

data science for (physical) scientists II

II: physics in a probabilistic world

dr.federica bianco | fbb.space |  fedhere |  fedhere

1 $P(\text{physics} \mid \text{data})$

2 NHRT

p-values

z-test

3 comparing distributions

Z, t, χ^2 , ks-test

KL divergence

this slide deck

http://bit.ly/dsps2019_2



Guiding principle of science practice

- *Theories* should be *falsifiable* (= make predictions)
- *Analysis* should be *reproducible* (share result, share raw data, share code to get result from raw data)

neap 2

probability

- *Frequentist* interpretation: fraction of occurrence
- *Bayesian* interpretation: degree of believe that it will happen
- Basic probability algebra rules

reap 3

statistics

- links between samples (observations) and populations (general rules)
- common distributions: binomial, Poisson, Gaussian, χ^2
- *Descriptive statistics*: central tendency, variance, symmetry
- Central limit theorem

reap

4

physics

- thermodynamics: the first deliberate example of application of statistics to physics

**if we know the properties of the *micro* system
statistically we can predict the *macro* system
deterministically**

descriptive statistics:

we summarize the properties of a distribution

$$\mu_n = \int_{-\infty}^{\infty} (x - c)^n f(x) \, dx.$$

reap

descriptive statistics:

we summarize the properties of a distribution

$$\mu_n = \int_{-\infty}^{\infty} (x - c)^n f(x) dx.$$

mean: $n=1$

$$\mu = \frac{1}{N} \sum_1^N x_i$$

other measures of central tendency:

median: 50% of the distribution is to the left,
50% to the right

mode: most popular value in the distribution

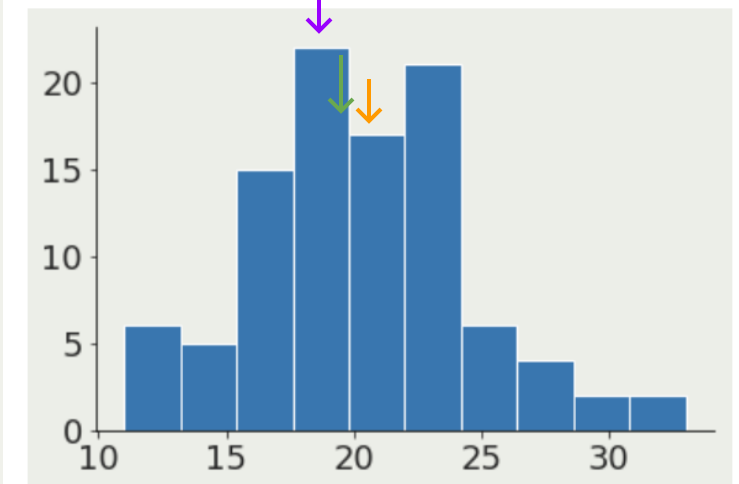
```
dist = sp.stats.poisson.rvs(size=100, mu=20)
pl.hist(dist)
print(dist.mean())
print(np.median(dist))
print(sp.stats.mode(dist))
|
```

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20.06

20.0

ModeResult(mode=array([18]), count=array([12]))



descriptive statistics:

we summarize the properties of a distribution

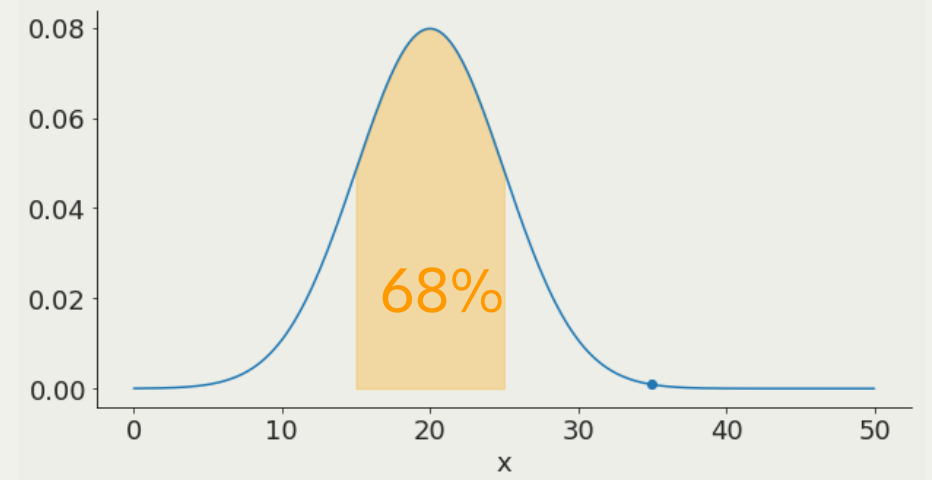
$$\mu_n = \int_{-\infty}^{\infty} (x - c)^n f(x) dx.$$

variance: $n=2$ $\text{Var}(X) = \text{E} [(X - \mu)^2] .$

standard deviation $\sigma(X) = \text{E} [(X - \mu)] .$

Gaussian distribution:

1σ contains 68% of the distribution



descriptive statistics:

we summarize the properties of a distribution

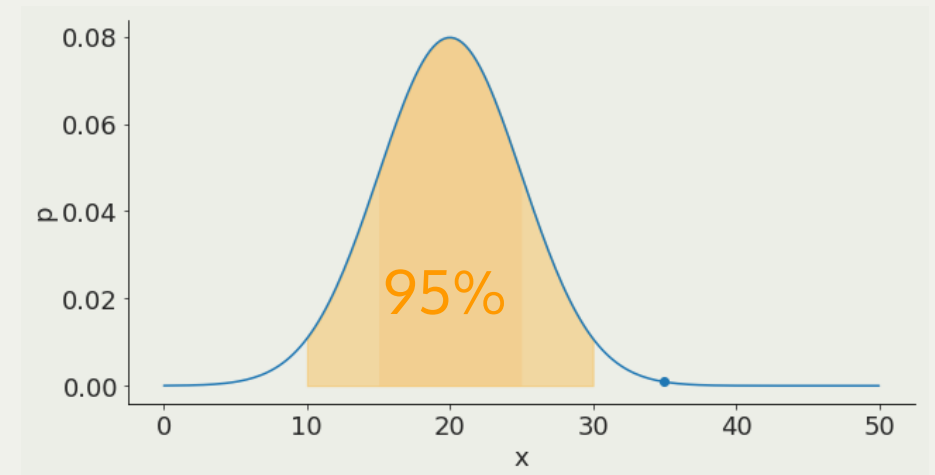
$$\mu_n = \int_{-\infty}^{\infty} (x - c)^n f(x) dx.$$

variance: $n=2$ $\text{Var}(X) = \text{E} [(X - \mu)^2] .$

standard deviation $\sigma(X) = \text{E} [(X - \mu)] .$

Gaussian distribution:

2σ contains 95% of the distribution



descriptive statistics:

we summarize the properties of a distribution

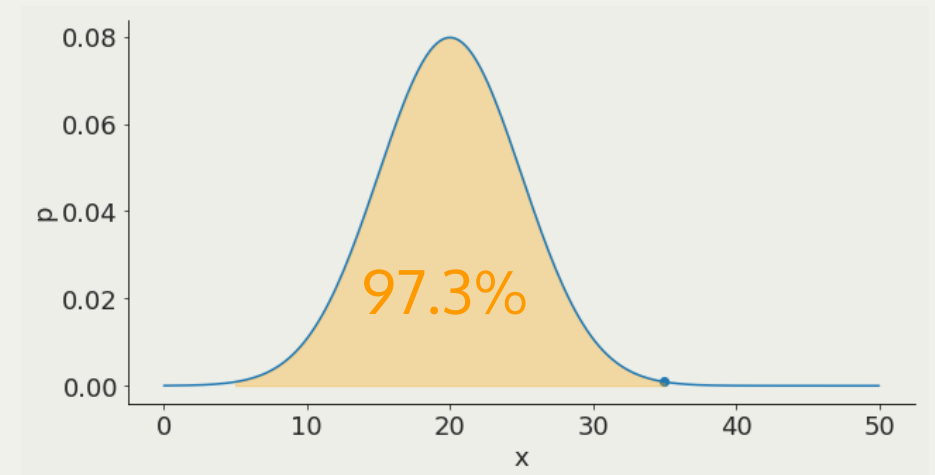
$$\mu_n = \int_{-\infty}^{\infty} (x - c)^n f(x) dx.$$

variance: $n=2$ $\text{Var}(X) = \mathbb{E} [(X - \mu)^2] .$

standard deviation $\sigma(X) = \mathbb{E} [(X - \mu)] .$

Gaussian distribution:

3σ contains 97.3% of the distribution



1

the scientific method
in a probabilistic context

p(physics | data)

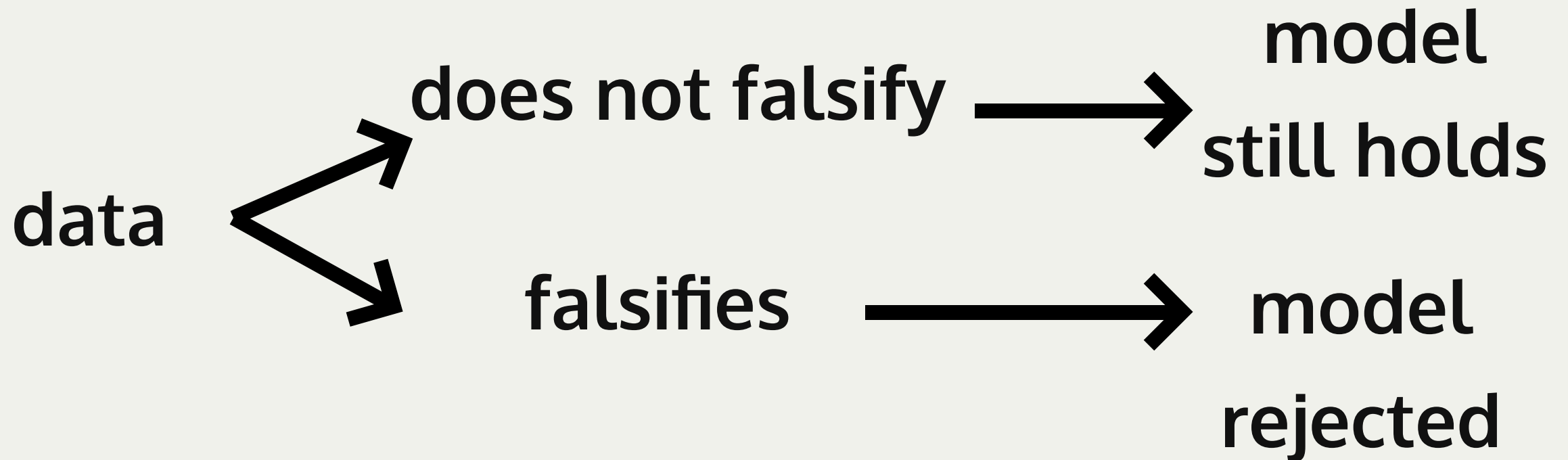
Bayesian Inference

Forward Modeling

Frequentist approach
(NHRT)

$p(\text{physics} \mid \text{data})$

model  **prediction**



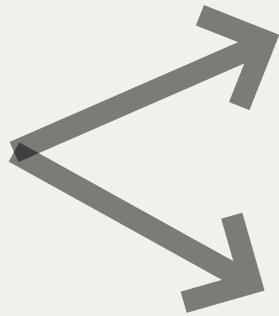
model



prediction

"Under the Null Hypothesis"
= if the model is true

data



does not falsify



**model
still holds**

falsifies



**model
rejected**

model

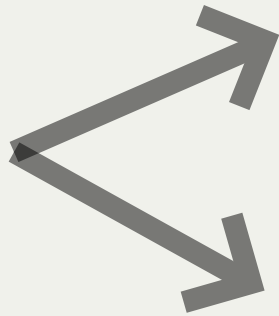


prediction

*"Under the Null Hypothesis"
= if the model is true*

*this has a high probability
of happening*

data



does not falsify



**model
still holds**

falsifies



**model
rejected**

model

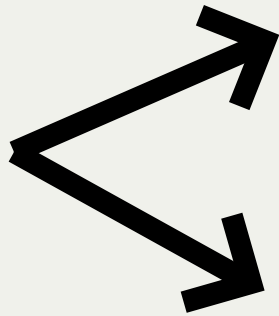


prediction

*"Under the Null Hypothesis"
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*this has a high probability
of happening*

data



does not falsify



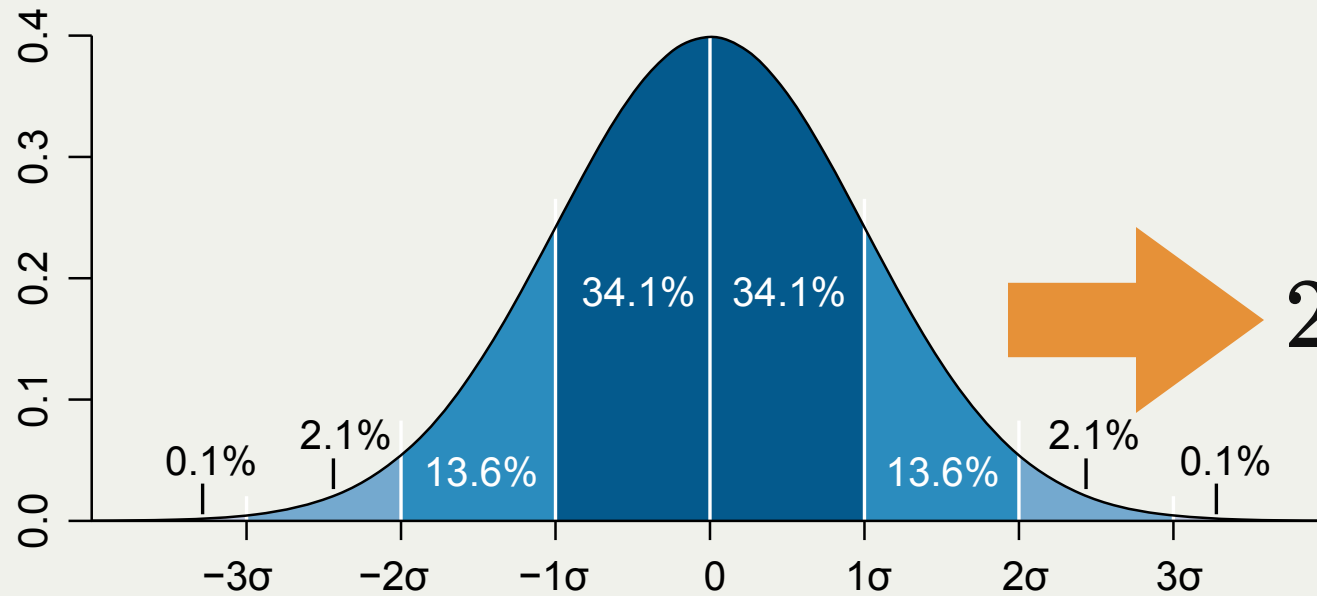
**model
still holds**

falsifies



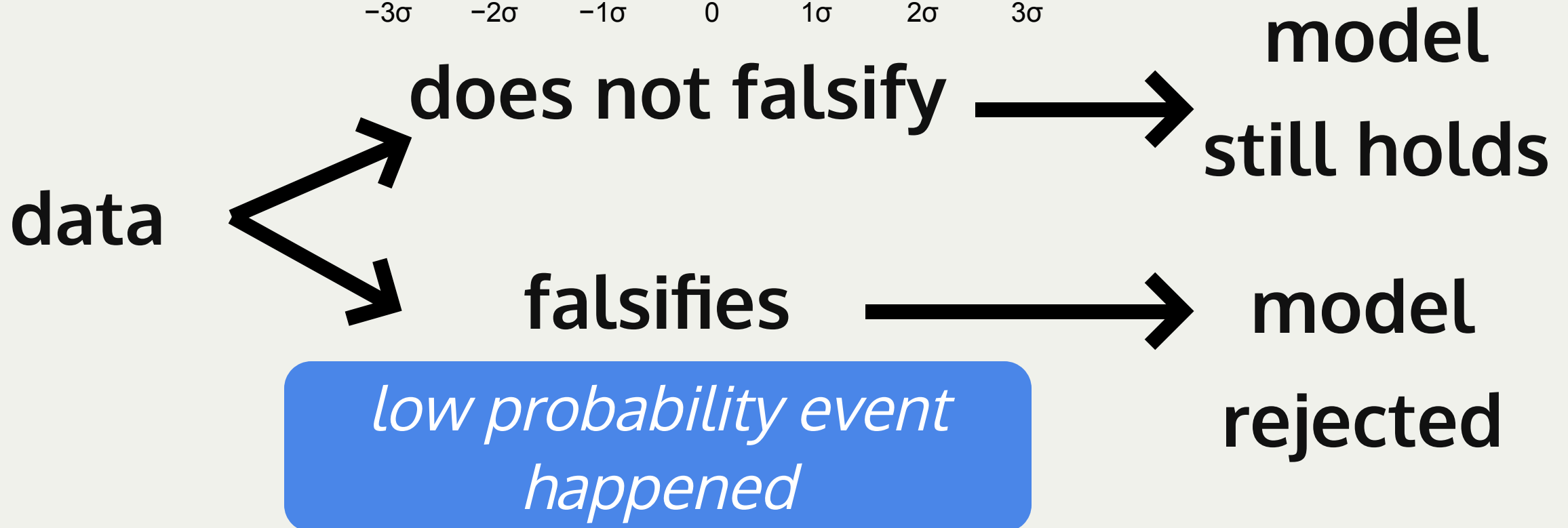
**model
rejected**

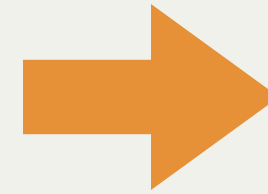
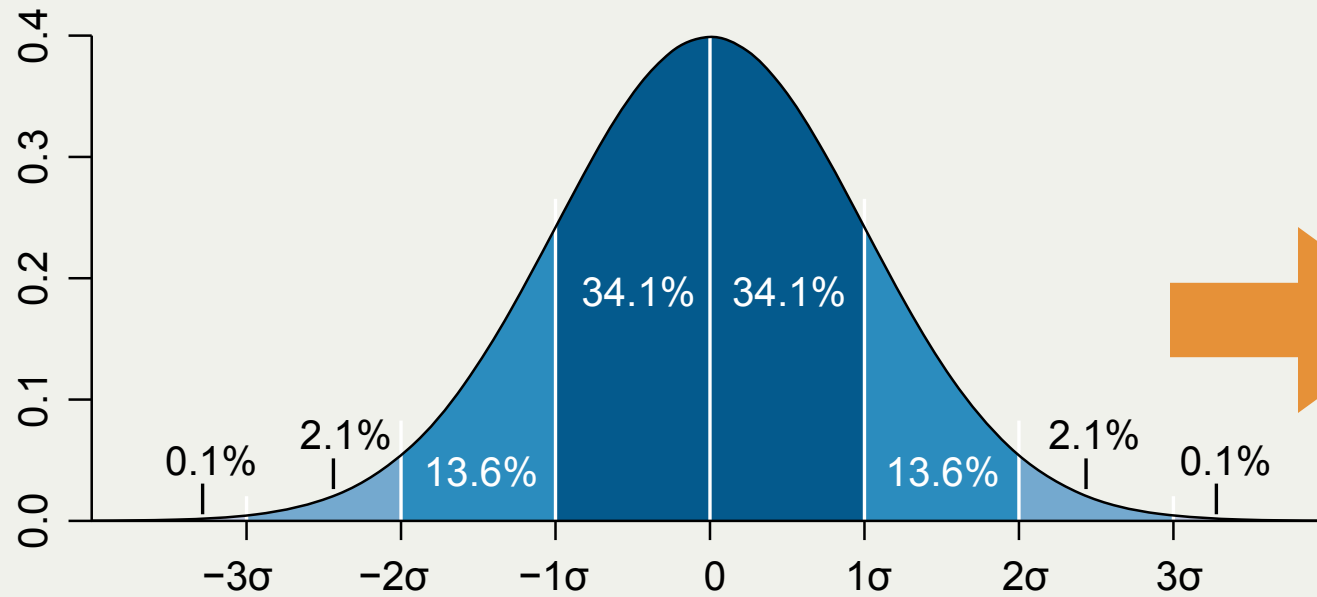
*low probability event
happened*



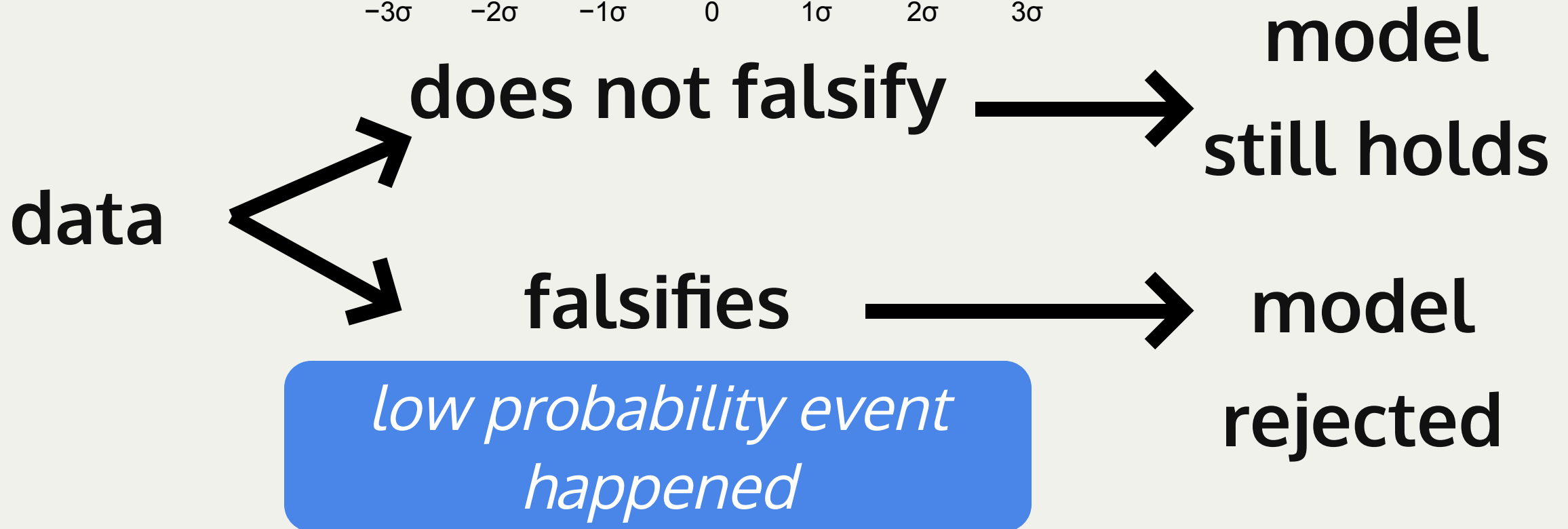
rejected at 95%
0.05 p-value
5% confidence

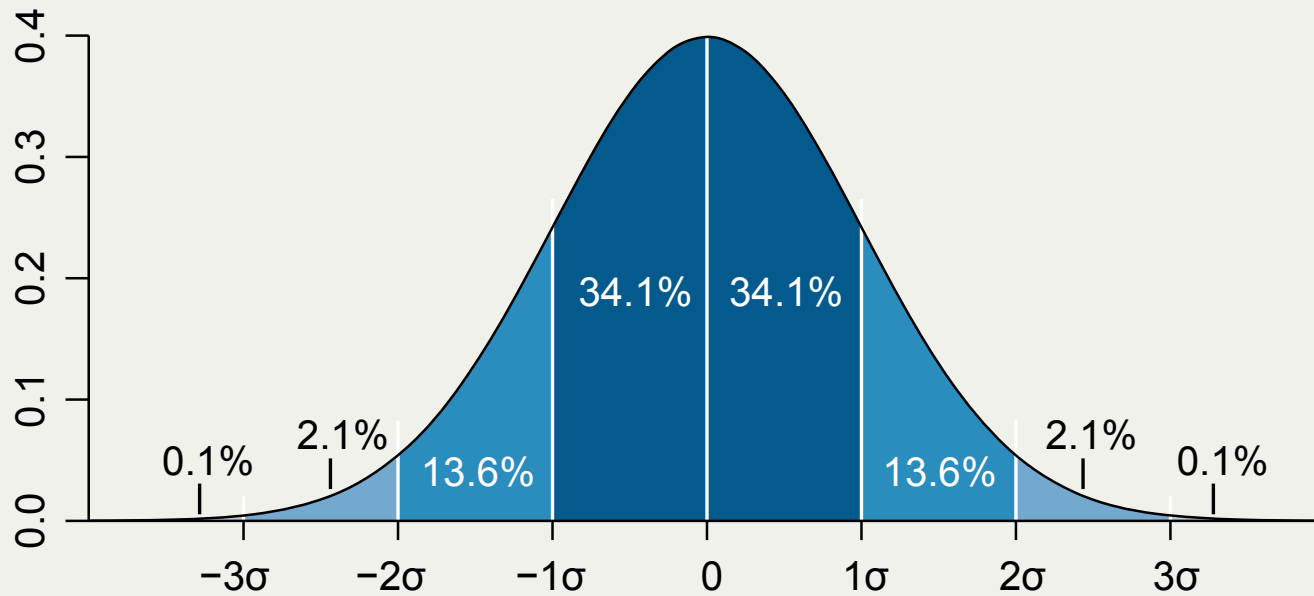
2σ





rejected at 99.7%
 3σ 0.003 p-value
0.3% confidence

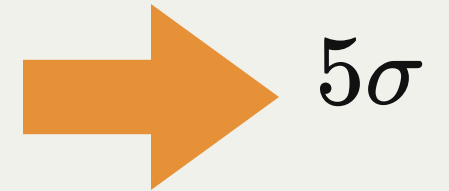




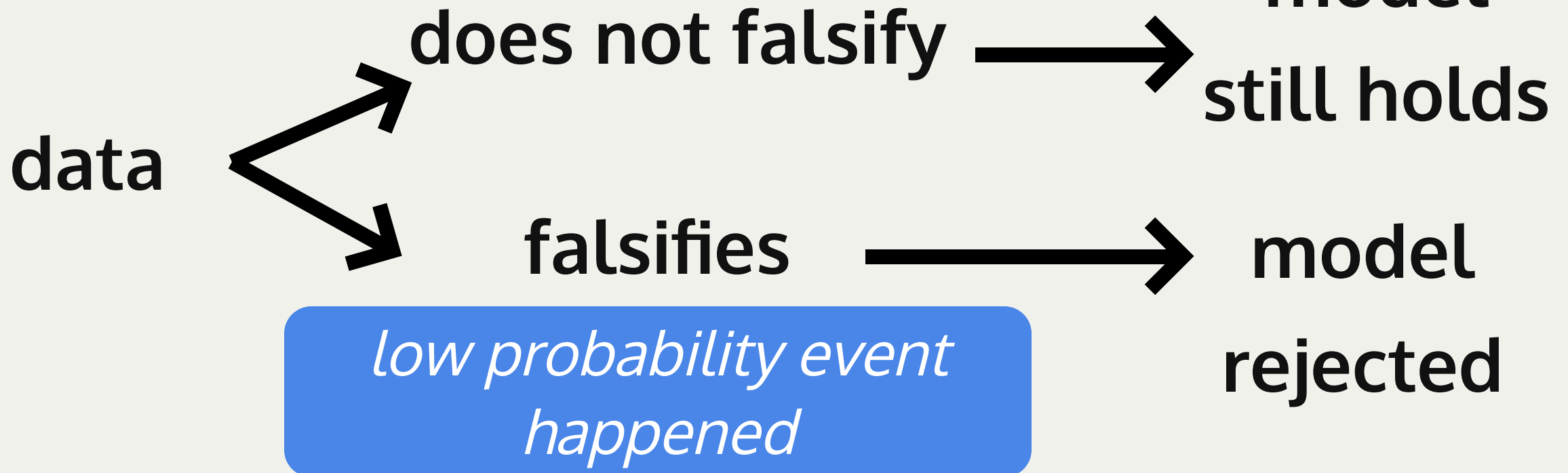
rejected at 99.99...%

3-e7 p-value

3-e5% confidence



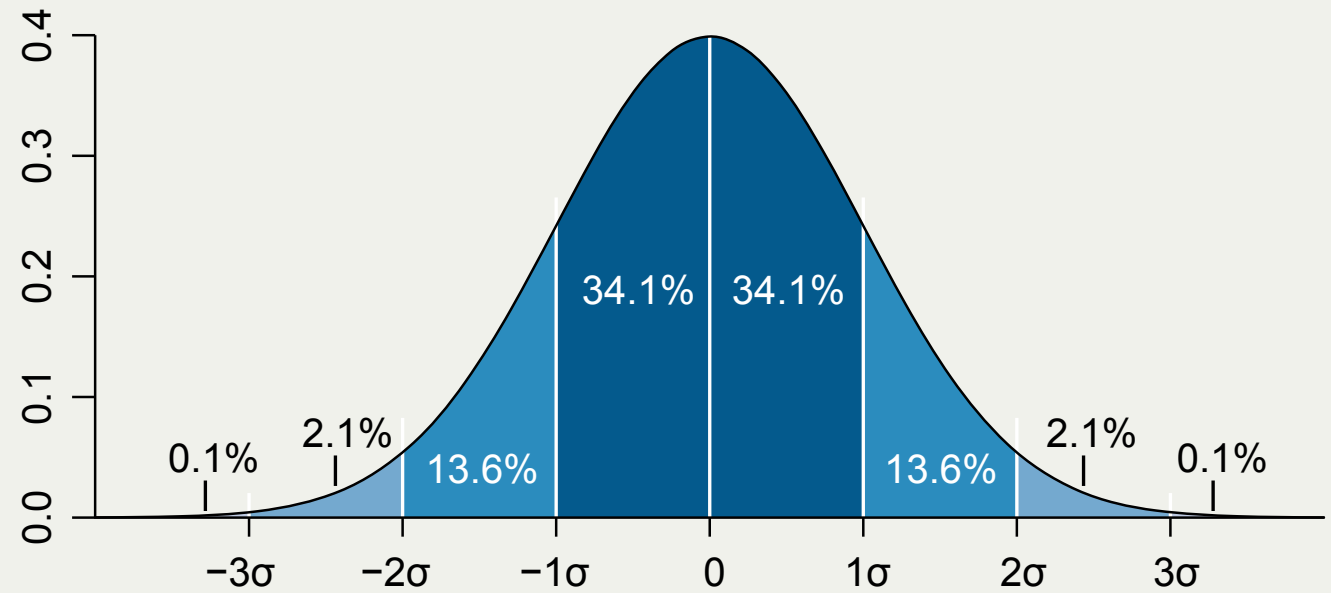
5σ



2

Null hypothesis rejection testing

Null
Hypothesis
Rejection
Testing



$p(\text{physics} \mid \text{data})$

Null

Hypothesis

Rejection

Testing

1

formulate your prediction

Null Hypothesis

Null

Hypothesis

Rejection

Testing

2

identify all alternative
outcomes

Alternative Hypothesis

Null

Hypothesis

Rejection

Testing



$$P(A) + P(\bar{A}) = 1$$

if *all alternatives* to our model are ruled out,
then our model must hold

2
identify all alternative
outcomes

Alternative Hypothesis

But instead of verifying a theory we want to falsify one
model  **prediction**

*"Under the **Null Hypothesis**"
= if the model is true*

*this has a **low** probability
of happening*



generally, our model about how the world works is the *Alternative* and we try to reject the non-innovative thinking as the *Null*!

But instead of verifying a theory we want to falsify one
model  **prediction**

*"Under the **Null Hypothesis**"
= if the model is true*

*this has a **low** probability
of happening*

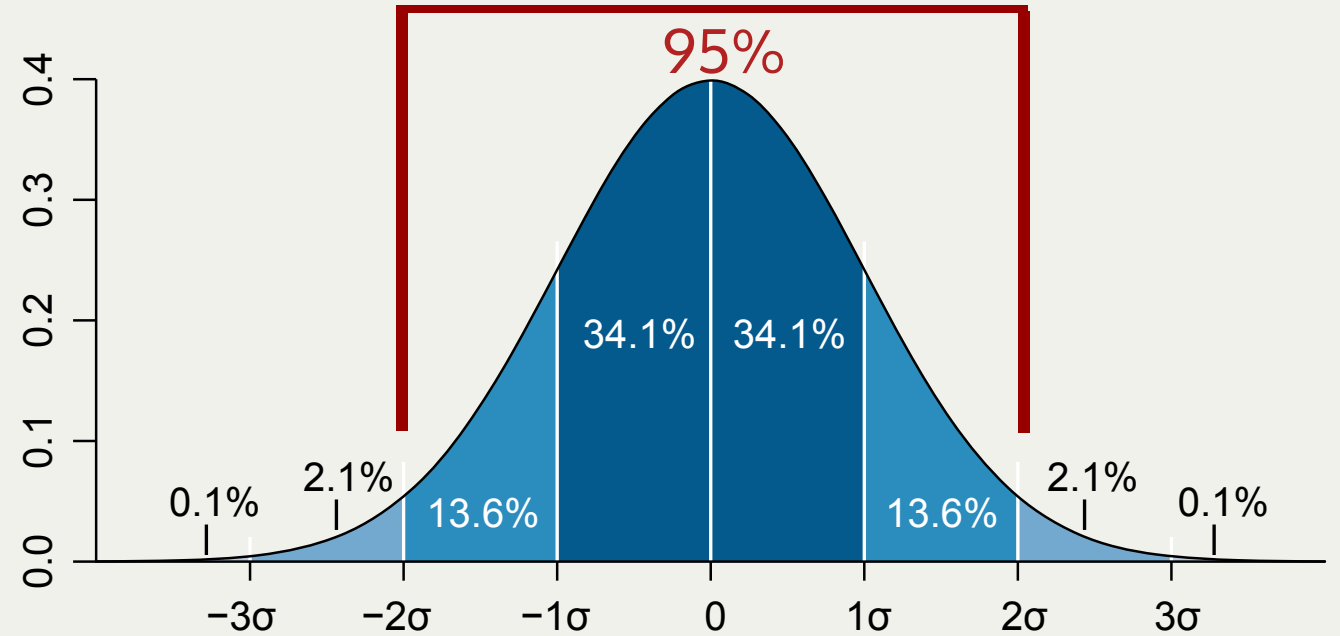


Earth is flat is Null

Earth is round is Alternative:

we reject the Null hypothesis that the Earth is flat ($p=0.05$)

Null Hypothesis Rejection Testing



3 set confidence threshold

2σ confidence level

0.05 p-value

95% α threshold

Null

Hypothesis

Rejection

Testing

pivotal quantities

4

find a measurable
quantity which
under the Null has
a known
distribution

Null

Hypothesis

Rejection

Testing

pivotal quantities

5

calculate it!

pivotal quantities

quantities that under the Null Hypothesis follow a known distribution

if a quantity follows a known distribution, once I measure its value I can what the probability of getting that value actually is! was it a likely or an unlikely draw?

pivotal quantities

quantities that under the Null
Hypothesis follow a known distribution

$$p(\text{pivotal quantity} | NH) \sim p(NH | D)$$

Null

Hypothesis

Rejection

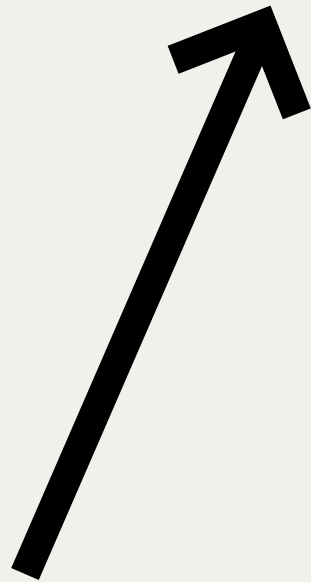
Testing

$$p(NH|D) < \alpha$$

prediction is unlikely

Null rejected

Alternative holds



test data against
alternative outcomes

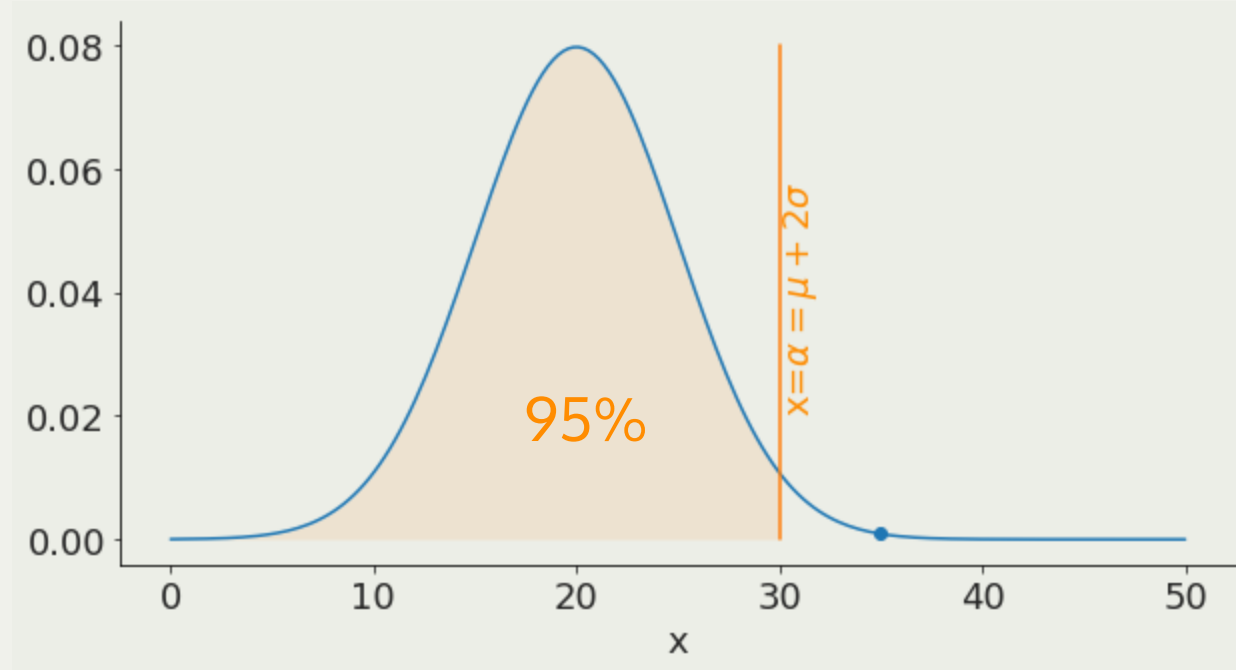
Null Hypothesis Rejection Testing



test data against
alternative outcomes

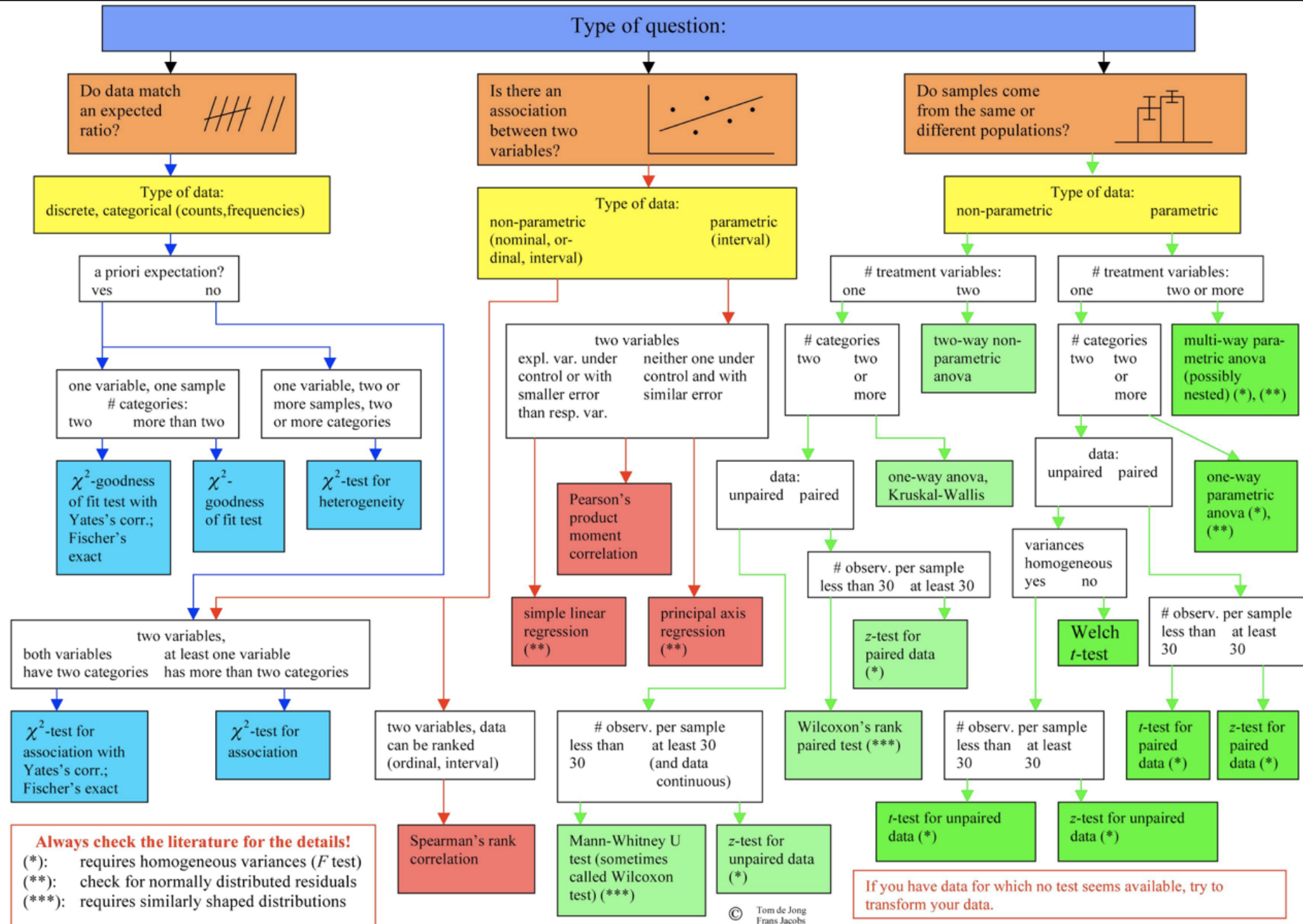
what is α ?

α is the x value corresponding to a chosen threshold



3

common tests and pivotal quantities



If you have data for which no test seems available, try to transform your data.

pivotal quantities

quantities that under the Null Hypothesis follow a known distribution

also called "statistics"

e.g.: χ^2 statistics: difference between expectation and reality squared

Z statistics: difference between means

$K-S$ statistics: maximum distance of cumulative distributions.

Z-test

Is the mean of a sample *with known variance* the same as that of a known population?

pivotal quantity

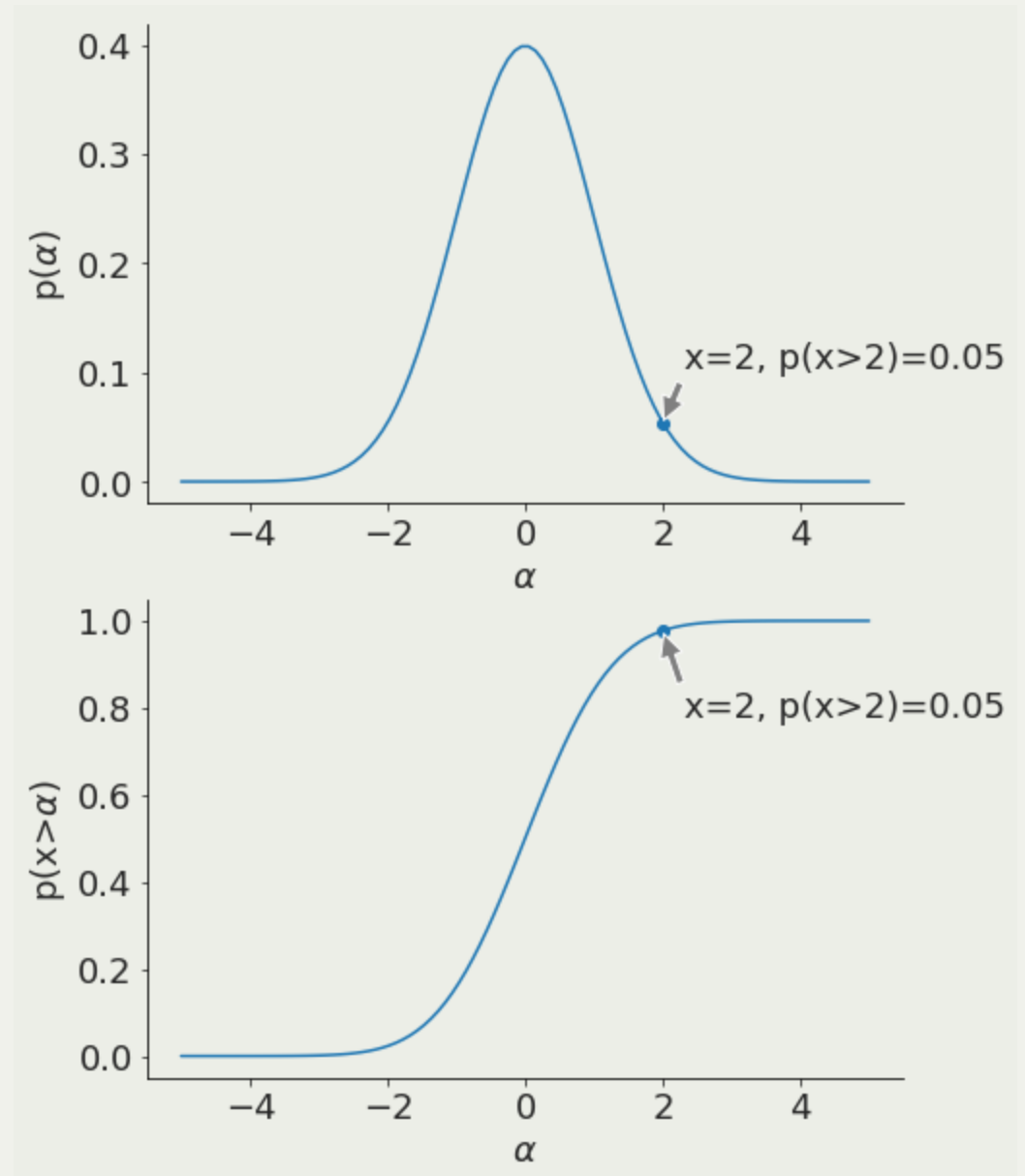
$$Z = (\bar{X} - \mu_0) / s$$

sample
mean

population
mean

sample
variance = σ / \sqrt{n}

$$Z \sim N(\mu = 0, \sigma = 1)$$



Z-test

Is the mean of a sample *with known variance* the same as that of a known population?

pivotal quantity

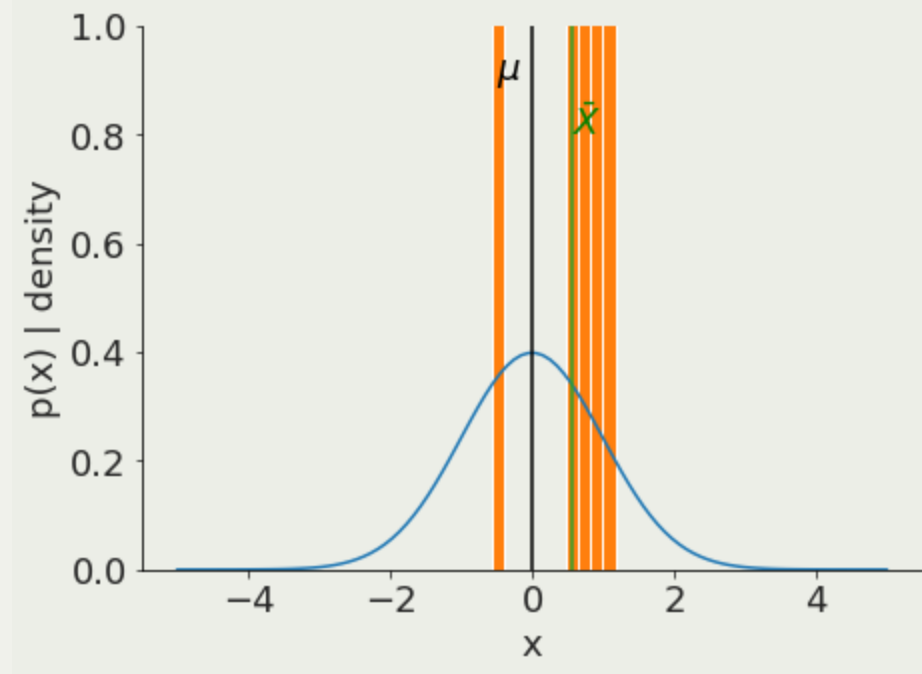
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sample
mean

population
mean

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variance = σ / \sqrt{n}

$$Z \sim N(\mu = 0, \sigma = 1)$$



why do we need a test? why
not just measuring the means
and seeing if they are the
same?

Z-test

Is the mean of a sample *with known variance* the same as that of a known population?

pivotal quantity

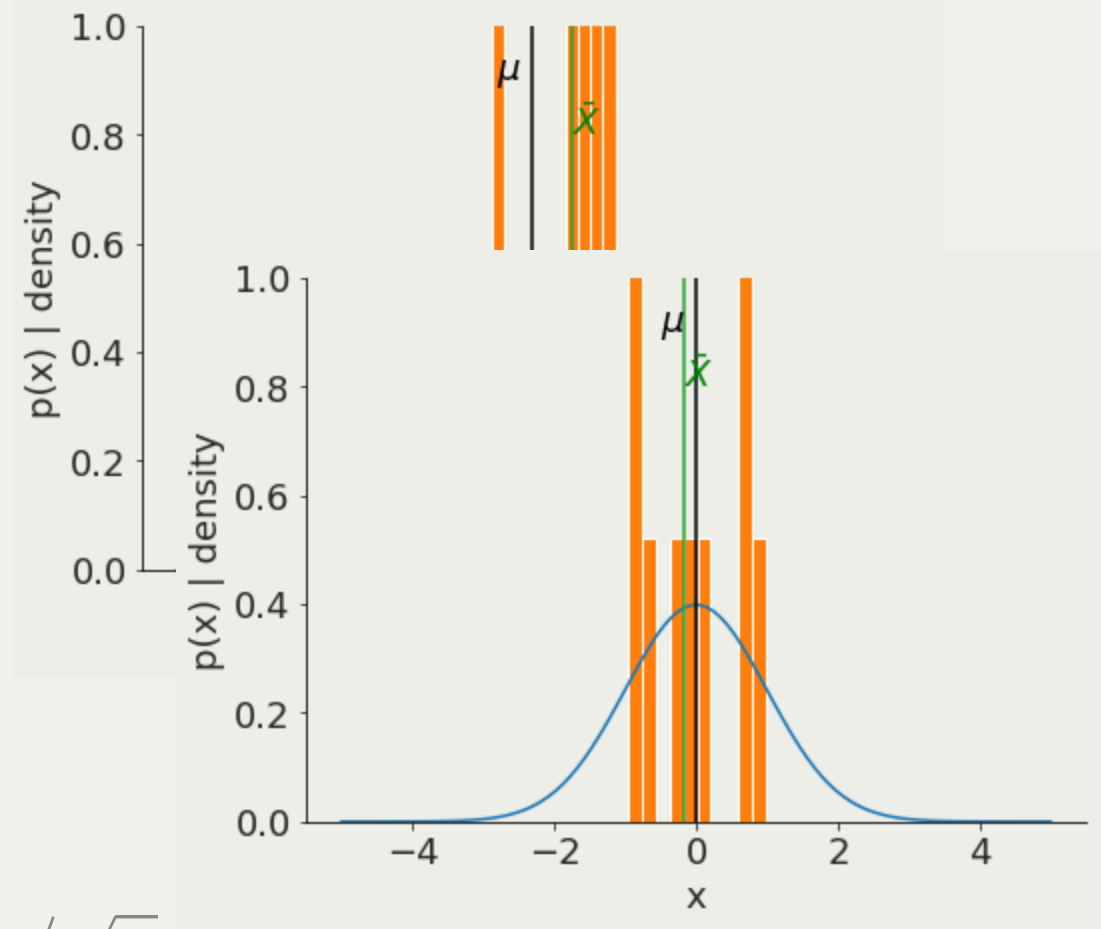
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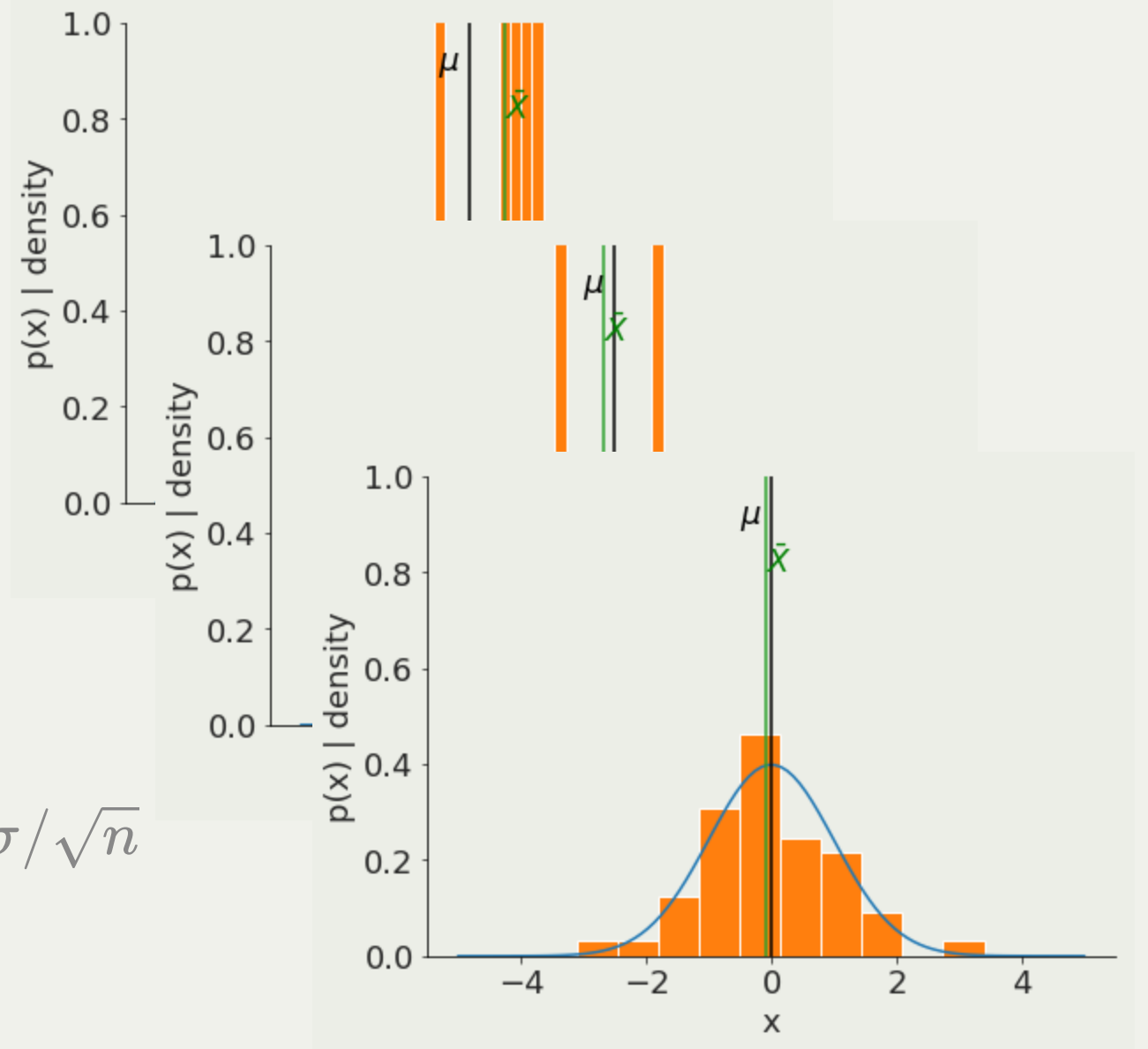
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Z-test

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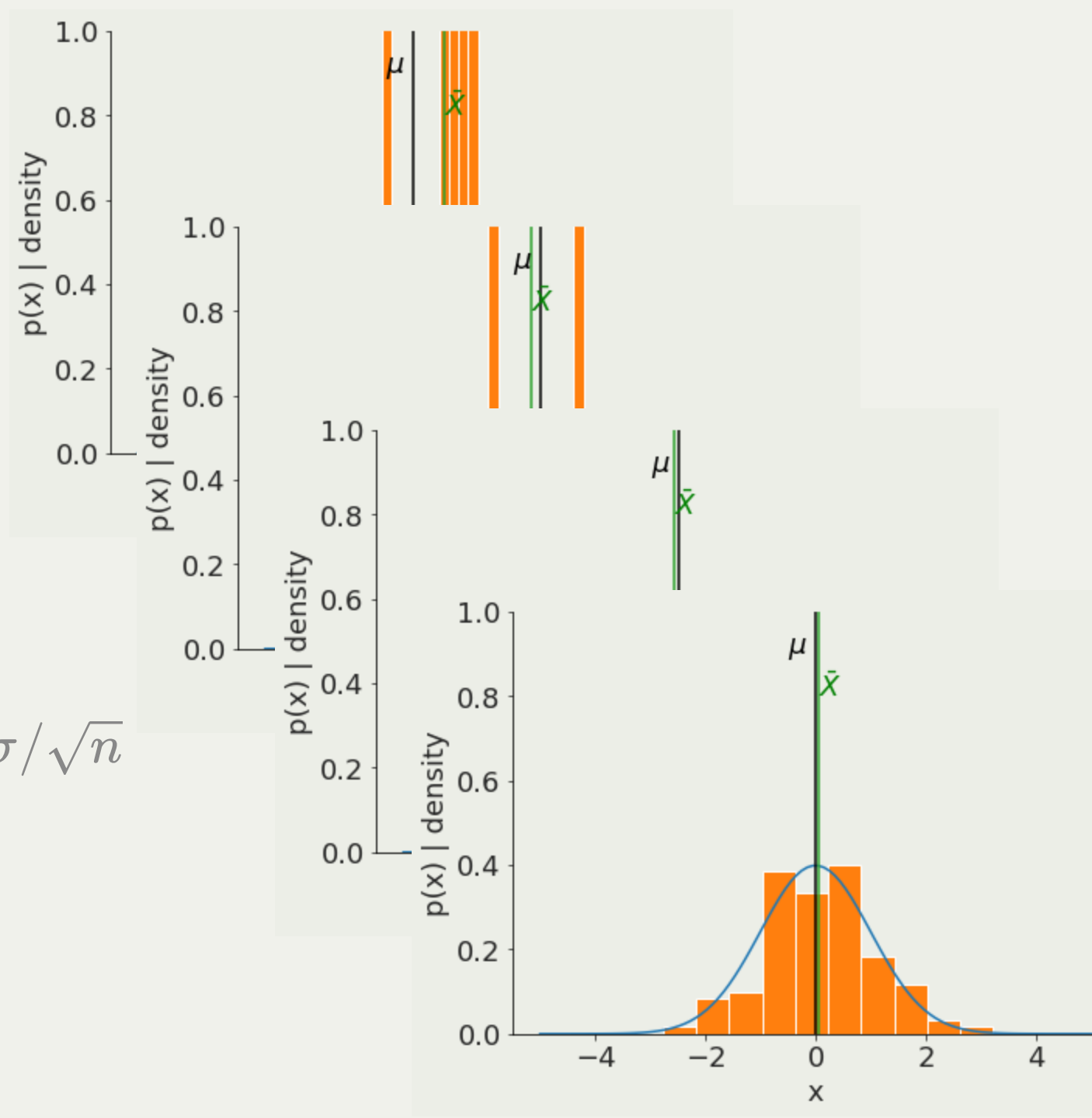
$$Z = (\bar{X} - \mu_0) / s$$

sample
mean

population
mean

sample
variance = σ / \sqrt{n}

$$Z \sim N(\mu = 0, \sigma = 1)$$



t- test

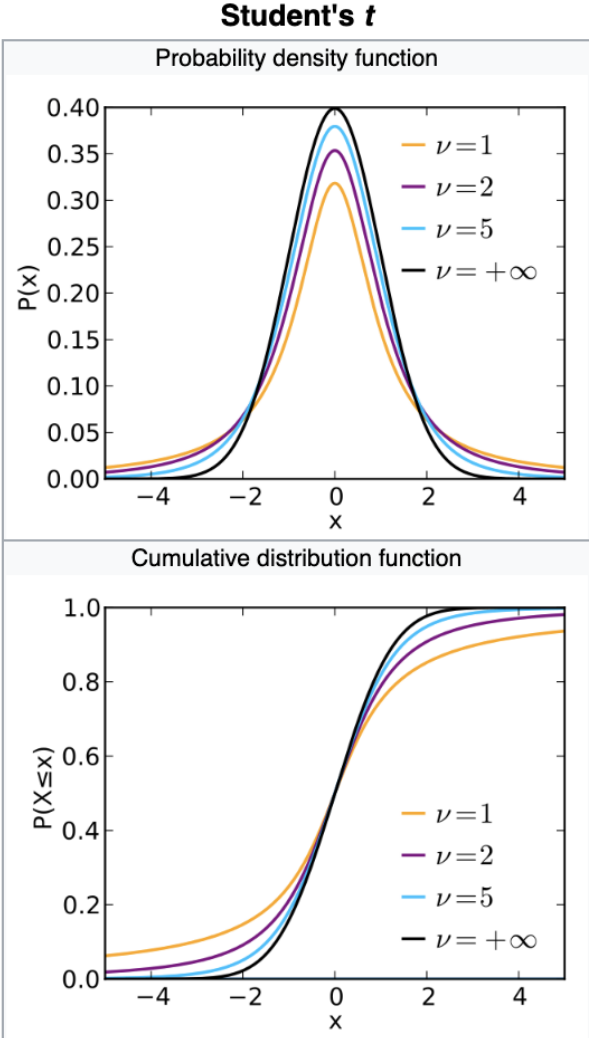
Are the means of 2 samples significantly different?

pivotal quantity

$$t = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}}$$

unbiased variance estimator
 size of sample

$$t \sim \text{Student's } t \left(\text{df} = \frac{\left(\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}\right)^2}{\frac{(s_1^2/n_1)^2}{n_1-1} + \frac{(s_2^2/n_2)^2}{n_2-1}} \right)$$



Parameters	$\nu > 0$ degrees of freedom (real)
Support	$x \in (-\infty, \infty)$
PDF	$\frac{\Gamma(\frac{\nu+1}{2})}{\sqrt{\nu\pi} \Gamma(\frac{\nu}{2})} \left(1 + \frac{x^2}{\nu}\right)^{-\frac{\nu+1}{2}}$
CDF	$\frac{1}{2} + x \Gamma\left(\frac{\nu+1}{2}\right) \times \frac{{}_2F_1\left(\frac{1}{2}, \frac{\nu+1}{2}; \frac{3}{2}; -\frac{x^2}{\nu}\right)}{\sqrt{\pi\nu} \Gamma(\frac{\nu}{2})}$ <p>where ${}_2F_1$ is the hypergeometric function</p>
Mean	0 for $\nu > 1$, otherwise undefined
Median	0
Mode	0
Variance	$\frac{\nu}{\nu-2}$ for $\nu > 2$, ∞ for $1 < \nu \leq 2$, otherwise undefined

t - test

Are the means of 2 samples significantly different?

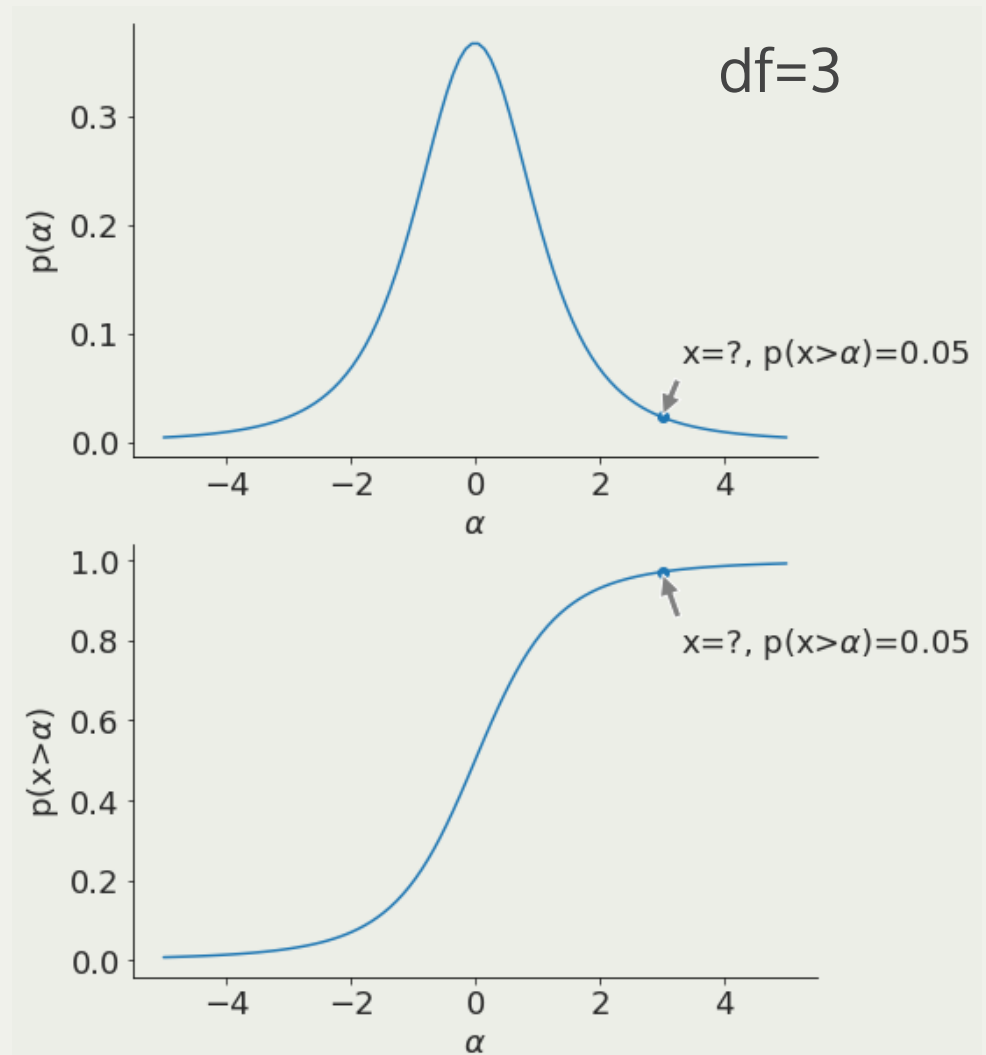
pivotal quantity

unbias
variance
estimator

$$t = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}}$$

size of sample

$$t \sim \text{Student's } t \left(df = \frac{\left(\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2} \right)^2}{\frac{(s_1^2/n_1)^2}{n_1 - 1} + \frac{(s_2^2/n_2)^2}{n_2 - 1}} \right)$$



t- test

Are the means of 2 samples significantly different?

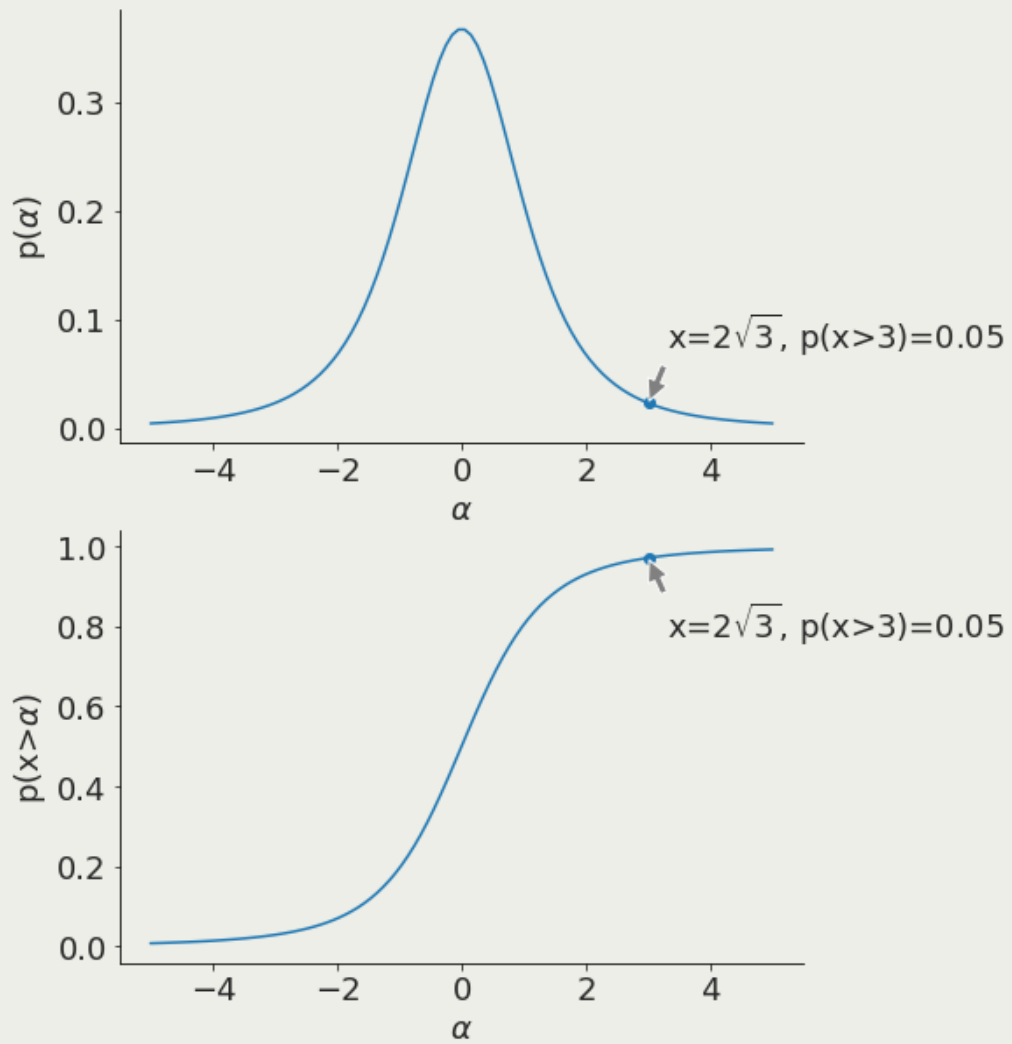
pivotal quantity

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unbias variance estimator

size of sample

$$t \sim \text{Student's } t \left(\text{df} = \frac{\left(\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2} \right)^2}{\frac{(s_1^2/n_1)^2}{n_1-1} + \frac{(s_2^2/n_2)^2}{n_2-1}} \right)$$



K-S test

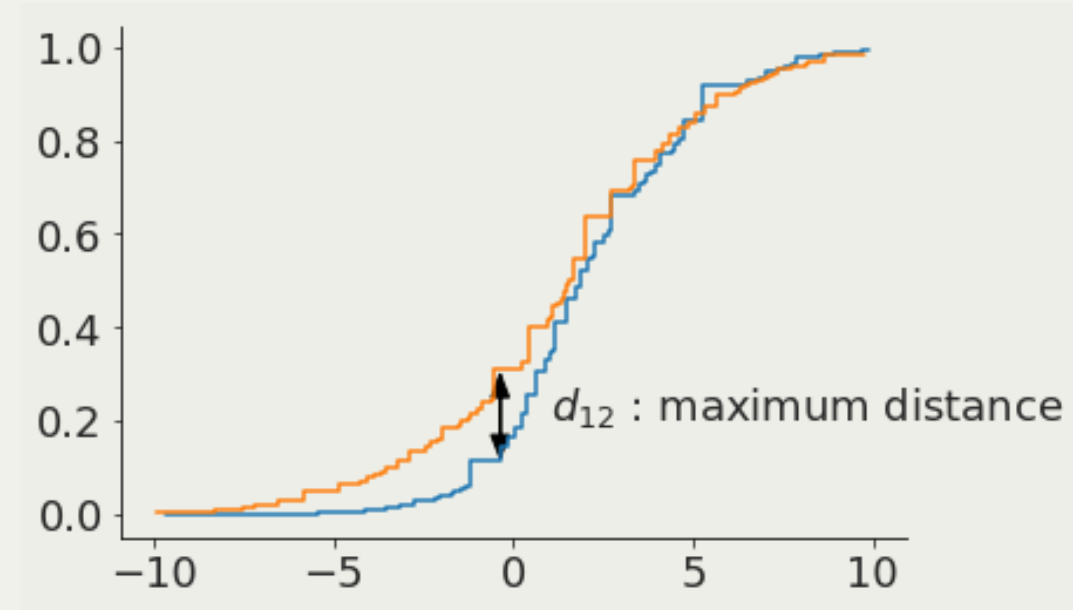
Kolmogorof-Smirnoff :

do two samples come from the same
parent distribution?

pivotal quantity

$$d_{12} \equiv \max_x |C_1(x) - C_2(x)|$$

↓ ↓
Cumulative Cumulative
distribution 1 distribution 2



$$P(d > \text{observed}) = 2 \sum_{j=1}^{\infty} (-1)^{j-1} e^{-2j^2 x^2} \sqrt{\frac{N_1 N_2}{N_1 + N_2}} D$$

K-S test

Kolmogorof-Smirnoff :

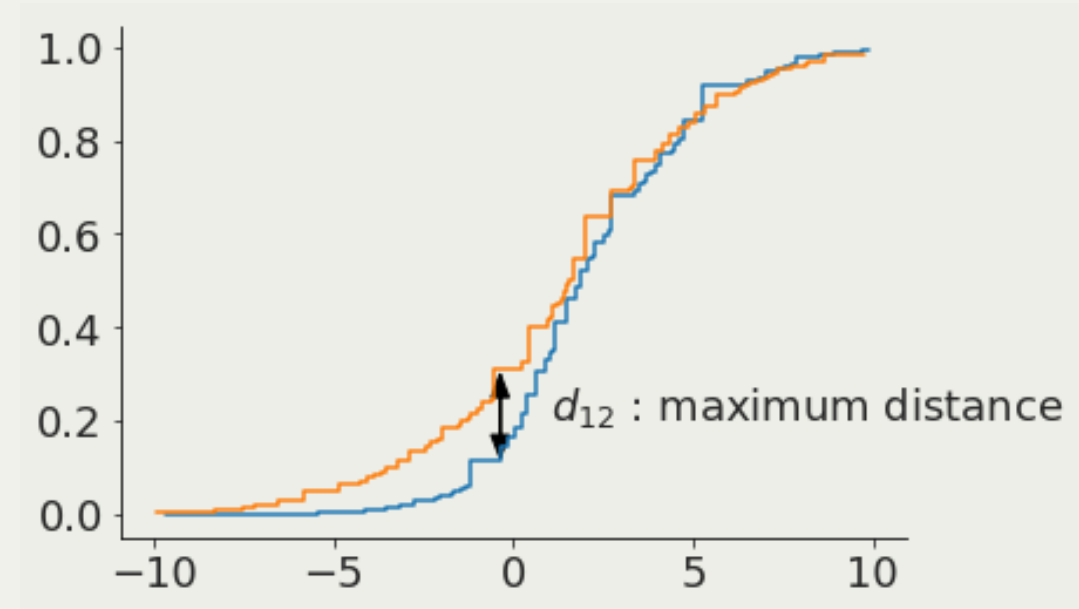
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pivotal quantity

$$d_{12} \equiv \max_x |C_1(x) - C_2(x)|$$

↓
Cumulative
distribution 1

↓
Cumulative
distribution 2



$P(d > \text{observed}) =$

```
sp.stats.ks_2samp(x, y)
```

```
executed in 7ms, finished 14:45:10 2019-09-09
```

```
Ks_2sampResult(statistic=0.4, pvalue=0.3128526760169558)
```

χ^2 test

are the data what is expected from the model (if likelihood is Gaussian... we'll see this later) - there are a few χ^2 tests. The one here is the "Pearson's χ^2 tests"

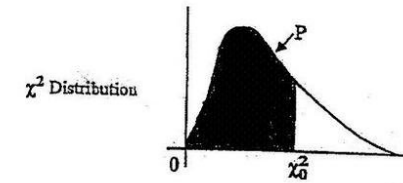
pivotal quantity

$$\chi^2 \equiv \sum_i \frac{(f(x_i) - y_i)^2}{\sigma_i^2}$$

model uncertainty observation

$$\chi^2 \sim \chi^2(df = n - 1)$$

number of observation



The table below gives the value χ_0^2 for which $P[\chi^2 < \chi_0^2] = P$ for a given number of degrees of freedom and a given value of P .

Degrees of Freedom	Values of P									
	0.005	0.010	0.025	0.050	0.100	0.900	0.950	0.975	0.990	0.995
1	---	---	0.001	0.004	0.016	2.706	3.841	5.024	6.635	7.879
2	0.01	0.020	0.051	0.103	0.211	4.605	5.991	7.378	9.210	10.597
3	0.072	0.115	0.216	0.352	0.584	6.251	7.815	9.348	11.345	12.838
4	0.207	0.297	0.484	0.711	1.064	7.779	9.488	11.143	13.277	14.860
5	0.412	0.554	0.831	1.145	1.610	9.236	11.070	12.833	15.086	16.750
6	0.676	0.872	1.237	1.635	2.204	10.645	12.592	14.449	16.812	18.548
7	0.989	1.239	1.690	2.167	2.833	12.017	14.067	16.013	18.475	20.278
8	1.344	1.646	2.180	2.733	3.490	13.362	15.507	17.535	20.090	21.955
9	1.735	2.088	2.700	3.325	4.168	14.684	16.919	19.023	21.666	23.589
10	2.156	2.558	3.247	3.940	4.865	15.987	18.307	20.483	23.209	25.188
11	2.603	3.053	3.816	4.575	5.578	17.275	19.675	21.920	24.725	26.757
12	3.074	3.571	4.404	5.226	6.304	18.549	21.026	23.337	26.217	28.300
13	3.565	4.107	5.009	5.892	7.042	19.812	22.362	24.736	27.688	29.819
14	4.075	4.660	5.629	6.571	7.790	21.064	23.685	26.119	29.141	31.319
15	4.601	5.229	6.262	7.261	8.547	22.307	24.996	27.488	30.578	32.801
16	5.142	5.812	6.908	7.962	9.312	23.542	26.296	28.845	32.000	34.267
17	5.697	6.408	7.564	8.672	10.085	24.769	27.587	30.191	33.409	35.718
18	6.265	7.015	8.231	9.390	10.865	25.989	28.869	31.526	34.805	37.156
19	6.844	7.633	8.907	10.117	11.651	27.204	30.144	32.852	36.191	38.582
20	7.434	8.260	9.591	10.851	12.443	28.412	31.410	34.170	37.566	39.997

χ^2 test

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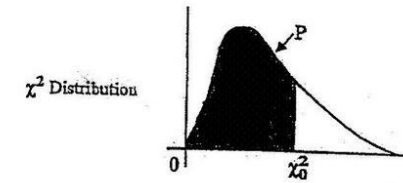
pivotal quantity

$$\chi^2 \equiv \sum_i \frac{(f(x_i) - y_i)^2}{\sigma_i^2}$$

model uncertainty observation

$$\frac{\chi^2}{n-1} \sim \chi^2(df = 1)$$

number of
observation



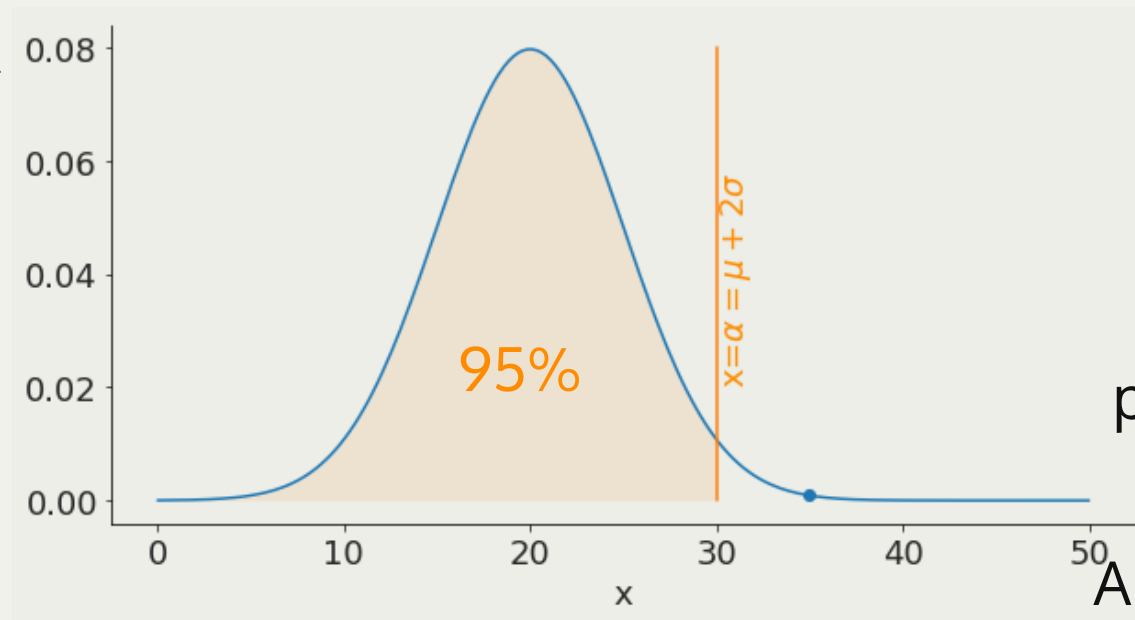
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2	0.01	0.020	0.051	0.103	0.211	4.605	5.991	7.378	9.210	10.597
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5	0.412	0.554	0.831	1.145	1.610	9.236	11.070	12.833	15.086	16.750
6	0.676	0.872	1.237	1.635	2.204	10.645	12.592	14.449	16.812	18.548
7	0.989	1.239	1.690	2.167	2.833	12.017	14.067	16.013	18.475	20.278
8	1.344	1.646	2.180	2.733	3.490	13.362	15.507	17.535	20.090	21.955
9	1.735	2.088	2.700	3.325	4.168	14.684	16.919	19.023	21.666	23.589
10	2.156	2.558	3.247	3.940	4.865	15.987	18.307	20.483	23.209	25.188
11	2.603	3.053	3.816	4.575	5.578	17.275	19.675	21.920	24.725	26.757
12	3.074	3.571	4.404	5.226	6.304	18.549	21.026	23.337	26.217	28.300
13	3.565	4.107	5.009	5.892	7.042	19.812	22.362	24.736	27.688	29.819
14	4.075	4.660	5.629	6.571	7.790	21.064	23.685	26.119	29.141	31.319
15	4.601	5.229	6.262	7.261	8.547	22.307	24.996	27.488	30.578	32.801
16	5.142	5.812	6.908	7.962	9.312	23.542	26.296	28.845	32.000	34.267
17	5.697	6.408	7.564	8.672	10.085	24.769	27.587	30.191	33.409	35.718
18	6.265	7.015	8.231	9.390	10.865	25.989	28.869	31.526	34.805	37.156
19	6.844	7.633	8.907	10.117	11.651	27.204	30.144	32.852	36.191	38.582
20	7.434	8.260	9.591	10.851	12.443	28.412	31.410	34.170	37.566	39.997

Null
Hypothesis
Rejection
Testing

$$p(NH|D) < \alpha$$

prediction is unlikely
Null rejected
Alternative holds



prediction is likely
Null holds
Alternative rejected



$$p(NH|D) \geq \alpha$$

test data against
alternative outcomes

Null

Hypothesis

Rejection

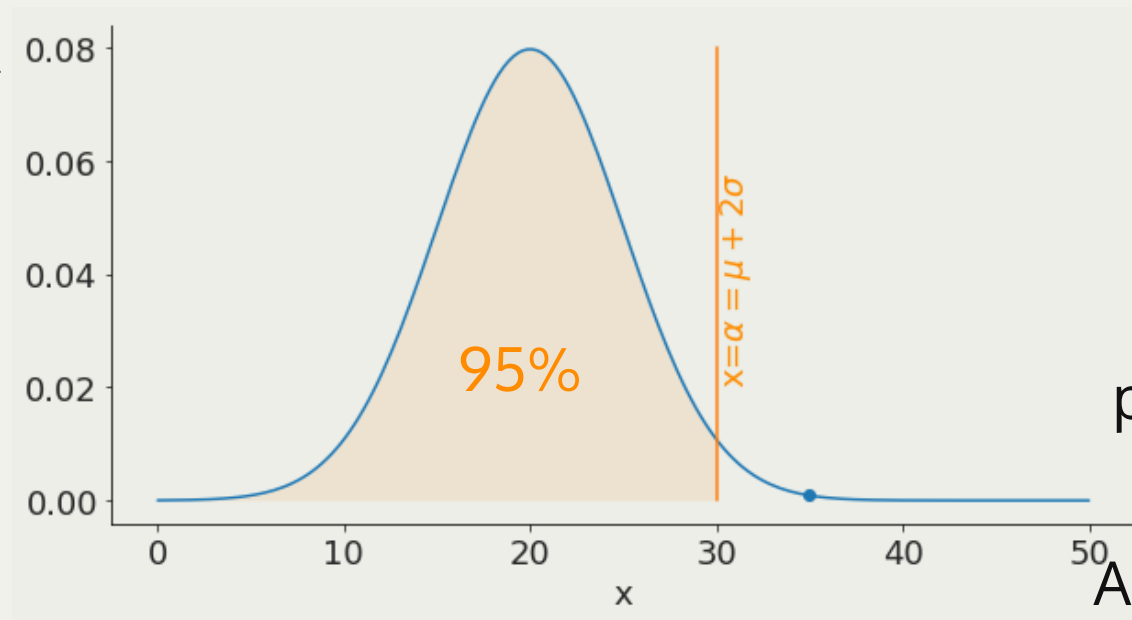
Testing

$$p(NH|D) < \alpha$$

prediction is unlikely

Null rejected

Alternative holds



prediction is likely

Null holds

Alternative rejected



$$p(NH|D) \geq \alpha$$



test data against
alternative outcomes

formulate the Null as the comprehensive opposite of your theory

model



prediction

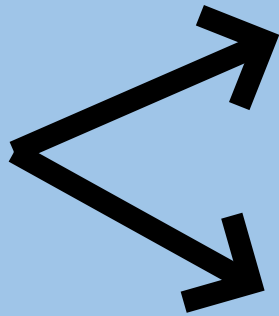
*"Under the **Null Hypothesis**" = if the model is **false***

this has a low probability of happening

everything

but model is rejected

data



**does not falsify
alternative**



**falsifies
alternative**



**model
holds**

Key Slide

low probability event happened

1

formulate your prediction (NH)

2

identify all alternative outcomes (AH)

3

set confidence threshold
(p -value)

4

find a measurable quantity which
under the Null has a known
distribution
(pivotal quantity)

5

calculate the pivotal quantity

6

calculate probability of value
obtained for the pivotal
quantity under the Null

Key Slide

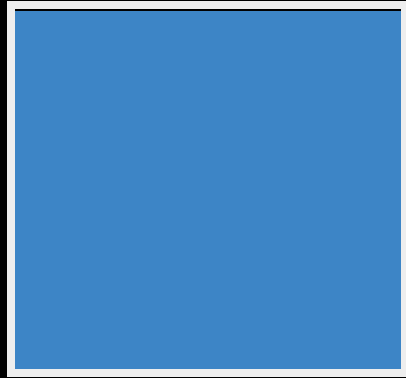
if probability < p -value : reject Null

4 scaling laws

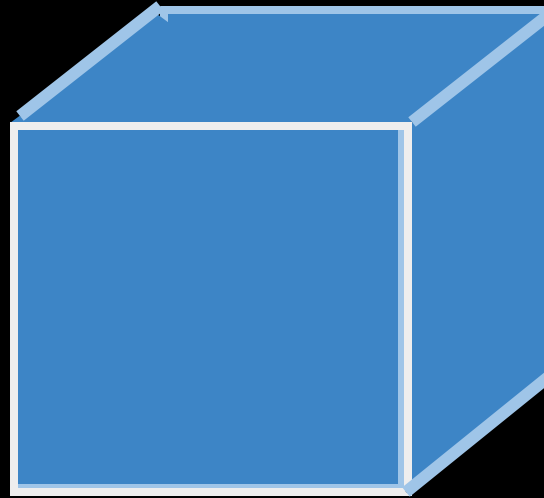
quantities that relate by powers

Example:

$$\underline{L = 1m}$$



$$A = 1m^2$$

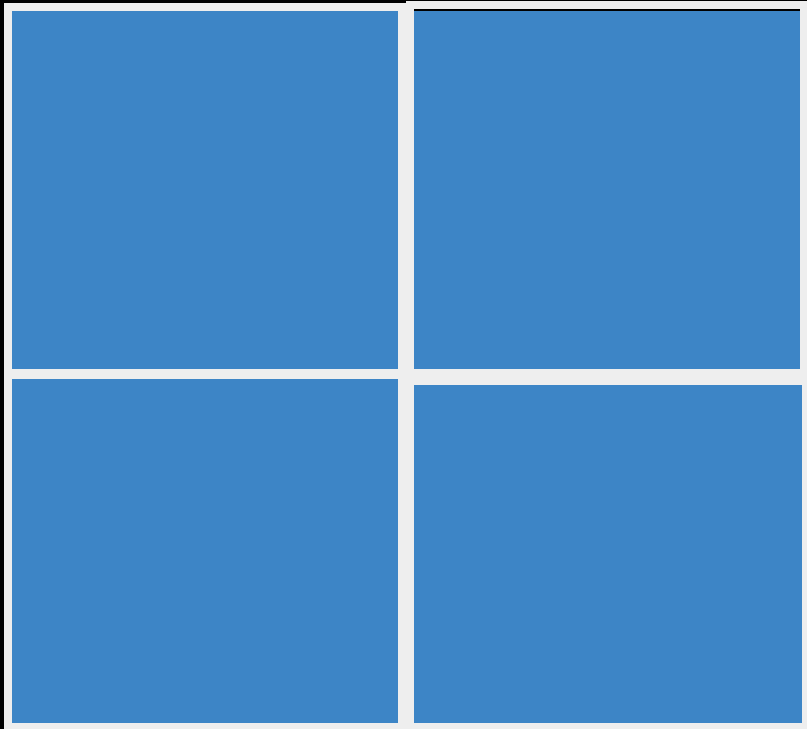


$$V = 1m^3$$

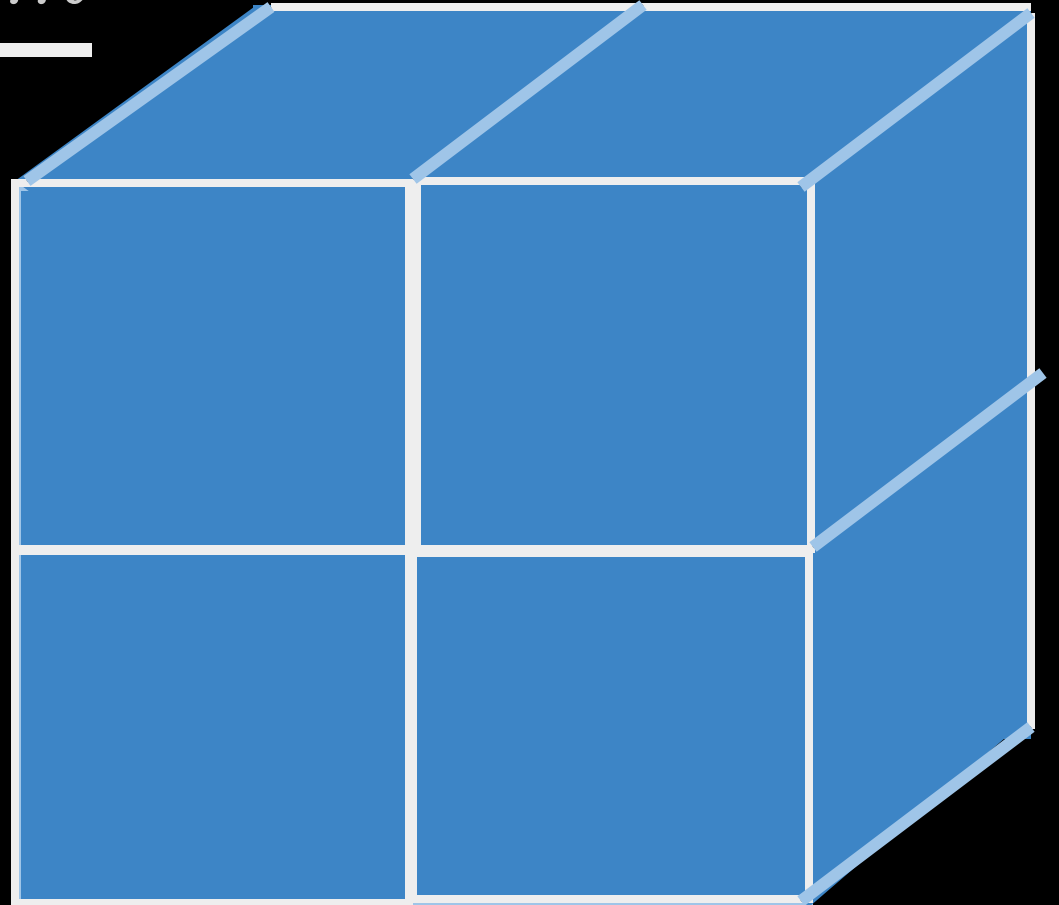
quantities that relate by powers

Example:

$$\underline{L = 2x = 2m}$$



$$A = 4x = 4m^2$$



$$V = 8x = 8m^3$$

quantities that relate by powers

Example:

scaling law: $(\text{ratio of areas}) = (\text{ratio of lengths})^2$

quantities that relate by powers

Example:

scaling law: $(\text{ratio of areas}) = (\text{ratio of lengths})^2$

scaling law: $(\text{ratio of volumes}) = (\text{ratio of lengths})^3$

quantities that relate by powers

Example:

scaling law: $(\text{ratio of areas}) = (\text{ratio of lengths})^2$

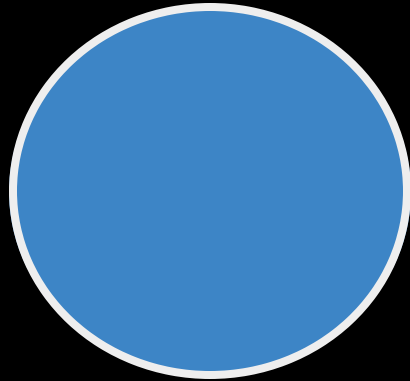
scaling law: $(\text{ratio of volumes}) = (\text{ratio of lengths})^3$

regardless of the shape!

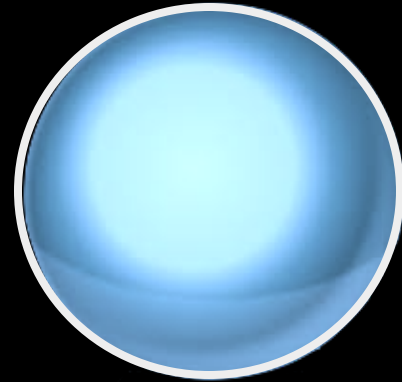
quantities that relate by powers

Example:

$$\underline{r = 1m}$$



$$A = 1m^2$$

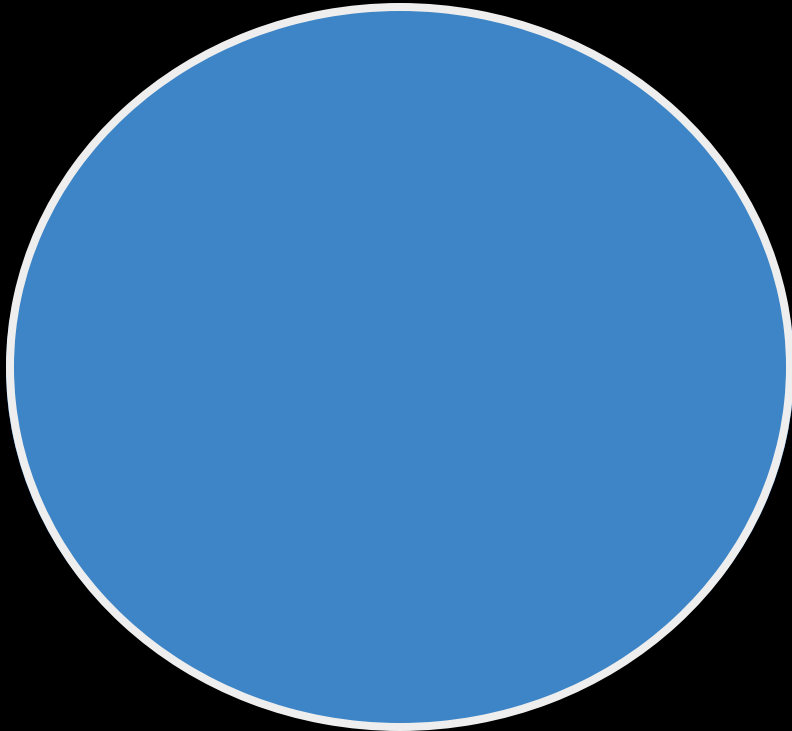


$$V = 1m^3$$

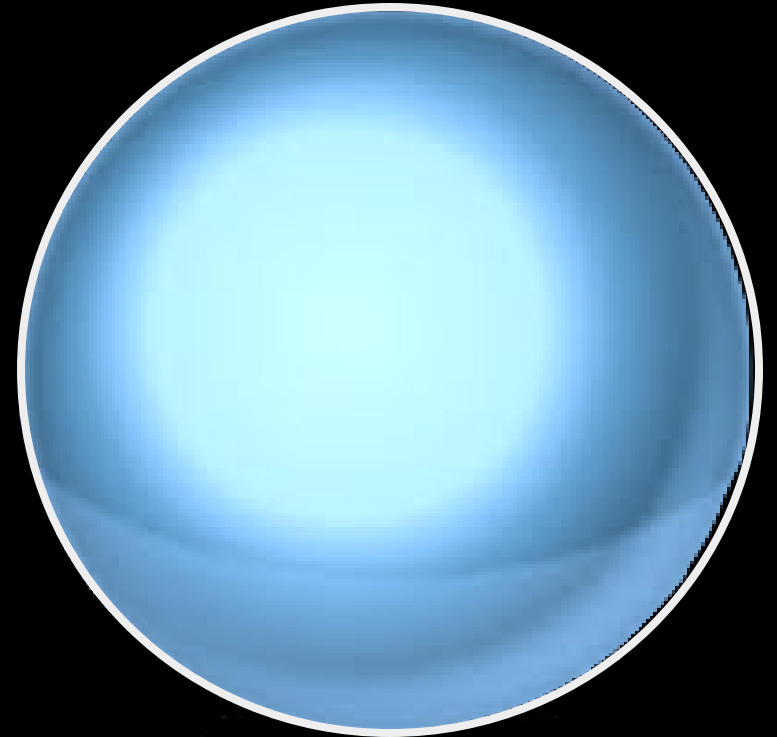
quantities that relate by powers

Example:

$$\underline{r = 1m}$$



$$V \sim 4x, V = \text{const } r^2$$



$$V \sim 8x, V = \text{const } r^3$$

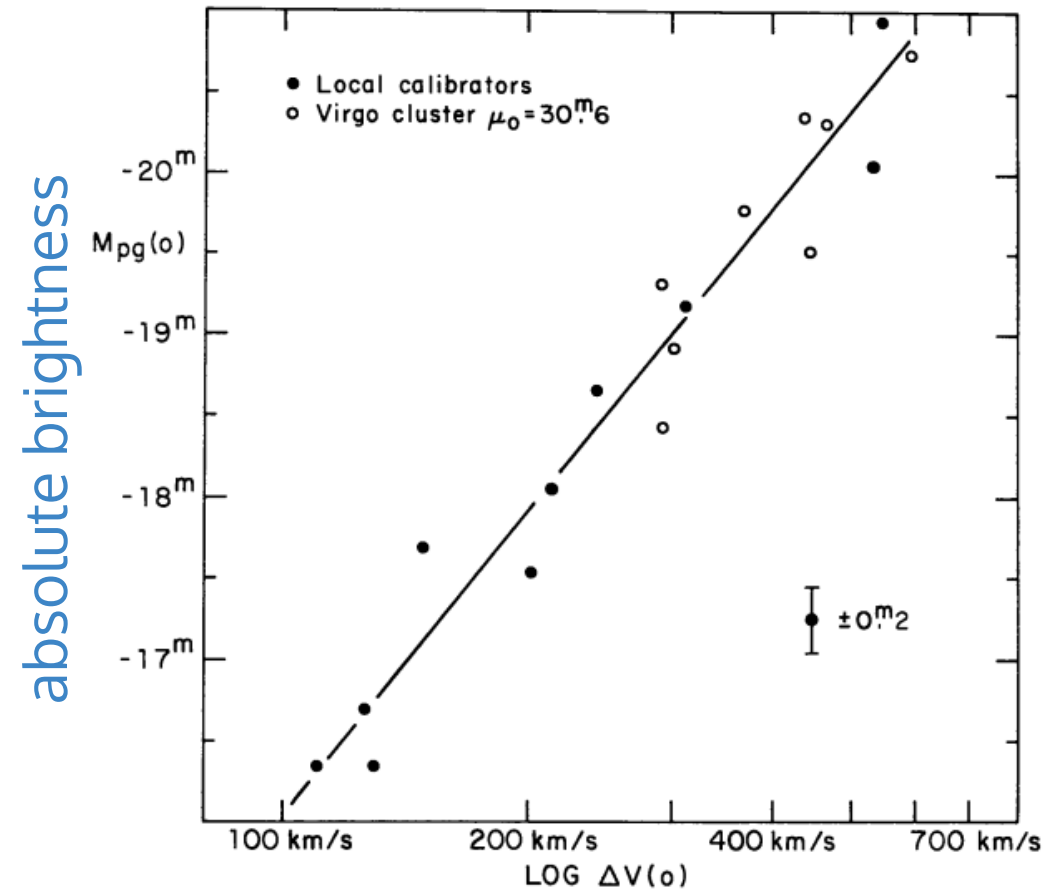
why is this important?

The existence of a **scaling** relationship between physical quantities reveals an underlying driving mechanism

Astrophysics

The **Tully–Fisher relation** is an *empirical relationship between the intrinsic luminosity of a spiral galaxy and its torational velocity*

R. Brent **Tully** and J. Richard **Fisher**, 1977
Astronomy and Astrophysics, 54, 661



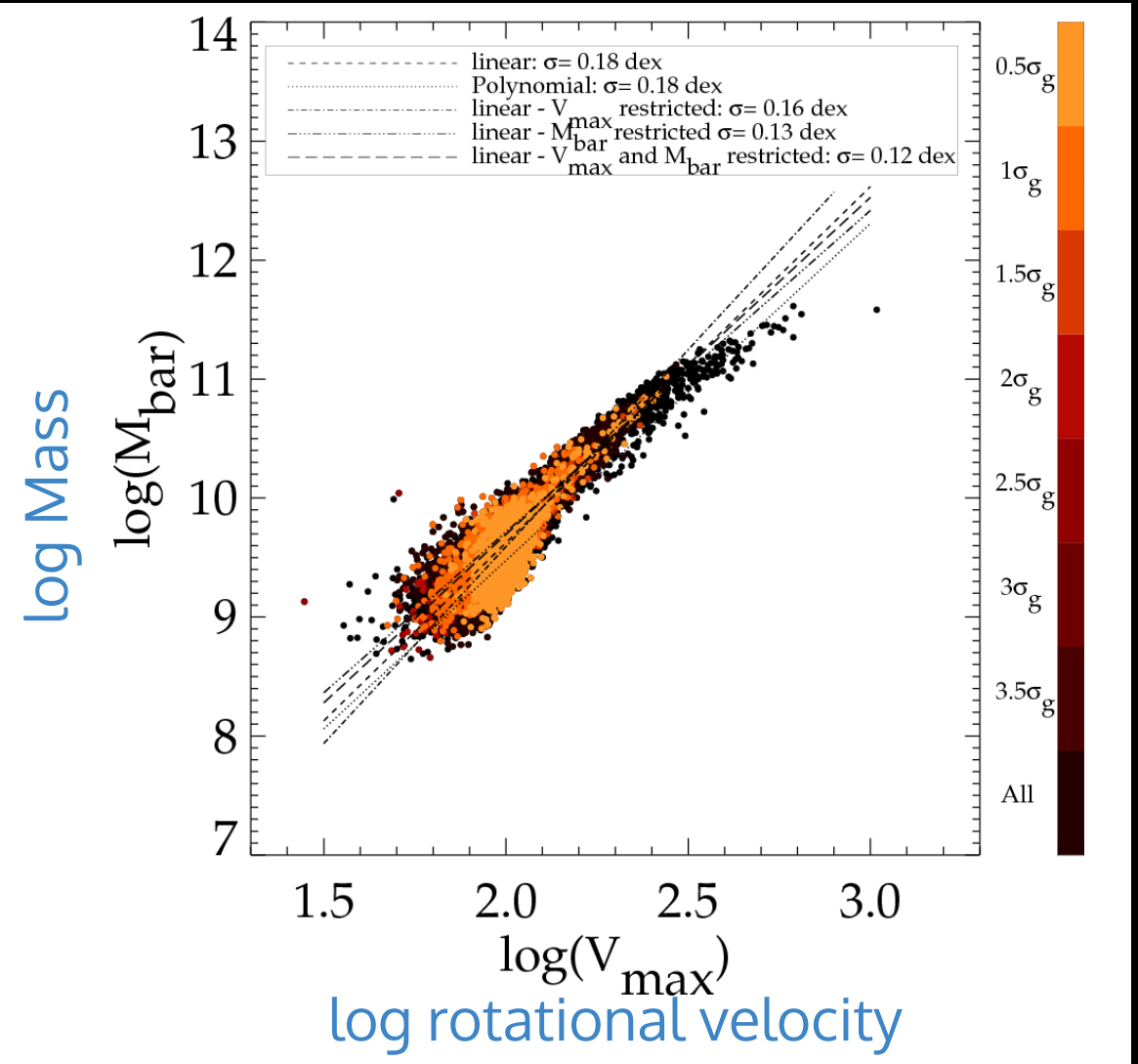
Astrophysics

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R. Brent **Tully** and J. Richard **Fisher**, 1977

GRAVITY

Sorce Jenny *et al.*

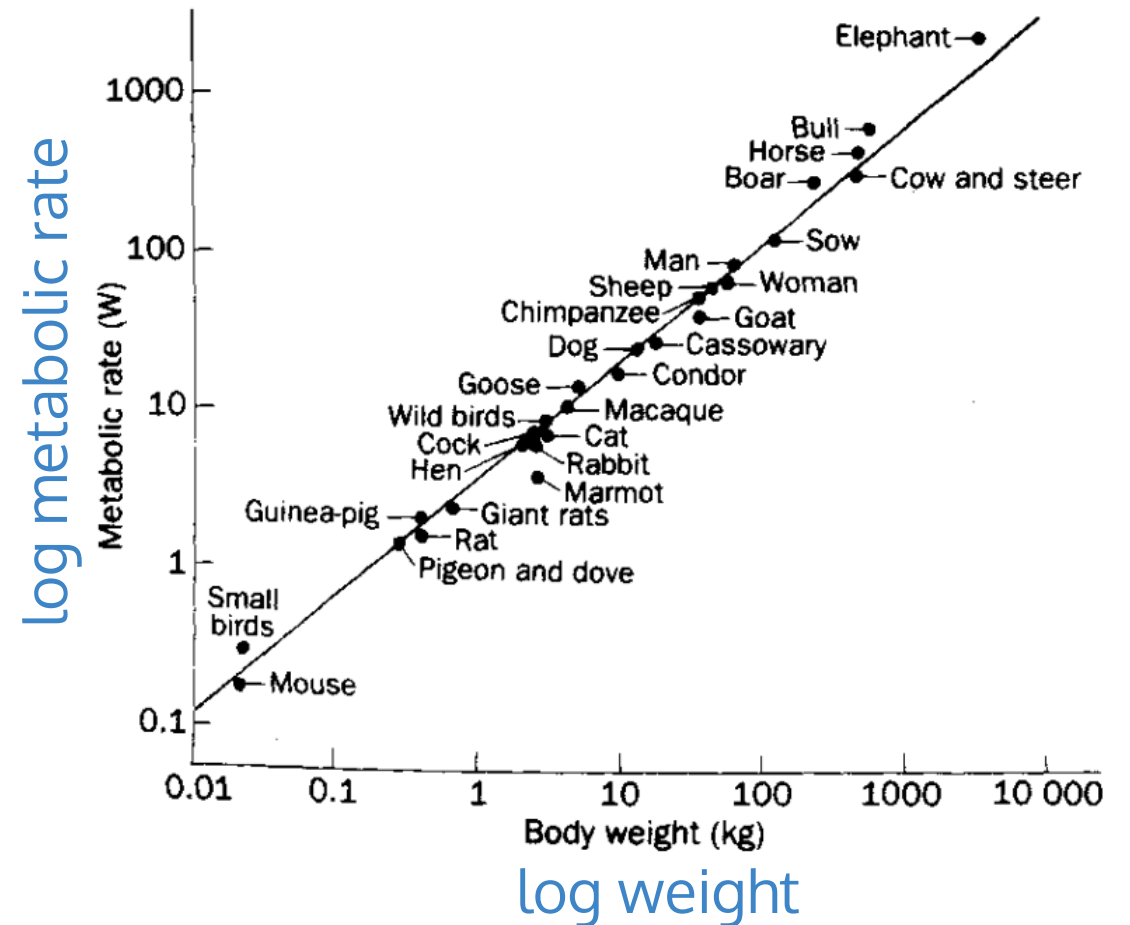


Biology

Basal metabolism of mammals (that is, the minimum rate of energy generation of an organism) has long been known to scale empirically as

$$B \propto M^{3/4}$$

KLEIBER, M. (1932). Body size and metabolism. [Hilgardia 6, 315](#)

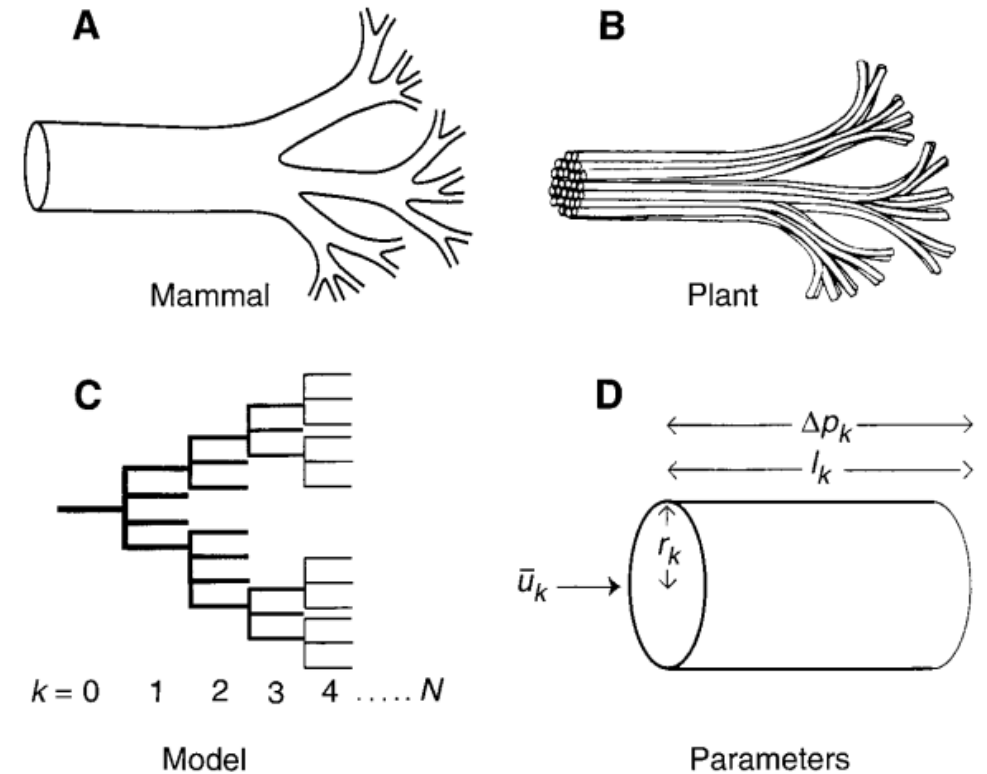


Biology

A general model that describes how essential materials are transported through space-filling fractal networks of branching tubes.

West, Brown, Enquist. 1997 [Science](#)

networks
G. West



Diagrammatic examples of segments of biological distribution networks

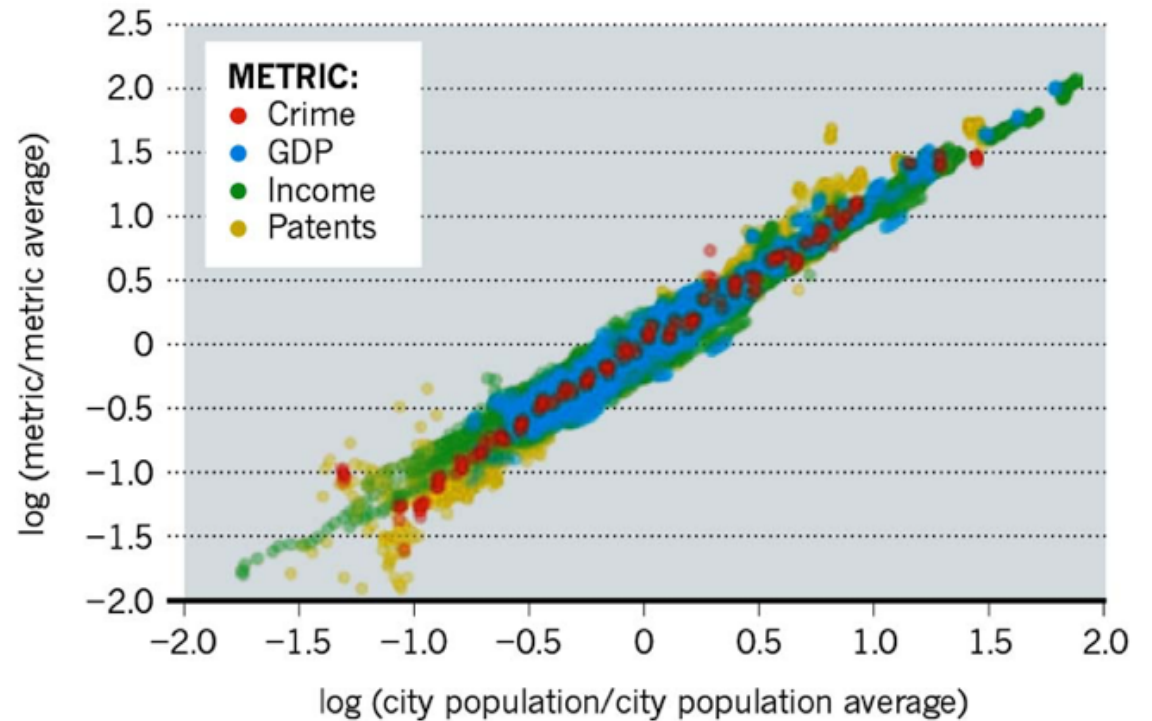
Cities are networks too! And they obey scaling laws on a ridiculous number of parameters!

Bettencourt, L. M. A., Lobo, J., Helbing, D., Kühnert, C. & West, G. B. Proc. Natl Acad. Sci. USA 104, 7301–7306 (2007)

Urban Science

PREDICTABLE CITIES

Data from 360 US metropolitan areas show that metrics such as wages and crime scale in the same way with population size.



<http://vermontcomplexsystems.org/share/papershredder/bettencourt-urban-nature-2010.pdf>

G. West

key concepts

descriptive statistics

null hypothesis rejection
testing setup

pivotal quantities

Z, t, χ^2 , K-S tests

the importance of scaling laws

HW1 : earthquakes and KS test:

reproduce the work of Carrell 2018 using a KS-test to demonstrate the existence of a scaling law in the frequency of earthquakes

<https://arxiv.org/pdf/0910.0055.pdf>

homework

<https://arxiv.org/pdf/0910.0055.pdf>

1

STATISTICAL TESTS FOR SCALING IN THE INTER-EVENT TIMES OF EARTHQUAKES IN CALIFORNIA

ÁLVARO CORRAL

Centre de Recerca Matemàtica, Edifici Cc, Campus UAB, E-08193 Bellaterra, Barcelona, Spain
ACorral at crm dot es

Received Day Month Year

Revised Day Month Year

We explore in depth the validity of a recently proposed scaling law for earthquake inter-event time distributions in the case of the Southern California, using the waveform cross-correlation catalog of Shearer *et al.* Two statistical tests are used: on the one hand, the standard two-sample Kolmogorov-Smirnov test is in agreement with the scaling of the distributions. On the other hand, the one-sample Kolmogorov-Smirnov statistic complemented with Monte Carlo simulation of the inter-event times, as done by Clauset *et al.*, supports the validity of the gamma distribution as a simple model of the scaling function appearing on the scaling law, for rescaled inter-event times above 0.01, except for the largest data set (magnitude greater than 2). A discussion of these results is provided.

Keywords: Statistical seismology; scaling; goodness-of-fit tests; complex systems.

https://www.ted.com/talks/geoffrey_west_the_surprising_math_of_cities_and_corporations?utm_campaign=tedsbread&utm_medium=referral&utm_source=tedcomshare¹

watching

https://embed.ted.com/talks/lang/en/geoffrey_west_the_surprising_math_of_cities_and_corporations

Sarah Boslaugh, Dr. Paul Andrew Watters, 2008

Statistics in a Nutshell (Chapters 3,4,5)

https://books.google.com/books/about/Statistics_in_a_Nutshell.html?id=ZnhgO65Pyl4C

David M. Lane et al.

Introduction to Statistics (XVIII)

http://onlinestatbook.com/Online_Statistics_Education.epub

<http://onlinestatbook.com/2/index.html>

Bernard J. T. Jones, Vicent J. Martínez, Enn Saar, and Virginia Trimble

Scaling laws in physics

https://ned.ipac.caltech.edu/level5/March04/Jones/Jones1_3.html

Bettencourt , Strumsky, West

Urban Scaling and Its Deviations: Revealing the Structure of Wealth, Innovation and Crime across Cities

<https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0013541>

resources