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\hat{p} is a value calculated from observed data

↳ A statistic

↳ probability distribution is called sampling distribution

If the mean $\hat{p} = p$ it is unbiased

Sampling without Replacement

$$E(\hat{p}) = p \text{ still}$$

$$\text{Var}[\hat{p}] = \langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2$$

$$\hat{p} = \left(\frac{x_1 + x_2 + \dots + x_n}{n} \right)$$

$$\langle \hat{p}^2 \rangle = \frac{1}{n^2} \langle x_1^2 + \dots + x_n^2 + 2x_1x_2 + \dots + 2x_{n-1}x_n \rangle$$

$$= \frac{1}{n^2} \langle n x_i^2 + \binom{n}{2} \langle 2x_i x_j \rangle \rangle$$

↑
Expected Values are
same for each x_i

$$= \frac{1}{n^2} \cdot \langle x_i^2 \rangle + \frac{n-1}{n} \langle 2x_i x_j \rangle$$

||
 $\langle x_i \rangle$
since $x_i = 0 \text{ or } 1$

||
 $P[x_i=1 \text{ and } x_j=1]$
 $= P[x_i=1] \cdot P[x_j=1 | x_i=1]$

$$= p \cdot \frac{p(N-1)}{N-1}$$

$$\text{Var}(\hat{p}) = \langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2$$

$$= \frac{1}{n} \cdot p + \frac{n-1}{n} \cdot p \cdot \frac{p(N-1)}{N-1}$$

$$= \frac{p(1-p)}{n} \left(1 - \frac{n-1}{N-1} \right)$$

⏟
Correction factor

Some stuff on Central Limit Theorem

Types of Inference Questions

- Hypothesis Testing: Asking a yes or no question about the distribution
- Estimation: Determining the distribution or some characteristic
- Confidence Interval

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Random Variables

Discrete: finite or countably infinite number of possible values

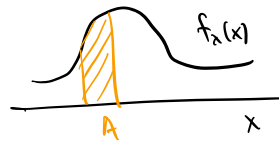
Probability Mass Function: $f_X(x) = P[X=x]$

For a set of values A $P[X \in A] = \sum_{x \in A} f_X(x) = 1$
when A is all possible

Continuous: takes any real value

Probability Density Function:

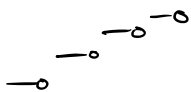
$$P[X \in A] = \int_A f_X(x) dx$$



$$\int_{\mathbb{R}} f_X(x) dx = P[X \in \mathbb{R}] = 1$$

Cumulative Distribution Function (CDF): $F_X(x) = P[X \leq x]$

Discrete CDF



$$F_X(x) = \sum_{y: y \leq x} f_X(y)$$

Continuous case: $F_X(x) = \int_{-\infty}^x f_X(y) dy$

Properties of CDF $F_X(x)$

Increasing: For any $x \leq y$ always $F_X(x) \leq F_X(y)$

As $x \rightarrow -\infty$ $F_X(x) \rightarrow 0$ as $x \rightarrow \infty$ $F_X(x) \rightarrow 1$

If $F_X(x)$ is strictly increasing and continuous, then $F_X(x)$ has an inverse function F_X^{-1}

: $(0,1) \rightarrow \mathbb{R}$ called quantile function of X

$F_X^{-1}(t)$ satisfies $P[X \leq x] = t$ i.e. $F_X^{-1}(t)$ is the t^{th} quantile of X

Expected Value and Variance

$$E[X] = \sum_{x \in X} x \cdot f_X(x)$$

$$E[X] = \int_{\mathbb{R}} x f_X(x) dx$$

$$g: \mathbb{R} \rightarrow \mathbb{R}$$

$$\mathbb{E}[g(x)] = \sum_{x \in X} g(x) f_x(x)$$

$$\mathbb{E}[g(x)] = \int_{\mathbb{R}} g(x) f_x(x) dx$$

Expectation is linear!!!

$$\text{Var}[X] = \mathbb{E}[(X - \mathbb{E}(X))^2] = \mathbb{E}[X^2] - \mathbb{E}(X)^2$$

Translation invariant: $\text{Var}[X+c] = \text{Var}[X]$

Multiply by constant: $\text{Var}[cX] = c^2 \text{Var}[X]$

Independent RV: $\text{Var}[X_1 + X_2] = \text{Var}[X_1] + \text{Var}[X_2]$

Dependent RV: $\text{Var}[X+Y] = \text{Var}[X] + \text{Var}[Y] + 2\text{Cov}[X,Y]$

The standard deviation of X is $\text{SD}(X) = \sqrt{\text{Var}(X)}$

A Bernoulli r.v. $X \sim \text{Bernoulli}(p)$ takes all possible values 0 and 1

The PMF is $f_x(1) = \mathbb{P}[X=1] = p$

$$f_x(0) = \mathbb{P}[X=0] = 1-p$$

Mean: $\mathbb{E}(X) = p \cdot 1 + (1-p) \cdot 0 = p$

Variance: $\text{Var}[X] = \mathbb{E}(X^2) - \mathbb{E}(X)^2$

$$= \mathbb{E}(X) - \mathbb{E}(X^2) \quad \text{since } X^2 = X \text{ when } X=0 \text{ or } 1$$

$$= p - p^2 = p(1-p)$$

A Binomial distribution is repeated Bernoulli trials

$$X = X_1 + X_2 + \dots + X_n \sim \text{Binomial}(n, p)$$

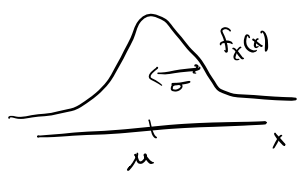
PMF is $f_x(x) = \binom{n}{x} p^x (1-p)^{n-x}$ for $x \in \{0, 1, \dots, n\}$

Mean: $\mathbb{E}(X) = \mathbb{E}(X_1 + \dots + X_n) = \mathbb{E}(X_1) + \dots + \mathbb{E}(X_n) = np$

Variance: $\text{Var}[X] = \text{Var}[X_1 + \dots + X_n] = \text{Var}[X_1] + \dots + \text{Var}[X_n] = np(1-p)$

A normal r.v. $X \sim \mathcal{N}(\mu, \sigma^2)$ is a continuous r.v. on \mathbb{R} ,

PDF $f_X(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$



$$E(X) = \int_{-\infty}^{\infty} x \cdot \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} = \mu$$

$$\text{Var}[X] = \int_{-\infty}^{\infty} (x-\mu)^2 \cdot \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} = \sigma^2$$

A Gamma r.v. $X \sim \text{Gamma}(\alpha, \beta)$ (for $\alpha, \beta > 0$) is continuous

$$f_X(x) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} e^{-\beta x} \quad \text{for } x > 0$$

$$\Gamma(\alpha) = \int_0^{\infty} x^{\alpha-1} e^{-x} dx$$

For integer $n \geq 1$, $\Gamma(n) = (n-1)!$

Joint Distributions

Discrete case: Joint PMF $f_{X_1, \dots, X_n}(x_1, \dots, x_n) = \mathbb{P}[X_1=x_1, \dots, X_n=x_n]$

Continuous case: Joint PDF $f_{X_1, \dots, X_n}(x_1, \dots, x_n)$

$$\mathbb{P}[(X_1, \dots, X_n) \in A] = \iint_A f_{X_1, \dots, X_n}(x_1, \dots, x_n) dx_1 \dots dx_n$$

Something about multi-nomial
↳ generalized binomial

$$f_{X_1, \dots, X_n}(x_1, \dots, x_n) = \binom{n}{x_1, \dots, x_n} p_1^{x_1} p_2^{x_2} \dots p_n^{x_n}$$

$$\frac{n!}{x_1! x_2! \dots x_n!}$$

Random Variable X_1, \dots, X_n are independent

$$f_{X_1, \dots, X_n}(x_1, \dots, x_n) = f_{X_1}(x_1) \times f_{X_2}(x_2) \dots \times f_{X_n}(x_n)$$

Properties of independent r.v

$$i) P[X_1 \in A_1 \text{ and } X_2 \in A_2 \text{ and } \dots X_n \in A_n]$$

$$= P[X_1 \in A_1] \times P[X_2 \in A_2] \times \dots \times P[X_n \in A_n]$$

ii) For any function $g_1 \dots g_n : \mathbb{R} \rightarrow \mathbb{R}$

$$E[g_1(X_1) \cdot g_2(X_2) \dots g_n(X_n)] = E[g_1(X_1)] \dots E[g_n(X_n)]$$

E.g. If X, Y are independent, then $E[XY] = E(X)E(Y)$

Covariance between r.v.'s X, Y

$$\text{Cov}[X, Y] = E[(X - E(X))(Y - E(Y))] = E(XY) - E(X)E(Y)$$

$$\text{Cov}[X, X] = \text{Var}[X]$$

Translationally Invariant: $\text{Cov}[X+a, Y+b] = \text{Cov}[X, Y]$

Bilinear: $\text{Cov}[aX, bY] = ab \text{Cov}[X, Y]$

If X_i and X_j are independent

$$\begin{aligned} \text{Cov}[X_i, X_j] &= E[X_i X_j] - E[X_i]E[X_j] \\ &= E(X_i)E(X_j) - E(X_i)E(X_j) = 0 \end{aligned}$$

Independent $\rightarrow \text{Cov} = 0$

Correlation

$$\text{Corr}(X, Y) = \frac{\text{Cov}[X, Y]}{\sqrt{\text{Var}(X)} \sqrt{\text{Var}(Y)}}$$

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Def: The moment generating function (MGF) of a random variable X is given by

$$M_X(t) = E[e^{tx}]$$

ex. Normal MGF

Let $X \sim \mathcal{N}(0,1)$. What is MGF of $M_X(t)$

$$\begin{aligned} M_X(t) &= E[e^{tx}] = \int_{-\infty}^{\infty} e^{tx} f_X(x) dx \\ &= \int_{-\infty}^{\infty} e^{tx} \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} dx \\ &= e^{-t^2/2} \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(x-t)^2} dx = e^{-t^2/2} \end{aligned}$$

PDF of $N(t, 1)$

If $M_X(t)$ is finite in a small interval around 0, then it uniquely determines the distribution of X

Theorem: Let X and Y be different random variables whose MGFs are finite in an interval $(-h, h)$ around 0, and

$$M_X(t) = M_Y(t) \text{ for all } t \in (-h, h). \text{ Then } X \text{ and } Y \text{ have the same distribution}$$

If X_1, \dots, X_n are independent r.v.'s then

$$\begin{aligned} M_{X_1 + \dots + X_n}(t) &= \mathbb{E}[e^{t(X_1 + \dots + X_n)}] \\ &= \mathbb{E}[e^{tX_1}] \times \dots \times \mathbb{E}[e^{tX_n}] = M_{X_1}(t) \times \dots \times M_{X_n}(t) \end{aligned}$$

Multivariate Normal Distribution

In k dimensions it is a continuous distribution for $(X_1, \dots, X_k) \in \mathbb{R}^k$

It is specified by

$$\text{mean vector: } \mu \in \mathbb{R}^k$$

$$\text{covariance matrix: } \Sigma \in \mathbb{R}^{k \times k}$$

k -dimensional generalization of the normal $\mathcal{N}(\mu, \sigma^2)$

Def: (X_1, \dots, X_k) are multivariate normal if for any constants $a_1, \dots, a_k \in \mathbb{R}$, the linear combination $a_1 X_1 + a_2 X_2 + \dots + a_k X_k$ has a normal distribution. More specifically, $(X_1, \dots, X_k) \sim \mathcal{N}(\mu, \Sigma)$ if in addition to this property

$$\mathbb{E}[X_i] = \mu_i \text{ and } \text{Var}[X_i] = \Sigma_{ii} \text{ for each } i = 1, \dots, k$$

$$\text{Cov}[X_i, X_j] = \Sigma_{ij} \text{ for } i \neq j$$

Note: This implies each individual r.v. is normal

You can prove this via expanding moment generating functions

$\text{Cov}(X, Y) = 0$ implies independence for bivariate normal

Theorem: If $\mathbf{X} = (X_1, \dots, X_k)$ is multivariate normal and \mathbf{X}_1 and \mathbf{X}_2 are two subvectors that are in pairwise uncorrelated, then \mathbf{X}_1 and \mathbf{X}_2 are independent.

Sampling Distribution of Statistics

For data X_1, \dots, X_n a statistic $T(X_1, \dots, X_n)$ is any value computed from this data

- Sample mean: $\bar{X} = \frac{1}{n} (X_1 + \dots + X_n)$

- Sample variance: $s^2 = \frac{1}{n-1} \left((X_1 - \bar{X})^2 + \dots + (X_n - \bar{X})^2 \right)$

- Sample Range: $R = \max(X_1, \dots, X_n) - \min(X_1, \dots, X_n)$

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A statistic is any function of data

Randomness of data induces a sampling distribution

Chi-Squared Distribution

$$X_1, \dots, X_n \stackrel{i.i.d.}{\sim} N(0,1)$$

Sampling distribution of $X_1^2 + \dots + X_n^2 \sim \chi_n^2$ with n degrees of freedom

$$M_{X_1^2 + \dots + X_n^2} = M_{X_1^2}(t) \times \dots \times M_{X_n^2}(t)$$

$$M_{X_1^2}(t) = \mathbb{E}[e^{tX_1^2}] = \int_{-\infty}^{\infty} e^{tx^2} \cdot \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} dx = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{(t-\frac{1}{2})x^2} dx$$

$t \geq 1/2$ blows up

$$M_{X_1^2}(t) = \frac{1}{\sqrt{1-2t}} \int_{-\infty}^{\infty} \sqrt{\frac{1-2t}{2\pi}} e^{-\frac{1}{2}(1-2t)x^2} dx$$

just MGF of $\text{Gamma}(\frac{1}{2}, \frac{1}{2})$ so $X_1^2 \sim \text{Gamma}(\frac{1}{2}, \frac{1}{2})$

$$M_{X_1^2 + \dots + X_n^2}(t) = \begin{cases} \infty & t \geq 1/2 \\ (1-2t)^{-n/2} & t < 1/2 \end{cases} \leftarrow \text{Gamma}(\frac{n}{2}, \frac{1}{2})$$

Distributions that are difficult to study will be studied by approximation

Simulate via R

Asymptotic approximations

- 1) Fastest
- 2) Theoretical Understanding

Weak Law of Large Numbers

Suppose X_1, \dots, X_n are IID, with $\mathbb{E}[X_i] = \mu$ and $\text{Var}[X_i] < \infty$. Let

$$\bar{X} = \frac{1}{n} (X_1 + \dots + X_n)$$

$$\bar{X} \rightarrow \mu \quad \text{as } n \rightarrow \infty$$

Central Limit Theorem

Suppose X_1, \dots, X_n are iid with $\mathbb{E}[X_i] = \mu$ and $\text{var}[X_i] = \sigma^2$

Let $\bar{X} = \frac{1}{n}(X_1 + \dots + X_n)$. Then

$$\sqrt{n} \left(\frac{\bar{X} - \mu}{\sigma} \right) \rightarrow N(0,1) \text{ is distribution as } n \rightarrow \infty$$

Normal Distribution Approximation accuracy depends on

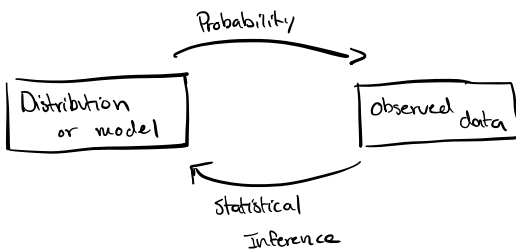
- i) Sample size
- ii) Skewness
- iii) Heaviness of tails

Continuous Mapping Theorem

Let $g(x)$ be a continuous function of x . As $n \rightarrow \infty$

- i) If $S_n \rightarrow z$ in distribution, then $g(S_n) \rightarrow g(z)$ in dist
- ii) Analogous for probability

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Einstein's Theory of Brownian Motion

Suppose the particle is at position $P_t \in \mathbb{R}^2$ at time t . Then at time $t + \Delta t$, the position $P_{t+\Delta t}$ is random and has a bivariate normal distribution around P_t

$$P_{t+\Delta t} - P_t \sim N\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \sigma^2 & 0 \\ 0 & \sigma^2 \end{pmatrix}\right)$$

$$\sigma^2 = \frac{RT}{3\pi\eta r N_A} (\Delta t) \quad \leftarrow \text{how tf he derive this}$$

Hypothesis test is a binary question about the distribution of the data

Accept/reject null hypothesis H_0 in favor of alternative hypothesis H_1

For the magicians die. Null hypothesis: die is fair

$$H_0: (X_1, \dots, X_6) \sim \text{Multinomial}(n, (1/6, \dots, 1/6))$$

$$H_1: (X_1, \dots, X_6) \sim \text{Multinomial}(n, (P_1, \dots, P_6))$$

$$P_1, \dots, P_6 \neq (1/6, \dots, 1/6)$$

Setting up notation for brownian motion experiment

$$(X_1, Y_1) = P_1 - P_0$$

$$(X_2, Y_2) = P_2 - P_1$$

⋮

$$(X_n, Y_n) = P_n - P_{n-1}$$

displacements
are measured every 30 sec

$$H_0: (X_1, Y_1) \dots (X_n, Y_n) \overset{iid}{\sim} \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 2.23e-7 & 0 \\ 0 & 2.23e-7 \end{pmatrix}\right) \leftarrow \text{Einstein's Theory}$$

$$H_1: (X_1, Y_1) \dots (X_n, Y_n) \overset{iid}{\sim} \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \sigma^2 & 0 \\ 0 & \sigma^2 \end{pmatrix}\right) \leftarrow \text{Variance is wrong}$$

Many other possibilities

Neyman Pearson Paradigm

Hypothesis testing is a binary test

Does that provide sufficiently strong evidence to reject H_0 , in favor of H_1 ?

Default assumption is that H_0 is true

A test statistic T is a statistic computed from data that provides evidence against H_0 when extreme values

- 1) How can we design a test statistic
- 2) How can you use it?

1) How can we design a test statistic?

For the brownian motion example:

$$\bar{R} = \frac{1}{n} (R_1 + R_2 + \dots + R_n) \quad R_i = X_i^2 + Y_i^2 \quad \text{average distance in 30 sec interval}$$

$$\mathbb{E}(\bar{R}) = \mathbb{E}(R_i) = \mathbb{E}(X_i^2) + \mathbb{E}(Y_i^2) = 4.46e-7$$

Extreme values of \bar{R} reject null hypothesis

Can also compare against $(2.23e-7) X_2^2$

Plot expected distribution against histogram

Hanging histogram plots $O_i - E_i$ for each histogram bin where O_i is the observed count in bin i and E_i is the theoretical expected count

$$\text{Test statistic } T = \sum_i (O_i - E_i)^2$$

Large T indicates rejection of null hypothesis

You can stabilize the variance by plotting $\frac{O_i - E_i}{\sqrt{E_i}} = \frac{O_i - E_i}{\sqrt{np_i}}$ so $\mathbb{E}\left[\left(\frac{O_i - E_i}{\sqrt{np_i}}\right)^2\right] = 1$

called hanging chi-gram

$T = \sum_i \frac{(O_i - E_i)^2}{E_i}$ is the Pearson chi-squared statistic for goodness of fit

Another alternative is to consider $\sqrt{O_i} - \sqrt{E_i}$

$$\sqrt{O_i} - \sqrt{E_i} \approx \frac{O_i - E_i}{2\sqrt{E_i}} \text{ via Taylor expansion}$$

Tukey's hanging histogram

QQ plot

plots sorted values R_1, \dots, R_n against $\frac{1}{n}, \frac{2}{n}, \dots, \frac{n}{n}$ quantiles of their hypothesized distribution

Values deviating from $y=x$ provide evidence against hypothesized distribution

Let $R_{(1)} < \dots < R_{(n)}$ be the sorted values of R_1, \dots, R_n . The maximum vertical deviation is

$$T = \max_{i=1}^n \left| R_{(i)} - F^{-1}\left(\frac{i}{n}\right) \right|$$

F^{-1} is the quantile function ← inverse cdf

more deviation is higher quantiles (not as squashed together)

Stabilize Quantile Spacing

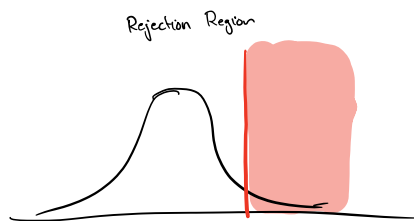
$$T = \max_{i=1}^n \left| F(R_{(i)}) - \frac{i}{n} \right|$$

Kolmogorov-Smirnov Statistic

2) What values of T would allow us to reject H_0 ?

Null distribution of T is the distribution of T under the assumption the null hypothesis is true

We divide space of possible T values into acceptance and rejection regions



Type I Error: probability that we reject H_0 when H_0 is true

In Neyman Pearson paradigm, we choose rejection error s.t.

$$\text{Type I error} \leq \alpha$$

for a specified significance level $\alpha \in (0,1)$

Generally don't want to specify a significance level

p-value is the smallest significance level that we would reject H_0

probability that the null distribution assigns values $\geq t_{obs}$ ← specifically for large T

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Recap:

H_0 : Null hypothesis

H_1 : Alternative hypothesis

① Designing a good test statistic

② Choosing rejection region

Type I error: $P_{H_0}[\text{reject } H_0] \leq \alpha$ ← significance level

What is the best choice of test statistic?

Simple hypothesis

Def: A hypothesis is simple if it completely specifies its distribution
no unknown parameters

Neyman Pearson Lemma

Simple H_0 vs. simple H_1

Def: The type II error for a simple alternative hypothesis H_1 is

$$B = P_{H_1}[\text{accept } H_0]$$

Power of the test is $1-B$

$$1-B = P_{H_1}[\text{reject } H_0]$$

Goal of hypothesis testing is to maximize power against H_1 while constraining type I error $\leq \alpha$

Example: Consider $X \in \{1, 2, 3, 4, 5\}$ Two hypotheses

X	1	2	3	4	5
$f_0(x)$	0.2	0.2	0.2	0.2	0.2
$f_1(x)$	0	0.1	0.2	0.3	0.4

Let's say we want a test w/ significance level $\alpha = 0.4$

A hypothesis is defined by a rejection region $R \in \{1, 2, 3, 4, 5\}$

If $x \in R$: Reject H_0

If $x \notin R$: Accept H_0

Type I Error: $P_{H_0}[X \in R]$

Power = $P_{H_1}[X \in R]$. To minimize power, set $R = \{4, 5\}$. Then power is 0.7

More generally: Suppose the data is

$$X = (X_1, \dots, X_n)$$

Takes values $x = (x_1, \dots, x_n) \in X$ is finite

H_0 : X has joint pmf $f_0(x)$

H_1 : X has joint pmf $f_1(x)$

To define a test, we need to define a region $R \subseteq X$

If $x \in R$: Reject H_0

If $x \notin R$: Accept H_0

Want to find points of high f_1 and low f_0

Intuition: R should contain points x that have the smallest values of

$$L(x) = \frac{f_0(x)}{f_1(x)} \leftarrow \text{increase in Type I error per unit increase in power}$$

$L(x)$ is the likelihood ratio. Test rejects H_0 for small $L(x)$ is the likelihood ratio test

Analogous for continuous distributions

Neyman-Pearson Lemma: Let H_0 and H_1 be simple hypotheses. The significance level $\alpha \in (0, 1)$. Suppose there is $c > 0$ s.t. the likelihood ratio test

rejects H_0 when $L(x) < c$

accepts H_1 when $L(x) \geq c$

has type I error of exactly α . Then for any other test of type I error $\leq \alpha$, its power is at most the power of LRT.

Proof: Consider the discrete case. Let $R = \{x: L(x) < c\}$ be the rejection region of LRT.

Then R maximizes

$$\sum_{x \in R} (c f_1(x) - f_0(x)) \text{ among all subsets of } X$$

b/c if $x \in R$ then $\frac{f_0(x)}{f_1(x)} < c$ so $c f_1(x) - f_0(x) > 0$

if $x \notin R$ then $\frac{f_0(x)}{f_1(x)} \geq c$ so $c f_1 - f_0 \leq 0$

Consider another test w/ rejection region R' .

$$\sum_{X \in R} c f_1(x) - f_0(x) \geq \sum_{X \in R'} c f_1(x) - f_0(x)$$

$$\Rightarrow c \left(\underbrace{\sum_{X \in R} f_1(x)}_{\text{power of LRT}} - \underbrace{\sum_{X \in R'} f_1(x)}_{\text{power of other test}} \right) \geq \underbrace{\sum_{X \in R} f_0(x)}_{\text{type I error of LRT}} - \underbrace{\sum_{X \in R'} f_0(x)}_{\text{type I error of other test}}$$

$$\geq 0$$

power of LRT \geq power of other test

Examples:

X_1, \dots, X_n are normal

$$H_0: X_1, \dots, X_n \stackrel{iid}{\sim} N(0,1)$$

$$H_1: X_1, \dots, X_n \stackrel{iid}{\sim} N(\mu,1)$$

for some fixed $\mu > 0$.

Let's apply N-P lemma

$$f_0(x) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi}} e^{-\frac{x_i^2}{2}} = \left(\frac{1}{\sqrt{2\pi}}\right)^n e^{-\left(\frac{x_1^2}{2} + \dots + \frac{x_n^2}{2}\right)}$$

$$f_1(x) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi}} e^{-\frac{(x_i - \mu)^2}{2}} = \left(\frac{1}{\sqrt{2\pi}}\right)^n e^{-\left(\frac{(x_1 - \mu)^2}{2} + \dots + \frac{(x_n - \mu)^2}{2}\right)}$$

$$L(x) = \frac{f_0(x)}{f_1(x)} = \frac{e^{-\left(\frac{x_1^2}{2} + \dots + \frac{x_n^2}{2}\right)}}{e^{-\left(\frac{(x_1 - \mu)^2}{2} + \dots + \frac{(x_n - \mu)^2}{2}\right)}} = e^{-\left(\frac{x_1^2}{2} + \dots + \frac{x_n^2}{2}\right) + \left(\frac{(x_1 - \mu)^2}{2} + \dots + \frac{(x_n - \mu)^2}{2}\right)}$$

$$= e^{\frac{n\mu^2}{2} - \mu(x_1 + \dots + x_n)}$$

By the N-P lemma: Want to pick $c > 0$ s.t.

$$\mathbb{P}_{H_0}[L(X) < c] = \alpha$$

↖ type I error

Then LRT which

rejects the null hypothesis when $L(X) < c$

accepts the null hypothesis when $L(X) \geq c$

is the most powerful test

Two observations:

$$L(x) = e^{\frac{n\mu^2}{2} - \mu(x_1 + \dots + x_n)} =: f(\bar{x})$$

$$\text{where } \bar{x} = \frac{(x_1 + \dots + x_n)}{n} \text{ and } f(x) = e^{\frac{n\mu^2}{2} - n\mu x}$$

This function is decreasing in y

$$\text{so } L(x) = f(\bar{x}) < c \Leftrightarrow \bar{x} > f^{-1}(c)$$

we want to pick $f^{-1}(c)$ s.t.

$$\mathbb{P}_{H_0}[\bar{X} > f^{-1}(c)] = \alpha$$

but we know under the null the $X_1, \dots, X_n \stackrel{iid}{\sim} N(0,1)$, $\bar{X} \sim N(0, 1/n)$. So $f^{-1}(c)$ should be the $(1-\alpha)^{\text{th}}$ quantile

of $N(0, 1/n)$. i.e. $\frac{1}{\sqrt{n}} z(\alpha)$ where $z(\alpha)$ is the upper portion of $N(0,1)$

So the most powerful test is:

$$\text{Reject } H_0 \text{ if } \bar{X} > \frac{1}{\sqrt{n}} Z(\alpha)$$

$$\text{Accept } H_0 \text{ if } \bar{X} \leq \frac{1}{\sqrt{n}} Z(\alpha)$$

(2) No dependence of n . The most powerful test is this same test for every $n > 0$

Lecture 7 (2/14/22)

Recap: Test $H_0 \sim f_0$

$$H_1 \sim f_1$$

most powerful test is to:

$$\text{Compute likelihood: } L(x) = \frac{f_0(x)}{f_1(x)}$$

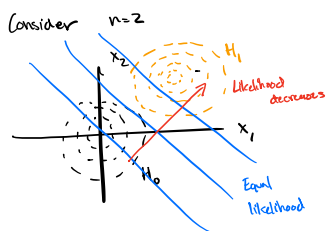
Pick a number $c > 0$ s.t. $P_{H_0}[L(x) < c] = \alpha$

Reject H_0 when $L(x) < c$, accept H_0 when $L(x) \geq c$

Example:

$$H_0: X_1, \dots, X_n \stackrel{iid}{\sim} N(0, 1)$$

$$H_1: X_1, \dots, X_n \stackrel{iid}{\sim} N(\mu, 1) \quad \mu > 0 \text{ fixed and known}$$



Most powerful test is equivalent to

$$\text{Compute } \bar{X} = \frac{X_1 + \dots + X_n}{n}$$

Pick $c \in \mathbb{R}$ s.t. $P_{H_0}[\bar{X} > c] = \alpha$

$$c = \frac{1}{\sqrt{n}} Z(\alpha)$$

Reject H_0 if $\bar{X} > c$, accept H_0 if $\bar{X} \leq c$

$$\text{EX: } H_0: X_1, \dots, X_n \stackrel{iid}{\sim} \text{Bernoulli}(1/2)$$

$$H_1: X_1, \dots, X_n \stackrel{iid}{\sim} \text{Bernoulli}(p)$$

$$L(x) = \frac{f_0(x)}{f_1(x)} = \left(\frac{1}{2(1-p)}\right)^n \cdot \left(\frac{1-p}{p}\right)^{x_1 + \dots + x_n}$$

Observation: $L(x)$ only depends on X_1, \dots, X_n via their sum

For $p > 1/2$ $\frac{1-p}{p} < 1$. So $L(x)$ is decreasing in $X_1 + \dots + X_n$

Likelihood procedure is equivalently:

- Compute $S = X_1 + \dots + X_n$
- Under H_0 $S \sim \text{Binomial}(n, 1/2)$
- pick c as the upper α point $b_n(\alpha)$ of binomial $(n, 1/2)$
- Reject H_0 when $S > c$, accept when $S \leq c$

Composite Hypothesis and pivotal statistic

A hypothesis (either H_0 or H_1) that is not simple is composite

EX. Let $n=250$ be the number of students in STAT 242

Does 242 improve student knowledge of statistics?

Suppose each student takes

- diagnostic exam at start
- final exam at end

Let X_i be the difference (final - diagnostic) for student i .

Two formulations:

$$H_0: X_1, \dots, X_n \stackrel{iid}{\sim} \mathcal{N}(0, \sigma^2)$$

$$H_1: X_1, \dots, X_n \stackrel{iid}{\sim} \mathcal{N}(\mu, \sigma^2) \quad \text{for some } \mu, \sigma^2 > 0$$

Both H_0 and H_1 are composite

$H_0: X_1, \dots, X_n$ are iid from some pdf f w/ median 0

$H_1: X_1, \dots, X_n$ are iid from some pdf f w/ median > 0

Both H_0 and H_1 are composite

When testing composite null H_0 :

• We want to ensure probability of Type I error is $\leq \alpha$ for every possible data distribution described H_0

• Simplify design of the test by picking test statistic T whose distribution is the same under every distribution in H_0

↑ pivotal or distribution free test statistic

When testing composite Alternative H_1 :

- Oftentimes no single test that maximizes power against all possible Alternatives
- We often design a test to balance the power against different alternatives

One-sample t-test

Setup: $X_1, \dots, X_n \stackrel{iid}{\sim} \mathcal{N}(\mu, \sigma^2)$ where both μ, σ^2 are unknown

$$H_0: \mu = 0 \quad H_1: \mu > 0$$

Q: What if σ^2 is known

In this case, we can first standardize our data: $Z_i = \frac{X_i}{\sigma}$

Then $Z_i \sim \mathcal{N}(\frac{\mu}{\sigma}, 1)$. The above is equivalent to testing $H_0: \frac{\mu}{\sigma} = 0$ vs. $H_1: \frac{\mu}{\sigma} > 0$ based on Z_1, \dots, Z_n

The Neyman Pearson Lemma implies Most powerful level- α test is to reject if $\bar{Z} = \frac{\bar{X}}{\sigma} > \frac{1}{\sqrt{n}} z(\alpha)$

Idea: If sigma is unknown, let's estimate it from the data

$$\text{Let } S^2 = \frac{1}{n-1} \left[(X_1 - \bar{X})^2 + \dots + (X_n - \bar{X})^2 \right]$$

Use instead

$$T = \frac{\sqrt{n} \bar{X}}{S} \quad \leftarrow \text{One sample t-statistic}$$

Pivotal statistic!

Thm: Let $X_1, \dots, X_n \stackrel{iid}{\sim} \mathcal{N}(\mu, \sigma^2)$. Let \bar{X} and S^2 be the sample mean and variance. Then

1) S^2 is independent of \bar{X}

2) $S^2 \sim \frac{\sigma^2}{n-1} \cdot \chi^2_{n-1}$

Proof: WLOG $\mu = 0$

1) It suffices to show \bar{X} is independent of $(X_1 - \bar{X}, \dots, X_n - \bar{X})$

↳ S_n is a simple function of $(X_1 - \bar{X}, \dots, X_n - \bar{X})$

$(\bar{X}, X_1 - \bar{X}, \dots, X_n - \bar{X})$ are all linear combinations of $X_1, \dots, X_n \stackrel{i.i.d.}{\sim} N(\mu, \sigma^2)$

$\Rightarrow (\bar{X}, X_1 - \bar{X}, \dots, X_n - \bar{X})$ is multivariate

So to show \bar{X} is independent of $(X_1 - \bar{X}, \dots, X_n - \bar{X})$ its enough $\text{Cov}[\bar{X}, X_i - \bar{X}] = 0$

We have:

$$\text{Cov}[\bar{X}, X_i] = \text{Cov}\left[\frac{1}{n} \sum_{j=1}^n X_j, X_i\right] = \frac{1}{n} \sum_{j=1}^n \underbrace{\text{Cov}[X_j, X_i]}_{=0 \text{ for } i \neq j} = \frac{1}{n} \text{Cov}[X_i, X_i] = \frac{1}{n} \text{Var}[X_i] = \frac{\sigma^2}{n}$$

$$\text{Cov}[\bar{X}, X_i] = \text{Var}[\bar{X}] = \frac{\sigma^2}{n}$$

$$\Rightarrow \text{Cov}[\bar{X}, X_i - \bar{X}] = \frac{\sigma^2}{n} - \frac{\sigma^2}{n} = 0 \text{ so } \bar{X} \text{ and } S^2 \text{ are independent}$$

2) For the distribution of S^2 , write $Z_i = \frac{X_i}{\sigma} \sim N(0,1)$

$$S^2 = \frac{1}{n-1} \left[(X_1 - \bar{X})^2 + \dots + (X_n - \bar{X})^2 \right]$$

$$\Rightarrow \frac{(n-1)}{\sigma^2} S^2 = (Z_1 - \bar{Z})^2 + \dots + (Z_n - \bar{Z})^2$$

$$= (Z_1^2 - 2Z_1\bar{Z} + \bar{Z}^2) + \dots + (Z_n^2 - 2Z_n\bar{Z} + \bar{Z}^2)$$

$$= (Z_1^2 + \dots + Z_n^2) - 2\bar{Z}(Z_1 + \dots + Z_n) + n\bar{Z}^2$$

$$= \underbrace{(Z_1^2 + \dots + Z_n^2)}_W - \underbrace{(\sqrt{n}\bar{Z})^2}_V$$

This shows that $W = U + V$

we know \bar{X} is independent of S^2

so V is independent of U

Here: $W \sim \chi_n^2$, $V \sim \chi_1^2$, b/c $\sqrt{n}\bar{Z} \sim N(0,1)$

$$\Rightarrow U \sim \chi_{n-1}^2$$

$$\text{Thus, } \frac{(n-1)}{\sigma^2} S^2 \sim \chi_{n-1}^2 \Rightarrow S^2 \sim \frac{\sigma^2}{n-1} \cdot \chi_{n-1}^2$$

$$\text{Returning to } T = \frac{\sqrt{n}\bar{X}}{S} = \frac{\sqrt{n} \bar{X}/\sigma}{S/\sigma}$$

• Under H_0 , $\frac{\sqrt{n}\bar{X}}{\sigma} \sim N(0,1)$ b/c $X_i \sim N(0, \sigma^2)$

• $\frac{S^2}{\sigma^2} \sim \frac{1}{n-1} \chi_{n-1}^2$

• And $\frac{\sqrt{n}\bar{X}}{\sigma}$ is independent of S/σ

Def: If $Z \sim N(0,1)$, $U \sim \chi_{n-1}^2$ and Z and U are independent, then the distribution of $\frac{Z}{\sqrt{\frac{1}{n}U}}$ is called the t -distribution

w/ n degrees of freedom

Remark: The preceding theorem explains why we use $\frac{1}{n-1}$ to define S^2 :

$$\mathbb{E}[S^2] = \mathbb{E}\left[\frac{\sigma^2}{n-1} \chi_{n-1}^2\right], \text{ hence } \mathbb{E}[\chi_{n-1}^2] = n-1 \text{ so } \mathbb{E}[S^2] = \sigma^2 \text{ so } S^2 \text{ is unbiased for } \sigma^2$$

Lecture 8 (2/16/22)

Recap: Data X_1, \dots, X_n iid samples. Test whether distribution of X_i 's is "centered around 0"

Formulation in Normal Setting:

$$H_0: X_1, \dots, X_n \stackrel{iid}{\sim} N(0, \sigma^2)$$

$$H_1: X_1, \dots, X_n \stackrel{iid}{\sim} N(\mu, \sigma^2), \mu > 0$$

One-sample t -statistic

$$T = \frac{\sqrt{n} \bar{X}}{S} \text{ where } \bar{X} \text{ is the average and } S^2 = \frac{1}{n-1} \left((X_1 - \bar{X})^2 + \dots + (X_n - \bar{X})^2 \right)$$

What is distribution of t under H_0 ?

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

$$\cdot \frac{S^2}{\sigma^2} \sim \frac{1}{n-1} \chi_{n-1}^2$$

• These two statistics are independent

So $T \sim t_{n-1}$, the t -distribution with $n-1$ degrees of freedom

T -test: Reject H_0 when $T > t_{n-1}$

Formulation in a non-parametric: $X_1, \dots, X_n \stackrel{iid}{\sim} f$

H_0 : Median of distribution is 0

H_1 : Median is greater than 0

Consider the sign statistic $S = \sum_{i=1}^n \mathbb{1}_{\{X_i > 0\}}$ ↖ Indicator

$$\mathbb{1}_{\{X_i > 0\}} = \begin{cases} 1 & \text{if } X_i > 0 \\ 0 & \text{if } X_i \leq 0 \end{cases}$$

Under the distribution f described by H_0 , $S \sim \text{Binomial}(n, 1/2)$

Let $b_n(\alpha)$ be upper α point of binomial $(n, 1/2)$. Then the test that rejects for $S > b_n(\alpha)$ is the sign test

Remark: For large n we can approximate this test via a normal approximation

$$\cdot \text{By the CLT: } \frac{S - \frac{n}{2}}{\sqrt{\frac{n}{4}}} \cdot \sqrt{n} \rightarrow N(0,1)$$

$$\frac{S}{n} - \frac{1}{2} \approx N\left(0, \frac{1}{4n}\right) \Rightarrow S \approx N\left(\frac{n}{2}, \frac{n}{4}\right)$$

• The $b_n(\alpha) \approx$ upper alpha point of $N(n/2, n/4)$

$$= \frac{n}{2} + \sqrt{\frac{n}{4}} \cdot z(\alpha)$$

↖ upper alpha point

Approximate sign test by rejecting H_0

$$S > \frac{n}{2} + \sqrt{\frac{n}{4}} z(\alpha) \iff \sqrt{4n} \left(\frac{S}{n} - \frac{1}{2} \right) > z(\alpha)$$

The type I error is not exactly α but under H_0

$$P[\text{Reject } H_0] \xrightarrow{n \rightarrow \infty} P[\mathcal{N}(0,1) > z(\alpha)] = \alpha$$

type I error approaches α

Two-sample Tests

Ex. X_1, \dots, X_n are differences in exam scores for $n = 250$ students

Q: What if the exams are not equally difficult?

A: Take a separate group of $m = 100$ students not in S&DS 242

Let Y_1, \dots, Y_m be the differences in scores

Informally, test whether the distribution of X_i 's is larger than the Y_i 's

Normal Model Function:

$$\begin{aligned} \text{Suppose } X_1, \dots, X_n &\stackrel{iid}{\sim} \mathcal{N}(\mu_x, \sigma^2) \\ Y_1, \dots, Y_m &\stackrel{iid}{\sim} \mathcal{N}(\mu_y, \sigma^2) \end{aligned}$$

$$H_0: \mu_x = \mu_y$$

$$H_1: \mu_x > \mu_y$$

More non-parametric formulation

$$\text{Suppose } X_1, \dots, X_n \stackrel{iid}{\sim} f, Y_1, \dots, Y_m \stackrel{iid}{\sim} g$$

$$H_0: f = g$$

$$H_1: f \text{ stochastically dominates } g$$

↑ If $x \sim f$ and $y \sim g$ then for any $x \in \mathbb{R}$ $P[X \geq x] \geq P[Y \geq x]$

Two-sample t-test

Intuition: Look at difference of sample means $\bar{X} - \bar{Y}$

Reject $H_0: \mu_x = \mu_y$ in favor $H_1: \mu_x > \mu_y$

if $\bar{X} - \bar{Y}$ is "large enough"

What is the null distribution of $\bar{X} - \bar{Y}$

$$\bar{X} = \frac{X_1 + \dots + X_n}{n} \sim \mathcal{N}\left(\mu_x, \frac{\sigma^2}{n}\right)$$

$$\bar{Y} = \frac{Y_1 + \dots + Y_m}{m} \sim \mathcal{N}\left(\mu_y, \frac{\sigma^2}{m}\right)$$

$$\bar{X} - \bar{Y} \sim \mathcal{N}\left(\mu_x - \mu_y, \frac{\sigma^2}{n} + \frac{\sigma^2}{m}\right)$$

Under $H_0: \mu_x = \mu_y$

$$\bar{X} - \bar{Y} \sim \mathcal{N}\left(0, \sigma^2 \left(\frac{1}{n} + \frac{1}{m}\right)\right)$$

$$\frac{\bar{X} - \bar{Y}}{\sigma \sqrt{\frac{1}{n} + \frac{1}{m}}} \sim \mathcal{N}(0,1)$$

If σ^2 were known, then reject H_0 if $\frac{\bar{X} - \bar{Y}}{\sigma \sqrt{\frac{1}{n} + \frac{1}{m}}} > z(\alpha)$

When σ^2 is unknown, estimate σ^2 from the data

$$s_{\text{pooled}}^2 = \frac{1}{m+n-2} \left(\sum_{i=1}^n (X_i - \bar{X})^2 + \sum_{j=1}^m (Y_j - \bar{Y})^2 \right)$$

Test statistic

$$T = \frac{\bar{X} - \bar{Y}}{\text{Spooled} \sqrt{\frac{1}{n} + \frac{1}{m}}} \leftarrow \text{pooled two-sample } t\text{-statistic}$$

Statistic is pivotal under H_0 : Let $\mu = \mu_x = \mu_y$

Write $X_i = \mu + \sigma Z_i$ where Z_i 's and W_j 's are now $N(0,1)$

$$Y_j = \mu + \sigma W_j$$

Substituting into T: μ cancels from $\bar{X} - \bar{Y}$
 σ cancels from $\frac{(\bar{X} - \bar{Y})}{\text{Spooled}}$

What is the distribution of T?

$$\left. \begin{aligned} \frac{\bar{X}}{\sigma} &\sim N\left(\frac{\mu}{\sigma}, \frac{1}{n}\right) \\ \frac{\bar{Y}}{\sigma} &\sim N\left(\frac{\mu}{\sigma}, \frac{1}{m}\right) \end{aligned} \right\} \frac{\bar{X} - \bar{Y}}{\sigma} \sim N\left(0, \frac{1}{n} + \frac{1}{m}\right)$$

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

$$\frac{1}{\sigma^2} \sum_{j=1}^m (Y_j - \bar{Y})^2 \sim \chi_{m-1}^2$$

$$\Rightarrow \frac{\text{Spooled}^2}{\sigma^2} = \frac{1}{m+n-2} \left(\frac{1}{\sigma^2} \sum_{i=1}^n (X_i - \bar{X})^2 + \frac{1}{\sigma^2} \sum_{j=1}^m (Y_j - \bar{Y})^2 \right)$$

$$\sim \frac{1}{m+n-2} \cdot \chi_{m+n-2}^2$$

This implies $E[\text{Spooled}^2] = \sigma^2$, so this is unbiased

$$\text{So } T = \frac{\bar{X} - \bar{Y}}{\text{Spooled} \sqrt{\frac{1}{n} + \frac{1}{m}}} = \frac{\frac{1}{\sigma \sqrt{\frac{1}{n} + \frac{1}{m}}} (\bar{X} - \bar{Y})}{\text{Spooled} / \sigma} = \frac{N(0,1)}{\sqrt{\frac{1}{m+n-2} \chi_{m+n-2}^2}}$$

$\sim t_{m+n-2}$, the t-distribution w/ $m+n-2$ degrees of freedom

The two sampled t-test rejects $H_0 = \mu_x = \mu_y$ in favor of $H_1: \mu_x > \mu_y$ when $T > t_{m+n-2}(\alpha)$

Remark: Assumed X_i and Y_j have the same variance

It's common to see applications where variances are not identical

$$\text{Suppose } X_1, \dots, X_n \stackrel{iid}{\sim} N(\mu_x, \sigma_x^2)$$

$$Y_1, \dots, Y_m \stackrel{iid}{\sim} N(\mu_y, \sigma_y^2)$$

Test $H_0: \mu_x = \mu_y$ vs. $H_1: \mu_x > \mu_y$

Idea: Look at $\bar{X} - \bar{Y}$. Under H_0 :

$$\bar{X} - \bar{Y} \sim N\left(0, \frac{\sigma_x^2}{n} + \frac{\sigma_y^2}{m}\right)$$

$$\text{Estimate } \sigma_x^2 \text{ by sample var. } S_x^2 = \frac{1}{n-1} \sum_{i=1}^n (X_i - \bar{X})^2$$

$$\sigma_y^2 \dots S_y^2$$

Define $T_{\text{Welch}} = \frac{\bar{X} - \bar{Y}}{\sqrt{\frac{1}{n} S_x^2 + \frac{1}{m} S_y^2}} \leftarrow \text{Not exactly pivotal under } H_0 \text{ and not exactly t-distributed}$

Mann-Whitney-Wilcoxon Rank-Sum Test

$$X_1 \dots X_n \stackrel{iid}{\sim} f \quad \text{and} \quad Y_1 \dots Y_m \stackrel{iid}{\sim} g$$

Test $H_0: f=g$ vs. $H_1: f$ stochastically dominates g

The M-W-W rank-sum statistic T is defined as:

① Pool all X_i 's and Y_j 's and rank them

Let smallest have rank 1

Largest have rank $m+n$

② Define T as the sum of ranks of only the Y_j 's

Lecture 9 (2/21/22) - Permutation Tests

$$X_1 \dots X_n \stackrel{iid}{\sim} f \quad Y_1 \dots Y_m \stackrel{iid}{\sim} g$$

$H_0: f=g$ vs. $H_1: f$ stochastically dominates g

↑ one-sided alternative
two-sided: $f \neq g$

Mann-Whitney-Wilcoxon Rank Sum

① Pool together $X_1 \dots X_n, Y_1 \dots Y_m$ and rank them smallest to largest

② $T = \text{sum of ranks } Y_1 \dots Y_m$

Under $H_0, X_1 \dots X_n, Y_1 \dots Y_m$ are all iid

By symmetry, equally likely for $Y_1 \dots Y_m$ to be any set of m ranks among $\{1, 2, \dots, m+n\}$

Then: Under $H_0: f=g$

$$a) \quad \mathbb{E}[T] = \frac{m(m+n+1)}{2} \quad \text{and} \quad \text{Var}[T] = \frac{mn(m+n+1)}{12}$$

$$b) \quad \frac{T - \mathbb{E}[T]}{\sqrt{\text{Var}[T]}} \rightarrow \mathcal{N}(0,1) \text{ in distribution as } n, m \rightarrow \infty$$

Proof of part a

Let $N = m+n$. Define

$$I_k = \begin{cases} 1 & \text{rank } k \text{ observation is a } Y \\ 0 & \text{rank } k \text{ observation is a } X \end{cases}$$

$$T = \sum_{k=1}^N k I_k$$

Have the values k when $I_k=1$ is a simple random sample from $\{1, \dots, N\}$ under H_0

$$\mathbb{E}[I_k] = \mathbb{P}[I_k=1] = \frac{m}{N}$$

$$\mathbb{E}[T] = \sum_{k=1}^N k \cdot \mathbb{E}[I_k] = \sum_{k=1}^N k \cdot \frac{m}{N} = \frac{N(N+1)}{2} \cdot \frac{m}{N} = \frac{m(m+n+1)}{2}$$

$$\text{Var}[T] = \mathbb{E}[T^2] - (\mathbb{E}[T])^2$$

$$\mathbb{E}[T^2] = \mathbb{E}\left[\left(\sum_{k=1}^N k I_k\right)\left(\sum_{j=1}^N j I_j\right)\right]$$

$$= \sum_{k=1}^N j k \mathbb{E}[I_k] \mathbb{E}[I_j]$$

$$= \sum_{k=1}^N k^2 \underbrace{\mathbb{E}[I_k^2]}_{\frac{m}{N}} + 2 \sum_{j \neq k} j k \underbrace{\mathbb{E}[I_k I_j]}_{\frac{m}{N} \cdot \frac{m-1}{N-1}}$$

$$\text{Apply: } \sum_{k=1}^N k^2 = \frac{N(N+1)(2N+1)}{6}$$

$$\begin{aligned} 2 \sum_{j \neq k} jk &= \left(\sum_{k=1}^N k \right)^2 - \sum_{k=1}^N k^2 \\ &= \left(\frac{N(N+1)}{2} \right)^2 - \frac{N(N+1)(2N+1)}{6} \end{aligned}$$

$$\Rightarrow \mathbb{E}[T^2] = \frac{m}{N} \cdot \frac{N(N+1)(2N+1)}{6} + \frac{m}{N} \cdot \frac{m-1}{N-1} \left[\left(\frac{N(N+1)}{2} \right)^2 - \frac{N(N+1)(2N+1)}{6} \right]$$

$$\begin{aligned} \text{Var}[T] &= \mathbb{E}[T^2] - \mathbb{E}[T]^2 \\ &= \frac{mn(m+n+1)}{12} \end{aligned}$$

To perform an asymptotic test

$$\text{For large } n, m \text{ distribution of } T \text{ is } \approx \mathcal{N}\left(\frac{m(m+n)}{2}, \frac{mn(m+n+1)}{12}\right)$$

To test against $H_1: f$ stochastically dominates g

The T takes smaller value under H_1

$$\text{Reject } H_0 \text{ when } T < \frac{m(m+n)}{2} - \sqrt{\frac{mn(m+n+1)}{12}} \cdot z(\alpha)$$

To test against $H_1: f \neq g$

$$\text{Reject when } \left| T - \frac{m(m+n)}{2} \right| > \sqrt{\frac{mn(m+n+1)}{12}} \cdot z\left(\frac{\alpha}{2}\right)$$

Permutation Tests

$$X_1, \dots, X_n \stackrel{iid}{\sim} f, Y_1, \dots, Y_m \sim g$$

$$\text{Test } H_0: f=g \text{ vs. } H_1: f \neq g$$

Symmetry Underlying rank-sum test

$$\text{Pool all observations as } \{Z_1, \dots, Z_{m+n}\}$$

(ignoring their ordering)

Given these pooled values $\{Z_1, \dots, Z_{m+n}\}$ under H_0 , it's equally likely for $X_1, \dots, X_n, Y_1, \dots, Y_m$ to be any permutation of these values

Idea: For any test statistic $T(X_1, \dots, X_n, Y_1, \dots, Y_m)$

The permutation null distribution of T is its distribution upon:

1) Take a random permutation $X_1^* \dots X_n^*, Y_1^* \dots Y_m^*$

2) Compute $T(X_1^*, \dots, X_n^*, Y_1^*, \dots, Y_m^*)$

↑ uniform distribution on all $(m+n)!$ possible possibilities

Can approximate this by simulation:

- Sample B uniformly random permutations
- Look at T distribution of the B values

A test of H_0 using T and this permutation null distribution is a permutation test

Permutation test is a conditional test

pivotal on H_0 conditional on $\{Z_1, \dots, Z_{m+n}\}$

The test guarantees

$$\mathbb{P}_{H_0} [\text{reject } H_0 \mid \{Z_1, \dots, Z_{m+n}\}] \leq \alpha \text{ for any set of } \{Z_1, \dots, Z_{m+n}\}$$

This also holds unconditionally

$$\mathbb{P}_{H_0} [\text{reject } H_0] \leq \alpha$$

Example: Suppose X_1, \dots, X_n are objects and Y_1, \dots, Y_m are a second sample

Suppose we have definite distance $d(x, x')$ on X

Here are 3 different statistics

• Average Distance Statistic

$$T_1 = 2 \frac{1}{mn} \sum_{i=1}^n \sum_{j=1}^m d(x_i, y_j) - \frac{1}{\binom{n}{2}} \sum_{\substack{i=1 \\ j=1}}^n d(x_i, x_j) - \frac{1}{\binom{m}{2}} \sum_{\substack{j=1 \\ i=1}}^m d(y_i, y_j)$$

• k-nearest neighbors

How many of its k-nearest neighbors from its sample

$T_2 =$ avg across all samples

• Friedman - Rafeky minimum spanning tree statistics

• Constructing a minimum spanning tree from the pooled observations

• Remove edges connected X with Y

$T_3 =$ number of connected components

T_1, T_2, T_3 are not necessarily pivotal under H_0

Their full null distributions are complicated

Fisher's exact test

Randomly shuffle outcomes in table

Lecture 10 (2/23/22) - Effect size, power, and experimental design

Steps of a Scientific Study

1. Identify and formulate question of interest
2. Design experiment to answer this question
3. Visualize and explore collected data
4. Apply statistical procedure

Questions

- Predict in advance whether the study will succeed
- Predict size of study
- Why does experimental design influence our ability to ID this effect

Case Study: Stanford Peer Grading Experiment

Divide course into peer grading and control groups

Predict the power

Rejecting H_0 at desired level of significance

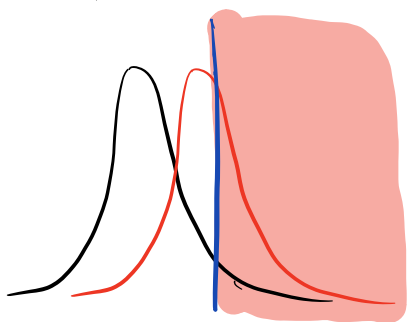
Power in the one-sample z-test

$$X_1, \dots, X_n \stackrel{iid}{\sim} N(\mu, \sigma^2)$$

$$H_0: \mu = 0 \text{ vs. } H_1: \mu > 0 \quad \text{assume } \sigma^2 \text{ is known}$$

Neyman-Pearson lemma tells us that the most powerful test rejects H_0 for large values of \bar{X} ← z test

$$\text{Null: } \bar{X} \sim N(0, \frac{\sigma^2}{n}) \quad \text{Alternative: } \bar{X} \sim N(\mu, \frac{\sigma^2}{n})$$



Analytically: z-test rejects H_0 when $\frac{\sqrt{n}}{\sigma} \bar{X} > z(\alpha)$

this ensures type I error = α

Under H_1 : $\bar{X} \sim N(\mu, \frac{\sigma^2}{n})$

$$\bar{X} = \mu + \frac{\sigma}{\sqrt{n}} z \quad \text{where } z \sim N(0,1)$$

$$\begin{aligned} \text{Power: } & \mathbb{P}_{H_1} \left[\frac{\sqrt{n}}{\sigma} \bar{X} > z(\alpha) \right] \\ &= \mathbb{P} \left[\frac{\sqrt{n}}{\sigma} \left(\mu + \frac{\sigma}{\sqrt{n}} z \right) > z(\alpha) \right] \\ &= \mathbb{P} \left[z > z(\alpha) - \sqrt{n} \frac{\mu}{\sigma} \right] \\ &= \Phi \left(\sqrt{n} \frac{\mu}{\sigma} - z(\alpha) \right) \end{aligned}$$

Power in comparing two samples

Consider $X_1, \dots, X_n \sim N(\mu_x, \sigma^2)$ $Y_1, \dots, Y_m \sim N(\mu_y, \sigma^2)$

$$H_0: \mu_x = \mu_y \quad H_1: \mu_x > \mu_y$$

pooled two-sample

$$T = \frac{\bar{X} - \bar{Y}}{\text{Spooled} \sqrt{\frac{1}{n} + \frac{1}{m}}}$$

$$\text{Power} = \mathbb{P}_{H_1} [T > t_{n+m-2}(\alpha)]$$

For large n, m

$$\approx \mathbb{P}_{H_1} \left[\frac{\bar{X} - \bar{Y}}{\sigma \sqrt{\frac{1}{n} + \frac{1}{m}}} > z(\alpha) \right]$$

Under H_1 : $\bar{X} - \bar{Y} \sim \mathcal{N}(\mu_X - \mu_Y, \sigma^2(\frac{1}{n} + \frac{1}{m}))$

$$\bar{X} - \bar{Y} = \mu_X - \mu_Y + \sigma \sqrt{\frac{1}{n} + \frac{1}{m}} \cdot Z \quad \text{where } Z \sim \mathcal{N}(0,1)$$

$$\text{Power} = \mathbb{P} \left[Z + \underbrace{\frac{1}{\sqrt{\frac{1}{n} + \frac{1}{m}}} \cdot \frac{\mu_X - \mu_Y}{\sigma}}_d > z(\alpha) \right] = \phi(d - z(\alpha))$$

Power is increasing in

$$d = \frac{1}{\sqrt{\frac{1}{n} + \frac{1}{m}}} \cdot \frac{\mu_X - \mu_Y}{\sigma} \Rightarrow \text{decreasing in } \frac{1}{n} + \frac{1}{m} \text{ so } \frac{1}{n} + \frac{1}{m} \text{ is minimized by}$$

$$n = m = \frac{N}{2}$$

Predicting typical p-value

$$\text{p-value} = \mathbb{P}_{H_0} [T > t_{\text{obs}}] \approx 1 - \phi(t_{\text{obs}})$$

Under H_1 ,

$$t_{\text{obs}} \approx \frac{\bar{X} - \bar{Y}}{\sigma \sqrt{\frac{1}{n} + \frac{1}{m}}} = z + \frac{1}{\sqrt{\frac{1}{n} + \frac{1}{m}}} \cdot \frac{\mu_X - \mu_Y}{\sigma}$$

median value of t_{obs} under H_1 is roughly d .

For $d=0.95$, this p-value is 0.17

Paired Design

split course into 2 units and swap groups between units

Consider paired differences

$$D_i = X_i - Y_i$$

If X_i, Y_i is bivariate normal then D_i has a normal distribution

$$\mathbb{E}(D_i) = \mu_X - \mu_Y$$

$$\text{Var}(D_i) = \text{Cov}(X_i - Y_i, X_i - Y_i) = 2\sigma^2(1-\rho)$$

Reduces problem to one-sample testing problem

Level α t-test

$$\frac{\sqrt{n}}{s} \bar{D} > t_{n-1}(\alpha)$$

$$s^2 = \frac{1}{n-1} \sum_{i=1}^n (D_i - \bar{D})^2 \text{ is sample variance}$$

Difference between paired and unpaired is a

$$\frac{1}{1-p} \text{ term}$$

$1-p$ is the relative efficiency of the unpaired design to the paired design

paired test with n pairs has the same power as an unpaired design with sample size $\frac{n}{1-p}$ per group

Confounding variables

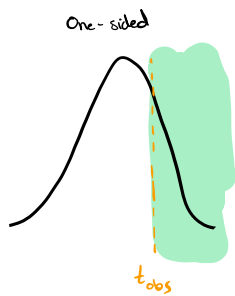
- Systematic bias
- Inflate variance

Lecture 11: Testing Multiple Hypotheses

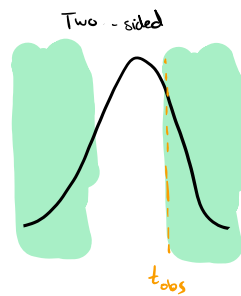
If I test n null hypotheses at level α , all of which are true, then on average I'll falsely reject αn of them

Most statistical multiple-testing procedures take p-values as inputs

p-value is the smallest significance value at which the test rejects the null hypothesis



p-val is 0.036 (smallest value that rejects null)



p-value is 0.072

For a one-sided test with continuous test statistic T , we reject H_0 when T exceeds upper- α point of its null distribution

$$P = \mathbb{P}_{H_0} [T > t_{obs}] = 1 - F(t_{obs})$$

For a two-sided test, we reject H_0 when T is larger than upper- $\frac{\alpha}{2}$ or less than lower- $\frac{\alpha}{2}$

$$P = 2 \cdot \min(F(t_{obs}), 1 - F(t_{obs}))$$

p-value is the probability under H_0 of observing a value of T that is more extreme than t_{obs} .

p-value can be considered as a test statistic itself

reject if $P \leq \alpha$

P is uniform $(0,1)$ under H_0

Bonferroni Method:

For n different null hypotheses, reject at α/n instead of α

Justification:

$$\begin{aligned} \mathbb{P}[\text{reject any null hypothesis}] &= \mathbb{P}[\{\text{reject } H_0^{(1)}\} \cup \dots \cup \{\text{reject } H_0^{(n)}\}] \\ &\leq \mathbb{P}[\text{reject } H_0^{(1)}] + \dots + \mathbb{P}[\text{reject } H_0^{(n)}] \leq \frac{\alpha}{n} + \dots + \frac{\alpha}{n} = \alpha \end{aligned}$$

Family Wise Error Rate

n null hypotheses, n_0 are true nulls

$$\text{FWER} = \mathbb{P}[\text{reject any true null hypothesis}]$$

Controls FWER at level α guarantees $\text{FWER} \leq \alpha$

Bonferroni Method controls FWER at α

False Discovery Rate

$$\text{False Discovery Proportion} = \frac{\text{number of true null hypotheses rejected}}{\text{number of total null hypotheses rejected}} = \frac{V}{R} \quad \leftarrow 0 \text{ when } V=0 \text{ and } R>0$$

Controls FDR at level α if $\text{FDR} \leq \alpha$

Controlling FWER is more appropriate if the consequences of a single type I error is high
result will be interpreted as truth

Controlling FDR is more appropriate if the best IDs candidate discoveries for further study
if false discoveries are acceptable as long most of the discoveries are correct

Estimating $\text{FDP} = \frac{V}{R}$ but we don't know V

We can estimate V since p -values are uniformly distributed $(0,1)$.

For a rejection value of t , we can expect $t n_0$ of the true nulls to have $p \leq t$

$$V \approx t n_0$$

We don't know n_0 so

$$\widehat{\text{FDP}} = \frac{t n}{R} \quad \leftarrow \text{estimate}$$

$$\text{Control } \widehat{\text{FDP}} = \frac{t n}{R(t)} \leq \alpha$$

\leftarrow number of rejections

goal is to find maximum t that satisfies this relation

For n rejections, $t = P_{(r)}$, the r^{th} smallest p -value and find largest r s.t.

$$\frac{P_{(r)}}{r} \cdot n \leq \alpha \iff P_{(r)} \leq \frac{\alpha r}{n} \quad \leftarrow \text{Benjamini-Hochberg}$$

1. Sort n p -values from smallest to largest

2. Find largest r s.t. $P_{(r)} \leq \frac{\alpha r}{n}$

3. Reject null hypothesis corresponding to $P_{(1)}, \dots, P_{(r)}$

Notice: $P_{(1)}$ is compared to $\frac{\alpha}{n}$, $P_{(2)} = \frac{2\alpha}{n}$, etc.

3/2: Parametric models and the method-of-moments

Def: A parametric model is a family of distributions indexed by a small number of unknown parameters

e.g. $N(\mu, \sigma^2)$

Notation: Vector of parameters $\Theta \in \mathbb{R}^k$

PDF/PMF as $f(x|\theta)$

not conditional

The set of allowable parameters is the parameter space

How to choose model to fit?

- What the data represents
- How the data arose?
- Visual examination of the data
- Considerations of complexity

Suppose we observe $X_1, \dots, X_n \stackrel{iid}{\sim} f(x|\theta)$

- How can we estimate θ
- How can we quantify our uncertainty

The Method of Moments

Suppose $\theta \in \mathbb{R}$ is a single unknown parameter

Pick θ so that the mean of $f(x|\theta)$ matches sample mean

$$\bar{X} = \frac{X_1 + \dots + X_n}{n}$$

Ex. The poisson distribution for parameter $\lambda > 0$ is a discrete distribution

over non-negative integer counts

$$\text{PMF: } f(x|\lambda) = \frac{e^{-\lambda} \lambda^x}{x!} \quad \text{for } x \in \{0, 1, 2, \dots\}$$

This distribution has mean λ . The M-O-M estimate is $\hat{\lambda} = \bar{X}$

Ex. The exponential distribution $\lambda > 0$

$$f(x|\lambda) = \lambda e^{-\lambda x} \quad \text{mean: } \frac{1}{\lambda}$$

$$\text{equate } \frac{1}{\lambda} = \bar{X}$$

More generally, suppose the parameters are $\Theta \in \mathbb{R}^k$. Equating the theoretical mean w/ sample avg. gives 1 equation

To get k equations, consider the first k moments of $X \sim f(x|\Theta)$

$$\left. \begin{array}{l} \mu_1 = \mathbb{E}[X] \\ \mu_2 = \mathbb{E}[X^2] \\ \vdots \\ \mu_k = \mathbb{E}[X^k] \end{array} \right\} \text{ depend on } \Theta$$

M-O-M estimate

- ① Compute μ_1, \dots, μ_k in terms of Θ
- ② Equate theoretical moments w/ sample moments
- ③ Solve for Θ

Ex. Let $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} N(\mu, \sigma^2)$

$$\mu_1 = \mathbb{E}[\bar{X}] = \mu$$

$$\mu_2 = \mathbb{E}[\bar{X}^2] = \text{Var}[\bar{X}] + (\mathbb{E}[\bar{X}])^2 = \frac{\sigma^2}{n} + \mu^2$$

$$\text{Set } \hat{\mu} = \frac{1}{n} (X_1 + \dots + X_n)$$

$$\hat{\sigma}^2 + \hat{\mu}^2 = \frac{1}{n} (X_1^2 + \dots + X_n^2)$$

Ex. $X_1, \dots, X_n \stackrel{iid}{\sim} \text{Gamma}(\alpha, \beta)$. Recall Mean is $\frac{\alpha}{\beta}$

Variance is $\frac{\alpha}{\beta^2}$

$$\mu_1 = \frac{\alpha}{\beta} \quad \mu_2 = \frac{\hat{\alpha} + \hat{\alpha}^2}{\hat{\beta}}$$

Bias, Variance, and mean-squared error

Any estimate $\hat{\theta}$ for $\theta \in \mathbb{R}^k$ is a statistic.

The bias of $\hat{\theta}$ is $\mathbb{E}_{\theta}[\hat{\theta}] - \theta$, where \mathbb{E}_{θ} means expectation when the parameter is θ .

"What's the difference between average value of $\hat{\theta}$ and θ "

Standard error is just standard deviation of $\hat{\theta}$

$$\sqrt{\text{Var}_{\theta}(\hat{\theta})}$$

"How far is $\hat{\theta}$ typically from its average value"

Mean-squared-error of $\hat{\theta}$ is $\mathbb{E}[(\hat{\theta} - \theta)^2]$

MSE combines bias and standard error

$$\text{MSE} = \text{Variance} + \text{Bias}^2$$

Usually, MSE, bias, and variance all depend on θ

An estimator is said to be unbiased if bias = $\mathbb{E}_{\theta}[\hat{\theta}] - \theta = 0$ for every possible θ in the parameter space

Ex. Consider $X_1, \dots, X_n \stackrel{iid}{\sim} \text{Poisson}(\lambda)$

Recall M-O-M estimate for $\hat{\lambda} = \bar{X}$

$$\textcircled{1} \text{ Bias: } \mathbb{E}_{\lambda}(\hat{\lambda}) = \mathbb{E}_{\lambda} \left[\frac{1}{n} (X_1 + \dots + X_n) \right] = \frac{1}{n} (\mathbb{E}(X_1) + \dots + \mathbb{E}(X_n)) = \lambda$$

so bias $\mathbb{E}_{\lambda}(\hat{\lambda}) - \lambda = 0$ $\hat{\lambda}$ is unbiased for λ

$$\textcircled{2} \text{ Standard error: } \text{Var}_{\lambda}[\hat{\lambda}] = \text{Var}_{\lambda} \left[\frac{1}{n} (X_1 + \dots + X_n) \right] = \frac{\lambda}{n}$$

$$s.e. = \sqrt{\frac{\lambda}{n}}$$

$$\textcircled{3} \text{ MSE} = (s.e.)^2 + (\text{bias})^2 = \frac{\lambda}{n}$$

3/7: Maximum Likelihood Estimator

Recap: Parametric model $f(x|\theta)$ parameterized by $\theta \in \mathbb{R}^k$

Estimate θ via method-of-moments

Compute $\mu_j = \mathbb{E}[X^j]$ in terms of θ for $j = 1 \dots k$

Equate values to sample values and solve

Def: The joint PMF or PDF of data X_1, \dots, X_n viewed as a function of the parameter $\theta \in \mathbb{R}^k$ is the likelihood function $\text{lik}(\theta)$

E.g. If $X_1, \dots, X_n \stackrel{iid}{\sim} f(x|\theta)$ then

$$\text{lik}(\theta) = f(x_1|\theta) \times \dots \times f(x_n|\theta)$$

Recall from NP

$$H_0: X \sim f_0 \quad \text{vs.} \quad H_1: X \sim f_1$$

$$\text{Likelihood ratio statistic} \quad L(X) = \frac{f_0(X)}{f_1(X)}$$

In the context of parametric models, if

$$f_0(x_1, \dots, x_n) = f(x_1|\theta_0) \times \dots \times f(x_n|\theta_0)$$

$$f_1(x_1, \dots, x_n) = f(x_1|\theta_1) \times \dots \times f(x_n|\theta_1)$$

$$\text{then} \quad L(X) = \frac{\text{lik}(\theta_0)}{\text{lik}(\theta_1)}$$

Maximum Likelihood Estimator of θ is the value of θ in the parameter space that maximizes $\text{lik}(\theta)$

Examples

How to compute MLE $\hat{\theta}$?

Note: It's equivalent to maximize log likelihood

$$\begin{aligned} \mathcal{Q}(\theta) &= \log \text{lik}(\theta) \\ &= \sum_{i=1}^n \log f(x_i|\theta) \quad \text{if } X_1, \dots, X_n \text{ are iid} \end{aligned}$$

Let $X_1, \dots, X_n \stackrel{iid}{\sim} \text{Poisson}(\lambda)$, Parameter space: $\lambda \in (0, \infty)$

$$\text{The PMF is } f(x|\lambda) = \frac{e^{-\lambda} \lambda^x}{x!}$$

Log Likelihood function

$$\mathcal{Q}(\theta) = \sum_{i=1}^n \log f(x_i|\lambda) = \sum_{i=1}^n -\lambda + x_i \log(\lambda) - \log(x_i!)$$

$$= -n\lambda + \log(\lambda) \sum_{i=1}^n x_i - \sum_{i=1}^n \log(x_i!)$$

To maximize λ , we want $0 = \mathcal{Q}'(\lambda)$

$$\mathcal{Q}'(\theta) = -n + \frac{1}{\lambda} \sum_{i=1}^n x_i = 0$$

$$\lambda = \frac{1}{n} \sum_{i=1}^n x_i = \bar{X}$$

First check: $\hat{\lambda}$ is in the parameter space

$$\hat{\lambda} = \bar{x} \text{ is in } (0, \infty) \text{ not all } x_i = 0$$

Second check: $\hat{\lambda}$ is a maximizer of the function

$$0 > \ell'(\lambda) \quad \lambda > \bar{x} \quad \text{and} \quad 0 < \ell'(\lambda)$$

$$\Downarrow$$

$$\hat{\lambda} > \hat{\lambda} = \bar{x}$$

$$\Downarrow$$

$$\lambda < \hat{\lambda} = \bar{x}$$

$\ell(\lambda)$ is decreasing left of \bar{x} and increasing right of \bar{x}

Alternatively check if $\ell''(\lambda) < 0$

$$\ell''(\lambda) = -\frac{1}{\lambda^2} \sum_{i=1}^n x_i$$

This is negative for all $\lambda \in (0, \infty)$ so $\ell(\lambda)$ is concave

If all x_i 's are 0, our estimate is $\hat{\lambda} =$

Example: Let $x_1, \dots, x_n \stackrel{iid}{\sim} N(\mu, \sigma^2)$. The log likelihood function is

$$\begin{aligned} \ell(\mu, \sigma^2) &= \sum_{i=1}^n \log f(x_i | \mu, \sigma^2) \\ &= \sum_{i=1}^n \log \left(\frac{1}{\sqrt{2\pi} \sigma} e^{-\frac{(x_i - \mu)^2}{2\sigma^2}} \right) \\ &= \sum_{i=1}^n \left[-\frac{1}{2} \log 2\pi - \frac{1}{2} \log \sigma^2 - \frac{(x_i - \mu)^2}{2\sigma^2} \right] \\ &= -\frac{n}{2} \log 2\pi - \frac{n}{2} \log \sigma^2 - \frac{1}{2\sigma^2} \sum_{i=1}^n (x_i - \mu)^2 \end{aligned}$$

Maximize: $\ell(\mu, \sigma^2)$

First order condition

$$\ell'(\theta) = 0$$

$$\frac{\partial \ell}{\partial \mu} = \frac{1}{\sigma^2} \sum_{i=1}^n (x_i - \mu) \quad \Leftrightarrow \quad 0 = \sum_{i=1}^n x_i - n\mu \Rightarrow \hat{\mu} = \frac{1}{n} \sum_{i=1}^n x_i = \bar{x}$$

$$\frac{\partial \ell}{\partial \sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4} \sum_{i=1}^n (x_i - \mu)^2 \quad \Leftrightarrow \quad 0 = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4} \sum_{i=1}^n (x_i - \bar{x})^2 \Rightarrow \hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2$$

Verifying Maximization

$$0 < \frac{\partial \ell}{\partial \mu} \Leftrightarrow \mu < \bar{x} \quad \text{and} \quad 0 > \frac{\partial \ell}{\partial \mu} \Leftrightarrow \mu > \bar{x}$$

Similarly for σ^2 by setting $\mu = \bar{x}$

Example: Let $X_1, \dots, X_n \stackrel{iid}{\sim} \text{Gamma}(\alpha, \beta)$ $\alpha, \beta > 0$

Log Likelihood

$$\begin{aligned} \mathcal{L}(\alpha, \beta) &= \sum_{i=1}^n \log f(X_i | \alpha, \beta) = \sum_{i=1}^n \log \left(\frac{\beta^\alpha}{\Gamma(\alpha)} X_i^{\alpha-1} e^{-\beta X_i} \right) = \sum_{i=1}^n \alpha \log \beta - \log \Gamma(\alpha) + (\alpha-1) \log(X_i) - \beta X_i \\ &= n\alpha \log \beta - n \log \Gamma(\alpha) + (\alpha-1) \sum_{i=1}^n \log(X_i) - \beta \sum_{i=1}^n X_i \end{aligned}$$

Maximize

$$\frac{\partial \mathcal{L}}{\partial \alpha} = n \log \beta - \frac{n \Gamma'(\alpha)}{\Gamma(\alpha)} + \sum_{i=1}^n \log X_i$$

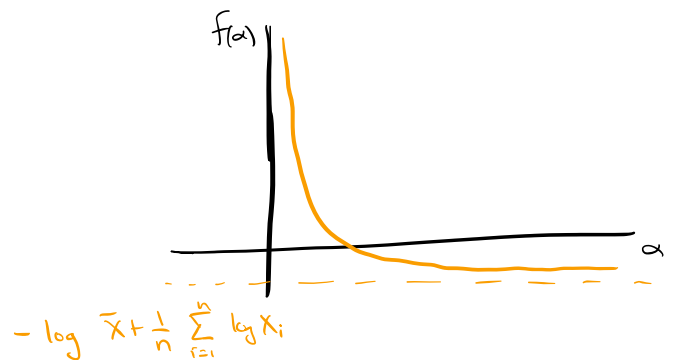
$$\frac{\partial \mathcal{L}}{\partial \beta} = \frac{n\alpha}{\beta} - \sum_{i=1}^n X_i$$

Solve 2nd equation in β so $\hat{\beta} = \frac{\hat{\alpha}}{\bar{X}}$

Substituting into first equation

$$0 = n \log \left(\frac{\hat{\alpha}}{\bar{X}} \right) - \frac{n \Gamma'(\hat{\alpha})}{\Gamma(\hat{\alpha})} + \sum_{i=1}^n \log(X_i)$$

$$0 = \underbrace{\log(\hat{\alpha}) - \frac{\Gamma'(\hat{\alpha})}{\Gamma(\hat{\alpha})} - \log \bar{X} + \frac{1}{n} \sum_{i=1}^n \log X_i}_{f(\hat{\alpha})}$$



Observe $f(\alpha)$ is decreasing

$$-\log(\bar{X}) + \frac{1}{n} \sum_{i=1}^n \log(X_i) < 0$$

by Jensen's Inequality

So there must be a unique root to $0 = f(\hat{\alpha})$

Then this $\hat{\alpha}$ and $\hat{\beta} = \frac{\hat{\alpha}}{\bar{X}}$ are the MLE's

You can check that these are the maximizers

Usually no explicit form for MLE, Instead compute via optimization algorithm

Newton-Raphson method is a common approach

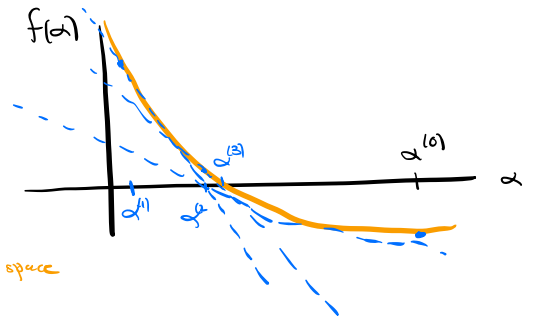
1. Initialize with a guess
Often use MOM estimate

2. Linearize $\alpha^{(t)}$ using a Taylor expansion

$$0 = f(\alpha^{(t)}) + (\alpha - \alpha^{(t)}) f'(\alpha^{(t)})$$

$$\hat{\alpha} = \alpha^{(t)} - \frac{f(\alpha^{(t)})}{f'(\alpha^{(t)})} \quad \leftarrow \text{reset } \alpha^{(t)} \text{ if } \alpha^{(t)} \text{ falls outside of the parameter space}$$

3. Use linearized estimate for next iteration



This is different from M-O-M estimator

Example: Let $X_1, \dots, X_K \sim \text{Multinomial}(n, (p_1, \dots, p_K))$

X_1, \dots, X_K are not IID, they sum to n

Log likelihood function is the log PMF for (X_1, \dots, X_K)

$$\begin{aligned} \ell(p_1, \dots, p_K) &= \log \left[\binom{n}{x_1, x_2, \dots, x_K} p_1^{x_1} p_2^{x_2} \dots p_K^{x_K} \right] \\ &= \log \binom{n}{x_1, \dots, x_K} + \sum_{i=1}^K x_i \log p_i \end{aligned}$$

The parameter space is the set (p_1, \dots, p_K) where $0 \leq p_i \leq 1$ and $p_1 + \dots + p_K = 1$

MLE maximizes $\ell(p_1, \dots, p_K)$ subject to these constraints

Easiest way to do this is via Lagrange Multiplier Method

$$\begin{aligned} \mathcal{L}(p_1, \dots, p_K, \lambda) &= \ell(p_1, \dots, p_K) + \lambda (p_1 + \dots + p_K - 1) \\ &= \log \binom{n}{x_1, \dots, x_K} + \sum_{i=1}^K x_i \log(p_i) + \lambda (p_1 + \dots + p_K - 1) \end{aligned}$$

Set all partials of \mathcal{L} to 0

$$0 = \frac{\partial \mathcal{L}}{\partial p_i} = \frac{x_i}{p_i} + \lambda$$

$$0 = \frac{\partial \mathcal{L}}{\partial \lambda} = p_1 + \dots + p_K - 1$$

Solve 1st eq to find $p_i = \frac{-x_i}{\lambda}$

Substitute into 2nd eqn:

$$0 = \frac{-x_1}{\lambda} - \frac{x_2}{\lambda} - \dots - \frac{x_K}{\lambda} - 1$$

$$\lambda = -(x_1 + \dots + x_K) = -n$$

$$\hat{p}_i = \frac{x_i}{n} \quad (\text{fraction of observations in class } i)$$

Rationale for Lagrange Multiplier

1) Fix any λ . Maximizing $\mathcal{L}(p_1, \dots, p_K, \lambda)$ subject to $p_1 + \dots + p_K = 1$ is equivalent to maximizing $\ell(p_1, \dots, p_K)$ under the same constraint

λ term cancels to 0

2) The unconstrained maximizer of $L(p_1, \dots, p_k, \lambda)$ over (p_1, \dots, p_k) is $p_i = -\frac{X_i}{\lambda}$ as calculated above

3) Choosing $\lambda = -(X_1 + \dots + X_k) = -n$, the unconstrained max satisfies the constraint

Implies that the solved p_i 's are also constrained maximizers

From 1) we have that this solution maximizes $L(p_1, \dots, p_k)$

Example: The genotypes AA, Aa, aa at a locus satisfy Hardy-Weinberg Equilibrium

Occur with probabilities

$$(1-\theta)^2, 2\theta(1-\theta) \text{ and } \theta^2$$

$\theta \in [0, 1]$ is the frequency of a

Count occurrences of AA, Aa, aa in n samples can be modeled as multinomial

$$(X_1, X_2, X_3) \sim \text{Multinomial}(n, [(1-\theta)^2, 2\theta(1-\theta), \theta^2])$$

Similar to previous example with single parameter $\theta \in [0, 1]$

Compute MLE for θ

$$\begin{aligned} \ell(\theta) &= \log \left[\binom{n}{X_1, X_2, X_3} ((1-\theta)^2)^{X_1} (2\theta(1-\theta))^{X_2} (\theta^2)^{X_3} \right] \\ &= \log \binom{n}{X_1, X_2, X_3} + (2X_1 + X_2) \log(1-\theta) + (X_2 + 2X_3) \log \theta \end{aligned}$$

Maximize over θ (constraint already accounted for)

$$0 = \ell'(\theta) = -\frac{2X_1 + X_2}{1-\theta} + \frac{X_2 + 2X_3}{\theta}$$

$$\hat{\theta} = \frac{2X_3 + X_2}{2n}$$

3/9: Normal Approximation, confidence Interval

Example: Poisson Model

$X_1, \dots, X_n \stackrel{iid}{\sim} \text{Poisson}(\lambda)$. Let λ_0 be the true parameter

Both M-O-M and MLE find $\hat{\lambda} = \bar{X}$

From lecture 12: $\mathbb{E}_{\lambda_0}[\hat{\lambda}] = \lambda_0$ unbiased estimator

$$\text{Var}_{\lambda_0}[\hat{\lambda}] = \frac{\lambda_0}{n} \text{ standard error of } \sqrt{\frac{\lambda_0}{n}}$$

By LLN: $\hat{\lambda} = \bar{X} \rightarrow \lambda_0$ in probability as $n \rightarrow \infty$

We say $\hat{\lambda}$ is consistent for λ

By CLT: $\sqrt{n}(\hat{\lambda} - \lambda_0) \rightarrow \mathcal{N}(0, \lambda_0)$ in distribution as $n \rightarrow \infty$

Informally, $\hat{\lambda}$ has approximate distribution $\mathcal{N}(\lambda_0, \frac{\lambda_0}{n})$ for large n

This allows us to make a confidence interval for λ_0

Random interval contains λ_0 w/ a pre-specified probability, $1 - \alpha \in (0, 1)$

Let $z(\alpha/2)$ be the upper $-\alpha$ point of $\mathcal{N}(0, 1)$

CLT implies $\mathbb{P} \left[-\sqrt{\frac{\lambda_0}{n}} z(\alpha/2) \leq \hat{\lambda} - \lambda_0 \leq \sqrt{\frac{\lambda_0}{n}} z(\alpha/2) \right] \approx 1 - \alpha$

Substituting $\sqrt{\hat{\lambda}_n}$ for $\sqrt{\lambda_0}$ we find

$$\mathbb{P} \left[-\sqrt{\frac{\hat{\lambda}}{n}} z(\alpha/2) \leq \hat{\lambda} - \lambda_0 \leq \sqrt{\frac{\hat{\lambda}}{n}} z(\alpha/2) \right] \approx 1 - \alpha$$

We have lower and upper bounds of λ_0

$$\Rightarrow \lambda_0 \text{ belongs to the interval } \hat{\lambda} \pm \sqrt{\frac{\hat{\lambda}}{n}} \cdot z(\alpha/2) \text{ w/ probability } 1 - \alpha$$

More formally: The coverage guarantee is

$$\mathbb{P}_{\lambda_0} \left[\lambda_0 \in \left[\hat{\lambda} - \sqrt{\hat{\lambda}_n} \cdot z(\alpha/2), \hat{\lambda} + \sqrt{\hat{\lambda}_n} \cdot z(\alpha/2) \right] \right] \rightarrow 1 - \alpha \text{ as } n \rightarrow \infty$$

Because

- $\cdot \sqrt{n}(\hat{\lambda} - \lambda_0) \rightarrow \mathcal{N}(0, \lambda_0)$ by CLT

- $\cdot \frac{1}{\sqrt{\hat{\lambda}}} \rightarrow \frac{1}{\sqrt{\lambda_0}}$ by LLN

- $\cdot \frac{\sqrt{n}(\hat{\lambda} - \lambda_0)}{\sqrt{\hat{\lambda}}} \rightarrow \frac{1}{\sqrt{\lambda_0}} \cdot \mathcal{N}(0, \lambda_0) = \mathcal{N}(0, 1)$ by Slutsky's Lemma

Asymptotic Normality of the MLE

Thm: Let $f(x|\theta)$ be a parametric model, where $\theta \in \mathbb{R}$. Let θ_0 be the true parameter, let $X_1, \dots, X_n \stackrel{iid}{\sim} f(x|\theta_0)$

Let $\hat{\theta}$ be the MLE.

Under some smoothness conditions for $f(x|\theta)$, as $n \rightarrow \infty$

a) $\hat{\theta}$ is a consistent estimator

$$\hat{\theta} \rightarrow \theta_0 \text{ in probability as } n \rightarrow \infty$$

b) $\hat{\theta}$ is asymptotic normal, and $\sqrt{n}(\hat{\theta} - \theta_0) \rightarrow \mathcal{N}(0, \frac{1}{I(\theta_0)})$ in distribution

$I(\theta)$ has two definitions

$$I(\theta) = \text{Var}_{\theta} \left[\frac{\partial}{\partial \theta} \log f(x|\theta) \right] = -\mathbb{E}_{\theta} \left[\frac{\partial^2}{\partial \theta^2} \log f(x|\theta) \right]$$

Single sample

- $\cdot I(\theta)$ is the Fisher Information

- $\cdot \frac{\partial}{\partial \theta} \log f(x|\theta)$ is the score

We will show $\mathbb{E}_{\theta} \left[\frac{\partial}{\partial \theta} \log f(x|\theta) \right] = 0$

so $I(\theta) = \mathbb{E}_{\theta} \left[\left(\frac{\partial}{\partial \theta} \log f(x|\theta) \right)^2 \right]$

- \cdot Implications

- Asymptotically $\hat{\theta}$ is unbiased. The bias is smaller scale than $1/\sqrt{n}$

$\mathbb{E}[\sqrt{n}(\hat{\theta} - \theta_0)] \rightarrow 0$, if bias was larger the constant term of the bias would be \mathbb{E} of expression

- For large n , the standard error of the MLE is

$$\text{S.E. } \hat{\theta} = \sqrt{\frac{1}{nI(\theta)}} \text{ . Is on the order of } 1/\sqrt{n}$$

MSE = (bias)² + (std. error)² is dominated by std. error for large n

- Distribution of $\hat{\theta}$ is $\approx \mathcal{N}(\theta_0, \frac{1}{nI(\theta_0)})$

- Confidence interval for θ_0 with coverage $1-\alpha$

$$\hat{\theta} \pm \sqrt{\frac{1}{nI(\hat{\theta})}} \cdot z(\frac{\alpha}{2}), \quad \sqrt{\frac{1}{I(\hat{\theta})}} \text{ estimates } \sqrt{\frac{1}{I(\theta_0)}}$$

Example: Consider again $X_1, \dots, X_n \stackrel{iid}{\sim} \text{Poisson}(\lambda_0)$

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

$$\log f(x|\lambda) = \log \frac{e^{-\lambda} \lambda^x}{x!} = -\lambda + \log \lambda - \log(x!)$$

$$\frac{\partial}{\partial \lambda} \log f(x|\lambda) = -1 + \frac{x}{\lambda} \quad \leftarrow \text{Score}$$

$$\frac{\partial^2}{\partial \lambda^2} \log f(x|\lambda) = -\frac{x}{\lambda^2}$$

$$\mathbb{E}_{\lambda_0} \left[\frac{\partial}{\partial \lambda} \log f(x|\lambda) \right] = \mathbb{E}_{\lambda_0} \left[-1 + \frac{x}{\lambda} \right] = 0$$

$$I(\lambda_0) = \text{Var}_{\lambda_0} \left[-1 + \frac{x}{\lambda_0} \right] = \text{Var} \left[\frac{x}{\lambda_0} \right] = \frac{1}{\lambda_0^2} \text{Var} [x] = \frac{1}{\lambda_0}$$

Alternatively,

$$I(\lambda_0) = -\mathbb{E}_{\lambda_0} \left[-\frac{x}{\lambda_0^2} \right] = -\frac{1}{\lambda_0^2} \mathbb{E} [-x] = \frac{1}{\lambda_0}$$

Theorem shows $\sqrt{n}(\hat{\lambda} - \lambda_0) \rightarrow \mathcal{N}(0, \frac{1}{I(\lambda_0)}) = \mathcal{N}(0, \lambda_0)$

Proof Sketch

Consistency: The MLE $\hat{\theta}$ maximizes

$$\frac{1}{n} \sum_{i=1}^n \log f(x_i|\theta)$$

Suppose θ_0 is the true parameter. For any fixed θ , this is the average of n IID random variables.

As $n \rightarrow \infty$, by LLN

$$\frac{1}{n} \sum_{i=1}^n \log f(x_i|\theta) \rightarrow \mathbb{E}_{\theta_0} [\log f(x_i|\theta)]$$

Implies under some conditions that the maximizer of LHS maximizes RHS

Maximizer of RHS is θ_0 .

$$\mathbb{E}_{\theta_0} [\log f(x_i|\theta)] - \mathbb{E}_{\theta_0} [\log f(x_i|\theta_0)] = \mathbb{E}_{\theta_0} \left[\log \frac{f(x_i|\theta)}{f(x_i|\theta_0)} \right] \leq \log \mathbb{E}_{\theta_0} \left[\frac{f(x_i|\theta)}{f(x_i|\theta_0)} \right]$$

$$= \log \int \underbrace{\frac{f(x|\theta)}{f(x|\theta_0)}}_{\text{PMF}} \cdot f(x|\theta_0) dx = \log \int f(x|\theta) dx = \log 1 = 0$$

↑
Jensen's Inequality since \log is concave

$$\Rightarrow \mathbb{E}_{\theta_0} [\log f(x; \theta)] - \mathbb{E}_{\theta_0} [\log f(x; \theta_0)] \leq 0$$

So this is maximized over θ at $\theta = \theta_0$

Fisher Information

$$\int f(x|\theta) dx = 1$$

$$\Rightarrow 0 = \frac{\partial}{\partial \theta} \int f(x|\theta) dx = \int \frac{\partial}{\partial \theta} f(x|\theta) dx$$

$$\frac{\partial}{\partial \theta} \log f(x|\theta) = \frac{\frac{\partial}{\partial \theta} f(x|\theta)}{f(x|\theta)} \Leftrightarrow \frac{\partial}{\partial \theta} f(x|\theta) = \left(\frac{\partial}{\partial \theta} \log f(x|\theta) \right) f(x|\theta)$$

$$\Rightarrow 0 = \int \left(\frac{\partial}{\partial \theta} \log f(x|\theta) \cdot f(x|\theta) \right) dx = \mathbb{E}_{\theta} \left[\frac{\partial}{\partial \theta} \log f(x|\theta) \right]$$

So the score has mean 0.

Differentiate a second time

$$0 = \frac{\partial}{\partial \theta} \int \left(\frac{\partial}{\partial \theta} \log f(x|\theta) \right) f(x|\theta) dx$$

$$\stackrel{\text{product rule}}{=} \int \left(\frac{\partial^2}{\partial \theta^2} \log f(x|\theta) \right) \cdot f(x|\theta) dx + \int \left(\frac{\partial}{\partial \theta} \log f(x|\theta) \right) \underbrace{\left(\frac{\partial}{\partial \theta} f(x|\theta) \right)}_{\frac{\partial}{\partial \theta} \log f(x|\theta) \cdot f(x|\theta)} dx$$

$$= \mathbb{E}_{\theta} \left[\frac{\partial^2}{\partial \theta^2} \log f(x|\theta) \right] + \mathbb{E}_{\theta} \left[\left(\frac{\partial}{\partial \theta} \log f(x|\theta) \right)^2 \right]$$

$$\Rightarrow - \mathbb{E}_{\theta} \left[\frac{\partial^2}{\partial \theta^2} \log f(x|\theta) \right] = \mathbb{E}_{\theta} \left[\left(\frac{\partial}{\partial \theta} \log f(x|\theta) \right)^2 \right] = \text{Var}_{\theta} \left[\frac{\partial}{\partial \theta} \log f(x|\theta) \right]$$

Asymptotical Normality

$$\sqrt{n} (\hat{\theta} - \theta_0) \rightarrow N(0, \frac{1}{I(\theta_0)})$$

The MLE $\hat{\theta}$ maximizes $l(\theta) = \sum_{i=1}^n \log f(x_i|\theta)$

so $0 = l'(\hat{\theta}) \approx l'(\theta_0) + (\hat{\theta} - \theta_0) \cdot l''(\theta_0) \leftarrow \text{Taylor Expansion}$

$$\hat{\theta} - \theta_0 \approx - \frac{l'(\theta_0)}{l''(\theta_0)}$$

$$\sqrt{n} (\hat{\theta} - \theta_0) \approx - \sqrt{n} \frac{l'(\theta_0)}{l''(\theta_0)} = \frac{-\frac{1}{\sqrt{n}} l'(\theta_0)}{-\frac{1}{n} l''(\theta_0)}$$

$$-\frac{1}{n} l''(\theta_0) = \frac{1}{n} \sum_{i=1}^n \left[-\frac{\partial^2}{\partial \theta^2} \log f(x_i|\theta_0) \right]$$

$$\text{iid w/ mean } -E_{\theta_0} \left[\frac{\partial}{\partial \theta} \log f(x_i; \theta) \right] = I(\theta_0) \text{ in pr}$$

$$\frac{1}{\sqrt{n}} \ell'(\theta_0) = \frac{1}{\sqrt{n}} \sum_{i=1}^n \underbrace{\frac{\partial}{\partial \theta} \log f(x_i; \theta_0)}_{\text{iid w/ mean } = 0}$$

iid w/ mean = 0

$$\text{Var}_{\theta_0} \left[\frac{\partial}{\partial \theta} \log f(x_i; \theta_0) \right] = I(\theta_0)$$

$$\rightarrow \mathcal{N}(0, I(\theta_0)) \text{ by CLT}$$

By Slutsky Lemma

$$\sqrt{n}(\hat{\theta} - \theta) \rightarrow \frac{1}{I(\theta_0)} \cdot \mathcal{N}(0, I(\theta_0)) = \mathcal{N}(0, \frac{1}{I(\theta)})$$

3/14: Plug-in Estimates, delta Method

Recap: $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} f(x|\theta), \theta \in \mathbb{R}^k$

① Method of Moments

write $M = h(\theta)$ $\begin{cases} \mu_1 = E_{\theta}[X] = \frac{1}{n} \sum_{i=1}^n X_i \\ \vdots \\ \mu_k = E_{\theta}[X^k] = \frac{1}{n} \sum_{i=1}^n X_i^k \end{cases}$ solve equations for θ

② Maximum Likelihood Estimation

$$\ell(\theta) = \sum_{i=1}^n \log f(x_i|\theta)$$

Maximize $\ell(\theta)$ over the parameter space to get $\hat{\theta}$

Thm: The MLE $\hat{\theta}$ is consistent for θ , as $n \rightarrow \infty$

$$\sqrt{n}(\hat{\theta} - \theta) \rightarrow \mathcal{N}(0, \frac{1}{I(\theta)}) \text{ for } \theta \in \mathbb{R}$$

$$I(\theta) = \text{Var}_{\theta} \left[\frac{\partial}{\partial \theta} \log f(X|\theta) \right] = -E_{\theta} \left[\frac{\partial^2}{\partial \theta^2} \log f(x|\theta) \right]$$

Asymptotic Confidence Interval level $1-\alpha$ for θ

$$\hat{\theta} \pm \sqrt{\frac{1}{n I(\theta)}} \cdot z(\frac{\alpha}{2})$$

Estimating a function of θ

First estimate θ by $\hat{\theta}$, then use $g(\hat{\theta})$ as an estimate for $g(\theta)$

Example: Binomial coin, heads prob is p

If heads lose \$1

If tails win \$X

What value of x makes this game fair

$$\text{Expected winnings: } p \cdot (-1) + (1-p)x = 0$$

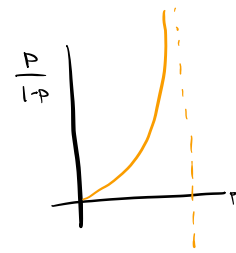
$$x = \frac{p}{1-p} \text{ is called the odds of this game}$$

often consider log-odds or logit

Estimate $\log \frac{p}{1-p}$ from $X_1, \dots, X_n \stackrel{iid}{\sim} \text{Bernoulli}(p)$

① First estimate p , by \bar{X}

② Plug-in to get $\log \frac{\bar{X}}{1-\bar{X}}$ as an estimate of $\log \frac{p}{1-p}$



Example: Pareto Distribution

$$\text{PDF: } f(x|\theta, x_0) = \theta x_0^\theta x^{-\theta-1} \text{ for } x \geq x_0$$

Suppose we know $x_0=1$, we don't know θ , so

$$f(x|\theta) = \theta x^{-\theta-1} \text{ for } x \geq 1$$

$$\text{Mean: } \frac{\theta}{\theta-1} \text{ when } \theta > 1$$

$$\text{Variance: } \frac{\theta}{(\theta-1)^2(\theta-2)} \text{ when } \theta > 2$$

How to estimate mean from $X_1, \dots, X_n \stackrel{iid}{\sim} f(x|\theta)$

① Estimate θ

$$\ell(\theta) = \sum_{i=1}^n \log f(x_i|\theta) = \sum_{i=1}^n \log \theta - (\theta+1) \log x_i$$

$$= n \cdot \log \theta - (\theta+1) \sum_{i=1}^n \log x_i$$

To maximize this over θ

$$0 = \ell'(\theta) = \frac{n}{\theta} - \sum_{i=1}^n \log x_i$$

$$\Rightarrow \hat{\theta} = \frac{n}{\sum_{i=1}^n \log x_i} \text{ is the MLE for } \theta$$

② Estimate the mean $\frac{\theta}{\theta-1}$ by $\frac{\hat{\theta}}{\hat{\theta}-1}$

Delta Method

Goal: Quantify the uncertainty (asymptotically) for $g(\hat{\theta})$ based on uncertainty of $\hat{\theta}$ itself

Thm: If $g: \mathbb{R} \rightarrow \mathbb{R}$ is continuously differentiable at θ , and if $\sqrt{n}(\hat{\theta} - \theta) \rightarrow N(0, v(\theta))$ in distribution as $n \rightarrow \infty$, then

$$\sqrt{n}(g(\hat{\theta}) - g(\theta)) \rightarrow N(0, g'(\theta)^2 \cdot v(\theta)) \text{ in distribution as } n \rightarrow \infty$$

Proof sketch: Apply Taylor expansion of $g(\hat{\theta})$ around $\hat{\theta} = \theta$

$$g(\hat{\theta}) \approx g(\theta) + (\hat{\theta} - \theta) g'(\theta)$$

$$\text{Then, } \sqrt{n} (g(\hat{\theta}) - g(\theta)) \approx \sqrt{n} (\hat{\theta} - \theta) g'(\theta)$$

$$\rightarrow g'(\theta) N(0, v(\theta)) = N(0, g'(\theta)^2 \cdot v(\theta))$$

Example: Let $X_1, \dots, X_n \stackrel{iid}{\sim} \text{Bernoulli}(p)$

We estimate $\log \frac{p}{1-p}$ by $\log \frac{\bar{X}}{1-\bar{X}}$

Apply Delta method:

$$\textcircled{1} \text{ By CLT: } \sqrt{n}(\bar{X} - p) \rightarrow N(0, p(1-p))$$

$$\textcircled{2} \text{ Let } g(p) = \log \frac{p}{1-p} = \log p - \log(1-p)$$

$$g'(p) = \frac{1}{p(1-p)}$$

$$\text{so, } \sqrt{n} \left(\log \frac{\bar{X}}{1-\bar{X}} - \log \frac{p}{1-p} \right) \rightarrow N\left(0, \frac{1}{p(1-p)}\right)$$

Suppose we toss $n=100$ coins with 60 heads

$$\bar{X} = 0.6$$

$$\log \text{ odds} \approx \frac{0.6}{1-0.6} = 0.41$$

$$\text{Standard error} = \sqrt{\frac{1}{n \bar{X}(1-\bar{X})}} \approx 0.2$$

Asymptotic Level $1-\alpha$, confidence interval is $0.41 \pm 0.2 \cdot z(\frac{\alpha}{2})$

Back to Pareto Example

Let $X_1, \dots, X_n \stackrel{iid}{\sim} \text{Pareto}(1, \theta)$

Recall: MLE is $\hat{\theta} = \frac{n}{\sum_{i=1}^n \log X_i}$

Plug in estimate for mean $\frac{\theta}{\theta-1}$ was $\frac{\hat{\theta}}{\hat{\theta}-1}$

Apply delta method:

$$\textcircled{1} \text{ Understand } \hat{\theta} \\ \sqrt{n}(\hat{\theta} - \theta) \rightarrow N(0, \frac{1}{I(\theta)})$$

Computing $I(\theta)$:

$$\log f(x|\theta) = \log \theta - (\theta+1) \log x$$

$$\frac{\partial}{\partial \theta} \log f(x|\theta) = \frac{1}{\theta} - \log x$$

$$\frac{\partial^2}{\partial \theta^2} \log f(x|\theta) = -\frac{1}{\theta^2}$$

$$I(\theta) = -\mathbb{E}_{\theta} \left[-\frac{1}{\theta^2} \right] = \frac{1}{\theta^2}$$

$$\sqrt{n}(\hat{\theta} - \theta) \rightarrow N(0, \theta^2)$$

② Set $g(\theta) = \frac{\theta}{\theta-1}$

$$g'(\theta) = -\frac{1}{(\theta-1)^2}$$

$$\text{so, } \sqrt{n} \left(\frac{\hat{\theta}}{\hat{\theta}-1} - \frac{\theta}{\theta-1} \right) \rightarrow N \left(0, \left[-\frac{1}{(\theta-1)^2} \right]^2 \theta^2 \right) = N \left(0, \frac{\theta^2}{(\theta-1)^4} \right)$$

An alternative estimate for the mean is \bar{X}

For \bar{X} estimate, we can apply CLT

$$\sqrt{n} \left(\bar{X} - \frac{\theta}{\theta-1} \right) \rightarrow N \left(0, \frac{\theta}{(\theta-1)^2(\theta-2)} \right)$$

Notice variance from MLE method is less than \bar{X} estimate

Reduces impact of extreme observations

Standard Error for Method of Moments

Consider $\theta \in \mathbb{R}$. Estimate $\mu = \mathbb{E}_{\theta} [X]$ by \bar{X}

Suppose $\mu = h(\theta)$ for some function $h(\cdot)$

Let g be the inverse function of h so $\theta = g(\mu)$

MOM estimate for $\theta = g(\mu)$ is $\hat{\theta} = g(\bar{x})$

For Standard Error

① By CLT, $\sqrt{n}(\bar{X} - \mu) \rightarrow N(0, v(\theta))$

$$v(\theta) = \text{var}_{\theta} [X_i]$$

② By delta method

$$\sqrt{n}(\hat{\theta} - \theta) = \sqrt{n}(g(\bar{X}) - g(h(\theta))) \rightarrow N(0, g'(h(\theta))^2 \cdot v(\theta))$$

Standard error of $\hat{\theta}$ is

$$\sqrt{\frac{g'(h(\theta))^2 \cdot v(\theta)}{n}}$$

Example: Consider $X_1, \dots, X_n \stackrel{iid}{\sim}$ Exponential(λ)

$$\text{PDF: } f(x|\lambda) = \lambda e^{-\lambda x} \text{ for } x > 0$$

$$\text{mean: } 1/\lambda \quad \text{var: } 1/\lambda^2$$

Inverse of $h(\cdot)$ is $\lambda = g(\mu) = 1/\mu$

$$g(\bar{x}) = 1/\bar{x}$$

Estimate std. error

$$\textcircled{1} \text{ By CLT, } \sqrt{n}(\bar{x} - 1/\lambda) \rightarrow N(0, 1/\lambda^2)$$

$$\textcircled{2} g'(\mu) = -1/\mu^2 \text{ so } g'(1/\lambda) = -\lambda^2$$

$$\sqrt{n}(1/\bar{x} - \lambda) = \sqrt{n}(g(\bar{x}) - g(1/\lambda)) \rightarrow N(0, g'(1/\lambda)^2 \cdot 1/\lambda^2) = N(0, \lambda^2)$$

Therefore std. error is $\approx \sqrt{\frac{\lambda^2}{n}}$ for large n , can estimate via $\sqrt{\frac{1}{n\bar{x}^2}}$

3/16: Cramer-Rao Bound, Asymptotic Efficiency

Recap: Pareto Model

$$\text{PDF: } f(x|\theta) = \theta x^{-\theta-1} \text{ for } x \geq 1$$

$$X_1, \dots, X_n \stackrel{iid}{\sim} f(x|\theta)$$

$$\text{MLE } \hat{\theta}: \frac{n}{\sum_{i=1}^n \log x_i}, \quad \sqrt{n}(\hat{\theta} - \theta) \rightarrow N(0, \theta^2)$$

$$\text{Mean in this model: } \mu = \frac{\theta}{\theta-1}, \quad \sqrt{n}\left(\frac{\hat{\theta}}{\hat{\theta}-1} - \frac{\theta}{\theta-1}\right) \rightarrow N\left(0, \frac{\theta^2}{(\theta-1)^2}\right)$$

Method-of-Moments Estimate for θ

$$\text{Solve } \mu = \frac{\theta}{\theta-1} \text{ for } \theta$$

$$\theta = g(\mu) = \frac{\mu}{\mu-1}$$

M-O-M Estimator $\hat{\theta} = \frac{\bar{X}}{\bar{X}-1}$

Delta Method

① By CLT, $\sqrt{n}(\bar{X} - \frac{\theta}{\theta-1}) \rightarrow N(0, \frac{\theta}{(\theta-1)^2(\theta-2)})$

② $g'(u) = \frac{1}{u-1} - \frac{u}{(u-1)^2} = \frac{-1}{(u-1)^2}$

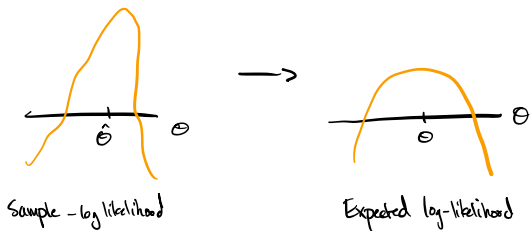
$\Rightarrow g'(\frac{\theta}{\theta-1}) = -(\theta-1)^{-2}$

so $\sqrt{n}(\hat{\theta} - \theta) = \sqrt{n}(g(\bar{X}) - g(\frac{\theta}{\theta-1})) \rightarrow N(0, \frac{\theta}{(\theta-1)^2(\theta-2)} \cdot [-(\theta-1)^{-2}]^2)$
 $= N(0, \frac{\theta(\theta-1)^2}{\theta-2})$

Geometry of the Fisher Information

Recall that as $n \rightarrow \infty$, fixing the parameter θ_0 ,

$\frac{1}{n} \sum_{i=1}^n \log f(x_i; \theta) \rightarrow E_{\theta_0}[\log f(x; \theta)]$ for every θ



Fisher information is the curvature of $\bar{Q}(\theta)$ at $\theta = \theta_0$

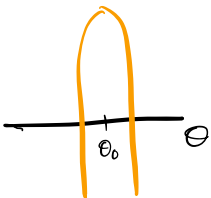
$\bar{Q}(\theta) = E_{\theta_0}[\log f(x; \theta)]$

Reason: $I(\theta) = -E_{\theta} \left[\frac{\partial^2}{\partial \theta^2} \log f(x; \theta) \right]$

For a fixed true parameter θ_0

$I(\theta_0) = -E_{\theta_0} \left[\frac{\partial^2}{\partial \theta^2} \log f(x; \theta) \Big|_{\theta=\theta_0} \right]$
 $= -\frac{\partial^2}{\partial \theta^2} E_{\theta_0} \left[\log f(x; \theta) \right] \Big|_{\theta=\theta_0} = -\bar{Q}''(\theta_0)$

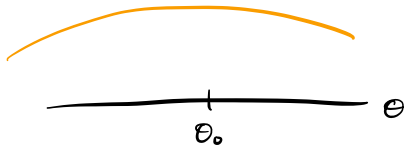
If $I(\theta_0)$ is large, then the curvature of \bar{Q} around θ_0 is big



If we perturb θ a bit from θ_0 , then $\bar{Q}(\theta)$ decreases a lot from $\bar{Q}(\theta_0)$

Data contains a lot of information about θ_0

If $I(\theta_0)$ is small, then \bar{L} would have small curvature around θ_0



perturbations from θ_0 do not result in large changes

Data contains less information about θ_0

Cramer-Rao Lower Bound

Thm: Consider a parametric model $f(x|\theta)$ where $\theta \in \mathbb{R}$ is a single parameter. Let T be any unbiased estimator of θ based on n observations $x_1, \dots, x_n \stackrel{iid}{\sim} f(x|\theta)$. Then (under smoothness conditions)

$$\text{Var}_{\theta} [T] \geq \frac{1}{nI(\theta)}$$

Interpretation: If $T = \hat{\theta}$ is the MLE, then for large n , $\text{Var} [T] \approx \frac{1}{nI(\theta)}$

Any unbiased estimator can't achieve a smaller variance

Proof: Let $Z \equiv \frac{\partial}{\partial \theta} \log f(x_1, \dots, x_n | \theta) = \sum_{i=1}^n \frac{\partial}{\partial \theta} \log f(x_i | \theta)$

$$\text{Recall: } \mathbb{E}_{\theta} \left[\frac{\partial}{\partial \theta} \log f(x|\theta) \right] = 0$$

$$\text{Var}_{\theta} \left[\frac{\partial}{\partial \theta} \log f(x|\theta) \right] = I(\theta)$$

$$\text{So, } \mathbb{E}_{\theta} [Z] = 0 \text{ and } \text{Var}_{\theta} [Z] = nI(\theta)$$

The correlation between Z and T belongs to $[-1, 1]$

$$\text{Cov}_{\theta} [Z, T]^2 \leq \text{Var}_{\theta} [Z] \text{Var} [T]$$

$$\text{Var}_{\theta} [Z] = nI(\theta)$$

$$\text{Cov}_{\theta} [Z, T] = \mathbb{E}_{\theta} [(Z - \mathbb{E}_{\theta} Z)(T - \mathbb{E}_{\theta} T)]$$

$$= \mathbb{E}_{\theta} [(Z - \mathbb{E}_{\theta} Z) T]$$

$$= \mathbb{E}_{\theta} [ZT] \quad \text{bc } \mathbb{E}_{\theta} Z = 0$$

Since T is unbiased for θ

$$\theta = \mathbb{E}_{\theta} [T] = \int T(x_1, \dots, x_n) f(x_1, \dots, x_n | \theta) dx_1 \dots dx_n$$

Derivative w/ respect to θ

$$1 = \int T(x_1, \dots, x_n) \cdot \frac{\partial}{\partial \theta} f(x_1, \dots, x_n | \theta) dx_1 \dots dx_n$$

Recall: $\left[\frac{\partial}{\partial \theta} \log f(x_1, \dots, x_n | \theta) \right] \cdot f(x_1, \dots, x_n | \theta) = \frac{\partial}{\partial \theta} f(x_1, \dots, x_n | \theta)$

$$\begin{aligned} &= \int \underbrace{T(x_1, \dots, x_n)}_T \cdot \underbrace{\left[\frac{\partial}{\partial \theta} \log f(x_1, \dots, x_n | \theta) \right]}_Z \cdot f(x_1, \dots, x_n | \theta) dx_1 \dots dx_n \\ &= E_{\theta} [TZ] \end{aligned}$$

Therefore, $\text{Cov}[T, Z] = 1$

$$\text{Var}_{\theta} [T] \geq \frac{1}{nI(\theta)} \quad \leftarrow \text{Plugging everything}$$

$\hat{\theta}$ is an asymptotically efficient estimator for θ

if $\sqrt{n}(\hat{\theta} - \theta) \rightarrow N(0, \frac{1}{I(\theta)})$ in distribution

MLE is asymptotically efficient

If two estimators $\hat{\theta}, \tilde{\theta}$ satisfy

$$\sqrt{n}(\hat{\theta} - \theta) \rightarrow N(0, \mu(\theta))$$

$$\sqrt{n}(\tilde{\theta} - \theta) \rightarrow N(0, \nu(\theta))$$

Then, $\frac{\nu(\theta)}{\mu(\theta)}$ is the asymptotic relative efficiency of $\hat{\theta}$ relative to $\tilde{\theta}$

Interpreted as ratio of sample sizes required

$$\text{Var}[\hat{\theta}] \approx \frac{\mu(\theta)}{n} \quad \text{Var}[\tilde{\theta}] = \frac{\nu(\theta)}{n}$$

For plug-in estimates

$$\sqrt{n}(g(\hat{\theta}) - g(\theta)) \rightarrow N(0, g'(\theta)^2 / I(\theta))$$

$$\text{Var}[g(\hat{\theta})] \approx \frac{g'(\theta)^2}{nI(\theta)}$$

Cramer-Rao Bound for plug-in estimates

In a parametric model $f(x|\theta)$ for $\theta \in \mathbb{R}$, if T is any unbiased estimator for $g(\theta)$ based on $X_1, \dots, X_n \stackrel{iid}{\sim} f(x|\theta)$

$$\text{then } \text{Var}_{\theta} [T] \geq \frac{g'(\theta)^2}{n \cdot I(\theta)}$$

Analogous proof as for traditional Cramer-Rao lower bound

Fisher Information for multiple parameters

$\theta \in \mathbb{R}^k$, the Fisher information matrix $I(\theta) \in \mathbb{R}^{k \times k}$ is the matrix w/

$$\begin{aligned} (i,j) \text{ entry: } I(\theta)_{ij} &= \text{Cov}_{\theta} \left[\frac{\partial}{\partial \theta_i} \log f(x|\theta), \frac{\partial}{\partial \theta_j} \log f(x|\theta) \right] \\ &= -\mathbb{E}_{\theta} \left[\frac{\partial^2}{\partial \theta_i \partial \theta_j} \log f(x|\theta) \right] \end{aligned}$$

Thm: Let $f(x|\theta)$ be a parametric model where $\theta \in \mathbb{R}^k$

Let $\hat{\theta}$ be the MLE for θ based on n observations $X_1, \dots, X_n \stackrel{iid}{\sim} f(x|\theta)$

then, under smoothness conditions and assuming $I(\theta)$ is invertible

$$\underbrace{\sqrt{n}(\hat{\theta} - \theta)}_{\in \mathbb{R}^k} \rightarrow \underbrace{\mathcal{N}(0, I(\theta)^{-1})}_{\substack{k\text{-dimension multivariate} \\ \text{normal}}} \quad \leftarrow \text{Inverse matrix}$$

Example: Consider $X_1, \dots, X_n \stackrel{iid}{\sim} \text{Gamma}(\alpha, \beta)$ $\alpha, \beta > 0$

We can compute α, β via MLE

Use $I(\alpha, \beta)$ to quantify their uncertainty

$$\log f(x|\alpha, \beta) = \alpha \log \beta - \log \Gamma(\alpha) + (\alpha-1) \log x - \beta x$$

$$\frac{\partial}{\partial \alpha} \log f(X|\alpha, \beta) = \log \beta - \frac{T'(\alpha)}{T(\alpha)} + \log X$$

$$\frac{\partial}{\partial \beta} \log f(X|\alpha, \beta) = \frac{\alpha}{\beta} - X$$

$$\frac{\partial^2}{\partial \alpha^2} \log f(X|\alpha, \beta) = \frac{T'(\alpha)^2}{T(\alpha)^2} - \frac{T''(\alpha)}{T(\alpha)} = -\Psi(\alpha)$$

← tri-gamma function

$$\frac{\partial^2}{\partial \alpha \partial \beta} \log f(X|\alpha, \beta) = 1/\beta$$

$$\frac{\partial^2}{\partial \beta^2} \log f(X|\alpha, \beta) = -\frac{\alpha}{\beta^2}$$

$$\text{so } I(\alpha, \beta) = - \begin{pmatrix} -\Psi(\alpha) & 1/\beta \\ 1/\beta & -\alpha/\beta^2 \end{pmatrix} = \begin{pmatrix} \Psi(\alpha) & -1/\beta \\ -1/\beta & \alpha/\beta^2 \end{pmatrix}$$

$$I(\alpha, \beta)^{-1} = \frac{1}{\Psi(\alpha)\frac{\alpha}{\beta} - 1/\beta^2} \begin{pmatrix} \alpha/\beta^2 & 1/\beta \\ 1/\beta & \Psi(\alpha) \end{pmatrix}$$

Errors are positively correlated

3128: Bayesian Inference

Parametric model: Data $\mathbf{X} = (X_1, \dots, X_n)$

Modeled by same distribution $f(\mathbf{X}, \theta)$ w/ parameter θ

Frequentist Perspective: Fixed true value we try to estimate

θ is non-random

Bayesian Perspective: Treat θ as a random variable with a distribution

Prior and Posterior Distributions

Review joint, marginal, and conditional distributions

Consider two r.v.'s $X+Y$

Joint PDF or PMF $f_{x,y}(x,y)$

Marginal Distribution of X is given by

$$f_x(x) = \int f_{x,y}(x,y) dy \quad \text{or} \quad f_x(x) = \sum_y f_{x,y}(x,y)$$

Continuous Discrete

Conditional distribution of Y given $X=x$ is then

$$f_{y|x}(y|x) = \frac{f_{x,y}(x,y)}{f_x(x)}$$

This is a PDF or PMF over values y , fixing the value x

Similarly define

$$f_{x|y}(x|y) = \frac{f_{x,y}(x,y)}{f_y(y)}$$

The Joint PDF/PMF factors in two ways

$$\begin{aligned} f_{x,y}(x,y) &= f_{y|x}(y|x) \cdot f_x(x) \\ &= f_{x|y}(x|y) \cdot f_y(y) \end{aligned}$$

Bayesian Inference: Observed data $\mathbf{X} = (X_1, \dots, X_n)$

Parametric model for \mathbf{X} with unknown parameter Θ

- Think about Θ as random

- Interpret the model for \mathbf{X} as the conditional distribution given $\Theta = \theta$

$$f_{\mathbf{X}|\Theta}(\mathbf{x}|\theta)$$

Θ is random w/ distribution $f_{\Theta}(\theta)$ — the prior distribution

\Rightarrow This defines a joint distribution over both Θ and \mathbf{X}

$$f_{\mathbf{X},\Theta}(\mathbf{x},\theta) = f_{\mathbf{X}|\Theta}(\mathbf{x}|\theta) \times f_{\Theta}(\theta)$$

We can factor this joint distribution

$$f_{\mathbf{X},\Theta}(\mathbf{x},\theta) = f_{\Theta|\mathbf{X}}(\theta|\mathbf{x}) \times f_{\mathbf{X}}(\mathbf{x})$$

$f_{\Theta}(\theta)$ is the prior distribution for Θ , i.e. marginal distribution of Θ

$f_{X|\Theta}(x|\theta)$ is our parametric model for X i.e. the likelihood function

$f_X(x) = \int f_{X|\Theta}(x|\theta) d\theta$ is the marginal distribution of X .

Distribution of data averaging over Θ

$f_{\Theta|X}(\theta|x)$ is the posterior distribution of Θ

This is our belief about the value of Θ , after seeing the data

Goal: Understand $f_{\Theta|X}(\theta|x)$

$$f_{\Theta|X}(\theta|x) = \frac{f_{X|\Theta}(x|\theta)}{f_X(x)} = \frac{f_{X|\Theta}(x|\theta) \times f_{\Theta}(\theta)}{f_X(x)}$$

$$f_{\Theta|X}(\theta|x) \propto f_{X|\Theta}(x|\theta) \times f_{\Theta}(\theta)$$

"posterior \propto likelihood \times prior"

Example: Coin, heads probability, P

Consider a prior distribution for P - Uniform $(0,1)$

Observe $X_1, \dots, X_n \stackrel{iid}{\sim} \text{Bernoulli}(p)$ given $P=p$

What is the posterior of P ?

Joint distribution of X_1, \dots, X_n, P is

$$\begin{aligned} f_{X,P}(X,P) &= f_{X|P}(X|P) \times f_P(P) \\ &= \prod_{i=1}^n p^{x_i} (1-p)^{1-x_i} \times 1 \quad \leftarrow \text{PDF uniform} \\ &= p^S (1-p)^{n-S} \quad \text{where } S = X_1 + \dots + X_n \end{aligned}$$

Marginal PMF of X is

$$\begin{aligned} f_X(X) &= \int_0^1 f_{X,P}(X,p) dp \\ &= \int_0^1 p^S (1-p)^{n-S} dp \end{aligned}$$

This is the beta integral

$$B(\alpha, \beta) = \int_0^1 x^{\alpha-1} (1-x)^{\beta-1} dx = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}$$

$$\Rightarrow f_X(X) = B(S+1, n-S+1)$$

Posterior Distribution of P given $X=x$ is

$$\begin{aligned} f_{P|X}(P|X) &= \frac{f_{X,P}(X,P)}{f_X(X)} \\ &= \frac{1}{B(S+1, n-S+1)} \cdot p^S (1-p)^{n-S} \quad \leftarrow \text{PDF of Beta}(S+1, n-S+1) \end{aligned}$$

Example: Can extend to a more general prior for P

Consider Beta (α, β) prior for P :

$$f_P(p) = \frac{1}{B(\alpha, \beta)} p^{\alpha-1} (1-p)^{\beta-1} \quad \text{for } p \in (0,1)$$

$\alpha = \beta = 1$ gives Uniform prior

Posterior for P satisfies

$$\begin{aligned} f_{P|X}(p|X) &\propto f_{X|P}(X|p) \times f_P(p) \\ &\propto p^s (1-p)^{n-s} \cdot p^{\alpha-1} (1-p)^{\beta-1} \\ &= p^{s+\alpha-1} (1-p)^{n-s+\beta-1} \end{aligned}$$

This is proportional to Beta $(s+\alpha, n-s+\beta)$

Beta distribution is the posterior for P

Example: Observe counts X_1, \dots, X_n model as $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Poisson}(\lambda)$

Treat parameter λ as random

Take the prior $\lambda \sim \text{Gamma}(\alpha, \beta)$. This has PDF $f_\lambda(\lambda) = \frac{\beta^\alpha}{\Gamma(\alpha)} \lambda^{\alpha-1} e^{-\beta\lambda}$ for $\lambda > 0$

What is the posterior distribution of λ ?

$$\begin{aligned} f_{\lambda|X}(\lambda|X) &\propto f_{X|\lambda}(X|\lambda) \times f_\lambda(\lambda) \\ &= \prod_{i=1}^n \frac{\lambda^{x_i} e^{-\lambda}}{x_i!} \times \frac{\beta^\alpha}{\Gamma(\alpha)} \lambda^{\alpha-1} e^{-\beta\lambda} \\ &\propto \lambda^{\sum_{i=1}^n x_i - n\lambda} e^{-\beta\lambda} \times \lambda^{\alpha-1} e^{-\beta\lambda} \\ &= \lambda^{\alpha + \sum_{i=1}^n x_i - 1} \times e^{-(\beta + \alpha)\lambda} \end{aligned}$$

This is proportional to the Gamma $(\alpha + \sum_{i=1}^n x_i, \beta + \alpha)$

So this Gamma distribution is the posterior for λ

Example: Observe $x_1, \dots, x_n \stackrel{\text{iid}}{\sim} \mathcal{N}(\theta, 1/\xi)$ where $\xi = 1/\sigma^2$ is the precision

① Assume that ξ is known, treat θ as random

Consider a normal prior for $\theta \sim \mathcal{N}(M_{\text{prior}}, 1/\xi_{\text{prior}})$

$$\begin{aligned} f_{\theta|x}(\theta|x) &\propto f_{x|\theta}(x|\theta) \times f_{\theta}(\theta) \\ &= \prod_{i=1}^n e^{-\frac{\xi}{2}(x_i - \theta)^2} \times e^{-\frac{\xi_{\text{prior}}}{2}(\theta - M_{\text{prior}})^2} \\ &\propto \exp\left(-\frac{n\xi}{2}\theta^2 + \xi\left(\sum_{i=1}^n x_i\right)\theta - \frac{\xi_{\text{prior}}}{2}\theta^2 + \xi_{\text{prior}}M_{\text{prior}}\theta\right) \end{aligned}$$

Suppose $\xi_{\text{post}} = n\xi + \xi_{\text{prior}}$ and $M_{\text{post}} = \frac{\xi \sum_{i=1}^n x_i + \xi_{\text{prior}} M_{\text{prior}}}{n\xi + \xi_{\text{prior}}}$

$$f_{\theta|x}(\theta|x)$$

Some more algebra i dont fucking know

$$\mathcal{N}(M_{\text{post}}, 1/\xi_{\text{post}})$$

② Assume mean θ is known, precision ξ is unknown

Consider Gamma prior $\frac{\Gamma}{\xi} \sim \text{Gamma}(\alpha, \beta)$

Then

$$\begin{aligned} f_{\frac{\Gamma}{\xi}|x}(\xi|x) &\propto \prod_{i=1}^n \sqrt{\frac{\xi}{2\pi}} e^{-\frac{\xi}{2}(x_i - \theta)^2} \times \frac{\alpha-1}{\xi} e^{-\beta\xi} \\ &\propto \frac{\xi^{\alpha+n-1}}{2} e^{-\left(\beta + \sum_{i=1}^n \frac{(x_i - \theta)^2}{2}\right)\xi} \end{aligned}$$

GAMMA!

Bayesian Point Estimates and Credible Intervals

To get a numeric estimate for Θ :

- Mean of the posterior distribution
- Mode of the posterior ("MAP estimate")

To get an interval estimate for Θ :

- Define a Bayesian credible interval
I w/ coverage level $1 - \alpha$

An interval containing $1 - \alpha$ portion of the posterior distribution

$$P[\Theta \in I | X=x] = \int_I f_{\Theta|X}(\theta|x) d\theta = 1 - \alpha$$

Common to use: lower $\frac{\alpha}{2}$ -point to upper $\frac{\alpha}{2}$ -point of the posterior

Example: $X_1, \dots, X_n \stackrel{iid}{\sim} \text{Bernoulli}(p)$

Prior $P \sim \text{Beta}(\alpha, \beta)$

Recall: Posterior $P|X=x \sim \text{Beta}(s+\alpha, n-s+\beta)$

where $s = X_1 + \dots + X_n$

Estimate \hat{p} by posterior mean

$$\hat{p} = \frac{s+\alpha}{n+\alpha+\beta}$$

Distinct from $\frac{s}{n}$ as calculated by M-O-M and MLE

\hat{p} is a weighted average of sample and prior means

Credible Interval

lower -0.05 point to upper -0.05 point of $\text{Beta}(s+\alpha, n-s+\beta)$

3/30: Bayesian Inference (cont'd)

Likelihood model: $X = (X_1, \dots, X_n) \sim f_{X|\Theta}(x|\theta)$

Prior: $f_{\Theta}(\theta)$

Posterior: $f_{\Theta|X}(\theta|x) \propto f_{X|\Theta}(x|\theta) \times f_{\Theta}(\theta)$

Examples:

① $X_1, \dots, X_n \stackrel{iid}{\sim} \text{Bernoulli}(p)$, prior $P \sim \text{Uniform}(0,1)$

$$\Rightarrow (P|X) \sim \text{Beta}(X_1 + \dots + X_n + 1, n - (X_1 + \dots + X_n) + 1)$$

② $X_1, \dots, X_n \stackrel{iid}{\sim} \text{Bernoulli}(p)$, prior $P \sim \text{Beta}(\alpha, \beta)$

$$\Rightarrow (P|X) \sim \text{Beta}(X_1 + \dots + X_n + \alpha, n - (X_1 + \dots + X_n) + \beta)$$

③ $X_1, \dots, X_n \stackrel{iid}{\sim} \text{Poisson}(\lambda)$, prior $\lambda \sim \text{Gamma}(\alpha, \beta)$

$$\Rightarrow (\lambda|X) \sim \text{Gamma}(X_1 + \dots + X_n + \alpha, n + \beta)$$

④ $X_1, \dots, X_n \stackrel{iid}{\sim} N(\theta, \frac{1}{\xi})$

known ξ , prior $\theta \sim N(\mu_{\text{prior}}, \frac{1}{\xi_{\text{prior}}})$

$$\Rightarrow (\Theta | \mathcal{X}) \sim \mathcal{N}(\mu_{\text{post}}, \frac{1}{\Sigma_{\text{post}}})$$

$$\mu_{\text{post}} = \frac{\sum_{i=1}^n X_i + \left(\frac{\Sigma_{\text{prior}}}{\Sigma}\right) \mu_{\text{prior}}}{n + \left(\frac{\Sigma_{\text{prior}}}{\Sigma}\right)}, \quad \Sigma_{\text{post}} = n \Sigma + \Sigma_{\text{prior}}$$

Posterior means:

$$\textcircled{3} \quad \hat{\lambda} = \frac{X_1 + \dots + X_n + \alpha}{n + \beta}$$

Different from MLE/MoM which is \bar{X}

- As if we had β extra samples summing to α

$$\hat{\lambda} = \frac{n}{n+\beta} \cdot \bar{X} + \frac{\beta}{n+\beta} \cdot \frac{\alpha}{\beta}$$

↑
sample mean
↑
prior mean

$$\textcircled{4} \text{ Posterior Mean: } \hat{\Theta} = \mu_{\text{post}}$$

$$\hat{\Theta} = \mu_{\text{post}} = \frac{n}{n + \left(\frac{\Sigma_{\text{prior}}}{\Sigma}\right)} \cdot \bar{X} + \frac{\frac{\Sigma_{\text{prior}}}{\Sigma}}{n + \left(\frac{\Sigma_{\text{prior}}}{\Sigma}\right)} \cdot \mu_{\text{prior}}$$

↑
sample mean
↑
prior mean

A 70% Bayesian credible interval for Θ would be

$$\mu_{\text{post}} \pm \sqrt{\frac{1}{\Sigma_{\text{post}}}} \cdot z(0.05)$$

Conjugate Priors and Improper Priors

A conjugate prior is a prior distribution when the resulting posterior has the same parametric form

- Beta prior → Binomial prob
- Gamma prior → Poisson rate
- Normal prior → Normal mean
- Gamma prior → Normal precision parameter

Unfortunately tend to be light-tailed (bias inference towards prior mean)

- Use heavier-tailed, non-conjugate priors for more robust inference

Goal is to use an uninformative prior

E.g. Poisson example $X_1, \dots, X_n \stackrel{iid}{\sim} \text{Poisson}(\lambda)$

$$\text{Gamma}(\alpha, \beta) \text{ prior} \Rightarrow \text{Posterior mean} = \frac{X_1 + \dots + X_n + \alpha}{n + \beta}$$

Uninformative prior would mean smaller values of α, β

$$\text{At its limit: } \text{Gamma}(0, 0) \propto \lambda^{-1}$$

↑
not a proper probability distribution

Since gamma(0,0) is not an actual distribution, we call it an improper prior

Improper priors can still yield proper posterior distributions

Bayesian vs. Frequentist Coverage Guarantees

Bayesian level- $(1-\alpha)$ credible interval guarantees

$$\mathbb{P}[\Theta \in I | \mathcal{X} = \mathbf{x}] = 1 - \alpha$$

Frequentist Confidence Interval

$$\mathbb{P}_{\Theta}[\Theta \in I] = 1 - \alpha \text{ where } \mathbb{P}_{\Theta} \text{ is over } X_1, \dots, X_n \stackrel{iid}{\sim} f(X|\Theta)$$

Example: Let $X_1, \dots, X_n \stackrel{iid}{\sim} \mathcal{N}(\theta, 1)$

MLE/MoM is that $\hat{\theta} = \bar{X}$

Under parameter θ , $\bar{X} \sim \mathcal{N}(\theta, 1/n)$ so a frequentist level- α confidence interval is

$$\bar{X} \pm \frac{1}{\sqrt{n}} \cdot z(\alpha/2)$$

This guarantees $\mathbb{P}_\theta \left[\theta \in \bar{X} \pm \frac{1}{n} \cdot z(\alpha/2) \right] = 1 - \alpha$

For a Bayesian analysis $\Theta \sim \mathcal{N}(0, \frac{1}{\xi_{\text{prior}}})$

$(\Theta | X) \sim \mathcal{N}(M_{\text{post}}, \frac{1}{\xi_{\text{post}}})$

$$M_{\text{post}} = \frac{\sum_{i=1}^n X_i}{n + \xi_{\text{prior}}} = \frac{n}{n + \xi_{\text{prior}}} \bar{X}$$

$$\xi_{\text{post}} = n + \xi_{\text{prior}}$$

Level $(1-\alpha)$ Bayesian credible interval is

$$\frac{n}{n + \xi_{\text{prior}}} \bar{X} \pm \sqrt{\frac{1}{n + \xi_{\text{prior}}}} \cdot z(\alpha/2)$$

$$\text{This guarantees: } \mathbb{P} \left[\Theta \in \frac{n}{n + \xi_{\text{prior}}} \bar{X} \pm \sqrt{\frac{1}{n + \xi_{\text{prior}}}} \cdot z(\alpha/2) \mid X = \bar{X} \right] = 1 - \alpha$$

Bayesian credible interval does guarantee that the frequentist coverage probability, averaged according to the prior for Θ is $1 - \alpha$

the average coverage probability with prior $f_\Theta(\theta)$ is $1 - \alpha$

Normal Approximation

Frequentist and Bayesian approach converge for large n

For a fixed prior, as $n \rightarrow \infty$, the influence of the prior vanishes
mean and shape of posterior distribution are determined by data

Posterior will approach $\mathcal{N}(\hat{\theta}, \frac{1}{nI(\theta)})$

$\hat{\theta}$ is MLE and $I(\theta)$ is Fisher Information

Bayesian Credible Interval will be $\hat{\theta} \pm \sqrt{\frac{1}{nI(\hat{\theta})}} \cdot z(\alpha/2)$

Heuristic Explanation

Let $X_1, \dots, X_n \stackrel{iid}{\sim} f(X|\theta)$ prior $f_\Theta(\theta)$

Define $\lambda(\theta) = \sum_{i=1}^n \log(f(x_i|\theta))$ the total log likelihood

Posterior:

$$f_{\Theta|X}(\theta|X) \propto \text{likelihood} \cdot \text{prior}$$

$$e^{\lambda(\theta)} \times f_\Theta(\theta)$$

Taylor Expand for θ close to MLE

$$\ell(\theta) = \ell(\hat{\theta}) + (\theta - \hat{\theta})\ell'(\hat{\theta}) + \frac{1}{2}(\theta - \hat{\theta})^2 \ell''(\hat{\theta})$$

$$\ell'(\hat{\theta}) = 0 \text{ by max}$$

$$\frac{1}{n} \ell''(\hat{\theta}) \approx \frac{1}{n} \ell''(\theta_0) = -I(\theta_0) \approx -I(\hat{\theta})$$

$$\ell(\theta) \approx \ell(\hat{\theta}) - \frac{1}{2}(\theta - \hat{\theta})^2 \cdot nI(\hat{\theta})$$

$\ell(\hat{\theta})$ depends on X so it can be absorbed into proportionality

4/4: MLE under misspecified models

$$X_1, \dots, X_n \stackrel{iid}{\sim} f(x|\theta_0)$$

Estimate θ , quantify uncertainty

- Bias, variance, MSE
- Consistency, asymptotic normality, efficiency

Kullback-Leibler divergence

for discrete distributions w/ PMFs f and g on the sample space X

$$D_{KL}(g||f) = \sum_{x \in X} g(x) \log \frac{g(x)}{f(x)}$$

For continuous distributions w/ PDFs f and g

$$D_{KL}(g||f) = \int g(x) \log \frac{g(x)}{f(x)} dx$$

Equivalent to

$$D_{KL}(g||f) = \mathbb{E}_g \left[\log \frac{g(x)}{f(x)} \right] = \mathbb{E}_g [\log g(x)] - \mathbb{E}_g [\log f(x)]$$

Asymmetric definition

↓
expectation
under true distribution $X \sim g(x)$

Properties:

if $f(x) = g(x)$ for all x , then $D_{KL}(g||f) = 0$ since $\log \frac{g(x)}{f(x)} = \log 1 = 0$

For any f and g , $D_{KL}(g||f) \geq 0$

Follows from applying Jensen's inequality

$$D_{KL}(g||f) = \mathbb{E}_g \left[-\log \frac{f(x)}{g(x)} \right] \geq -\log \mathbb{E}_g \left[\frac{f(x)}{g(x)} \right] = -\log \int g(x) \cdot \frac{f(x)}{g(x)} dx = -\log 1 = 0$$

f and g don't need to come from the same family

Ex. Let f be $N(\mu_0, \sigma^2)$ and g be $N(\mu_1, \sigma^2)$. What is $D_{KL}(g||f)$?

$$\log \frac{g(x)}{f(x)} = \log \left[\frac{\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu_1)^2}{2\sigma^2}}}{\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu_0)^2}{2\sigma^2}}} \right] = \frac{-(x-\mu_1)^2}{2\sigma^2} + \frac{(x-\mu_0)^2}{2\sigma^2} = \frac{2(\mu_1 - \mu_0)x - (\mu_1^2 - \mu_0^2)}{2\sigma^2}$$

$$D_{KL}(g||f) = \mathbb{E}_g \left[\log \frac{g(x)}{f(x)} \right] = \frac{2(\mu_1 - \mu_2) \mathbb{E}_g[X] - (\mu_1^2 - \mu_2^2)}{2\sigma^2} \quad \text{where } \mathbb{E}_g[X] = \mu_1$$

$$= \frac{1}{2\sigma^2} (\mu_1 - \mu_2)^2$$

KL divergence is the squared difference of means, normalized by variance

In this example KL divergence is symmetric

Ex. Let f be Bernoulli(p) What is $D_{KL}(g||f)$
 g be Bernoulli(q)

$$\text{Then } \log \frac{g(x)}{f(x)} = \begin{cases} \log \frac{q}{p} & x=1 \\ \log \frac{1-q}{1-p} & x=0 \end{cases}$$

$$D_{KL}(g||f) = \mathbb{E}_g \left[\log \frac{g(x)}{f(x)} \right] = q \log \frac{q}{p} + (1-q) \log \frac{1-q}{1-p}$$

If $p=q$, we can approximate this by Taylor expansion

$$\log p \approx \log q + (p-q) \cdot \frac{1}{q} + \frac{1}{2}(p-q)^2 \cdot \left(-\frac{1}{q^2}\right)$$

$$\log(1-p) \approx \log(1-q) + (p-q) \left(-\frac{1}{1-q}\right) + \frac{1}{2}(p-q)^2 \cdot \left(-\frac{1}{(1-q)^2}\right)$$

$$\begin{aligned} D_{KL}(g||f) &= q(\log q - \log p) + (1-q)(\log(1-q) - \log(1-p)) \\ &\approx q \cdot \left(-\frac{p-q}{q} + \frac{1}{2}(p-q)^2 \cdot \frac{1}{q^2}\right) + (1-q) \left(\frac{p-q}{1-q} + \frac{1}{2}(p-q)^2 \cdot \frac{1}{(1-q)^2}\right) \\ &= \frac{1}{2}(p-q)^2 \cdot \left(\frac{1}{q} + \frac{1}{1-q}\right) = \frac{(p-q)^2}{2q(1-q)} \end{aligned}$$

Ex. f is binomial (n, p)

g is binomial (n, q)

$$\text{Then } \log \frac{g(x)}{f(x)} = \log \left(\frac{\binom{n}{x} q^x (1-q)^{n-x}}{\binom{n}{x} p^x (1-p)^{n-x}} \right) = x \log \frac{q}{p} + (n-x) \log \frac{1-q}{1-p}$$

$$D_{KL}(g||f) = \mathbb{E}_g \left[\log \frac{g(x)}{f(x)} \right] = \mathbb{E}_g[X] \cdot \log \frac{q}{p} + (n - \mathbb{E}_g[X]) \log \frac{1-q}{1-p}$$

$$= n \left(q \cdot \log \frac{q}{p} + (1-q) \log \frac{1-q}{1-p} \right)$$

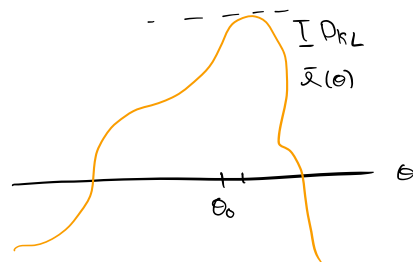
↳ exactly n times KL divergence in Bernoulli example

For $p=q$

$$D_{KL}(g||f) = n \cdot \frac{(p-q)^2}{2q(1-q)}$$

Generally, for $f(x) = f(x|\theta)$ and $g(x) = f(x|\theta_0)$

$$\begin{aligned} D_{KL}(f(x|\theta_0)||f(x|\theta)) &= \mathbb{E}_{\theta_0} \left[\log \frac{f(x|\theta_0)}{f(x|\theta)} \right] \\ &= \mathbb{E}_{\theta_0} [\log f(x|\theta_0)] - \mathbb{E}_{\theta_0} [\log f(x|\theta)] \\ &= \bar{\chi}(\theta_0) - \bar{\chi}(\theta) \end{aligned}$$



$$\bar{\lambda} = \mathbb{E}_{\theta_0} [\log f(x|\theta)]$$

Using a Taylor expansion we find

$$D_{KL}(f(x|\theta_0) \| f(x|\theta)) \approx \frac{1}{2} (\theta - \theta_0)^2 \cdot I(\theta_0)$$

Interpretation of $I(\theta_0)$: scale factor that relates $(\theta - \theta_0)^2$ in parameter space to the theoretical "differences" D_{KL}

Consistency of MLE in misspecified model

Suppose $X_1, \dots, X_n \stackrel{iid}{\sim} g(x)$, the pdf of the true distribution

We fit a parametric model $f(x|\theta)$ that doesn't contain $g(x)$

What happens to the MLE?

By definition the MLE $\hat{\theta}$ maximizes

$$\frac{1}{n} \ell(\theta) = \frac{1}{n} \sum_{i=1}^n \log f(x_i|\theta)$$

By LLN, $\frac{1}{n} \ell(\theta) \rightarrow \bar{\ell}(\theta)$ in probability

$$\bar{\ell}(\theta) = \mathbb{E}_g [\log f(x|\theta)]$$

Here, if g doesn't belong to our model

$$\bar{\ell}(\theta) = \underbrace{\mathbb{E}_g [\log g(x)]}_{\text{independent of } \theta} - \underbrace{\mathbb{E}_g \left[\log \frac{g(x)}{f(x|\theta)} \right]}_{D_{KL}(g \| f(x|\theta))}$$

therefore we maximize $\bar{\ell}(\theta)$ by maximizing $D_{KL}(g \| f(x|\theta))$

Suppose $\theta \mapsto D_{KL}(g(x) \| f(x|\theta))$ has a unique maximizer θ^*

Under some smoothness assumptions as $n \rightarrow \infty$, the MLE $\hat{\theta}$ converges to θ^* in probability

Example: Suppose we observe $x_1, \dots, x_n > 0$ and fit a model Exponential λ

$$f(x|\lambda) = \lambda e^{-\lambda x} \text{ for } x > 0$$

In reality $x_1, \dots, x_n \stackrel{iid}{\sim} \text{Gamma}(\alpha, 1)$, $g(x) = \frac{1}{\Gamma(\alpha)} x^{\alpha-1} e^{-x}$ only exponential if $\alpha=1$

This tells us that maximizing $D_{KL}(g(x) \| f(x|\lambda^*))$ estimates λ^*

$$\log \frac{g(x)}{f(x|\lambda)} = \log \left(\frac{\frac{1}{\Gamma(\alpha)} x^{\alpha-1} e^{-x}}{\lambda e^{-\lambda x}} \right) = -\log \Gamma(\alpha) + (\alpha-1) \log x - \log \lambda - (\lambda-1)x$$

Minimizing λ

$$0 = -\frac{1}{\lambda} + \mathbb{E}_g[X] \Rightarrow \lambda^* = \frac{1}{\mathbb{E}_g[X]} = \frac{1}{\alpha}$$

MLE $\hat{\lambda} \rightarrow \frac{1}{\alpha}$ in probability

Could solve this more directly through traditional methods

Ex. What is the asymptotic variance of \hat{X} ?

We have explicit $\hat{X} = \frac{1}{\bar{X}}$ so we can apply the delta method

$$\sqrt{n}(\bar{X} - \alpha) \rightarrow N(0, \text{Var}_g[X]) \text{ where } \text{Var}_g[X] = \alpha$$

Apply delta method w/ $h(\alpha) = \frac{1}{\alpha} \Rightarrow h'(\alpha)^2 = \frac{1}{\alpha^4}$

$$\text{So, } \sqrt{n}(\hat{X} - \frac{1}{\alpha}) = \sqrt{n}(h(\bar{X}) - h(\alpha)) \\ \rightarrow N(0, \alpha \cdot \frac{1}{\alpha^4}) = N(0, \frac{1}{\alpha^3})$$

Variance \hat{X} for large n is $\frac{1}{n\alpha^3}$

Fisher information estimate would be incorrect

$$I(\lambda) = \frac{1}{\lambda^2}$$

$\frac{1}{nI(\hat{\lambda})}$ to estimate variance

$$\hat{\lambda} \approx \lambda^* = \frac{1}{\alpha}$$

$I(\hat{\lambda}) \approx I(\lambda^*) = \alpha^2$ and $\frac{1}{nI(\hat{\lambda})} = \frac{1}{n\alpha^2}$ instead of correct variance $\frac{1}{n\alpha}$

4/6: The bootstrap

Simulation based approach to quantify uncertainty of statistical estimates

Can estimate standard error or a confidence interval

Given $X_1, \dots, X_n \stackrel{iid}{\sim} f(X|\theta)$, what is the standard error for an estimator $\hat{\theta}$ for θ

Idea of the bootstrap is to simulate new data and compute $\hat{\theta}$ from each dataset

Unfortunately, you can't simulate $f(X|\theta)$ without knowing θ

Bootstrap method involves simulations from an estimate of the true distribution

Parametric Bootstrap

Assume $X_1, \dots, X_n \stackrel{iid}{\sim} f(X|\theta)$

Estimate θ by $\hat{\theta}$ and simulate $X_1^*, \dots, X_n^* \stackrel{iid}{\sim} f(X|\hat{\theta})$

Analogous to the plug-in principle

Non-parametric bootstrap

No assumption of a parametric model

Instead, we sample X_1^*, \dots, X_n^* independently with replacement from the original X_1, \dots, X_n

Sample size is n

Likely to have repeated values

Some samples will be lost (unsampled)

63.2% of samples are expected to be present

Rationale for the nonparametric bootstrap

Estimated distribution is the empirical distribution

each observation places a mass of $\frac{1}{n}$

Draw new data from this estimated distribution

Key differences between the distribution and empirical distribution

Empirical distribution is always discrete

Some statistics don't make sense to compare
mode, max value, min value

The empirical CDF very closely resembles the true CDF

$$\hat{F}_n(t) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}\{X_i \leq t\}$$

as $n \rightarrow \infty$, this converges to CDF

Mean translates well between empirical and true distributions

Bootstrap and Misspecified Models

Suppose $X_1, \dots, X_n \stackrel{iid}{\sim} g(x)$. We fit $g(x)$ with Poisson λ

Fisher Information:

$$I(\lambda) = 1/\lambda$$

$$\sqrt{\frac{1}{n I(\lambda)}} = \sqrt{\frac{\lambda}{n}} = \sqrt{\frac{\bar{X}}{n}}$$

so the standard error is $\sqrt{\frac{\sigma^2}{n}}$

If Poisson were correct then $\sigma^2 = \lambda$ so $\sqrt{\frac{\bar{X}}{n}}$ is an accurate estimate of standard error

Non-parametric bootstrap guards against model misspecification

Bootstrap Confidence Intervals

Let $\hat{\theta}$ be an estimator of θ and \hat{se} be the bootstrap standard error estimate of $\hat{\theta}$

$\hat{\theta} \pm z(\alpha/2) \hat{se}$ for $100 - \alpha$ confidence interval \leftarrow Normal

Percentile bootstrap interval

Let $\hat{\theta}_1^*, \dots, \hat{\theta}_B^*$ be the values of $\hat{\theta}$ computed in B simulations

Let $\hat{\theta}^{*(\alpha/2)}$ and $\hat{\theta}^{*(1-\alpha/2)}$ be the empirical $\alpha/2$ and $1-\alpha/2$ quantiles of the simulated values

$$[\hat{\theta}^{*(\alpha/2)}, \hat{\theta}^{*(1-\alpha/2)}]$$

Requires symmetry?

Basic Bootstrap Interval

Let $q^{(\alpha/2)}$ and $q^{(1-\alpha/2)}$ be the $\alpha/2$ and $1-\alpha/2$ quantiles of $\hat{\theta}_1^* - \hat{\theta}, \dots, \hat{\theta}_B^* - \hat{\theta}$

Use this to approximate true distribution of $\hat{\theta} - \theta$

$$\left[\hat{\theta} - q^{(1-\alpha/2)}, \hat{\theta} - q^{(\alpha/2)} \right]$$

since $\hat{\theta} - \theta \in [q^{(\alpha/2)}, q^{(1-\alpha/2)}] \Leftrightarrow$

Same as percentile confidence interval if it is symmetric

Advantages and Disadvantages of bootstrap

- Easy to apply
- Obtains estimates valid under misspecification
- Can be computationally prohibitive
- Validity of bootstrap requires analytic proofs

4/11: Generalized Likelihood Ratio Test

- ① Simple Null Hypothesis
- ② Sub-model null hypothesis

Generalized Likelihood Ratio Test for Simple null hypothesis

Observe: $X_1, \dots, X_n \stackrel{iid}{\sim} f(X|\theta)$

$$H_0: \theta = \theta_0$$

$$H_1: \theta \neq \theta_0$$

The GLRT rejects H_0 for small values of \mathcal{L}

$$\mathcal{L} = \frac{\text{lik}(\theta_0)}{\max_{\theta} \text{lik}(\theta)} \quad \text{where } \text{lik}(\theta) = \prod_{i=1}^n f(X_i|\theta)$$

H_1 is composite, so you replace $\text{lik}(\theta)$ with $\max_{\theta} \text{lik}(\theta)$

$$\max_{\theta} \text{lik}(\theta) = \text{lik}(\hat{\theta}) \text{ where } \hat{\theta} \text{ is the MLE}$$

By definition of MLE

$$\text{lik}(\hat{\theta}) \geq \text{lik}(\theta_0) \text{ so } \Lambda \leq 1$$

If H_0 were true, we expect $\hat{\theta} \approx \theta_0$ for large n

Rejecting H_0 for small Λ is the same as rejecting H_0 for large $-2 \log \Lambda$

$$-2 \log \Lambda = 2\lambda(\hat{\theta}) - 2\lambda(\theta_0)$$

$$\lambda(\theta) = \log \text{lik}(\theta) = \sum_{i=1}^n \log(f(x_i; \theta))$$

Since $\Lambda \leq 1$, $-2 \log \Lambda \geq 0$

We reject H_0 when

$$-2 \log \Lambda \geq \chi_k^2(\alpha) \leftarrow \text{upper } \alpha \text{ point of } \chi_k^2$$

k is the dimension of the parameter space

Example: Let $X_1, \dots, X_n \stackrel{iid}{\sim} N(\theta, 1)$. Test null hypothesis $\theta = 0$ and $H_1: \theta \neq 0$

MLE for θ is $\hat{\theta} = \bar{X}$. We compute

$$\text{lik}(\theta) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi}} e^{-\frac{x_i^2}{2}}$$

$$\text{lik}(\hat{\theta}) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi}} e^{-\frac{(x_i - \bar{x})^2}{2}}$$

$$\Lambda = \frac{\text{lik}(\theta)}{\text{lik}(\hat{\theta})} = \exp\left(-\sum_{i=1}^n \frac{x_i^2}{2} + \sum_{i=1}^n \frac{(x_i - \bar{x})^2}{2}\right)$$

$$= \exp\left(-\frac{n}{2} \bar{x}^2\right) \leftarrow \text{expand square and combine terms}$$

$$-2 \log \Lambda = n \bar{x}^2 = (\sqrt{n} \bar{x})^2$$

Under $H_0: \theta = 0$ — $\bar{x} \sim N(0, 1/n)$ so $\sqrt{n} \bar{x} \sim N(0, 1)$

$$\text{so } -2 \log \Lambda = (\sqrt{n} \bar{x})^2 \sim \chi_1^2$$

For more general non-parametric models

Thm: Let $X_1, \dots, X_n \stackrel{iid}{\sim} f(x|\theta)$, a parametric model with parameter space of dimension k . Let θ_0 be in the interior of the parameter space. Under smoothness conditions

$$H_0: \theta = \theta_0 \text{ vs. } H_1: \theta \neq \theta_0$$

$$-2 \log \Lambda \rightarrow \chi_k^2 \text{ in distribution as } n \rightarrow \infty \text{ under } H_0$$

So, the GLRT that rejects $-2 \log \Lambda \geq \chi_k^2(\alpha)$ is an asymptotic level- α test

Proof sketch: Suppose $k=1$ when $\theta \in \mathbb{R}$ is a single parameter

$$-2 \log \Lambda = 2\lambda(\hat{\theta}) - 2\lambda(\theta_0)$$

Taylor Expansion: $\lambda(\theta_0)$ around $\hat{\theta}$

$$\lambda(\theta_0) \approx \lambda(\hat{\theta}) + (\theta_0 - \hat{\theta}) \cdot \lambda'(\hat{\theta}) + \frac{1}{2} (\theta_0 - \hat{\theta})^2 \cdot \lambda''(\hat{\theta})$$

Recall: $\lambda'(\hat{\theta}) = 0$ since it is at a maximizing point

$$\lambda''(\hat{\theta}) = -n I(\hat{\theta}) = -n I(\theta_0) \leftarrow \text{from earlier}$$

$$\Rightarrow \lambda(\theta_0) \approx \lambda(\hat{\theta}) - \frac{n}{2} I(\theta_0) (\theta_0 - \hat{\theta})^2$$

$$\Rightarrow -2 \log \Lambda = n I(\theta_0) \cdot (\theta_0 - \hat{\theta})^2$$

Under $H_0: \sqrt{n}(\hat{\theta} - \theta_0) \rightarrow N(0, 1/I(\theta_0))$ in distribution, by asymptotic normality for MLE

$$\sqrt{n I(\theta_0)} (\hat{\theta} - \theta_0) \rightarrow N(0, 1)$$

$$n I(\theta_0) (\hat{\theta} - \theta_0)^2 \rightarrow \chi_1^2$$

Dimension is the number of parameters minus the number of equality constraints

Example: Consider $(X_1, \dots, X_k) \sim \text{Multinomial}(n, (P_1, P_2, \dots, P_k))$

$$H_0: (P_1, \dots, P_k) = (P_{01}, \dots, P_{0k})$$

$$H_1: (P_1, \dots, P_k) \neq (P_{01}, \dots, P_{0k})$$

Likelihood function:

$$\text{lik}(P_1, \dots, P_k) = \binom{n}{X_1, \dots, X_k} P_1^{X_1} P_2^{X_2} \dots P_k^{X_k}$$

$$\ell(P_1, \dots, P_k) = \log \binom{n}{X_1, \dots, X_k} + X_1 \log P_1 + \dots + X_k \log P_k$$

$$\text{The MLE is } (\hat{P}_1, \dots, \hat{P}_k) = \left(\frac{X_1}{n}, \dots, \frac{X_k}{n} \right)$$

$$\begin{aligned} \Rightarrow -2 \log \Lambda &= 2\ell(\hat{P}_1, \dots, \hat{P}_k) - 2\ell(P_{01}, \dots, P_{0k}) \\ &= 2X_1 \left(\log \frac{X_1}{n} - \log P_{01} \right) + \dots + 2X_k \left(\log \frac{X_k}{n} - \log P_{0k} \right) \end{aligned}$$

Dimension is $k-1$ (1 equality constraint)

$$\text{GLRT rejects when } -2 \log \Lambda \geq \chi_{k-1}^2(\alpha)$$

GLRT for a sub-model

Let $X_1, \dots, X_n \stackrel{iid}{\sim} f(X|\theta)$. Let Ω be the parameter space.

$$H_0: \theta \in \Omega_0$$

$\Omega_0 \subset \Omega$ is a lower dimensional space in Ω

$$H_1: \theta \notin \Omega_0$$

Example: Consider $X_1, \dots, X_n \stackrel{iid}{\sim} N(\mu, \sigma^2)$

$\Omega = \{(\mu, \sigma^2) : \sigma^2 > 0\}$ is a region of the plane \mathbb{R}^2

$$H_0: \mu = 0$$

$$H_1: \mu \neq 0$$

Then $\Omega_0 = \{(\mu, \sigma^2) : \mu = 0, \sigma^2 > 0\}$ ← a line inside Ω

Ω_0 has dimension 1 while Ω has dimension 2

GLRT rejects H_0 for small values of

$$\Lambda = \frac{\max_{\theta \in \Omega_0} \text{lik}(\theta)}{\max_{\theta \in \Omega} \text{lik}(\theta)}$$

$$\text{In other words, } \Lambda = \frac{\text{lik}(\hat{\theta}_0)}{\text{lik}(\hat{\theta})} \quad \begin{array}{l} \hat{\theta}_0 \text{ is MLE in } \Omega_0 \\ \hat{\theta} \text{ is MLE in } \Omega \end{array}$$

Once again we consider $-2 \log \Lambda$

GLRT rejects for

$$-2 \log \Lambda \geq \chi_k^2(\alpha)$$

where k is the difference in dimension between Ω and Ω_0

If $\Omega_0 = \Theta_0$ we have dimension = 0, so the submodel generalization simplifies to the simple null example

Example: (One-sample t-test)

$$X_1, \dots, X_n \stackrel{iid}{\sim} N(\mu, \sigma^2)$$

log-likelihood:

$$\begin{aligned} \mathcal{L}(\mu, \sigma^2) &= \sum_{i=1}^n \log \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i - \mu)^2}{2\sigma^2}} \\ &= -\frac{n}{2} \log(2\pi\sigma^2) - \sum_{i=1}^n \frac{(x_i - \mu)^2}{2\sigma^2} \end{aligned}$$

Full model MLE:

$$(\hat{\mu}, \hat{\sigma}^2) = (\bar{X}, \frac{1}{n} \sum_{i=1}^n (x_i - \bar{X})^2)$$

$$\Rightarrow \mathcal{L}(\hat{\mu}, \hat{\sigma}^2) = -\frac{n}{2} (\log(2\pi\hat{\sigma}^2) + 1)$$

Sub-model MLE:

$$\mu=0$$

$$\text{MLE is } (\hat{\mu}_0, \hat{\sigma}_0^2) = (0, \frac{1}{n} \sum_{i=1}^n x_i^2) \quad \leftarrow \text{from HW6}$$

$$\Rightarrow \mathcal{L}(\hat{\mu}_0, \hat{\sigma}_0^2) = -\frac{n}{2} \log(2\pi\hat{\sigma}_0^2) - \frac{n}{2}$$

$$-2 \log \mathcal{L} = 2\mathcal{L}(\hat{\mu}, \hat{\sigma}^2) - 2\mathcal{L}(\hat{\mu}_0, \hat{\sigma}_0^2)$$

$$= n \log \left(\frac{\hat{\sigma}_0^2}{\hat{\sigma}^2} \right)$$

$$\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{X})^2 \quad \hat{\sigma}_0^2 = \frac{1}{n} \sum_{i=1}^n x_i^2 \quad \text{so } \hat{\sigma}^2 = \hat{\sigma}_0^2 - \bar{X}^2$$

$$\Rightarrow -2 \log \mathcal{L} = n \log \frac{\hat{\sigma}_0^2}{\hat{\sigma}^2} = n \log \left(1 + \frac{\bar{X}^2}{\hat{\sigma}^2} \right) = n \log \left(1 + \frac{1}{n-1} T^2 \right)$$

$$\text{recall: } T = \frac{\sqrt{n}\bar{X}}{\sqrt{\frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{X})^2}}$$

This is increasing in $|T|$ so rejecting for large $-2 \log \mathcal{L}$ is the same as rejecting large $|T|$

Except, for 2-sided t-test we reject H_0 when $|T| \geq t_{n-1}(\frac{\alpha}{2})$

for GLRT we reject H_0 when $-2 \log \mathcal{L} \geq \chi^2_{\alpha}$

for large n $-2 \log \mathcal{L} \approx \chi^2_{\alpha}$

$$-2 \log \mathcal{L} = n \log \left(1 + \frac{1}{n-1} T^2 \right)$$

$$\approx n \cdot \frac{1}{n-1} T^2 \approx T^2 = Z^2 \text{ where } Z \sim N(0,1)$$

4/18: Chi-squared tests for categorical data

Recap: GLRT

$$H_0: \Theta \in \Omega_0 \text{ vs. } H_1: \Theta \notin \Omega_0$$

Generalized Neyman Pearson Lemma

$$\mathcal{L} = \frac{\text{lik}(\hat{\Theta}_0)}{\text{lik}(\hat{\Theta})} \text{ where: } \hat{\Theta}_0 \text{ the MLE in } \Omega_0$$

$\hat{\Theta}$ the MLE in full model

Test statistic: $-2 \log \mathcal{L}$

For large sample distribution is $\approx \chi^2_k$ where k is the difference in dimension between Ω and Ω_0

Example: Hardy-Weinberg Equilibrium

Genotypes at single locus $\in \{AA, Aa, aa\}$ in n individuals with observed counts N_{AA} , N_{Aa} , and N_{aa}

Full model: $(N_{AA}, N_{Aa}, N_{aa}) \sim \text{Multinomial}(n, (p_{AA}, p_{Aa}, p_{aa}))$

$$H_0: p_{AA} = (1-\theta)^2, p_{Aa} = 2\theta(1-\theta), p_{aa} = \theta^2 \text{ for some } \theta \in (0,1)$$

$$lik(P_{AA}, P_{Aa}, P_{aa}) = \binom{n}{N_{AA}, N_{Aa}, N_{aa}} \times P_{AA}^{N_{AA}} P_{Aa}^{N_{Aa}} P_{aa}^{N_{aa}}$$

$$\Rightarrow \log \binom{n}{N_{AA}, N_{Aa}, N_{aa}} + N_{AA} \log P_{AA} + N_{Aa} \log P_{Aa} + N_{aa} \log P_{aa}$$

$$\begin{aligned} \Rightarrow -2 \log \mathcal{L} &= 2 \mathcal{L}(\hat{P}_{AA}, \hat{P}_{Aa}, \hat{P}_{aa}) - 2 \mathcal{L}(\hat{P}_{0AA}, \hat{P}_{0Aa}, \hat{P}_{0aa}) \\ &= 2N_{AA} \left(\log \frac{\hat{P}_{AA}}{\hat{P}_{0AA}} \right) + 2N_{Aa} \left(\log \frac{\hat{P}_{Aa}}{\hat{P}_{0Aa}} \right) + 2N_{aa} \left(\log \frac{\hat{P}_{aa}}{\hat{P}_{0aa}} \right) \end{aligned}$$

Full Model MLE: $\hat{P}_{AA} = \frac{N_{AA}}{n}$ $\hat{P}_{Aa} = \frac{N_{Aa}}{n}$ $\hat{P}_{aa} = \frac{N_{aa}}{n}$

Sub-model MLE: $\hat{\theta} = \frac{2N_{aa} - N_{Aa}}{2n}$

$$P_{0AA} = (1-\hat{\theta})^2, \quad P_{0Aa} = 2\hat{\theta}(1-\hat{\theta}), \quad P_{0aa} = \hat{\theta}^2$$

Dimensions: Full model: 2 (3 params w/ 1 constraint)

Sub-model: 1 (single param θ)

$$k=1$$

Compare $-2 \log \mathcal{L}$ to $\chi_1^2(\infty)$

Test of Independence

Example: General Social Survey

Random sample of 1972 people

	Dem	Repub	Indep
M	422	381	273
F	299	365	232

Want to test whether gender is independent of party affiliation

$$\text{Model: } \begin{pmatrix} N_{11} & N_{12} & N_{13} \\ N_{21} & N_{22} & N_{23} \end{pmatrix} \sim \text{Multinomial} \left(n, \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \end{pmatrix} \right)$$

$$\text{Let } p_{i.} = \sum_j P_{ij} \quad (\text{row sums})$$

$$P_{.j} = \sum_i P_{ij} \quad (\text{column sums})$$

$$H_0: P_{ij} = p_{i.} \times P_{.j} \quad \text{for every } ij \quad \text{vs.} \quad H_1:$$

Dimensions:

Full model: 5 (6 params, 1 constraint $\sum_{ij} P_{ij} = 1$)

Sub model: 3 (5 params, 2 constraints)

Parameters: $p_{1.}, p_{2.}, P_{.1}, P_{.2}, P_{.3}$

Constraints: $p_{1.} + p_{2.} = 1$ $P_{.1} + P_{.2} + P_{.3} = 1$

$k=2$ so $-2 \log \mathcal{L}$ compare against $\chi_2^2(\infty)$

Consider more generally,

$$(N_1, \dots, N_k) \sim \text{Multinomial}(n, (p_1, \dots, p_k))$$

Test $H_0: (p_1, \dots, p_k) \in \mathcal{L}_0$

Multinomial likelihood

$$\text{lik}(p_1, \dots, p_k) = \binom{n}{N_1, \dots, N_k} \times \prod_{i=1}^k p_i^{N_i}$$

Let \hat{p}_i and $\hat{p}_{0,i}$ be the full model and submodel MLEs.

$$\begin{aligned} -2 \log \mathcal{L} &= 2 \log \text{lik}(\hat{p}_1, \dots, \hat{p}_k) - 2 \log \text{lik}(\hat{p}_{0,1}, \dots, \hat{p}_{0,k}) \\ &= 2 \sum_{i=1}^k N_i \cdot \log \frac{\hat{p}_i}{\hat{p}_{0,i}} \end{aligned}$$

Recall: $\hat{p}_i = \frac{N_i}{n}$

Expected counts in sub-model $E_i = n \cdot \hat{p}_{0,i}$

$$\Rightarrow -2 \log \mathcal{L} = 2 \sum_{i=1}^k N_i \log \frac{N_i}{E_i}$$

Return to $k=6$ example

$$\begin{aligned} \text{lik}(p_1, p_2, p_3, p_{12}, p_{23}) &= \binom{n}{N_{11}, N_{12}, \dots, N_{23}} \times \prod_{i=1}^2 \prod_{j=1}^3 (p_i \dots p_j)^{N_{ij}} \\ &= \binom{n}{N_{11}, N_{12}, \dots, N_{23}} \times \prod_{i=1}^2 p_i^{N_i} \times \prod_{j=1}^3 p_j^{N_j} \end{aligned}$$

where $N_i = N_{i1} + N_{i2} + N_{i3}$

$$N_j = N_{1j} + N_{2j}$$

Take a log and maximize subject to $\sum_i p_i = 1$, $\sum_j p_j = 1$

$$\mathcal{J} = \text{Lagrangian: } \log \binom{n}{N_{11}, \dots, N_{23}} + \sum_{i=1}^2 N_i \log p_i + \sum_{j=1}^3 N_j \log p_j + \lambda \left(\sum_{i=1}^2 p_i - 1 \right) + \mu \left(\sum_{j=1}^3 p_j - 1 \right)$$

$$0 = \frac{\partial \mathcal{J}}{\partial p_i} = \frac{N_i}{p_i} + \lambda \Rightarrow p_i = \frac{-N_i}{\lambda}$$

$$0 = \frac{\partial \mathcal{J}}{\partial p_j} = \frac{N_j}{p_j} + \mu \Rightarrow p_j = \frac{-N_j}{\mu}$$

$$\begin{aligned} 0 = \frac{\partial \mathcal{J}}{\partial \lambda} &= p_1 + p_2 - 1 \Rightarrow \frac{-N_1}{\lambda} - \frac{N_2}{\lambda} = \frac{-n}{\lambda} = 1 \\ &\Rightarrow \lambda = -n \end{aligned}$$

$$\Rightarrow \hat{p}_i = \frac{N_i}{n}$$

$$0 = \frac{\partial \mathcal{J}}{\partial \mu} = p_1 + p_2 + p_3 - 1 = \frac{-N_{11}}{\mu} - \frac{N_{12}}{\mu} - \frac{N_{21}}{\mu} - \frac{N_{22}}{\mu} = \frac{-n}{\mu} = 1$$

$$\Rightarrow \mu = -n$$

$$\Rightarrow \hat{p}_{ij} = \frac{N_{ij}}{n}$$

$$\Rightarrow \hat{p}_{0,ij} = \hat{p}_i \times \hat{p}_j = \frac{N_i \cdot N_j}{n^2}$$

Expected counts: $E_{ij} = n \cdot \hat{p}_{0,ij} = \frac{N_i \cdot N_j}{n}$

Plug in into $-2 \log \Lambda = 2 \sum_{r=1}^2 \sum_{j=1}^3 N_{rj} \log \frac{N_{rj}}{E_{rj}} = 8.31$

Compare to χ^2_2 so we find a p-value of 0.016

Pearson chi-squared test

Alternative to GLRT

$$X^2 = \sum_{r=1}^k \frac{(N_r - E_r)^2}{E_r}$$

Test rejects H_0 when X^2 exceeds $\chi^2_{\text{dof}}(\alpha)$ value
↑
difference in dimension of
the models

X^2 is similar to $-2 \log \Lambda$

See via a Taylor expansion (4/13 lecture 22)

Test of Homogeneity

Setting: $(N_1, \dots, N_k) \sim \text{Multinomial}(n, (p_1, \dots, p_k))$

$(M_1, \dots, M_k) \sim \text{Multinomial}(m, (q_1, \dots, q_k))$

$H_0: p_i = q_i$ for all $i=1, \dots, k$

Example: Jane Austen + Emulator

	a	an	this	that	with	without
Ch. 1 + 6	101	11	15	37	23	10
Ch. 12 + 24	83	29	15	22	43	4

Ch 1 + 6 \sim Multinomial(202, (p_1, \dots, p_6))

Ch 12 + 24 \sim Multinomial(196, (q_1, \dots, q_6))

Test $H_0: p_i = q_i$ for all $i=1, \dots, 6$

GLRT statistic

$$-2 \log \Lambda = 2 \sum_{r=1}^k N_r \log \frac{N_r}{E_r} + M_r \log \frac{M_r}{F_r}$$

N_i, m_i are the observed counts

$$E_i = n \cdot \hat{p}_{0,i} \quad F_i = m \cdot \hat{q}_{0,i}$$

MLEs are $\hat{p}_{0,i} = \frac{N_i + M_i}{n+m}$

Dimension of full model: $5+5 = 10$

Dimension of sub model: 5

$k = 10 - 5 = 5$ so compare against $\chi^2_5(\alpha)$

Find p-value to be 0.0014 \leftarrow very different!

4/11/18: The Bradley-Terry Model

Data: $\mathcal{Y} = (Y_1, \dots, Y_n)$

Parametric model - $f(\mathcal{Y}|\theta)$ is the joint PDF/PMF of our data dependent on $\theta \in \mathbb{R}^k$

Log-likelihood function - $\ell(\theta) = \sum_{i=1}^n \log f(Y_i|\theta)$

MLE - $\hat{\theta}$ that maximizes $\ell(\theta)$

Recall: If $Y_1, \dots, Y_n \stackrel{iid}{\sim} f(Y|\theta)$

$$J(\theta) = \text{Var}_{\theta} \left[\frac{\partial}{\partial \theta} \log f(Y|\theta) \right] = -\mathbb{E}_{\theta} \left[\frac{\partial^2}{\partial \theta^2} \log f(Y|\theta) \right]$$

For large n , the MLE $\hat{\theta}$ is approximately distributed as

$$N(\theta_0, \frac{1}{n} J(\theta_0))$$

$$\begin{aligned} \text{Define } I_{\mathcal{Y}}(\theta) = n J(\theta) &= \text{Var}_{\theta} \left[\sum_{i=1}^n \frac{\partial}{\partial \theta} \log f(Y_i|\theta) \right] = \text{Var}_{\theta} [\mathcal{L}'(\theta)] \\ &= -\mathbb{E}_{\theta} \left[\sum_{i=1}^n \frac{\partial^2}{\partial \theta^2} \log f(Y_i|\theta) \right] = -\mathbb{E}_{\theta} [\mathcal{L}''(\theta)] \end{aligned}$$

Generally for $\mathcal{Y} \sim f(\mathcal{Y}|\theta)$, define Fisher information of all observations

$$I_{\mathcal{Y}}(\theta) = \text{Var}_{\theta} [\mathcal{L}'(\theta)] = -\mathbb{E}_{\theta} [\mathcal{L}''(\theta)]$$

Under regularity assumptions, the MLE $\hat{\theta}$ has approximately distribution $N(\theta_0, \frac{1}{I_{\mathcal{Y}}(\theta_0)})$ ← Estimate when data isn't iid

For multiple parameters $\theta \in \mathbb{R}^k$, we define $I_{\mathcal{Y}}(\theta) \in \mathbb{R}^{k \times k}$

$$\begin{aligned} I_{\mathcal{Y}}(\theta)_{ij} &= \text{Cov}_{\theta} \left[\frac{\partial}{\partial \theta_i} \mathcal{L}(\theta), \frac{\partial}{\partial \theta_j} \mathcal{L}(\theta) \right] \\ &= -\mathbb{E}_{\theta} \left[\frac{\partial^2}{\partial \theta_i \partial \theta_j} \mathcal{L}(\theta) \right] \end{aligned}$$

Again, $\hat{\theta}$ is $\approx N(\theta_0, I_{\mathcal{Y}}(\theta_0)^{-1})$

Bradley Terry Model

Example: NBA has 30 basketball teams
Each team plays 82 games
How can we rank teams?

① Naively: Count number of wins against number of losses

However, each team plays each other team between 2 and 4 times

② Bradley-Terry: Represent strength of team i by $B_i \in \mathbb{R}$

If game played between teams i and j , outcome is random and depends on B_i and B_j

Outcome - Bernoulli (P_{ij})

$$\log \frac{P_{ij}}{1-P_{ij}} = B_i - B_j \Rightarrow P_{ij} = \frac{e^{B_i - B_j}}{1 + e^{B_i - B_j}} = \frac{e^{B_i}}{e^{B_i} + e^{B_j}}$$

- Each B_i is only meaningful relative to other B_j 's

We can add any constant $C \in \mathbb{R}$ to all B_i 's without changing the model

Allows us to select a team as a standard (set to 0)
in this case B_j is relative strength to the standardized teams

- Can specify order of each game sit. the first team is always the home team

Incorporate home team advantage by adding an additional intercept

$$\log \frac{P_{ij}}{1-P_{ij}} = \alpha + B_i + B_j$$

Estimation and Inference

$K=30$ (number of teams)

$n=150$ (number of total games)

Questions: Estimate α and B_1, B_2, \dots, B_K (constraining $B_{i,i} = B_i = 0$)

Test the null hypothesis $H_0: \alpha = 0$ (no home team advantage)

Obtain confidence interval

We observe n games $(i_1, j_1), (i_2, j_2), \dots, (i_n, j_n)$ where i is always the home team

Outcomes: $Y_1, Y_2, \dots, Y_n \in \{0, 1\}$

$$Y_m = \begin{cases} 1 & \text{if } i \text{ beat } j \text{ in the } m^{\text{th}} \text{ game} \\ 0 & \text{otherwise} \end{cases}$$

Log-likelihood:

$$L(\alpha, B_1, \dots, B_K) = \prod_{m=1}^n P_{i_m j_m}^{Y_m} (1 - P_{i_m j_m})^{1 - Y_m} = \prod_{m=1}^n (1 - P_{i_m j_m}) \left(\frac{P_{i_m j_m}}{1 - P_{i_m j_m}} \right)^{Y_m}$$

$$\begin{aligned} \ell(\alpha, B_1, \dots, B_K) &= \sum_{m=1}^n Y_m \log \frac{P_{i_m j_m}}{1 - P_{i_m j_m}} + \log(1 - P_{i_m j_m}) \\ &\quad \underbrace{\hspace{10em}}_{\text{log-odds}} \\ &= \alpha + B_{i_m} + B_{j_m} \end{aligned}$$

$$= \sum_{m=1}^n Y_m [\alpha + B_{i_m} + B_{j_m}] - \log(1 + e^{\alpha + B_{i_m} + B_{j_m}})$$

① Common approach to estimate $\Theta(\alpha, B_1, \dots, B_K)$ via MLE

Solve:

$$0 = \frac{\partial \ell}{\partial \alpha} = \sum_{m=1}^n \left[Y_m - \frac{e^{\alpha + B_{i_m} + B_{j_m}}}{1 + e^{\alpha + B_{i_m} + B_{j_m}}} \right]$$

$$0 = \frac{\partial \ell}{\partial B_i} = \sum_{m: i_m=i} \left[Y_m - \frac{e^{\alpha + B_{i_m} + B_{j_m}}}{1 + e^{\alpha + B_{i_m} + B_{j_m}}} \right] + \sum_{m: j_m=i} \left[-Y_m + \frac{e^{\alpha + B_{i_m} + B_{j_m}}}{1 + e^{\alpha + B_{i_m} + B_{j_m}}} \right]$$

No closed form so we solve it numerically

Gradient: $\nabla \ell(\theta) = \left(\frac{\partial \ell}{\partial \alpha}, \dots, \frac{\partial \ell}{\partial B_K} \right)$

Hessian: $\nabla^2 \ell(\theta) = \begin{pmatrix} \frac{\partial^2 \ell}{\partial \alpha^2} & \dots & \frac{\partial^2 \ell}{\partial \alpha \partial B_K} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 \ell}{\partial \alpha \partial B_K} & \dots & \frac{\partial^2 \ell}{\partial B_K^2} \end{pmatrix}$

Newton-Raphson: $\theta^{(t+1)} = \theta^{(t)} - (\nabla^2 \ell(\theta^{(t)}))^{-1} \nabla \ell(\theta^{(t)})$

② To test $H_0: \alpha = 0$

Use the GLRT sub-model where $\alpha = 0$

$$0 = \frac{\partial \ell}{\partial B_i} = \sum_{m: i_m=i} \left[Y_m - \frac{e^{B_{i_m} + B_{j_m}}}{1 + e^{B_{i_m} + B_{j_m}}} \right] + \sum_{m: j_m=i} \left[-Y_m + \frac{e^{B_{i_m} + B_{j_m}}}{1 + e^{B_{i_m} + B_{j_m}}} \right]$$

Solve numerically using Newton-Raphson

$$\text{Compute } -2 \log \Lambda = 2\ell(\hat{\alpha}, \hat{\beta}_1, \dots, \hat{\beta}_K) - 2\ell(0, \hat{\beta}_1, \dots, \hat{\beta}_K)$$

Compare against $\chi^2_1(\alpha)$

③ Confidence Interval for $\beta_i - \beta_j$:

Center the interval at $\hat{\beta}_i - \hat{\beta}_j$ with the MLE's

Estimate standard error of $\hat{\beta}_i - \hat{\beta}_j$

$$\begin{aligned}\text{Var}[\hat{\beta}_i - \hat{\beta}_j] &= \text{Cov}[\hat{\beta}_i - \hat{\beta}_j, \hat{\beta}_i - \hat{\beta}_j] \\ &= \text{Cov}[\hat{\beta}_i, \hat{\beta}_i] - \text{Cov}[\hat{\beta}_i, \hat{\beta}_j] - \text{Cov}[\hat{\beta}_j, \hat{\beta}_i] + \text{Cov}[\hat{\beta}_j, \hat{\beta}_j] \\ &= \text{Var}[\hat{\beta}_i] + \text{Var}[\hat{\beta}_j] - 2 \text{Cov}[\hat{\beta}_i, \hat{\beta}_j] \\ &\approx (\mathbb{I}_Y(\theta)^{-1})_{ii} + (\mathbb{I}_Y(\theta)^{-1})_{jj} - 2 (\mathbb{I}_Y(\theta)^{-1})_{ij}\end{aligned}$$

Holds for large n

$$\mathbb{I}_Y(\theta) = -\mathbb{E}_{\theta}[\nabla^2 \ell(\theta)] \text{ where } \nabla^2 \ell(\theta) \text{ is the Hessian}$$

Can estimate standard error of $\hat{\beta}_i - \hat{\beta}_j$ as

$$\hat{se} = \sqrt{(\mathbb{I}_Y(\theta)^{-1})_{ii} + (\mathbb{I}_Y(\theta)^{-1})_{jj} - 2 (\mathbb{I}_Y(\theta)^{-1})_{ij}}$$

We expect $\hat{\beta}_i - \hat{\beta}_j$ to be approx. normal for large n .

$$\hat{\beta}_i - \hat{\beta}_j \pm \hat{se} \cdot z\left(\frac{\alpha}{2}\right)$$

② Test $H_0: \alpha = 0$

Randomly permute (i_m, j_m) for each gene

Compute a test statistic T on the permuted data

$$T = -2 \log \Lambda$$

③ Non parametric bootstrap

Resample (i_m^*, j_m^*) with replacement

Estimate $\hat{\beta}_i - \hat{\beta}_j$ using bootstrap samples

Avoid model misspecification

4/20: Logistic Regression

Model for binary classification

Example: Predict whether a user will click on an ad

Have n ad impressions

Binary response $Y_i = \begin{cases} 1 & \text{if clicked} \\ 0 & \text{otherwise} \end{cases}$

Other features

- size of ad
- user age
- etc.

represented by a collection of p covariates

Logistic Regression: n responses are independent

$$Y_i \sim \text{Bernoulli}(p)$$

$$\log \frac{p_i}{1-p_i} = \alpha + \beta_1 X_{i1} + \dots + \beta_p X_{ip}$$

α is the intercept or baseline log-odds

β_j represents the change in log odds for a one unit change in X_j

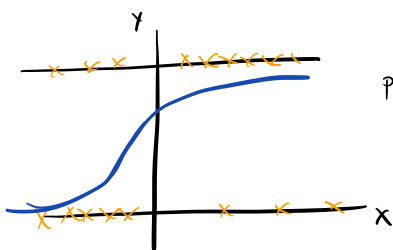
Parameters: $(\alpha, \beta_1, \dots, \beta_p)$

$$P[Y_i = 1] = p_i = \frac{e^{\alpha + \beta_1 X_{i1} + \dots + \beta_p X_{ip}}}{1 + e^{\alpha + \beta_1 X_{i1} + \dots + \beta_p X_{ip}}}$$

Assume one covariate $p=1$ for simplicity

$$\beta = B, \text{ and } X_i = X_i$$

Data = $(X_1, Y_1), \dots, (X_n, Y_n)$



$$p(x) = \frac{e^{\alpha + Bx}}{1 + e^{\alpha + Bx}}$$

Estimation and Inference

① Estimating the regression coefficients

② Estimating the "conversion" probability $p(x) = \frac{e^{\alpha + Bx}}{1 + e^{\alpha + Bx}}$ for a new impression with covariate x

③ Provide a 95% confidence interval for B

④ Test a null hypothesis $H_0: B=0$

① Estimating (α, B) via MLE

$$\text{lik}(\alpha, B) = \prod_{i=1}^n p_i^{Y_i} (1-p_i)^{1-Y_i} \quad \text{where } p_i = \frac{e^{\alpha + Bx_i}}{1 + e^{\alpha + Bx_i}}$$

$$= \prod_{i=1}^n (1-p_i)^{1-Y_i} \left(\frac{p_i}{1-p_i} \right)^{Y_i}$$

$$\Rightarrow \ell(\alpha, B) = \sum_{i=1}^n Y_i \underbrace{\log \frac{p_i}{1-p_i}}_{\alpha + Bx_i} + \log(1-p_i) \underbrace{-\log(1 + e^{\alpha + Bx_i})}_{-\log(1 + e^{\alpha + Bx_i})}$$

$$= \sum_{i=1}^n \left(Y_i (\alpha + Bx_i) - \log(1 + e^{\alpha + Bx_i}) \right)$$

MLE: set derivatives to 0

$$0 = \frac{\partial \ell}{\partial \alpha} = \sum_{i=1}^n (Y_i - p_i)$$

$$0 = \frac{\partial \mathcal{L}}{\partial \beta} = \sum_{i=1}^n (Y_i - P_i) X_i$$

No closed form solution so we once again use Newton-Raphson Method

$$\begin{pmatrix} \alpha^{(k+1)} \\ \beta^{(k+1)} \end{pmatrix} = \begin{pmatrix} \alpha^{(k)} \\ \beta^{(k)} \end{pmatrix} - \left(\nabla^2 \mathcal{L}(\alpha^{(k)}, \beta^{(k)}) \right)^{-1} \cdot \nabla \mathcal{L}(\alpha^{(k)}, \beta^{(k)})$$

$$\nabla \mathcal{L}(\alpha, \beta) = \begin{pmatrix} \frac{\partial \mathcal{L}}{\partial \alpha} \\ \frac{\partial \mathcal{L}}{\partial \beta} \end{pmatrix} = \sum_{i=1}^n (Y_i - P_i) \begin{pmatrix} 1 \\ X_i \end{pmatrix}$$

$$\nabla^2 \mathcal{L}(\alpha, \beta) = \begin{pmatrix} \frac{\partial^2 \mathcal{L}}{\partial \alpha^2} & \frac{\partial^2 \mathcal{L}}{\partial \alpha \partial \beta} \\ \frac{\partial^2 \mathcal{L}}{\partial \alpha \partial \beta} & \frac{\partial^2 \mathcal{L}}{\partial \beta^2} \end{pmatrix} = \sum_{i=1}^n -P_i(1-P_i) \begin{pmatrix} 1 & X_i \\ X_i & X_i^2 \end{pmatrix}$$

Skipped Algebra

Interpretation: The update $(\alpha^{(k+1)}, \beta^{(k+1)})$ solves a least-squares problem

$$\arg \min_{\alpha, \beta} \sum_{i=1}^n P_i^{(k)}(1-P_i^{(k)}) (Z_i^{(k)} - (\alpha + \beta X_i))^2$$

$$Z_i^{(k)} = \alpha^{(k)} + \beta^{(k)} X_i + \frac{Y_i - P_i^{(k)}}{P_i^{(k)}(1-P_i^{(k)})}$$

Check: To minimize, we would set derivatives α, β to 0

$$0 = \sum_{i=1}^n P_i^{(k)}(1-P_i^{(k)}) \cdot 2(\alpha + \beta X_i - Z_i^{(k)})$$

$$= 2 \left[(\alpha - \alpha^{(k)}) \cdot \sum_{i=1}^n P_i^{(k)}(1-P_i^{(k)}) + (\beta - \beta^{(k)}) \cdot \sum_{i=1}^n P_i^{(k)}(1-P_i^{(k)}) X_i - \sum_{i=1}^n (Y_i - P_i^{(k)}) \right]$$

$$0 = \sum_{i=1}^n P_i^{(k)}(1-P_i^{(k)}) \cdot 2 X_i (\alpha + \beta X_i - Z_i^{(k)})$$

$$= 2 \left[(\alpha - \alpha^{(k)}) \cdot \sum_{i=1}^n P_i^{(k)}(1-P_i^{(k)}) X_i + (\beta - \beta^{(k)}) \sum_{i=1}^n P_i^{(k)}(1-P_i^{(k)}) X_i^2 - \sum_{i=1}^n (Y_i - P_i^{(k)}) X_i \right]$$

$$\Leftrightarrow \sum_{i=1}^n (Y_i - P_i^{(k)}) \cdot \begin{pmatrix} 1 \\ X_i \end{pmatrix} = \begin{bmatrix} \sum_{i=1}^n P_i^{(k)}(1-P_i^{(k)}) & \sum_{i=1}^n P_i^{(k)}(1-P_i^{(k)}) X_i \\ \sum_{i=1}^n P_i^{(k)}(1-P_i^{(k)}) X_i & \sum_{i=1}^n P_i^{(k)}(1-P_i^{(k)}) X_i^2 \end{bmatrix} \cdot \begin{pmatrix} \alpha - \alpha^{(k)} \\ \beta - \beta^{(k)} \end{pmatrix}$$

Also called Iterative Reweighted Least Squares (glm in R)

② Estimate $p(x) = \frac{e^{\alpha + \beta x}}{1 + e^{\alpha + \beta x}}$: Use plug-in estimates

$$\hat{p}(x) = \frac{e^{\hat{\alpha} + \hat{\beta} x}}{1 + e^{\hat{\alpha} + \hat{\beta} x}}$$

③ Confidence Interval for β

Model Based Approach: Compute Fisher information to estimate std error of $\hat{\beta}$

Fisher Information for all n observations is

$$I_Y(\alpha, \beta) = -E \left[\nabla^2 \ell(\alpha, \beta) \right] = \sum_{i=1}^n p_i(1-p_i) \begin{pmatrix} 1 & x_i \\ x_i & x_i^2 \end{pmatrix} \quad p_i = \frac{e^{\alpha + \beta x_i}}{1 + e^{\alpha + \beta x_i}}$$

Covariance of $(\hat{\alpha}, \hat{\beta})$ is approximately $I_Y(\alpha, \beta)^{-1}$ for large n

Estimate p_i by $\hat{p}_i = \frac{e^{\hat{\alpha} + \hat{\beta} x_i}}{1 + e^{\hat{\alpha} + \hat{\beta} x_i}}$ and estimate $I_Y(\alpha, \beta)$ by

$$I_Y(\hat{\alpha}, \hat{\beta}) = \sum_{i=1}^n \hat{p}_i(1-\hat{p}_i) \begin{pmatrix} 1 & x_i \\ x_i & x_i^2 \end{pmatrix}$$

$$\hat{SE} = \sqrt{(I_Y(\hat{\alpha}, \hat{\beta})^{-1})_{22}}$$

95% confidence interval is $\hat{\beta} \pm Z(0.025) \cdot \hat{SE}$

④ To test $H_0: \beta = 0$

GLRT: Need to compute MLE $\hat{\alpha}_0$ for α in the null model where $\beta = 0$

log-likelihood:

$$\ell(\alpha) = \sum_{i=1}^n y_i \underbrace{\log \frac{p_i}{1-p_i}}_{\alpha} + \underbrace{\log(1-p_i)}_{-\log(1+e^{\alpha})}$$

$$= \sum_{i=1}^n (y_i \alpha - \log(1+e^{\alpha}))$$

$$0 = \frac{\partial \ell}{\partial \alpha} = \sum_{i=1}^n \left(y_i - \frac{e^{\alpha}}{1+e^{\alpha}} \right)$$

$$\Leftrightarrow \hat{\alpha}_0 = \log \frac{\bar{Y}}{1-\bar{Y}}$$

GLRT test statistic is $-2 \log \Lambda = 2\ell(\hat{\alpha}, \hat{\beta}) - 2\ell(\hat{\alpha}_0, 0)$

Compare against χ^2_1 null distribution

⑤ Diagnostic of model-fit is based on residual

$$\text{Pearson Residual} = \frac{Y_i - \hat{p}_i}{\sqrt{\hat{p}_i(1-\hat{p}_i)}}$$

If logistic regression is correct, we expect

mean 0

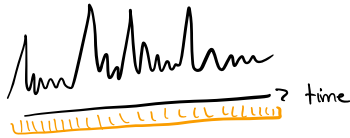
variance 1 ← Common to not follow this

uncorrelated w/ covariate X_i

Overdispersion is a common misspecified model outcome
variance greater than 1

4/25: Poisson Log-linear Model + Generalized Linear Model

Example: Neuron spiking overtime



Basic Model: Poisson Process

spikes in the i^{th} bin = $Y_i \sim \text{Poisson}(\lambda_i, \Delta)$ independent for $i=1, 2, \dots, n$

• WLOG $\Delta = 1$

• λ_i is the spiking rate in the i^{th} bin (Depends on external stimuli)

• Encode stimuli using p covariates

Poisson Log-linear model

$$\log \lambda_i = \alpha + B_1 X_{i1} + \dots + B_p X_{ip}$$

α is the intercept, B_1, \dots, B_p are the regression coefficients

Equivalently,

$$\alpha + B_1 X_{i1} + B_p X_{ip}$$

$$\lambda_i = e$$

The responses are then $Y_i \sim \text{Poisson}(\lambda_i)$ independent for $i=1, \dots, n$

To simplify notation, $p=1$

Data: $(X_1, Y_1), \dots, (X_n, Y_n)$

Consider fixed X 's with random responses Y_i

$$\text{Model: } Y_i \sim \text{Poisson}(\lambda_i) \quad \lambda_i = e^{\alpha + B X_i}$$

Estimation and Inference

- Estimate regression coefficients
- Provide 95% confidence interval for B

Likelihood Function:

$$\text{lik}(\alpha, B) = \prod_{i=1}^n \frac{\lambda_i^{Y_i} e^{-\lambda_i}}{Y_i!} \quad \text{where } \lambda_i = e^{\alpha + B X_i}$$

$$\begin{aligned} \mathcal{L}(\alpha, B) &= \sum_{i=1}^n Y_i \log(\lambda_i) - \lambda_i - \log(Y_i!) \\ &= \sum_{i=1}^n Y_i (\alpha + B X_i) - e^{\alpha + B X_i} - \log(Y_i!) \end{aligned}$$

Solving MLE via derivatives

$$0 = \frac{\partial \mathcal{L}}{\partial \alpha} = \sum_{i=1}^n (Y_i - e^{\alpha + B X_i}) = \sum_{i=1}^n (Y_i - \lambda_i)$$

$$0 = \frac{\partial \mathcal{L}}{\partial B} = \sum_{i=1}^n (Y_i - \lambda_i) X_i$$

No closed form so we can apply Newton-Raphson Method

Gradient of $\mathcal{L}(\alpha, \beta)$:

$$\nabla \mathcal{L}(\alpha, \beta) = \begin{pmatrix} \frac{\partial \mathcal{L}}{\partial \alpha} \\ \frac{\partial \mathcal{L}}{\partial \beta} \end{pmatrix} = \sum_{i=1}^n (y_i - \lambda_i) \begin{pmatrix} 1 \\ x_i \end{pmatrix}$$

Hessian of $\mathcal{L}(\alpha, \beta)$

$$\nabla^2 \mathcal{L}(\alpha, \beta) = \begin{pmatrix} \frac{\partial^2 \mathcal{L}}{\partial \alpha^2} & \frac{\partial^2 \mathcal{L}}{\partial \alpha \partial \beta} \\ \frac{\partial^2 \mathcal{L}}{\partial \alpha \partial \beta} & \frac{\partial^2 \mathcal{L}}{\partial \beta^2} \end{pmatrix} = - \sum_{i=1}^n w_i \begin{pmatrix} 1 & x_i \\ x_i & x_i^2 \end{pmatrix} \quad w_i = \lambda_i = e^{\alpha + \beta x_i}$$

\Rightarrow Newton Raphson Iterations

$$\begin{pmatrix} \alpha^{(t+1)} \\ \beta^{(t+1)} \end{pmatrix} = \begin{pmatrix} \alpha^{(t)} \\ \beta^{(t)} \end{pmatrix} - \left(\nabla^2 \mathcal{L}(\alpha^{(t)}, \beta^{(t)}) \right)^{-1} \cdot \nabla \mathcal{L}(\alpha^{(t)}, \beta^{(t)})$$

Newton-Raphson update solves a weighted least-squares regression

Also called iterative reweighted least square

To make a model based 95% confidence interval for β

• Fisher Information of all n observations

$$\begin{aligned} \mathbf{I}_y(\alpha, \beta) &= -\mathbb{E} \left[\nabla^2 \mathcal{L}(\alpha, \beta) \right] && \leftarrow \text{full log-likelihood} \\ &= \sum_{i=1}^n \lambda_i \begin{pmatrix} 1 & x_i \\ x_i & x_i^2 \end{pmatrix} && (\text{can't use } n \cdot \mathbf{I} \text{ since each is different}) \end{aligned}$$

Use plug-in estimate

$$\mathbf{I}_y(\hat{\alpha}, \hat{\beta}) = \sum_{i=1}^n \hat{\lambda}_i \begin{pmatrix} 1 & x_i \\ x_i & x_i^2 \end{pmatrix}$$

Estimate standard error of $\hat{\beta}$ by

$$\hat{\text{se}} = \sqrt{(\mathbf{I}_y(\hat{\alpha}, \hat{\beta}))^{-1}_{22}}$$

Model Diagnostics:

• Based on normalized Residuals

$$\text{Pearson Residual: } \frac{y_i - \hat{\lambda}_i}{\sqrt{\hat{\lambda}_i}}$$

If model is correctly specified we expect

mean 0

variance 1

uncorrelated with x_i

Generalized Linear Model

A GLM is a model for responses $Y_1 \dots Y_n$ where $Y_i \sim f(Y|\theta)$, $\theta \in \mathbb{R}$

θ_i is the value for observation i

For observation i we observe p covariates $X_1 \dots X_p$

GLM assumes

$$g(\theta_i) = \alpha + B_1 X_{i1} + \dots + B_p X_{ip}$$

$g: \mathbb{R} \rightarrow \mathbb{R}$ is the link function

In logistic regression, $g \rightarrow \log$ odds

Poisson log-linear, $g \rightarrow \log \mu$

Alternative link functions

$$g(p) = \Phi^{-1}(p)$$

Φ is the standard normal quantile function

Choice of link function

- Goodness of model fit to data
- Interpretation of model/parameters
- Mathematical convenience

Change of variable $\theta \rightarrow \eta(\theta)$ so pdf/pmf has the form

$$f(y|\eta) = e^{\eta y - A(\eta)} \cdot h(y)$$

← Canonical or natural link

• For Bernoulli(p): The PMF is

$$\begin{aligned} f(y) &= p^y (1-p)^{1-y} = (1-p) \left(\frac{p}{1-p}\right)^y \\ &= e^{\log\left(\frac{p}{1-p}\right)y + \log(1-p)} \end{aligned}$$

Set $\eta(p) = \log \frac{p}{1-p}$, $A(\eta) = -\log(1-p) = \log(1 + e^\eta)$ and $h(y) = 1$

$$p = \frac{e^\eta}{1 + e^\eta}$$

• For Poisson: The PMF is

$$f(y) = \frac{\lambda^y e^{-\lambda}}{y!} = e^{(\log \lambda)y - \lambda} \cdot \frac{1}{y!}$$

Set $\eta(\lambda) = \log \lambda$, $A(\eta) = \lambda$ and $h(y) = \frac{1}{y!}$

$$\lambda = e^\eta$$

$f(y|\eta) = e^{\eta y - A(\eta)} h(y)$ is called the exponential family form of the model

η is the natural parameter of the model

For a GLM based on a parametric model $f(y|\theta)$, the natural/canonical link is the choice $g(\theta) = \eta(\theta)$ where η is natural parameter

If we use the natural link:

Log-likelihood function for $(x_1, y_1), \dots, (x_n, y_n)$ is

$$\begin{aligned} \ell(\alpha, \beta) &= \log \prod_{i=1}^n e^{\eta_i y_i - A(\eta_i)} h(y_i) \\ &= \sum_{i=1}^n y_i \eta_i - A(\eta_i) + \log(h(y_i)) \\ &\quad \uparrow \\ &\quad \alpha + \beta x_i \text{ when we use the natural link} \\ &= \sum_{i=1}^n y_i (\alpha + \beta x_i) - A(\alpha + \beta x_i) + \log h(y_i) \end{aligned}$$

Computing MLE:

$$0 = \frac{\partial \ell}{\partial \alpha} = \sum_{i=1}^n y_i - A'(\eta_i)$$

$$\eta_i = \alpha + \beta x_i$$

$$0 = \frac{\partial \ell}{\partial \beta} = \sum_{i=1}^n y_i x_i - x_i A'(\eta_i)$$

$$\Rightarrow 0 = \sum_{i=1}^n (y_i - A'(\eta_i)) \begin{pmatrix} 1 \\ x_i \end{pmatrix}$$

What is $A'(\eta)$

$$1 = \sum_y f(y|\eta) = \sum_y e^{\eta y - A(\eta)} h(y)$$

differentiate wrt y

$$0 = \sum_y (y - A'(\eta)) \cdot \underbrace{e^{\eta y - A(\eta)} h(y)}_{f(y|\eta)}$$

$$= \mathbb{E}[Y] - A'(\eta)$$

$$\Rightarrow A'(\eta) = \mathbb{E}[Y]$$

For GLM, $A'(\eta) = \mathbb{E}[Y_i]$ is the model prediction for mean of Y_i and $Y_i - A'(\eta)$ is a residual

Fisher Information is

$$I_y(\alpha, B) = -E[V^2 \ell(\alpha, B)]$$

$$= \sum_{i=1}^n w_i \begin{pmatrix} 1 & X_i \\ X_i & X_i^2 \end{pmatrix} \quad \text{where } X_i = A^T(a_i)$$

4/27: Proportional Hazards Model

Example: Clinical trial studying the effect of a cancer drug process data

T_1, T_2, \dots, T_n

where T_i is the time of remission

For the i^{th} patient we have p covariates

- ex. Treatment vs. Control
- stage of cancer
- Age
- Family history

Goal: Model T_i via X_i, \dots, X_{ip}

Let T be a continuous variable

Hazard Function

$$\lambda(t) = \lim_{\delta \rightarrow 0} \frac{1}{\delta} \mathbb{P}[T \in [t, t+\delta] | T \geq t] \quad \leftarrow \text{Instantaneous Risk}$$

$$\lambda(t) = \lim_{\delta \rightarrow 0} \frac{\frac{1}{\delta} \mathbb{P}[T \in [t, t+\delta] | T \geq t]}{\mathbb{P}[T \geq t]} = \frac{f(t)}{1-F(t)}$$

Conditional probability

Example: When $T \sim \text{Exponential}(\Theta)$

$$f(t) = \Theta e^{-\Theta t}$$

$$F(t) = 1 - e^{-\Theta t}$$

$$\lambda(t) = \frac{\Theta e^{-\Theta t}}{1 - (1 - e^{-\Theta t})} = \Theta$$

Hazard function is constant in time \leftarrow Memoryless Property!!

In general the hazard may depend on time and covariates for each patient

Model T_i via



$$\lambda_i(t) = \lambda(t) \exp(B_1 X_{i1} + \dots + B_p X_{ip})$$

↑
time
dependence

↑
covariates

Same time dependence for each patient

Shape of hazard function will have the same shape over time but it will be scaled based on the covariates

Origin of the name proportional hazards

This model is semi-parametric

parametric component: Regression Coefficient

Non-parametric component: hazard function

Usually we care more about B_1, \dots, B_p than $\lambda(t)$

Idea: Condition on the set of all observed recurrence times

$$t_{(1)} < t_{(2)} < \dots < t_{(n)}$$

Fixes times at which the n recurrence events occurred but not the patient

Inference for B_1, \dots, B_p will then be based on only the information about which patient had recurrence

Akin to permutation tests

For each $t_{(k)}$, let $R_{(k)}$ be the at risk set immediately before time $t_{(k)}$ (Patients still in remission before $t_{(k)}$)

Conditional on some patient in $R_{(k)}$ having recurrence at time $t_{(k)}$, the probability it is patient i for $i \in R_{(k)}$

$$\frac{\lambda_i(t_{(k)})}{\sum_{j \in R_{(k)}} \lambda_j(t_{(k)})} \leftarrow \text{Ratio of the instantaneous rate of recurrence in patient } i \text{ to the sum of risk for all patients}$$

The baseline $\lambda(t)$ cancels and we find

$$\frac{\lambda_i(t_{(k)})}{\sum_{j \in R_{(k)}} \lambda_j(t_{(k)})} = \frac{\exp(B_1 x_{i1} + \dots + B_p x_{ip})}{\sum_{j \in R_{(k)}} \exp(B_1 x_{j1} + \dots + B_p x_{jp})}$$

For each time $t_{(k)}$ $k=1, \dots, n$

Partial likelihood function

$$p_{lik}(B_1, \dots, B_p) = \prod_{k=1}^n \frac{\exp(B_1 x_{i_k 1} + \dots + B_p x_{i_k p})}{\sum_{j \in R_{(k)}} \exp(B_1 x_{j1} + \dots + B_p x_{jp})}$$

Use partial likelihood in place of actual likelihood

Note: Typically the responses T_1, \dots, T_n are right-censored

If the i th patient is still in remission by the end of the trial we do not know T_i

just that $T_i \geq \mathcal{L}_i$

\mathcal{L}_i is the duration of the trial

If cancer never occurs, then $T_i = \infty$

When some responses are right-censored, the at risk set $R_{(k)}$ is defined as the set of patients

- still in remission
- Not right censored

Maximum Likelihood Estimation

Assume $p=1$ for simplicity

Data: $(X_1, T_1) \dots (X_n, T_n)$

$$\text{log-partial-likelihood} \quad \mathcal{L}(B) = \log \prod_{k=1}^n \frac{\exp(BX_{i_k})}{\sum_{j \in R_{(k)}} \exp(BX_j)} = \sum_{k=1}^n \left(BX_{i_k} - \log \sum_{j \in R_{(k)}} \exp(BX_j) \right)$$

$$\hat{\beta} = \arg \max \ell(\beta)$$

Solve via Newton-Raphson

Variance is estimated by

$$I(\hat{\beta})^{-1} \approx \left(-\frac{\partial^2 \ell(\hat{\beta})}{\partial \beta^2} \right)^{-1}$$

Test of $H_0: \beta = 0$ based on GLRT statistic

$$-2 \log \Lambda = 2\ell(\hat{\beta}) - 2\ell(0)$$

w/ distribution χ^2_1

Course Review

Hypothesis Testing: Deciding whether a particular null hypothesis about the underlying distribution is true/false

Estimation: Estimating quantities/parameters related to this distribution

Hypothesis Testing

Binary decision to accept/reject H_0 based on data X_1, \dots, X_n using a test statistic $T(X_1, \dots, X_n)$

Step 1: How to choose T ?

Step 2: Deciding whether H_0 is true/false based on T ?

Neyman-Pearson Lemma: Maximize power via likelihood ratio statistic

If monotonic increasing/decreasing we can use its input in its place

Simple Alternatives

Composite Alternatives: