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Randomness and Simulation

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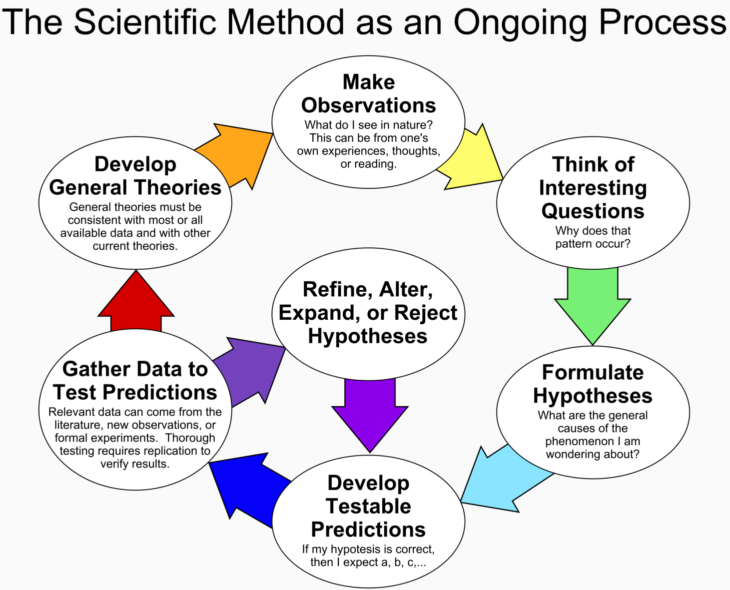
- randomness
- reproducibility
- designing an experiment


The Scientific Method as an Ongoing Process
Make Observations
What do I see in nature? This can be from one's own experiences, thoughts, or reading.
Think of Interesting Questions
Why does that pattern occur?
Formulate Hypotheses
What are the general causes of the phenomenon I am wondering about?
Develop Testable Predictions
If my hypotesis is correct, then I expect a, b, c,...
Gather Data to Test Predictions
Relevant data can come from the literature, new observations, or formal experiments. Thorough testing requires replication to verify results.
Develop General Theories
General theories must be consistent with most or all available data and with other current theories.
Refine, Alter, Expand, or Reject Hypotheses

errors

- How do I classify my method?
- Goal: determine how the error $|f(x) - p_n(x)|$ behaves relative to n (and f).
- Goal: determine how the cost of computing $p_n(x)$ behave relative to n (and f).
- for $f(x) = \frac{1}{1-x}$ we have

$$p_n = \sum_{k=0}^{n} x^k = 1 + x + x^2 + \dots$$

- so

$$e_n = |f(x) - p_n(x)|$$

- Is $e_n \sim 1/n^r$?
- Is $e_n \sim 1/\sqrt{n}$?
- Is $e_n \sim 1/n!$?

timing

- `mymethod()` takes x seconds
- How long does it take in general?
- If the data input is of size n, how long should it take?
  - n^2?
  - $n!$?
  - 10^n?

big-o

How to measure the impact of n on algorithmic cost?

$\mathcal{O}(\cdot)$

Let $g(n)$ be a function of n. Then define

$$\mathcal{O}(g(n)) = \{f(n) \,|\, \exists c, n_0 > 0 \,:\, 0 \leq f(n) \leq cg(n), \forall n \geq n_0\}$$

That is, $f(n) \in \mathcal{O}(g(n))$ if there is a constant c such that $0 \leq f(n) \leq cg(n)$ is satisfied.

- assume non-negative functions (otherwise add $|\cdot|$) to the definitions
- $f(n) \in \mathcal{O}(g(n))$ represents an asymptotic upper bound on $f(n)$ up to a constant
- example: $f(n) = 3\sqrt{n} + 2\log n + 8n + 85n^2 \in \mathcal{O}(n^2)$

big-o (omicron)

$\mathcal{O}(\cdot)$

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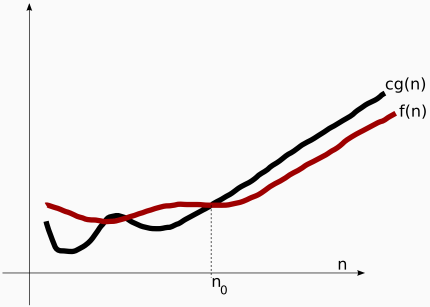


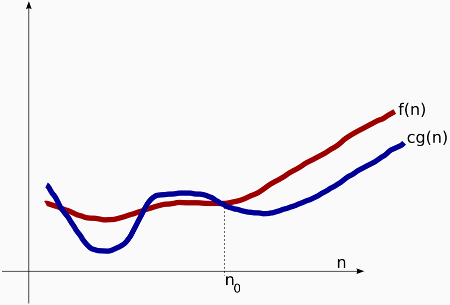
big-omega

$\Omega(\cdot)$

Let $g(n)$ be a function of n. Then define

$$\Omega(g(n)) = \{f(n) \,|\, \exists c, n_0 > 0 \,:\, 0 \leq cg(n) \leq f(n),\, \forall n \geq n_0\}$$

That is, $f(n) \in \Omega(g(n))$ if there is a constant c such that $0 \leq cg(n) \leq f(n)$ is satisfied.



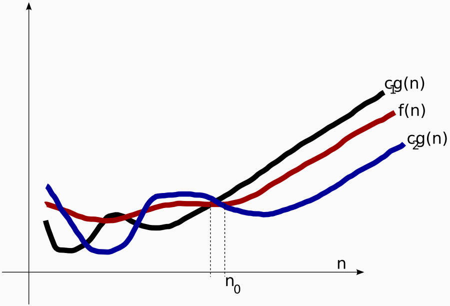
big-theta

$\Theta(\cdot)$

Let $g(n)$ be a function of n. Then define

$$\Theta(g(n)) = \{f(n) \mid \exists c_1, c_2, n_0 > 0 \, : \, 0 \leq c_1 g(n) \leq f(n) \leq c_2 g(n), \, \forall n \geq n_0\}$$

Equivalently, $\Theta(g(n)) = \mathcal{O}(g(n)) \cap \Omega(g(n))$.



algebraic convergence (j. p. boyd)

Definition

The Algebraic Index of Convergence α is the largest number for which

$$\lim_{n \to \infty} |a_n| n^{\alpha} < \infty$$

where a_n are the coefficients in the sequence. Alternatively, α is the algebraic index if

$$a_n \sim \mathcal{O}(1/n^{\alpha})$$

exponential convergence (j. p. boyd)

Definition

If the algebraic index α is unbounded (i.e. a_n decrease faster than $1/n^\alpha$ for any finite α), then the sequence converges exponentially (a.k.a. spectrally).

Alternatively, the sequence converges exponentially if for constants q and β

$$a_n \sim \mathcal{O}(e^{-qn^\beta})$$

where β is the exponential index of convergence and

$$\beta = \lim_{n \to \infty} \frac{\log|\log(|a_n|)|}{\log(n)}$$

rates of exponential convergence (j. p. boyd)

Definition

A sequence a_n has supergeometric, geometric, or subgeometric if

$$\lim_{n\to\infty} \log(|a_n|)/n = \begin{cases} \infty, & \text{supergeometric} \\ contant, & \text{geometric} \\ 0, & \text{subgeometric} \end{cases}$$

or, alternatively,

$$a_n \sim \mathcal{O}(e^{-(n/j)\log(n)}) : \text{ supergeometric}$$
$$a_n \sim \mathcal{O}(e^{-qn}) : \text{ geometric}$$
$$\beta < 1 : \text{ subgeometric}$$

asymptotic rate of geometric convergence (j. p. boyd)

definition

If a sequence a_n has geometric convergence ($\beta = 1$) so that

$$a_n \sim \mathcal{O}(e^{-n\mu})$$

then the asymptotic rate of geometric convergence is μ. Alternatively,

$$\mu = \lim_{n \to \infty} \{-\log |a_n|/n\}$$

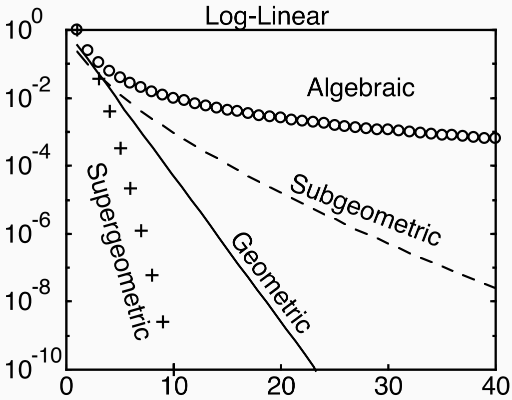


Figure 2.5: $\log | a_n |$ versus n for four rates of convergence. Circles: algebraic convergence, such as $a_n \sim 1/n^2$. Dashed: subgeometric convergence, such as $a_n \sim \exp(-1.5\ n^{2/3})$. Solid: geometric convergence, such as $\exp(-\mu\ n)$ for any positive μ. Pluses: supergeometric, such as $a_n \sim \exp(-n\ \log(n)\ )$ or faster decay.

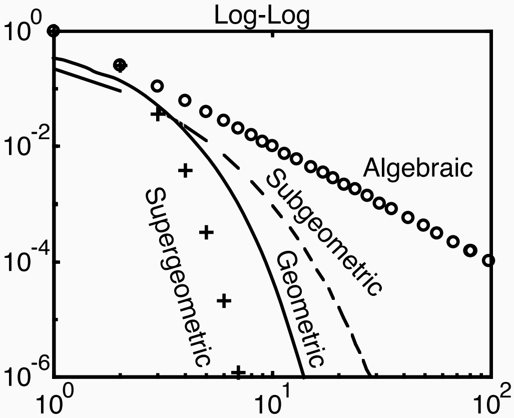


Figure 2.6: Same as previous figure except that the graph is log-log: the degree of the spectral coefficient n is now plotted on a logarithmic scale, too.

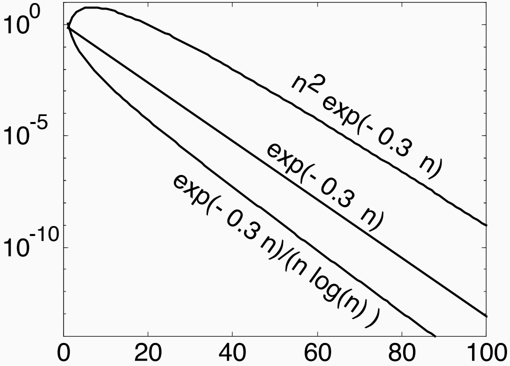
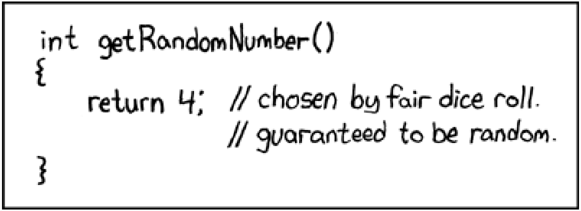


Figure 2.8: Spectral coefficients for three geometrically converging series. Although the three sets of coefficients differ through algebraic coefficients — the top curve is larger by n^2 than the middle curve, which in turn is larger by a factor of $n \log(n)$ than the bottom curve — the *exponential* dependence on n is the same for all. Consequently, all three sets of coefficients asymptote to parallel lines on this log-linear plot.

randomness

- Randomness ≈ unpredictability
- One view: a sequence is random if it has no shorter description
- Physical processes, such as flipping a coin or tossing dice, are deterministic with enough information about the governing equations and initial conditions.
- But even for deterministic systems, sensitivity to the initial conditions can render the behavior practically unpredictable.
- we need random simulation methods

`http://www.xkcd.com/221/`



randomness is easy, right?

- In May, 2008, Debian announced a vulnerability with OpenSSL: the OpenSSL pseudo-random number generator
  - the seeding process was compromised (2 years)
  - only 32,767 possible keys
  - seeding based on process ID (this is not entropy!)
  - all SSL and SSH keys from 9/2006 - 5/2008 regenerated
  - all certificates recertified
- Cryptographically secure pseudorandom number generator (CSPRNG) are necessary for some apps
- Other apps rely less on true randomness

repeatability

- With unpredictability, true randomness is not repeatable
- ...but lack of repeatability makes testing/debugging difficult
- So we want repeatability, but also independence of the trials

```
>>>> np.random.seed(1234)
```

pseudorandom numbers

Computer algorithms for random number generations are deterministic

- ...but may have long periodicity (a long time until an apparent pattern emerges)
- These sequences are labeled *pseudorandom*
- Pseudorandom sequences are predictable and reproducible (this is mostly good)

random number generators

Properties of a good random number generator:

Random pattern:	passes statistical tests of randomness
Long period:	long time before repeating
Efficiency:	executes rapidly and with low storage
Repeatability:	same sequence is generated using same initial states
Portability:	same sequences are generated on different architectures

random number generators

- Early attempts relied on complexity to ensure randomness
- "midsquare" method: square each member of a sequence and take the middle portion of the results as the next member of the sequence
- ...simple methods with a statistical basis are preferable

linear congruential generators

- Congruential random number generators are of the form:

$$x_k = (ax_{k-1} + c) \pmod{M}$$

  where a and c are integers given as input.
- x_0 is called the *seed*
- Integer M is the largest integer representable (e.g. $2^{31} - 1$)
- Quality depends on a and c. The period will be at most M.

Example

Let $a = 13$, $c = 0$, $m = 31$, and $x_0 = 1$.

$$1, 13, 14, 27, 10, 6, \ldots$$

This is a permutation of integers from $1, \ldots, 30$, so the period is $m - 1$.

history

- IBM used Scientific Subroutine Package (SSP) in the 1960's the mainframes.
- Their random generator, `rnd` used $a = 65539$, $c = 0$, and $m = 2^{31}$.
- arithmetic mod 2^{31} is done quickly with 32 bit words.
- multiplication can be done quickly with $a = 2^{16} + 3$ with a shift and short add.
- Notice (mod m):

$$x_{k+2} = 6x_{k+1} - 9x_k$$

...strong correlation among three successive integers

history

- Matlab used $a = 7^5$, $c = 0$, and $m = 2^{31} - 1$ for a while
- period is $m - 1$.
- this is no longer sufficient

what's used?

Two popular methods:

1. Method of Marsaglia (period $\approx 2^{1430}$).

Initialize $x_0, \ldots, x_3$ **and** c to random values given a seed

Let $s = 2111111111x_{n-4} + 1492x_{n-3}1776x_{n-2} + 5115x_{n-1} + c$

Compute $x_n = s \mod 2^{32}$

$c = \mathit{floor}(s/2^{32})$

2. *rand()* in Unix uses $a = 1103515245$, $c = 12345$, $m = 2^{31}$.

Even the Marsaglia method produces points in $n - D$ on only a small number of hyperplanes.

linear congruential generators

- sensitive to a and c
- be careful with supplied random functions on your system
- period is M
- standard division is necessary if generating floating points in $[0, 1)$.

fibonacci

- produce floating-point random numbers directly using differences, sums, or products.
- Typical subtractive generator:

$$x_k = x_{k-17} - x_5$$

  with "lags" of 17 and 5.
- Lags much be chosen very carefully
- negative results need fixing
- more storage needed than congruential generators
- no division needed
- very very good statistical properties
- long periods since repetition does not imply a period

sampling over intervals

If we need a uniform distribution over $[a, b)$, then we modify x_k on $[0, 1)$ by

$$(b - a)x_k + a$$

non-uniform distributions

- sampling nonuniform distributions is much more difficult
- if the cumulative distribution function is invertible, then we can generate the non-uniform sample from the uniform:

$$f(t) = \lambda e^{-\lambda t}, \quad t > 0$$

thus

$$y_k = -\log(1 - x_k)/\lambda$$

where x_k is uniform in $[0, 1)$.
- ...not so easy in general

quasi-random sequences

- For some applications, reasonable uniform coverage of the sample is more important than the “randomness”
- True random samples often exhibit clumping
- Perfectly uniform samples uses a uniform grid, but does not scale well at high dimensions
- quasi-random sequences attempt randomness while maintaining coverage

quasi-random sequences

- quasi random sequences are not random, but give random appearance
- by design, the points avoid each other, resulting in no clumping