Master Program in *Data Science and Business Informatics*

Statistics for Data Science

Lesson 31 - Two-sample tests of the mean and applications to classifier comparison

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Tests and confidence intervals for classifier performance

The Caret package

```
Define sets of model parameter values to evaluate
for each parameter set do
    for each resampling iteration do
        Hold–out specific samples
        [Optional] Pre–process the data
        Fit the model on the remainder
        Predict the hold–out samples
    end
    Calculate the average performance across hold–out predictions
end
Determine the optimal parameter set
Fit the final model to all the training data using the optimal parameter set
```

See R script

Binary classifier performance metrics

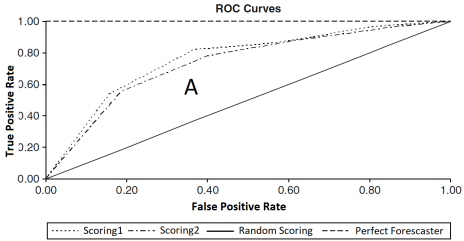
Confusion matrix (in R packages, it is transposed)

		Predicted condition			
	Total population $= P + N$	**Positive (PP)**	**Negative (PN)**	Informedness, bookmaker informedness (BM) $= TPR + TNR - 1$	Prevalence threshold (PT) $= \frac{\sqrt{TPR \times FPR} - FPR}{TPR - FPR}$
Actual condition	**Positive (P)**	**True positive (TP),** **hit**	**False negative (FN),** **type II error, miss,** **underestimation**	True positive rate (TPR), recall, sensitivity (SEN), probability of detection, hit rate, power $= \frac{TP}{P} = 1 - FNR$	False negative rate (FNR), miss rate $= \frac{FN}{P} = 1 - TPR$
	Negative (N)	**False positive (FP),** **type I error, false alarm,** **overestimation**	**True negative (TN),** **correct rejection**	False positive rate (FPR), probability of false alarm, fall-out $= \frac{FP}{N} = 1 - TNR$	True negative rate (TNR), specificity (SPC), selectivity $= \frac{TN}{N} = 1 - FPR$
	Prevalence $= \frac{P}{P + N}$	Positive predictive value (PPV), precision $= \frac{TP}{PP} = 1 - FDR$	False omission rate (FOR) $= \frac{FN}{PN} = 1 - NPV$	Positive likelihood ratio (LR+) $= \frac{TPR}{FPR}$	Negative likelihood ratio (LR−) $= \frac{FNR}{TNR}$
	Accuracy (ACC) $= \frac{TP + TN}{P + N}$	False discovery rate (FDR) $= \frac{FP}{PP} = 1 - PPV$	Negative predictive value (NPV) $= \frac{TN}{PN} = 1 - FOR$	Markedness (MK), deltaP (Δp) $= PPV + NPV - 1$	Diagnostic odds ratio (DOR) $= \frac{LR+}{LR-}$
	Balanced accuracy (BA) $= \frac{TPR + TNR}{2}$	F_1 score $= \frac{2PPV \times TPR}{PPV + TPR} = \frac{2TP}{2TP + FP + FN}$	Fowlkes–Mallows index (FM) $= \sqrt{PPV \times TPR}$	Matthews correlation coefficient (MCC) $= \sqrt{TPR \times TNR \times PPV \times NPV} - \sqrt{FNR \times FPR \times FOR \times FDR}$	Threat score (TS), critical success index (CSI), Jaccard index $= \frac{TP}{TP + FN + FP}$

Metrics computed on a test set are intended to estimate some parameter over the general distribution.

- $X = (W, C) \sim F$, i.e., F is the (unknown) multivariate distribution of predictive features and class
- Accuracy ACC of a classifier y_θ^+ is a point estimate of $E_F[\mathbb{1}_{y_\theta^+(W)=C}] = P_F(y_\theta^+(W) = C)$

Binary classifier performance metrics



- Binary classifier score $s_\theta(w) \in [0,1]$ where $s_\theta(w)$ estimates $\eta(w) = P_{\theta_{TRUE}}(C = 1|W = w)$
- ROC Curve
  - $TPR(p) = P(s_\theta(w) \geq p|C = 1)$ and $FPR(p) = P(s_\theta(w)|C = 0)$
  - ROC Curve is the scatter plot $TPR(p)$ over $FPR(p)$ for p ranging from 1 down to 0
  - AUC-ROC is the area below the curve **What does AUC-ROC estimate?**
- Squared error loss or L_2 loss or Brier score: $\frac{1}{n}\sum_i (s_\theta(w_i) - c_i)^2$
- Classifier is calibrated if $P(C = 1|s_\theta(w) = p) = p$ **classifier-calibration.github.io**
  - Binary Expected Calibration Error (binary-ECE): $\sum_b \frac{|B_b|}{n}|Y_b - S_b|$
    - B_b is the set of i's in the b^{th} bin, $Y_b = |\{i|\ i \in B_b, c_i = 1\}|/|B_b|$, $S_b = (\sum_{i \in B_b} s_\theta(w_i))/|B_b|$

Two sample test of the mean

- Dataset $x_1, \ldots, x_n$ realization of $X_1, \ldots, X_n \sim F_1$ with $E[X_i] = \mu_1$ and $Var(X_i) = \sigma_X^2$
- Dataset $y_1, \ldots, y_m$ realization of $Y_1, \ldots, Y_m \sim F_2$ with $E[Y_i] = \mu_2$ and $Var(Y_i) = \sigma_Y^2$
  - measurements for control and (medical) treatment groups of patients
  - performances on benchmark datasets/folds of two different classifiers
- $H_0 : \mu_1 = \mu_2 \qquad H_1 : \mu_1 \neq \mu_2$
- Wald test statistics: $T = \frac{\bar{X}_n - \bar{Y}_m}{\sqrt{Var(\bar{X}_n - \bar{Y}_m)}} = \frac{\bar{X}_n - \bar{Y}_m}{\sqrt{\frac{\sigma_X^2}{n} + \frac{\sigma_Y^2}{m}}}$
- We distinguish a few cases:
  - F_1, F_2 are normal distributions
    - σ_X^2 and σ_Y^2 are known *[z-test]*
    - σ_X^2 and σ_Y^2 are unknown and $\sigma_X^2 = \sigma_Y^2$ *[t-test]*
    - σ_X^2 and σ_Y^2 are unknown and $\sigma_X^2 \neq \sigma_Y^2$ *[Welch test]*
  - F_1, F_2 are general distributions
    - Large sample *[t-test]*
    - $F_1(x - \Delta) = F_2(x)$ location-shift *[Wilcoxon test]*
    - Bootstrap two sample test
  - Paired data *[paired t-test]*

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

- $X_1, \ldots, X_n \sim N(\mu_1, \sigma_X^2)$ and $Y_1, \ldots, Y_m \sim N(\mu_2, \sigma_Y^2)$
- $H_0 : \mu_1 = \mu_2$
- $H_1 : \mu_1 \neq \mu_2$ *[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]*
- $Z = \frac{\bar{X}_n - \bar{Y}_m}{\sqrt{\frac{\sigma_X^2}{n} + \frac{\sigma_Y^2}{m}}} \sim N(0,1)$ 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 $P(Z \geq z_{\alpha/2}) = \alpha/2$ *[Critical values]*
- Output of the test at confidence level $100(1-\alpha)\%$ using critical values
  - $|z| \geq z_{\alpha/2}$: H_0 is rejected *[Critical region]*
  - otherwise: H_0 cannot be rejected

See R script

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

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

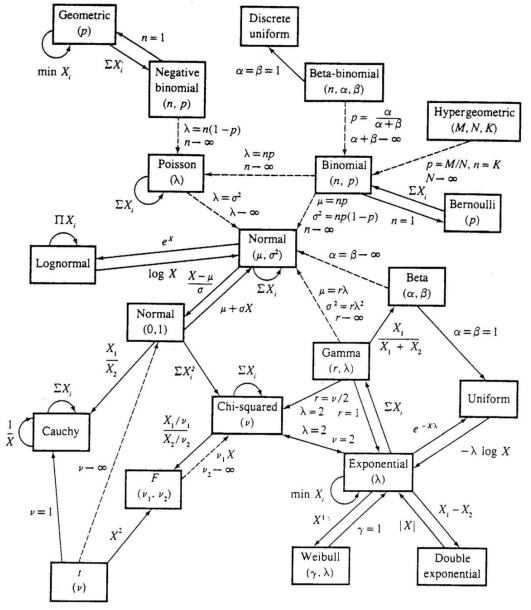
Testing equal variances for normal data: F-test

- $X_1, \ldots, X_n \sim N(\mu_1, \sigma_X^2)$ and $Y_1, \ldots, Y_m \sim N(\mu_2, \sigma_Y^2)$
- $H_0 : \sigma_X^2 = \sigma_Y^2$
- $H_1 : \sigma_X^2 \neq \sigma_Y^2$ *[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 $P(F \geq u) = \alpha/2$ *[Critical values]*
- Output of the test at confidence level $100(1-\alpha)\%$ using critical values
  - $f \leq l$ or $f \geq u$: H_0 is rejected *[Critical region]*
  - otherwise: H_0 cannot be rejected

See R script

Common distributions

- **Probability distributions at Wikipedia**
- **Probability distributions in R**
- C. Forbes, M. Evans, N. Hastings, B. Peacock (2010) Statistical Distributions, 4th Edition Wiley



Relationships among common distributions. Solid lines represent transformations and special cases, dashed lines represent limits. Adapted from Leemis (1986).

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

- $X_1, \ldots, X_n \sim N(\mu_1, \sigma^2)$ and $Y_1, \ldots, Y_m \sim N(\mu_2, \sigma^2)$
- $H_0 : \mu_1 = \mu_2$
- $H_1 : \mu_1 \neq \mu_2$ *[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 $p = P(|T_p| \geq |t|)$
- $P(T_p \leq -t_{n+m-2,\alpha/2}) = \alpha/2$ 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
  - $|t| \geq t_{n+m-2,\alpha/2}$: H_0 is rejected *[Critical region]*
  - 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 $Var(\bar{X}_n - \bar{Y}_m) = \frac{\sigma_X^2}{n} + \frac{\sigma_Y^2}{m}$

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

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

- $X_1, \ldots, X_n \sim N(\mu_1, \sigma_X^2)$ and $Y_1, \ldots, Y_m \sim N(\mu_2, \sigma_Y^2)$
- $H_0 : \mu_1 = \mu_2$
- $H_1 : \mu_1 \neq \mu_2$ *[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]*
- $T_d = \frac{\bar{X}_n - \bar{Y}_m}{S_d} \approx t(\upsilon)$ test statistics when H_0 is true, with $\upsilon = \frac{\left(\frac{1}{n} + \frac{u}{m}\right)^2}{\frac{1}{n^2(n-1)} + \frac{u^2}{m^2(m-1)}}$ 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 $p = P(|T_d| \geq |t|)$
- $P(T_d \leq -t_{\upsilon,\alpha/2}) = \alpha/2$ and $P(T_d \geq t_{\upsilon,\alpha/2}) = \alpha/2$ *[Critical values]*
- Output of the test at confidence level $100(1-\alpha)\%$ using critical values
  - $|t| \geq t_{\upsilon,\alpha/2}$: H_0 is rejected *[Critical region]*
  - otherwise: H_0 cannot be rejected

See R script

General data, large sample: t-test

- $X_1, \ldots, X_n \sim F_1$ and $Y_1, \ldots, Y_m \sim F_2$
- $H_0 : \mu_1 = \mu_2$
- $H_1 : \mu_1 \neq \mu_2$ *[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]*
- $T_d = \frac{\bar{X}_n - \bar{Y}_m}{S_d} \approx N(0,1)$
- t value is $\frac{\bar{x}_n - \bar{y}_m}{\sqrt{\frac{s_X^2}{n} + \frac{s_Y^2}{m}}}$ and p-value $p = P(|T_d| \geq |t|)$
- $P(T_d \leq -z_{\alpha/2}) = \alpha/2$ and $P(T_d \geq z_{\alpha/2}) = \alpha/2$ *[Critical values]*
- Output of the test at confidence level $100(1-\alpha)\%$ using critical values
  - $|t| \geq z_{\alpha/2}$: H_0 is rejected *[Critical region]*
  - otherwise: H_0 cannot be rejected

See R script

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

- Also called as: **Mann–Whitney U test** or Mann–Whitney–Wilcoxon (MWW)
- $X_1, \ldots, X_n \sim F_1$ and $Y_1, \ldots, Y_m \sim F_2$
- $H_0 : \mu_1 = \mu_2$
  - actually, $H_0 : F_1(x - \Delta) = F_2(x)$ where $\Delta = \mu_2 - \mu_1$ *[Location-shift model]*
  - we should test that empirical distributions have **the same shape**
- $H_1 : \mu_1 \neq \mu_2$ *[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$(X_1, \ldots, X_n, Y_1, \ldots, Y_m)$
  - `pwilcox` in R, or large sample Normal approx
- w value is $\sum_{i=1}^{n} s_i$ and p-value $p = P(|W| \geq |w|)$
- $P(W \leq -w_{\alpha/2}) = \alpha/2$ 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

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

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

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

See R script

Paired data

- Datasets $x_1, \ldots, x_n$ and $y_1, \ldots, y_n$ 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 $x_1 - y_1, \ldots, x_n - y_n$ 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

Optional reference

- On confidence intervals and statistical tests (with R code)

Myles Hollander, Douglas A. Wolfe, and Eric Chicken (2014)
Nonparametric Statistical Methods.
3rd edition, *John Wiley & Sons, Inc.*