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Chapter 1

Goodness of Fit Tests and Categorical Data Analysis

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1.1 Introduction

The *a priori* assumption of a probability model governing an observed phenomenon is central to the analysis of samples from an underlying population. The measure appropriateness for this assumed probability model is done through *goodness-of-fit* tests.

The null hypothesis to be tested is that a sample has the specified probability distribution. The parameters of this probability distribution may not be fully specified, leading to a more complex problem.

1.2 Goodness of fit tests with all parameters specified

Consider a set of n independent random variables $\{Y_j\}$ each of which can take on discrete values in the integer set $\{1, \ldots, k\}$. The null hypothesis to test is that they all have the same underlying PMF, specified as

$$H_0: P\{Y = i\} = p_i \qquad \forall \ i \in \{1, \dots, k\}$$
 (0.1)
 $H_1: P\{Y = i\} \neq p_i \qquad \text{for some } i \in \{1, \dots, k\}$

Defining the set $\{X_i\}$ as the number of RVs $\{Y_j\}$ which have the value i, it follows that the set $\{X_i\}$ are independent binomial RVs with parameters $\{(n, p_i)\}$ under H_0

$$X_i \sim \text{Binom}(n, p_i)$$
 (0.2)

$$\mathbb{E}[X_i] = np_i \tag{0.3}$$

A method of judging how close p_i is to the actual probability $P\{Y = i\}$, is to look at a standardized sum of squared errors, and use it to define a test statistic.

Using a significance threshold α , and the fact that T approaches a χ^2 RV with (k-1) DOF as $n \to \infty$,

$$T = \sum_{i=1}^{k} \frac{(X_i - np_i)^2}{np_i} \tag{0.4}$$

$$\lim_{n \to \infty} T \to \chi_{k-1}^2 \tag{0.5}$$

reject
$$H_0$$
 if $T > \chi^2_{\alpha,k-1}$
accept H_0 otherwise (0.6)

A rule of thumb for sample sizes in the test above is to ensure that in the set $\{np_i\}$, all values exceed 1 and most exceed 5.

A simpler expression for T exploits the fact that $\sum X_i = n$ and $\sum p_i = 1$. This constraint on the X_i is also responsible for the χ^2 RV having (k-1) DOF.

$$T = \sum_{i=1}^{k} \frac{(X_i - np_i)^2}{np_i} = \sum_{i=1}^{k} \frac{X_i^2}{np_i} - n$$
 (0.7)

Simulation-based methods of determining critical region : Until the modern computer age led to computing power being cheap and widely available, the above χ^2 approximation was

the only method of defining critical regions for the goodness-of-fit test.

Consider a set of randomly generated variables $\{Y_1^{(1)}, \dots, Y_n^{(1)}\}$, each having the PMF $P\{Y_j^{(1)}=i\}=p_i$ for $i\in\{1,\dots,k\}$.

Defining the set $\{X_i^{(1)}\}\$ and test statistic $T^{(1)}$ as above,

$$X_i^{(1)} = \text{number of } j: Y_j^{(1)} = i$$
 (0.8)

$$T^{(1)} = \sum_{i=1}^{k} \frac{(X_i^{(1)} - np_i)^2}{np_i}$$
 (0.9)

Using the above procedure to generate a large number of test statistics $\{T^{(1)}, \ldots, T^{(r)}\}$ by repetition of the above procedure yields an approximation to the probability distribution of T.

$$P_{H_0}(T \ge t) \approx \frac{\text{number of } l : T^{(l)} \ge t}{r}$$
 (0.10)

The above approximation becomes very accurate for large r and can also be used then to calculate a p-value for the test. The generation of a random set $\{Y^{(r)}\}$ exploits the Monte-Carlo system of using a standard uniform RV transformed using the set of probabilities $\{p_i\}$ to output the discrete value of $Y_i^{(r)}$.

1.3 Goodness of fit tests with some parameters unspecified

When the underlying probability distribution is not fully specified, a general strategy is to divide the possible continuous set of outcomes into a few discrete regions. Using the observed set of data points to calculate an estimate for the unspecified parameters, an estimated test statistic can then be calculated.

$$P\{Y_i = i\} = p_i \quad \text{where} \quad \widehat{p_i} \approx p_i$$
 (0.11)

$$T = \sum_{i=1}^{k} \frac{(X_i - n\widehat{p}_i)^2}{n\widehat{p}_i} \tag{0.12}$$

$$\lim_{n \to \infty} T \to \chi^2_{k-1-m} \tag{0.13}$$

reject
$$H_0$$
 if $T > \chi^2_{\alpha,k-1-m}$
accept H_0 otherwise (0.14)

In the calculation of \widehat{p}_i above, the CDF of the underlying probability distribution assumed by H_0 , with estimated parameters $\{\widehat{\lambda}\}$ is used along with the user-defined discrete outcomes. The χ^2 RV has (k-1-m) DOF if there are m unspecified parameters to be estimated.

For example, a set of observed data with a null hypothesis of the underlying distribution being Poisson, would involve estimating the unspecified mean of the Poisson distribution $\hat{\lambda}$ using the observations and then calculating the test statistic and p-value.

1.4 Tests of independence in contingency tables

Consider a population whose members are governed by two characteristics (X, Y) each of which can take (r, s) possible values. The marginal probabilities can then be calculated as,

$$P_{ij} = P\{X = i, Y = j\}$$
 $i \in \{1, \dots, r\}$ $j \in \{1, \dots, s\}$ (0.15)

$$p_i = P\{X = i\} = \sum_j P_{ij} \quad i \in \{1, \dots, r\}$$
 (0.16)

$$q_j = P\{Y = j\} = \sum_i P_{ij} \qquad j \in \{1, \dots, s\}$$
 (0.17)

The null hypothesis of interest here is to test the independence of the X and Y characteristics.

$$H_0: P_{ij} = p_i q_j \qquad \forall \text{ possible pairs } (i, j)$$
 (0.18)

$$H_1: P_{ij} \neq p_i q_j$$
 for some pair (i, j)
$$(0.19)$$

Let the set of n observations be arranged into a contingency table where each element N_{ij} represents the number of observations with X = i, Y = j. The marginal probabilities can be estimated from the data set as

$$N_i = \sum_{i} N_{ij} \qquad \qquad \widehat{p}_i = \frac{N_i}{n} \tag{0.20}$$

$$M_j = \sum_i N_{ij} \qquad \qquad \widehat{q}_j = \frac{M_j}{n} \tag{0.21}$$

When H_0 is true, a test statistic can be set up as,

$$\mathbb{E}[N_{ij}] = nP_{ij} = p_i q_j \qquad \text{assuming } H_0 \text{ true}$$
 (0.22)

$$T = \sum_{i=1}^{r} \sum_{j=1}^{s} \frac{(N_{ij} - n\widehat{p}_i\widehat{q}_j)^2}{n\widehat{p}_i\widehat{q}_j}$$

$$= \sum_{i=1}^{r} \sum_{j=1}^{s} \frac{N_{ij}^{2}}{n\widehat{p}_{i}\widehat{q}_{j}} - n$$
 (0.23)

The reduction in DOF is (1+(r-1)+(s-1)). This leads to $T \sim \chi^2_{(r-1)(s-1)}$ since there are a total of $r \times s$ possible categories into which each observation can belong.

$$\lim_{n \to \infty} T \to \chi^2_{(r-1)(s-1)} \tag{0.24}$$

reject
$$H_0$$
 if $T > \chi^2_{\alpha,(r-1)(s-1)}$
accept H_0 otherwise (0.25)

1.5 Tests of independence in contingency tables with fixed marginal totals

If the sample is chosen such that the row sum and/or column sum is fixed across all rows and/or columns, the procedure used in the above section is largely unchanged. Defining the sample incidence of each pair of characteristics \hat{e}_{ij} , and then a test statistic,

$$\widehat{e}_{ij} = n\widehat{p}_i\widehat{q}_j = \frac{N_i M_j}{n} \tag{0.26}$$

$$T = \sum_{i} \sum_{j} \frac{(N_{ij} - \hat{e}_{ij})^2}{\hat{e}_{ij}}$$
 (0.27)

Here, N_i and M_j are the row-sums and column-sums respectively. The rest of the test is also unchanged with the use of a χ^2 RV with (r-1)(s-1) DOF used to calculate the critical regions.

An extension of the above procedure can be used to test the hypothesis that m populations with each member taking on one of n possible values, all have the same discrete population distribution.

Value		Po	pulat	ion		Row Sum
					n	
1	N_{11}	N_{12}		N_{1j}	$egin{array}{c} N_{1n} & & & & & & & & & & & & & & & & & & &$	M_1
2	N_{21}	N_{22}		N_{2j}	N_{2n}	M_2
÷	÷	:	٠.,	:	÷	:
i	N_{i1}	N_{i2}		N_{ij}	N_{in}	M_i
m	N_{m1}	N_{m2}		N_{mj}	N_{mn}	M_m
Column Sum						I

The hypothesis above now reduces to the absence of a row effect in the table of observations. $H_0: p_{1j} = p_{2j} = \cdots = p_{mj}$

1.6 Kolmogorov-Smirnov goodness of fit test for continuous data

Given a set of samples $\{Y_i\}$ from an underlying population distribution, the hypothesis testing whether this distribution is some continuous CDF given by F can be performed using the discretization procedure from the previous section.

Let the range $(-\infty, \infty)$ be broken up into k parts. Now, the observations can belong to one of these k categories as

$$Y_i^d = i$$
 if $Y_j \in (y_{i-1}, y_i)$ (0.28)

$$P\{Y_j^d = i\} = F(y_i) - F(y_{i-1}) \qquad \forall i \in \{1, \dots, k\}$$
 (0.29)

This creates a model that is amenable to the χ^2 goodness-of-fit test outlined in the above sections.

Consider the alternative approach which involves estimating the CDF as an empirical distribution function F_e ,

$$F_e(x) = \frac{\text{number of } i: Y_i \le x}{n} \tag{0.30}$$

Here, $F_e(x)$ is the proportion of observations that are less than or equal to x. Since $F_e(x)$ is an estimator of F(x) when H_0 is true, the Kolmogorov-Smirnov test statistic is

$$D \equiv \max_{x} \left| F_e(x) - F(x) \right| \tag{0.31}$$

 $F_e(x)$ is a step-like function with step size 1/n and jumps at each of the data points $\{Y_j\}$ after they have been rearranged into ascending order as $\{Y_{(j)}\}$.

$$F_{e}(x) = \begin{cases} 0 & \text{if } x \in (-\infty, Y_{(1)}) \\ 1/n & \text{if } x \in (Y_{(1)}, Y_{(2)}) \\ \dots & \\ (n-1)/n & \text{if } x \in (Y_{(n-1)}, Y_{(n)}) \\ 1 & \text{if } x \in (Y_{(n)}, \infty) \end{cases}$$
(0.32)

Since F(x) itself is a monotonically increasing function, the expression $|F_e(x) - F(x)|$ must have its maximum close to one of the points $x = \{Y_{(i)}\}$.

$$D = \max_{j} \left\{ \frac{j}{n} - F(y_{(j)}), \ F(y_{(j)}) - \frac{j-1}{n} \right\}$$
 (0.33)

A p-value defined using this statistic does not depend on the choice of underlying distribution F,

$$p = P_F(D \ge d) = P_F \left\{ \max_{x} \left| \frac{\#i : Y_i \le x}{n} - F(x) \right| \ge d \right\}$$
 (0.34)

$$= P\left\{ \max_{x} \left| \frac{\#i : U_i \le F(x)}{n} - F(x) \right| \ge d \right\}$$
 (0.35)

The above uses the fact that if Y has a continuous CDF F, then F(Y) is a standard uniform RV. This enables the use of independent standard uniform RVs $\{U_i\}$ to ease the Monte-Carlo simulation of the p-value.

The Monte-Carlo procedure involves defining y = F(x) for the hypothesized CDF F and then performing many repeats of checking whether the following inequality holds,

MC iteration is
$$\max_{0 \le y \le 1} \left| \frac{\#i : U_i \le y}{n} - y \right| \ge d$$
 (0.36)

$$\max_{y} \left| \frac{\#i : U_i \le y}{n} - y \right| = \max_{j} \left| \frac{j}{n} - U_{(j)}, \ U_{(j)} - \frac{j-1}{n} \right|$$
 (0.37)

Chapter 2

Goodness of Fit Tests and Categorical Data Analysis

1 Table of observations and results of goodness-of-fit tests are tabulated below.

	X_i	p_i
White	141	0.25
Pink	291	0.5
Red	132	0.25
Total	564	1

Goodness of Fit	Test
Test Statistic	8.62e-01
p value %	65.00
Significance (α) %	5.00
null hypothesis (H_0)	accepted
minimum np_i	141

2 Table of observations and results of goodness-of-fit tests are tabulated below.

	X_i	p_i
1	158	0.1667
2	172	0.1667
3	164	0.1667
4	181	0.1667
5	160	0.1667
6	165	0.1667
Total	1000	1

Goodness of Fit	Test
Test Statistic	1.98e + 00
p value %	85.20
Significance (α) %	5.00
null hypothesis (H_0)	accepted
$\underline{\text{minimum } np_i}$	167

3 Table of observations and results of goodness-of-fit tests for an underlying Poisson distribution are tabulated below.

Failures	X_i	p_i
0	0	0.015
1	5	0.063
2	22	0.1323
3	23	0.1852
4	32	0.1944
5	22	0.1633
6	19	0.1143
7	13	0.0686
8	6	0.036
9	4	0.0168
10	4	0.0071
11	0	0.0027
Total	150	1

Goodness of Fit	Test
Test Statistic	1.66e+01
p value %	12.16
Significance (α) %	5.00
null hypothesis (H_0)	accepted
minimum np_i	0

- 4 No data given.
- 5 Table of observations and results of goodness-of-fit tests for an underlying exponential distribution with mean 50 are tabulated below.

Lifetime	X_i	p_i
< 30	41	0.4512
30 - 60	31	0.2476
60 - 90	13	0.1359
> 90	15	0.1653
Total	100	1

Goodness of Fit	Test
Test Statistic	2.11e+00
p value %	54.89
Significance (α) %	5.00
null hypothesis (H_0)	accepted
minimum np_i	14

6 Table of observations and results of goodness-of-fit tests are tabulated below.

Grade	X_i	p_i
Top	234	0.4
High	117	0.3
Medium	81	0.2
Low	68	0.1
Total	500	1

Goodness of Fit	Test
Test Statistic	2.31e+01
p value %	0.00
Significance (α) %	5.00
null hypothesis (H_0)	rejected
$\underline{\text{minimum } np_i}$	50