Discoveries in Experimental Mathematics

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Mathematical Discovery

- Where do theorems come from?
- We are never taught this. We learn to prove theorems, not invent them
- Some theorems are easy to conjecture and easy to prove
  - $\sqrt{2}$ is irrational (not a fraction, known to Plato, 360 B.C.)
- Theorem easy to conjecture, hard to prove (hundreds of years)
  - Four-color theorem (124 years)
  - Fundamental theorem of algebra (every non-constant polynomial has at least one zero). Took 180 years.
  - Fermat's last theorem (357 years)

Mathematical Discovery

- Difficult to conjecture; easy to prove
  - Hadamard three-circles theorem
- Difficult to invent; difficult to prove
  - Gödel's Theorem (there are theorems, i.e., true statements, which have no proof)
  - Riemann hypothesis

Outline

- The problem
  - Closed-form expression for $\zeta(3) = \sum_{k=1}^{\infty} \frac{1}{k^3} \approx 1.2020569031...$
- The approach
  - Build a catalog of real-valued expressions indexed by first 20 digits
  - Equivalent expressions will "collide"
  - Look up 1.2020569031595942853
- The discoveries
  - The Partial Sum Theorem
  - Overcounting functions
  - How many ways can *n* be expressed as an integer power k^j?
  - Expression for $\sum_{k=1}^{\infty} \frac{1}{2^{2^k}}$
  - . . .

The Problem

- Find a closed form expression for odd values of the zeta function:

$$\zeta(s) = \sum_{k=1}^{\infty} \frac{1}{k^s}$$

- In 1739, Euler found an expression for all even values of *s* and showed that:

$\zeta(2s)$ is a rational multiple of π^{2s}

$$\zeta(2) = \sum_{k=1}^{\infty} \frac{1}{k^2} = \frac{1}{6}\pi^2; \qquad \zeta(4) = \sum_{k=1}^{\infty} \frac{1}{k^4} = \frac{1}{90}\pi^4$$

- BUT: no expression is known for even a single odd value, e.g.

$$\zeta(3) = \sum_{k=1}^{\infty} \frac{1}{k^3}$$

(this is the only odd value even known to be irrational)

Concept of the Catalog

$$1.0000009539\ 6203387279\ 41 \approx \zeta(20) = \frac{176411\,\pi^{20}}{1531329465\ 290625}$$

$$1.08232323\ 3711138191\ 5160 \approx \zeta(4) = \frac{\pi^4}{90}$$

$$1.20202249\ 1761611317\ 1527 \approx \frac{1}{2Catalan - 1}$$

$$1.20205690\ 3159594285\ 3997 \approx \zeta(3) = \ ?$$

$$1.64493406\ 6848226436\ 4724 \approx \zeta(2) = \frac{\pi^2}{6}$$

$$0.91596559\ 4177219015\ 05 \approx Catalan = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)^2}$$

Other Catalogs

- Sloane's Encyclopedia of Integer Sequences
  – Terrific, but for integer sequences, not reals
- Plouffe's Inverter
  – Huge (215 million entries), but not "natural" expressions from actual mathematical work
- Simon Fraser Inverse Symbolic Calculator
  – 50 million constants

Discovery A

$$\sum_{k=1}^{\infty} \frac{\pi(k)}{2^k} = 2 \sum_{p\ prime}^{\infty} \frac{1}{2^p}$$

where $\pi(k)$ is the number of primes $\leq k$

- Is this a coincidence?
- Why the factor of 2?
- Is there a general principle at work?
  – In fact,

$$\sum_{k=1}^{\infty} \frac{\pi(k)}{a^k} = \frac{a}{a-1} \sum_{p\ prime}^{\infty} \frac{1}{a^p}$$

Observation

$\pi(k)$ is a partial sum function, i.e., $\pi(k) = \sum_{\substack{p\ prime \\ p \le k}} 1$

More generally, $\pi(k)$ is the partial sum function of the indicator function of the property "primeness":

$$\pi(k) = \sum_{j=1}^{k} I_{prime}(j), \quad where \quad I_{prime}(j) = \begin{cases} 1, & j\ prime \\ 0, & otherwise \end{cases}$$

So $\sum_{k=1}^{\infty} \frac{\pi(k)}{2^k} = 2 \sum_{p\ prime} \frac{1}{2^p} = \sum_{p\ prime} \frac{1}{2^{p-1}}$ can be rewritten as:

$$\sum_{k=1}^{\infty} \pi(k) f(k) = \sum_{p\ prime} g(k) = \sum_{k=1}^{\infty} I_{prime}(k) g(k)$$

where f and g are "related"

The Partial Sum Theorem (New)

- Given a sequence *S* of complex numbers *s*(*k*), let $t(n) = \sum_{k=1}^{n} s(k)$ be the sequence of partial sums of S.
- Given a function *f*, if certain convergence criteria are satisfied, then

$$\sum_{k=1}^{\infty} t(k) f(k) = \sum_{j=1}^{\infty} s(j) g(j)$$

PARTIAL TAILS OF *f*(*k*)

PARTIAL SUMS OF *s*(*j*)

where

$$g(j) = \sum_{k=j}^{\infty} f(k)$$

(the partial tails of *f*) is a transform of *f* independent of *s* & *t*

Partial Sum Functions

- Many sequences are partial sum functions:

$$H(n) = \sum_{k=1}^{n} \frac{1}{k}$$ **the harmonic function**

$$H^{(s)}(n) = \sum_{k=1}^{n} \frac{1}{k^s}$$ **generalized harmonic function**

$$1 - 2^{-n} = \sum_{k=1}^{n} \frac{1}{2^n}$$

$$6 - \frac{n^2 + 4n + 6}{2^n} = \sum_{k=1}^{n} \frac{k^2}{2^k}$$

$$\log \Gamma(n) = \sum_{k=1}^{n} \log k$$

- Actually, every sequence is the partial sum function of some other sequence

Some Partial Sum Transforms

$f(k) \Leftrightarrow$	$g(j) = \sum_{k=j}^{\infty} f(k)$	$f(k) \Leftrightarrow$	$g(j)$
$\frac{1}{a^k}$	$\frac{1}{(a-1)a^{j-1}}$	$\frac{1}{k!}$	$e\left(1 - \frac{\Gamma(j,1)}{\Gamma(j)}\right)$
$\frac{1}{k^2+k}$	$\frac{1}{j}$	$\frac{k^2+k-1}{(k+2)!}$	$\frac{j}{(j+1)!}$
$\frac{1}{k^3-k}$	$\frac{1}{2j(j-1)}$	$\frac{\sin k}{a^k}$	$\frac{\sin(1-j) + a \sin j}{a^{j-1}\left(1+a^2-2a\cos 1\right)}$
$\frac{(-1)^k}{k^2-1}$	$\frac{(-1)^j}{2j(j-1)}$	$\frac{1}{k\,a^k}$	$\beta\left(\frac{1}{a}, j, 0\right)$
$\prod_{i=0}^{n} \frac{1}{(k+i)}$	$\frac{1}{n-1}\left(\sum_{i=1}^{n} (-1)^i S_1(n,i)\, j^{i-1}\right)^{-1}$	$\frac{1}{\binom{2k}{k}}$	$\frac{\sqrt{\pi}\,\Gamma(j)}{4^j\,\Gamma(j+½)}\, {}_2F_1\left(1, j+1, j+½, ¼\right)$

Partial Sum Theorem (Proof)

- Consider the upper triangular matrix $m_{i,j} = s(i)f(j), \quad i \le j$:

$$\begin{pmatrix} s(1)f(1) & s(1)f(2) & s(1)f(3) & s(1)f(4) & s(1)f(5) & \cdots \\ 0 & s(2)f(2) & s(2)f(3) & s(2)f(4) & s(2)f(5) & \\ 0 & 0 & s(3)f(3) & s(3)f(4) & s(3)f(5) & \cdots \\ 0 & 0 & 0 & s(4)f(4) & s(4)f(5) & \\ 0 & 0 & 0 & 0 & s(5)f(5) & \\ 0 & 0 & 0 & 0 & 0 & \\ 0 & 0 & & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

TAILS OF *f* = *g(j)*

Row sums are $\sum s(j)g(j)$

HEADS OF s = *t(i)*

Column sums are $\sum t(k)f(k)$

The Convergence Criteria

$$\sum_{k=1}^{\infty} t(k)f(k) = \sum_{k=1}^{\infty} s(k)g(k) \quad \text{iff}$$

1. All sums *g*(*k*) converge
2. $\sum_{k=1}^{\infty} s(k)g(k)$ converges; and
3. $\lim_{n\to\infty} t(n)g(n) = 0$

Proof: By Markoff's theorem on convergence of double series

Further Applications

- The number of perfect n^{th} powers $\le k$ is $\lfloor \sqrt[n]{k} \rfloor$
- The number of positive integers powers of $a \le k$ is $\lfloor \log_a k \rfloor$
- Therefore, by inspection,

$$\sum_{k=2}^{\infty} \frac{\lfloor \log_a k \rfloor}{k^2+k} = \sum_{\substack{n \text{ a positive} \\ \text{power of } a}} \frac{1}{n} = \sum_{j=1}^{\infty} \frac{1}{a^j} = \frac{1}{a-1} \quad *$$

$$\sum_{k=1}^{\infty} \frac{\lfloor \sqrt[m]{k} \rfloor}{k^2+k} = \sum_{\substack{n \text{ a perfect} \\ m^{th} \text{ power}}} \frac{1}{n} = \sum_{j=1}^{\infty} \frac{1}{j^m} = \zeta(m) \quad *$$

$$\sum_{k=2}^{\infty} \frac{2\pi(k)}{k^3-k} = \sum_{p \text{ prime}} \frac{1}{p(p-1)} \quad *$$

$$\sum_{k=2}^{\infty} \frac{k\pi(k)}{(k+1)!} = \sum_{p \text{ prime}} \frac{1}{p!} \quad *$$

$$\sum_{k=2}^{\infty} \frac{(2k+1)\pi(k)}{k^2(k+1)^2} = \sum_{p \text{ prime}} \frac{1}{p^2} \quad *$$

The Partial Integral Theorem *

- Given a function $s(x)$, let $t(y)$ be the "left integral" of s :

$$t(y) = \int_0^y s(x)\,dx$$

- Given a function $f(y)$, if certain convergence criteria are satisfied, then

RIGHT INTEGRAL OF $f(y)$

$$\int_0^{\infty} t(y) f(y)\,dy = \int_0^{\infty} s(x) g(x)\,dx$$

LEFT INTEGRAL OF $s(x)$

where

$$g(x) = \int_x^{\infty} f(y)\,dx$$

(the right integral of f) is a transform of f independent of s & t

Discovery B

$$\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}\frac{1}{(k+j)^3} = \zeta(2) - \zeta(3) = \sum_{k=1}^{\infty}\left(\frac{1}{k^2}-\frac{1}{k^3}\right)$$

- $\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}\frac{1}{(k+j)^3}$ must exceed $\sum_{k=2}^{\infty}\frac{1}{k^3} = \zeta(3) - 1$,

  but by how much?

- Is there a general principle at work?
  – In fact,

$$\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}\frac{1}{(k+j)^s} = \zeta(s-1) - \zeta(s)$$

Overcounting Functions

Let $S = \sum_{k=1}^{\infty} f(k)$ and $S^+ = \sum_{j=1}^{\infty}\sum_{k=1}^{\infty} f(g(k,j))$,

where $g(k,j)$ ranges over the natural numbers

1. Every term of S^+ occurs at least once in S.
2. In general, S^+ overcounts S, since some terms of S occur many times in S^+
3. If $K_g(k)$ is the number of times $f(k)$ is included in S^+, then

$$S^+ = \sum_{j=1}^{\infty}\sum_{k=1}^{\infty} f(g(k,j)) = \sum_{k=1}^{\infty} K_g(k) f(k)$$

where $K_g(k)$ depends only on g and not on f .

Examples

- Let $g(k, j) = k + j$. How many ordered pairs (k, j) of natural numbers give $k + j = n$? Answer: $K_{k+j}(n) = n - 1$
- Therefore, by inspection,

$$\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}\frac{1}{(k+j)^s} = \sum_{n=1}^{\infty}\frac{n-1}{n^s} = \sum_{n=1}^{\infty}\left(\frac{1}{n^{s-1}} - \frac{1}{n^s}\right) = \zeta(s-1) - \zeta(s)$$

$$\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}\frac{\zeta(k+j)}{2^{k+j}} = \sum_{n=1}^{\infty}\frac{n-1}{2^n}\zeta(n) = \frac{\pi^2}{8}$$

$$\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}\frac{1}{(k+j)!} = \sum_{n=1}^{\infty}\frac{n-1}{n!} = e-(e-1) = 1$$

Examples

- Let $g(k, j) = k \bullet j$. How many ordered pairs (k, j) give $k \bullet j = n$?

  Answer: $K_{k \bullet j}(n) = d(n)$, the number of divisors of n.
- Therefore, by inspection

$$\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}\frac{1}{(k\cdot j)^s} = \sum_{n=1}^{\infty}\frac{d(n)}{n^s} = \zeta^2(s)$$

$$\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}\frac{1}{a^{k\cdot j}} = \sum_{j=1}^{\infty}\frac{1}{a^j - 1} = \sum_{n=1}^{\infty}\frac{d(n)}{a^n}$$

$$\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}\frac{1}{(k\cdot j)!} = \sum_{n=1}^{\infty}\frac{d(n)}{n!} \approx 2.4810610197907626979 \ldots$$

Enumerating Non-Trivial Powers

- Let $g(k, j) = k^j$.
- How many ordered pairs (k, j) give $k^j = n$?
  Or, how many ways $K(n)$ can n be expressed as a positive integral power of a positive integer?
- Example: $16 = 16^1 = 8^2 = 2^4$, so $K(16) = 3$
- If n is prime, $K(n) = 1$
- If n is a square, then, $K(n) \geq 2$; $36 = 36^1 = 6^2$
- But many non-primes have $K(n) = 1$ also, such as
  6, 8,10, 11, 12, 14, 15, 18, 20, 21, 22, 24, 26, 27,
  $45 = 3^2 \cdot 5$; $55125 = 3^2 \cdot 5^3 \cdot 7^2$
- How to compute $K(n)$?

Enumerating Non-Trivial Powers

- Let $n = p_1^{e_1} p_2^{e_2} \ldots$ be the prime factorization of n
- n can be a non-trivial power of an integer > 1 iff
  $G(n) = \gcd(e_1, e_2, \ldots)$ exceeds 1; otherwise $K(n) = 1$.
- Suppose $b > 1$ divides $G(n)$. Then ,
  where each of the e_i/b is a natural number, so n is the b^th^ power of a natural number
- Suppose $c > 1$ does not divide $G(n)$. Then at least one of the exponents e_i/c is not a natural number and n is not the c^th^ power of a natural number. Therefore,

$$n = \left(p_1^{e_1/b} p_2^{e_2/b} \ldots\right)^b$$

$$K_{k^j}(n) = d(\text{gcd(exponents of the prime factorization of n)})$$ *

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A Remarkable Series

- Let $S = \sum_{k=2}^{\infty} \frac{1}{k^s} = \zeta(s) - 1.$ Then

(Old)

$$S^+ = \sum_{j=1}^{\infty}\sum_{k=2}^{\infty} \frac{1}{(k^j)^s} = \sum_{k=2}^{\infty}\sum_{j=1}^{\infty} k^{-js} = \sum_{k=2}^{\infty} \frac{1}{k^s - 1} = \sum_{n=1}^{\infty}\left(\zeta(ns) - 1\right)$$

the "overcounting" function

$$S^+ - S = \sum_{n=1}^{\infty}\left(K_{k^j}(n) - 1\right)k^{-s} = \sum_{n=1}^{\infty} \Omega_{k^j}(n)\, k^{-s}$$

$\frac{1}{k^s - 1} = \frac{1}{k^{2s} - k^s} + \frac{1}{k^s}$ yields $S^+ - S = \sum_{n=2}^{\infty} \Omega(n) n^{-s} = \sum_{n=2}^{\infty} \frac{1}{n^{2s} - n^s}$

$$\sum_{n=2}^{\infty} \frac{\Omega(n)}{n} = \sum_{n=2}^{\infty} \frac{d(G(n)) - 1}{n} = \sum_{n=2}^{\infty} \frac{1}{n^2 - n} = 1 \quad *$$

$$1 = \frac{1}{4} + \frac{1}{8} + \frac{1}{9} + \frac{2}{16} + \frac{1}{25} + \frac{1}{27} + \frac{1}{32} + \frac{1}{36} + \frac{1}{49} + \frac{3}{64} + \ldots$$

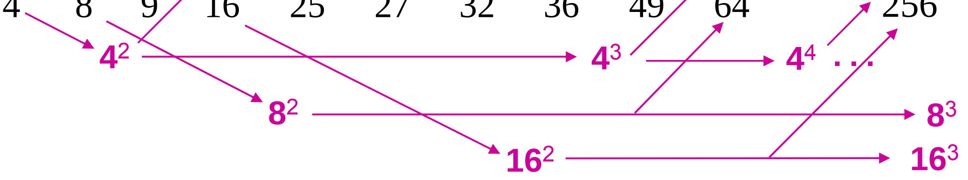
Goldbach's Theorem

- In 1729, Christian Goldbach proved that

$$\sum_{\substack{q \text{ a non-trivial} \\ \text{integer power}}} \frac{1}{q - 1} = 1 = \frac{1}{3} + \frac{1}{7} + \frac{1}{8} + \frac{1}{15} + \frac{1}{24} + \frac{1}{26} + \ldots$$

- We just showed that $\sum_{k=1}^{\infty} \frac{\Omega(k)}{k} = 1$

$$1 = \frac{1}{4} + \frac{1}{8} + \frac{1}{9} + \frac{2}{16} + \frac{1}{25} + \frac{1}{27} + \frac{1}{32} + \frac{1}{36} + \frac{1}{49} + \frac{3}{64} + \ldots \qquad \frac{3}{256}$$

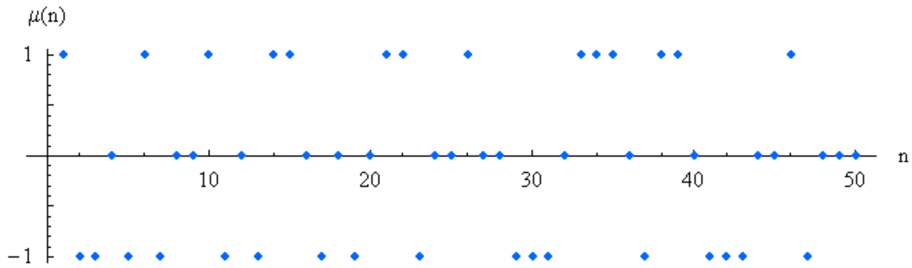


Mobius Function Review

The Mobius function, $\mu(k)$, useful in combinatorics, was defined in 1831

$$\mu(k) = \begin{cases} 1, & k = 1 \\ (-1)^n, & k \text{ a product of } n \text{ distinct primes} \\ 0, & k \text{ has a repeated prime factor} \end{cases}$$

$\mu(2) = -1$; $\mu(3) = -1$; $\mu(4) = 0$; $\mu(6) = \mu(2 \cdot 3) = 1$



Discovery C

For $c > 1$ real and p prime,

$$\sum_{k=1}^{\infty}\frac{1}{c^{p^k}} = -\sum_{m=1}^{\infty}\frac{\mu(mp)}{c^{mp}-1}$$

In particular,

$$\sum_{k=1}^{\infty}\frac{1}{2^{2^k}} = -\sum_{m=1}^{\infty}\frac{\mu(2m)}{4^m-1}$$

$$\sum_{k=0}^{\infty}\frac{1}{2^{2^k}} = \sum_{k=1}^{\infty}\frac{\lceil \log_2 k \rceil}{2^k} = \sum_{j=1}^{\infty}\frac{1}{\sqrt{2}^{2^j}}$$

Results from Counting Functions

The counting function $K_{\mathbf{max}}(n)$ of max(k, j) is 2n-1. So

$$\sum_{k=1}^{\infty}\sum_{j=1}^{\infty}\frac{1}{2^{\max(k,j)}} = \sum_{k=1}^{\infty}\frac{2k-1}{2^k} = 3$$

$$\sum_{k=1}^{\infty}\sum_{j=1}^{\infty}\frac{1}{\max(k,j)!} = \sum_{k=1}^{\infty}\frac{2k-1}{k!} = e+1$$

$$\sum_{k=1}^{\infty}\sum_{j=1}^{\infty}\frac{1}{\max(k,j)^3} = \sum_{k=1}^{\infty}\frac{2k-1}{k^3} = \frac{\pi^2}{3} - \zeta(3)$$

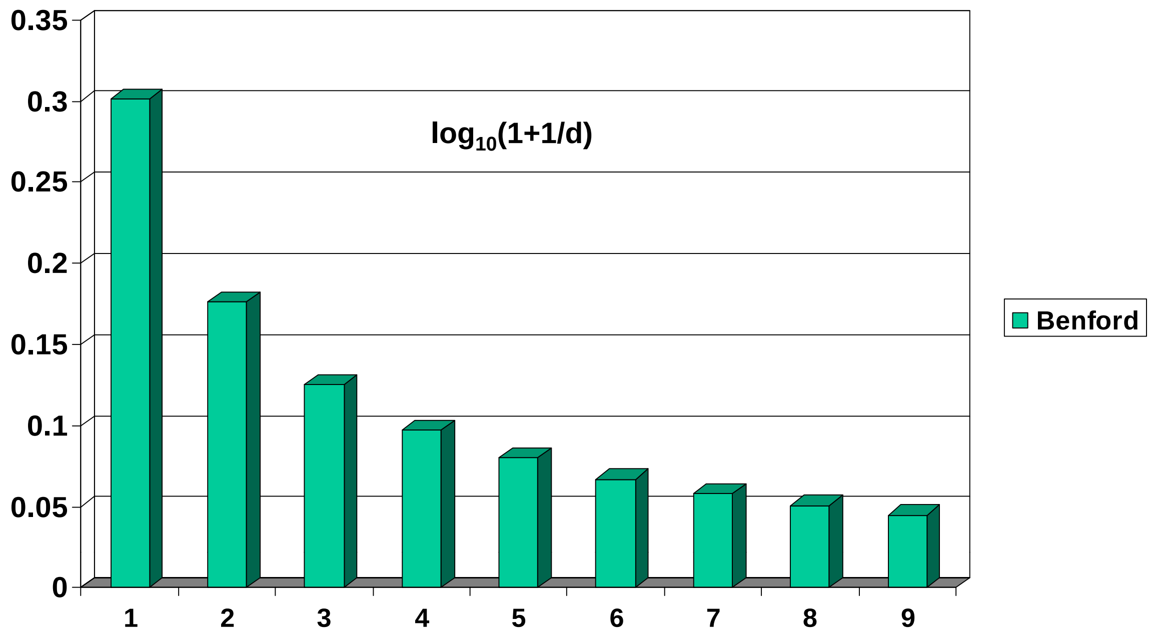
The counting function $K_{\mathbf{lcm}}(n)$ of lcm(k, j) is d(n^2). So

$$\sum_{k=1}^{\infty}\sum_{j=1}^{\infty}\frac{1}{\mathrm{lcm}(k,j)^s} = \sum_{k=1}^{\infty}\frac{d(k^2)}{k^a} = \frac{\zeta^3(s)}{\zeta(2a)}$$

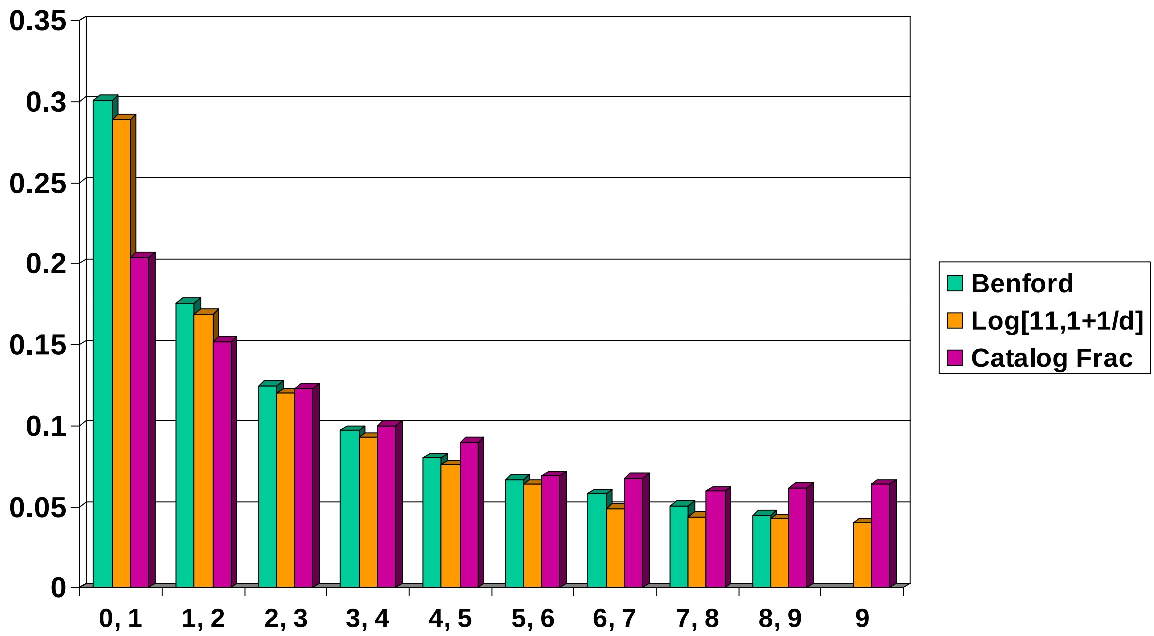
The First-Digit Phenomenon

- Given a random integer, what is the probability that its leading digit is a 1?
- Answer: depends on the distribution from which k is chosen.
- If k is chosen uniformly in [1, n], then let p(d, n) be the probability that the leading digit of k is d
- For n = 19^+, 5/9 < p(1,n) < .579; 1/19 $\leq$ p(9,n) < 1/18
- For n = 9^+, p(1,n) = 1/9; p(9,n) = 1/9
- The “average” is $\log_{10}(1+1/d)$
- {.301, .176, .124, .097, .079, .066, .058, .051, .046}

Relative Digit Frequency (Benford's Law)



First-Digit Phenomenon



Major Ideas

- Theorems can be discovered with the aid of machines
- For mathematicians:
  - How to populate the catalog
  - How to generalize from discoveries
- For computer scientists:
  - Use in symbolic manipulation systems
- For data miners:
  - How to mine the catalog, i.e. how to find new relations
- For statisticians:
  - How to use the fact that $\int_0^\infty P(y)f(y)\,dy = \int_0^\infty p(x)g(x)\,dx$

    where *P* is the cumulative distribution of density *p*

A Parting Philosophy

"The object of mathematical rigor is to sanction and legitimize the conquests of intuition, and there was never any other object for it."

Jacques Hadamard
(as quoted by Borel in 1928)

Q&A

