Reject H_0 with p-value $p \leq S$ if $P(M \geq m \mid H_0) \leq S$
  Caveat: the p-value corresponds to $P(m \mid H_0)$, *not* $P(H_0 \mid m)$

p-Values

Commonly used *p*-values are:

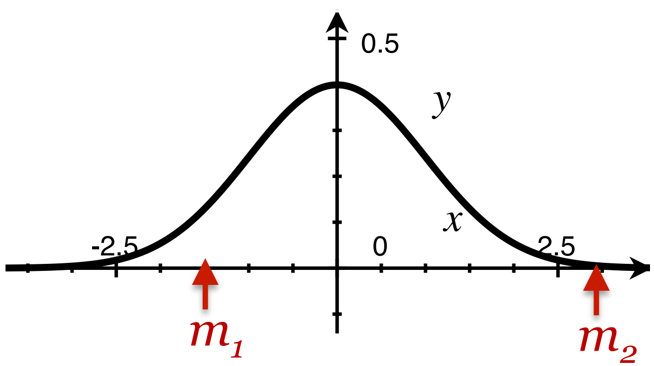
– 0.05: There is a 5% (1/20) chance to get the observed results under the null hypothesis.

Corollary: If you run 20 or more experiments, at least one of them will yield results that fall in the "statistically significant range" with p=0.05, even if the null hypothesis is actually true.

– 0.01: There is a 1% (1/100) chance to get the observed results under the null hypothesis.

Null hypothesis

Null hypothesis:
We assume the data comes from a (normal) distribution $P(M \mid H_o)$ with mean $\mu=0$ and (unknown) variance σ^2/N.



From the data (sample) $X = \{x^1 \ldots x^N\}$, we compute the **sample mean** $m = \sum_i x^i/N$

How likely is it that m came from $P(M \mid H_o)$?

For m_1: very likely. For m_2: pretty unlikely

Confidence intervals

One-tailed test:

Test whether the accuracy of A is higher than B with probability p

Two-tailed test:

Test whether the accuracies of A and B are different (lower or higher) with probability p

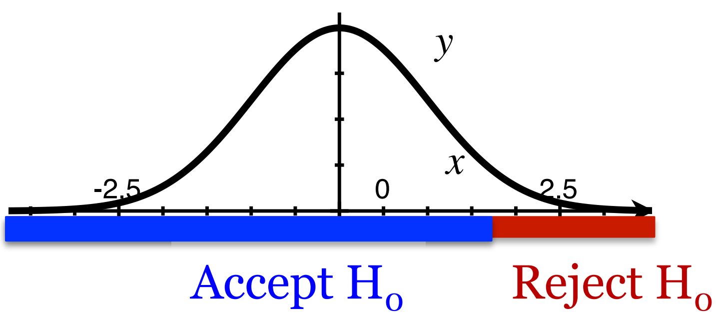
This is the stricter test.

Confidence intervals

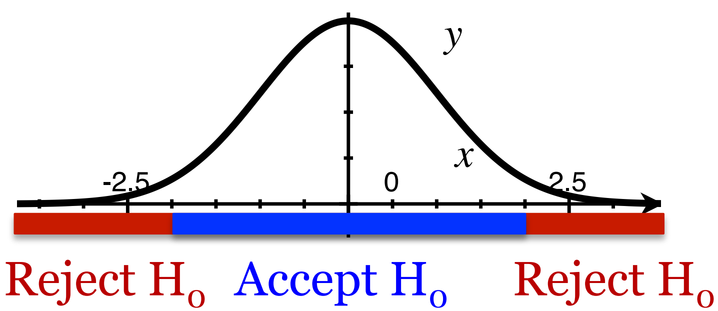
One-tailed test:
We fail to reject H_0 if *m* is inside the asymmetric 100(1-p) percent confidence interval (-∞, a)

Two-tailed test:
We fail to reject H_0 if *m* lies in the symmetric 100(1-p) percent confidence interval (-a, +a) around the mean.

p=0.05%; Confidence 95%
One-tailed test



p=0.05%; Confidence 95%
Two-tailed test



Hypothesis tests to evaluate classifiers

Paired t-test:

Compare the performance of two classifiers on N test sets (e.g. N-fold cross-validation).

Uses the t-statistic to compute confidence intervals.

McNemar's test:

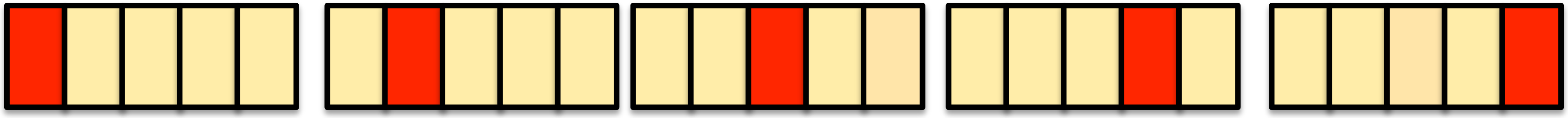
Compare the performance of two classifiers on N items from a single test set.

N-fold cross validation: Paired t-test

N-fold cross validation

Instead of a single test-training split:

– Split data into N equal-sized parts



– Train and test N different instances of the same classifier

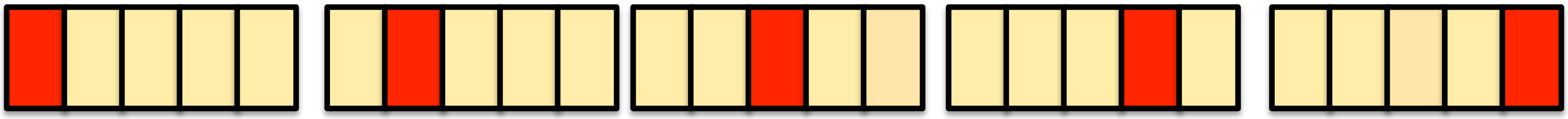
– This gives N different accuracies

Evaluating N-fold cross validation

	test set 1	**test set 2**	**test set 3**	**test set 4**	**test set 5**
A	80%	82%	85%	78%	85%
B	81%	81%	86%	80%	88%
diff (A–B)	*-1%*	*+1%*	*-1%*	*-2%*	*-3%*

The paired t-test tells us whether there is a (statistically significant) difference between the accuracies of classifiers A and B, based on their difference in accuracy on N different test sets.

Paired t-test for cross-validation



Two different classifiers, A and B are trained and tested using N-fold cross-validation

For the *n*-th fold:

$$accuracy(\mathrm{A}, n),\ accuracy(\mathrm{B}, n)$$
$$diff_{\mathrm{n}} = accuracy(\mathrm{A}, n) - accuracy(\mathrm{B}, n)$$

Null hypothesis: *diff* comes from a distribution with mean (expected value) = 0.

Paired t-test

Null hypothesis (H_0; to be rejected), informally:
There is no difference between A and B's accuracy.

- Statistically, we treat accuracy(A) and accuracy(B) as random variables drawn from some distribution.
- H_0 says that accuracy(A) and accuracy(B) are drawn from the same distribution.
- If H_0 is true, then the expected difference (over all possible data sets) between their accuracies is 0.

Null hypothesis (H_0; to be rejected), formally:
The difference between accuracy(A) and accuracy(B) on the same test set is a random variable with mean = 0.

$$H_0: E[\text{accuracy(A)} - \text{accuracy(B)}] = E[\mathit{diff}_D] = 0$$

Paired t-test

Null hypothesis (H_0; to be rejected), formally:
The difference between accuracy(A) and accuracy(B) on the same test set is a random variable with mean = 0.

$$H_0: E[\text{accuracy(A)} - \text{accuracy(B)}] = E[diff_D] = 0$$

- $E[diff_D]$ is the expected value (mean) over all possible data sets. We don't (can't) know that quantity.
- But N-fold cross-validation gives us N samples of $diff_D$

We can ask instead: How likely are these N samples to come from a distribution with mean = 0?

Paired t-test

Paired t-test: The accuracy of A on test set *i* is paired with the accuracy of B on test set *i*

Assumption: Accuracies are drawn from a normal distribution (with unknown variance)

Null hypothesis: The accuracies of A and B are drawn from the same distribution.

Hence, the *difference* of the accuracies on test set *i* comes from a normal distribution with mean = 0

Alternative hypothesis: The accuracies are drawn from two different distributions: E[*diff*] ≠ 0

Paired t-test

Given: **a sample of *N* observations**

We assume these come from a normal distribution with fixed (but unknown) mean and variance

- Compute the **sample mean** and **sample variance** for these observations
- This allows you to compute the **t-statistic**.
- The **t-distribution for *N-1* degrees of freedom** can be used to estimate how likely it is that the true mean is in a given range

Reject H_o at significance level p if the t-statistic does not lie in the interval $(-t_{p/2,\, n-1}, +t_{p/2,\, n-1})$.

There are tables where you can look this up

Computing the t-statistic

Difference in accuracy on the n-th test set:

$$diff_n = Accuracy_n(\mathrm{A}) - Accuracy_n(\mathrm{B})$$

Sample mean m of $diff_D$, based on N samples of $diff_D$:

$$m = \frac{1}{N}\sum_{n=1}^{N} diff_n$$

Sample standard deviation S of $diff_D$:

$$S = \sqrt{\frac{\sum_{n=1}^{N}(diff_n - m)^2}{N-1}}$$

t-statistic for N samples of $diff_D$:

$$t = \frac{\sqrt{N}\cdot m}{S}$$

Can we reject H_o?

1. Compute the t-statistic t for your N samples.
2. Define a p-value $p \in \{0.05, 0.01, 0.001\}$.
3. Look up $t_{p/2,N-1}$ for N−1 degrees of freedom (df)
4. If $t > t_{N\text{-}1,p}$: Reject H_o with p-value p

For our example:

	test set 1	test set 2	test set 3	test set 4	test set 5
A	80%	82%	85%	78%	85%
B	81%	81%	86%	80%	88%
diff (A–B)	*-1%*	*+1%*	*-1%*	*-2%*	*-3%*

$m = (-1 + 1 - 1 - 2 - 3)/5 = -6/5 = -1.2$

$S = \sqrt{\frac{(-2.2)^2 + 2.2^2 + (-2.2)^2 + (-3.2)^2 + (-4.2)^2}{4}} \approx 3.256$

Our t-statistic $t = -0.824$

With p=0.05 and N–1 = 4: $t_{0.025,4} = 2.776$

We cannot reject H$_0$: t is between $-t_{0.025,4}$ and $+t_{0.025,4}$

$-t_{0.025,4} = -2.776 < t = -0.824 < +t_{0.025,4} = 2.776$

Summary t-test

The t-test can be used to to compare two classifiers on N-fold cross-validation.

Caveat: N should be at least 30.

Alternative: 5x2 Cross-validation

A single test set: McNemar’s test

McNemar's test

Compares classifiers A and B on a single test set.

Considers the number of test items where
either A or B make errors:

n_{11}: number of items classified correctly by both A and B

n_{00}: number of items misclassified by both A and B

n_{01}: number of items misclassified by A but not by B

n_{10}: number of items misclassified by B but not by A

Null hypothesis:
A and B have the same error rate. Hence, $n_{01} = n_{10}$

McNemar's test

Observed data:

n_{00}	n_{01}
n_{10}	n_{11}

Expected counts under H_0:

n_{00}	$(n_{01} + n_{10})/2$
$(n_{01} + n_{10})/2$	n_{11}

Compute the χ^2 statistic

$$\chi^2 = \frac{\left(|n_{01} - n_{10}| - 1\right)^2}{n_{01} + n_{10}}$$

McNemar's test

Two-tailed test:

– Reject H_0 with p=0.05 if $\chi^2 > \chi_{.05}{}^2 = 3.84$

– Reject H_0 with p=0.01 if $\chi^2 > \chi_{.05}{}^2 = 6.63$

One-tailed test:

– Reject H_0 with p=0.05 if $\chi^2 > \chi_{.05}{}^2 = 2.71$

– Reject H_0 with p=0.01 if $\chi^2 > \chi_{.05}{}^2 = 5.43$

McNemar’s test

McNemar’s test is used to compare the performance of two classifiers on the same test set.

This test works if there are a large number of items on which A and B make different predictions.

Today's key concepts

Using significance tests to compare the performance of two classifiers:

t-test (Cross-validation)

McNemar's test (single test set)