Master Program in *Data Science and Business Informatics*

Statistics for Data Science

Lesson 34 - Fitting distributions. Testing independence/association

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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** $H_0 : X \sim F \quad H_1 : X \nsim F$ 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

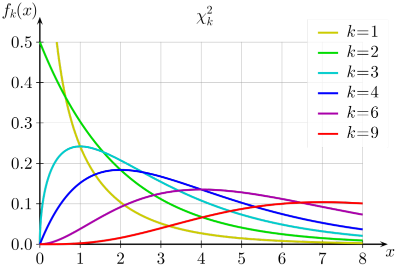
Chi-square distribution

Chi-square distribution

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

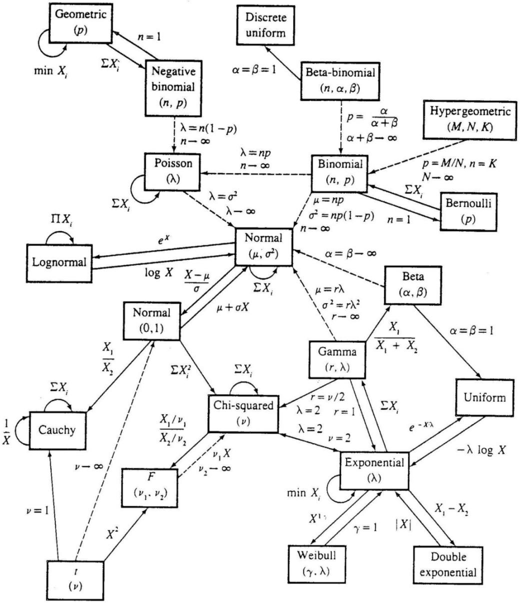
$$f(x) = \frac{1}{2^{k/2}\Gamma(k/2)} x^{k/2-1} e^{-x/2}$$

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 $Y_1, \ldots, Y_n \sim F_2$
- $H_0 : F_1 = F_2 \qquad H_1 : F_1 \neq F_2$
- Continuous data: KS statistics

$$D = \sup_{a \in \mathbb{R}} |F_1(a) - F_2(a)| \sim K$$

- Discrete data: χ^2 statistics

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

  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, $df = |\{i \,|R_i > 0 \vee S_i > 0\}| - 1$

- Useful to detect **covariate drift** (data stability) from source to target datasets (training set vs deployment set) *[See also Lessons 16 and 33 for association measures]*

See R script

Testing independence/association: discrete data

- **Pearson's Chi-Square test** of independence
- X and Y discrete (finite) distributions
- $(x_1, y_1) \dots, (x_n, y_n)$ bivariate observed dataset
- $H_0 : X \perp\!\!\!\perp Y \qquad H_1 : X \not\perp\!\!\!\perp Y$
- 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

Association between nominal variables: χ^2-based

- Association measures based on Pearson χ^2 *[See [Lesson 16]*
  - **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

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 statistic:

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

  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

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:

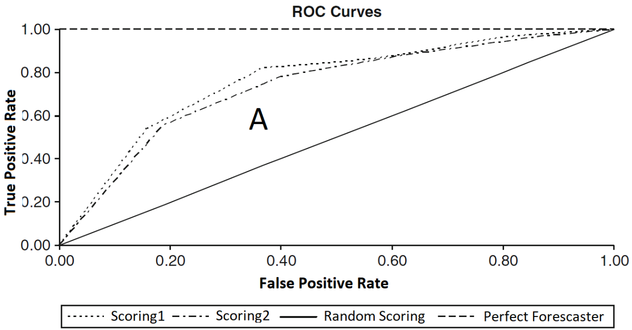
$$r = \frac{\sum_{i=1}^{n} (x_i - \bar{x}) \cdot (y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n} (x_i - \bar{x})^2 \cdot \sum_{i=1}^{n} (y_i - \bar{y})^2}}$$

- 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:

$$T = \frac{r\sqrt{n-2}}{\sqrt{1-r^2}} \sim t(n-2)$$

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