ST2132 Goodness-of-fit

Semester 1 2022/23

Introduction

- Assuming a statistical model for data, we can estimate parameters, SEs, and construct CI's. But these do not indicate how well the model fits the data.

- Goodness-of-fit of models is often check ed using a hypothesis test. We will look at:
  1. Pearson's X^2, for multinomial data
  2. Likelihood ratio (LR)

Possibilities for a die

Roll a die n times independently and in the same way:

$$(X_1, \dots, X_6) \sim \text{Multinomial}(n, (p_1, \dots, p_6))$$

1. It could be that $p_1 = p_2 = p_3$, $p_4 = p_5$, i.e., there are at most 3 different probabilities.
2. Or $p_1 = p_2 = p_3$, $p_4 = p_5 = p_6$.
3. Or $p_1 = \cdots = p_6$, i.e., die is fair.

The three models are nested in the general multinomial model. Which might be preferred?

Models as subsets

A general die can be represented as

$$\Omega = \{(p_1, \ldots, p_6) : p_i > 0, \sum_{i=1}^{6} p_i = 1\}$$

1. $p_1 = p_2 = p_3$, $p_4 = p_5$ correspond to a subset of Ω:

$$\{(\theta_1, \theta_1, \theta_1, \theta_2, \theta_2, \theta_3) : \theta_i > 0, 3\theta_1 + 2\theta_2 + \theta_3 = 1\}$$

2. $p_1 = p_2 = p_3$, $p_4 = p_5 = p_6$:

$$\{(\theta_1, \theta_1, \theta_1, \theta_2, \theta_2, \theta_2) : \theta_i > 0, \theta_1 + \theta_2 = 1/3\}$$

Let $(X_1, \ldots, X_r) \sim \text{Multinomial}(n, \mathbf{p})$, with n, r fixed. Set of all distributions:

Ω Ω_1 Ω_0

$$\Omega = \{(p_1, \ldots, p_r) : p_i > 0, \sum_{i=1}^{r} p_i = 1\}$$

Consider a subset where $\mathbf{p}$ depends on $\theta \in \Theta \subset \mathbb{R}^k$, $k < r - 1$:

$$\Omega_0 = \{(p_1(\theta), \ldots, p_r(\theta)) : \theta \in \Theta\}$$

Given realisations $(x_1, \ldots, x_r)$, to judge whether $\mathbf{p} \in \Omega_0$.

Assume (342, 500, 187) is a realisation of $\mathbf{X} \sim$ Trinomial(1029,$\mathbf{p}$).

$$\Omega = \{(p_1, p_2, p_3) : p_i > 0, \sum_{i=1}^{3} p_i = 1\}$$

Ω

HWE says $\mathbf{p}$ is in

$$\Omega_0 = \{(1-\theta)^2, 2\theta(1-\theta), \theta^2) : 0 < \theta < 1\}$$

Goodness-of-fit test:

1. Null hypothesis $H_0 : \mathbf{p} \in \Omega_0$.
2. Alternative hypothesis $H_1 : \mathbf{p} \in \Omega_1 = \Omega - \Omega_0$.
3. Calculate test statistic and P-value, then conclude.

Observed vs expected counts

If H_0 is true, we expect X_1 to be

$$E(X_1) = 1029 \times (1-\theta)^2 \approx 1029 \times (1-0.42)^2 \approx 340.6$$

if H_0 is true

Observed	*Expected*	$(O-E)^2/E$
342	340.6	0.006
500	502.8	0.016
187	185.6	0.011
1029	1029	0.033

The P-value is roughly $\Pr(\chi_1^2 \geq 0.033) \approx 0.86$.

0.033 measures a distance between observed and expected frequencies. If H_0 is true, the chance is quite high to get data that are more extreme than (342,500,187). HWE seems to fit well.

Pearson's X^2

Assumption.

$(X_1, \ldots, X_r) \sim \text{Multinomial}(n, \mathbf{p}(\theta))$, $\theta \in \Theta \subset \mathbb{R}^k$, $k < r - 1$.

Definitions.

$\hat{\theta}$: ML estimator of θ. $n\mathbf{p}(\hat{\theta})$: random expected counts.

Chi-square statistic:

$$X^2 = \sum_{i=1}^{r} \frac{(X_i - np_i(\hat{\theta}))^2}{np_i(\hat{\theta})}$$

Theorem. As $n \to \infty$, the distribution of X^2 converges to χ^2_{r-1-k}.

Strictly speaking, the dimension of Θ has to be k.

X^2 goodness-of-fit test

$(X_1, \ldots, X_r) \sim \text{Multinomial}(n, \mathbf{p}), \mathbf{p} \in \Omega$, with n large.

$\Omega_0 = \{\mathbf{p}(\theta) : \theta \in \Theta \subset \mathbb{R}^k\}$. $\Omega_1 = \Omega - \Omega_0$.

1. $H_0 : \mathbf{p} \in \Omega_0$ (assumption in previous slide).
2. $H_1 : \mathbf{p} \in \Omega_1$.

   HWE 0.42

3. Substituting each X_i by x_i, and $\hat{\theta}$ by the ML estimate, we get a realisation x^2 of X^2.

   = 0.033

4. The P-value:

   calculated assuming H_0 $\rightarrow$

$$\Pr(X^2 \geq x^2) \approx \Pr(\chi^2_{r-1-k} \geq x^2)$$

   The smaller it is, the more suspicious we are of H_0.

Examples

- HWE: $r = 3$. $k = 1$, since the probabilities are modelled as functions of θ. $r - 1 - k = 1$.
- k can be 0, in which case Ω_0 is a single point. Then the expected counts are exact, not estimated.

  For a die, if H_0 says it is fair, i.e., $p_i = 1/6$, then there is no parameter to estimate. $r - 1 - k = 5$.

  Tutorial 9 Question 3: $x^2 = 14.2$, $P(X^2 \geq 14.2) \approx \Pr(\chi_5^2 \geq 14.2) \approx 0.01$. The die is likely unfair.

G statistic

- Define
$$G = 2\sum_{i=1}^{r} X_i \log\left(\frac{X_i}{np_i(\hat{\theta})}\right)$$
- In the following, g is very close to x^2.

Example	n	x^2	g
HWE	1209	0.033	0.032
T8Q3	60	14.20	14.15
T8Q4	3839	2.02	2.02

- G is a **likelihood ratio** statistics.

Likelihood ratio and G

$(X_1, \ldots, X_r) \sim \text{Multinomial}(n, \mathbf{p})$. $\Pr(\underset{\sim}{X} = \underset{\sim}{x}) = \binom{n}{x_1 \cdots x_r} p_1^{x_1} \cdots p_r^{x_r}$

- Maximum of likelihood $L(\mathbf{p}) = \prod_{i=1}^{r} p_i^{X_i}$ over Ω:

$$\hat{p}_i = \frac{X_i}{n} \qquad L_1 = L(\hat{p}) = \prod_{i=1}^{r} \left(\frac{X_i}{n}\right)^{X_i}$$

- Maximum of likelihood $L(\theta) = \prod_{i=1}^{r} p_i(\theta)^{X_i}$ over Ω_0:

$$L_0 = L(\hat{\theta}) = \prod_{i=1}^{r} p_i(\hat{\theta})^{X_i}$$

- Always, $L_1/L_0 \geq 1$. The larger the ratio, the more we doubt H_0, which says that $\mathbf{p} \in \Omega_0$.

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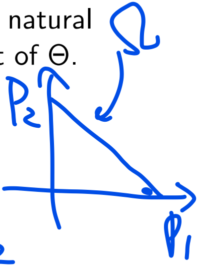
$$2\log\left(\frac{L_1}{L_0}\right) = 2\log\left(\prod_{i=1}^{r}\left(\frac{X_i}{np_i(\hat{\theta})}\right)^{X_i}\right)$$

$$= 2\sum_{i=1}^{r} X_i \log\left(\frac{X_i}{np_i(\hat{\theta})}\right)$$

Ω and parameter space

In applications, we often identify the big model Ω with a natural parameter space Θ. Then the small model Ω_0 is a subset of Θ.



- For the general trinomial distribution, we can define

$$\Omega = \{(p_1, p_2) : p_i > 0, p_1 + p_2 < 1\}$$

- The HWE model is the subset Ω_0 with

$$p_1 = (1-t)^2, p_2 = 2t(1-t), \qquad p_3 = t^2 \qquad 0 < 1 < t$$

- Let $\Omega_1 = \Omega - \Omega_0$ and $\theta = (p_1, p_2)$. The goodness-of-fit test of the HWE model can be stated as follows:

$$H_0 : \theta \in \Omega_0 \qquad H_1 : \theta \in \Omega_1$$

LR statistic G

Assumption.

n IID RV's density defined by $\theta \in \Omega$ with k_1 independent parameters.
L_1: maximum likelihood value over Ω.

Nested in Ω is Ω_0 with $k_0 < k_1$ independent parameters.
L_0: maximum likelihood value over Ω_0.

Theorem. Suppose $\theta \in \Omega_0$. As $n \to \infty$, the distribution of

$$G = 2 \log \left(\frac{L_1}{L_0} \right)$$

converges to $\chi^2_{k_1 - k_0}$.

Letting $\ell_0 = \log L_0, \ell_1 = \log L_1,\ G = 2(\ell_1 - \ell_0)$.

LR goodness-of-fit test

Assumption as in previous slide. $\Omega_1 = \Omega - \Omega_0$.

1. $H_0 : \theta \in \Omega_0$.
2. $H_1 : \theta \in \Omega_1$.
3. L_0 and L_1 are the maximum likelihood values under Ω_0 and Ω.

   $$g = 2 \log \left(\frac{L_1}{L_0} \right)$$

   is a realisation of G.
4. The P-value is calculated with distribution of G under H_0:

   $$\Pr(G \geq g) \approx \underbrace{\Pr(\chi^2_{k_1 - k_0} \geq g)}_{1 - \mathrm{pchisq}(g,\, k_1 - k_0)}$$

Multinomial goodness-of-fit

- To judge whether multinomial data $(x_1, \ldots, x_r)$ might have come from a simpler model with $k < r - 1$ parameters, either

$$G = 2\sum_{i=1}^{r} X_i \log\left(\frac{X_i}{np_i(\hat{\theta})}\right), \qquad X^2 = \sum_{i=1}^{r} \frac{(X_i - np_i(\hat{\theta}))^2}{np_i(\hat{\theta})}$$

  can be used. For large $n = \sum_{i=1}^{r} x_r$, under H_0, both are approximately χ^2_{r-1-k}.

- If the simpler model consists of a distribution specified by θ_0, then $k = 0$ and $\hat{\theta}$ should be replaced by θ_0.

- For multinomial data, there is no need to evaluate L_0 and L_1 to compute G. Other examples may also yield such shortcuts.

Bacterial clumps in milk (pg 344)

- Assume 400 counts of bacterial clumps are realisations of IID Poisson(λ) RV's. By ML estimate of λ is the mean number: 2.44.

Number	0	1	2	3	4	5	6	≥ 7
Frequency	56	104	80	62	42	27	9	20
Expected	34.9	85.1	103.8	84.4	51.5	25.1	10.2	5.0

- The model looks bad. We will assess how bad it is relative to a larger model:

  For $i = 1, \ldots, 400$, x_i is a realisation of $X_i \sim \text{Poisson}(\lambda_i)$, which are independent.

Poisson likelihood ratio

1. Ω: For $i = 1, \ldots, n$, $X_i \sim \text{Poisson}(\lambda_i)$ are independent.

$x_i \log \lambda_i - \lambda_i$ $\quad \frac{\lambda^x e^{-\lambda}}{x!}$

$\hat{\lambda}_i = X_i$

$$\ell(\lambda_1, \ldots, \lambda_n) = \sum_{i=1}^n X_i \log \lambda_i - \sum_{i=1}^n \lambda_i$$

Maximum loglikelihood under Ω : $\ell_1 =$ $\ell(X_1, \ldots, X_n) = \boxed{\sum_{i=1}^n X_i \log X_i - \sum_{i=1}^n X_i}$

2. Ω_0: Every $\lambda_i = \lambda$.

$\hat{\lambda} = \bar{X}$

$$\ell(\lambda) = \sum_{i=1}^n X_i \log \lambda - n\lambda$$

Maximum likelihood under Ω_0 : $\ell_0 = \ell(\bar{X}) = \boxed{\sum_{i=1}^n X_i \log \bar{X} - n\bar{X}}$

$$G = 2 \sum_{i=1}^n X_i \log \left(\frac{X_i}{\bar{X}} \right) \approx \frac{\sum_{i=1}^n (X_i - \bar{X})^2}{\bar{X}}$$

Suppose every $\lambda_i = \lambda$. For large n, $G \sim \chi^2_{n-1}$ approximately.

Poisson dispersion test

$Y \sim \chi^2_{399}$

$E(Y) = 399$

$SD(Y) \approx \sqrt{800}$

$\approx 30.$

1. H_0: rates are all equal.
2. H_1: rates are not all equal.
3. Sample mean and variance are 2.44 and 4.59.

$$g \approx \frac{\sum_{i=1}^{400}(x_i - \bar{x})^2}{\bar{x}} = \frac{399 \times 4.59}{2.44} \approx 751$$

4. The P-value is approximately

$$\Pr(\chi^2_{399} \geq 751) \approx 0$$

The rates are likely different.

Normal data

Based on $\mathrm{N}(\mu, \sigma^2)$ realisations $x_1, \ldots, x_n$, might we conclude that $\mu = 0$?

- Idea: if $\bar{X}$ is far from 0, reject $H_0 : \mu = 0$. $H_1 : \mu \neq 0$.
- Suppose σ is known. Under H_0,

$$\frac{\sqrt{n}\bar{X}}{\sigma} \sim \mathrm{N}(0,1)$$

- The P-value

$$\Pr\left(|Z| \geq \frac{\sqrt{n}|\bar{x}|}{\sigma}\right) = \Pr\left(Z^2 \geq \frac{n\bar{x}^2}{\sigma^2}\right)$$

The P-value is called two-tailed. One-tailed P-values correspond to H_1 saying $\mu > 0$ or $\mu < 0$.

LR test on normal data

$H_0 : \mu = 0$. $H_1 : \mu \neq 0$.

$\Omega = \mathbb{R}$, $\Omega_0 = \{0\}$. LR test can be applied.

1. σ is known.

$$G = \frac{n\bar{X}^2}{\sigma^2}$$

   Under H_0, $G \sim \chi_1^2$ exactly. Identical to previous slide.

2. σ is unknown. For large n,

$$G \approx \frac{n\bar{X}^2}{\hat{\sigma}^2}$$

   Under H_0, $G \sim \chi_1^2$ approximately.

1. Ω:

$$\ell(\mu) = -\frac{\sum_{i=1}^{n}(X_i - \mu)^2}{2\sigma^2}$$

$$\ell_1 = -\frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{2\sigma^2} = -\frac{n\hat{\sigma}^2}{2\sigma^2}$$

2. Ω_0:

$$\ell_0 = -\frac{\sum_{i=1}^{n} X_i^2}{2\sigma^2} = -\frac{n\hat{\mu}_2}{2\sigma^2}$$

3.

$$G = \frac{n(-\hat{\sigma}^2 + \hat{\mu}_2)}{\sigma^2} = \frac{n\bar{X}^2}{\sigma^2}$$

Suppose $\mu = 0$. $G \sim \chi_1^2$.

Normal data: unknown σ

1. Ω:

$$\ell(\mu, \sigma) = -n \log \sigma - \frac{\sum_{i=1}^{n}(X_i - \mu)^2}{2\sigma^2}$$

$$\ell_1 = -\frac{n}{2} \log \hat{\sigma}^2 - \frac{n}{2}$$

2. Ω_0:

$$\ell(\sigma) = -n \log \sigma - \frac{\sum_{i=1}^{n} X_i^2}{2\sigma^2}$$

$$\ell_0 = -\frac{n}{2} \log \hat{\mu}_2 - \frac{n}{2}$$

3.

$$G = n \log \left(\frac{\hat{\mu}_2}{\hat{\sigma}^2} \right) \approx \frac{n\bar{X}^2}{\hat{\sigma}^2}$$

Suppose $\mu = 0$. For large n, $G \sim \chi_1^2$ approximately.

Conclusion (1)

- The LR test applies in many situations where the investigator wants to know the goodness-of-fit of a model *relative* to a larger model. If n is large, the P-value can be computed using a χ^2 distribution.
- The test assumes the larger model is valid, and does not assess *its* goodness-of-fit.
- A P-value is not a probability that H_0 is true. H_0 is either true or false. P-value is computed assuming H_0 is true.
- Even if a model seems to fit the data, it may not mean the data were generated randomly according to the model. Plotting data in sequence is an important diagnosis. But for prediction, this point may not be so important.

Conclusion (2)

- Statistical inference consists of two main areas: parameter estimation and hypothesis testing.
- MOM and ML are general estimation methods. To apply to data, a statistical model is needed. The procedures are blind to the goodness-of-fit of the model.
- We only test hypotheses relating to goodness-of-fit. But the general framework applies similarly when testing other hypotheses.
- Statistical inference can be quite procedural. Watch out for pitfalls in other aspects of data analysis, such as the choice of a model.