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Computational Statistics

Lecture 6: Two distributions, are they of the same kind ?

Raymond Bisdorff

University of Luxembourg

29 novembre 2019

Content of Lecture 6

1. Methodology
    Comparing statistical distributions
    Methodological approach
    Statistical tests

2. Comparing histograms
    Chi-square test against a known distribution
    Comparing two binned data sets
    Testing uniform randomness

3. Comparing continuous distributions
    Kolmogorov-Smirnov Test
    Kolmogorov-Smirnov Test in R

Comparing statistical distributions

- Given two sequences of random numbers, we can ask the question : "*Are the two sequences drawn from a same random number generator, or from different generators ?*"

- In proper statistical terms : "*Can we disprove, to a certain required level of significance that two data sets are drawn from the same population distribution function ?*"

- Disproving the null hypothesis proves that the data are from different random distributions.

- Failing to disprove, on the othe hand, only shows that the data sets appear to be consistent with being generated from a same distribution function.

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Methodological approach

Four problems may appear from two dichotomies :

1. The data are either :

    1.1 continuous, or

    1.2 binned.

2. We wish to compare either

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Four problems may appear from two dichotomies :

1. The data are either :
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2. We wish to compare either
   2.1 one data set to a known distribution, or
   2.2 two data sets with each other.

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1. The data are either :
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Statistical tests

- The usual test for differences between binned data is the Chi-square *goodness-of-fit* test.

- For continuous data as a function of a single variable, the usual test is the Kolmogorov-Smirnov test.

- One can always turn continuous data into binned data, by grouping the observed data into specified ranges of the continuous variable(s).

- There is however often some arbitrariness as how the bins should be chosen; how many bins, with equal sizes or not?

- Furthermore, binning always involves some loss of information. Even more, when uniform distributions of observations are not verified within all bins.

- Mind that statistical summaries are not truthful per se. They are merely numerical or graphical arguments supporting one or the other hypothesis concerning the observed data.

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Chi-square test against a known distribution

- Consider a random sequence grouped into υ bins.

- Suppose that N_i is the number of events observed in the ith bin, and that n_i is the number of expected events according to some known distribution. Note that the N_i's are integers, while the n_i's may not be.

- Then the Chi-square "*goodness-of-fit*" test statistic is :

$$\chi^2 = \sum_{i=1}^{\upsilon} \frac{(N_i - n_i)^2}{n_i}$$

where the sum runs over all υ bins.

- A value of $\chi^2 \gg \upsilon$ indicates that a "*goodness-of-fit*" is rather unlikely.

Chi-square test against a known distribution

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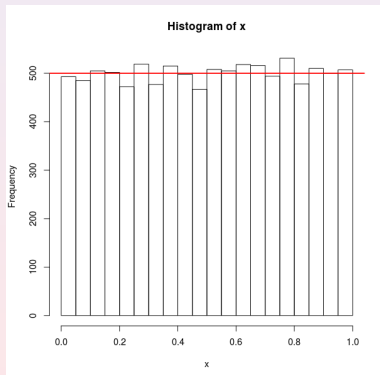
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Uniformity Chi-Square *goodness-of-fit* Test in R

Let us test if the R `runif` generator is giving consistent data with a uniform distribution. The R `chisq.test` method implements this *goodness-of-fit* test.

```
> nSim = 10^4
> x = runif(nSim)
> freq = hist(x)
> Ni = freq$counts
> upsilon = length(Ni)
  [1] 20
> ni = rep(nSim/upsilon,upsilon)
> chi2 = sum((Ni-ni)^2/ni)
  [1] 18.4988
> df = upsilon - 1
> pvalue = 1.0 - pchisq(chi2,df)
  [1] 0.4893842
> chisq.test(Ni)
  X-squared = 18.4988 df = 19
  p-value = 0.4893842
```

Chi-square Test – continue

- Any term i with $0 = n_i = N_i$ should be omitted from the sum.

- A term with $n_i = 0$ and $N_i \neq 0$ gives an infinite χ^2, as it should, since in this case the N_i's cannot possibly be drawn from these n_i's.

- The $P(\chi^2|\upsilon)$ probability function with degree of freedom υ is the probability that the sum of the squares of υ standard Gaussian variables of unit variance and 0 mean will be greater than χ^2.

- The terms in the sum of the χ^2 measure are only good approximations of squares of random standard normal variables when $N_i \gg 1$ in each bin.

- Usually, the binning process gives a constrained last bin content. Hence, the degree of freedom of $P(\chi^2|\upsilon)$ is only $\upsilon - 1$!

Chi-square Test – continue

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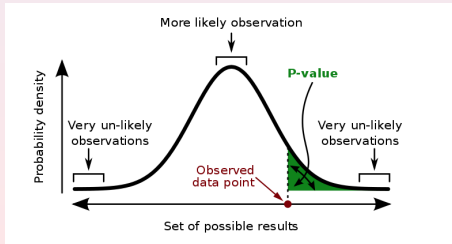
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- The $P(\chi^2|v)$ probability function with degree of freedom v is the probability that the sum of the squares of v standard Gaussian variables of unit variance and 0 mean will be greater than χ^2.

- The terms in the sum of the χ^2 measure are only good approximations of squares of random standard normal variables when $N_i \gg 1$ in each bin.

- Usually, the binning process gives a constrained last bin content. Hence, the degree of freedom of $P(\chi^2|v)$ is only $v - 1$!

Significance of the *goodness-of-fit* test

- The $P(\chi^2|v)$ probability function gives via the *p*-value a good estimate for the actual significance of the chi-square goodness-of-fit test.

- The *p*-value equals the probability that the Chi-square test may give, under the "*goodness-of-fit*" hypothesis, a result greater or equal than x :
$\mathcal{P}(\chi^2|v \geq x) = 1.0 - \mathcal{P}(\chi^2|v \leq x)$.

- The higher, resp. the smaller, the *p*-value, the more the goodness-of-fit is likely, resp. unlikely.

- If a certain significance level is required, like 95% for instance, then the *goodness-of-fit* hypothesis is rejected if the *p*-value is smaller than 5%.
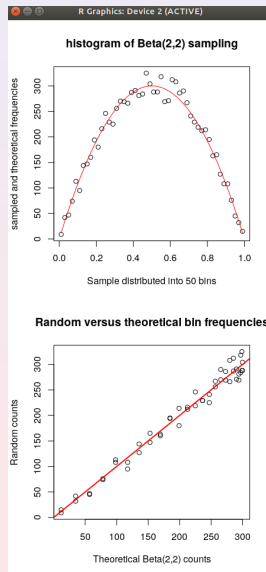

Source : https ://en.wikipedia.org/wiki/P-value

Exercise (Chi-square "*goodness-of-fit*" tests)

1. *How to apply a Chi-square "goodness-of-fit" tests to samples taken with a $\mathcal{B}(2,2)$ random number generator ?*

2. *How to check the accuracy of random sampling from the empirical random law shown on slide 12/34 of lecture 3 ?*

3. *May the random sequences obtained with a Mersenne twister RNG versus the ones obtained from a linear congruational RNG be discriminated by the Chi-square "goodness-of-fit" test ?*

4. *What is the distribution of p-values for samples of size $n = 10^4$ of uniform random numbers generated with* `runif(n)` *?*

Checking *goodness-of-fit* of a $\mathcal{B}(2,2)$ sample

```
> par(mfrow=c(2,1))
> nSim = 10^4
> xb = rbeta(nSim,2,2)
> h = hist(xb,breaks=50,plot=F)
> plot(h$mids,h$counts)
> thcounts =
+    dbeta(h$mids,2,2)*0.02*nSim
> lines(h$mids,thcounts,col="red")
> plot(thcounts,h$counts)
> abline(0,1,col="red",lwd=2)
> Ki2=sum((h$counts-thcounts)^2/thcounts)
[1] 46.494
> pval = 1-pchisq(Ki2,length(h$counts)-1)
[1] 0.5753
> chisq.test(h$counts,
+ p=dbeta(h$mids,2,2)*0.02,rescale.p=T)
X-squared = 46.503, df = 49,
p-value = 0.5749
```

Comparing *two* binned data sets of same size

- Let R_i be the number of events observed in the ith bin for the first data set, and let S_i be the number of events in the same bin for data set two.

- Then the chi-square "*goodness-of-fit*" test statistic is :

$$\chi^2 = \sum_{i=1}^{v} \frac{(R_i - S_i)^2}{R_i + S_i}$$

  where the sum runs over all v bins.

- If the data were collected in such a way that the sum of R_i's is necessarily equal to the sum of the S_i's, then the number of degrees of freedom is one less than the number v of bins.

Comparing *two* binned data sets of different size

- Let R_i be the number of events observed in the ith bin for the first data set, and let S_i be the number of events in the same bin for data set two.

- Then the chi-square "*goodness-of-fit*" test statistic is :

$$\chi^2 = \sum_{i=1}^{\upsilon} \frac{(\sqrt{S/R}R_i - \sqrt{R/S}S_i)^2}{R_i + S_i}$$

  where $R := \sum_i R_i$ and $S := \sum_i S_i$.

- The number of degrees of freedom is still one less than the number υ of bins.

Problem with small number of counts

- When significant fractions of bins have a small number of counts ($\leqslant 10$, say), then χ^2 statistics are not well approximated by a chi-square probability function.

- Under the "*goodness-of-fit*" hypothesis, the count in an individual bin, N_i, is following a Poisson law with $\lambda = n_i$ and each term $(N_i - n_i)^2/n_i$ has $\mu = 1$ and $\sigma^2 = 2 + 1/n_i$.

- Each term in the χ^2 statistic adds, on average, 1 to its value, and slightly more than 2 to its variance.

- But, the variance of the chi-square probability function is exactly twice its mean. If a significant fraction of n_i's are small, then quite probable values of the χ^2 statistic will appear to lie farther out on the tail than they actually are.

- Thus, the "*goodness-of-fit*" hypothesis may be rejected even when it is true.

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- Thus, the "*goodness-of-fit*" hypothesis may be rejected even when it is true.

Remedies with small number of counts

- Regroup the bins with small number of counts.

- When υ, the number of bins, is large (> 30), the central limit theorem implies that the χ^2 statistic gets approximately a Gaussian distribution :

$$\chi^2 \rightsquigarrow \mathcal{N}\Big(\upsilon, \big[2\upsilon + \sum_i n_i^{-1}\big]^{1/2}\Big),$$

  and p-values may be computed as a complement of the corresponding cumulated Gaussian distribution function.

- In the case of *two* binned data sets :

$$\sum_i n_i^{-1} \to \Big[\frac{(R-S)^2}{RS} - 6\Big] \sum_i \frac{1}{R_i + S_i}$$

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- When v, the number of bins, is large (> 30), the central limit theorem implies that the χ^2 statistic gets approximately a Gaussian distribution :

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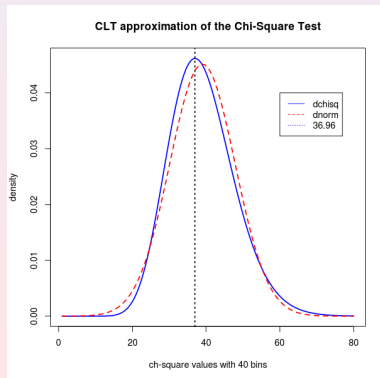
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$$\sum_i n_i^{-1} \rightarrow \Big[\frac{(R-S)^2}{RS} - 6\Big] \sum_i \frac{1}{R_i + S_i}$$

Remedies for small number of counts in R

A $P(\chi^2|\upsilon)$ cdf may be approximated with a Gaussian cdf when $\upsilon > 30$ as shown in R plot below.

```
> breaks = seq(0,1,0.025)
> freq = hist(x,breaks)
> Ni = freq$counts
> upsilon = length(freq$breaks)-1
> ni = rep(Nsim/upsilon,upsilon)
> chi2 = sum((Ni-ni)^2/ni)
  [1] 36.96
> df = upsilon - 1
> pvalue = 1.0 - pchisq(chi2,df)
  [1] 0.5632565
> sigma = sqrt(2*df+sum(1/ni))
> npvalue = 1.0 -
+        pnorm(chi2,df,sigma)
  [1] 0.5912447
```


CLT approximation of the Chi-Square Test

legend:
— dchisq
--- dnorm
···· 36.96

ch-square values with 40 bins

RNG Quality : Testing equidistribution

Let $\langle U_n \rangle = [u_0, u_1, u_2, ...]$ be a sequence of random numbers from the float interval $[0.0; 1.0)$ apparently generated in a uniformly manner.

To test the quality of the random generator, we consider the auxiliary sequence $\langle Y_n \rangle = [y_0, y_1, y_2, ...]$ defined by the rule $y_n = \lfloor d \times u_n \rfloor$, where d is a positive integer – usually 64, 100, or 128 – also called the *discrete grain* of the generator.

When sequence $\langle U_n \rangle$ is indeed uniformly distributed, we will observe a sequence $\langle Y_n \rangle$ of equidistributed integers between 0 and $d-1$.

The quality of a given random generator may now be assessed with a two-tailed Chi-square "*goodness-of-fit*" test between the empirical N_i distribution and the theoretical uniform $n_i = 1/d$ distribution.

A p -value below 5% or above 95% indicates the very likeliness of a suspicious non-randomness in $\langle U_n \rangle$.

RNG Quality : Serial test

- We reconsider the auxilliary $\langle Y_n \rangle$ sequence with discrete grain d and count the number of times the pair $(y_{2j}, y_{2j+1}) = (q, r)$ occurs, for $0 \leq j < n/2$, $q \neq r$ and $0 \leq q, r \leq d$.

- These counts are to be made for each pair of integers (q, r) with $0 \leq q, r \leq d$, and the Chi-square "*goodness-of-fit*" test is applied to these $k = d^2$ categories with theoretical uniform relative frequency $1/d^2$ in each category.

- To keep the length n of the random sequence large compared to k, d will be chosen of smaller value than for the equidistributional test.

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RNG Quality : Gap test

- Another test is to examine the length of "gaps" between occurences of u_j in a certain range. If α and β are two real numbers with $0 \leq \alpha < \beta \leq 1$, we want to consider the lengths of consecutive subsequences $[u_j, u_{j+1}, ..., u_{j+r}]$ in which the consecutive r values u_{j+k}, for $k = 1, ...r$, remain between α and β. This situation will be counted as a gap of length r.

- With given values α and β and a maximal gap length t, let C_r for $r = 0, ..., t-1$ count the occurences of gaps of length $0, ..., t-1$, and C_t the gaps of length $r \geq t$. If $p = \beta - \alpha$, the theoretical counts for each gap length r, is $p_r = p(1-p)^r$ for $0 \leq r < t-1$ and $p_t = (1-p)^t$.

- Again, a Chi-square "*goodness-of-fit*" test, comparing the C_r with the p_r distribution may be used in order to assess the likeliness of a suspicious non-randomness of the gap lengths observed in the sequence $\langle U_n \rangle$.

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RNG Quality : Coupon collector's test

- This test relates the frequency test to the previous gap test. We use the auxiliary sequence $\langle Y_n \rangle$ and we observe the lengths of subsequences $y_{j+1}, y_{j+2}, ..., y_{j+r}$ that are required to get a complete set of integers – a coupon collector seqment – from 0 to $d-1$.

- With a given maximal subsequence length t, let C_r for $r = d, ..., t-1$ count the occurences of coupon collector segments of length $d, d+1, ..., t-1$, and C_t the segments of length $r \geq t$.

- The theoretical count for each coupon collector segment of length r, is

$$p_r = \frac{d!}{d^r} \left\{ \begin{matrix} r-1 \\ d-1 \end{matrix} \right\}, \quad d \leq r < t-1; \quad p_t = 1 - \frac{d!}{d^r} \left\{ \begin{matrix} r \\ d \end{matrix} \right\}.$$

- Similarly, a Chi-square "*goodness-of-fit*" test, comparing the empirical C_r with the theoretical p_r distribution, may be used in order to assess the likeliness of a suspicious non-randomness of the coupon collector segments.

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RNG Quality : Up and down runs test

- A sequence $\langle U_n \rangle$ of uniform random numbers may also be tested for "*runs up*" and "*runs down*" segments, by examining the length of monotone portions of it. Let $[u_{j+0}, u_{j+1}, ..., u_{j+r}]$ be a subsequence of length r such that either $u_{j+0} \geq u_{j+1} \geq ... \geq u_{j+r}$, or, $u_{j+0} \leq u_{j+1} \leq ... \leq u_{j+r}$.

- Given a maximal subsequence length t, let C_r for $r = 1, ..., t-1$ count the occurences of separated monotone, either up, or, down runs of length $1, 2, ..., t-1$, and C_t the same runs of length $r \geq t$.

- Assuming that a monotone run of length r occurs with probability $1/r! - 1/(r+1)!$, the theoretical relative count for each length r, gives $p_r = 1/r! - 1/(r+1)!$ for $r < t$ and $p_t = 1/t!$.

- And, again, we may use a Chi-square "*goodness-of-fit*" test, comparing the empirical C_r with the theoretical p_r distribution, for assessing the likeliness of a suspicious non-randomness of "*runs up*" or "*runs down*" segments.

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Kolmogorov-Smirnov Test

- The ordered list of data points is converted into a cumulative distribution function of the probability distribution from which it has been drawn.

- If the N events are located at points x_i, $i = 1, ..., N$, then $S_N(x)$ is giving the fraction of points to the left of a given value x.

- The Kolmogorov-Smirnov statistic D is defined as the maximum value of the absolute difference between two cumulative distribution functions.

- When comparing $S_N(x)$ to a known cdf $P(x)$, the K-S statistic is

$$D = \max_{-\infty < x < +\infty} |S_N(x) - P(x)|$$

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Kolmogorov-Smirnov Test – continue

- Testing the p-value significance of the K-S test is done with the complement $Q_{KS}(z) = 1 - P_{KS}(z)$ of the cdf $P_{KS}(z)$ of the K-S distribution for $z > 0$:

$$P_{KS}(z) \ = \ 1 - 2 \sum_{j=1}^{\infty} (-1)^{j-1} exp(-2j^2 z^2)$$

- The K-S statistic is invariant under reparametrization of the data set points. D remains the same when locally stretching and sliding the x axis. Using for instance x or $\log x$ in D will result in the same significance of the test.

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Kolmogorov-Smirnov Test in R

- The D observed and its p-value as disproof of the null hypothesis that the distributions under review are the same is given by the R `ks.test` procedure.

```
> x = rnorm(50)
> ks.test(x,"pnorm")
  D = 0.101, p-value = 0.6498
> y = runif(30,-2.5,2.5)
> plot(ecdf(x),col="blue")
> plot(ecdf(y),add=T,col="red")
> ks.test(x,y,exact=T)
  D = 0.3267, p-value = 0.02926
```


Comparing two continuous distributions

K-S test
D = 0.3267
p-value = 0.02926

rnorm(0,1)
runif(-3,3)

Cumulative distribution functions

sample data from a Gaussian and a uniform generator