Algorithms, Evidence, and Data Science Cookbook

Part I: Classic Statistical Inference

* **Population:** the entire group
* **Sample:** a subset of the population
* **Mean:** μ is the mean of the population; $\bar{x}$ is the mean of the sample

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

* **Variance:** the dispersion around the mean

Variance of a population:

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

Variance of a sample:

$$s^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2$$

* **Standard Deviation:** square root of the variance
* **Standard Error:** an estimate of the standard deviation of the sampling distribution

For a mean:

$$se(\bar{x}) = \sqrt{\frac{s^2}{n}}$$

For the difference between two means:

$$se(\bar{x_1}, \bar{x_2}) = \sqrt{\frac{{s_1}^2}{n_1} + \frac{{s_2}^2}{n_2}}$$

Algorithms and Inference

* **Algorithm:** set of data probability-steps to produce an estimator
* **Inference:** measuring the uncertainty around the estimator *e.g.:* $\bar{x}$ the algorithm, while $se(\bar{x})$ is the inference

A Regression Example

Linear Regression

any regression is a conditional mean $\hat{Y}_i = E(Y_i|X_i)$
* Y : response variable
* X : covariate/predictor/feature
* $\hat{\beta_0}, \hat{\beta_1}$: regression coefficients

$$\hat{\beta_0} = \hat{Y} - \hat{\beta_1}\hat{X}$$

$$\hat{\beta_1} = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})}{\sum_{i=1}^{n}(X_i - \bar{X})^2}$$

$$se(\hat{\beta_0}) = \hat{\sigma}^2\left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(X_i - \bar{X})^2}\right] \quad se(\hat{\beta_1}) = \frac{\hat{\sigma}^2}{\sum_{i=1}^{n}(X_i - \bar{X})^2}$$

* predicted values = fitted curve given x:

$$\hat{Y}(x) = \hat{\beta_0} + \hat{\beta_1}x$$

* residuals $\hat{\epsilon}$:

$$\hat{\epsilon_i} = Y_i - \hat{Y_i} = Y_i - \hat{\beta_0} + \beta_1 X_i$$

* residual sum of squares RSS

$$RSS(\hat{\beta_0}, \hat{\beta_1}) = \sum_{i=1}^{n}{\hat{\epsilon_i}}^2$$

* mean square error $\hat{\sigma}^2$

$$\hat{\sigma}^2 = \frac{RSS(\hat{\beta_0}, \hat{\beta_1})}{n-2}$$

LOWESS & LOESS

* 1) specify the number of points within the range/window n
* 2) neighbour weightings $w(x_k)$

$$w(x_k) = \left(1 - \left|\frac{x_i - x_k}{d}\right|^3\right)^3 \quad \begin{array}{l} for k = 1, ..., n \\ d \text{ is the distance between } x_i \\ \text{and the } k^{th} \text{ neighbouring point} \end{array}$$

* 3) for each range, estimate a regression function

LOWESS: $\hat{y_k} = a + bx_k$
LOESS: $\hat{y_k} = a + bx_k + c{x_k}^2$
* 4) robust weightings $G(x_k)$

$$G(x_k) = \begin{cases} \left(1 - \left(\frac{|y_i - \hat{y_i}|}{6median(|y_i - \hat{y_i}|)}\right)^2\right)^2, & \left|\frac{|y_i - \hat{y_i}|}{6median(|y_i - \hat{y_i}|)}\right| < 1 \\ 0, & \left|\frac{|y_i - \hat{y_i}|}{6median(|y_i - \hat{y_i}|)}\right| \geq 1 \end{cases}$$

LOWESS: $\hat{y_k} = \sum_k w(x_k)G(x_k)(a + bx_k)^2$

LOESS: $\hat{y_k} = \sum_k w(x_k)G(x_k)(a + bx_k + c{x_k}^2)^2$

* 5) A series of new smoothed values is the result. The procedure can be repeated to get a more precise curve fitting.

Bootstrapping

* bootstrap principle:

$\sigma_{\text{(sampling w/replacemnt)}} = \sigma_{\text{(across samples)}}$
* bootstrap iterations: B
* original sample: $(x_i, y_i)_{i=1}^N$
* bootstrap samples: $(x_{j(b)}, y_{j(b)})_{j \epsilon I}$ for $b = 1, ..., B$, $I = \{1, ..., N\}$, and j is the index that is randomly sampled from I
* for each b, compute $\hat{y_{j(b)}}$ using LOWESS or any other model

j \ b	1	2	3	$\cdots$	B
1	$\hat{y_{1(1)}}$	$\hat{y_{1(2)}}$	$\hat{y_{1(3)}}$	$\cdots$	$\hat{y_{1(B)}}$
2	$\hat{y_{2(1)}}$	$\hat{y_{2(2)}}$	$\hat{y_{2(3)}}$	$\cdots$	$\hat{y_{2(B)}}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
N	$\hat{y_{N(1)}}$	$\hat{y_{N(2)}}$	$\hat{y_{N(3)}}$	$\cdots$	$\hat{y_{N(B)}}$

* for each j row, the standard deviation σ_j^{boot} is

$$\sigma_j^{boot} = \sqrt{\frac{(\hat{y_j} - \bar{\hat{y_j}})^2}{B-1}}$$

* sort $i(\hat{b})$ by value from min to max $\rightarrow$ get the 5^{th} and 95^{th} values to get a 90% confidence interval

Hypothesis Testing

T-test, one-sample

* null hypothesis $H_o : \mu = \mu_0$
* alternative hypothesis $H_a : \mu\{=, > or <\}\mu_0$
* $t - statistict$ standarices the difference between $\bar{x}$ and μ_0

$$t = \frac{\bar{x} - \mu_0}{se(\bar{x})}$$

degrees of freedom $df = n - 1$
* $p - value$: probability that $\bar{x}$ was obtained by chance given $\mu_0 = \mu$.
* **algorithm:** read the t-distribution critical values (chart) for the $p - value$ using t and df
* if($p - value < \alpha$){ reject H_o and accept H_a }
else { can't reject H_o }
* α is the predetermined value of significance (usually 0.05)
* if(t is of the 'wrong' sign)$p - value = 1 - p - value_{chart}$

paired two-sample t-test

each value of one group corresponds to a value in the other group
* **algorithm:** subtract the values for each sample to get one set of values and use μ_0 to perform a one-sample t-test

unpaired two-sample t-test

the two populations are independent
* $H_o : \mu_1 = \mu_2$
* $H_a : \mu_1\{=, > or <\}\mu_2$
* $t - statistict$

$$t = \frac{\bar{x_1} - \bar{x_2}}{se(\bar{x_1}, \bar{x_2})}$$

degrees of freedom $df = (n_1 - 1) + (n_2 - 1)$
* **algorithm:** same as in one-sample t-test
* double the $p - value$ for $H_a : \mu_1 \neq \mu_2$

* **Type I error** α**:** probability of rejecting a true H_o
* **Type II error** β**:** probability of failing to reject a false H_o

Notes

* the OLS confidence intervals work asymptotically $\rightarrow$ they assume the number of available observations is infinite, but it assumes normality
* in LOWESS, n is not infinite, but it does not assume any distribution

Frequentist Inference

* assumes the observed data comes from a probability distribution F
* $x = (x_1, ..., x_n)$ is the data vector (aka. *the sample's values*)
* $X = (X_1, ..., X_n)$ is the vector of random variables (aka. *a sample, individual draws of F*)
* the expectation property $\theta = E_F(X_i)$ (aka. the true expectation value of any draw X_i)
* $\hat{\theta}$ is the best estimate of θ

usually,

$$\hat{\theta} = t(x) \qquad t(x) = \bar{x}$$

where $t(x)$ is the algorithm

* $\hat{\theta}$ is sample specific, is a realization of $\hat{\Theta} = t(x)$. Typically,

$$E_F(\hat{\Theta}) = \mu$$

μ is the expected value of producing an estimate using $t(x)$ when x comes from F

* **Bias-Variance Trade-Off:** models with lower bias will have higher variance and vice versa.
* **Bias:** error from incorrect assumptions to make target function easier to learn (high bias → missing relevant relations or under-fitting)
* **Variance:** error from sensitivity to fluctuations in the dataset, or how much the target estimate would differ if different training data was used (high variance → modelling noise or over-fitting)

$$bias = \mu - \theta$$

(aka. $expected - true values$) $\qquad var = E_F\{(\hat{\Theta} - \mu)^2\}$

Frequentist principles

* usually defines parameters with infinite sequence of trials → hypothetical data sets $X^{(1)}, X^{(2)}, \ldots$ generate infinite samples $\hat{\Theta}^{(1)}, \hat{\Theta}^{(2)}, \ldots$
* 1) Plug-in principle: relate the sample $se(\bar{x})$ with the true variance.

$$var_F(x) = \hat{var}_F = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$$

$$se(\bar{x}) = \left[\frac{var_F(x)}{n}\right]^{\frac{1}{2}}$$

* 2) Taylor series approximations: relate $t(x)$ by local linear approximations (aka. compute $\bar{se}(x)$ of the transformed estimator)

$$se(\hat{\theta}) = se(\bar{x})\frac{d\hat{\theta}}{d\bar{x}} = se(\bar{x})\frac{dt(x)}{d\bar{x}}$$

* 3.1) Parametric Families: given $x = (x_1, ..., x_n)$, the Likelihood Function $L(x)$ (aka. the probability to observe x) is given by:

e.g. $\hat{\theta} = \mu$ for a normal distribution

$$P(x|N(\mu, \sigma^2)) = P(x_1|N(\mu, \sigma^2))...P(x_n|N(\mu, \sigma^2))$$

$$P(x|N(\mu, \sigma^2)) = \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^n \prod_{1=1}^{n} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}} = L(x)$$

$$L(x) = \prod_{1=1}^{n} f_\theta(x_i)$$

where f_θ is the density function

* 3.2) MLE (maximum likelihood estimate): find $\hat{\theta}$ such that $L(x)$ is maximized

e.g.

$$\max_{\hat{\theta}} L(x) \Rightarrow \max_{\mu} L(x) = \hat{\mu}^{MLE}$$

* 4) Simulation and Bootstrap: estimate F as $\hat{F}$, then simulate values from $\hat{F}$ to get a prior sample $\hat{\Theta}^{(k)} = t(x^{(b)})$ The empirical standard deviation of the $\hat{\Theta}'s$ is the frequentist estimate for $se(\hat{\theta})$
* 5) Pivotal Statistics: Frequentist use pivotal statistics whenever they are available to conduct stat. tests

e.g. t-test is a pivotal statistic as it does not depend on parameters the distribution might have.

Frequentist Optimality

Neyman-Pearson lemma optimum hypothesis-testing algorithm:

purpose: choose one of the two possible density functions for observed data x

* null hypothesis density $f_0(x)$
* alternative density $f_1(x)$

let $L(x)$ be the Likelihood Ratio

$$L(X) = \frac{f_1(X)}{f_0(X)}$$

let the testing rule $t_c x$ be:

$$t_c x = \begin{cases} 1(pic f_1(x)), & ln(L(X)) \geq c \\ 0(pic f_0(x)), & ln(L(X)) < c \end{cases}$$

* only rules in the $t_c x$ form can be optimal *problem Steps*
* 1) define the density functions $f_0(x_i)$ and $f_1(x_i)$ for $f_0(x)$ and $f_1(x)$

e.g.

$$f_0 \sim N(\mu_0, {\sigma^2}_0) \qquad f_1 \sim N(\mu_1, {\sigma^2}_1)$$

$$f_0 \sim N(0, 1) \qquad f_1 \sim N(0.5, 1)$$

$$f_0(x_i) = \frac{1}{\sqrt{2\pi}} e^{-\frac{{x_i}^2}{2}} \qquad f_1(x_i) = \frac{1}{\sqrt{2\pi}} e^{-\frac{{x_i-0.5}^2}{2}}$$

* 2) calculate the likelihood functions $f_0(X)$ and $f_1(X)$

e.g.

$$f_0(X) = \left[\frac{1}{\sqrt{2\pi}}\right]^n e^{-\frac{1}{2}\sum_{i=1}^{n} {x_i}^2}$$

$$f_1(X) = \left[\frac{1}{\sqrt{2\pi}}\right]^n e^{-\frac{1}{2}\sum_{i=1}^{n} ((x_i-0.5)^2)}$$

* 3) calculate the likelihood ratio

e.g.

$$L(X) = \frac{e^{-\frac{1}{2}\sum_{i=1}^{n}((x_i-0.5)^2)}}{e^{-\frac{1}{2}\sum_{i=1}^{n} {x_i}^2}}$$

$$L(X) = e^{-\frac{1}{2}\left[n\bar{x} - \frac{n}{4}\right]}$$

* 4) remove all independent variables *e.g.*

$$L(X) > c \Rightarrow \begin{aligned} e^{-\frac{1}{2}\left[n\bar{x} - \frac{n}{4}\right]} &> c_1 \\ -\frac{1}{2}\left[n\bar{x} - \frac{n}{4}\right] &> C_2 \\ n\bar{x} - \frac{n}{4} &> c_3 \\ \bar{x} &> c_4 \\ \bar{x} &> c \end{aligned}$$

only the mean depends on the sample x

* 5) the *most powerful* hypothesis test at any type I error rate α is to compare c to a constant.

e.g.

$$\alpha = P(\bar{x} > c|\mu = \mu_0)$$
$$\alpha = P((\bar{x} - \mu)\sqrt{n} > (c - \mu)\sqrt{n}|\mu = 0)$$
$$\alpha = 1 - P(\bar{x}\sqrt{n} \leq c\sqrt{n}|\mu = 0)$$
$$\alpha = 1 - \Phi(c\sqrt{n})$$

Φ is the cumulative density function (CDF) of a normal distribution $N(\mu_0, {\sigma^2}_0)$

* 6) calculate c

e.g.

$$\Phi(c\sqrt{n}) = 1 - \alpha$$
$$c\sqrt{n} = \Phi^{-1}(1 - \alpha)$$
$$c = 0 + \frac{1}{\sqrt{n}}\Phi^{-1}(1 - \alpha)$$

In general:

$$c = \mu_0 + \frac{1}{\sqrt{n}}\Phi^{-1}(1 - \alpha)$$

* 7) calculate β, such that it's minimized

e.g.

$$\beta = P(\bar{x} \leq c|\mu = \mu_1)$$
$$\beta = P((\bar{x} - \mu)\sqrt{n} \leq (c - \mu)\sqrt{n}|\mu = 0.5)$$
$$\beta = \Phi((c - 0.5)\sqrt{n})$$

Notes and Details

* $1 - \beta$ is the power of the hypothesis test (probability of correctly rejecting $f_0(x)$

Bayesian Inference

Bayes Rule

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

* Bayes Rule (for one μ) can be written as:

$$g(\mu|x) = c_x L_x(\mu)\Pi(\mu)$$

where:
μ : an unobserved point in the parameter space Ω
x : a point in the sample space X
c_x : normalization constant of the posterior distribution
$g(\mu|x)$: posterior distribution
$L_x(\mu)$: likelihood function
$\Pi(\mu)$: prior distribution

* Bayes Rule (for two μ_1, μ_2) can be written as:

$$\frac{g(\mu_1|x)}{g(\mu_2|x)} = \frac{g(\mu_1)}{g(\mu_2)}\frac{L_x(\mu_1)}{L_x(\mu_2)}$$

The posterior odds ratio is the prior odds ratio times the likelihood ratio

$$L_x(\mu) = \prod_{i=1}^{n} e^{-\frac{1}{2}(x_i-\mu)^2}$$

Warm-up example

e.g. Find the probability of identical twins. The doctor says that $\frac{1}{3}$ of twin births are identical. A sonogram observed same sex. identical twins are of the same sex, while fraternals have 0.5 probability to be of the same sex.

$$\frac{g(identical|sameSex)}{g(fraternal|sameSex)} = \frac{g(identical)}{g(fraternal)} \times \frac{L_{identical}(sameSex)}{L_{fraternal}(sameSex)}$$

$$\frac{g(identical|sameSex)}{g(fraternal|sameSex)} = \frac{\frac{1}{3}}{1-\frac{1}{3}} \times \frac{1}{\frac{1}{2}}$$

Flaws in Frequentist Inference

* In Frequentist, if the algorith changes (even if the data points stay exactly the same), the significance level is different for each algorithm.
* On Bayesian inference, the algorithm stays the same → the significance level does not change.

A Bayesian/Frequentist Comparison List

Bayesian:

* attention is in choosing an algorithm $t(x)$
* operates only in one sample with the whole parameter space
* answers all posible questions at once, since the posterior is a distribution

Frequentist:

* attention is in choosing a prior Π
* operates with one parameter (specific question) in many samples
* only computes the expected value and the variance (each answer requires an specific algorithm)
* is more flexible than Bayes as we can come up with many algorithms

Bayesian Reasoning - estimate μ from x if $\mu \sim N(m, A)$

normal likelihood function (assume a variance of 1):

$$x|\mu \sim N(\mu, 1)$$

the normal posterior:

$$\mu|x \sim N(m + B(x-m), B)$$

where $B = \frac{A=\text{prior variance}}{A+1=\text{total variance}}$, m = prior parameter therefore:

$$\hat{\mu}^{Bayes} = m + B(x-m)$$

Notes and Details

* like in frequentist, the fundamental unit of inference is a family of probability densities.
* Bayesian inferences assumes the knowledge of a prior density $g(\mu), \mu\epsilon\Omega$

Fisherian Inference and Maximum Likelihood Estimation

* The log-likelihood function is defined as:

$$\ell_x(\theta) = Log\{f_\theta(x)\}$$

$\ell_x(\theta)$: gets the most likely parameters to get the sample x
$f_\theta(x)$: likelihood function (aka. family probability densities) θ : vector of parameters

for a fixed x and a variable θ

* The MLE is the value of $\theta\epsilon\Omega$ that maximizes $\ell_x(\theta)$

$$MLE: \hat{\theta} = \overset{argmax}{\theta\epsilon\Omega} \{\ell_x(\theta)\}$$

* Estimate functions of the true parameter: $\hat{\gamma} = T(\hat{\theta})$
* Good frequentist properties (good bias & variance):

$$bias = \mu - E(\hat{\mu})$$

$$variance = \sum_{i=1}^{I}(\hat{\mu}^{(i)} - E(\hat{\mu}))^2$$

μ : true value of the parameter
$E(\hat{\mu})$: expected value of the estimate

$$variance = E_F\{(\hat{\mu}^{(i)} - E(\hat{\mu}))^2\}$$

* Reasonable Bayesian justification

$$P(\theta|x) = c_x\Pi(\theta)e^{\ell_x(\theta)}$$

$P(\theta|x)$: posterior
c_x : constant
$\Pi(\theta)$: prior
$e^{\ell_x(\theta)}$: maximum likelihood estimation

* Fisherian inference assumes a flat prior (aka. unknown prior), so that the MLE $\hat{\theta}^{MLE}$ is a maximizer of $P(\theta|x)$. (The MLE is the highest point of the posterior distribution)
* As the algorithm does not change, the significance level is not affected by unexpected changes in the algorithm.

e.g. - for a Normal density function
* let $\theta = (\mu, \sigma^2)$
* density function $f_\theta = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{x_i-\mu}{\sigma}\right)^2}$ * Since: $L(x) = \prod_{1=1}^{n} f_\theta(x_i)$ Log-Likelihood function

$$\ell_x(\theta) = \sum_{i=1}^{n} Log\{f_\theta(x_i)\} = \sum_{i=1}^{I} \ell_x(\theta)$$

$$\hat{\mu^{MLE}} = \bar{x}$$

$$\sigma^{MLE} = \sqrt{\frac{\sum_{i=1}^{n}(x_i - \bar{x})^2}{n}}$$

* MLE can cause over-fitting identification problems when we fit a lot of parameters in θ (it would become very specific to our sample → may not represent the population)

Fisher Information and the MLE

Log-Likelihood Function

$$\ell_x(\theta) = Log f_\theta(x)$$

Score Function

how higher or lower is the likelihood function value of the sample as θ varies?

$$\dot{\ell}_x(\theta) = \frac{\dot{f}_\theta(x)}{f_\theta(x)}$$

Expectation of $\dot{\ell}_x(\theta)$

$f(x)$: density function

$$E(x) = \int_x x f(x)\, dx$$

$$E[\dot{\ell}_x(\theta)] = 0$$

Variance of $\dot{\ell}_x(\theta)$

$$V[x] = \int_x [x - E(x)]^2 f(x)\, dx$$

$$V[\dot{\ell}_x(\theta)] = \int_x \left[\dot{\ell}_x(\theta)\right]^2 f_\theta(x)\, dx$$

Fisher Information I_0

$$I_0 = V[\dot{\ell}_x(\theta)]$$

$$\ddot{\ell}_x(\theta) = \frac{\ddot{f}_\theta(x)}{f_\theta(x)} - \left(\frac{\dot{f}_\theta(x)}{f_\theta(x)}\right)^2 \qquad E(\ddot{\ell}_x(\theta)) = -I_0$$

MLE estimator of $\hat{\theta}$: $\hat{\theta}^{MLE}$

$$\hat{\theta}^{MLE} \sim N\left(\theta, \frac{1}{I_0}\right)$$

e.g. for a normal dist.
let $x_i \sim N(\theta, \sigma^2)$
* 1) compute $\ell_x(\theta)$

density function $f_\theta(x) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$

likelihood function $\ell_x(\theta) = -\frac{1}{2}\sum_{i=1}^{n}\frac{(x_i-\theta)^2}{\sigma^2} - \frac{n}{2}Log(2\pi\sigma^2)$

* 2) score function $\dot{\ell}_x(\theta) = \frac{1}{\sigma^2}\sum_{i=1}^{n}(x_i - \theta)$

$\ddot{\ell}_x(\theta) = -\frac{n}{\sigma^2}$
* 3) compute I_0
as $E(\ddot{\ell}_x(\theta)) = -I_0$, Fisher Information $I_0 = \frac{n}{\sigma^2}$
* 4) compute $\hat{\theta}^{MLE}$

$E(\dot{\ell}_x(\theta)) = \frac{1}{\sigma^2}\sum_{i=1}^{n}(x_i - \theta) = 0$, such that

$\sum_{i=1}^{n} x_i = n\theta \Rightarrow \hat{\theta}^{MLE} = \frac{\sum_{i=1}^{n} x_i}{n} = \bar{x}$
* 5) compute $se(\hat{\theta}^{MLE})$
for a large n,
$\hat{\theta}^{MLE} \sim N\left(\theta, \frac{1}{I_0}\right) \Rightarrow \hat{\theta}^{MLE} \sim N\left(\theta, \frac{\sigma^2}{n}\right)$

$$se(\hat{\theta}^{MLE}) = \frac{1}{I_0} = \frac{\sigma^2}{n}$$

* 6) $se(\hat{\theta}^{MLE}) = \frac{1}{nI_0}$, by Cramer-Rao lower bound.
The MLE has variance at least as small as the best unbiased estimate of θ

Conditional Inference

e.g. An *iid* sample $x \sim N(\theta, 0)$ has produced estimate $\hat{\theta} = \bar{x}$. however,

$$n = 25 \text{ was declined}$$

$$n = \begin{cases} 25, & \text{prob } \frac{1}{2} \\ 100, & \text{prob } \frac{1}{2} \end{cases}$$

* Classical Frequentist rational:

$$sd(\bar{x}) = \sigma_{\bar{x}} = \sqrt{\frac{1}{2}\frac{\sigma^2}{100} + \frac{1}{2}\frac{\sigma^2}{25}} = 0.158$$

* Conditional Inference rational:

$$sd(\bar{x}) = \sqrt{\frac{\sigma^2}{25}} = 0.2$$

* use the likelihood function (based on observation) without the prior
* "just take the sample you have"

1) more relevant inferences (w/what really happened)
2) simpler inferences (no correlation between the result and the sample size selection)

e.g. Observed Fisher Information $I_{(x)}$

$$I_{(x)} = -\ddot{\ell_x}(\hat{\theta}^{MLE})$$

In large samples $I_{(x)} = I_0$. Use $I_{(x)}$ in small samples

$$E[I_{(x)}] = nI_0$$

* 1) compute the log-likelihood

$$f_\theta(x) = \frac{1}{\pi}\frac{1}{1+(x+\theta)^2} \Rightarrow \text{Cauchi density function}$$

$$\ell_x(\theta) = Log\left(\frac{1}{\pi}\right) + Log(1) - Log(1+(x+\theta)^2)$$

* 2) get its derivative

$$\dot{\ell_x}(\theta) = \frac{2(x-\theta)}{1+(x+\theta)^2}$$

* 3) get the 2nd derivative

$$\ddot{\ell_x}(\theta) = \frac{-2(1+(x-\theta)^2) + 4(x-\theta)^2}{(1+(x-\theta)^2)^2}$$

* 4) get the observed fisher information

$$I_{(x)} = -\ddot{\ell_x}(\hat{\theta}^{MLE})$$

* 5) get the variance of the estimate, even if the distribution does not have a defined variance or expected value

- for 10000 samples of size n with $\theta = 0$, compute $1/I_{(x)}$ and $\hat{\theta}^{MLE}$
- group the 10000 $\hat{\theta}^{MLE}$ values according to quantiles of $1/I_{(x)}$ and calculate the empirical variance for each sample.

* for all samples, the unconditional variance $1/nI_0$ is the same because all the samples are of the same size.
* on the other hand, $I_{(x)}$ will vary from sample to sample ($\hat{\theta}^{MLE}$ is different for each sample). * $I_{(x)}$ is related to the variance.

Permutation and Randomization

* when performing a t-test, it's assumed that the data samples come from a normal distribution.
* small samples may follow a different distribution.

Randomization removes the normality assumption

* Randomization is: taking random groups from the data that are of the same size as the tested groups.

* 1) compute the t-statistic for each randomly sampled pair of groups
* 2) get the t-statistic histogram

Utilizing random generated groups, it's expected the t-values not to be very high → construct an empirical distribution of t-values

Parametric Models and Exponential Families

Univariate Families

Name Notation	Density	X	Ω	E Var
Normal $N(\mu, \sigma^2)$	$\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}}$	$\mathbb{R}^{(1)}$	$\mu \epsilon \mathbb{R}^{(1)}$ $\sigma^2 \epsilon \mathbb{R}^+$	μ σ^2

* has two parameters, but they are very specific. μ is the location parameter, and σ^2 is the wide/narrow parameter
* model quatities that take positive and/or negative continuous values, if the distribution is symetric and if there are no too many extreme values

Name Notation	Density	X	Ω	E Var
Poisson $Poi(\lambda)$	$\frac{e^{-\lambda}\lambda^x}{x!}$	$\mathbb{N}_0$	$\lambda \epsilon \mathbb{R}^+$	λ λ

* if the mean grows/shrinks the variance also grows/shrinks proportionally
* λ must stay positive and is the interval of time of an exponential distribution, which is continuous → the expected number of successes can have decimals
* model a quantity that is discrete, it's the number of counts of something
* It's not very flexible as only has one parameter to tweak

Name Notation	Density	X	Ω	E Var
Binomial $Bi(n, \theta)$	$\binom{n}{x}\theta^n(1-\theta)^{n-x}$	$\{0, ... , n\}$	$0 \leq$ $\theta \leq 1$	$n\theta$ $n\theta(1-\theta)$

* model the count of successes as Poisson, but we know the number of trials n

Name Notation	Density	X	Ω	E Var
Gamma $Ga(\nu, \sigma)$	$\frac{x^{\nu-1}e^{-\frac{x}{\sigma}}}{\sigma^\nu \Gamma(\nu)}$	$\mathbb{R}^+$	$\nu > 0$ $\sigma > 0$	$\sigma\nu$ $\sigma^2\nu$

* the Gamma is used to model positive quantities. its common to use the inverse Gamma to model variances.

Name Notation	Density	X	Ω	E Var
Beta $Be(\alpha, \beta)$	$\frac{x^{\alpha-1}(1-x)^{\beta-1}}{B(\alpha,\beta)}$	$0 \leq x \leq 1$	$\alpha > 0$ $\beta > 0$	$\frac{\alpha}{\alpha+\beta}$ var

$var = \frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}$

* as x goes from 0 to 1, it's mostly used to talk about probabilities (aka. probability distribution)

* both the Gamma and Beta have two parameters that convey some degree of flexibility
* Gamma is flexible but not as flexible as Beta
* The Binomial can approximate a Poisson with a large n and small probability.

Multinomial Distribution (a.k.a. multidimensional binomial)

Used when observations take take a finite number of possible outcome values L.

* let $\underline{x} = (x_1, \ldots, x_L)$ be the vector of counts given the possible outcomes, where x_l is de number of cases/counts having outcome l. *e.g.* $\underline{x} = (150, 300, 1000, 50)$, where outcome $l = 1$ happened 150 times, and outcome $l = 4$ happened 50 times
* code the outcomes in terms of unit vectors of length L. *e.g.* $e_l = (0, \ldots, 0, 1, 0, \ldots, 0)^T$, where the 1 is in the l^{th} place.
* encode the outcomes as unit vectors with assigned probabilities in π_l, a vector of probabilities.

$$\pi_l = P\{e_l\}, l = 1, 2, 3, \ldots, L$$

$\underline{x}$ follows a multinomial distribution f_π

$$f_\pi(\underline{x}) = \underline{x} \sim Mult_L(n, \pi) = \frac{n!}{x_1!x_2!\ldots x_L!} \cdot \prod_{l=1}^{L} \pi_l{}^{x_l}$$

where L is the no. of outcomes, n the no. of observations, and π is the prob. vector.
* The multinomial distribution assumes the probabilities are constant.

The parameter space Ω of π is S_L; a set of probability vectors π such that the components of π are positive quantities for all $l's$

$$S_L = \{\pi : \pi_l \geq 0 \forall l \text{ and } \sum_{l=1}^{L} \pi_l = 1\}$$

The sample space X for $\underline{x}$ is a subset of nS_L with integer components. *e.g.* for $L = 2$ (a Binomial dist.), $(\pi_1, \pi_2) = (\pi, 1-\pi)$; $(x_1, x_2) = (x, n-x)$

The mean vector $E(x) = n\pi$

The covariance matrix Σ is given by:

$$\Sigma = n \cdot \left(\begin{bmatrix} \pi_1 & & \text{zeros} \\ & \pi_2 & \\ & \ddots & \\ \text{zeros} & & \pi_L \end{bmatrix} - \pi \cdot \pi^T \right)$$

The variance of x_l is:

$$V(x_l) = n \cdot \pi_l \cdot (1 - \pi_l)$$

The covariance of x_l is:

$$Cov(x_l, x_j) = -n\pi_l \cdot \pi_j$$

Multinomial-Poisson relationship

IF {
$S_1, S_2, \ldots, S_L$ are independent Poisson distributions/counts; meaning that the counts of each category follow the distribution: $S_l \overset{ind}{\sim} Poi(\mu_l), l = 1, 2, \ldots, L$.
Each Poisson has a different μ_l parameter, which is a vector of mean/rate parameters.
}
THEN {
the vector of successes is given by:

$$\underline{S} | \sum_{l=1}^{L} S_l \sim Mult_L \left(\sum_{l=1}^{L} S_L, \frac{\underline{\mu}}{\sum_{l=1}^{L} \mu_l} \right)$$

}

IF {
the number of trials N is distributed Poisson with parameter n

$$N \sim Poi(n)$$

}
THEN {

$$Mult_L(N, \underline{\pi}) \sim Poi(n \cdot \underline{\pi})$$

}
where $\underline{\pi}$ is the probability vector, and $n \cdot \underline{\pi}$ is a vector of expected values (means).

For a large n, the approximation

$$\underline{x} \overset{a}{\sim} Poi(n \cdot \underline{\pi})$$

removes the need to compute multinomial correlations

* the multinomial distribution contains all distributions on sample space X composed of $\underline{L}$ discrete categories $\rightarrow$ the multinomial dist. can model any distribution

Exponential Families - Poisson Dist.

$$f_\mu(x) = \frac{\mu^x e^{-\mu}}{x!}$$

From the ratio of two Poissons $\frac{f_\mu(x)}{f_{\mu_o}(x)}$,

$$f_\mu(x) = e^{-(\mu - \mu_o)} \cdot \left(\frac{\mu}{\mu_o} \right)^x \cdot f_{\mu_o}(x)$$

given: $\alpha = log(\frac{\mu}{\mu_o})$, then: $\left(\frac{\mu}{\mu_o} \right)^x = e^{\alpha x}$ and $\mu = e^\alpha \mu_o$
therefore:

$$f_\mu(x) = e^{\alpha x} - \Psi(\alpha) \cdot f_{\mu_o}(x)$$
$$\Psi(\alpha) = \mu_o(e^{\alpha - 1})$$

Exponential Families - Gamma Dist.

$$f_{\underline{\alpha}}(x) = \frac{x^{\nu-1} \cdot e^{-\frac{x}{\sigma}}}{\sigma^\nu \Gamma(\nu)}$$

$\underline{\alpha} = (\alpha_1, \alpha_2) = \left(-\frac{1}{\sigma}, \nu\right) \epsilon A \subseteq \{\alpha_1 < 0; \alpha_2 > 0\}$
$\underline{y} = (y_1, y_2) = (\gamma, log(x))$
$\Psi(\underline{\alpha}) = \alpha_2 log(-\alpha_1) + log(\Gamma(\alpha_2))$

IF {
$\underline{x} = (x_1, \ldots, x_n)$ is iid from $f_\mu(x) = e^{\underline{\alpha}^T \underline{y} - \Psi(\underline{\alpha})} \cdot f_{\mu_o}(x)$ and $y_i = t(x_i)$
}
THEN {

$$f_{\underline{\alpha}}(\underline{x}) = e^{n(\underline{\alpha}^T \bar{y} - \Psi(\underline{\alpha})) \cdot f_o(\underline{x})}$$

with: $\bar{y} = \sum_{i=1}^{n} \frac{y_i}{n}$
}

$\Psi(\alpha)$ can be computed numerically by doing:

$$\Psi(\alpha) = log \int_{\text{sample space } X} e^{\underline{\alpha} \underline{y}} f_o(x) dx$$

where $f_o(x)$ is the *pdf* in question

James-Stein Estimator vs Bayes vs MLE

Estimate μ from x if $\mu \sim N(m, A)$

$$\hat{\underline{\mu}}^{Bayes} = \underline{M} + B(\underline{x} - \underline{M})$$

where m = prior parameter, $B = \frac{A}{A+1} = \frac{\text{prior variance}}{\text{total variance}}$,
$\underline{M} = [m, m, \ldots, m]$

$$\hat{\underline{\mu}}^{MLE} = \underline{x}$$

$$\hat{\underline{\mu}}^{JS} = \hat{\underline{M}} + \hat{B}(\underline{x} - \hat{M})$$

where $\hat{M} = \bar{x}$, $\hat{\underline{M}} = [\hat{M}, \hat{M}, \ldots, \hat{M}]$, $\hat{B} = \frac{1 - N - 3}{\sum_{i=1}^{N} (x_i - \bar{x})^2}$
(for N points)

Expected Squared Error

$$E\{\| \hat{\underline{\mu}}^{Bayes} - \underline{\mu} \|^2\} = NB$$

$$E\{\| \hat{\underline{\mu}}^{MLE} - \underline{\mu} \|^2\} = N$$

$$E\{\| \hat{\underline{\mu}}^{JS} - \underline{\mu} \|^2\} = NB + 3(1 - B)$$

$\hat{\underline{\mu}}^{JS}$ has a bigger ESE than $\hat{\underline{\mu}}^{Bayes}$ as $\underline{M}$ and B are estimated, but still better than $\hat{\underline{\mu}}^{MLE}$ if $N \leq 4$ observations.

James-Stein Theorem

IF $x_i | \mu_i \sim N(\mu_i, 1)$ for $i = 1, 2, \ldots, N$ with $N \geq 4$; THEN

$$E\{\| \hat{\underline{\mu}}^{JS} - \underline{\mu} \|^2\} < E\{\| \hat{\underline{\mu}}^{MLE} - \underline{\mu} \|^2\}$$

for all choices of $\underline{\mu} \epsilon \mathbb{R}^N$ (not Bayesian reasoning any more)

* JS gets observations from Normal distributions which have different means for each observation (estimate different means for each observation). * JS is a shrinks the effects of individual observations towards the common mean * extreme shrinkage is to say each observation is the average of all observations * void shrinkage is to say each observation is its own average (as in MLE) * JS is in between.

Ridge Regression vs Linear Regression

Linear Regression

based on MLE, it assumes a n-dimensional vector
$\underline{y} = (y_1, \ldots, y_n)^T$ from a linear model $\underline{y} = x\beta + \underline{\epsilon}$
where:
β a unknown p-dimensional parameter vector
$\underline{\epsilon}$ uncertain values (aka. independent random variables or independent draws from a dist.)
x known data points
$\underline{y}$ outcomes taken from the linear model

Thus: $\epsilon \sim (0, \sigma^2 I_n)$ where:
$mean = 0$
the variance I_n is the identity matrix of size n

$$\hat{\beta} = \overset{argmin}{\beta} \{\| \epsilon \|^2\} = \overset{argmin}{\beta} \{\| \underline{y} - x\beta \|^2\}$$

differentiating:

$$\hat{\beta}^{OLS} = S^{-1} \cdot x^T y$$

where: $S = x^T x$

standard error:

$$\hat{\beta}^{OLS} \sim (\beta, \sigma^2 \cdot S^{-1})$$

Ridge Regression

$$\hat{\beta} = \overset{argmin}{\beta} \{\| y - x \cdot \beta \|^2 + \lambda \cdot \| \beta \|^2\}$$
where: $\| \beta \|^2 = {\beta_1}^2 + {\beta_2}^2 + \ldots + {\beta_p}^2$

if β coefficients are small, the better the results $\rightarrow$ as the variance decreases by introducing some bias. λ is how much the sum of squares is penalized.

differentiating:

$$\hat{\beta}^{Ridge} = (S + \lambda \cdot I_n)^{-1} \cdot x^T y$$

standard error:

$$\hat{\beta}^{Ridge} \sim ((S+\lambda \cdot I_n)^{-1} \cdot S \cdot \beta, \sigma^2 \cdot (S+\lambda \cdot I_n)^{-1} \cdot S \cdot (S+\lambda \cdot I_n)^{-1})$$

Ridge is a regularized regression, meaning that the variables need to be rescaled as the coefficients have to be on the same scale.

OLS is a special case of Rigde where $\lambda = 0$

Logistic Regression

In OLS y can take values in $\mathbb{R}$, or $y \epsilon \mathbb{R}$. However, to predict proportions then $y = p$ should $y_i = p_i \epsilon \{0, 1\} \forall i$

for each observation the odds ratio is: $\lambda_i = log\left(\frac{p_i}{1-p_i}\right)$

for the 1-dimension case, $\lambda_i = log\left(\frac{p_i}{1-p_i}\right) = \beta_0 + \beta_1 \cdot x_i + \epsilon_i$
using MLE, estimate β_0, β_1 and therefore λ_i
$\hat{\lambda}(x) = \hat{\beta_0} + \hat{\beta_1} \cdot x_i$

$$\hat{\lambda_i} = log\left(\frac{\hat{p_i}}{1-\hat{p_i}}\right)$$

$$\hat{p_i} = (1 + e^{-(\hat{\beta_0} + \hat{\beta_1} \cdot x_i)})^{-1}$$

This transformation does not work well when $x = 0$ or $x = 1$ as the OLS loss function $\overset{min}{\beta} \parallel \lambda - x\beta \parallel^2$ increases with the right prediction and decreases with a wrong prediction.

The Deviance Function has the opposite behaviour...

$$D = p_i \cdot log\left(\frac{p_i}{\hat{p_i}}\right) + (1 - p_i) \cdot log\left(\frac{1-p_i}{1-\hat{p_i}}\right)$$

multiply assuming independent sampling to get the loss function:

$$D(\hat{p_i}|p_i) = 2n_i \left[p_i \cdot log\left(\frac{p_i}{\hat{p_i}}\right) + (1 - p_i) \cdot log\left(\frac{1-p_i}{1-\hat{p_i}}\right)\right]$$

Then minimize the loss function to estimate $(\hat{\beta_0}, \hat{\beta_1})$

Generalized Linear Models - GLMs

GLMs extend linear regression to Binomial, Poisson, Gamma or any exponential distribution.
* GLMs transform an estimation problem in to a regression problem where the regression parameters are to be estimated.

GLM - exponential family

start with 1-parameter exponential family:

$$f_\lambda(y) = e^{\lambda y - \gamma(\lambda)} \cdot f_o(y)$$

where: the observed data $\underline{y} = (y_1, y_2, \ldots, y_N)^T$ is assumed to come from $y_i \overset{ind}{\sim} f_{\lambda_i}(\cdot)$ for $i = 1, \ldots, N$

write $\underline{\lambda}$ as a regression equation to avoid N estimations (one for each λ_i)

$$\underline{\lambda} = \underline{x} \cdot \underline{\alpha}$$

where:
α is a coefficients vector to assess the importance of each x
x the covariance matrix from the data

the likelihood of $\underline{y}$ for an exponential family is:

$$f_{\underline{\lambda}}(\underline{y}) = e^{\underline{\lambda} \cdot \underline{y} - \gamma(\underline{\lambda})} \cdot f_o(\underline{y})$$

let $\underline{\lambda} = \underline{x} \cdot \underline{\alpha}$, $\underline{z} = \underline{x}^T y$, $\Psi(\alpha) = \sum_{i=1}^{N} \gamma({x_i}^T \cdot \alpha)$ such that

$$f_{\underline{\alpha}}(\underline{y}) = e^{\underline{\alpha}^T \underline{z} - \Psi(\alpha)} \cdot f_o(\underline{y})$$

GLM - Binomial Distribution

$$\lambda = log\left(\frac{\pi}{1+\pi}\right)$$

$$\gamma(\lambda) = nlog(1 + e^{\lambda})$$

GLM - Poisson Distribution

$$\lambda = log(\mu)$$

$$\gamma(\lambda) = e^{\lambda}$$

GLM - Parameter Estimation

$(\mu\lambda, {\sigma_\lambda}^2)$ denotes the expectation and variance of a univariate density $f_\lambda(y)$ in terms of the exponential family properties

$$y \sim (\mu\lambda, {\sigma_\lambda}^2)$$

a N-dimensional vector y from $f_{\underline{\alpha}}(y)$ has mean and covariance matrix:

$$y \sim (\underline{\mu}(\underline{\alpha}), \Sigma(\underline{\alpha}))$$

where:

$$\underline{\mu}(\underline{\alpha}) = [\mu_{\lambda_1}, \mu_{\lambda_2}, \ldots, \mu_{\lambda_N}]$$

$$\Sigma(\underline{\alpha}) = \begin{bmatrix} {\sigma_{\lambda_1}}^2 & & & \text{zeros} \\ & {\sigma_{\lambda_2}}^2 & & \\ & & \ddots & \\ \text{zeros} & & & {\sigma_{\lambda_N}}^2 \end{bmatrix}$$