18.650 – Fundamentals of Statistics

4. Hypothesis testing

Goals

We have seen the basic notions of hypothesis testing:

- Hypotheses H_0/H_1, not symmetric, H0:status quo, H1: discovery
- Type 1/Type 2 error, level and power
- Test statistics and rejection region
- p-value

Our tests were based on CLT (and sometimes Slutsky)...

- What if data is Gaussian, σ^2 is unknown and Slutsky does not apply? T-test 需要假设样本服从正态分布
- Can we use asymptotic normality of MLE? Wald's test
  不止有CLT可以有渐进正态，MLE也可以有渐进协方差矩阵（I^-1）。 如果感兴趣的不是均值，就不能用CLT了。
- Tests about multivariate parameters $\theta = (\theta_1, \ldots, \theta_d)$ (e.g.: $\theta_1 = \theta_2$)? Implicit hypotheses
- More complex tests: "Does my data follow a Gaussian distribution"? Goodness of fit.

Parametric hypothesis testing

Clinical trials

Let us go through an example to remind the main notions of hypothesis testing.

- Pharmaceutical companies use hypothesis testing to test if a new drug is efficient.
- To do so, they administer a drug to a group of patients (test group) and a placebo to another group (control group).
- We consider testing a drug that is supposed to lower LDL (low-density lipoprotein), a.k.a "bad cholesterol" among patients with a high level of LDL (above 200 mg/dL)

Notation and modelling

- Let $\Delta_{\mathrm{d}} > 0$ denote the expected decrease of LDL level (in mg/dL) for a patient that has used the drug.
- Let $\Delta_{\mathrm{c}} \geqslant 0$ denote the expected decrease of LDL level (in mg/dL) for a patient that has used the placebo.
- We want to know if $\Delta_{\mathrm{d}} > \Delta_{\mathrm{c}}$
- We observe two independent samples:
  - $X_1, \ldots, X_n \overset{iid}{\sim} \mathcal{N}(\Delta_{\mathrm{d}}, \sigma_{\mathrm{d}}^2)$ from the test group and
  - $Y_1, \ldots, Y_m \overset{iid}{\sim} \mathcal{N}(\Delta_{\mathrm{c}}, \sigma_{\mathrm{c}}^2)$ from the control group.

Hypothesis testing

- Hypotheses:

$$H_0 : \Delta_c = \Delta_d \quad \text{vs.} \quad H_1 : \Delta_d > \Delta_c$$

- Since the data is Gaussian by assumption we don't need the CLT

- We have

$$\bar{X}_n \sim \mathcal{N}\left(\Delta_d, \frac{\sigma_d^2}{n}\right) \quad \text{and} \quad \bar{Y}_m \sim \mathcal{N}\left(\Delta_c, \frac{\sigma_c^2}{m}\right)$$

- Therefore

$$\frac{\bar{X}_n - \bar{Y}_m - (\Delta_{\mathrm{d}} - \Delta_{\mathrm{c}})}{\sqrt{\frac{\sigma_d^2}{n} + \frac{\sigma_c^2}{m}}} \sim \mathcal{N}(0,1)$$

方差可加

Asymptotic test

- Assume that $m = cn$ and $n \to \infty$
- Using Slutsky's lemma, we also have

$$\frac{\bar{X}_n - \bar{Y}_m - (\Delta_d - \Delta_c)}{\sqrt{\frac{\hat{\sigma}_d^2}{n} + \frac{\hat{\sigma}_c^2}{m}}} \xrightarrow[n\to\infty]{(d)} \mathcal{N}(0,1)$$

我们并不知道这个，但是在H0下，他们相等（alpha水平是假设在H0下拒绝的概率）。

m也要
但是这里assume m is a constant times n

$$\frac{\bar{X}_n - \bar{Y}_m - (\Delta_d - \Delta_c)}{\sqrt{\frac{\sigma_d^2}{n} + \frac{\sigma_c^2}{m}}} \xrightarrow{(d)} \mathcal{N}(0,1) \quad (\text{actually equal})$$

$$\times \frac{\sqrt{\frac{\sigma_d^2}{n} + \frac{\sigma_c^2}{m}}}{\sqrt{\frac{\hat{\sigma}_d^2}{n} + \frac{\hat{\sigma}_c^2}{m}}} \xrightarrow[n\to\infty]{\mathbb{P}} 1 \quad \text{by CMT}$$

$\to$ Slutsky

where

scaling by 1/(n-1) leads to an unbiased estimator

$$\hat{\sigma}_{\mathrm{d}}^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X}_n)^2 \quad \text{and} \quad \hat{\sigma}_{\mathrm{c}}^2 = \frac{1}{m-1}\sum_{i=1}^{m}(Y_i - \bar{Y}_m)^2$$

- We get the the following test at asymptotic level α:

$$R_\psi = \left\{ \frac{\bar{X}_n - \bar{Y}_m}{\sqrt{\frac{\hat{\sigma}_d^2}{n} + \frac{\hat{\sigma}_c^2}{m}}} > q_\alpha \right\} = \left\{ \frac{\bar{X}_n - \bar{Y}_m}{\sqrt{\frac{\hat{\sigma}_d^2}{n} + \frac{\hat{\sigma}_c^2}{m}}} > q_\alpha \right\}$$

q_α is $(1-\alpha)$ quantile of $\mathcal{N}(0,1)$

- This is one-sided, two-sample test.

Asymptotic test

- Example $n = 70, m = 50$, $\bar{X}_n = 156.4$, $\bar{Y}_m = 132.7$, $\hat{\sigma}^2_{\mathrm{d}} = 5198.4$, $\hat{\sigma}^2_{\mathrm{c}} = 3867.0$,

$$\frac{156.4 - 132.7}{\sqrt{\frac{5198.4}{70} + \frac{3867.0}{50}}} = 1.57$$

Since $q_{5\%} = 1.645$, we fail to reject H_0

- We can also compute the p-value:

$$\text{p-value} = \mathbb{P}(N(0,1) > 1.57) = 0.0582$$

p-value is the probability that i would reject even more than that i'm currently doing
It's probability that the distribution of my test statistic is larger than the actual value of my test statistic


PHARMACOLOGICAL
DRUG TRIAL RESULTS
OUR TRIALS SHOW THAT
THE NEW DRUG PERFORMS
NO BETTER THAN PLACEBO
MAYBE WE SHOULD
INVEST IN PLACEBOS
CHRIS
MADDEN

Small sample size

- What if $n = 20, m = 12$?
- We cannot realistically apply Slutsky's lemma
- We needed it to find the (asymptotic) distribution of quantities of the form

如果你的数据是正态分布，那么X_bar - mu也是正态分布。相当于一个均值为0的正态分布。（linear combination）

$$\bar{X}_n - \mu$$

样本小，所以用不了Slutsky
CLT需要用Slutsky，但是我们并不需要它
我们只需要用样本方差替代总体方差的时候，使用Slutsky

$$\sqrt{\hat{\sigma}^2}$$

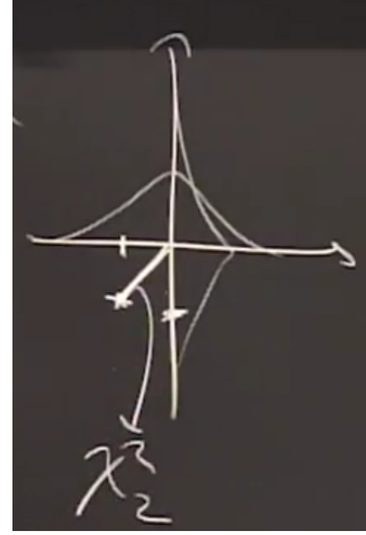
when $X_1, \ldots, X_n \overset{iid}{\sim} \mathcal{N}(\mu, \sigma^2)$.

- It turns out that this distribution *does not depend on* μ *or* σ so we can compute its quantiles

The χ^2 distribution

measuring the length of Gaussian vector(square length)

二维正态分布点离原点的距离的平方。



Definition

For a positive integer d, the χ^2 *(pronounced "Kai-squared") distribution with* d *degrees of freedom* is the law of the random variable $Z_1^2 + Z_2^2 + \ldots + Z_d^2$, where $Z_1, \ldots, Z_d \overset{iid}{\sim} \mathcal{N}(0,1)$.

这里的d是几个变量

Examples:

这里的d是维度

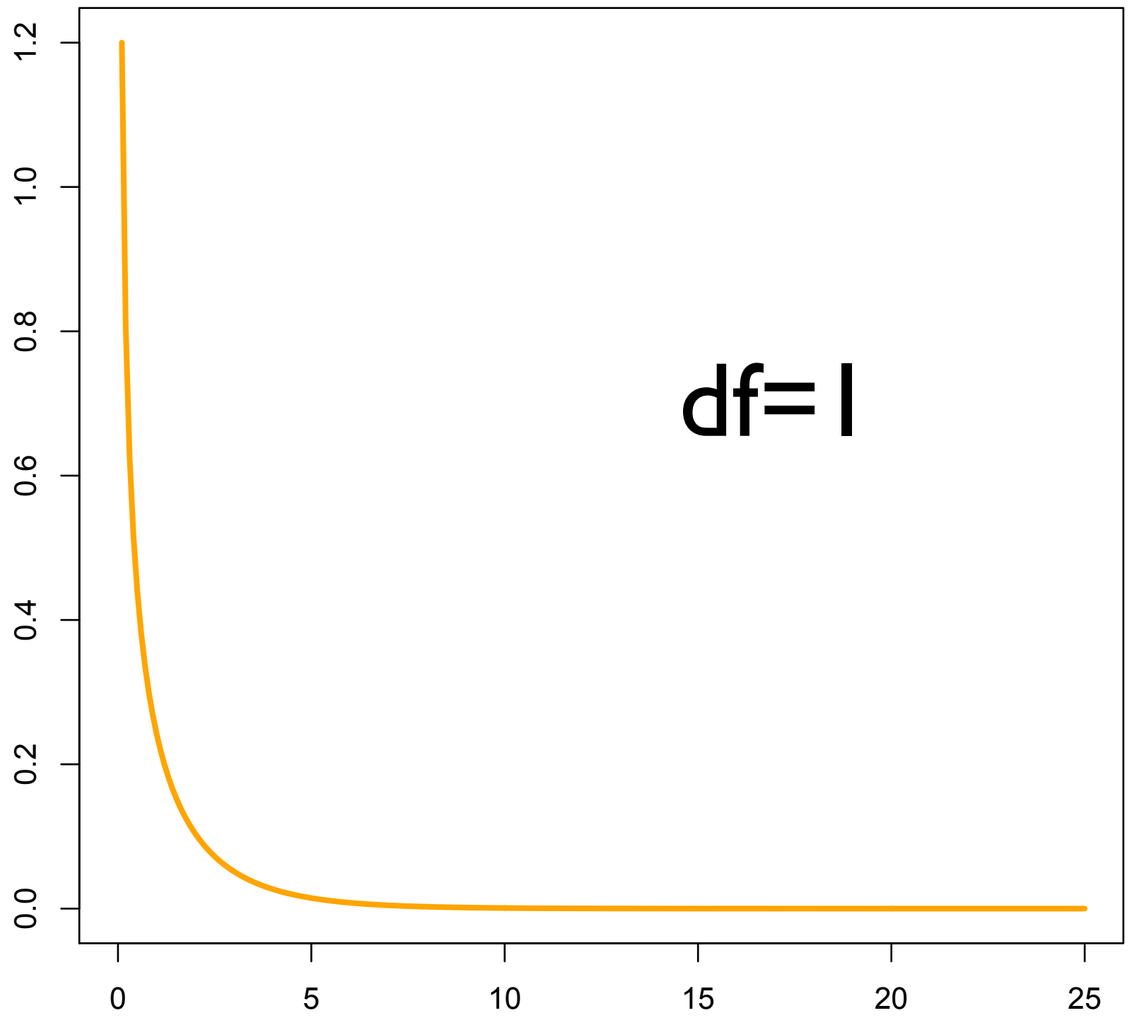
- If $Z \sim \mathcal{N}_d(\mathbf{0}, I_d)$, then $\|Z\|_2^2 \sim \chi_d^2$

L2 norm
Euclidean norm

- $\chi_2^2 = \mathsf{Exp}(1/2)$.

pdf of $X \sim \chi_k^2 = \Gamma(\frac{k}{2}, \frac{1}{2})$

$\frac{1}{2^{k/2}\Gamma(\frac{k}{2})} x^{k/2-1} e^{-x/2}, \; x > 0$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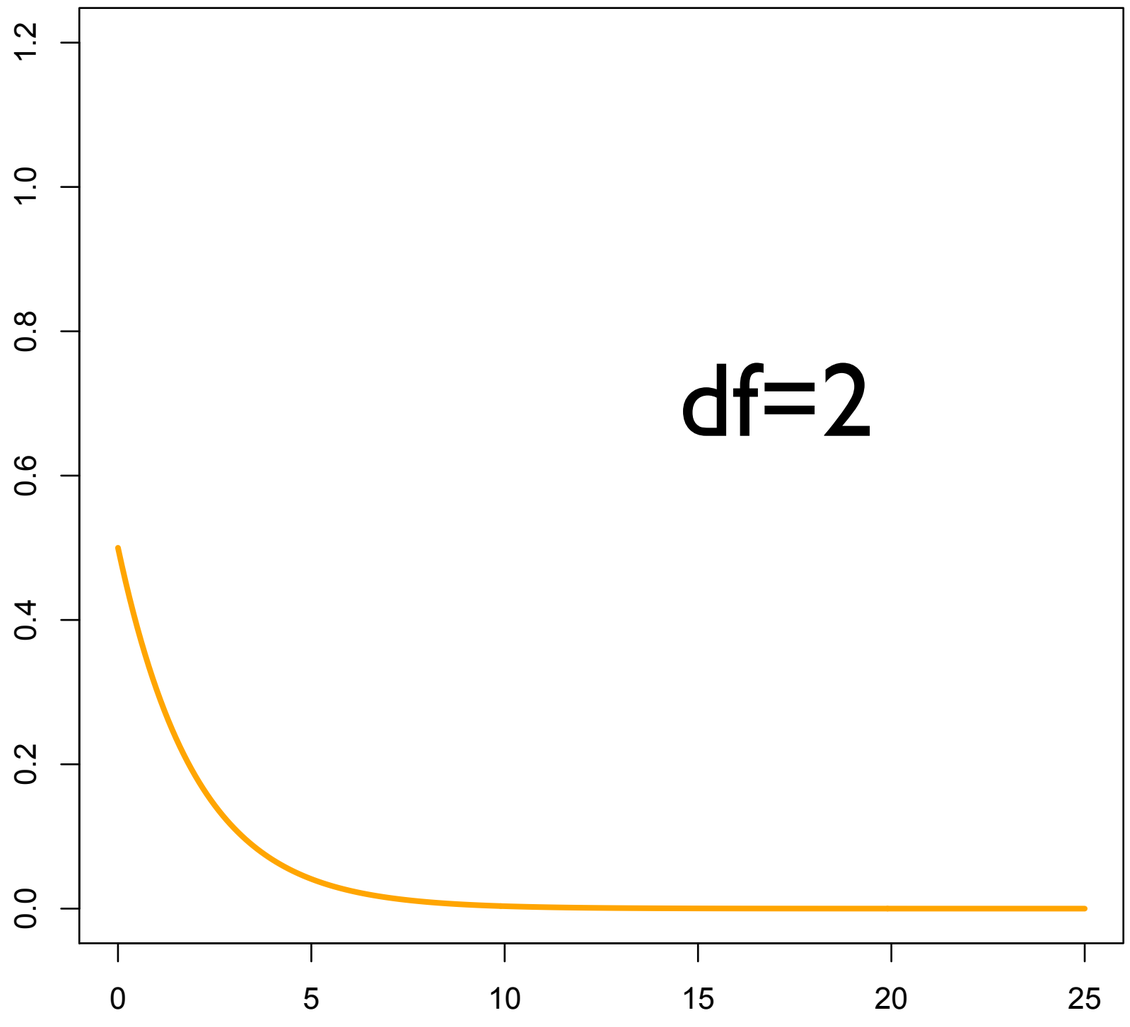
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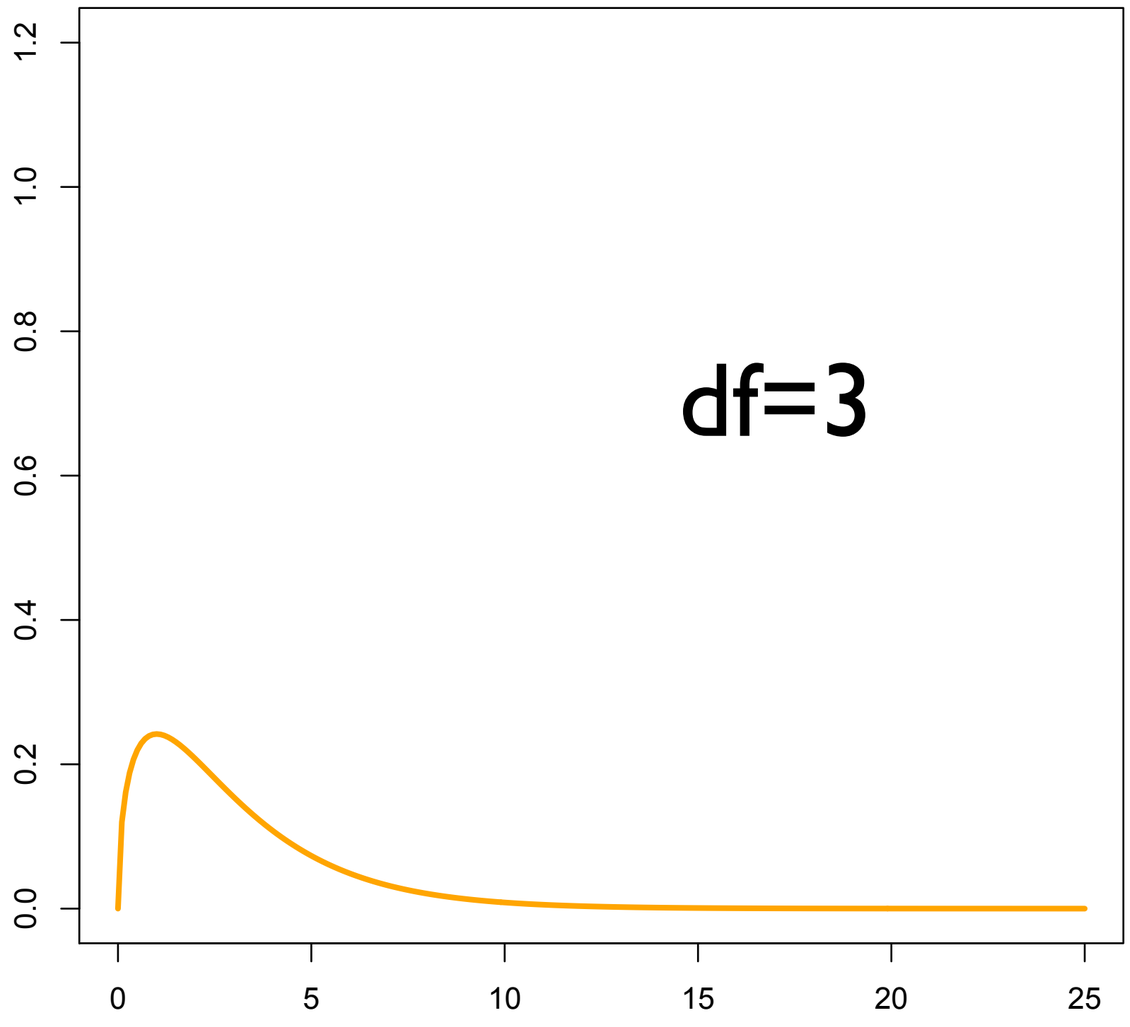
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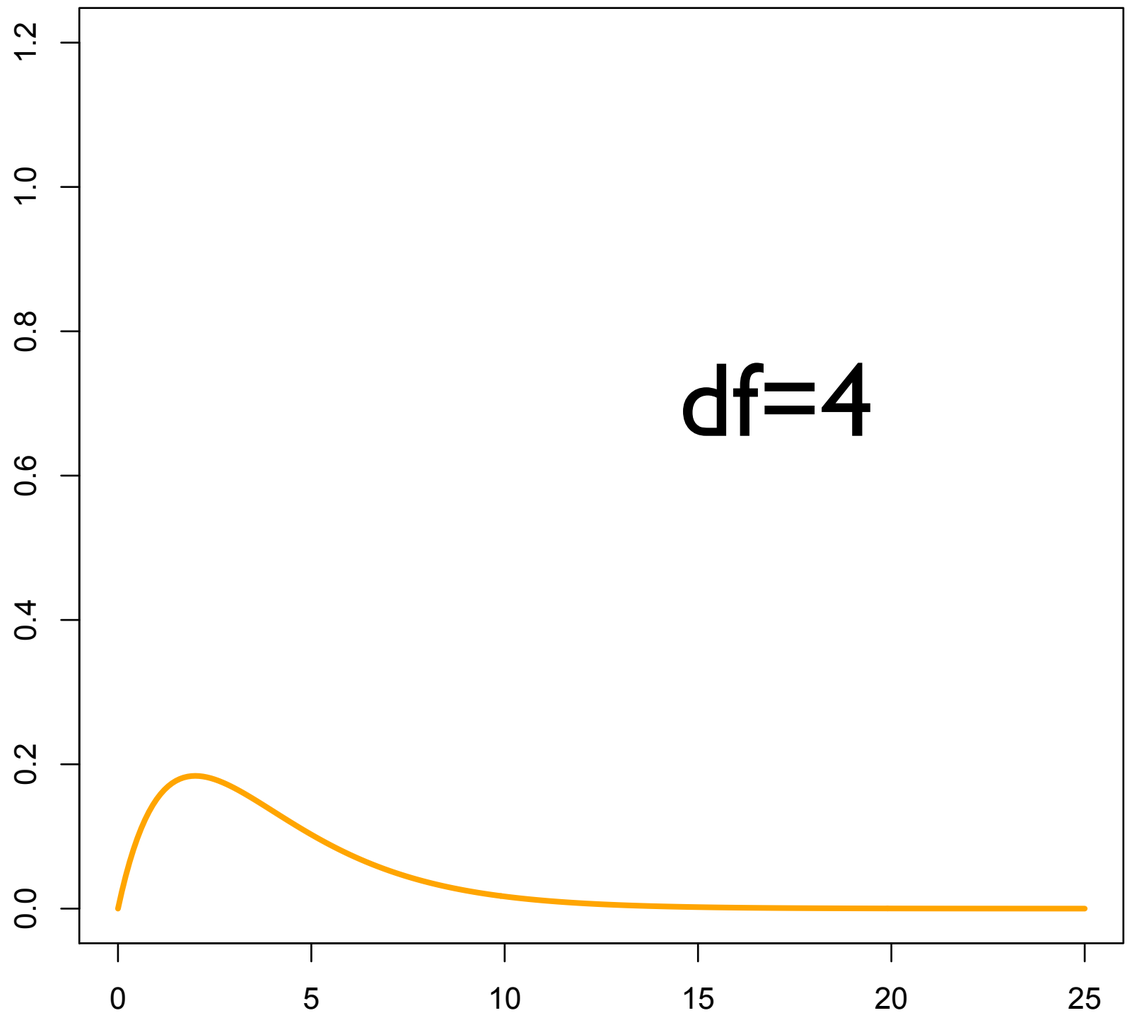
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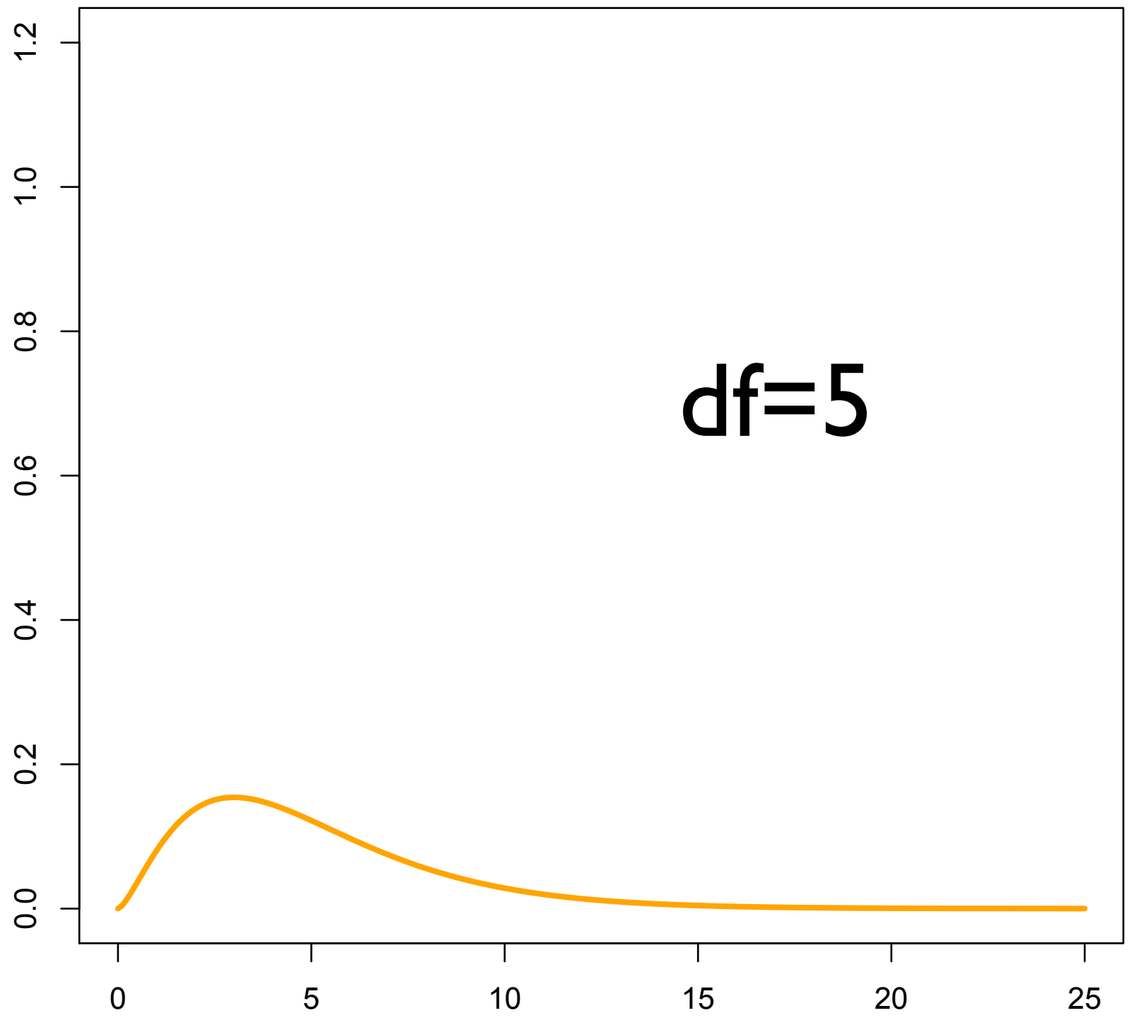
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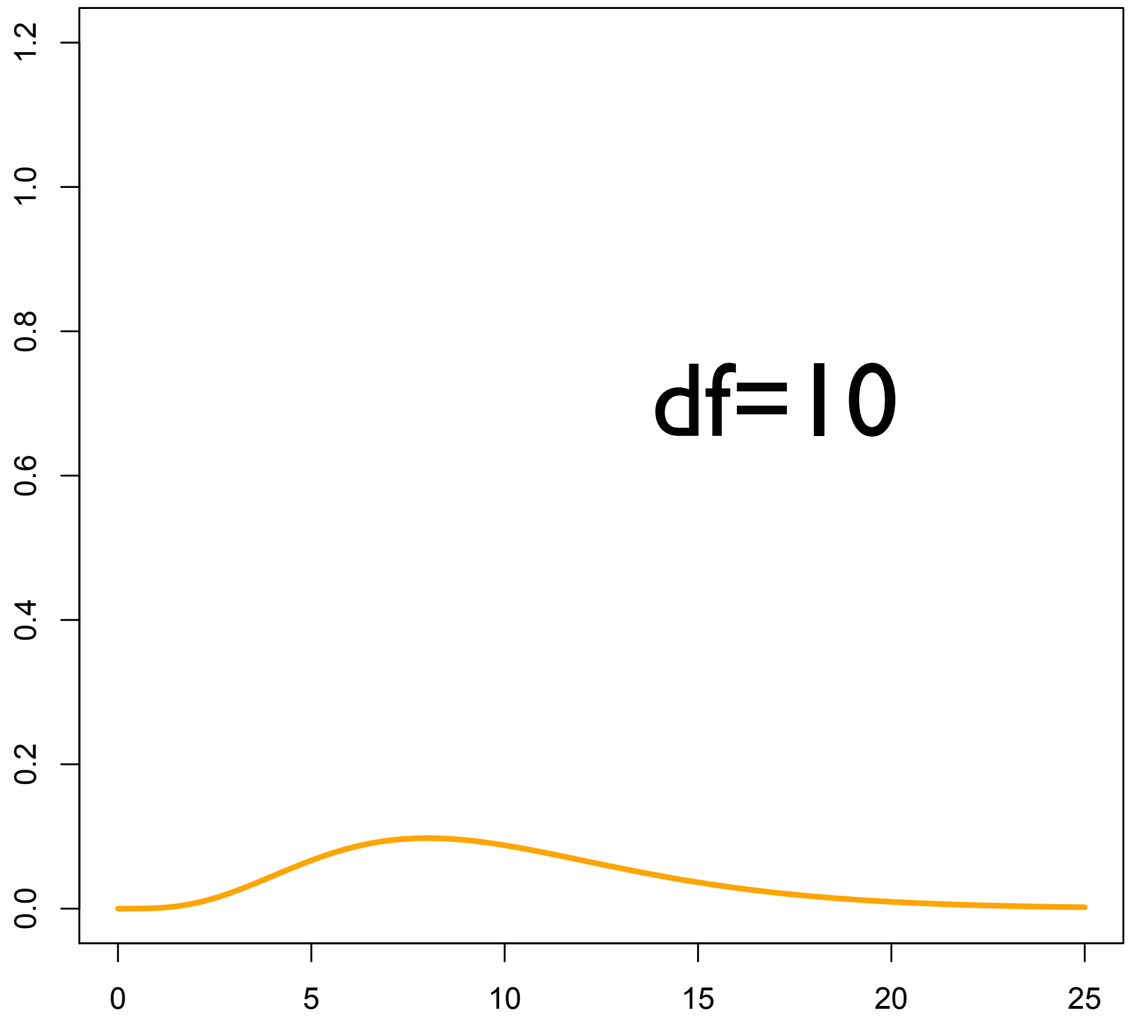
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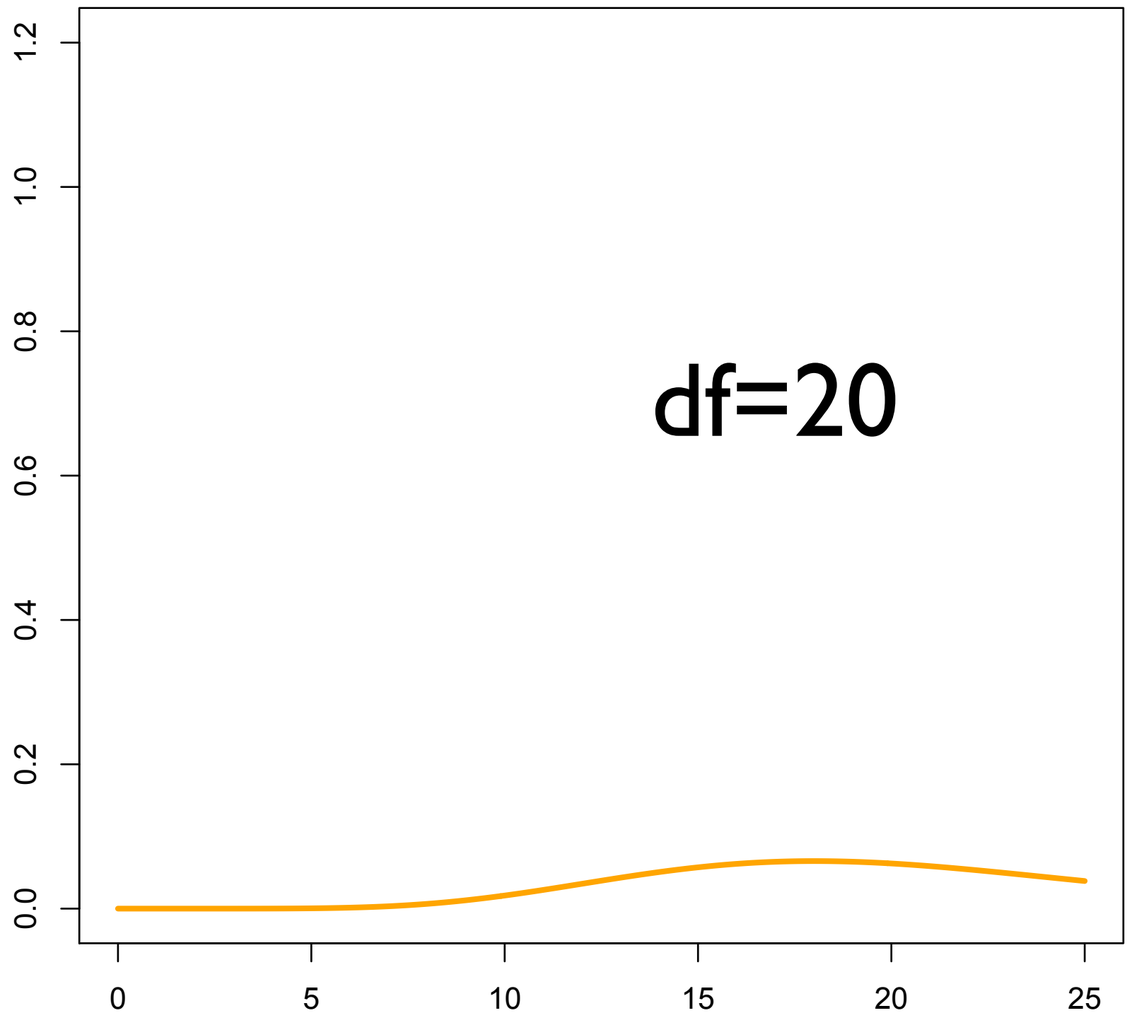
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Properties χ^2 distribution (2)

Definition

For a positive integer d, the χ^2 *(pronounced "Kai-squared") distribution with d degrees of freedom* is the law of the random variable $Z_1^2 + Z_2^2 + \ldots + Z_d^2$, where $Z_1, \ldots, Z_d \overset{iid}{\sim} \mathcal{N}(0,1)$.

Properties: If $V \sim \chi^2_k$, then

- $\mathbb{E}[V] =$ $E[Z_1^2] + \cdots + E[Z_d^2] = d$
- $\text{var}[V] =$ $Var[Z_1^2] + \cdots + Var[Z_d^2] = 2d$

$Var[Z_1^2] = E[Z_1^4] - 1 = 3 - 1 = 2$

third moment is measuring skewedness
forth moment is measuring kurtosis

如果d很大，那么chi^2 -> N(d,2d) CLT

Important example: the sample variance

- Recall that the sample variance is given by
$$S_n = \frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X}_n)^2 = \frac{1}{n}\sum_{i=1}^{n} X_i^2 - (\bar{X}_n)^2$$
- Cochran's theorem states that for $X_1, \ldots, X_n \overset{iid}{\sim} \mathcal{N}(\mu, \sigma^2)$, if S_n is the sample variance, then
  - $\bar{X}_n \perp\!\!\!\perp S_n$; (independent) for all n.
  - $\frac{nS_n}{\sigma^2} \sim \chi^2_{n-1}$

remove the mean and variance of N(mu,sigma^2). and times n. Get the sum of the squared r.v from N(0,1)

这个是自由度，n个r.v.只有n-1个自由度。他不是n个独立的正态分布变量，有一个自由度丢失了。因为你知道，这些数加起来是0，但是你当你把n个独立的正态分布变量加起来的时候，你几乎肯定得不到0。

$\mathbb{E}[S_n] = \frac{n-1}{n}\sigma^2$

- We often prefer the unbiased estimator of σ^2:

$$\tilde{S}_n = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X}_n)^2 = \frac{n}{n-1} S_n$$

$$\mathbb{E}[\tilde{S}_n] = \frac{n}{n-1}\,\mathbb{E}\left[\frac{\sigma^2}{n}\chi^2_{n-1}\right] = \frac{n\sigma^2}{n-1}\cdot\frac{n-1}{n} = \sigma^2$$

Student's T distribution

Definition

For a positive integer d, the *Student's T distribution with d degrees of freedom* (denoted by t_d) is the law of the random variable $\frac{Z}{\sqrt{V/d}}$, where $Z \sim \mathcal{N}(0,1)$, $V \sim \chi^2_d$ and $Z \perp\!\!\!\perp V$ (Z is independent of V).

这个是定义

这个的sample variance就是 V

VOLUME VI MARCH, 1908 No. 1

BIOMETRIKA.

THE PROBABLE ERROR OF A MEAN.

BY STUDENT.

Introduction.

ANY experiment may be regarded as forming an individual of a "population" of experiments which might be performed under the same conditions. A series of experiments is a sample drawn from this population.

Now any series of experiments is only of value in so far as it enables us to form a judgment as to the statistical constants of the population to which the experiments belong. In a great number of cases the question finally turns on the value of a mean, either directly, or as the mean difference between the two quantities.

Who was Student?

This distribution was introduced by **William Sealy Gosset** (1876–1937) in 1908 while he worked for the Guinness brewery in Dublin, Ireland.

$$\bar{X}_n \sim N\left(\mu, \frac{\sigma^2}{n}\right)$$

$$\frac{\bar{X}_n - \mu}{\sqrt{\sigma^2/n}} = \frac{\sqrt{n}\,\frac{\bar{X}_n - \mu}{\sigma}}{\sqrt{\frac{S_n}{\sigma^2}}}$$

$$\sqrt{n} \cdot \frac{\bar{x} - \mu}{\sqrt{\sigma^2}} \sim N(0,1)$$

if $\bar{x}$ is Gaussian.

$$\Rightarrow \sqrt{n} \cdot \frac{\bar{x} - \mu}{\sqrt{\hat{\sigma}^2}} \sim t_{n-1}$$

Student's T test (one sample, two-sided)

两种t检验的理解方式
1，N(0,1)除以chi^2_n-1
2，x_bar是正态分布时，如果想用样本方差估计总体方差，就要将标准正态分布换成自由度为n-1的t分布

non-asymptotic: you don't know the distribution, have to assume.

- Let $X_1, \ldots, X_n \overset{iid}{\sim} \mathcal{N}(\mu, \sigma^2)$ where both μ and σ^2 are unknown
- We want to test:

$$H_0 : \mu = 0, \quad \text{vs} \quad H_1 : \mu \neq 0$$

- Test statistic:

$$T_n = \frac{\bar{X}_n}{\sqrt{\tilde{S}_n/n}} =$$

under H_0 所以是0

$$\sim \mathcal{N}(0,1)$$

$$\frac{\sqrt{n}(\bar{X}_n - \mu)/\sigma}{\sqrt{\tilde{S}_n/\sigma^2}}$$

- Since $\sqrt{n}\bar{X}_n/\sigma \sim \mathcal{N}(0,1)$ (under H_0) and $\tilde{S}_n/\sigma^2 \sim \frac{\chi^2_{n-1}}{n-1}$ are independent by Cochran's theorem, we have:

$$T_n \sim t_{n-1}$$

- Student's test with (non asymptotic) level $\alpha \in (0,1)$:

$$\psi_\alpha = \mathbb{1}\{|T_n| > q_{\alpha/2}\},$$

where $q_{\alpha/2}$ is the $(1-\alpha/2)$-quantile of t_{n-1}.

Student's T test (one sample, one-sided)

- We want to test:

等于mu0和小于mu0其实是一个意思，因为是无论mu取什么值，都小于mu0

$$H_0 : \mu \leq \mu_0, \quad \text{vs} \quad H_1 : \mu > \mu_0$$

- Test statistic:

$$T_n = \sqrt{n}\frac{\bar{X}_n - \mu_0}{\sqrt{\tilde{S}_n}} \sim t_{n-1} \quad \text{under } H_0$$

under H_0.

- Student's test with (non asymptotic) level $\alpha \in (0, 1)$:

$$\psi_\alpha = \mathbb{1}\Big\{ T_n > q_\alpha \Big\},$$

where q_α is the $(1-\alpha)$-quantile of t_{n-1}

Two-sample T-test

- Back to our cholesterol example. What happens for small sample sizes?
- We want to know the distribution of

$$\frac{\bar{X}_n - \bar{Y}_m - (\Delta_{\mathrm{d}} - \Delta_{\mathrm{c}})}{\sqrt{\frac{\hat{\sigma}_{\mathrm{d}}^2}{n} + \frac{\hat{\sigma}_{\mathrm{c}}^2}{m}}}$$

- We have approximately

$$\frac{\bar{X}_n - \bar{Y}_m - (\Delta_{\mathrm{d}} - \Delta_{\mathrm{c}})}{\sqrt{\frac{\hat{\sigma}_{\mathrm{d}}^2}{n} + \frac{\hat{\sigma}_{\mathrm{c}}^2}{m}}} \sim t_N$$

where

$$N = \frac{\left(\hat{\sigma}_{\mathrm{d}}^2/n + \hat{\sigma}_{\mathrm{c}}^2/m\right)^2}{\frac{\hat{\sigma}_{\mathrm{d}}^4}{n^2(n-1)} + \frac{\hat{\sigma}_{\mathrm{c}}^4}{m^2(m-1)}} \geq \min(n, m)$$

observation

N越大，越接近正态。
N越小，越保守。

(Welch-Satterthwaite formula)

Non-asymptotic test

- Example $n = 70, m = 50$, $\bar{X}_n = 156.4$, $\bar{Y}_m = 132.7$, $\hat{\sigma}_{\mathrm{d}}^2 = 5198.4$, $\hat{\sigma}_{\mathrm{c}}^2 = 3867.0$,

$$\frac{156.4 - 132.7}{\sqrt{\frac{5198.4}{70} + \frac{3867.0}{50}}} = 1.57$$

- Using the shorthand formula $N = \min(n, m) = 50$, we get $q_{5\%} = 1.68$ and

more conservative than normal
tail has more weight

$$\text{p-value} = \mathbb{P}[t_{50} > 1.57] = 0.0614$$

- Using the W-S formula

$$N = \frac{\left(\frac{5198.4}{70} + \frac{3867.0}{50}\right)^2}{\frac{5198.4^2}{70^2(70-1)} + \frac{3867.0^2}{50^2(50-1)}} = 113.78$$

we round to 113 .

- We get

$$\text{p-value} = \mathbb{P}[t_{113} > 1.57] = 0.0596$$

随着N增加，p值变小到和正态中的一样。(Slutsky)

Non-asymptotic test

- Example $n = 20$, $m = 12$, $\bar{X}_n = 156.4$, $\bar{Y}_m = 132.7$, $\hat{\sigma}_{\mathrm{d}}^2 = 5198.4$, $\hat{\sigma}_{\mathrm{c}}^2 = 3867.0$,

$$\frac{156.4 - 132.7}{\sqrt{\frac{5198.4}{20} + \frac{3867.0}{12}}} = 0.982$$

- Using the shorthand formula $N = \min(n, m) = 12$, we get $q_{5\%} = 1.78$ and

$$\text{p-value} = \mathbb{P}[t_{12} > 0.982] = 17.27\,\%$$

- Using the W-S formula

$$N = \frac{\left(\frac{5198.4}{20} + \frac{3867.0}{12}\right)^2}{\frac{5198.4^2}{20^2(20-1)} + \frac{3867.0^2}{12^2(12-1)}} = 26.07$$

  we round to 26.

- We get

$$\text{p-value} = \mathbb{P}[t_{26} > 0.982] = 16.16\,\%$$

Discussion

Advantage of Student's test: Non asymptotic / Can be run on small samples + Can always use it for large sample sizes.

large data + CLT 就可以使用

Drawback of Student's test: It relies on the assumption that the sample is Gaussian (soon we will see how to test this assumption)

A test based on the MLE

- Consider an i.i.d. sample $X_1, \ldots, X_n$ with statistical model $(E, (\mathbb{P}_\theta)_{\theta \in \Theta})$, where $\Theta \subseteq \mathbb{R}^d$ $(d \geq 1)$ and let $\theta_0 \in \Theta$ be fixed and given. θ^* is the true parameter
- Consider the following hypotheses:

$$\begin{cases} H_0 : & \theta^* = \theta_0 \\ H_1 : & \theta^* \neq \theta_0. \end{cases}$$

- Let $\hat{\theta}^{MLE}$ be the MLE. Assume the MLE technical conditions are satisfied.

- If H_0 is true, then

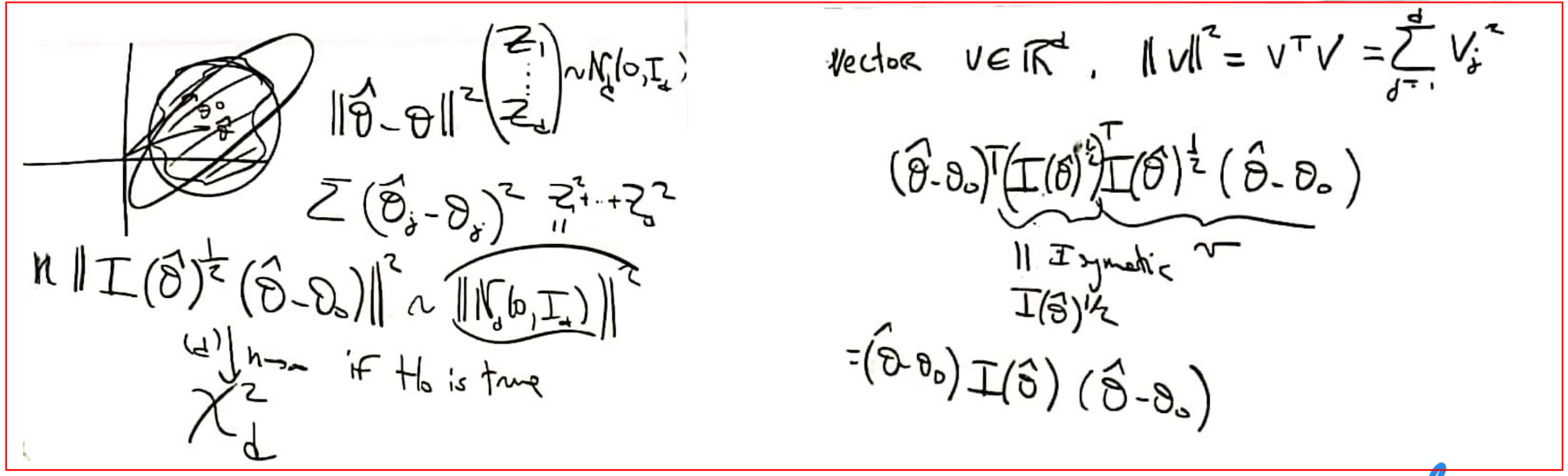
MLE converges to true parameter, so we can plug in the theta

sample(under H0) $\sqrt{n}\, I(\theta_0)^{1/2} \times \left(\hat{\theta}_n^{MLE} - \theta_0\right) \xrightarrow[n\to\infty]{(d)} \mathcal{N}_d(0, I_d)$

true $\sqrt{n}\, I(\theta^*)^{1/2}$

MLE(under H0) $\sqrt{n}\, I(\hat{\theta}_n^{MLE})^{1/2}$

Wald's test



- Hence,

$$\underbrace{n \left(\hat\theta_n^{MLE} - \theta_0\right)^\top I(\hat\theta^{MLE}) \left(\hat\theta_n^{MLE} - \theta_0\right)}_{T_n} \xrightarrow[n\to\infty]{(d)} \chi^2_d$$

- Wald's test with asymptotic level $\alpha \in (0,1)$:

$$\psi = \mathbb{1}\{T_n > q_\alpha\},$$

where q_α is the $(1-\alpha)$-quantile of χ^2_d (see tables).

- Remark: Wald's test is also valid if H_1 has the form "$\theta > \theta_0$" or "$\theta < \theta_0$" or "$\theta = \theta_1$"...

But less powerful

A test based on the log-likelihood

- Consider an i.i.d. sample $X_1, \ldots, X_n$ with statistical model $(E, (\mathbb{P}_\theta)_{\theta \in \Theta})$, where $\Theta \subseteq \mathbb{R}^d$ $(d \geq 1)$.

- Suppose the null hypothesis has the form

$$H_0 : (\theta_{r+1}, \ldots, \theta_d) = (\theta_{r+1}^{(0)}, \ldots, \theta_d^{(0)}),$$

for some fixed and given numbers $\theta_{r+1}^{(0)}, \ldots, \theta_d^{(0)}$.

- Let

$$\hat{\theta}_n = \underset{\theta \in \Theta}{\operatorname{argmax}} \ \ell_n(\theta) \quad \text{(MLE)}$$

and

$$\hat{\theta}_n^c = \underset{\theta \in \Theta_0}{\operatorname{argmax}} \ \ell_n(\theta) \quad \text{(“constrained MLE”)}$$

where $\Theta_0 =$ $\{\theta \in \Theta : (\theta_{r+1}, \ldots, \theta_d) = (\theta_{r+1}^{(0)}, \ldots, \theta_d^{(0)})\}$

Likelihood ratio test

Test statistic:

$$T_n = 2\left(\ell_n(\hat{\theta}_n) - \ell_n(\hat{\theta}_n^c)\right).$$

Wilks' Theorem

Assume H_0 is true and the MLE technical conditions are satisfied. Then,

$$T_n \xrightarrow[n\to\infty]{(d)} \chi^2_{d-r}$$

Likelihood ratio test with asymptotic level $\alpha \in (0,1)$:

$$\psi = \mathbb{1}\{T_n > q_\alpha\},$$

where q_α is the $(1-\alpha)$-quantile of χ^2_{d-r} (see tables).

Implicit hypotheses

- Let $X_1, \ldots, X_n$ be i.i.d. random variables and let $\theta \in \mathbb{R}^d$ be a parameter associated with the distribution of X_1 (e.g. a moment, the parameter of a statistical model, etc...)

- Let $g : \mathbb{R}^d \to \mathbb{R}^k$ be continuously differentiable (with $k < d$).

- Consider the following hypotheses:

$$\begin{cases} H_0 : & g(\theta) = 0 \\ H_1 : & g(\theta) \neq 0. \end{cases}$$

- E.g. $g(\theta) = (\theta_1, \theta_2)$ $(k = 2)$, or $g(\theta) = \theta_1 - \theta_2$ $(k = 1)$, or...

Delta method

- Suppose an asymptotically normal estimator $\hat{\theta}_n$ is available:

$$\sqrt{n}\left(\hat{\theta}_n - \theta\right) \xrightarrow[n\to\infty]{(d)} \mathcal{N}_d(0, \Sigma(\theta)).$$

- Delta method:

$$\sqrt{n}\left(g(\hat{\theta}_n) - g(\theta)\right) \xrightarrow[n\to\infty]{(d)} \mathcal{N}_k\left(0, \Gamma(\theta)\right),$$

where $\Gamma(\theta) = \nabla g(\theta)^\top \Sigma(\theta) \nabla g(\theta) \in \mathbb{R}^{k\times k}$.

- Assume $\Sigma(\theta)$ is invertible and $\nabla g(\theta)$ has rank k. So, $\Gamma(\theta)$ is invertible and

$$\sqrt{n}\,\Gamma(\theta)^{-1/2}\left(g(\hat{\theta}_n) - g(\theta)\right) \xrightarrow[n\to\infty]{(d)} \mathcal{N}_k\left(0, I_k\right).$$

Wald's test for implicit hypotheses

- Then, by Slutsky's theorem, if $\Gamma(\theta)$ is continuous in θ,

$$\sqrt{n}\,\Gamma(\hat{\theta}_n)^{-1/2}\left(g(\hat{\theta}_n) - g(\theta)\right) \xrightarrow[n\to\infty]{(d)} \mathcal{N}_k\left(0, I_k\right).$$

- Hence, if H_0 is true, i.e., $g(\theta) = 0$,

$$\underbrace{n g(\hat{\theta}_n)^\top \Gamma^{-1}(\hat{\theta}_n) g(\hat{\theta}_n)}_{T_n} \xrightarrow[n\to\infty]{(d)} \chi^2_k.$$

- Test with asymptotic level α:

$$\psi = \mathbb{1}\{T_n > q_\alpha\},$$

where q_α is the $(1-\alpha)$-quantile of χ^2_k (see tables).

Goodness of fit

Goodness of fit tests

Let X be a r.v. Given i.i.d copies of X we want to answer the following types of questions:

- Does X have distribution $\mathcal{N}(0, 1)$? (Cf. Student's T distribution)
- Does X have distribution $\mathcal{U}([0, 1])$?
- Does X have PMF $p_1 = 0.3,\ p_2 = 0.5,\ p_3 = 0.2$

These are all *goodness of fit* (GoF) tests: we want to know if the hypothesized distribution is a good fit for the data.

Key characteristic of GoF tests: no parametric modeling.

The zodiac sign of the most powerful people is....

Can your zodiac sign predict how successful you will be later in life?
Fortune magazine collected the signs of 256 heads of the Fortune 500.

Fyi:
256/12
=21.33

Sign	Count
Aries	23
Taurus	20
Gemini	18
Cancer	23
Leo	20
Virgo	19
Libra	18
Scorpio	21
Sagittarius	19
Capricorn	22
Aquarius	24
Pisces	29

The zodiac sign of the most successful people is....

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Capricorn	22
Aquarius	24
Pisces	29

In view of this data, is there statistical evidence that successful people are more likely to be born under some sign than others?

$$p^0 = \underbrace{\left(\frac{1}{12}, \ldots, \frac{1}{12}\right)}_{12 \text{ times}} \in \Delta_{12}$$

275 jurors with identified racial group.
We want to know if the jury is representative of the population of this county.

$p^0 = (0.72, 0.07, 0.12, 0.09)$

$K = 4$

Race	White	Black	Hispanic	Other	Total
# jurors	205	26	25	19	275
proportion in county	0.72	0.07	0.12	0.09	1

Discrete distribution

Let $E = \{a_1, \ldots, a_K\}$ be a finite space and $(\mathbb{P}_{\mathbf{p}})_{\mathbf{p} \in \Delta_K}$ be the family of all probability distributions on E:

$p_j = \mathbb{P}[X = a_j]$

- $\Delta_K = \left\{ \mathbf{p} = (p_1, \ldots, p_K) \in (0,1)^K : \sum_{j=1}^{K} p_j = 1 \right\}.$

- For $\mathbf{p} \in \Delta_K$ and $X \sim \mathbb{P}_{\mathbf{p}}$,

$$\mathbb{P}_{\mathbf{p}}[X = a_j] = p_j, \qquad j = 1, \ldots, K.$$

Goodness of fit test

- Let $X_1, \ldots, X_n \overset{iid}{\sim} \mathbb{P}_{\mathbf{p}}$, for some unknown $\mathbf{p} \in \Delta_K$, and let $\mathbf{p}^0 \in \Delta_K$ be fixed.

- We want to test:

$$H_0\colon\ \mathbf{p} = \mathbf{p}^0 \text{ vs. } H_1\colon\ \mathbf{p} \neq \mathbf{p}^0$$

  with asymptotic level $\alpha \in (0, 1)$.

- Example: If $\mathbf{p}^0 = (1/K, 1/K, \ldots, 1/K)$, we are testing whether $\mathbb{P}_{\mathbf{p}}$ is the uniform distribution on E.

Multinomial likelihood

K = # of modalities

- Likelihood of the model:

$X \sim \text{Multinomial}(\underbrace{p_1, \dots, p_K}_{\vec{p}})$

$$L_n(X_1, \dots, X_n, \mathbf{p}) = p_1^{N_1} p_2^{N_2} \dots p_K^{N_K},$$

where $N_j = \#\{i = 1, \dots, n : X_i = a_j\}$.

- Let $\hat{\mathbf{p}}$ be the MLE:

$$\hat{\mathbf{p}}_j = \frac{N_j}{n}, \quad j = 1, \dots, K.$$

⚠ $\hat{\mathbf{p}}$ maximizes $\log L_n(X_1, \dots, X_n, \mathbf{p})$ **under the constraint**

χ^2 test

- If H_0 is true, then $\sqrt{n}(\hat{\mathbf{p}} - \mathbf{p}^0)$ is asymptotically normal, and the following holds.

$\sqrt{n}\, I(p^0)^{1/2}(\hat{p} - p^0) \xrightarrow[n\to\infty]{} \mathcal{N}_{K-1}(0, I_{K-1})$

Theorem Under H_0:

$$n \sum_{j=1}^{K} \frac{\left(\hat{\mathbf{p}}_j - \mathbf{p}_j^0\right)^2}{\mathbf{p}_j^0} \xrightarrow[n\to\infty]{(d)} \chi^2_{K-1}.$$

T_n

- χ^2 test with asymptotic level α: $\psi_\alpha = \mathbb{1}\{T_n > q_\alpha\}$, where q_α is the $(1-\alpha)$-quantile of χ^2_{K-1}.
- Asymptotic p-value of this test: $p - \text{value} = \mathbb{P}\left[Z > T_n | T_n\right]$, where $Z \sim \chi^2_{K-1}$ and $Z \perp\!\!\!\perp T_n$.

CDF and empirical CDF

Let $X_1, \ldots, X_n$ be i.i.d. real random variables. Recall the cdf of X_1 is defined as:

$$F(t) = \mathbb{P}[X_1 \leq t], \qquad \forall t \in \mathbb{R}.$$

It completely characterizes the distribution of X_1.

Definition

The *empirical cdf* (a.k.a sample cdf) of the sample $X_1, \ldots, X_n$ is defined as:

$$\begin{aligned} F_n(t) &= \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}\{X_i \leq t\} \\ &= \frac{\#\{i = 1, \ldots, n : X_i \leq t\}}{n}, \qquad \forall t \in \mathbb{R}. \end{aligned}$$

Consistency

By the LLN, for all $t \in \mathbb{R}$,

$$F_n(t) \xrightarrow[n\to\infty]{a.s.} F(t).$$

Glivenko-Cantelli Theorem (*Fundamental theorem of statistics*)

$$\sup_{t\in\mathbb{R}} |F_n(t) - F(t)| \xrightarrow[n\to\infty]{a.s.} 0.$$

Asymptotic normality

By the CLT, for all $t \in \mathbb{R}$,

$$\sqrt{n}\ (F_n(t) - F(t)) \xrightarrow[n\to\infty]{(d)} \mathcal{N}\big(0, F(t)\,(1 - F(t))\big).$$

Donsker's Theorem

If F is continuous, then

$$\sqrt{n}\ \sup_{t\in\mathbb{R}}\ |F_n(t) - F(t)| \xrightarrow[n\to\infty]{(d)} \sup_{0\le t\le 1}\ |\mathbb{B}(t)|,$$

where $\mathbb{B}$ is a Brownian bridge on $[0, 1]$.

Goodness of fit for continuous distributions

- Let $X_1, \ldots, X_n$ be i.i.d. real random variables with unknown cdf F and let F^0 be a **continuous** cdf.

- Consider the two hypotheses:

$$H_0 : F = F^0 \quad \text{v.s.} \quad H_1 : F \neq F^0.$$

- Let F_n be the empirical cdf of the sample $X_1, \ldots, X_n$.

- If $F = F^0$, then $F_n(t) \approx F^0(t)$, for all $t \in [0, 1]$.

Kolmogorov-Smirnov test

- Let $T_n = \sup_{t \in \mathbb{R}} \sqrt{n} \left| F_n(t) - F^0(t) \right|$.

- By Donsker's theorem, if H_0 is true, then $T_n \xrightarrow[n \to \infty]{(d)} Z$, where Z has a known distribution (supremum of a Brownian bridge).

- **KS test with asymptotic level α:**

$$\delta_\alpha^{KS} = \mathbb{1}\{T_n > q_\alpha\},$$

where q_α is the $(1-\alpha)$-quantile of Z (obtained in tables).

- p-value of KS test: $\mathbb{P}[Z > T_n | T_n]$.

Computatinal issues

- In practice, how to compute T_n ?
- F^0 is non decreasing, F_n is piecewise constant, with jumps at $t_i = X_i, i = 1, \ldots, n$.
- Let $X_{(1)} \leq X_{(2)} \leq \ldots \leq X_{(n)}$ be the reordered sample.
- The expression for T_n reduces to the following practical formula:

$$T_n = \sqrt{n} \max_{i=1,\ldots,n} \left\{ \max \left(\left| \frac{i-1}{n} - F^0(X_{(i)}) \right|, \left| \frac{i}{n} - F^0(X_{(i)}) \right| \right) \right\}.$$

Pivotal distribution

- T_n is called a *pivotal statistic*: If H_0 is true, the distribution of T_n does not depend on the distribution of the X_i's and it is easy to reproduce it in simulations.

- Indeed, let $U_i = F^0(X_i), i = 1, \ldots, n$ and let G_n be the empirical cdf of $U_1, \ldots, U_n$.

- If H_0 is true, then $U_1, \ldots, U_n \overset{i.i.d.}{\sim}$ Unif([0,1])

  and $T_n = \sup_{0 \leq x \leq 1} \sqrt{n}\,|G_n(x) - x|$.

Quantiles and p-values

- For some large integer M:
  - Simulate M i.i.d. copies $T_n^1, \ldots, T_n^M$ of T_n;
  - Estimate the $(1-\alpha)$-quantile $q_\alpha^{(n)}$ of T_n by taking the sample $(1-\alpha)$-quantile $\hat{q}_\alpha^{(n,M)}$ of $T_n^1, \ldots, T_n^M$.
- Test with approximate level α:

$$\delta_\alpha = \mathbb{1}\{T_n > \hat{q}_\alpha^{(n,M)}\}.$$

- Approximate p-value of this test:

$$\text{p-value} \approx \frac{\#\{j = 1, \ldots, M : T_n^j > T_n\}}{M}.$$

K-S table

Kolmogorov–Smirnov Tables

Critical values, $d_{alpha};(n)^{a}$, of the maximum absolute difference between sample $F_n(x)$ and population $F(x)$ cumulative distribution.

Number of trials, n	Level of significance, α 0.10	0.05	0.02	0.01
1	0.95000	0.97500	0.99000	0.99500
2	0.77639	0.84189	0.90000	0.92929
3	0.63604	0.70760	0.78456	0.82900
4	0.56522	0.62394	0.68887	0.73424
5	0.50945	0.56328	0.62718	0.66853
6	0.46799	0.51926	0.57741	0.61661
7	0.43607	0.48342	0.53844	0.57581
8	0.40962	0.45427	0.50654	0.54179
9	0.38746	0.43001	0.47960	0.51332
10	0.36866	0.40925	0.45662	0.48893

Other goodness of fit tests

We want to measure the distance between two functions: $F_n(t)$ and $F(t)$. There are other ways, leading to other tests:

- Kolmogorov-Smirnov:

$$d(F_n, F) = \sup_{t \in \mathbb{R}} |F_n(t) - F(t)|$$

- Cramér-Von Mises:

$$d^2(F_n, F) = \int_{\mathbb{R}} [F_n(t) - F(t)]^2 \, dF(t)$$

- Anderson-Darling:

$$d^2(F_n, F) = \int_{\mathbb{R}} \frac{[F_n(t) - F(t)]^2}{F(t)(1 - F(t))} dF(t)$$

Composite goodness of fit tests

What if I want to test: "Does X have Gaussian distribution?" but I don't know the parameters?
Simple idea: plug-in

$$\sup_{t\in\mathbb{R}} \left|F_n(t) - \Phi_{\hat{\mu},\hat{\sigma}^2}(t)\right|$$

where

$$\hat{\mu} = \bar{X}_n, \qquad \hat{\sigma}^2 = S_n^2$$

and $\Phi_{\hat{\mu},\hat{\sigma}^2}(t)$ is the cdf of $\mathcal{N}(\hat{\mu},\hat{\sigma}^2)$.

In this case Donsker's theorem is *no longer valid*. This is a common and serious mistake!

Kolmogorov-Lilliefors test (1)

Instead, we compute the quantiles for the test statistic:

$$\sup_{t \in \mathbb{R}} \left| F_n(t) - \Phi_{\hat{\mu}, \hat{\sigma}^2}(t) \right|$$

They do not depend on unknown parameters!

This is the Kolmogorov-Lilliefors test.

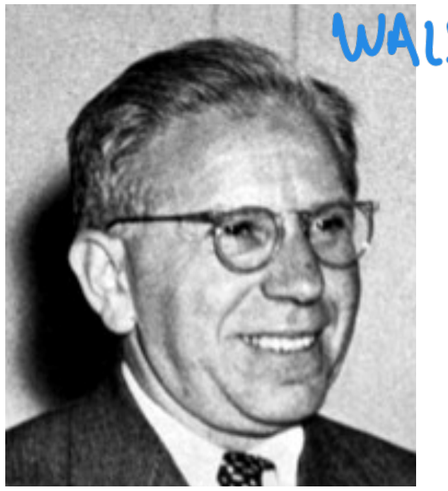
K-L table

Sample Size N	Level of Significance for $D = \text{Max} \left\| F^*(X) - S_N(X) \right\|$				
	.20	.15	.10	.05	.01
4	.300	.319	.352	.381	.417
5	.285	.299	.315	.337	.405
6	.265	.277	.294	.319	.364
7	.247	.258	.276	.300	.348
8	.233	.244	.261	.285	.331
9	.223	.233	.249	.271	.311
10	.215	.224	.239	.258	.294
11	.206	.217	.230	.249	.284
12	.199	.212	.223	.242	.275
13	.190	.202	.214	.234	.268
14	.183	.194	.207	.227	.261
15	.177	.187	.201	.220	.257
16	.173	.182	.195	.213	.250
17	.169	.177	.189	.206	.245
18	.166	.173	.184	.200	.239
19	.163	.169	.179	.195	.235
20	.160	.166	.174	.190	.231

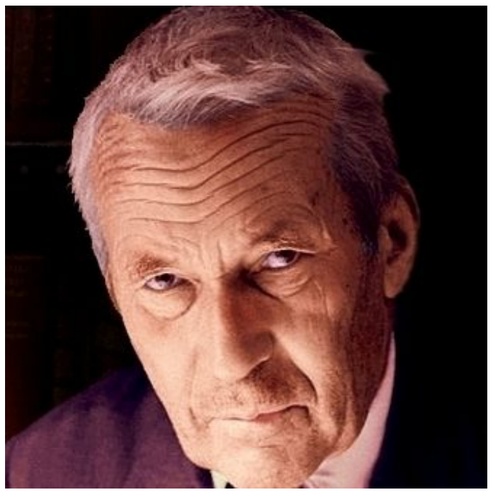
LILLIEFORS

VON MISES

WALD

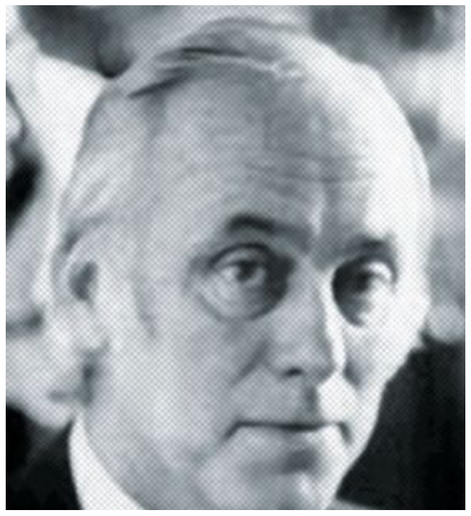


KOLMOGOROV



SMIRNOV

WILKS



ANDERSON

DARLING

CRAMÉR

Quantile-Quantile (QQ) plots (1)

- Provide a visual way to perform GoF tests
- Not formal test but quick and easy check to see if a distribution is plausible.
- Main idea: we want to check visually if the plot of F_n is close to that of F or equivalently if the plot of F_n^{-1} is close to that of F^{-1}.
- More convenient to check if the points

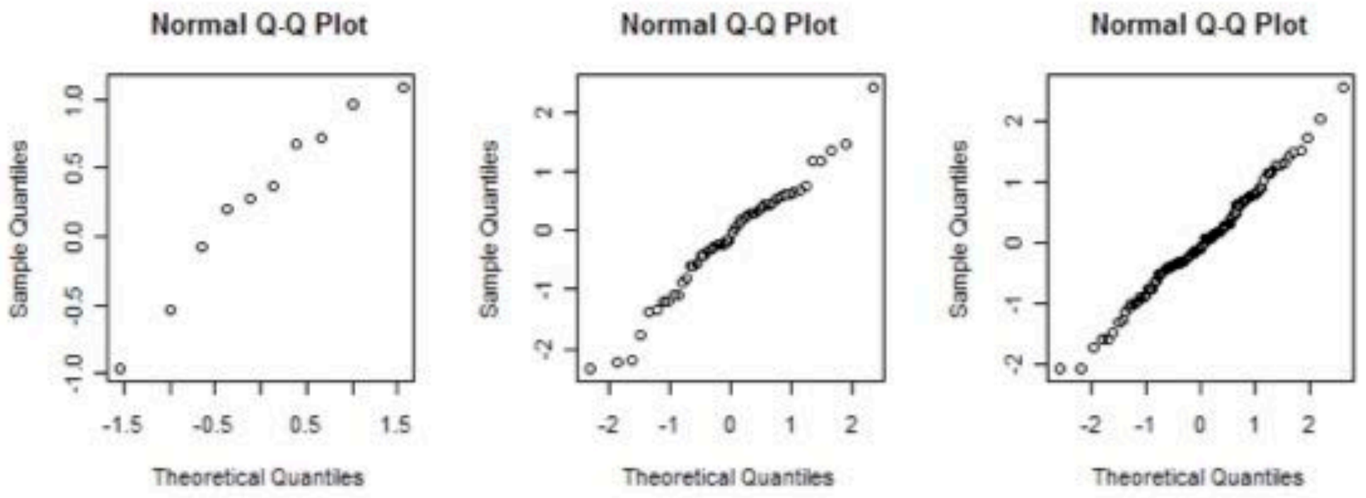
$$\left(F^{-1}(\frac{1}{n}), F_n^{-1}(\frac{1}{n})\right), \left(F^{-1}(\frac{2}{n}), F_n^{-1}(\frac{2}{n})\right), \ldots, \left(F^{-1}(\frac{n-1}{n}), F_n^{-1}(\frac{n-1}{n})\right)$$

  are near the line $y = x$.
- F_n is not technically invertible but we define

$$F_n^{-1}(i/n) = X_{(i)},$$

  the ith largest observation.

Quantile-Quantile (QQ) plots (2)



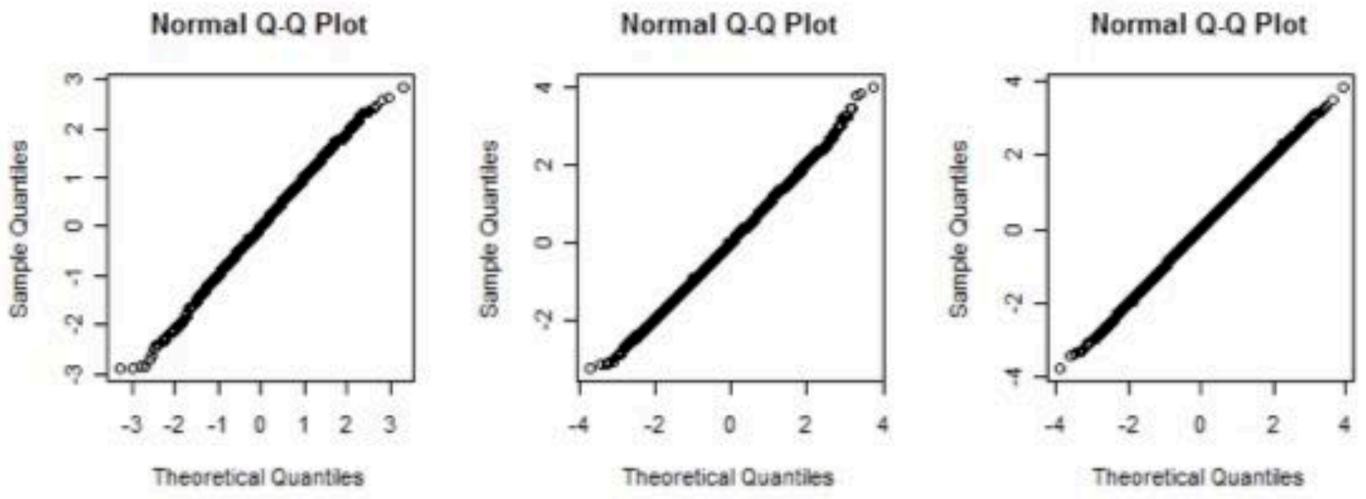
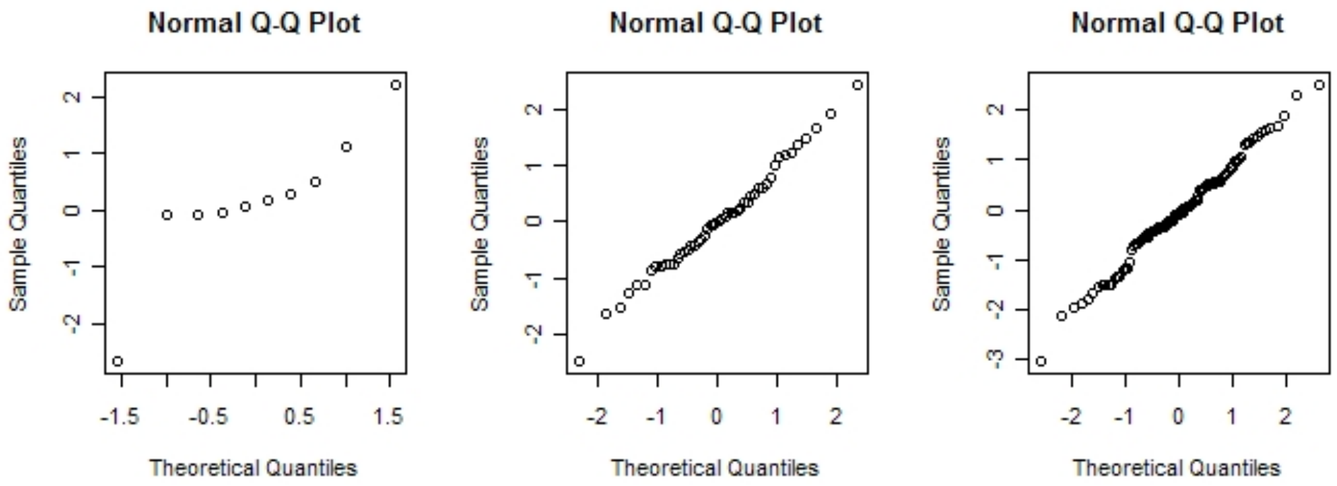


Figure 1: QQ-plots for samples of sizes $10, 50, 100, 1000, 5000, 10000$ from a standard normal distribution. The upper-left figure is for sample size 10, the lower-right is for sample 10000.

Quantile-Quantile (QQ) plots (3)



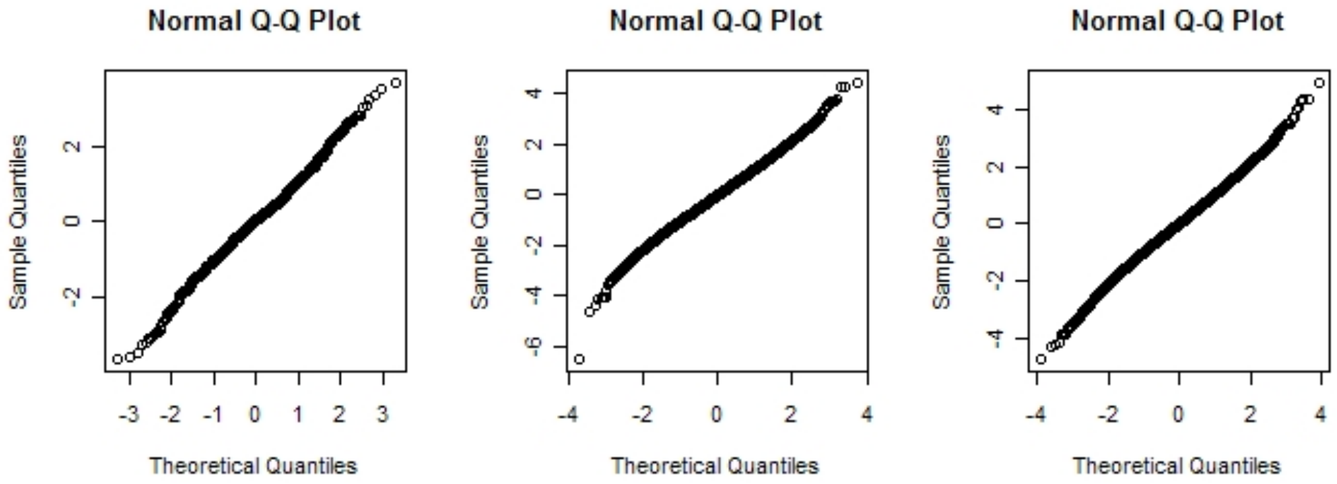


Figure 2: QQ-plots for samples of sizes $10, 50, 100, 1000, 5000, 10000$ from a t_{15} distribution. The upper-left figure is for sample size 10, the lower-right is for sample 10000.