DATA 606: Statistical Methods in Data Science

—— Introduction of categorical data analysis

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Lecture 7

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General intro

Definition 1 (Categorical variable)

A categorical variable has a measurement scale consisting of a set of categories.

Example 1

1. Political philosophy: liberal, moderate or conservative.
2. Diagnoses regarding some cancer: normal, benign or malignant.

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A categorical variable

- Could be either response or explanatory variable.
- Could be binary, nominal or ordinal scale.
- Could be discrete or continuous.
- Could be qualitative or quantitative.

Distributions

Three key distributions for categorical data: **binomial, multinomial and Poisson**.

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1. Binomial distribution (π, n)
   - Fixed number of observations, e.g. n.
   - Observations $(y_i, i = 1, 2, \ldots, n)$ are binary, e.g. $y_i = 1$ or $y_i = 0$.
   - Fixed probability, e.g. $\mathbf{P}(Y_i = 1) = \pi$.
   - Observations are independent.

   Let $Y = \sum_{i=1}^{n} Y_i$, then Y is said to follow the binomial distribution, denoted as $\text{bin}(n, \pi)$.

Binomial distribution

The statistical properties of a binomial distribution

- The probability mass function

$$\mathbf{P}(Y = y) = \binom{n}{k} \pi^y (1-\pi)^{n-y}, \quad y = 0, 1, \ldots, n.$$

- The mean and variance

$$\mathbf{E}[Y] = n\pi, \quad \mathrm{Var}(Y) = n\pi(1-\pi).$$

Multinomial distribution

2. Multinomial distribution $(\pi_1, \dots, \pi_c)$
   - Fixed number of observations/trials, e.g. n.
   - c categories of outcomes $(1, 2, \dots, c)$.
   - Each kind of outcome appears with fixed probability, e.g. $\pi_1, \dots, \pi_c$.

Let $N_1, \dots, N_c$ count the number of appearance of each kind of outcome, then $(N_1, \dots, N_c)$ is said to follow the multinomial distribution.

- The probability mass function $(n_1 + n_2 + \cdots + n_c = n)$

$$\mathbf{P}(N_1 = n_1, \dots, N_c = n_c) = \frac{n!}{n_1! \cdots n_c!} \pi_1^{n_1} \cdots \pi_c^{n_c},$$

- Statistical properties

$$\mathbf{E}[N_i] = n\pi_i, \quad \mathrm{Var}(N_i) = n\pi_i(1 - \pi_i), \quad \mathrm{Cov}(N_i, N_j) = -n\pi_i\pi_j.$$

Poisson distribution

3. Poisson distribution (μ) Rare events?
   - Count data do not result from a fixed number of observations/trials.
   - There is no upper bound for the number of appearance of the outcome.

- The probability mass function

$$\mathbf{P}(Y = y) = \frac{e^{-\mu}\mu^{y}}{y!}, \quad y = 0, 1, 2 \ldots .$$

- Statistical properties

$$\mathbf{E}[Y] = \mu, \quad \mathrm{Var}(Y) = \mu.$$

Overdispersion

Definition 2 (Overdispersion)

count observations often exhibit variability exceeding that predicted by the preset distribution.

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An example:

- We assume each day there is a fixed probability for the tornado to occur.
- The probability actually is changing w.r.t other factors, such as temperature, moisture, whether it is rainy or windy, etc..
- Suppose Y is a random variable which is Poisson distributed conditional on μ. This μ is not fixed in reality.
- Using conditional mean and variance formulas

$$\mathbf{E}[Y] = \mathbf{E}[\mathbf{E}[Y|\mu]] = \mathbf{E}[\mu],$$
$$\mathrm{Var}(Y) = \mathbf{E}[\mathrm{Var}(Y|\mu)] + \mathbf{E}[\mathrm{Var}(Y|\mu)] = \mathbf{E}[\mu] + \mathbf{E}[\mathrm{Var}(Y \mid \mu)].$$

An alternative

4. Negative binomial (π, k)
   - Each time binary outcome, success or failure.
   - Each time, fixed probability for success, e.g. π.
   - Y is the number of failures before k successes occur.

- The probability mass function

$$\mathbf{P}(Y = y) = \binom{y + k - 1}{y} (1 - \pi)^y \pi^k, \quad y = 0, 1, 2 \ldots .$$

- Statistical properties

$$\mathbf{E}[Y] = \frac{\pi k}{1 - \pi}, \quad \mathrm{Var}(Y) = \frac{\pi k}{(1 - \pi)^2}$$

Likelihood function

Definition 2 (Likelihood function)

A likelihood function is the probability of the observed data.

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Example 3

Suppose Y_1, Y_2, Y_3 all follow Poisson distribution with parameter μ, then given $Y_1 = 4, Y_2 = 2, Y_3 = 1$, the likelihood function is

$$L(\mu) = \frac{e^{-\mu}\mu^4}{4!} \cdot \frac{e^{-\mu}\mu^2}{2!} \cdot \frac{e^{-\mu}\mu}{1!} = \frac{e^{-3\mu}\mu^7}{48}$$

Maximum likelihood estimation

Maximum likelihood estimation (MLE)

Find the parameters which could maximize the likelihood function.

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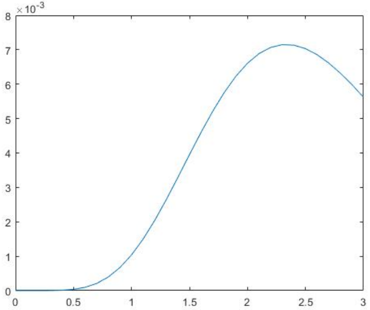
Example 4 (Cont.)



$$L'(\mu) = -\frac{e^{-3\mu}\mu^7}{16} + \frac{7e^{-3\mu}\mu^6}{48} = 0 \Longrightarrow \hat{\mu} = \frac{7}{3}.$$

Maximum likelihood function

Note that maximizing the likelihood function is **equivalent to** maximizing its log version:

$$\max \ L(\mu) \iff \max \ l(\mu) = \log(L(\mu)).$$

It is easier to calculate based on the log-likelihood function.

Example 5 (Cont.)

$$\log(L(\mu)) = \log(e^{-3\mu}) + \log(\mu^7) - \log(48) = -3\mu + 7\log(\mu) - \log(48),$$

$$\frac{d\log(L(\mu))}{d\mu} = -3 + \frac{7}{\mu} = 0 \Longrightarrow \hat{\mu} = \frac{7}{3}.$$

MLE for binomial distribution

Suppose Y follows binomial distribution (n, π) where π is unknown, and we observe $Y = y$, then

$$L(\pi) = \binom{n}{y} \pi^y (1-\pi)^{n-y},$$

$$l(\pi) = \log L(\pi) = \log \binom{n}{y} + y \log \pi + (n-y) \log(1-\pi).$$

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Then

$$\frac{dl(\pi)}{d\pi} = \frac{y}{\pi} - \frac{n-y}{1-\pi} = 0 \Longrightarrow \hat{\pi} = \frac{y}{n}.$$

More about MLE

In the previous examples, the estimator $\hat{\mu}$ and $\hat{\pi}$ are both **random**.

Question: without parametric form, can you tell the variance of the MLE estimator?

Answer:

- *Information matrix*: $\nu(\mu) = -\mathbf{E}\left(l''(\mu)\right) = -\mathbf{E}\left(\frac{d^2 l(\mu)}{d\mu^2}\right)$.
- The asymptotic variance of $\hat{\mu}$ is $\frac{1}{\nu(\mu)}$.

Variance for binomial MLE

In binomial example, the log-likelihood function is (neglecting the constant term)

$$l(\pi) = Y \log \pi + (n - Y) \log(1 - \pi).$$

Its second-order derivative is

$$l''(\pi) = -\frac{Y}{\pi^2} - \frac{n - Y}{(1 - \pi)^2}.$$

Then the information matrix of π is

$$\nu(\pi) = -\mathbf{E}(l''(\pi)) = \frac{n\pi}{\pi^2} + \frac{n - n\pi}{(1 - \pi)^2} = \frac{n}{\pi(1 - \pi)}.$$

Therefore, the asymptotic variance is $\frac{\pi(1-\pi)}{n}$[1].

[1]The MLE estimator $\hat{\pi} = \frac{y}{n}$, its variance is also $\frac{\pi(1-\pi)}{n}$.

More about MLE

Asymptotic property of MLE estimator: when the number of observations n is large, the estimator is more close to normal distributed.

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Asymptotic property of MLE estimator: when the number of observations n is large, the estimator is more close to normal distributed.

In other words, if β is the parameter to be estimated, then when $n \to \infty$,

$$\hat{\beta} \sim \text{Normal}(\mathbf{E}[\hat{\beta}], \sigma(\hat{\beta})),$$

where $\hat{\beta}$ is the MLE estimator.

Several tests

Motivation: in daily life, we always encounter hypothesis tests, such that

$$\begin{aligned} \mathcal{H}_0: &\quad \beta = \beta_0 \\ \mathcal{H}_1: &\quad \beta \neq \beta_0. \end{aligned}$$

β is some parameter in the model we apply to the practical problem.

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How to test whether $\mathcal{H}_0$ is acceptable or not?
We use MLE estimator and the following three constructed tests.

Wald statistic

- With MLE, we could obtain $\hat{\beta}$, as well as its information $\nu(\hat{\beta}) - \mathbf{E}[\frac{\partial^2 l(\beta)}{\partial \beta^2}|_{\beta=\hat{\beta}}]$.
- Under the NULL hypothesis $\mathcal{H}_0$, the following statistic is proved to asymptotically follow standard normal distribution

$$Z = \frac{\hat{\beta} - \beta_0}{\sigma(\hat{\beta})}$$

where

$$\sigma^2(\hat{\beta}) = \frac{1}{\nu(\hat{\beta})}.$$

- As $Z \sim \text{Normal}(0, 1)$, if Z is too small or too large, then the null hypothesis should be rejected.

Likelihood ratio test

- You have a vector of parameters to estimate: $\boldsymbol{\beta} = (\beta_0, \beta_1)$.
- You are given a hypothesis: $\mathcal{H}_0 : \beta_0 = 0$ and want to test if this hypothesis is acceptable.
- You apply MLE to the data and obtain the following parameters:

$$\mathcal{H}_0 \text{ is assumed : } \quad (0, \tilde{\beta}_1),$$

$$\mathcal{H}_0 \text{ is NOT assumed : } \quad (\hat{\beta}_0, \hat{\beta}_1).$$

- You get two likelihoods:

$$L_0 = L(\boldsymbol{x}; 0, \tilde{\beta}_1), \quad L_1 = L(\boldsymbol{x}; \hat{\beta}_0, \hat{\beta}_1).$$

Likelihood ratio test

- Apparently, $L_1 \geq L_0$. Furthermore, the following statistic

$$-2\log\Delta = -2\log\frac{L_0}{L_1} = -2(l_0 - l_1)$$

  follows χ^2_q distribution, where q is equal to the difference between the dimensions of the two different parameter spaces[2].

- We hope L_0 is not far away from L_1, therefore, if $-2\log\Delta$ is too large, then $\mathcal{H}_0$ should be rejected.

[2] In this case, the df is equal to 1.

Score test

- You are given the hypothesis: $\mathcal{H}_0 : \beta = \beta_0$
- The first-order derivative of the log-likelihood function evaluated at β_0:

$$u(\beta_0) = \frac{\partial l(\beta)}{\partial \beta}\Big|_{\beta=\beta_0}.$$

- The expected second-order derivative of the log-likelihood function evaluated at β_0:

$$\nu(\beta_0) = -\mathbf{E}\Big[\frac{\partial^2 l(\beta)}{\partial \beta^2}\Big|_{\beta=\beta_0}\Big].$$

- The score statistic is $\frac{u(\beta_0)}{\sqrt{\nu(\beta_0)}}$[3] and it is proved to approximately follow standard normal distribution.

[3] Understand it as slope/curvature.

An illustrative graph

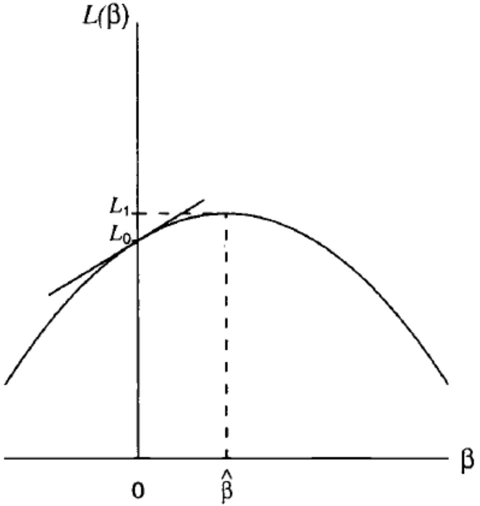

Figure 1.1 Log-likelihood function and information used in three tests of H_0: $\beta = 0$.

Tests about a binomial distribution

In a binomial distribution, the parameter to be estimated is π.

The MLE estimator for π is $\hat{\pi} = \frac{y}{n}$, its statistical characteristics are

$$\mathbf{E}[\hat{\pi}] = \pi, \quad \mathrm{Var}(\hat{\pi}) = \frac{\pi(n - \pi)}{n}.$$

Now we have our hypothesis:

$$\mathcal{H}_0 : \quad \pi = \pi_0,$$

$$\mathcal{H}_1 : \quad \pi \neq \pi_0.$$

Tests about a binomial distribution

- The Wald statistics

$$z_W = \frac{\hat{\pi} - \pi_0}{\sqrt{\hat{\pi}(1-\hat{\pi})/n}}$$

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$$z_W = \frac{\hat{\pi} - \pi_0}{\sqrt{\hat{\pi}(1-\hat{\pi})/n}}$$

- The slope and curvature

$$u(\pi_0) = \frac{y}{\pi_0} - \frac{n-y}{1-\pi_0}, \quad \nu(\beta_0) = \frac{n}{\pi_0(1-\pi_0)}.$$

The score statistic simplifies to

$$z_S = \frac{u(\pi_0)}{\sqrt{\nu(\pi_0)}} = \frac{\hat{\pi} - \pi_0}{\sqrt{\pi_0(1-\pi_0)/n}}$$

Tests about a binomial distribution

- Under $\mathcal{H}_0$,

$$l_0 = \log L_0 = y \log \pi_0 + (n - y) \log(1 - \pi_0).$$

- Without $\mathcal{H}_0$,

$$l_1 = \log L_1 = y \log \hat{\pi} + (n - y) \log(1 - \hat{\pi}).$$

- The likelihood-ratio test statistic is

$$-2(l_0 - l_1) = 2 \left[y \log \frac{\hat{\pi}}{\pi_0} + (n - y) \log \frac{1 - \hat{\pi}}{1 - \pi_0} \right].$$

  As here the difference between the dimensions of parameter spaces is 1. Therefore

$$-2(l_0 - l_1) \sim \chi_1^2.$$

CI for binomial distribution

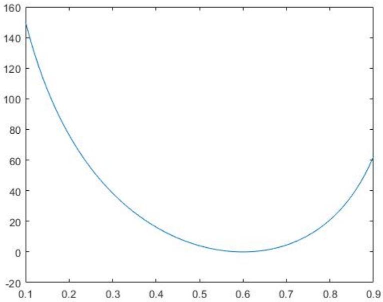
We could again utilize the aforementioned three constructed tests to obtain the *confidence intervals* for π.

- *Wald statistic* $|z_W| \leq z_{1-\alpha/2}$:

$$\left[\hat{\pi} - z_{1-\alpha/2}\sqrt{\frac{\hat{\pi}(1-\hat{\pi})}{n}},\ \hat{\pi} + z_{1-\alpha/2}\sqrt{\frac{\hat{\pi}(1-\hat{\pi})}{n}}\right].$$

CI for binomial distribution

- *Likelihood ratio test*



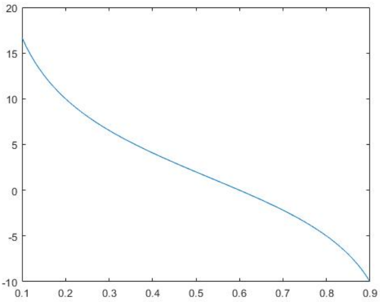
$$-2(l_0 - l_1) \leq \chi_1^2(0.95) \implies [\pi_0(1),\ \pi_0(2)],$$

where $\pi_0(1)$ and $\pi_0(2)$ are the roots of

$$2\left[y \log \frac{\hat{\pi}}{\pi_0} + (n-y)\log \frac{1-\hat{\pi}}{1-\pi_0}\right] = \chi_1^2(0.95).$$

CI for binomial distribution

- *Score statistic*



$$|z_S| \le z_{1-\alpha/2} \implies [\pi_0(1),\ \pi_0(2)],$$

where $\pi_0(1)$ and $\pi_0(2)$ are the roots of

$$\frac{\hat{\pi} - \pi_0}{\sqrt{\frac{\pi_0(1-\pi_0)}{n}}} = \pm z_{1-\alpha/2}.$$

An example

Example 6 (The proportion of vegetarians)

The instructor questioned the students in one class whether he or she was a vegetarian. Of $n = 25$ students, $y = 0$ answered "yes". Give a 95% confidence interval for the proportion of vegetarians over the whole student population on campus.

An example

Example 6 (The proportion of vegetarians)

The instructor questioned the students in one class whether he or she was a vegetarian. Of $n = 25$ students, $y = 0$ answered "yes". Give a 95% confidence interval for the proportion of vegetarians over the whole student population on campus.

- Since $y = 0$, the MLE estimate $\hat{\pi} = \frac{0}{25} = 0$. With the *Wald method*, the 95% CI for π is

$$\left[\hat{\pi} - 1.96\sqrt{\hat{\pi}(1-\hat{\pi})/n},\ \hat{\pi} + 1.96\sqrt{\hat{\pi}(1-\hat{\pi})/n}\right]$$

which is $[0, 0]$.

An example

- With *Score statistic*, we first need to solve the equation

$$|\hat{\pi} - \pi| = 1.96\sqrt{\pi(1-\pi)/n},$$

which yields $\pi(1) = 0$ and $\pi(2) = 0.133$. Therefore the CI based on score statistics is $[0, 0.133]$

An example

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- With *likelihood ratio test*, as we know the likelihood function is

$$l(\pi) = \pi^2(1-\pi)^{25} = (1-\pi)^{25},$$

The likelihood-ratio-based 95% CI is given by

$$-2(l_0 - l_1) = -2(l(\pi) - l(\hat{\pi})) = -50\log(1-\pi) \leq \chi_1^2(0.95) = 3.84$$

which gives $\pi \in [0, 0.074]$.

MLE for multinomial distribution

In a multinomial distribution, the parameters to be estimated are $\pi_1, \ldots, \pi_c$.

- We have observations $\pi_1, \ldots, \pi_c$ such that $n = n_1 + \cdots + n_c$.
- The likelihood function is $L(\pi_1, \ldots, \pi_c) = \pi_1^{n_1} \cdots \pi_c^{n_c}$, where the log-likelihood function is

$$l(\pi_1, \ldots, \pi_c) = \log L(\pi_1, \ldots, \pi_c) = \sum_{i=1}^{c} n_i \log \pi_i.$$

- Note that $\pi_1 + \cdots + \pi_c = 1$, therefore only first $c - 1$ parameters need to be estimated and $\pi_c = 1 - \pi_1 - \cdots - \pi_{c-1}$.

MLE for multinomial distribution

- Write $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_c)$, for $j \in \{1, 2, \ldots, c-1\}$, we have

$$\frac{\partial \log \pi_i}{\partial \pi_j} = \begin{cases} 0, & i \neq j \text{ and } i \neq c, \\ \frac{1}{\pi_j}, & i = j, \\ -\frac{1}{\pi_c}, & i = c. \end{cases}$$

and

$$\frac{\partial l(\boldsymbol{\pi})}{\partial \pi_j} = \frac{n_j}{\pi_j} - \frac{n_c}{\pi_c}.$$

Hence $\frac{\hat{\pi}_j}{\hat{\pi}_c} = \frac{n_j}{n_c}$. Recall $\sum_{i=1}^{c} \hat{\pi}_i = 1$, therefore $\hat{\pi}_j = n_j/n$.

Pearson Chi-square test

Now we are faced with another hypothesis test problem

$$\mathcal{H}_0 : \quad \pi_1 = a_1, \ldots, \pi_c = a_c.$$

With observations $n_1, \ldots, n_c$, how to check whether $\mathcal{H}_0$ is acceptable?

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$$\mathcal{H}_0: \quad \pi_1 = a_1, \ldots, \pi_c = a_c.$$

With observations $n_1, \ldots, n_c$, how to check whether $\mathcal{H}_0$ is acceptable?

Let $n = n_1 + \cdots + n_c$ and $\mu_i = n \times a_i$. Pearson proposed the following test statistic

$$X^2 = \sum_{i=1}^{c} \frac{(n_i - \mu_i)^2}{\mu_i}$$

If the null hypothesis is wrong, then at least one term of the above sum is large.

Pearson Chi-square test

For large samples, the above test statistic

$$X^2 \sim \chi^2_{c-1}.$$

Hence, if $\underline{X^2 > \chi^2_{c-1}(0.95)}$, the hypothesis $\mathcal{H}_0$ could be rejected.