

Bayesian Hypotheses Testing

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Null hypothesis significance testing

NHST in machine learning

Pitfalls of NHST

Bayesian tests

Bibliography

Based on tutorial by Benavoli et al.

<http://ipg.idsia.ch/tutorials/2016/bayesian-tests-ml/>

Experiments:

- ▶ Comparing Adaboost (ada) vs. Gradient boosting classifier (gbc)
- ▶ scikit-learn implementation
- ▶ `max_depth=1, n_estimators=100`
- ▶ `learning_rate=1.0` (gbc)

Data

Table: 27 UCI data sets

	Name	Size	No. of features
0	heart-statlog	270	13
1	mushroom	5644	22
2	segment	2310	19
3	cleveland-14-heart-disease	296	13
4	zoo	101	17
	...		
23	ionosphere	351	34
24	pima_diabetes	768	8
25	vote	232	16
26	vehicle	846	18

Procedure of NHST

1. State the null and the alternative hypotheses H_0 and H_1
2. Based on statistical assumption about data, choose a statistical test
3. Under the null hypothesis, the test statistic T follows a known probability distribution
4. Calculate observed test statistic $t(\mathbf{x})$
5. Calculate the probability that T is “more extreme” than observed $t(\mathbf{x})$ (the p -value)
6. If $p < \alpha$, reject H_0

Correlated t -test

- ▶ Used to test two algorithms on one data set
- ▶ Calculates a score (e. g., accuracy) on p runs of k -fold cross-validation
- ▶ Sample size: $n = pk$
- ▶ Observations: $\mathbf{x} = (x_i)_{i=1}^n$, the score differences on each fold
- ▶ The standard t -test assumes x_i to be independently, identically and normally distributed
- ▶ Correlated t -test accounts for correlations between $x_i, x_j, i \neq j$ due to cross-validation

Correlated t -test (II)

The test statistic:

$$t(\mathbf{x}, \mu) = \frac{\bar{\mathbf{x}} - \mu}{\sqrt{\hat{\sigma}^2 \left(\frac{1}{n} - \frac{\rho}{1-\rho} \right)}}$$

- ▶ t follows Student's distribution with $n - 1$ degrees of freedom
- ▶ ρ – correlation between results from overlapping training sets
- ▶ $\frac{\rho}{1-\rho} = \frac{n_{te}}{n_{tr}}$ – a heuristic for the correlation correction parameter (Nadeau and Bengio, 2003)
- ▶ Two-sided test: $H_0 : \mu = 0, H_1 : \mu \neq 0$
- ▶ One-sided test: $H_0 : \mu \leq 0, H_1 : \mu > 0$

Example

Table: p -values of the two-sided correlated t -test. 14 out of 27 results are significant at $\alpha = 0.05$.

	Name	p-val
0	heart-statlog	0.51
1	mushroom	0.00*
2	segment	0.00*
3	cleveland-14-heart-disease	0.42
4	zoo	0.00*
	...	
23	ionosphere	0.23
24	pima_diabetes	0.29
25	vote	0.39
26	vehicle	0.00*

Wilcoxon signed-rank test

- ▶ Used to compare two classifiers on multiple data sets
- ▶ Counts ranks of differences, not their magnitudes
- ▶ z_i – the mean score difference on i th data set, $i = 1, \dots, q$
- ▶ z_i assumed to be i.i.d. samples from a symmetric distribution

Wilcoxon signed-rank test (II)

- ▶ The test statistic is

$$t = \min \left\{ \begin{aligned} &\sum_{i:z_i>0} \text{rank}(|z_i|) + \frac{1}{2} \sum_{i:z_i=0} \text{rank}(|z_i|), \\ &\sum_{i:z_i<0} \text{rank}(|z_i|) + \frac{1}{2} \sum_{i:z_i=0} \text{rank}(|z_i|) \end{aligned} \right\}$$

- ▶ Critical value tables exist for q small enough, e. g., $q < 25$
- ▶ Otherwise $w = \frac{t - \frac{1}{4}q(q+1)}{\sqrt{\frac{1}{24}q(q+1)(2q+1)}}$ follows an approximately normal distribution

Example

Wilcoxon signed-rank test of mean accuracy difference between ada and gbc:

$$w = 120, p\text{-value} = 0.10.$$

p -value not what researchers want

- ▶ p -value is not the probability of the null hypothesis

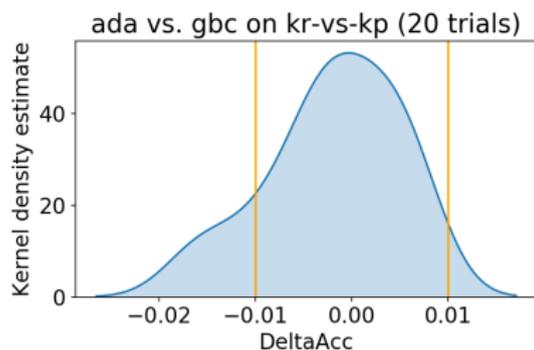
$$p(T > t(\mathbf{x})|H_0) \neq p(H_0|\mathbf{x})$$

- ▶ Similarly, $1 - p$ is not the probability of the alternative hypothesis

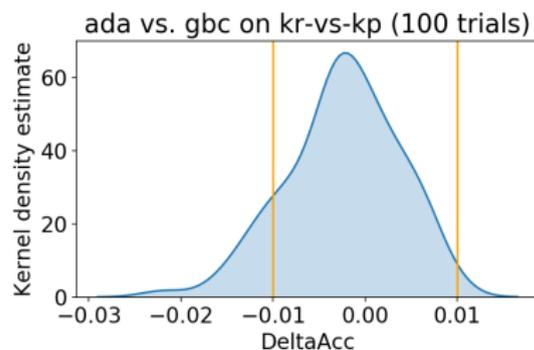
$$p(T \leq t(\mathbf{x})|H_0) \neq p(H_1|\mathbf{x})$$

p -value depends on sample size

- ▶ The difference between classifiers is never zero
- ▶ Arbitrarily small effects can be confirmed on large enough samples



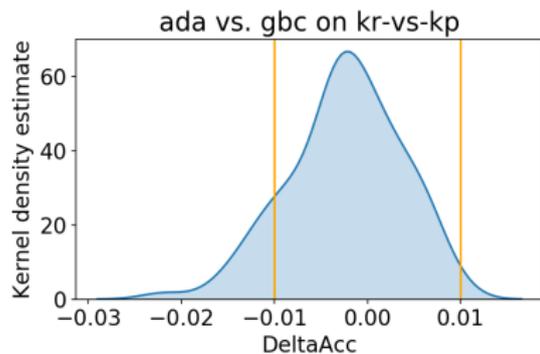
20 trials, p -value = 0.24



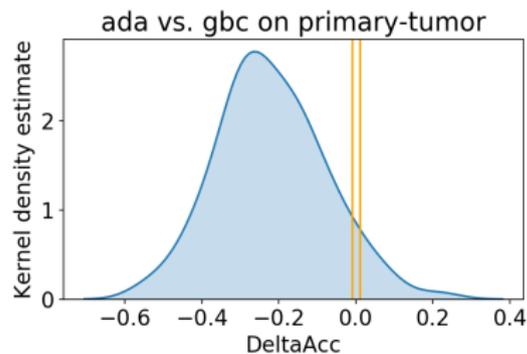
100 trials, $pr < 10^{-3}$

NHST cannot measure effect size

- ▶ Statistical significance does not imply practical significance



$$p < 10^{-3}$$



$$p < 10^{-3}$$

And more . . .

- ▶ If null hypothesis is not rejected, the result is inconclusive
- ▶ Significance level cannot be reasonably decided
- ▶ NHST assumes certain sampling intentions

Bayesian analysis

Bayesian inference:

1. Formulating a joint probability model of observable data \mathbf{x} and unknown parameters θ :

$$p(\theta, \mathbf{x}) = p(\mathbf{x}|\theta)p(\theta)$$

2. Inferring $\theta|\mathbf{x}$ by Bayes' theorem:

$$p(\theta|\mathbf{x}) = \frac{p(\theta, \mathbf{x})}{p(\mathbf{x})} = \frac{p(\mathbf{x}|\theta)p(\theta)}{p(\mathbf{x})}$$

3. Summarizing the posterior distribution

Bayesian correlated t -test

Likelihood:

$$\mathbf{x} \mid \mu, \tau \sim \text{MVN}(\mu \mathbf{1}, \Sigma)$$
$$\Sigma = \begin{pmatrix} 1/\tau & \rho/\tau & \cdots & \rho/\tau \\ \rho/\tau & 1/\tau & \cdots & \rho/\tau \\ \vdots & \vdots & \ddots & \vdots \\ \rho/\tau & \rho/\tau & \cdots & 1/\tau \end{pmatrix}$$

Prior:

$$\mu, \tau \sim \text{NormalGamma}(\mu_0, k_0, a, b)$$

$$\mu \mid \tau \sim \mathcal{N}(\mu_0, k_0/\tau)$$

$$\tau \sim \text{Gamma}(a, b)$$

Bayesian correlated t -test (II)

- ▶ NormalGamma is conjugate to MVN
- ▶ The posterior is a NormalGamma distribution
- ▶ Marginalizing out precision τ , the posterior of μ is a Student t -distribution
- ▶ For $\mu_0 = 0, k_0 \rightarrow \infty, a = -1/2, b = 0$ (matching prior):

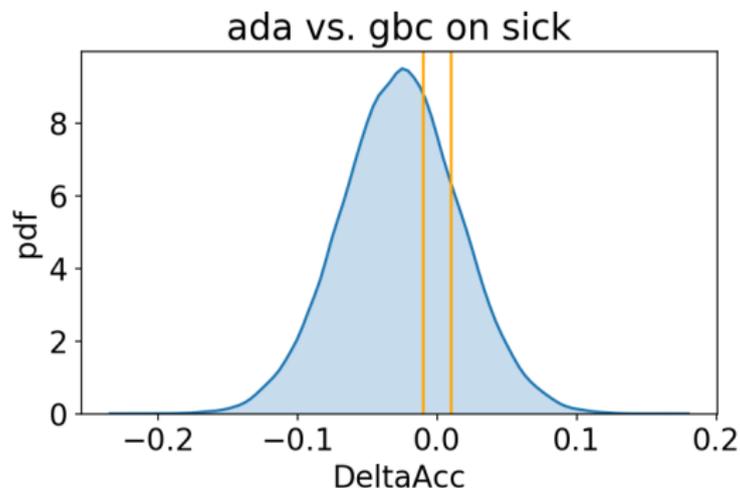
$$\mu \sim St \left(n - 1, \bar{\mathbf{x}}, \sqrt{\hat{\sigma}^2 \left(\frac{1}{n} + \frac{\rho}{1 - \rho} \right)} \right)$$

- ▶ What is the difference then?

Example

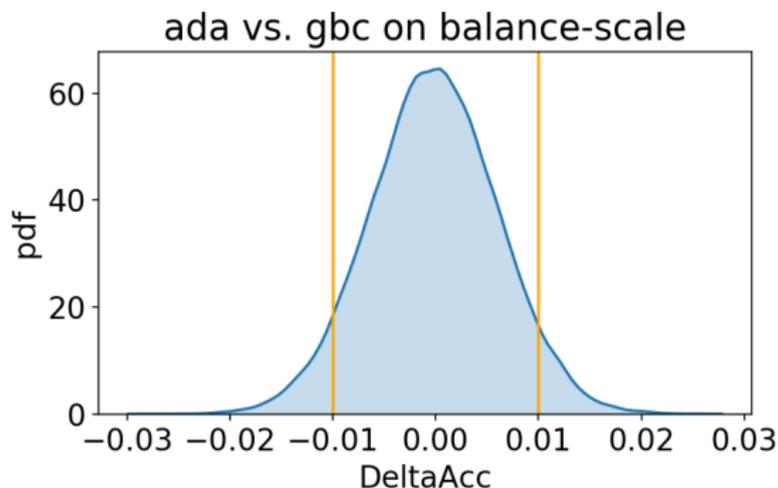
Region of practical equivalence (rope): 0.01

$$P(ada) > gbc) = 0.65 \quad P(rope) = 0.15 \quad P(gbc > ada) = 0.20$$



Example

- ▶ Can show practically significant differences ($1 - P(\text{rope})$)
- ▶ Can quantify uncertainty (high density intervals)
- ▶ Posterior probability of the null: $P(\text{rope})$
- ▶ Provides basis for decisions (expected loss minimization)



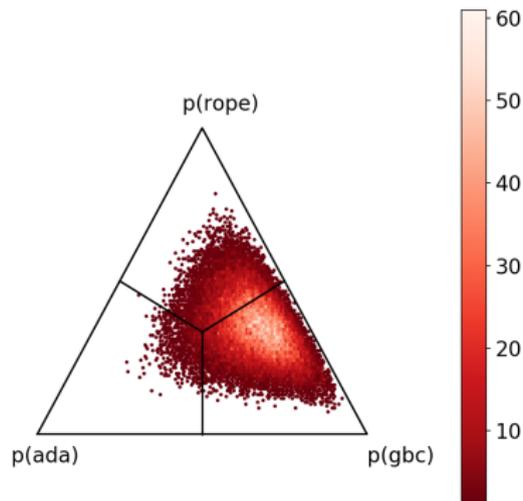
Bayesian signed-rank test

- ▶ Let $\mathbf{z} = (z_1, \dots, z_q)$ be i.i.d. samples of z
- ▶ Place Dirichlet process prior on z parameterized by strength $s > 0$ and mean z_0
- ▶ The posterior is a Dirichlet mixture
- ▶ Can be reformulated to a ternary distribution of test outcomes
- ▶ Monte Carlo sampling used to approximate the posterior

Example

Rope = 0.01

$$P(ada > gbc) = 0.02 \quad P(rope) = 0.24 \quad P(gbc > ada) = 0.75$$



Posterior for Bayesian signed-rank test for ada vs. gbc on 27 UCI data sets

Conclusion

- ▶ NHST has many drawbacks
- ▶ Bayesian tests:
 - ▶ claimed significant differences are practical
 - ▶ are able to detect practical equivalence
 - ▶ provide estimate with uncertainty
 - ▶ allow to automatize decisions

Bibliography

-  A. Benavoli, G. Corani, J. Demsar, and M. Zaffalon, *Time for a change: a tutorial for comparing multiple classifiers through Bayesian analysis*, ArXiv e-prints (2016).
-  J. Demšar, *Statistical comparisons of classifiers over multiple data sets*, J. Mach. Learn. Res. **7** (2006), 1–30.

Thank you!
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