

Statistical Methods for Data Science

Lesson 23 - Two sample testing of the mean, and F -test.

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Tests and confidence intervals for classifier performance

The Caret package

- 1 Define sets of model parameter values to evaluate
- 2 **for** *each parameter set* **do**
- 3 | **for** *each resampling iteration* **do**
- 4 | | Hold-out specific samples
- 5 | | [Optional] Pre-process the data
- 6 | | Fit the model on the remainder
- 7 | | Predict the hold-out samples
- 8 | **end**
- 9 | Calculate the average performance across hold-out predictions
- 10 **end**
- 11 Determine the optimal parameter set
- 12 Fit the final model to all the training data using the optimal parameter set

The binomial test

- Dataset x_1, \dots, x_n realization of $X_1, \dots, X_n \sim \text{Ber}(\theta)$
- $H_0 : \theta = \theta_0$ $H_1 : \theta \neq \theta_0$
- Test statistics: $T = \sum_{i=1}^n X_i \sim \text{Bin}(n, \theta_0)$ *[Asymmetric distribution]*
- t -value is $t = \sum_{i=1}^n x_i$
- Critical values (exact test):

$$P(T \leq l) = \sum_{i=0}^l \binom{n}{i} \theta_0^i (1 - \theta_0)^{n-i} = P(T \leq b) = \sum_{i=u}^n \binom{n}{i} \theta_0^i (1 - \theta_0)^{n-i} = \alpha/2$$

- Normal approximation $\text{Bin}(n, \theta_0) \approx N(\theta_0, \theta_0(1 - \theta_0))$: use z-test (or even t-test)

See R script

Two sample test of the mean

- Dataset x_1, \dots, x_n realization of $X_1, \dots, X_n \sim F_1$ with $E[X_i] = \mu_1$ and $\text{Var}(X_i) = \sigma_X^2$
- Dataset y_1, \dots, y_m realization of $Y_1, \dots, Y_m \sim F_2$ with $E[Y_i] = \mu_2$ and $\text{Var}(Y_i) = \sigma_Y^2$
 - ▶ measurements for control and (medical) treatment groups of patients
 - ▶ performances on benchmark datasets/folds of two different classifiers

- $H_0 : \mu_1 = \mu_2$ $H_1 : \mu_1 \neq \mu_2$
- Test statistics:
$$T = \frac{\bar{X}_n - \bar{Y}_m}{\sqrt{\text{Var}(\bar{X}_n - \bar{Y}_m)}} = \frac{\bar{X}_n - \bar{Y}_m}{\sqrt{\frac{\sigma_X^2}{n} + \frac{\sigma_Y^2}{m}}}$$

- We distinguish a few cases:

- ▶ F_1, F_2 are normal distributions
 - σ_X^2 and σ_Y^2 are known
 - σ_X^2 and σ_Y^2 are unknown and $\sigma_X^2 = \sigma_Y^2$
 - σ_X^2 and σ_Y^2 are unknown and $\sigma_X^2 \neq \sigma_Y^2$

[z-test]

[t-test]

[Welch test]

- ▶ F_1, F_2 are general distributions
 - Large sample
 - $F_1(x - \Delta) = F_2(x)$ location-shift
 - Bootstrap two sample test

[t-test]

[Wilcoxon test]

- ▶ Paired data

[paired t-test]

Normal data with known σ_X^2 and σ_Y^2 : z-test

• $X_1, \dots, X_n \sim N(\mu_1, \sigma_X^2)$ and $Y_1, \dots, Y_m \sim N(\mu_2, \sigma_Y^2)$

• $H_0 : \mu_1 = \mu_2$

• $H_1 : \mu_1 \neq \mu_2$

• $100(1 - \alpha)\%$, e.g., 95% or 99% or 99.9%

▶ i.e., $\alpha = 0.05$ or $\alpha = 0.01$ or $\alpha = 0.001$

• $Z = \frac{\bar{X}_n - \bar{Y}_m}{\sqrt{\frac{\sigma_X^2}{n} + \frac{\sigma_Y^2}{m}}} \sim N(0, 1)$ test statistics when H_0 is true

• z value is $\frac{\bar{x}_n - \bar{y}_m}{\sqrt{\frac{\sigma_X^2}{n} + \frac{\sigma_Y^2}{m}}}$ and p-value $p = P(|Z| \geq |z|) = 2(1 - \Phi(|z|))$

• $P(Z \leq -z_{\alpha/2}) = \alpha/2$ and $P(Z \geq z_{\alpha/2}) = \alpha/2$

• Output of the test at confidence level $100(1 - \alpha)\%$ using critical values

▶ $|z| \geq z_{\alpha/2}$: H_0 is rejected

▶ otherwise: H_0 cannot be rejected

[Two-tailed test]

[Confidence level]

[Significance level]

[Critical values]

[Critical region]

See R script

Unknown $\sigma_X^2 = \sigma_Y^2 = \sigma^2$ and pooled variance

- We need to estimate $\text{Var}(\bar{X}_n - \bar{Y}_m) = \sigma^2 \left(\frac{1}{n} + \frac{1}{m}\right)$
- Recall

$$S_X = \frac{1}{n-1} \sum_{i=1}^n (X_i - \bar{X}_n)^2 \quad \text{and} \quad S_Y = \frac{1}{m-1} \sum_{i=1}^m (Y_i - \bar{Y}_m)^2$$

are unbiased estimators of σ_X^2 and σ_Y^2

- The *pooled variance*:

$$S_p^2 = \frac{(n-1)S_X^2 + (m-1)S_Y^2}{n+m-2} \left(\frac{1}{n} + \frac{1}{m}\right) = \frac{\sum_{i=1}^n (X_i - \bar{X}_n)^2 + \sum_{i=1}^m (Y_i - \bar{Y}_m)^2}{n+m-2} \left(\frac{1}{n} + \frac{1}{m}\right)$$

is an unbiased estimator of $\sigma^2 \left(\frac{1}{n} + \frac{1}{m}\right)$

F-test for normal data

- $X_1, \dots, X_n \sim N(\mu_1, \sigma_X^2)$ and $Y_1, \dots, Y_m \sim N(\mu_2, \sigma_Y^2)$
- $H_0 : \sigma_X^2 = \sigma_Y^2$
- $H_1 : \sigma_X^2 \neq \sigma_Y^2$ *[Two-tailed test]*
- $100(1 - \alpha)\%$, e.g., 95% or 99% or 99.9% *[Confidence level]*
 - ▶ i.e., $\alpha = 0.05$ or $\alpha = 0.01$ or $\alpha = 0.001$ *[Significance level]*
- $F = \frac{S_X^2}{S_Y^2} \sim F(n - 1, m - 1)$ test statistics when H_0 is true *[Fisher-Snedecor distribution]*
- f value is $\frac{S_X^2}{S_Y^2}$ and p -value is $p = 2 \min \{P(F \leq f), 1 - P(F \leq f)\}$ *[Asymmetric]*
- $P(F \leq l) = \alpha/2$ and $P(F \geq r) = \alpha/2$ *[Critical values]*
- Output of the test at confidence level $100(1 - \alpha)\%$ using critical values *[Critical region]*
 - ▶ $t \leq l$ or $t \geq r$: H_0 is rejected
 - ▶ otherwise: H_0 cannot be rejected

See R script

Normal data with unknown $\sigma_X^2 = \sigma_Y^2 = \sigma^2$: t-test

- $X_1, \dots, X_n \sim N(\mu_1, \sigma^2)$ and $Y_1, \dots, Y_m \sim N(\mu_2, \sigma^2)$
- $H_0 : \mu_1 = \mu_2$
- $H_1 : \mu_1 \neq \mu_2$ *[Two-tailed test]*
- $100(1 - \alpha)\%$, e.g., 95% or 99% or 99.9% *[Confidence level]*
 - ▶ i.e., $\alpha = 0.05$ or $\alpha = 0.01$ or $\alpha = 0.001$ *[Significance level]*
- $T_p = \frac{\bar{X}_n - \bar{Y}_m}{S_p} \sim t(n + m - 2)$ test statistics when H_0 is true
- t value is $\frac{\bar{x}_n - \bar{y}_m}{\sqrt{\frac{(n-1)s_X^2 + (m-1)s_Y^2}{n+m-2} \left(\frac{1}{n} + \frac{1}{m}\right)}}$ and p -value $p = P(|T_p| > |t|)$
- $P(T_p \leq -t_{n+m-2, \alpha/2}) = \alpha/2$ and $P(T_p \geq t_{n+m-2, \alpha/2}) = \alpha/2$ *[Critical values]*
- Output of the test at confidence level $100(1 - \alpha)\%$ using critical values *[Critical region]*
 - ▶ $|t| \geq t_{n+m-2, \alpha/2}$: H_0 is rejected
 - ▶ otherwise: H_0 cannot be rejected

See R script

Normal data with unknown $\sigma_X^2 \neq \sigma_Y^2$

- The *nonpooled variance*:

$$S_d^2 = \frac{S_X^2}{n} + \frac{S_Y^2}{m}$$

is an unbiased estimator of $\text{Var}(\bar{X}_n - \bar{Y}_m) = \frac{\sigma_X^2}{n} + \frac{\sigma_Y^2}{m}$

- The test statistics $T_d = \frac{\bar{X}_n - \bar{Y}_m}{S_d}$ is not t -distributed!
- Possible solution: empirical bootstrap (see textbook Sect. 28.3)
- Another solution: Welch t -test

Normal data with unknown $\sigma_X^2 \neq \sigma_Y^2$: Welch t-test

- $X_1, \dots, X_n \sim N(\mu_1, \sigma_X^2)$ and $Y_1, \dots, Y_m \sim N(\mu_2, \sigma_Y^2)$
- $H_0 : \mu_1 = \mu_2$
- $H_1 : \mu_1 \neq \mu_2$ *[Two-tailed test]*
- $100(1 - \alpha)\%$, e.g., 95% or 99% or 99.9% *[Confidence level]*
 - ▶ i.e., $\alpha = 0.05$ or $\alpha = 0.01$ or $\alpha = 0.001$ *[Significance level]*
- $T_d = \frac{\bar{X}_n - \bar{Y}_m}{S_d} \approx t(v)$ test statistics when H_0 is true, with $v = \frac{(\frac{1}{n} + \frac{u}{m})^2}{\frac{1}{n^2(n-1)} + \frac{u^2}{m^2(m-1)}}$ and $u = \frac{s_Y^2}{s_X^2}$
- t value is $\frac{\bar{x}_n - \bar{y}_m}{\sqrt{\frac{s_X^2}{n} + \frac{s_Y^2}{m}}}$ and p -value $p = P(|T_d| > |t|)$
- $P(T_d \leq -t_{v, \alpha/2}) = \alpha/2$ and $P(T_d \geq t_{v, \alpha/2}) = \alpha/2$ *[Critical values]*
- Output of the test at confidence level $100(1 - \alpha)\%$ using critical values *[Critical region]*
 - ▶ $|t| \geq t_{v, \alpha/2}$: H_0 is rejected
 - ▶ otherwise: H_0 cannot be rejected

See R script

General data, large sample: t-test

- $X_1, \dots, X_n \sim F_1$ and $Y_1, \dots, Y_m \sim F_2$
- $H_0 : \mu_1 = \mu_2$
- $H_1 : \mu_1 \neq \mu_2$
- $100(1 - \alpha)\%$, e.g., 95% or 99% or 99.9%
 - ▶ i.e., $\alpha = 0.05$ or $\alpha = 0.01$ or $\alpha = 0.001$

[Two-tailed test]
[Confidence level]
[Significance level]

- $T_d = \frac{\bar{X}_n - \bar{Y}_m}{S_d} \approx N(0, 1)$
- t value is $\frac{\bar{x}_n - \bar{y}_m}{\sqrt{\frac{s_X^2}{n} + \frac{s_Y^2}{m}}}$ and p -value $p = P(|T_d| > |t|)$

- $P(T_d \leq -z_{\alpha/2}) = \alpha/2$ and $P(T_d \geq z_{\alpha/2}) = \alpha/2$
- Output of the test at confidence level $100(1 - \alpha)\%$ using critical values
 - ▶ $|t| \geq z_{\alpha/2}$: H_0 is rejected
 - ▶ otherwise: H_0 cannot be rejected

[Critical values]
[Critical region]

See R script

General data, location-shift: Wilcoxon rank-sum test

- Also called as: **Mann–Whitney U test**, Mann–Whitney–Wilcoxon (MWW), or Wilcoxon–Mann–Whitney test
- $X_1, \dots, X_n \sim F_1$ and $Y_1, \dots, Y_m \sim F_2$
- $H_0 : \mu_1 = \mu_2$, actually, $H_0 : F_1(x - \Delta) = F_2(x)$ where $\Delta = \mu_2 - \mu_1$ [*Location-shift model*]
- $H_1 : \mu_1 \neq \mu_2$ [*Two-tailed test*]
- $W = \sum_{i=1}^n S_i \sim W(n, m)$ when H_0 is true
 - ▶ where S_i is the rank of X_i in sorted($X_1, \dots, X_n, Y_1, \dots, Y_m$)
 - ▶ `pwilcox` in R, or large sample Normal approx, or $U = W - \frac{n(n+1)}{2}$ statistic
- w value is $\sum_{i=1}^n s_i$ and p -value $p = P(|W| > |w|)$
- $P(W \leq -w_{\alpha/2}) = \alpha/2$ and $P(T_p \geq w_{\alpha/2}) = \alpha/2$ [*Critical values*]
- Output of the test at confidence level $100(1 - \alpha)\%$ using critical values
 - ▶ $|w| \geq w_{\alpha/2}$: H_0 is rejected [*Critical region*]
 - ▶ otherwise: H_0 cannot be rejected

See R script

General data: bootstrap test

- Equal variance ($\sigma_X^2 = \sigma_Y^2$)
 - ▶ bootstrap of pooled studentized mean difference

$$t_p^* = \frac{(\bar{x}_n^* - \bar{y}_m^*) - (\bar{x}_n - \bar{y}_m)}{s_p^*}$$

- Non-equal variance ($\sigma_X^2 \neq \sigma_Y^2$)
 - ▶ bootstrap of nonpooled studentized mean difference

$$t_d^* = \frac{(\bar{x}_n^* - \bar{y}_m^*) - (\bar{x}_n - \bar{y}_m)}{s_d^*}$$

See R script

Paired data

- Datasets x_1, \dots, x_n and y_1, \dots, y_n are measurement for the same experimental unit
 - ▶ unit: a person before and after a (medical) treatment
 - ▶ unit: a dataset/fold used to train two different classifiers
- The theory is essentially based on taking differences $x_1 - y_1, \dots, x_n - y_n$ and thus reducing the problem to that of a one-sample test.
- $H_0 : \mu_1 = \mu_2 \Rightarrow H_0 : \mu_1 - \mu_2 = 0$
- Advantage: better power / lower Type II risk of the test w.r.t. unpaired version
 - ▶ $P_{paired}(p \leq \alpha | H_1) \geq P_{unpaired}(p \leq \alpha | H_1)$

See R script

Reference handbook (with R code)

