# Simple Random Sampling: Not So Simple

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# Permutation Tests for Complex Data

## Theory, Applications and Software

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# Simple Random Sampling

**Simple random sampling:** drawing $k$ objects from a group of $n$ in such a way that all $\binom{n}{k}$ possible subsets are equally likely

If there is a problem generating SRSs, it will be even worse for other methods: permutation, bootstrap samples, MCMC, Monte Carlo integration...

Number of possibilities for $n = 100$, $k = 50$

| | | |
|---|---|---|
| SRSs | $\binom{n}{k}$ | $\binom{100}{50} \approx 10^{29}$ |
| Bootstrap Samples | $n^k$ | $100^{50} = 10^{100}$ |
| Permutations | $n!$ | $100! \approx 10^{158}$ |

# Simple Random Sampling

In practice, it is difficult to draw truly random samples.

Instead, people tend to draw samples using

- A **pseudorandom number generator** (PRNG)
- An algorithm that maps a set of pseudorandom numbers into a subset of the population

Most people take for granted that this procedure is a sufficient approximation to simple random sampling.

# Pigeons and Pigeonholes

**Theorem (Pigeonhole Principle)**

*If there are $n$ pigeonholes and $m > n$ pigeons, then there exists at least one pigeonhole containing more than one pigeon.*

(Wikipedia)

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## Corollary (Too few pigeons)

*If $\binom{n}{k}$ is greater than the size of a PRNG's state space, then the PRNG cannot possibly generate all samples of size $k$ from a population of $n$.*

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Period of 32-bit linear congruential generators (e.g. RANDU):
$2^{32} \approx 4 \times 10^9$
Samples of size $10$ from $50$: $\binom{50}{10} \approx 10^{10}$
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Period of Mersenne Twister (standard PRNG in Statistics):
$2^{32 \times 624} \approx 2 \times 10^{6010}$
Permutations of $2084$ objects: $2084! \approx 3 \times 10^{6013}$
**Less than $0.01\%$ of permutations can be generated**

# Pigeons and Pigeonholes

But does it *really* matter in practice?

- Social applications may require the PRNG to produce all possible samples – e.g. jury duty summons, gaming machines, lottery tickets (Marsaglia [2003])
- Impossibility bounds show that this introduces a nontrivial amount of bias into statistics estimated from Monte Carlo distributions here

# Sampling Algorithms

Given a sequence of (pseudo)random numbers, how do we use them to draw a SRS?

Two general strategies:

- "Shuffle the deck" and take the top $k$ as the sample
- Number the population, select $k$ random integers, and take the corresponding items

# PIKK

**Algorithm 1** PIKK: Permute indices and keep $k$

1: Assign IID uniform values on $[0, 1]$ to the $n$ elements of the population
2: Sort the population according to these values (break ties randomly)
3: Take the top $k$ to be the sample

- Relies on assumption that all permutations are equally likely
- Inefficient: requires $n$ PRNs and $O(n \log n)$ sorting operation
- Sort: Stata uses a random sort function to break ties! Not reproducible! TO DO: cite http://www.stata-journal.com/sjpdf.html?articlenum=dm0019

# Shuffling algorithms

- Knuth shuffle: requires $n-1$ random integers, but no sorting. This is what `np.random.choice` does.

**Algorithm 2** Fisher-Yates-Knuth-Durstenfeld shuffle

**for** $i = 2, \ldots, n$ **do**
    $J \leftarrow$ random integer uniformly distributed on $1, \ldots, i$
    $(a[J], a[i]) \leftarrow (a[i], a[J])$
**end for**
Take the first $k$ to be the sample

TO DO: PUT PROOF THAT SHUFFLE WORKS IN APPENDIX

- Reservoir algorithms: Algorithm R (Waterman, Knuth 1997), Algorithm Z (Vitter 1985) are related to shuffling and don't require knowing the population size a priori

# Using random integers

**Algorithm 3** Uniform random integers

$\tilde{n} \leftarrow n$
Population indices $\leftarrow \{1, \ldots, n\}$
**for** $i = 1, \ldots, k$ **do**
    $w \leftarrow$ A random integer on $\{1, \ldots, \tilde{n}\}$
    $j \leftarrow$ The $w$th element in Population indices
    Sample indices $\leftarrow$ Sample indices $\cup \{j\}$
    Population indices $\leftarrow$ Put last remaining index in place $w$
    $\tilde{n} \leftarrow \tilde{n} - 1$
**end for**
Take the items with selected Sample indices

- Method used by R `sample`, Python `random.sample`
- More efficient: uses only $k$ PRNs and no sorting

# Generating (non)uniform integers

- Algorithm 2 relies on uniformly distributed integers
- A common way to get integers in the range $\{1, \ldots, m\}$ is $X = \lfloor mU \rfloor + 1$, $U \sim U[0, 1)$.
- Unless $m$ is a multiple of $2^w$, $\lfloor mU \rfloor$ will not truly be uniform!

**Lemma**

*For $m < 2^w$, the ratio of the largest to smallest selection probability is, to first order, $1 + m2^{-w}$. (See, e.g., Knuth v2 3.4.1.A.)*

TO DO: PROPER CITATION, PUT PROOF IN APPENDIX

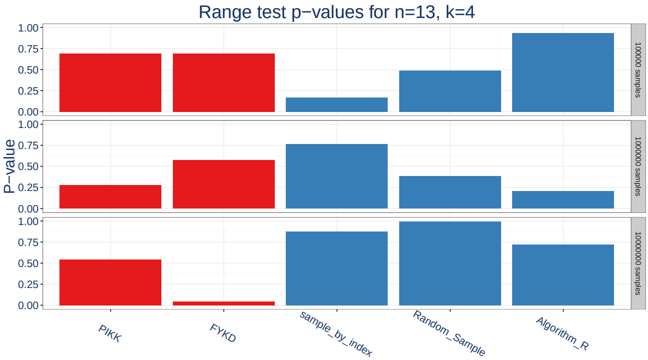
# Generating (non)uniform integers

A better way to generate integers on $\{1, \ldots, m\}$:

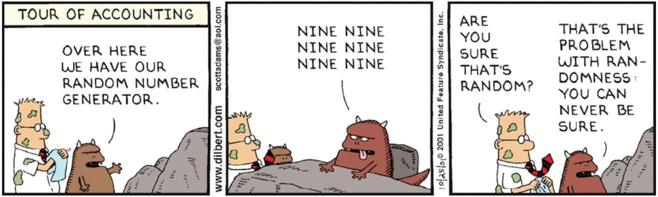
- Let $w = \lfloor \log_2 m \rfloor + 1$
- Generate a $w$-bit integer $J$
- If $J > m$, discard and repeat.

# Sampling Algorithms

- Red: require $n$ PRNs
- Blue: require $k$ PRNs
- No straightforward pattern in how uniform the samples are



# Pseudorandomness

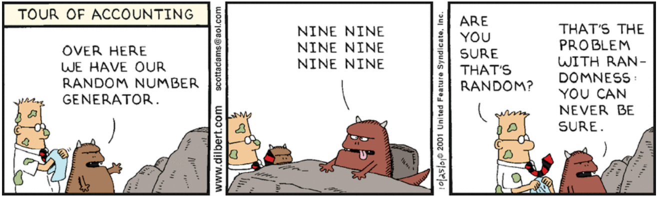



Dilbert

**Pseudorandom**: deterministic, but having the same relevant statistical properties as if random

- Uniformity: Values and sequences of values should be equiprobable
- Independence: Lack of serial correlation, unpredictable

# Pseudorandomness

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PRNGs can't do this perfectly.

- They are deterministic. Knowing input tells you the output.
- Most are **periodic**: they eventually produce the same sequence of values.
- They have some predictable mathematical structure.

## What makes a PRNG

- Fast and memory efficient
- Mimics a random sequence (statistically indistinguishable)
- Unpredictable. this is different from random - if it's deterministic, then it's predictable to some degree
- Jump-ahead feature so we can efficiently skip random numbers, generate multiple streams for parallel applications

# Testing PRNGs

TO DO:

- List and cite test suites
- Describe a few interesting/important tests
- Argue that for statistical use, PRNGs should be able to produce samples uniformly and this ought to be a test
- Describe chi-squared test and range test
- Mention Spearman correlation test of permutations?

# Bad seeds

- **Seed**: an initial value to set the internal state of a PRNG.
- Mersenne Twister has problems with seeds with too many zeros (Saito and Matsumoto [2008])
- LCGs may not achieve their full period with certain seeds (Park and Miller [1988])

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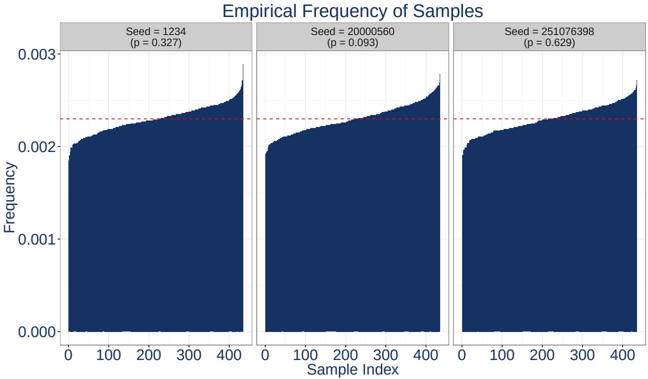


$10^5$ samples of size $2$ from a population of $30$ (Mersenne Twister in R)

# Linear Congruential Generators

LCGs have the form

$$X_{n+1} = (aX_n + c) \mod m$$

Smart choices of $a$,$c$, and $m$ can make the LCG fast to compute and more or less random

**Theorem (Hull-Dobell Full Period Theorem)**

*The period of an LCG is $m$ for all seeds $X_0$ if and only if*

- $m$ *and* $c$ *are relatively prime,*
- $a - 1$ *is divisible by all prime factors of* $m$*, and*
- $a - 1$ *is divisible by 4 if* $m$ *is divisible by 4.*

# The good, the bad, and the ugly

**(Knuth, 1997)**

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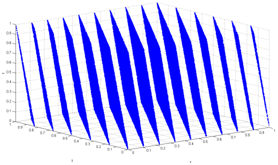
Marsaglia [1968] proved that $n$-tuples of numbers generated by any LCG will lie on parallel hyperplanes, making them especially non-random.



Triples of RANDU lie on 15 planes in 3D space

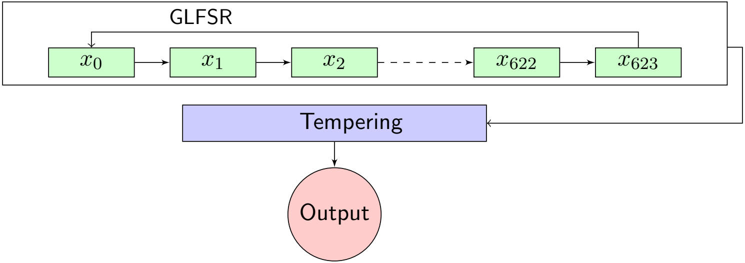
$$x_{n+1} = (65539 x_n) \mod 2^{31}$$

(Wikipedia)

# Linear Congruential Generators

- Fast to compute and requires little memory
- Some LCGs are more random than others – depends on choosing good constants
- Not unpredictable. We only need 2 values to determine the constants.
- Possible to do jump ahead using mathematical formulas.

# Mersenne Twister (Matsumoto and Nishimura [1998])




- A "twisted" generalized linear feedback shift register: a complicated sequence of bitwise and linear operations
- Enormous period of $2^{19937} - 1$, a Mersenne prime
- $k$-distributed to 32-bit accuracy for $1 \leq k \leq 623$, i.e. tuples of up to length $623$ occur with equal frequency over the entire period
- Integer seed is used to set the state, a $624 \times 32$ binary matrix

# Mersenne Twister

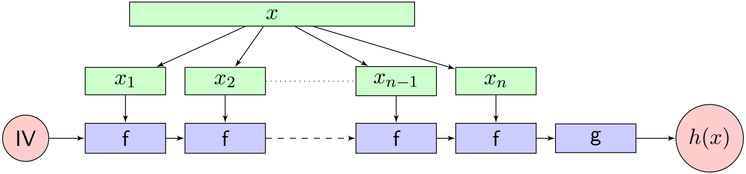
- Fast to compute but has a large state space, not the most memory efficient
- Generally considered “random” enough for Statistics, but fails some TestU01 tests
- Completely predictable after we’ve seen 624 values
- No good jump ahead feature

# A better alternative

**One solution:** Find a class of PRNGs with infinite state space

# Hash function PRNGs

**Hash functions** take in a message $x$ of arbitrary length and return a value $h(x)$ of fixed size (e.g. 256 bits)




Cryptographic hash functions:

- computationally infeasible to invert
- difficult to find two inputs that map to the same output
- small input changes produce large, unpredictable changes to output
- resulting bits are uniformly distributed

# Hash function PRNGs

Procedure for using a cryptographic hash function as PRNG:

1. Set a seed, a large random integer
2. Set the counter to $0$
3. Set the state to be "seed,counter"
4. Hash the state value. This is your random number.
5. Increment the counter
6. Repeat Steps 2-5 as many times as needed

# Hash function PRNGs

- Efficient: based on fast, pre-existing hash function code
- Memory efficient: only need to store the seed and counter
- Unpredictable: small changes to input produce large unpredictable changes to output. The only way to figure out the sequence is to know the hashing function
- Jump ahead: add the desired number of steps to the counter

## Simulations

TO DO:

- Compare MT/CSPRNG/LCG with different seeds
- For the unique sample frequencies, report
  - Range statistic $p$-value
  - Chi-squared test $p$-value
- Do this for various numbers of samples - 1e6 up to 1e8. How do $p$-values change? How does this relate to equidistribution?

# Next steps

TO DO:

Theoretical:

- Understand how the equidistribution of a PRNG relates to how uniformity of sampling frequencies over different segments of the period
- Study the properties of hash function PRNGs

Practical:

- Find examples where results of a study would change from using a better SA/PRNG
- Add these statistical tests to a more thorough test battery for PRNGs for Statistics
- Create plug-in hash function PRNGs for R and Python

# Impossibility bounds

Let $F$ be the uniform distribution on all samples of size $k$ from a population of $n$. For some subset of samples $S$, define $\mathcal{G} = \{G : G(S) = 0, S \in \mathcal{S}\}$ and $\nu = |S|$.

## Lemma

*For any $G \in \mathcal{G}$, $\|F - G\|_1 \geq \frac{2\nu}{\binom{n}{k}}$*

For any bounded function $\psi : \Omega \to \mathbb{R}$ and for any $G \in \mathcal{G}$,

$$\left| \int \psi dG - \int \psi dF \right| \leq \|F - G\|_1 \|\psi\|_\infty$$

## Corollary

*There exists a statistic $\psi$ such that*

$$|\mathbb{E}_F(\psi) - \mathbb{E}_G(\psi)| \geq \frac{2\nu \|\psi\|_\infty}{\binom{n}{k}}$$

# Proof of Lemma.

Fix $S$ and choose $G \in \mathcal{G}$ such that $G(S) = 0$, $G(\omega) > 0$ for $\omega \in S^c$.

$$\begin{aligned}
\|F - G\|_1 &= \sum_{\omega \in \Omega} |F(\omega) - G(\omega)| \\
&= \sum_{\omega \in S} |F(\omega) - G(\omega)| + \sum_{\omega \in S^c} |F(\omega) - G(\omega)| \\
&= \sum_{\omega \in S} |F(\omega)| + \sum_{\omega \in S^c} |F(\omega) - G(\omega)| \\
&= \frac{|S|}{\binom{n}{k}} + \sum_{\omega \in S^c} |F(\omega) - (F(\omega) + \varepsilon_\omega)|
\end{aligned}$$

where $\varepsilon_\omega \in [-\binom{n}{k}^{-1}, 1 - \binom{n}{k}^{-1}]$ and $\sum_{\omega \in S^c} \varepsilon_\omega = \sum_{\omega \in S} F(\omega) = \frac{|S|}{\binom{n}{k}}$. NB this must be the case to ensure that $\sum_\omega G(\omega) = 1$, since

$$\sum_\omega G(\omega) = \sum_{\omega \in S^c} G(\omega) = \sum_{\omega \in S^c} F(\omega) + \varepsilon_\omega = \sum_{\omega \in S^c} F(\omega) + \sum_{\omega \in S} F(\omega) = 1.$$

Therefore,

$$\begin{aligned}
\|F - G\|_1 &= \frac{|S|}{\binom{n}{k}} + \sum_{\omega \in S^c} |\varepsilon_\omega| \\
&= \frac{|S|}{\binom{n}{k}} + \sum_{\omega \in S} |F(\omega) \\
&= \frac{2|S|}{\binom{n}{k}}
\end{aligned}$$

$\square$

back

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