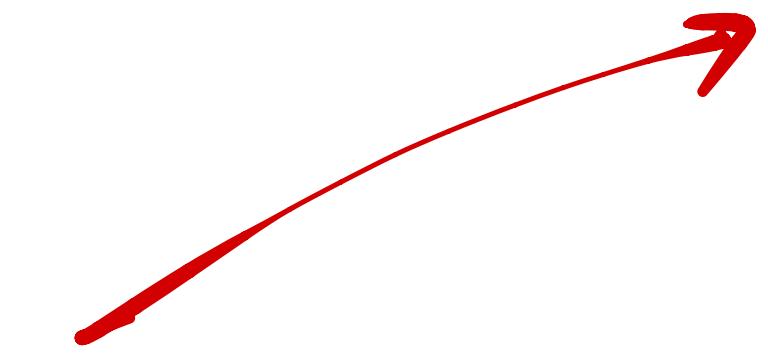


Lecture 4

Least Squares, Percentiles, and Regression

History of Data Science, Spring 2022 @ UC San Diego
Suraj Rampure

Announcements



Office hours : Friday 12-1 PM
SDSC 2nd floor
Zoom

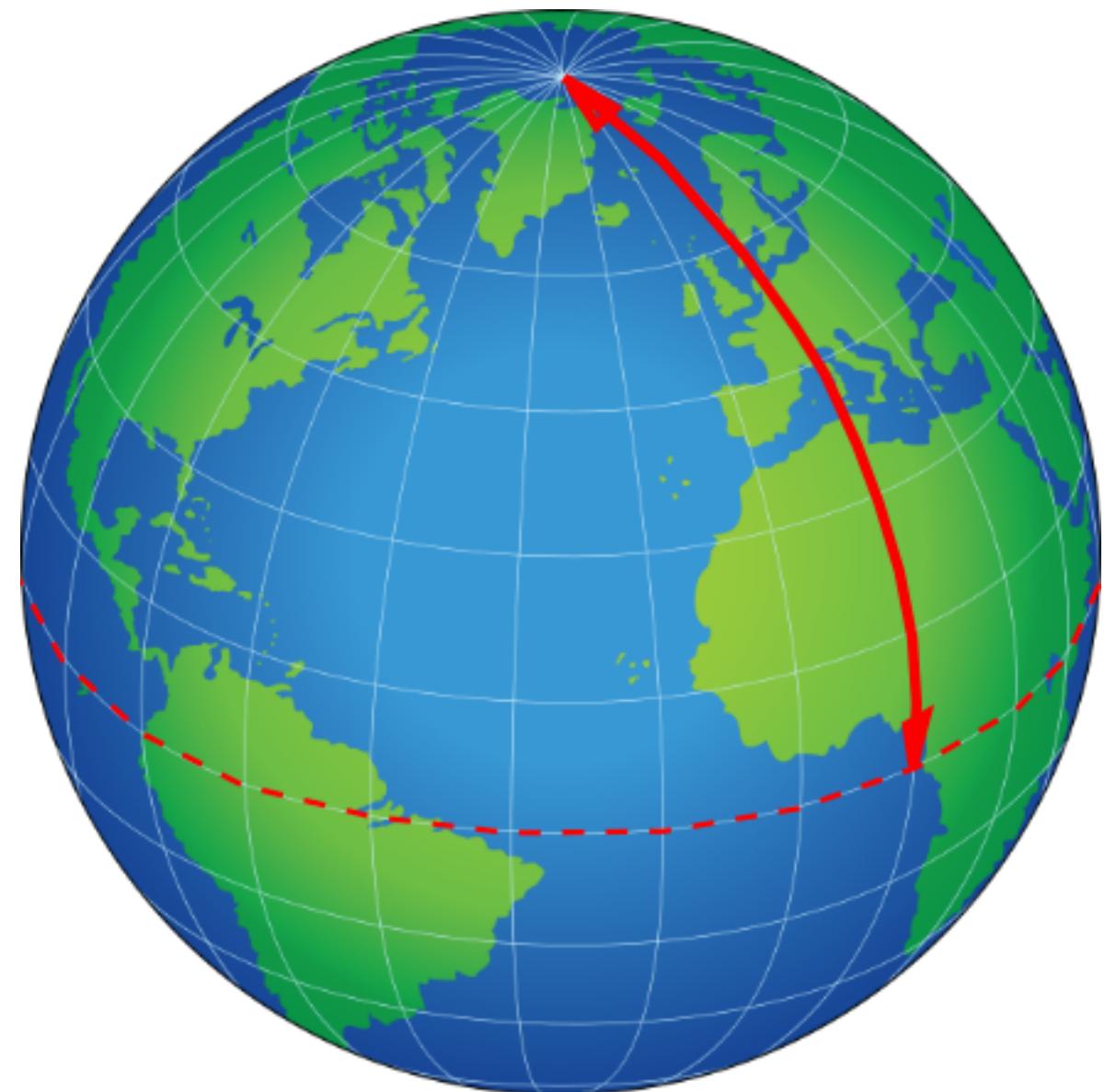
- Homework 4 is released and is due on **Sunday, April 24th at 11:59PM**.
- Homework 2 is graded! Make sure to look at the solutions, posted on Slack and on the course website.

Agenda

- Legendre and Gauss' development of least squares.
- Quetelet and the “average man”.
- Galton's development of regression.
- Pearson.

Least squares

Legendre



- Adrien-Marie Legendre (1752-1833) was a French mathematician who was also active in the field of geodesy¹.
- In 1791, the French Academy of Science defined a meter as being one **ten millionth** of the length of the meridian arc starting at the North Pole, passing through Paris, and ending at the equator.
- He helped measure the length of a meter.

1. <https://www.britannica.com/biography/Adrien-Marie-Legendre>

Legendre's least squares

- In a 1805 paper about measuring the orbits of comets, Legendre published an appendix titled “Sur la Methode des moindres quarres”, which detailed a general procedure for estimating coefficients of linear equations.
- He wrote (translated):

“Of all the principles which can be proposed for [making estimates from a sample], I think there is none more general, more exact, and more easy of application, than that of which we have made use... which consists of rendering the sum of the squares of the errors a minimum.”

→ minimizing sum of squared errors ↗ MSE

Gauss

- Carl Friedrich Gauss (1777-1855)¹ was a German mathematician, and is one of the most accomplished mathematicians of all time.
- He is known for developing or contributing to:
 - Least squares.
 - The normal (Gaussian) distribution.
 - Algebra and number theory.
 - He supposedly summed the positive integers between 1 and 100 very quickly.
 - Electromagnetism.
 - **Not** Gaussian elimination!

1. <https://www.britannica.com/biography/Carl-Friedrich-Gauss>

$$S = 1 + 2 + 3 + 4 + \dots + 98 + 99 + 100$$

$$+ S = 100 + 99 + 98 + 97 + \dots + 3 + 2 + 1$$

$$+ S = \overbrace{101 + 101 + 101 + 101 + \dots + 101 + 101 + 101}^{\text{101 terms}}$$

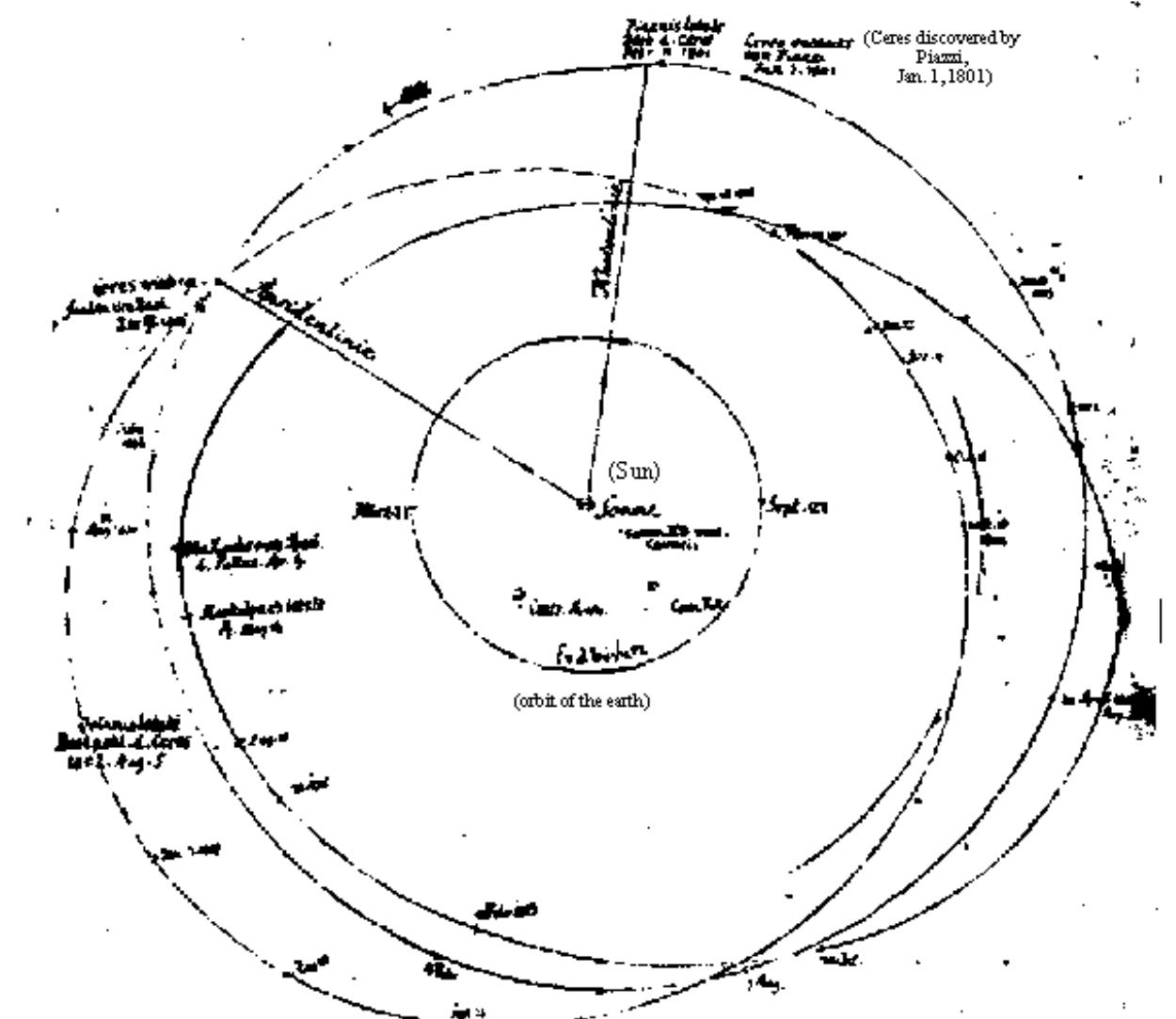
$$2S = 101 \cdot 100$$

$$\Rightarrow 2S = 101 \cdot 100$$

$$S = \frac{101 \cdot 100}{2} = 50 \cdot 101 = \boxed{5050}$$

Gauss and least squares

- In 1809, Gauss published "Theory of the Motion of the Heavenly Bodies Moving About the Sun in Conic Sections", and in it he used the method of least squares to calculate the shapes of orbits.
- Legendre published about least squares in 1805, 4 years before. However, Gauss claimed to have known about least squares in 1795.
- **Evidence:** Gauss was able to predict the precise location of planetoid Ceres using his method of least squares.
- Ceres was observed on January 1st, 1801 for a period of 40 days. Several astronomers competed to predict where it would be spotted again, and Gauss' guess was the only correct one².



Sketch of the orbits of Ceres and Pallas (nachlaß Gauß, Handb. 4). Courtesy of Universitätsbibliothek Göttingen.

[Source](#)

1. <https://www.britannica.com/biography/Carl-Friedrich-Gauss>
2. <https://blog.bookstellyouwhy.com/carl-friedrich-gauss-and-the-method-of-least-squares>

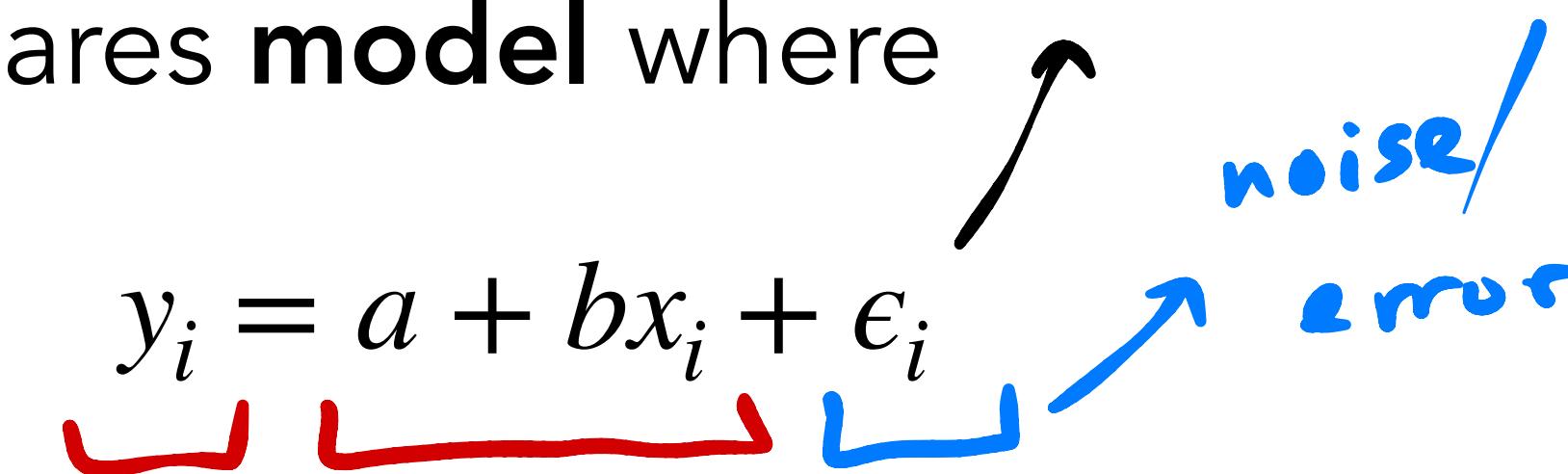
Error distributions

- One of the key differences between the approaches to least squares by Gauss and Legendre was that Gauss linked the theory of least squares to probability theory.

mean = 0

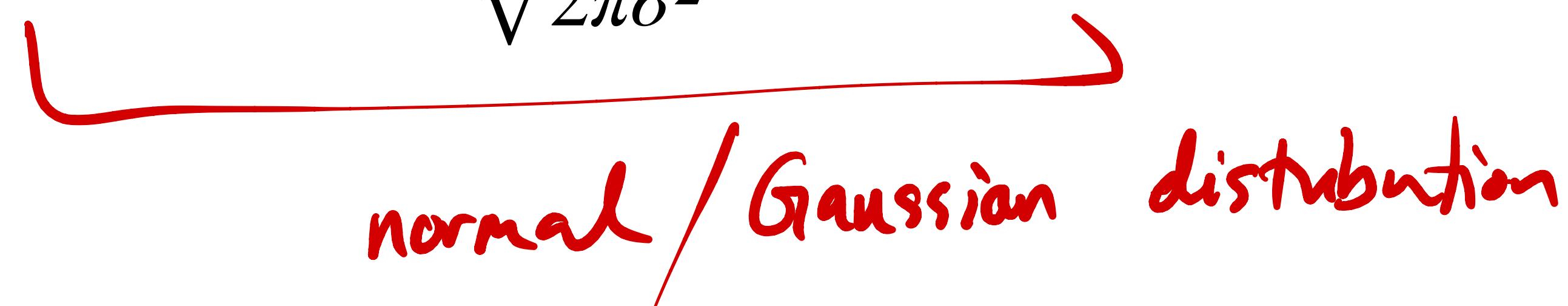
- Specifically, he posed the least squares **model** where

$$y_i = a + b x_i + \epsilon_i$$

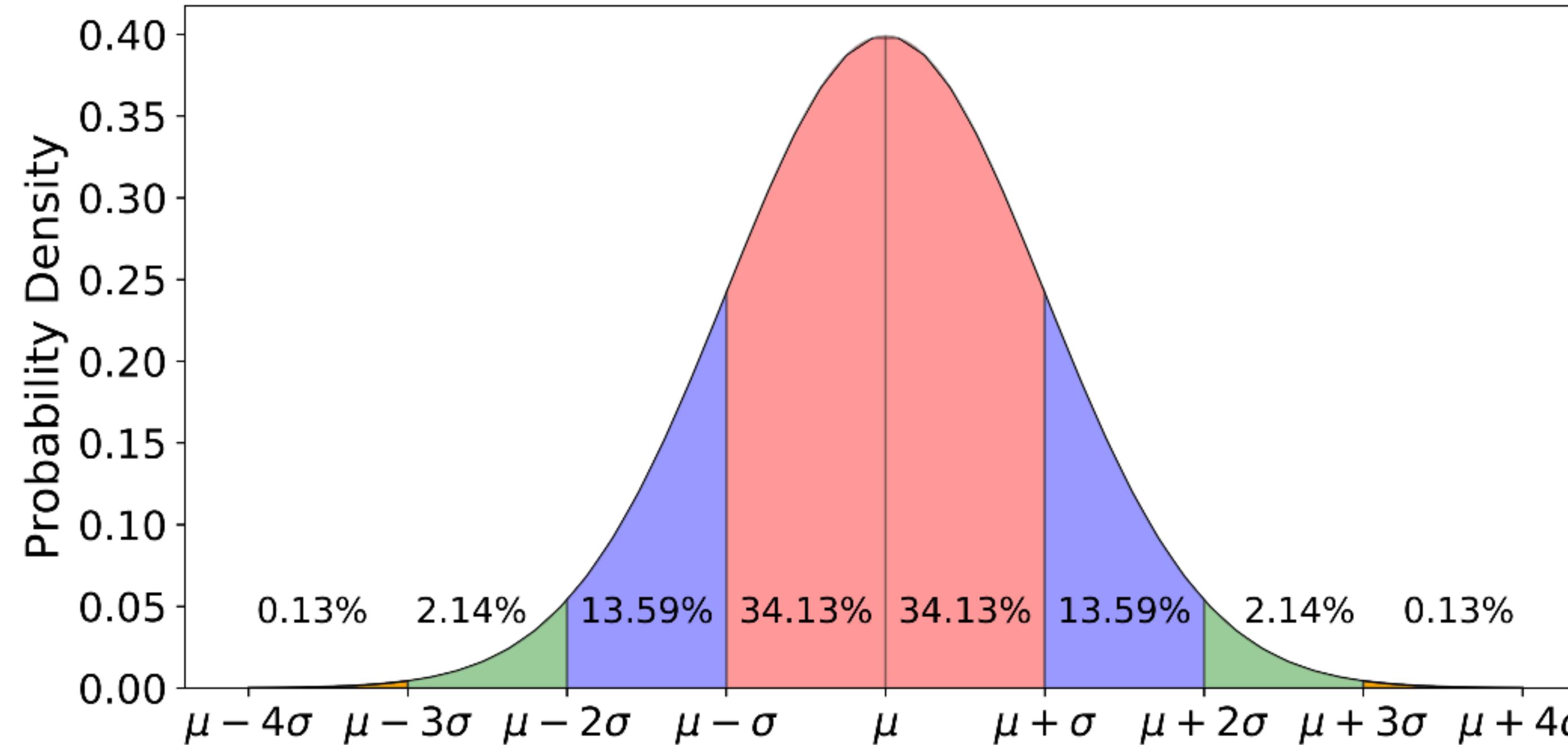


where ϵ_i is a **random variable** that follows the following **error distribution**:

$$\phi(x | \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x - \mu)^2}{2\sigma^2}}$$


normal / Gaussian distribution

Normal Distribution



We will study Gauss' derivation of the (now-called) Gaussian/normal distribution in Lecture 5.

Maximum likelihood estimation (MLE)

- To illustrate the power of Gauss' contribution, we need to describe the concept of **maximum likelihood estimation**.
→ probability it flips heads
- Suppose we have a coin, whose **bias**, p , is unknown. We flip the coin 10 times, and see the sequence HTTHTTTTTTH.
- Question: what is the best guess for the value of p ?

*reasonable
guess* = $\frac{3}{10} = 0.3$, *proportion of
heads in
sample*

Sequence

HTTH TTTTTH

What if $p=0.6$

$$\begin{aligned} P(\text{sequence}) &= 0.6 \cdot 0.4 \cdot 0.4 \cdot 0.6 \cdot 0.4^5 \cdot 0.6 \\ &= 0.6^3 \cdot 0.4^7 \end{aligned}$$

What if $p=0.2$

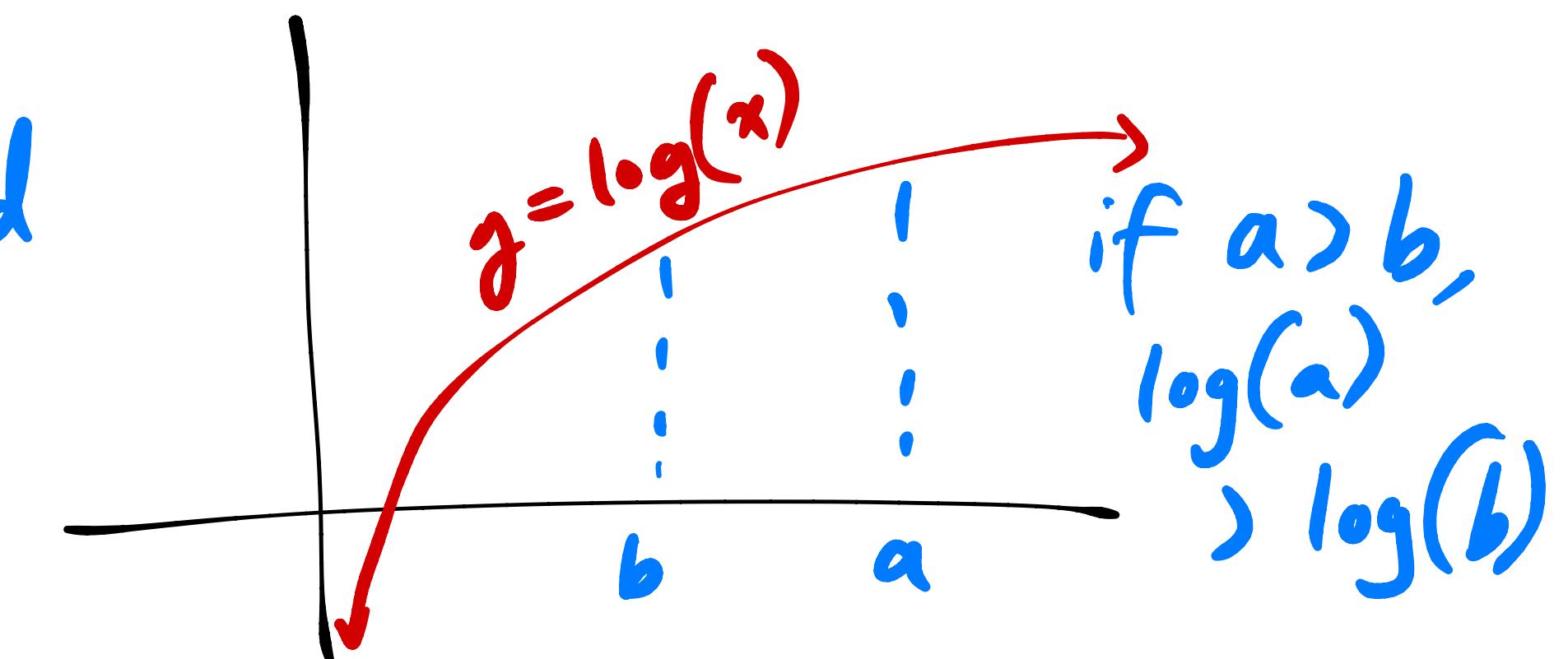
$$P(\text{sequence}) = 0.2^3 \cdot 0.8^7$$

Likelihood : $L(p) = P(\text{sequence if bias is } p)$

$$= p^3 (1-p)^7 \rightarrow \text{maximize } L(p)!$$

idea: maximize LOG of likelihood

maximize $LL(p) = \log(p^3(1-p)^7)$
is this allowed?



$$\text{LL}(p) = \log(p^3(1-p)^7)$$

$$= \log(p^3) + \log((1-p)^7)$$

$$\text{LL}(p) = 3\log(p) + 7\log(1-p)$$

$$\frac{d}{dp} \text{LL}(p) = 3 \cdot \frac{1}{p} + 7 \cdot \frac{1}{1-p}(-1) = 0$$

$$\frac{3}{p} = \frac{7}{1-p}$$

$$3(1-p) = 7p$$

$$3 = 10p \Rightarrow$$

$$p = \frac{3}{10}$$

log rules
 $\log(ab) = \log(a) + \log(b)$
 $\log(a^n) = n \log(a)$

Maximum likelihood estimation (MLE)

- In general, if we flip a fair coin n times and see x heads, to find the “best guess” for p , we **maximize** the **likelihood function**

$$L(p) = p^x(1 - p)^{n-x}$$

- It is hard to maximize this directly, so instead we maximize the **log-likelihood**:

$$LL(p) = x \log p + (n - x) \log(1 - p)$$

- This is maximized when $p = \frac{x}{n}$, which matches our intuitive guess.

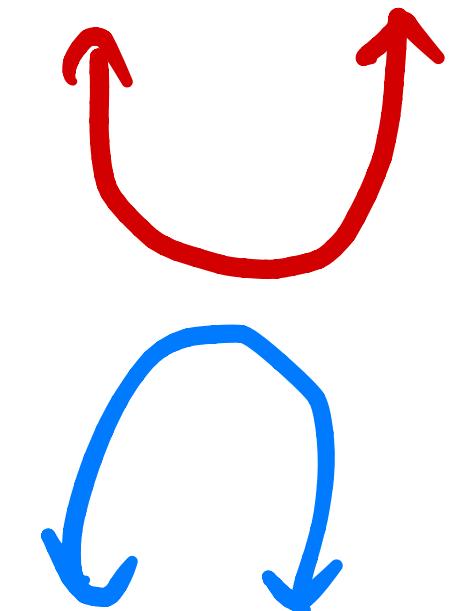
MLE and regression

$$LL(a, b, \sigma^2) = -\frac{1}{n} \sum_{i=1}^n (y_i - a - bx_i)^2$$

$\max_{\text{LLL(p)}} = \min_{\text{MSE}}$

$$y_i = a + bx_i + \epsilon_i$$

$$\epsilon_i \sim N(0, \sigma^2)$$



- **Key point:** if you use the assumption that the errors in a linear regression model are independent and follow a Normal distribution, then **maximizing (log-)likelihood** is equivalent to minimizing **mean squared error**.
- This is a big reason why least squares is so prevalent – not only is it computationally easy to minimize mean squared error, but it is consistent with this **assumption of normality**.
- You're not expected to fully grasp this concept just yet, but it is valuable context to have throughout the rest of today's lecture, for tomorrow's lecture, and for the rest of your data science career.

Statistics in biology and sociology

Quetelet

- Adolphe Quetelet (1796-1874)¹ was a Belgian astronomer, mathematician, statistician, and sociologist.
- He was born in Ghent (picture to the right).
- Originally an **astronomer**, he is known for being one of the first people to apply statistical methods to ideas in the **social sciences**.



Photo taken in Ghent by Suraj

1. <https://www.britannica.com/biography/Adolphe-Quetelet>

From astronomy to social science

- Astronomers took the **average** of several observations to estimate the **true value** of some quantity, i.e. to reduce observational error.
 - e.g. measuring the speed of Saturn.
- Quetelet was the first to apply the average to data on humans and societies.
 - For instance, he obtained a dataset containing the chest circumferences of thousands of Scottish soldiers¹.
 - He computed the **average** of the chest circumferences of these soldiers, yielding ~39.75 inches.
 - **What does this mean?**

1. <https://www.theatlantic.com/business/archive/2016/02/the-invention-of-the-normal-person/463365/>

The “average man”

- Possible interpretations:
 - 39.75 inches is the chest size we'd expect if we selected a random soldier.
 - 39.75 inches is roughly the chest size of a normal soldier.
- Quetelet's interpretation: 39.75 inches is the **true** chest size of soldiers, and any differences in an individual's chest size is due to error.
 - Later, Quetelet described the concept of the “average man” (in his words, *l'homme moyen*), who is defined by having an average measurement in several biological and sociological characteristics.
 - He believed that with more data, we could get closer and closer to approximating the “true” human.

Quetelet index

- To quantify the weight and height of the average man, Quetelet devised the **Quetelet index**, defined as

$$\text{Quetelet index} = \frac{\text{mass in kg}}{(\text{height in m})^2} = \text{BMI}$$

(Body Mass Index)

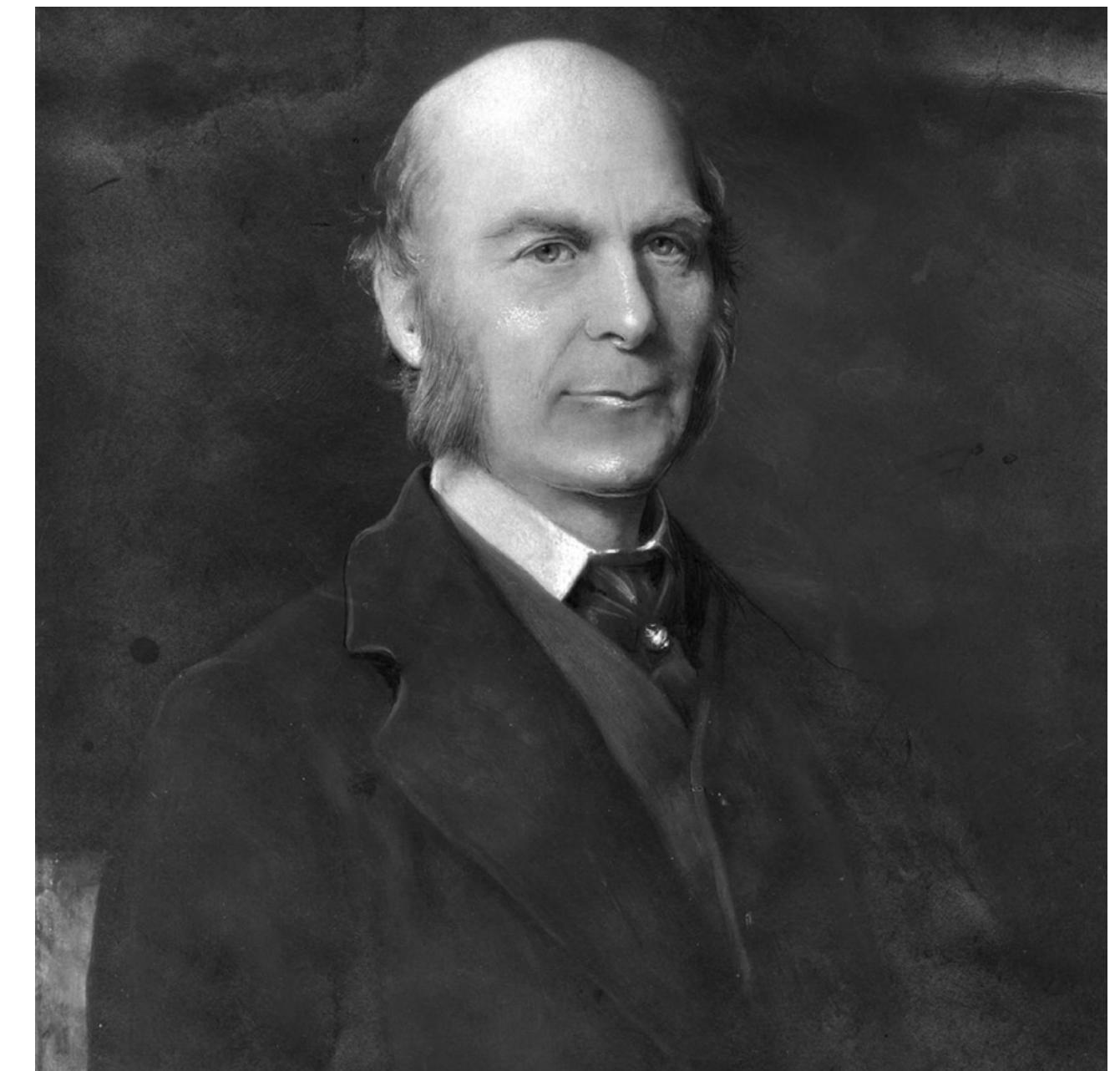
- Quetelet never intended it to be a measure of obesity.
- However, in the 1900s, the Quetelet index began to be used for this purpose by insurance companies.

Galton

Galton

Legendre: 1805
Gauss: 1809

- Sir Francis Galton (1822-1911) was a British polymath.
 - He was knighted in 1909, hence the "Sir".
- He was Charles Darwin's half-cousin. As we will see, this played a pivotal role in the ideas he decided to study.
 - Example: Galton was the first to discover that everyone has unique fingerprints, and thus that fingerprints can be used for identification.
- galton.org contains excerpts of many of his original works.
- Note that Galton was only born years after Legendre and Gauss formulated least squares.



Aside: Darwin and the “Rule of Three”

- Charles Darwin is well-known for his development of the **theory of evolution**, though he was supposedly not found of mathematics.
- He wrote to a colleague,

“I have no faith in anything short of actual measurement and the Rule of Three.”¹

- The “Rule of Three” in question is that if $\frac{a}{b} = \frac{c}{d}$, then given any three of a, b, c, d , one can find the fourth by cross-multiplication.
- **Question:** does the Rule of Three work when there is measurement error in any of a, b, c, d ?

1. Stigler, *The Seven Pillars of Statistical Wisdom*, p.107

$$\frac{10 \text{ miles}}{20 \text{ min}} = \frac{15 \text{ miles}}{\text{???}}$$

$$\frac{10.5 \text{ miles}}{19 \text{ min}} = \frac{15 \text{ miles}}{\text{???}}$$

Galton's motivation

- Galton was interested in studying how traits were passed from parents to children.
- He created the field of **eugenics**, and wrote:

"Eugenics is the science which deals with all influences that improve the inborn qualities of a race; also with those that develop them to the utmost advantage. The improvement of the inborn qualities, or stock, of some one human population, will alone be discussed here."¹

- In other words, he believed that the traits that made people successful were inheritable, and so only people with those characteristics should have children.
- Along these lines, he “ranked” the worth of each race.
- Virtually all of the statistical techniques he developed were to further his study of eugenics.

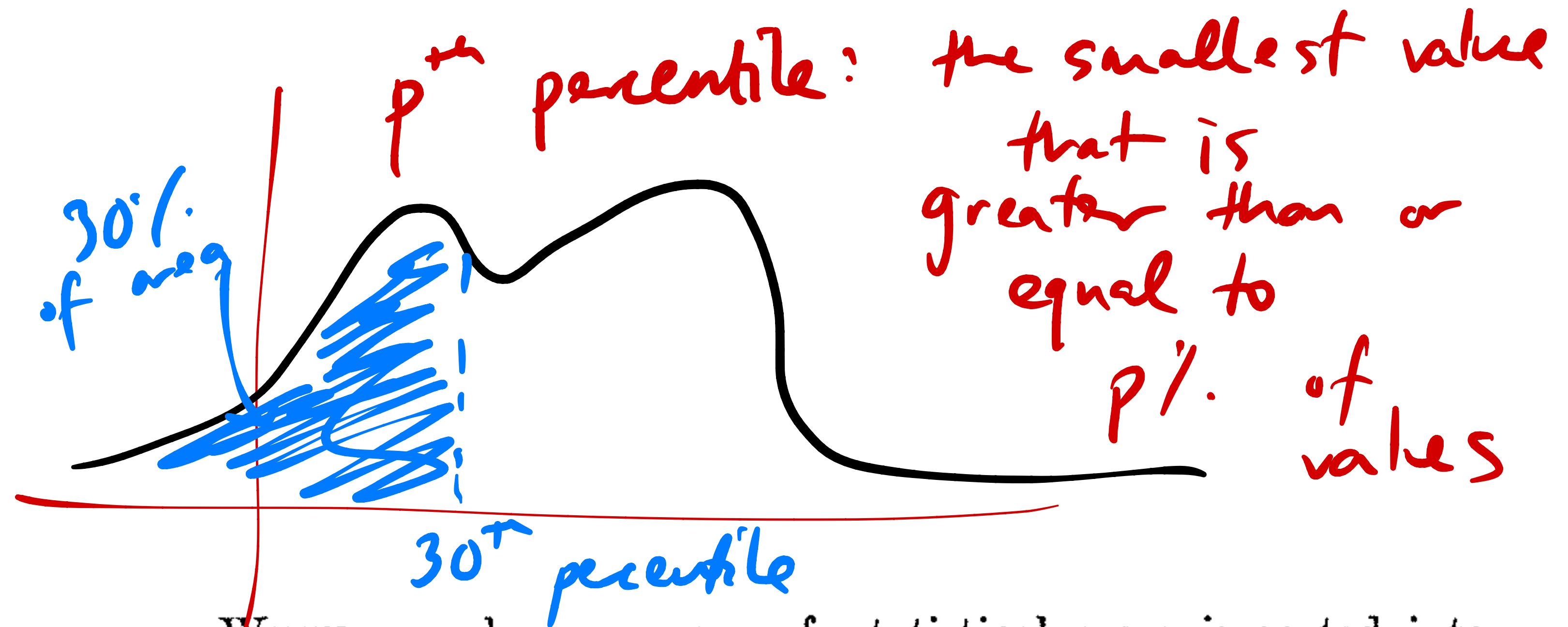
1. <https://galton.org/essays/1900-1911/galton-1905-socpapers-eugenics-definition-scope-aims.pdf>



Galton coined the phrase “nature vs. nurture.” ([graphic source](#))

Percentiles

- Galton developed the idea of a **percentile**.
- He collected data on the physical measurements of many individuals and summarized the data using percentiles, quartiles, and deciles.



WHEN any large group of statistical cases is sorted into a hundred classes equal in number, and progressively increasing in value, the dividing values between the classes are called Percentiles;² or, if into ten classes, they are called Deciles; or if into four classes, they are called Quartiles. The fiftieth percentile, the fifth decile, and the second quartile are consequently the same as the median. All other deciles, &c., are calculated on the

etc. = et cetera

(The value that is un-reached by n per cent. of any large group of measurements, and surpassed by $100-n$ of them, is called its n th percentile)

Subject of measurement	Age	Unit of measurement	Sex	No. of persons in the group	Values surpassed by per-cent. as below										
					95	90	80	70	60	50	40	30	20	10	5
					5	10	20	30	40	50	60	70	80	90	95
Height, standing, without shoes ...	23-51	Inches {	M. F.	811 770	63.2 58.8	64.5 59.9	65.8 61.3	66.5 62.1	67.3 62.7	67.9 63.3	68.5 63.9	69.2 64.6	70.0 65.3	71.3 66.4	72.4 67.3
Height, sitting, from seat of chair ...	23-51	Inches {	M. F.	1013 775	33.6 31.8	34.2 32.3	34.9 32.9	35.3 33.3	35.4 33.6	36.0 33.9	36.3 34.2	36.7 34.6	37.1 34.9	37.7 35.6	38.2 36.0
Span of arms ...	23-51	Inches {	M. F.	811 770	65.0 58.6	66.1 59.5	67.2 60.7	68.2 61.7	69.0 62.4	69.9 63.0	70.6 63.7	71.4 64.5	72.3 65.4	73.6 66.7	74.8 68.0
Weight in ordinary indoor clothes ...	23-26	Pounds {	M. F.	520 276	121 102	125 105	131 110	135 114	139 118	143 122	147 129	150 132	156 136	165 142	172 149
Breathing capacity	23-26	Cubic inches {	M. F.	212 277	161 92	177 102	187 115	199 124	211 131	219 138	226 144	236 151	248 164	277 177	290 186
Strength of pull as archer with bow	23-26	Pounds {	M. F.	519 276	56 30	60 32	64 34	68 36	71 38	74 40	77 42	88 44	82 47	89 51	96 54
Strength of squeeze with strongest hand	23-26	Pounds {	M. F.	519 276	67 36	71 39	76 43	79 47	82 49	85 52	88 55	91 58	95 62	100 67	104 72
Swiftness of blow.	23-26	Feet per second {	M. F.	516 271	13.2 9.2	14.1 10.1	15.2 11.3	16.2 12.1	17.3 12.8	18.1 13.4	19.1 14.0	20.0 14.5	20.9 15.1	22.3 16.3	23.6 16.9
Sight, keenness of —by distance of reading diamond test-type ...	23-26	Inches {	M. F.	398 433	13 10	17 12	20 16	22 19	23 22	25 24	26 26	28 27	30 29	32 31	34 32

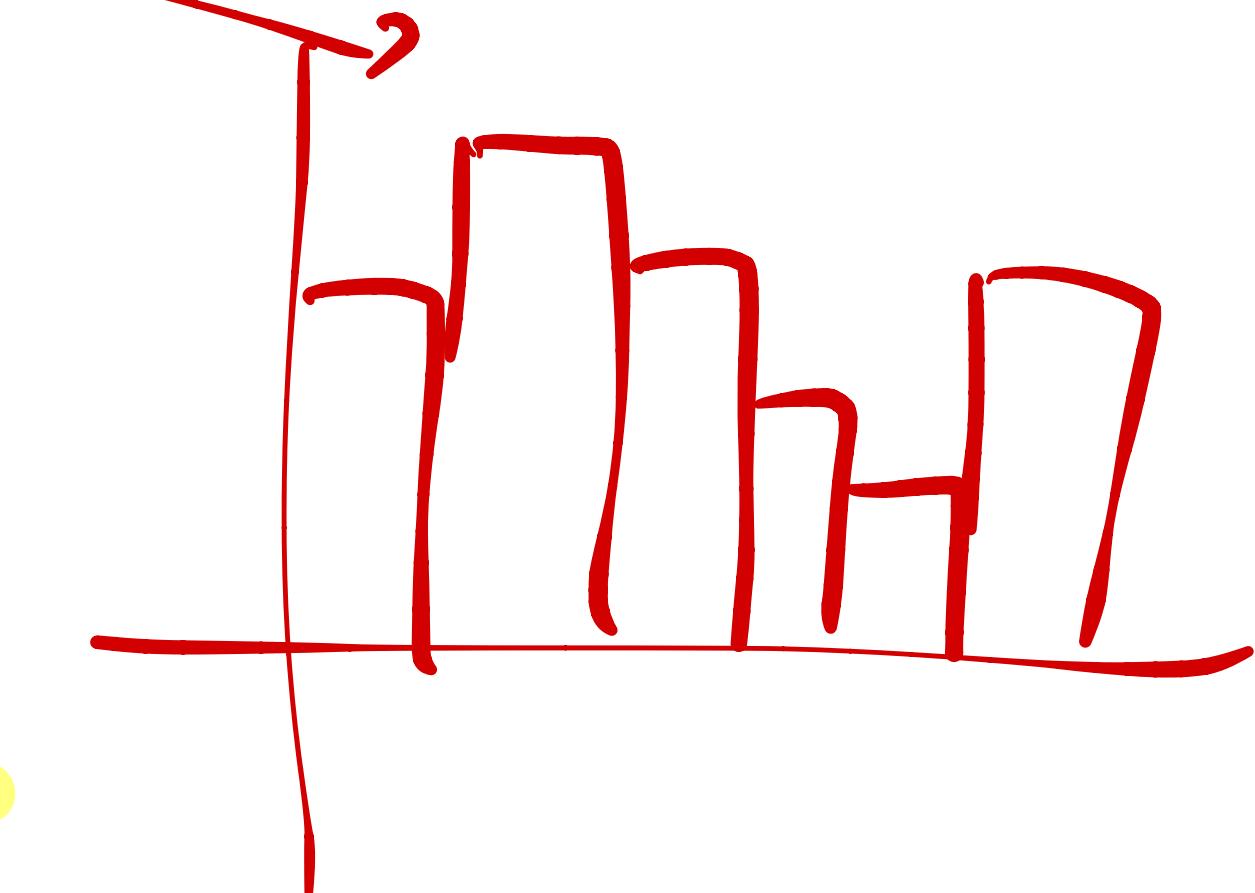
Poverty

TABLE A.

(A.) Pauperism. Per Cent.	(B.) No. of Unions.	(C.) Sums of B from top.	(D.) Successive tenths of the total of B.	(E.) D - C (in each row).	(F.) D - C multiplied into 0·5.	(G.) D - C × (0·5) and divided by B ₁ *.	Interpolated Deciles	
							Order.	Value (G + A)†
Below 1·75	1·75	7	7	—	—	—	—	—
1·75 to 2·25	2·25	7	14	—	—	—	—	—
2·25 „ 2·75	2·75	11	25	—	—	—	—	—
2·75 „ 3·25	3·25	21	46	59	13	6·5	0·23	1st 3·48
3·25 „ 3·75	3·75	28	74	—	—	—	—	—
3·75 „ 4·25	4·25	33	107	118	11	5·5	0·12	2nd 4·37
4·25 „ 4·75	4·75	46	153	176	23	11·5	0·21	3rd 4·96
4·75 „ 5·25	5·25	55	208	235	27	13·5	0·34	4th 5·59
5·25 „ 5·75	5·75	40	248	—	—	—	—	—
5·75 „ 6·25	6·25	45	293	294	1	0·5	0·01	5th 6·26
6·25 „ 6·75	6·75	44	337	353	16	8·0	0·23	6th 6·98
6·75 „ 7·25	7·25	35	372	412	40	20·0	0·45	7th 7·70
7·25 „ 7·75	7·75	44	416	—	—	—	—	—
7·75 „ 8·25	8·25	31	447	470	23	11·5	0·43	8th 8·68
8·25 „ 8·75	8·75	27	474	—	—	—	—	—
8·75 „ 9·25	9·25	34	508	—	—	—	—	—
9·25 „ 9·75	9·75	21	529	529	0	0·0	0·00	9th 9·75
9·75 „ 10·25	10·25	11	540	—	—	—	—	—
Above 10·25	10·25	48	588	—	—	—	—	—
		588	—	—	—	—	—	—

* B₁ in column G means the entry in column B that lies *one line below* that on which the entry in F is standing. Thus 6·5 is divided by 28, and 5·5 by 46.

† The second decimal is approximate.



Here is an example of how Galton applied his **method of deciles**. Let's see if we can understand how it works.

TABLE A.

(A.)	(B.)	(C.)	(D.)	(E.)	(F.)	(G.)	Interpolated Deciles	
Pauperism. Per Cent.	No. of Unions.	Sums of B from top.	Successive tenths of the total of B.	D - C (in each row).	D - C multiplied into 0.5.	D - C × (0.5) and divided by B ₁ *.	Order.	Value (G + A) †
Below 1.75 ...	7	7	—	—	—	—	—	—
1.75 to 2.25 ...	7	14	—	—	—	—	—	—
2.25 „ 2.75 ...	11	25	—	—	—	—	—	—
2.75 „ 3.25 ...	21	46	59	13	6.5	0.23	1st	3.48
3.25 „ 3.75 ...	28	74	—	—	—	—	—	—
3.75 „ 4.25 ...	33	107	118	11	5.5	0.12	2nd	4.37
4.25 „ 4.75 ...	46	153	176	23	11.5	0.21	3rd	4.96
4.75 „ 5.25 ...	55	208	235	27	13.5	0.34	4th	5.59
5.25 „ 5.75 ...	40	248	—	—	—	—	—	—
5.75 „ 6.25 ...	45	293	294	1	0.5	0.01	5th	6.26
6.25 „ 6.75 ...	44	337	353	16	8.0	0.23	6th	6.98
6.75 „ 7.25 ...	35	372	412	40	20.0	0.45	7th	7.70
7.25 „ 7.75 ...	44	416	—	—	—	—	—	—
7.75 „ 8.25 ...	31	447	470	23	11.5	0.43	8th	8.68
8.25 „ 8.75 ...	27	474	—	—	—	—	—	—
8.75 „ 9.25 ...	34	508	—	—	—	—	—	—
9.25 „ 9.75 ...	21	529	529	0	0.0	0.00	9th	9.75
9.75 „ 10.25 ...	11	540	—	—	—	—	—	—
Above 10.25 ...	48	588	—	—	—	—	—	—
		588	—	—	—	—	—	—

D - CB,

= fraction of
the next
bin to
"cover"

0.5 = size
of bin

* B₁ in column G means the entry in column B that lies *one line below* that on which the entry in F is standing. Thus 6.5 is divided by 28, and 5.5 by 46.

† The second decimal is approximate.

height	count	cumulative counts
52-56	4	4
56-60	8	12
60-64	12	24
64-68	15	39
68-72	12	51
72-76	8	59
76-80	1	60
		60

Suppose we want to find quartiles.

60 numbers total

→ # at position 15

→ # at position 30

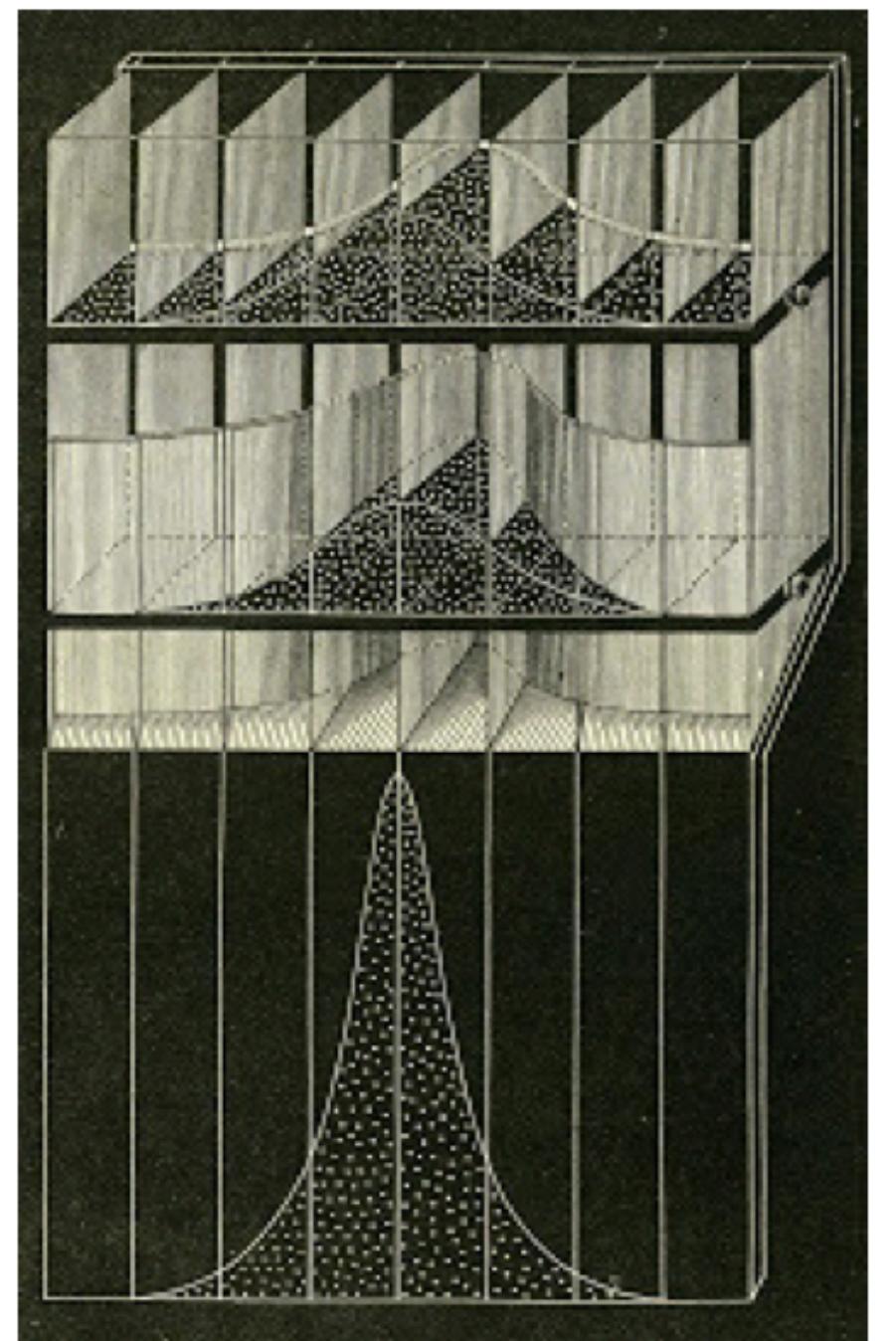
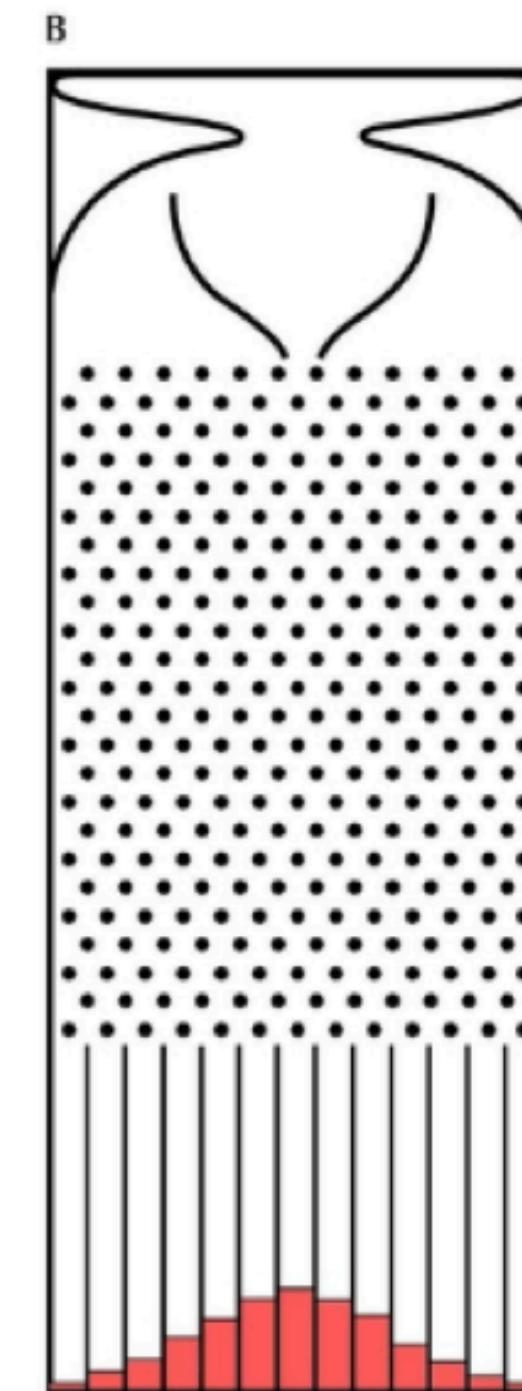
→ # at position

45

$$60 + \left(\frac{15 - 12}{12} \right) 4 = 60 + \frac{1}{4} \cdot 4 = 61$$

Human characteristics are “normally” distributed

- While he did not derive the normal distribution (Gauss did), Galton was the first to call it by the name “normal” distribution, rather than the name “error distribution”.
- He observed that many human characteristics, such as human height, roughly follow a **normal** distribution.
- In order to demonstrate why this is the case, he constructed what is known as a **quincru**x.
- See an animated quincru [here](#).



Heights

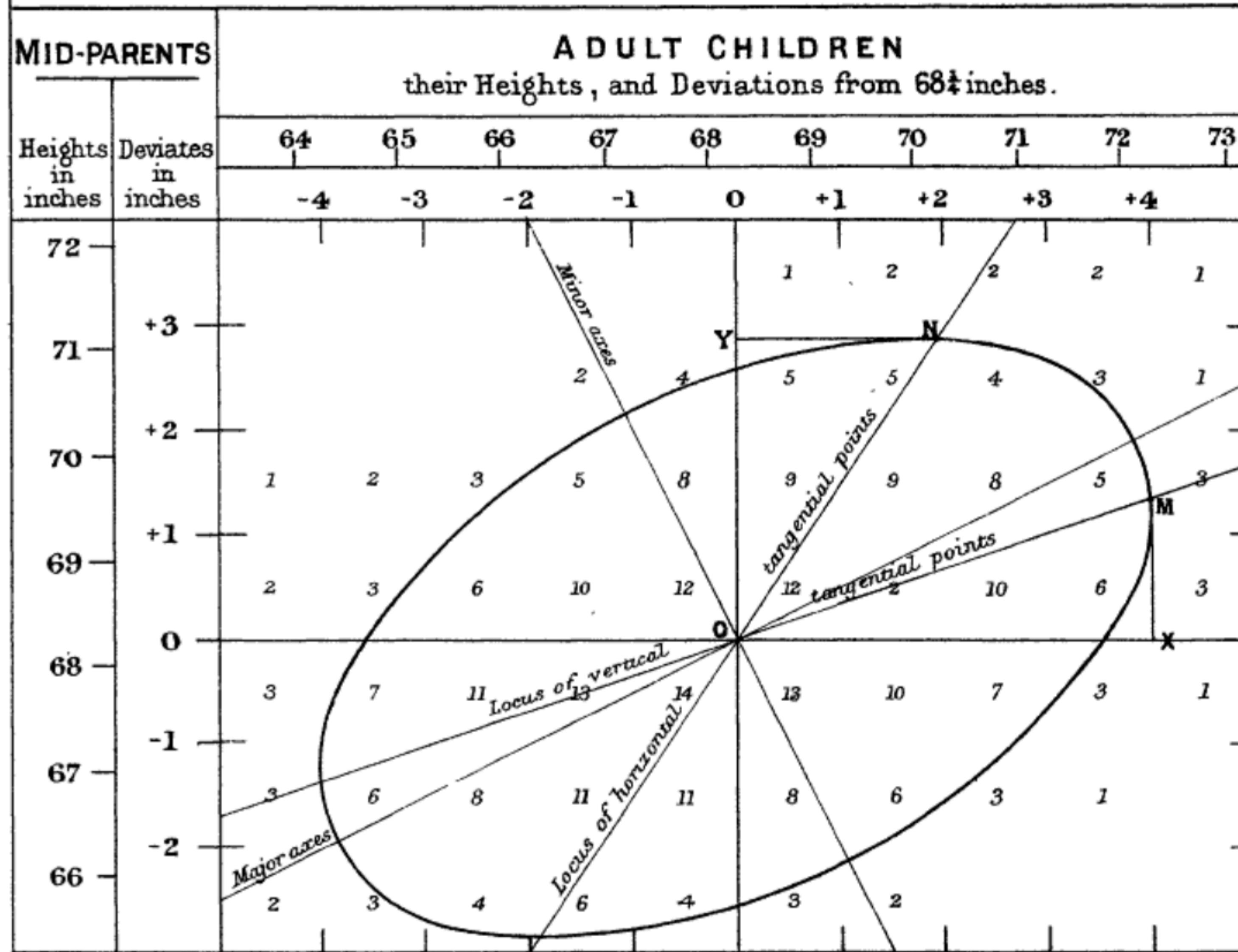
- One trait Galton was interested in studying was the difference in heights between parents and their children.
- He defined a new quantity, “midparent height”, as being the average of a child’s mother’s and father’s heights, after the mother’s height was multiplied by 1.08.
 - He also multiplied the heights of daughters by 1.08.
- After collecting data, he estimated that the **correlation** between the **deviations of midparent heights** and the **deviations of child heights** was $\frac{2}{3}$.

TABLE I.
NUMBER OF ADULT CHILDREN OF VARIOUS STATURES BORN OF 205 MID-PARENTS OF VARIOUS STATURES.
(All Female heights have been multiplied by 1·08).

Heights of the Mid- parents in inches.	Heights of the Adult Children.														Total Number of		Medians.	
	Below	62·2	63·2	64·2	65·2	66·2	67·2	68·2	69·2	70·2	71·2	72·2	73·2	Above	Adult Children.	Mid- parents.		
Above	1	3	4	4	5	..	
72·5	1	2	1	2	7	2	4	19	6	72·2	
71·5	1	3	4	3	5	10	4	9	2	2	43	11	69·9	
70·5	1	..	1	..	1	1	3	12	18	14	7	4	3	3	68	22	69·5	
69·5	1	16	4	17	27	20	33	25	20	11	4	5	183	41	68·9	
68·5	1	..	7	11	16	25	31	34	48	21	18	4	3	..	219	49	68·2	
67·5	..	3	5	14	15	36	38	28	38	19	11	4	211	33	67·6	
66·5	..	3	3	5	2	17	17	14	13	4	78	20	67·2	
65·5	1	..	9	5	7	11	11	7	7	5	2	1	66	12	66·7	
64·5	1	1	4	4	1	5	5	..	2	23	5	65·8	
Below	..	1	..	2	4	1	2	2	1	1	14	1	..	
Totals	..	5	7	32	59	48	117	138	120	167	99	64	41	17	14	928	205	..
Medians	66·3	67·8	67·9	67·7	67·9	68·3	68·5	69·0	69·0	70·0

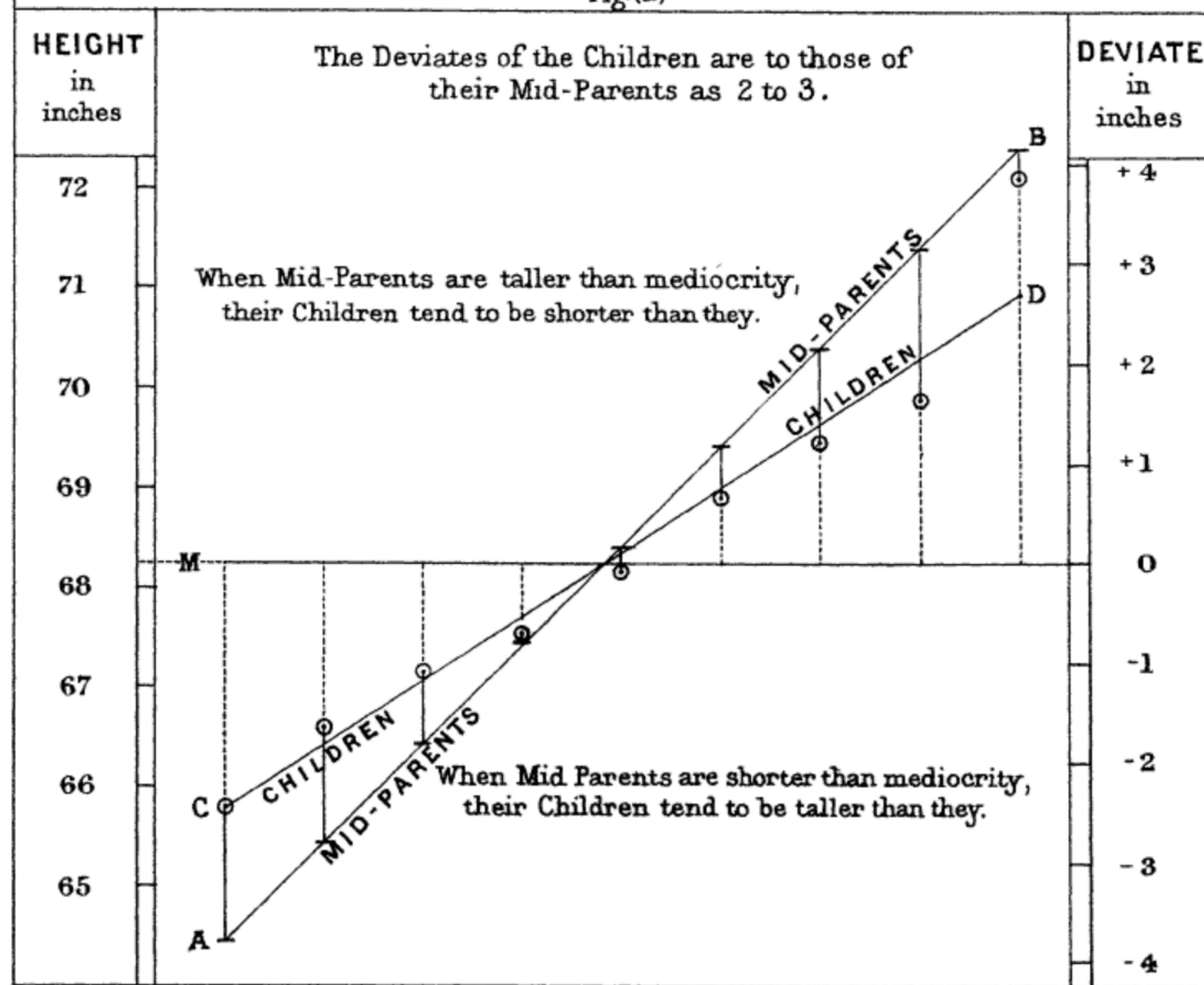
NOTE.—In calculating the Medians, the entries have been taken as referring to the middle of the squares in which they stand. The reason why the headings run 62·2, 63·2, &c., instead of 62·5, 63·5, &c., is that the observations are unequally distributed between 62 and 63, 63 and 64, &c., there being a strong bias in favour of integral inches. After careful consideration, I concluded that the headings, as adopted, best satisfied the conditions. This inequality was not apparent in the case of the Mid-parents.

DIAGRAM BASED ON TABLE I.
 (all female heights are multiplied by 1.08)



RATE OF REGRESSION IN HEREDITARY STATURE.

Fig.(a)



and breadth (0·45). The concluding passage of the memoir is worth citing for its historical interest :—“The prominent characteristics of any two correlated variables, so far at least as I have as yet tested them, are four in number. It is supposed that their respective measures have been first transmuted into others of which the unit is in each case equal to the probable error of a single measure in its own series. Let y = the deviation of the subject, whichever of the two variables may be taken in that capacity; and let $x_1, x_2, x_3, \&c.$, be the corresponding deviations of the relative, and let the mean of these be X . Then we find (1) that $y = rX$ for all values of y , (2) that r is the same whichever of the two variables is taken for the subject, (3) that r is always less than 1, (4) that r measures the closeness of the co-relation.” Galton determined r by a simple graphic method,

TABLE OF DATA FOR CALCULATING TABLES OF DISTRIBUTION OF
STATURE AMONG THE KINSMEN OF PERSONS WHOSE STATURE IS
KNOWN.

From group of persons of the same Stature, to their Kinsmen in various near degrees.	Mean regression= w .	$Q = f$ $= p \times \sqrt{(1 - w^2)}$.
Mid-parents to Sons	2 / 3	1.27
Brothers to Brothers	2 / 3	1.27
Fathers or Sons to } Sons or Fathers }	1 / 3	1.60
Uncles or Nephews to } Nephews or Uncles }	2 / 9	1.66
Grandsons to Grandparents...	1 / 9	{ Practically that of Popu- lation, or 1.7 inch.
Cousins to Cousins	2 / 27	

Regression to the mean

- The effect that Galton observed was that **children tended to have heights that were closer to average than their parents.**
 - Tall parents tended to have children that were still tall, but closer to the average child's height.
 - Short parents tended to have children that were still short, but closer to the average child's height.
 - The same effect holds true in the opposite direction – remember, the correlation coefficient is symmetric!
- He called this “**reversion** to the mean”, and later “**regression** to the mean”.
- **The presence of regression to the mean depends on random variability in the distributions from which observations are drawn.**

Pearson

- Karl Pearson (1857-1936), a British statistician, was one of Galton's disciples.
 - He was also a staunch eugenicist.
 - He further developed the theory of correlation, and defined the correlation coefficient as we know it now.
- He founded the world's first Statistics department, at University College London, in 1911.
 - Started as part of UCL's Eugenics department.
 - Fun fact: UCSD has the world's first Cognitive Science department!

Summary, next time

Summary, next time

- Both Legendre and Gauss developed the theory of least squares, but Gauss tied it to probability theory.
 - Both used least squares in the development of planetary models.
- Quetelet was one of the first to apply tools from statistics to the social sciences, and was interested in studying the composition of the “average man”.
- Galton pioneered many now-ubiquitous ideas in statistics, including that of the percentile and the term “regression”.
 - He was motivated by the study of inheritance, and more specifically **eugenics**.