

Computational Physics 2022

Sommersemester, 3th April, 2023 – 14th Juli, 2023

1)Introduction

2)Numbers and errors

3)Differentiation and integration

4)Ordinary differential equations

5)Molecular dynamics simulations

6)Partial differential equations

7)Iteration processes

8)Matrixdiagonalisation & Eigenvalue problems

9)Minimization

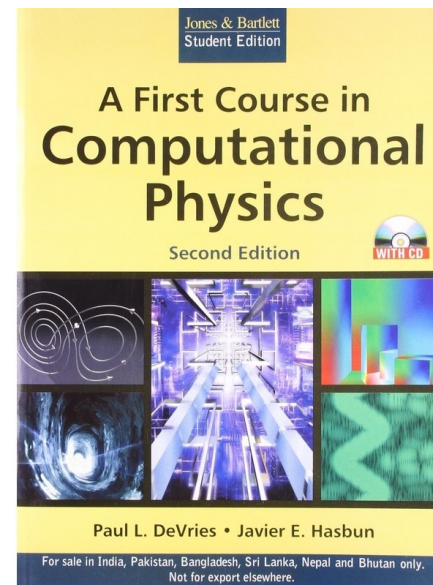
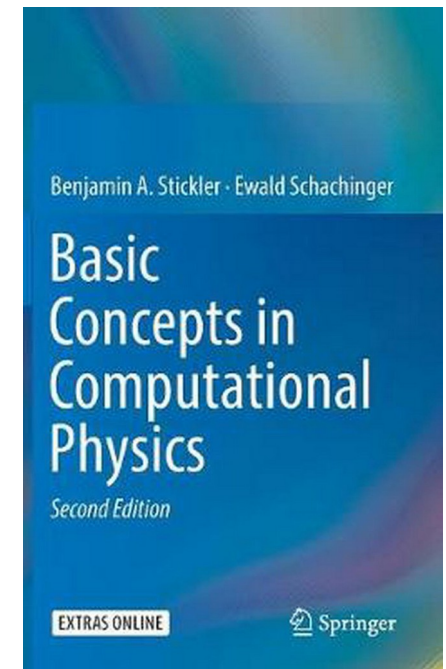
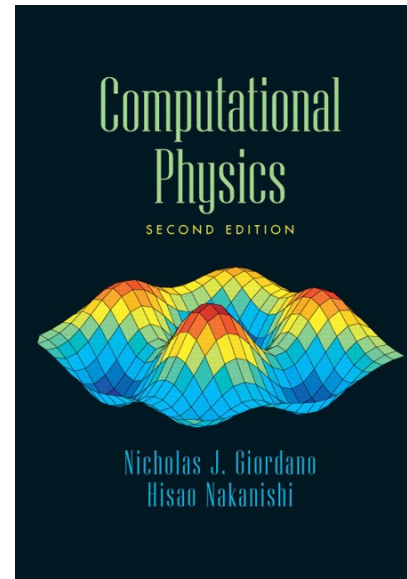
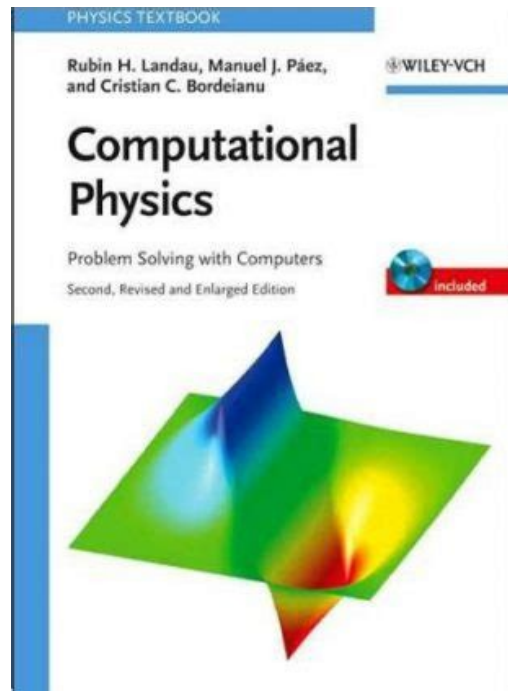
10) Random numbers

11) Monte Carlo (MC) Simulations

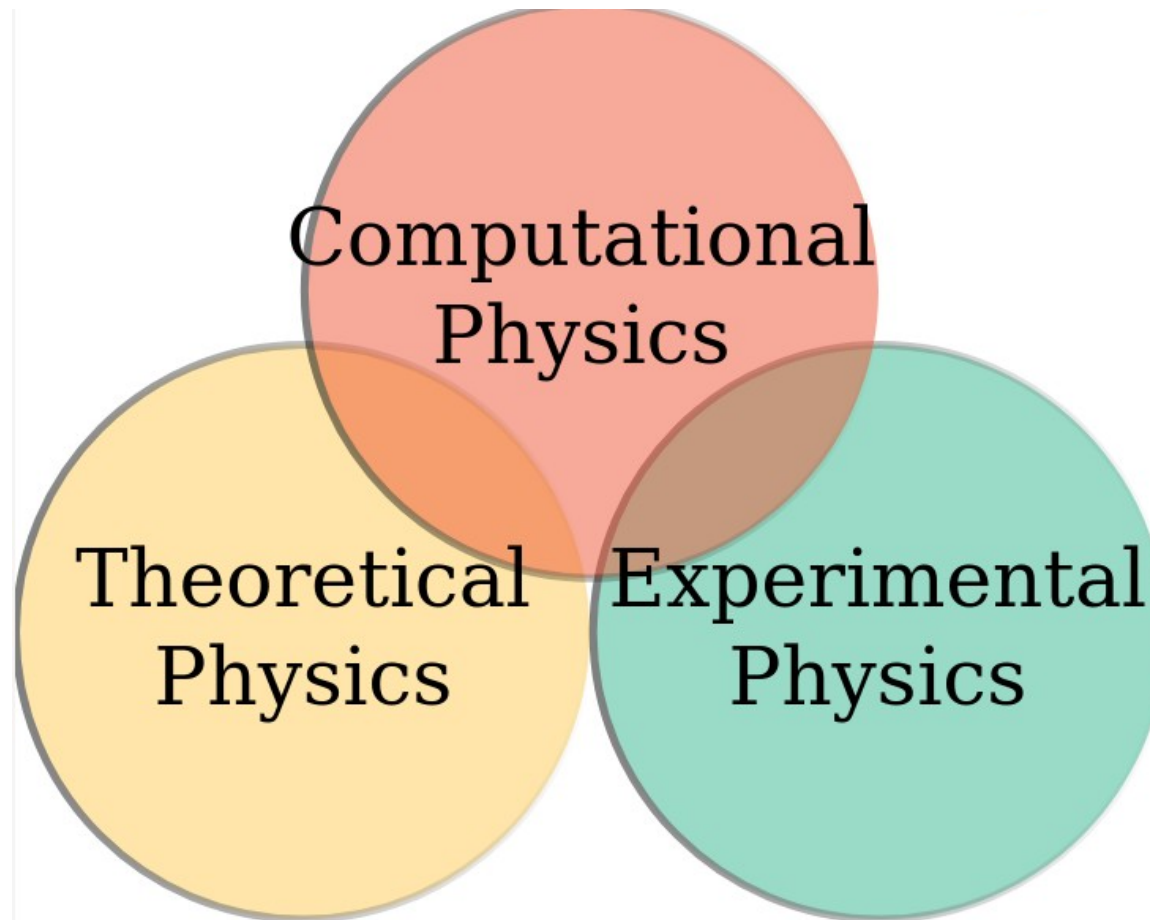
12)Perkolation ~

13)Stochastic Dynamics?

Introduction: Computational Physics



Introduction: Computational Physics



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The word "computer" was first used in 1613 in the book *The Yong Mans Gleanings* by Richard Braithwaite and originally described a human who performed calculations or computations.

The definition of a computer remained the same until the end of the 19th century, when the industrial revolution gave rise to mechanical machines whose primary purpose was calculating.



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~100 B.C.!!!!

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Decoding the ancient Greek astronomical calculator known as the Antikythera Mechanism

[T. Freeth](#), [Y. Bitsakis](#), [X. Moussas](#), [J. H. Seiradakis](#), [A. Tselikas](#), [H. Mangou](#), [M. Zafeiropoulou](#), [R. Hadland](#),
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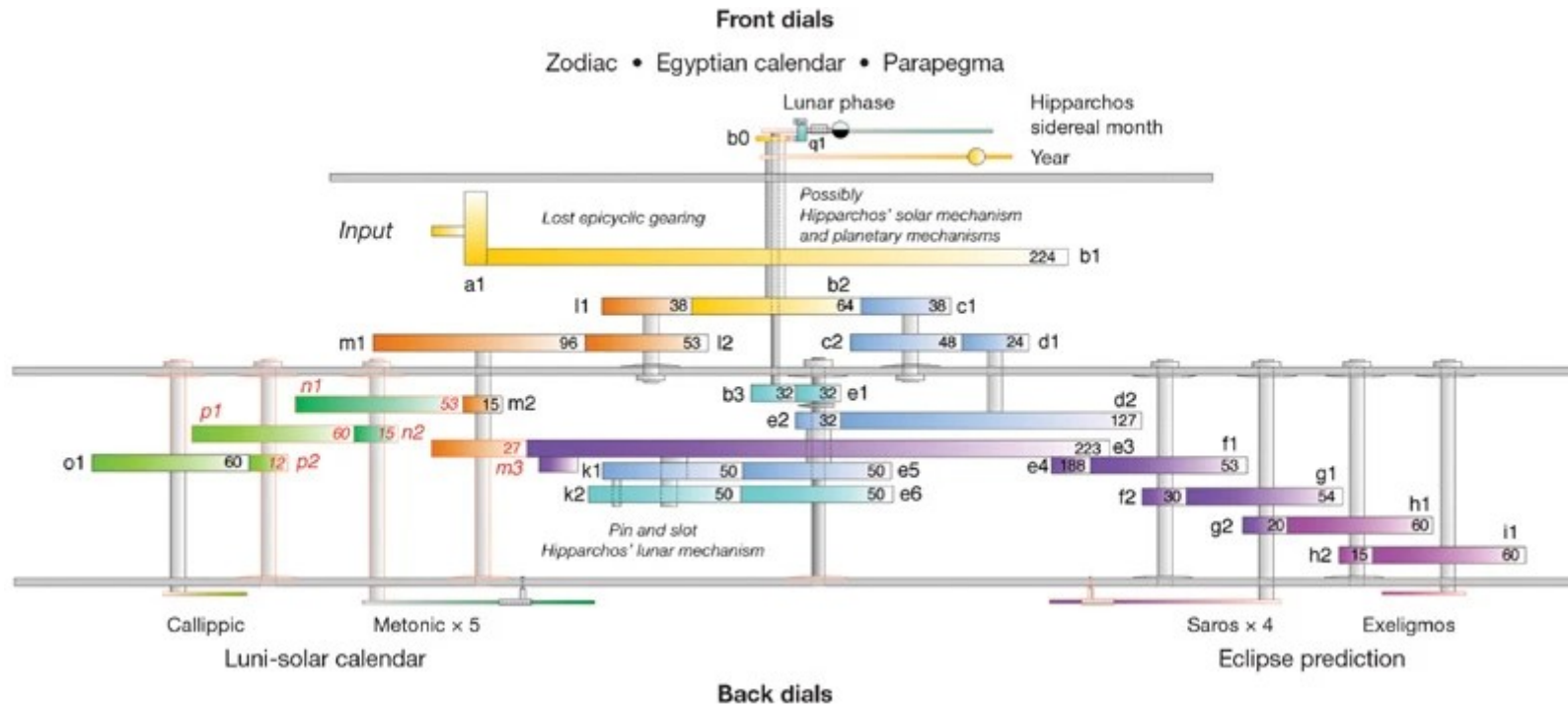
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“Can predict [astronomical](#) positions and [eclipses](#) decades in advance”

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“technically more complex than any known device for at least a millennium afterwards.”



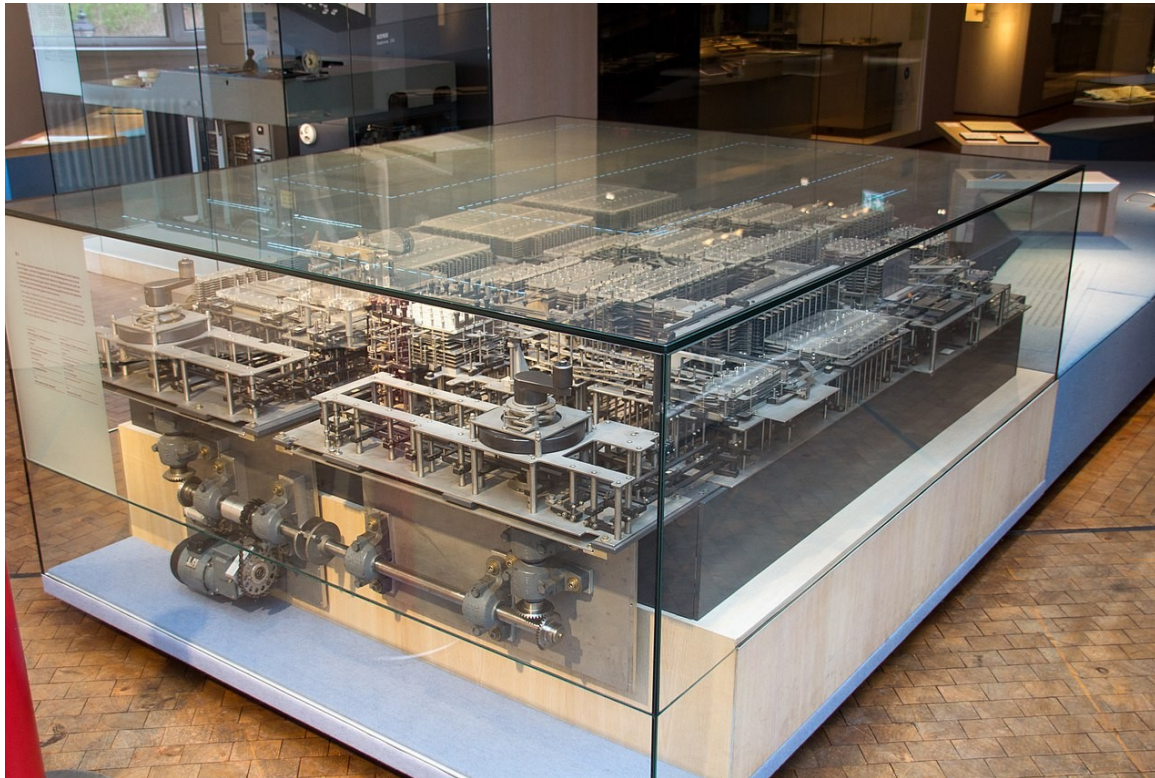
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The Antikythera Mechanism: known gears and accuracy of computation

Gear name ^[table 1]	Function of the gear/pointer	Expected simulated interval of a full circular revolution	Mechanism formula ^[table 2]	Computed interval	Gear direction ^[table 3]
x	Year gear	1 tropical year	1 (by definition)	1 year (presumed)	cw ^[table 4]
b	the Moon's orbit	1 sidereal month (27.321661 days)	$\text{Time}(b) = \text{Time}(x) * (c1 / b2) * (d1 / c2) * (e2 / d2) * (k1 / e5) * (e6 / k2) * (b3 / e1)$	27.321 days ^[table 5]	cw
r	lunar phase display	1 synodic month (29.530589 days)	$\text{Time}(r) = 1 / (1 / \text{Time}(b2 \text{ [mean sun] or sun3 [true sun]}) - (1 / \text{Time}(b)))$	29.530 days ^[table 5]	
n*	Metonic pointer	Metonic cycle () / 5 spirals around the dial = 1387.94 days	$\text{Time}(n) = \text{Time}(x) * (l1 / b2) * (m1 / l2) * (n1 / m2)$	1387.9 days	ccw ^[table 6]
o*	Games dial pointer	4 years	$\text{Time}(o) = \text{Time}(n) * (o1 / n2)$	4.00 years	cw ^{[table 6][table 7]}
q*	Callippic pointer	27758.8 days	$\text{Time}(q) = \text{Time}(n) * (p1 / n3) * (q1 / p2)$	27758 days	ccw ^[table 6]
e*	lunar orbit precession	8.85 years	$\text{Time}(e) = \text{Time}(x) * (l1 / b2) * (m1 / l2) * (e3 / m3)$	8.8826 years	ccw ^[table 8]
g*	Saros cycle	Saros time / 4 turns = 1646.33 days	$\text{Time}(g) = \text{Time}(e) * (f1 / e4) * (g1 / f2)$	1646.3 days	ccw ^[table 6]
i*	Exeligmos pointer	19755.8 days	$\text{Time}(i) = \text{Time}(g) * (h1 / g2) * (i1 / h2)$	19756 days	ccw ^[table 6]
The following are proposed gearing from the 2012 Freeth and Jones reconstruction:					
sun3*	True sun pointer	1 mean year	$\text{Time}(\text{sun3}) = \text{Time}(x) * (\text{sun3} / \text{sun1}) * (\text{sun2} / \text{sun3})$	1 mean year ^[table 5]	cw ^[table 9]
mer2*	Mercury pointer	115.88 days (synodic period)	$\text{Time}(\text{mer2}) = \text{Time}(x) * (\text{mer2} / \text{mer1})$	115.89 days ^[table 5]	cw ^[table 9]
ven2*	Venus pointer	583.93 days (synodic period)	$\text{Time}(\text{ven2}) = \text{Time}(x) * (\text{ven1} / \text{sun1})$	584.39 days ^[table 5]	cw ^[table 9]
mars4*	Mars pointer	779.96 days (synodic period)	$\text{Time}(\text{mars4}) = \text{Time}(x) * (\text{mars2} / \text{mars1}) * (\text{mars4} / \text{mars3})$	779.84 days ^[table 5]	cw ^[table 9]
jup4*	Jupiter pointer	398.88 days (synodic period)	$\text{Time}(\text{jup4}) = \text{Time}(x) * (\text{jup2} / \text{jup1}) * (\text{jup4} / \text{jup3})$	398.88 days ^[table 5]	cw ^[table 9]
sat4*	Saturn pointer	378.09 days (synodic period)	$\text{Time}(\text{sat4}) = \text{Time}(x) * (\text{sat2} / \text{sat1}) * (\text{sat4} / \text{sat3})$	378.06 days ^[table 5]	cw ^[table 9]

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Z1 Konrad Zuse (1936-1937)



“..a binary electrically driven mechanical calculator with limited programmability, reading instructions from punched celluloid film.

The “Z1” was the first freely programmable computer in the world which used [Boolean logic](#) and binary [floating-point numbers](#), however it was unreliable in operation”

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1982 (64kB memory, BASIC)

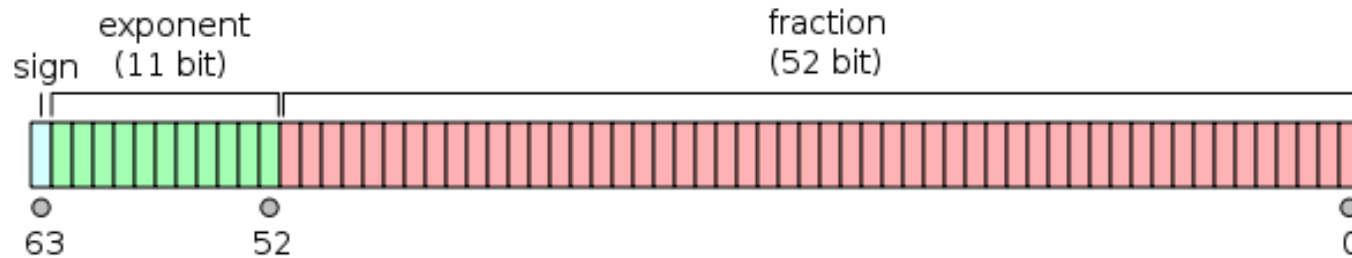
“It has been listed in the [Guinness World Records](#) as the highest-selling single computer model of all time”



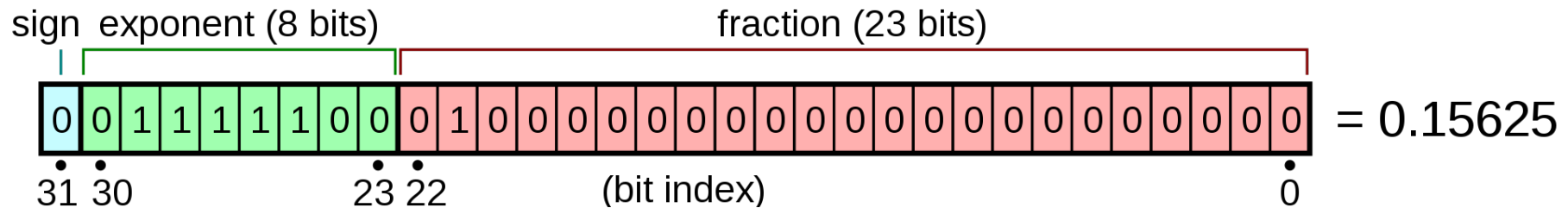
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IEEE Standard for Floating-Point Arithmetic

64 bits



32 bits



Computational Physics 2022

Sommersemester, 4th April, 2022 – 15th Juli, 2022

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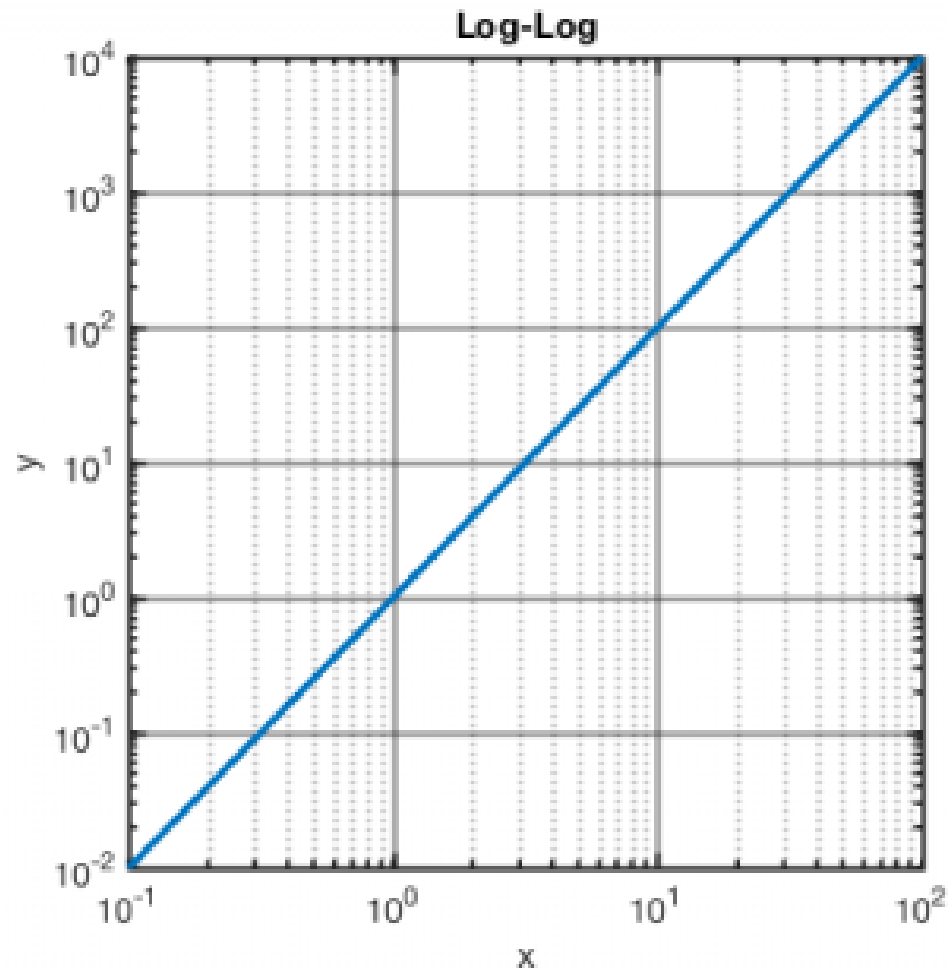
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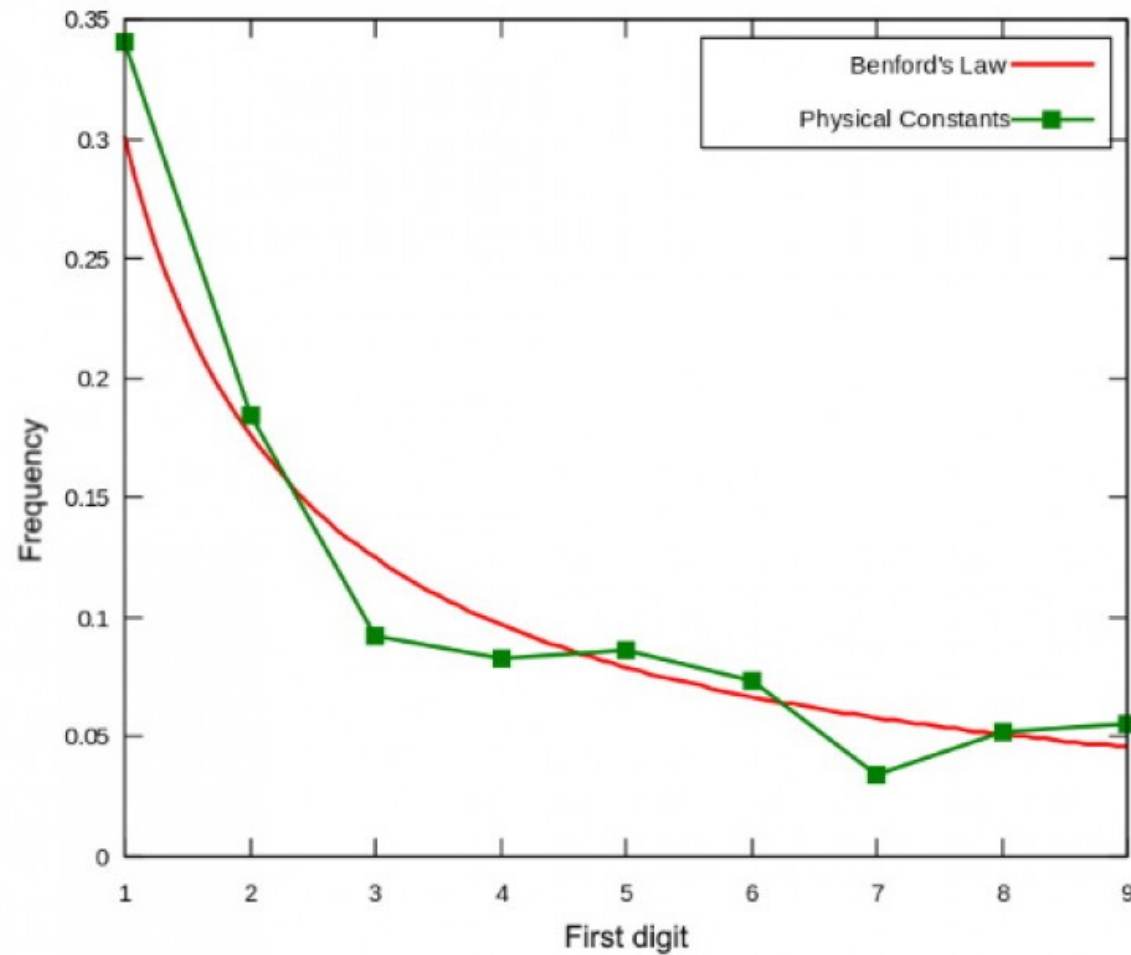
12) Perkolations

13) Stochastic Dynamics

Numbers & Errors : Benford's Law



Numbers & Errors : Benford's Law



Numbers & Errors : Benford's Law

Original Articles

A first-digit anomaly in the 2009 Iranian presidential election

Boudewijn F. Roukema 

Pages 164-199 | Received 23 Nov 2012, Accepted 24 Aug 2013, Published online: 18 Oct 2013

 Download citation  <https://doi.org/10.1080/02664763.2013.838664>

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Abstract

A local bootstrap method is proposed for the analysis of electoral vote-count first-digit frequencies, complementing the Benford's Law limit. The method is calibrated on five presidential-election first rounds (2002–2006) and applied to the 2009 Iranian presidential-election first round. Candidate K has a highly significant ($p < 0.15\%$) excess of vote counts starting with the digit 7. This leads to other anomalies, two of which are individually significant at $p \sim 0.1\%$ and one at $p \sim 1\%$. Independently, Iranian pre-election opinion polls significantly reject the official results unless the five polls favouring candidate A are considered alone. If the latter represent normalised data and a linear, least-squares, equal-weighted fit is used, then either candidates R and K suffered a sudden, dramatic ($70\% \pm 15\%$) loss of electoral support just prior to the election, or the official results are rejected ($p \sim 0.01\%$).

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Numbers & Errors : Benford's Law

2. Method. Benford's Law (Newcomb 1881; Benford 1938) for the relative frequency of the occurrence of the first digit i in a set of real numbers

$$(1) \quad f(i) = \log_{10} \left(1 + \frac{1}{i} \right)$$

should be valid for real world samples that can be considered approximately uniform over several orders of magnitude.¹ The degree to which this assumption is accurate depends on the degree to which

$$(2) \quad \{\log_{10} v_j - \lfloor \log_{10} v_j \rfloor\},$$

i.e. the folding of a sample $\{v_j\}$ to a single decade, is uniform, where $\lfloor x \rfloor$ is the greatest integer $\leq x$. This illustrates why data sets do not necessarily need to span many orders of magnitude in order to approximately satisfy Benford's Law. The most striking characteristic follows from Eq. (1): the first digit is 1 with a frequency of $\log_{10} 2 \approx 30\%$, i.e. much more frequently than any other digit.

Mebane (Mebane 2009) has pointed out that use of Benford's Law for distributions of the first digit is problematic. Hence, in order to apply an equivalent probability distribution to Benford's Law, an empirical version of the law can be constructed as follows. Let the total numbers of votes in voting area j be v_j and the global fraction of votes received by candidate $X = A, R, K, \text{ and } M$ be $\alpha_X = (\sum v_{Xj}) / (\sum v_j)$, where v_{Xj} is the vote count for candidate X in the j -th voting area. If voters in different areas vote fractionally in exactly identical ways independently of geography, then the distributions of first digits should follow the total vote

counts, apart from a constant logarithmic shift. That is, let us define $f_X(i)$ as the relative frequency of the digit i in the set of digits

$$(3) \quad \{\lfloor 10^{\log_{10}(\alpha_X v_j) - \lfloor \log_{10}(\alpha_X v_j) \rfloor} \rfloor\}.$$

¹Powers of 10.

Numbers & Errors : Benford's Law

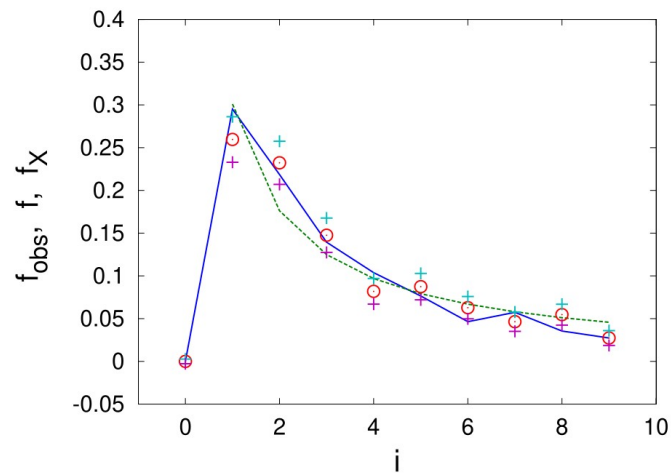


FIG 4. As for Fig. 3, for candidate A vote counts only.

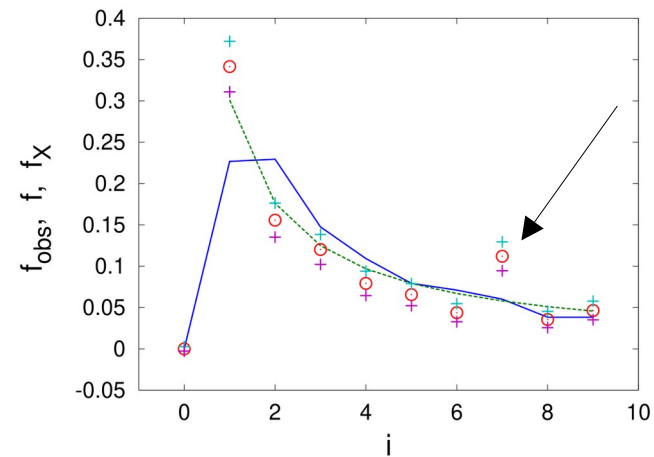
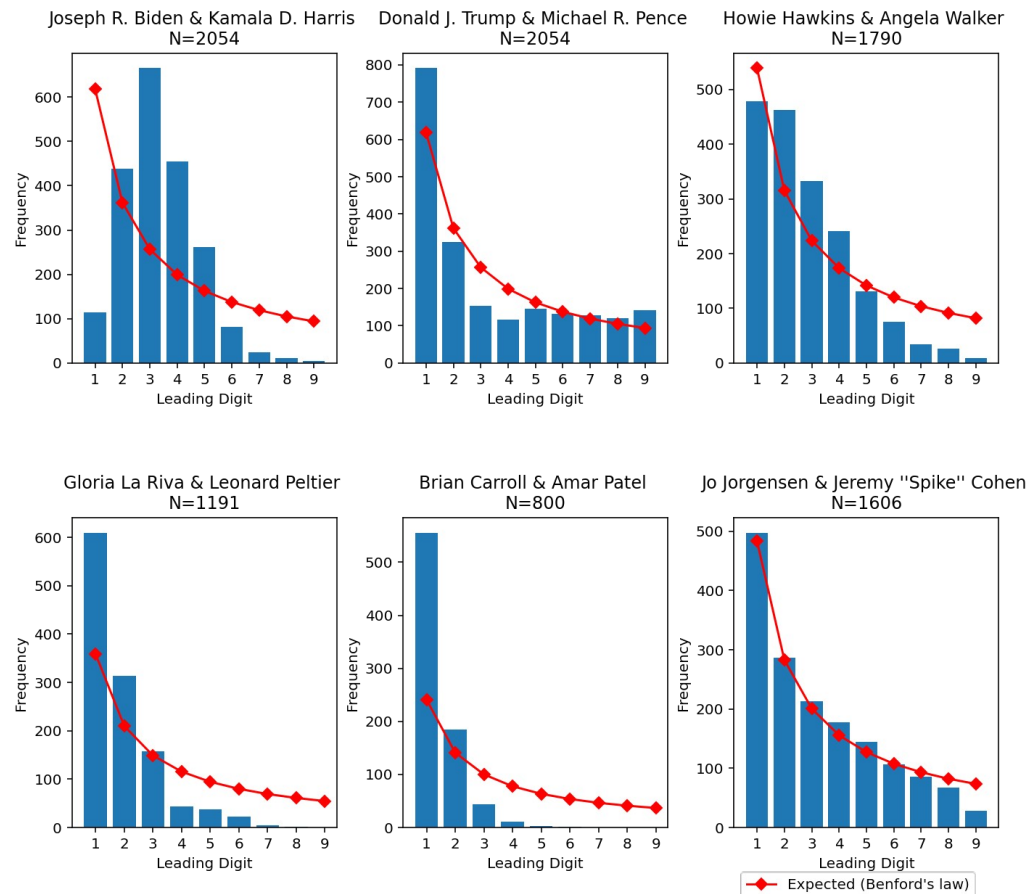


FIG 6. As for Fig. 4, for candidate K. The excess number of 7's is about 3 standard deviations in excess of the expected values for both the idealised and empirical Benford's Laws.

Numbers & Errors : Benford's Law

Chicago



“Benford's law has also been misapplied to claim election fraud. When applying the law to [Joe Biden's](#) election returns for [Chicago](#), [Milwaukee](#), and other localities in the [2020 United States presidential election](#), the distribution of the first digit did not follow Benford's law. The misapplication was a result of looking at data that was tightly bound in range, which violates the assumption inherent in Benford's law that the range of the data be large”