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

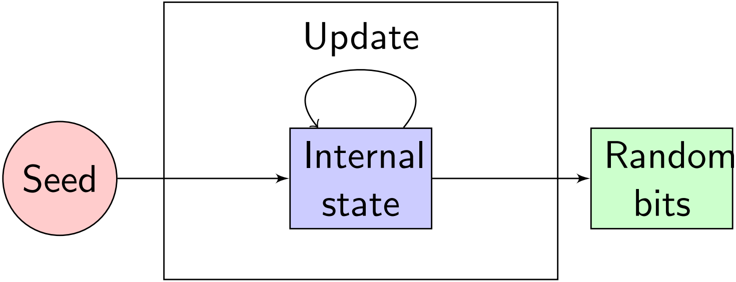
- A **pseudorandom number generator** (PRNG) that produces sequences of bits
- An algorithm that maps a set of pseudorandom numbers into a subset of the population

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

PRNGs

A PRNG is a deterministic function with several components:

- A user-supplied seed value used to set the internal state
- A function that maps the internal state to random bits
- A function that updates the internal state



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.

Pigeons and Pigeonholes

Period of 32-bit linear congruential generators:

at most $2^{32} \approx 4 \times 10^9$

Samples of size 10 from 50:

$\binom{50}{10} \approx 10^{10}$

More than half of samples cannot be generated

Pigeons and Pigeonholes

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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])
- TO DO: THINK ABOUT IF I WANT TO INCLUDE THIS
  Impossibility bounds show that some statistics estimated from Monte Carlo distributions will have nontrivial bias (though we don't know which statistics) here

Arguments

- Some sampling algorithms are better than others – look under the hood of your software
- Inputs to your PRNGs matter for producing "good" PRNs
- PRNGs for Statistical applications should be judged on how well they produce random samples when passed into a reasonable sampling algorithm

Contents

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
- Possibly the basis for the `sample` function in Stata

TO DO: who else recommends PIKK? do a lit search

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

Random indices

Algorithm 3 Uniform random indices

$\tilde{n} \leftarrow n$
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 wth 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

- These algorithms depend 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! (Knuth [1997])

Lemma

For $m < 2^w$, the ratio of the largest to smallest selection probability is, to first order, $1 + m2^{-w}$.

Proof

Generating (non)uniform integers

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

$$w = \begin{cases} \log_2(m) & \text{if } m \text{ is a power of 2} \\ \lfloor \log_2(m) \rfloor + 1 & \text{otherwise} \end{cases}$$

  Generate a w-bit integer J. If $J > m$, discard and repeat.

- Possibly slow: will discard nearly half of draws when m is close to 2^{w-1}
- Resulting integers will truly be uniform

Sampling Algorithms

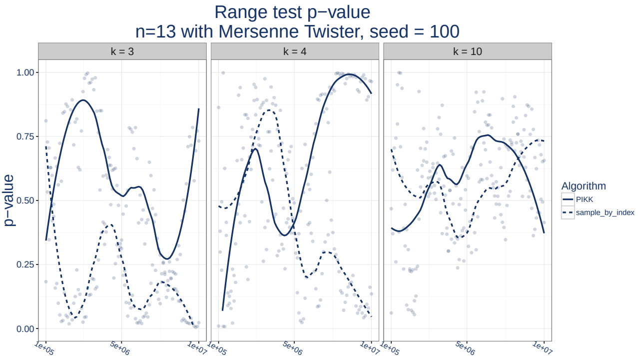
Package	Sampling algorithm	Random integer algorithm
R	random indices	variant of floor method
Python `random`	random indices	discard method
Numpy `random`	shuffle and keep k	discard method
Stata	?	?

- Stata blogs recommend people use PIKK when coding up sampling themselves. But Stata's sort function is randomized by default. Not reproducible! (Schumm [2006])
- TO DO: R bug report

Sampling Algorithms

TO DO: May want to remove this slide or move it later

- Generate samples using a single PRNG and single seed, various sampling algorithms and number of samples TO DO: what's the seed
- Red require n PRNs; Blue require only k PRNs
- No straightforward pattern in how uniform the samples are



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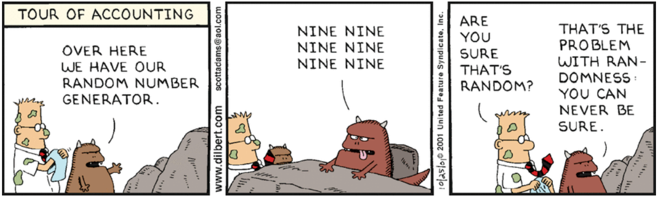
Pseudorandomness

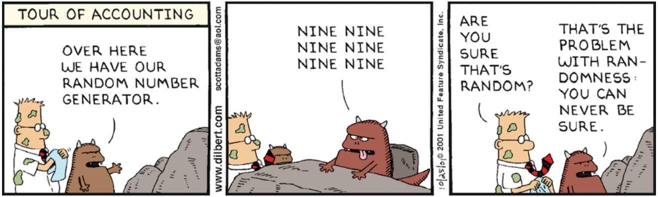


Dilbert

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



Dilbert

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

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- Independence: lack of serial correlation, unpredictable

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

- Mimics a random sequence (statistically indistinguishable)
- Unpredictable. This is different from random - if it's deterministic, then it's predictable to some degree
- Fast and memory efficient
- Desirable, but not essential:
  - Jump-ahead feature to efficiently skip through random numbers, generate multiple streams for parallel applications
  - TO DO:

Testing PRNGs

- "Independent" and "uniform" are broad criteria – many ways to define and check for these properties
  - Uniformity at varying levels of granularity
  - Correlations within and between subsequences
- Test batteries:
  - Diehard battery (Marsaglia [1995])
  - NIST Statistical Test Suite (Soto [1999], Rukhin et al. [2010])
  - TestU01 suite (L'Ecuyer and Simard [2007])

Testing for uniformity

1. Kolmogorov-Smirnov test: values should appear IID $U[0,1]$

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Testing for uniformity

1. Kolmogorov-Smirnov test: values should appear IID $U[0, 1]$
2. Chi-squared test: break values or sequences of values into categories with known frequencies under the null
3. **New proposal:** Range test
   Break values into equally probable categories and compute the range of observed frequencies

$$R = \max_i O_i - \min_i O_i$$

R has a complicated distribution based on multinomial distribution... use asymptotic approximation from Young [1962]:

$$\mathbb{P}(R \le r) \approx P(W_N \le (r - (2B)^{-1})(N/B)^{1/2})$$

where W_N denotes the sample range of N independent standard normal random variables.

Testing for independence

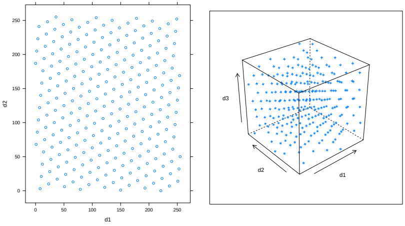
1. Gap test: count length of sequence between values in a given range
2. Permutation test: look at ordering of values in subsequences of length t
3. Serial correlation test: correlation between consecutive pairs of values
4. Many more possibilities!

Geometric tests

- Some PRNGs generate points with geometric structure (more on this later)
- The **spectral test** in dimension d considers a set of parallel hyperplanes that covers all points $(x_n, \ldots, x_{n+d-1})$.

$$\nu_d = 1/\max \text{distance between parallel hyperplanes}$$

Idea: More information needed to describe structure $\iff$ less correlation between consecutive PRNs



$$X_{n+1} = (137X_n + 187) \mod 256$$

Testing PRNGs

- Some sampling algorithms use PRNGs in ways that are not covered by these tests
- E.g. Algorithm 3 for sampling by uniform random indices
  - To generate a SRS of size k from n, obtain PRNs $(U_1, \ldots, U_k)$ where U_j is uniform on $\{1, \ldots, n-j+1\}$
  - The sequences $(U_1, \ldots, U_k)$ should themselves be equiprobable

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  - The sequences $(U_1, \ldots, U_k)$ should themselves be equiprobable
- Test by generating a large "sample" of B SRSs

$$H_0 : \mathbb{P}(\mathsf{SRS}_i) = \frac{1}{\binom{n}{k}} \text{ for all } \binom{n}{k} \text{ possible SRSs}$$
$$H_1 : \mathbb{P}(\mathsf{SRS}_i) \neq \frac{1}{\binom{n}{k}} \text{ for some SRS}$$

- Under H_0, the number of times each SRS is observed follows a multinomial distribution with B trials and equal selection probabilities $1/\binom{n}{k}$

Testing PRNGs

Test proposals:

- Chi-squared or range test
- Sequential probability ratio test

SPRT

TO DO:

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)

> "Random numbers should not be generated with a method chosen at random."

The good, the bad, and the ugly

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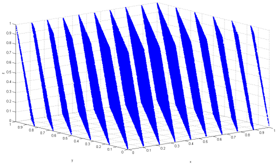
> “Random numbers should not be generated with a method chosen at random.”

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)

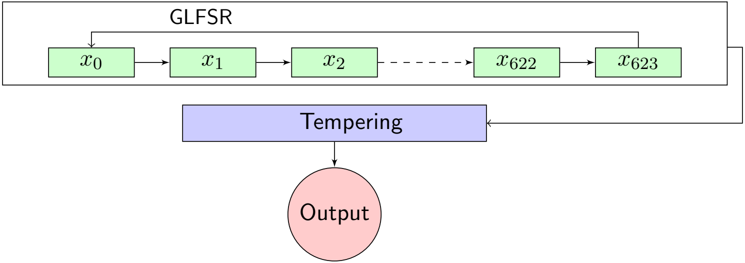
Better LCGs

- Super-Duper: $X_{n+1} = (69069 X_n) \mod 2^{32}$
  - $69069 = 3 \times 7 \times 11 \times 13 \times 23$
  - Considered a good LCG, passes spectral tests in low dimensions
- MINSTD: $X_{n+1} = (16807 X_n) \mod (2^{31} - 1)$
  - $16807 = 7^5$
  - The "minimum standard" against which other PRNGs should be judged (Park and Miller [1988])
- KISS: combines Super-Duper with two other PRNGs
  - Was previously the only PRNG in Stata
  - Period length over 2^{210}
- Wichman-Hill PRNG: a sum of 3 LCGs
  - Was previously the only PRNG in Excel
  - Faulty implementation didn't allow seeding and sometimes produced negative values (McCullough [2008])

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 624×32 binary matrix

Mersenne Twister

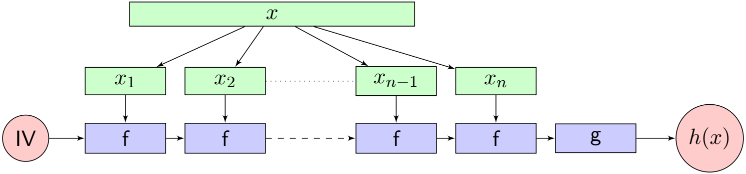
- Fast to compute but has a large state space, not the most memory efficient
- Fails some TestU01 tests but has been generally considered "random" enough for Statistics... (but stay tuned)
- Completely predictable after we've seen 624 values
- No good jump ahead feature

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:

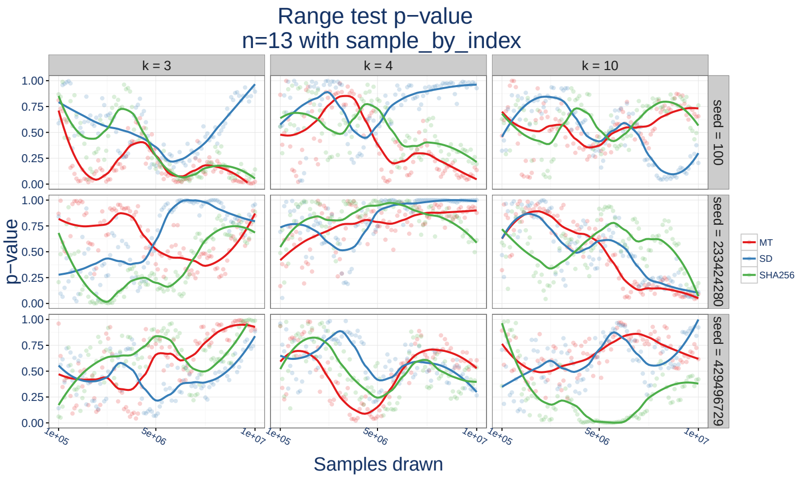
1. Set a seed, a large random integer
2. Set the counter to 0
3. Set the state to be "seed,counter"
4. Hash the state value. This is your random number (expressed in hexadecimal).
5. Increment the counter
6. Repeat Steps 2-5 as many times as needed

This PRNG passes the tests described. see appendix

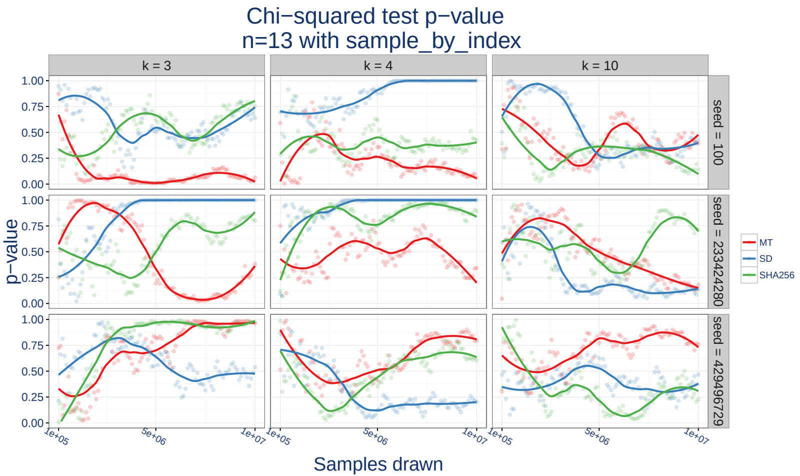
Hash function PRNGs

- Efficient: based on fast, pre-existing hash function code. Some cryptographic hash functions are even built into hardware (e.g. AES and Intel)
- 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 seed.
- Jump ahead: add the desired number of steps to the counter

Simulations



Simulations



Simulations

TO DO: SUMMARIZE SIM RESULTS

- Even though sampling k from n is complementary to sampling $n-k$ from n, the resulting samples are not equally uniform
- None of the 3 PRNGs is best overall – results vary by seed value
- p-value curves tend to dip around 5×10^6 samples – trade-off between statistical power and equidistribution of PRNG?

Next steps

Theoretical:

- Study the properties of hash function PRNGs
- Understand how the equidistribution of a PRNG relates to how uniformity of sampling frequencies over different segments of the period
- Implement a sequential hypothesis test for uniformity of samples

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 ψ such that

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

back

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,

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

$\square$

Proof.

Define $Y = \lfloor mX \rfloor + 1$ and $\tilde{X}$ to be a uniform random integer on $\{0, 1, \ldots, 2^w - 1\}$ (while X has the same distribution scaled by 2^{-w}). The selection probability for a particular integer value is

$$\begin{aligned}
\mathbb{P}(Y = y) &= \mathbb{P}(1 + \lfloor mX \rfloor = y) \\
&= \mathbb{P}(y - 1 \leq mX < y) \\
&= \mathbb{P}\left(\tilde{X} < \frac{y2^w}{m}\right) - \mathbb{P}\left(\tilde{X} < \frac{(y-1)2^w}{m}\right) \\
&= \mathbb{P}\left(\tilde{X} < \left\lceil \frac{y2^w}{m} \right\rceil\right) - \mathbb{P}\left(\tilde{X} \leq \left\lceil \frac{(y-1)2^w}{m} \right\rceil\right) \\
&= 2^{-w}\left(k^-(y) - k^-(y-1) + 1\right) = 2^{-w}\left(k^+(y-1) - k^-(y-1)\right)
\end{aligned}$$

where, for fixed m, we define $k^-(i) \equiv \min\{k : k2^{-w} \geq i/m\}$ for all i,
$k^+(i) \equiv \max\{k : k2^{-w} < i/m\} = k^-(i+1) - 1$ for $i = 0, \ldots, m-1$ and $k^+(m) \equiv 2^w$. The maximum ratio of selection probabilities is

$$\begin{aligned}
\max_{i,j \in \{0,\ldots,m-1\}} \frac{k^+(i) - k^-(i)}{k^+(j) - k^-(j)} &= \frac{\max_{i=0}^{m-1}(k^+(i) - k^-(i))}{\min_{i=0}^{m-1}(k^+(i) - k^-(i))} \\
&= \frac{\max_{i=0}^{m-1}(k^+(i) - k^+(i+1) + 1)}{\min_{i=0}^{m-1}(k^-(i+1) - k^-(i) - 1)} \\
&= \frac{\lceil 2^w/m \rceil + 1}{\lfloor 2^w/m \rfloor - 1} \\
&= 1 + 2^{-w}m + \ldots
\end{aligned}$$

□

back

TO DO: Insert table of p-values for several tests + several seeds back

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