Master Program in *Data Science and Business Informatics*

Statistics for Data Science

Lesson 34 - Fitting distributions. Testing independence/association

Salvatore Ruggieri

Department of Computer Science
University of Pisa
salvatore.ruggieri@unipi.it

Distribution fitting and quality of fitting

- Dataset $x_1, \ldots, x_n$ realization of $X_1, \ldots, X_n \sim F$
- **Distribution fitting**: What is a plausible F?
  - Useful in Data Science for understanding the data generation process, for checking assumptions (e.g., normality of noise in LR), for checking data distribution changes, etc.
  - Parametric approaches:
    - Assume $F = F(\lambda)$ for some family F, and estimate λ as $\hat{\lambda}$
    - Maximum Likelihood Estimation (point estimate): *[See Lesson 19]*

$$\hat{\lambda} = argmax_{\lambda} L(\lambda)$$

    - Parametric bootstrap (p-value): *[See Lesson 28]*

$$T_{ks} = \sup_{a \in \mathbb{R}} |F_n^*(a) - F_{\hat{\Lambda}^*}(a)|$$

  - Non-parametric approaches:
    - Empirical distribution F_n *[**Glivenko-Cantelli Thm**]*
    - Kernel Density Estimation *[See Lesson 15]*
- **Quality of fitting**: Among several fits $F_1, \ldots, F_k$, which one is the best?
  - Goodness of fit: measure of how good/bad is F_i in fitting the data?
  - Comparison: which one between two F_1 and F_2 is better?

Quality of fitting

- Loss functions (to be minimized)
  - Akaike information criterion (AIC), balances model fit against model simplicity

$$AIC(F(\lambda)) = 2|\lambda| - 2\ell(\lambda)$$

  - Bayesian information criterion (BIC), stronger balances over model simplicity

$$BIC(F(\lambda)) = |\lambda| \log n - 2\ell(\lambda)$$

- Statistics (continuous data):
  - **KS test** $H_0 : X \sim F \quad H_1 : X \not\sim F$ with Kolmogorov-Smirnov (KS) statistic:

$$D = \sup_{a \in \mathbb{R}} |F_n(a) - F(a)| \sim K$$

  - **LR test** $H_0 : X \sim F_1 \quad H_1 : X \sim F_2$ with the likelihood-ratio test:

$$\lambda_{LR} = \log \frac{L(F_1(\lambda_1))}{L(F_2(\lambda_2))} = \ell(F_1(\lambda_1)) - \ell(F_2(\lambda_2)) \quad \text{with} \quad -2\lambda_{LR} \sim \chi^2(1)$$

See R script

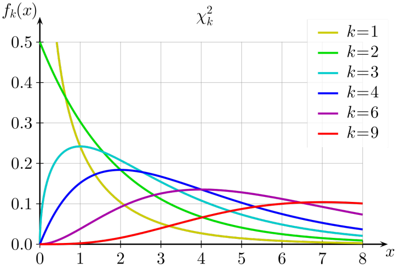
Chi-square distribution

Chi-square distribution

The Chi-square distribution with k degrees of freedom $\chi^2(k)$ has density:

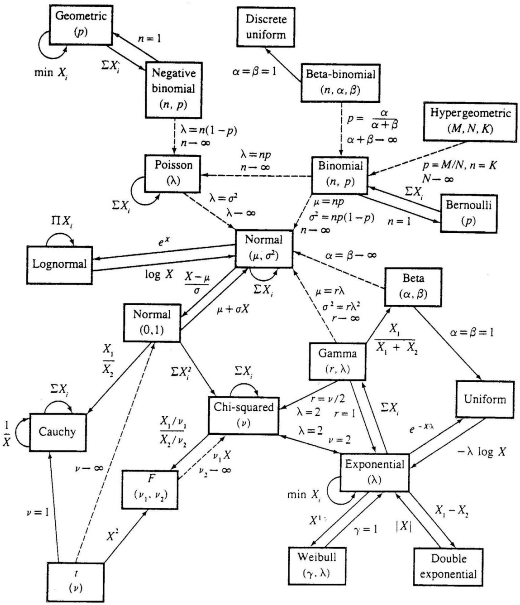
$$f(x) = \frac{1}{2^{k/2}\Gamma(k/2)} x^{k/2-1} e^{-x/2}$$

Let $X_1, \ldots, X_k \sim N(0,1)$. Then $Y = \sum_{i=1}^{k} X_i^2 \sim \chi^2(k)$



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).

Quality of fitting

- Statistics (discrete data):
  - **Pearson's Chi-Square test**
    $H_0 : X \sim F \quad H_1 : X \not\sim F$ with χ^2 statistic:
    $$\chi^2 = \sum_{N_i>0} \frac{(N_i - n_i)^2}{n_i} = n \cdot \sum_{N_i>0} \frac{(N_i/n - p(i))^2}{p(i)} \sim \chi^2(df)$$
    where N_i number of observations of value i, $n_i = n \cdot p(i)$ expected number of observations (rescaled), and $df = |\{i \mid N_i > 0\}| - 1$ is the number of observed values minus 1.
    $\chi^2 = \infty$ if for some i: $n_i = 0$
  - **Yates's correction for continuity**
    It corrects for approximating the discrete probability of observed frequencies by the continuous chi-squared distribution
    $$\chi^2 = \sum_{N_i>0} \frac{(|N_i - n_i| - 0.5)^2}{n_i}$$
    It increases Type II error, so do not use it!

See R script

Comparing two datasets

- Dataset $x_1, \ldots, x_n$ realization of $X_1, \ldots, X_n \sim F_1$
- Dataset $y_1, \ldots, y_m$ realization of $Y_1, \ldots, Y_n \sim F_2$
- $H_0 : F_1 = F_2 \quad H_1 : F_1 \neq F_2$
  - Useful to detect **covariate drift** (data stability) from source to target datasets
- Univariate data:
  - Continuous data: KS statistics $D = \sup_{a \in \mathbb{R}} |F_1(a) - F_2(a)| \sim K$
  - Discrete data: χ^2 statistics

$$\chi^2 = \sum_{R_i > 0 \vee S_i > 0} \frac{\left(\sqrt{\frac{m}{n}} R_i - \sqrt{\frac{n}{m}} S_i\right)^2}{R_i + S_i} \sim \chi^2(df)$$

    where R_i (resp., S_i) is the number of variables in $X_1, \ldots, X_n$ (resp., $Y_1, \ldots, Y_m$) which are equal to i, $df = |\{i \,|R_i > 0 \vee S_i > 0\}| - 1$
  - Other tests in the R package **twosamples**
- Multivariate data: see classifier 2-sample test and others in the R package **Ecume**

See R script

Testing independence:

- **Pearson's Chi-Square test** of independence
- X and Y discrete (finite) distributions
- $(x_1, y_1) \ldots, (x_n, y_n)$ bivariate observed dataset
- $H_0 : X \perp\!\!\!\perp Y \quad H_1 : X \not\perp\!\!\!\perp Y$
- Test statistic:
$$\chi^2 = \sum_{i,j} \frac{(O_{i,j} - E_{i,j})^2}{E_{i,j}} = n \sum_{i,j} \frac{(O_{i,j}/n - p_{i,.}p_{.,j})^2}{p_{i,.}p_{.,j}} \sim \chi^2(df)$$
where $O_{i,j}$ is the number of observations of value $X = i$ and $Y = j$, $E_{i,j} = np_{i,.}p_{.,j}$ where $p_{i,.} = \sum_j O_{i,j}/n$ and $p_{.,j} = \sum_i O_{i,j}/n$. $df = (n_x - 1)(n_y - 1)$ where n_x (resp., n_y) is the size of the support of X (resp., Y)
- Exact test when n is small: **Fisher's exact test**
- Paired data (e.g., before and after taking a drug): **McNemar's test**

See R script

The G-test and Mutual Information

- **G-test** of independence
- X and Y discrete (finite) distributions
- $(x_1, y_1) \ldots, (x_n, y_n)$ bivariate observed dataset
- $H_0 : X \perp\!\!\!\perp Y \qquad H_1 : X \not\perp\!\!\!\perp Y$
- Test statistics:

$$G = 2 \sum_{i,j} O_{i,j} \log \frac{O_{i,j}}{E_{i,j}} = 2 \sum_{i,j} O_{i,j} \log \frac{O_{i,j}}{np_{i,.}p_{.,j}} \sim \chi^2(df)$$

  where $O_{i,j}$ is the number of observations of value $X = i$ and $Y = j$, $E_{i,j} = np_{i,.}p_{.,j}$ where $p_{i,.} = \sum_j O_{i,j}/n$ and $p_{.,j} = \sum_i O_{i,j}/n$. $df = (n_x - 1)(n_y - 1)$ where n_x (resp., n_y) is the size of the support of X (resp., Y)
- Preferrable to Chi-Squared when numbers (O_{ij} or E_{ij}) are small, asymptotically equivalent
- $G = 2 \cdot n \cdot I(O, E)$ where $I(O, E)$ is the mutual information between O and E *[See Lesson 16]*

See R script

Other tests of independence

- $(x_1, y_1) \ldots, (x_n, y_n)$ bivariate observed dataset
- Permutation tests:
  - reduces to comparing two datasets: $(x_1, y_1) \ldots, (x_n, y_n)$ and $(x_1, y_{\pi_1}) \ldots, (x_n, y_{\pi_n})$, where $\pi_1, \ldots, \pi_n$ is a permutation of $1, \ldots, n$ *[see slide on comparing two datasets]*
- Continuous X and Y:
  - discretize both X and Y and then apply independence tests for discrete r.v.'s, or
  - test correlation (see later), or
  - **Hoeffding's test**, see R package **independence**
- Continuous X and discrete Y:
  - discretize X and then apply independence tests for discrete r.v.'s, or
  - a direct approach **Yang and Kim**, or
  - special case Y binary: $X \perp\!\!\!\perp Y$ iff $P(X|Y) = P(X)$ iff $P(X|Y=0) = P(X|Y=1)$ *[see slide on comparing two datasets]*

Measures of association (from Lesson 16)

- *Association*: one variable provides information on the other
  - $X \perp\!\!\!\perp Y$ independent, i.e., $P(X|Y) = P(X)$: zero information
  - $Y = f(X)$ deterministic association with f invertible: maximum information
- *Correlation*: the two variables show an increasing/decreasing trend
  - $X \perp\!\!\!\perp Y$ implies $Cov(X, Y) = 0$
  - the converse is not always true

	Variable X		
Variable Y	Nominal	Ordinal	Continuous
Nominal	φ or λ	Rank biserial	Point biserial
Ordinal	Rank biserial	τ_b or Spearman	τ_b or Spearman
Continuous	Point biserial	τ_b or Spearman	Pearson or Spearman

φ = phi coefficient, λ = Goodman and Kruskal's lambda,
τ_b = Kendall's τ_b.

Association between nominal variables: Pearson χ^2-based

- ϕ **coefficient** (or MCC, Matthews correlation coefficient)
  - For 2×2 contingency tables: *[Exercise. Show $\phi = |r_{xy}|$]*

$$\phi = \sqrt{\frac{\chi^2}{n}} \in [0, 1]$$

- **Cramer's V**
  - For contingency tables larger than 2×2:

$$V = \sqrt{\frac{\chi^2}{n \cdot \min\{r-1, c-1\}}} \in [0, 1]$$

  where r and c are the number of rows and columns

- **Tschuprov's T** *[sames as V if $r = c$]*
  - For contingency tables larger than 2×2:

$$T = \sqrt{\frac{\chi^2}{n \cdot \sqrt{(r-1)(c-1)}}} \in [0, 1]$$

  where r and c are the number of rows and columns

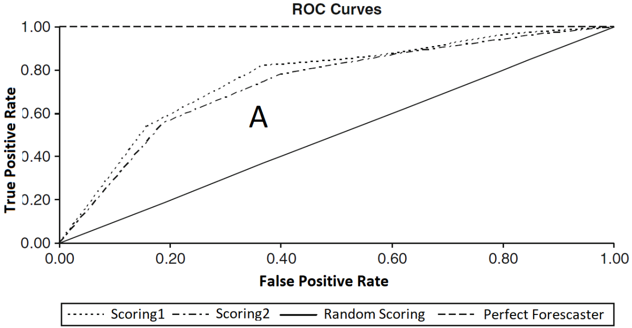
See R script

Testing correlation: continuous data

- Population correlation:
$$\rho = \frac{E[(X-\mu_X)\cdot(Y-\mu_Y)]}{\sigma_X \cdot \sigma_Y}$$
- Pearson's correlation coefficient:
$$r = \frac{\sum_{i=1}^n (x_i-\bar{x})\cdot(y_i-\bar{y})}{\sqrt{\sum_{i=1}^n (x_i-\bar{x})^2 \cdot \sum_{i=1}^n (y_i-\bar{y})^2}}$$
- Assumption: joint distribution of X, Y is bivariate normal (or large sample)
- $(x_1, y_1)\ldots,(x_n, y_n)$ bivariate observed dataset
- $H_0 : \rho = 0 \qquad H_1 : \rho \neq 0$
- Test statistics:
$$T = \frac{r\sqrt{n-2}}{\sqrt{1-r^2}} \sim t(n-2)$$
  - Recall that $X \perp\!\!\!\perp Y$ implies $\rho = 0$: if H_0 can be rejected, then $X \perp\!\!\!\perp Y$ can be rejected

See R script

Testing AUC-ROC



- Binary classifier score $s_\theta(w) \in [0,1]$ where $s_\theta(w)$ estimate $\eta(w) = P_{\theta_{TRUE}}(C = 1|W = w)$
- 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?**
  - Linearly related to Somer's D correlation index (a.k.a. Gini coefficient) *[See Lesson 16]*

Testing AUC-ROC

- AUC is the probability of correct identification of the order between two instances:

$$AUC = P_{\theta_{TRUE}}(s_\theta(W1) < s_\theta(W2) | C_{W1} = 0, C_{W2} = 1)$$

  where $(W1, C_{W1}) \sim f_{\theta_{TRUE}}$ and $(W2, C_{W2}) \sim f_{\theta_{TRUE}}$

- $s_\theta(W_1), \ldots, s_\theta(W_n) \sim F_{\theta_{TRUE}}|_{C=1}$ and $s_\theta(V_1), \ldots, s_\theta(V_m) \sim F_{\theta_{TRUE}}|_{C=0}$

$$U = \sum_{i=1}^{n} \sum_{j=1}^{m} S(s_\theta(W_i), s_\theta(V_j)) \qquad S(X, Y) = \begin{cases} 1 & \text{if } X > Y \\ 1/2 & \text{if } X = Y \\ 0 & \text{if } X < Y \end{cases}$$

  - AUC-ROC $= U/(n \cdot m)$ is an estimator of AUC

- Related to $W = U + \frac{n(n+1)}{2}$, where W is the **Wilcoxon rank-sum test statistics** *[See Lesson 31]*
- Normal approximation, DeLong's algorithm or bootstrap for confidence interval estimation

See R script