Simulation

Random numbers

Random numbers

- ”Anyone who considers arithmetic methods of producing random digits is, of course, in a state of sin”, John v. Neumann
- Only seemingly random (pseudo random numbers) are used in simulation
- Random numbers should be
  - Reproducable and efficiently generated
  - Reflect the desired properties of the intended truely random sequence (apparent independency, statistics)
- Intended use dictates which features are important

History

- Need to generate random numbers boomed after invention of computers
  - Simulation of nuclear reactions, Los Alamos
- Simplicity and computational efficiency were emphasized in the beginning
  - Simple arithmetics, simple parameters
- Later portability and quality issues
  - Efficient implementation with high level languages
  - Statistical properties

Generation of random numbers

- Divided in two stages
  - Generation of Uniform (0,1) random numbers
    - Generate uniformly (0,m-1) distributed integers and divide with m
  - Generation of random numbers with given probability density function
    - Is done using Unif(0,1) random streams

Mid square method

- One of first ad hoc ideas (von Neumann)
  - Let x be k-digit number.
    - Take k=5, x=12345
  - Compute x*2 (2k-digits)
    - 0016604025
  - Take k digits from the middle
    - 16604 ->x, U=0,16604
  - Etc

Mid square method

```
integer,parameter :: m0=100,m1=10000
integer :: seed

real function random()
seed=seed*seed
seed=seed/m0
seed=modulo(seed,m1)
random=real(seed)/real(m1)
return
end function random
```

```
3456
0.9439 9.47000E-02 0.8968 0.425 6.25000E-02 0.3906 0.2568 0.5946
   0.3549 0.5954 0.4501 0.259 0.7081 0.1405 0.974 0.8676 0.2729
   0.4474 1.66000E-02 2.75000E-02 7.56000E-02 0.5715 0.6612 0.7185
   0.6242 0.9625 0.6406 3.68000E-02 0.1354 0.8333 0.4388 0.2545
   0.477 0.7529 0.6858 3.21000E-02 0.103 6.09000E-02 0.3708 0.7492
   0.13 0.69 0.61 0.21 0.41 0.81 0.61 0.21 0.41 0.81 0.61 0.21
```

Mid square - analysis

- Produces an endless stream of k-digit numbers.
- First numbers often apparently independent
- Method ends up to repeating a finite cycle
  - Cycle is too short for simulation purposes
  - Length and statistical properties are not easy to analyze/control

”Good” random numbers

- Generated stream should
  - Be ”random”
    - Same sequence must not occur systematically during the simulation
    - In practice the cycle length must be bigger than number of needed numbers in the experiment series
  - Have right distribution
    - Generally OK, if all possible values can be reached (maximal cycle) .

”Good” random numbers

– Consequtive values should be independent
  - Never true literally, must be tested carefully
  - For example distribution of k succesfull values within the unit cube of R^k or distribution of max(x_i,…,x_(i+k-1)).
  - Spectral test(sequence must be orthogonal with all sinusoidal forms)
  - Way of using defines the criteria – numbers used as single values, pairs, -tuplets etc.
  - See Knuth vol II

Lehmer generator

- Developed in 40s (D Lehmer) for first computers (Eniac)
- Basic operations: addition, multiplication and taking reminder
    - $X = (a X + c) \bmod m$
    - Parameters a, c and m influence the properties of the sequence
    - Original generator was implemented as a separate physical unit. Random stream was read when needed (-> additional randomness)

Lehmer generator

- Original Eniac generator
    - m= 10^8 +1
    - A= 23
    - C= 0
  - Simple and efficient to implement
  - Modest statistical quality (small multiplier, sequential correlation)

Lehmer generator

- Next X is uniquely defined from the previous value.
  - Sequence starts to repeat at first reoccurence of X
  - Domain of X:n defines the theoretical maximum for the length of sequence (=m)
- Conditions for reaching the maximum cycle are known
  - If q divides m (being prime or 4), a-1 =0 mod q
  - C and m have no common divisors (and c is nonzero)

Lehmer generator

- (Counter)examples for maximum cycle conditions
  - Let m=8, c=3
  - If a-1 =0 mod 2 and a-1=0 mod 4=> a=5
    - 0->3->18=2->13=5->28=4->23=7->38=6->33=1->0
  - If a=3 (a-1=0 mod 2)
    - 0->3->12=4->15=7->24=0
  - If c=0, 0->0 for all m, a

Lehmer generator

- If c=0, maximal cycle is not possible X=0 maps to 0 always)
- Theoretical maximal cycle (when c=0) is m-1.
- Can be reached if and only if
  - m is prime
  - a is so called primitive element mod m
- In practice a can be defined only experimentally
  - Prime modulus multiplicative congruental generator

Lehmer generator

– Popular basic generators in practice
– Conceptually simple arithmetics
– 2^31-1 (maxint) is prime
– Portable implementation simple (for a small enough using double precision arithmetics if 64 bit integers are not supported)
– Well studied and known

Lehmer generator

```
real(dp),parameter :: m=2._dp**31-1._dp

m_1=1._dp/m
a=16807._dp

real(wp) function random()
seed=modulo(seed*a,m)
random=seed*m_1
return
end function random
```

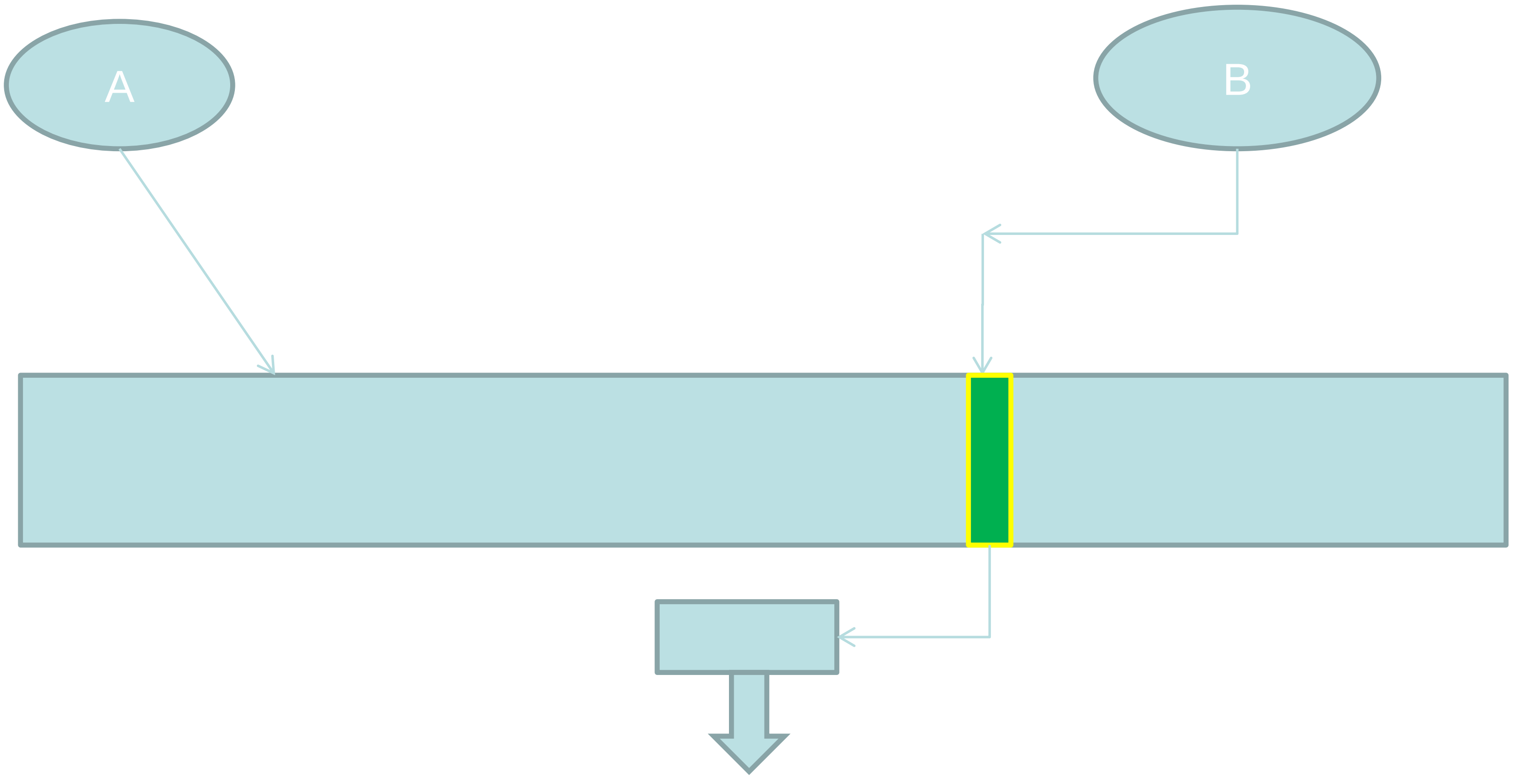
Combined generators

- Needed in the era of 16-bit processors, (Wichman-Hill)
- Uses several generators with short cycles
  - Take cycles m_1, m_2 ja m_3
  - Produce streams X_i and $U_i = X_i/m_i$
  - Set $U = U_1+U_2+U_3 \mod 1$
- With appropriate choices the cycle is $m_1*m_2*m_3$
  - Fully standard (32-bit) arithmetics (if $m_i<2^{14}$)

Shuffled generators

- Used both for longer cycles and reduced serial correlation
  - Generate random numbers with method A to a table
  - Using generator B to select value from the table (for output) and replace it with new value from A
  - Requires an initialization, some memory and two random number for each output value
  - Cycle can be longer (but how much)

Shuffled generator



State of the Art

– Current de facto standard is Mersenne Twister
  - Developed at late1990s
  - Very long cycle (2^ 19937 -1)
  - Best known serial correlation properties
  - Needs a working memory (and initialization) of 624-words
  - Available for several languages

Mersenne twister

- The main ideas
  - X_(N+1) = F(X_N,…, X_(N-623))
    - ”State vector” has 624*32 = 19968 bits
    - Theoretical maximal cycle would go through all states
    - Ruling out some bits of X_(N-623) and the zero state from possible states we get the wanted length of theoretical maximal cycle (Mersenne prime which gives the name)

Mersenne twister

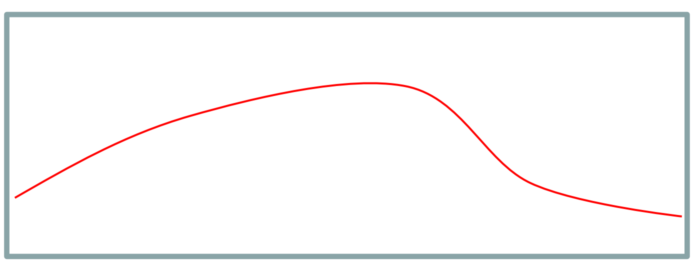
- We need an F, that
  - Is computationally light
  - Leads to reaching the maximal cycle
- Can be found in the family of
  - X_(N+1) = X_N*A_0 + … X_(N-k) * A_k
  - A_i:s are coefficient matrices
  - The family has theory for maximum cycles
  - Found F with only three A:s with non zero values
    - I.e. only three distinct old X values are used on each round.

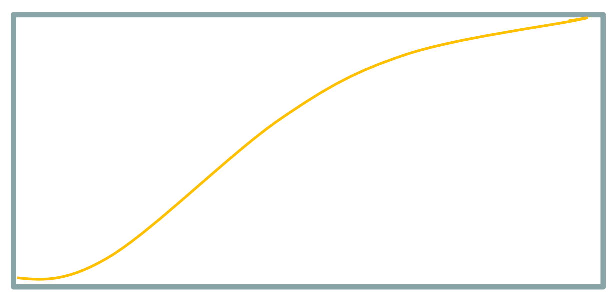
Mersenne Twister

– Method produces a very long cycle
– Is computationally relatively light
– Serial correlation has to be addresed
  • K-test: take k significant bits from successive random numbers
  • For how many successive numbers the above sequence is uniformy distributed (for given k)
  • This can be affected shuffling bits in the output
  • Cycle (and X values) are not touched, only output

Random numbers and probability distributions

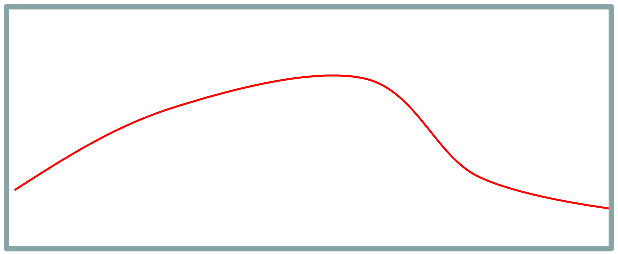
- How to generate random numbers with given probability distribution function (pdf).
- Method of inverse probability
  - Let f be a given pdf. It has a cumulative probability function F: x-> (0,1).

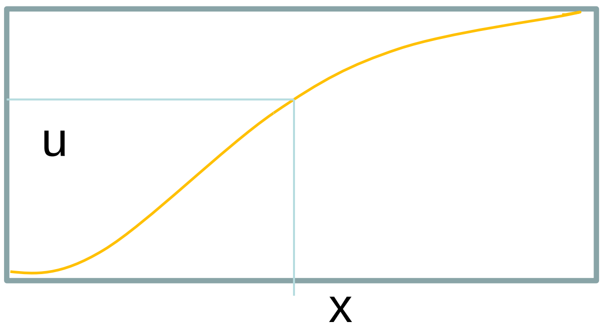




Inverse probability method

- Pick u from Unif (0,1)
- Set x = F^(-1) (u).
- Pdf of x is f.
- We have to know F^(-1) in closed form



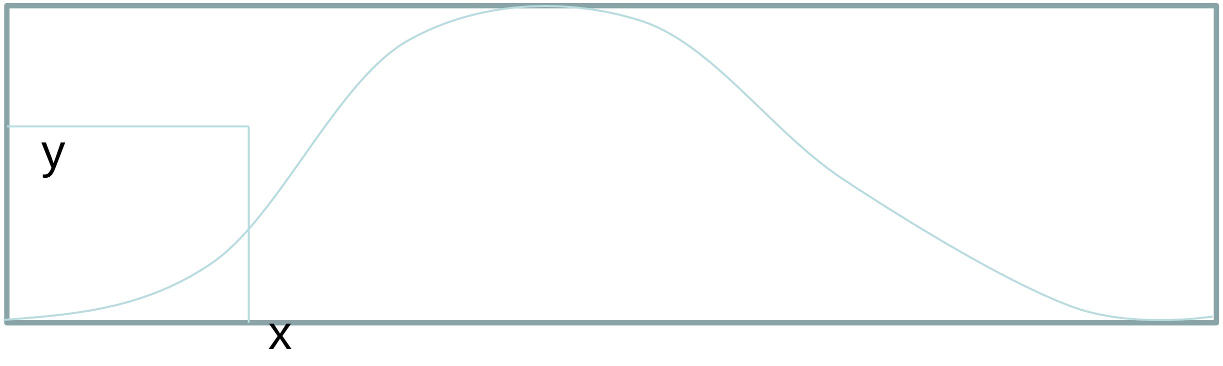


Inverse probability method

- Consider exponential distribution
  - Pdf f. is f(x) = a e^(-ax)
  - Cumulative pf is F(x) = 1- e^(-ax)
  - So F^(-1) (U) = - ln(1-U)/a
  - Numbers obeying exponential pdf are obtained generating U ~ Unif(0,1) and reporting
    - Either –ln(1-U)/a
    - Or –ln (U)/a if U>0 always

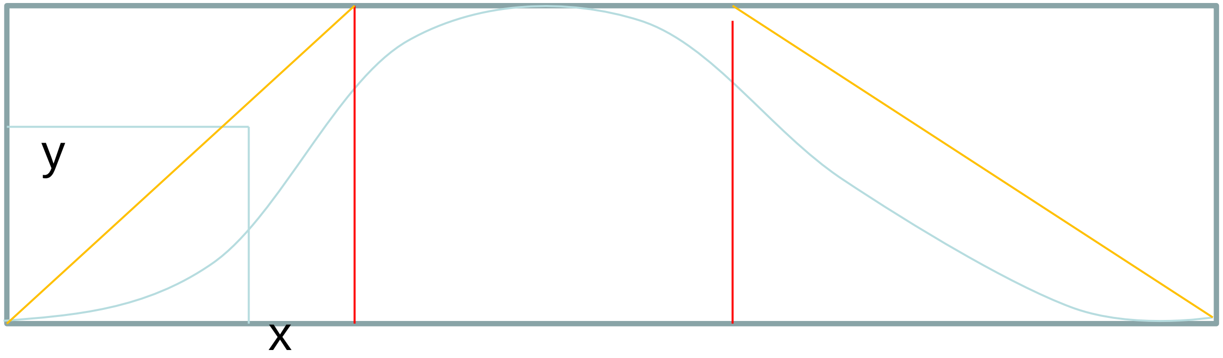
Elimination method

– General method that requires only pdf values
  - Let f be a pdf supported on (a,b) with values 0<f<c.
  - Pick x in Unif(a,b), y in Unif(0,c).
  - If y< f(x), accept x.
  - Else reject x and pick new values for x,y



Elimination method

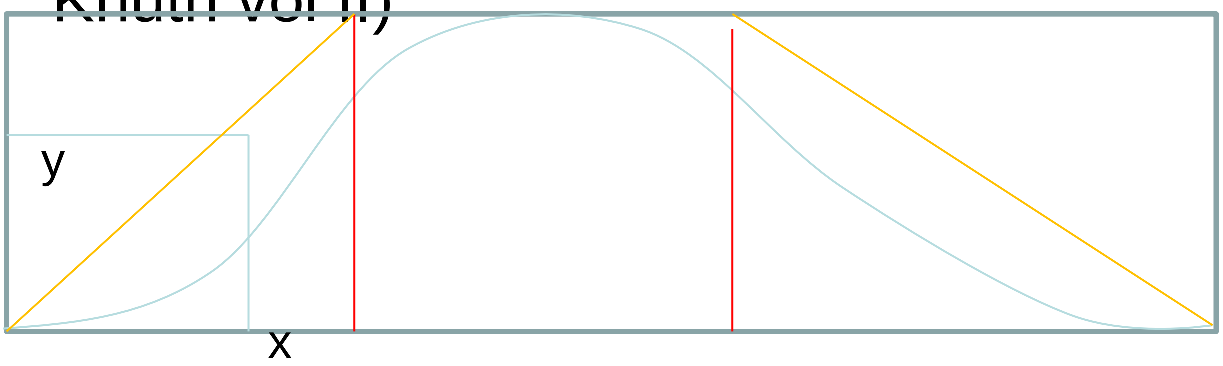
– Method is most efficient when there is least amount of rejections
  - One can divide (a,b) to subintervals and/or change the pdf of y to approximate f better.
  - If f< cg (on some subinterval), g is a known pdf, pick x from g-distribution and y from Unif(0, cg(x))



Elimination method

– When using subintervals

- First one has to draw which subinterval to select for x (probabilites computed beforehand)
- Then draw x from g corresponding to subinterval and y Unif(0,cg(x)) and test for y<f(x).
- Subdivision of interval can be an art (Marsaglia, ks Knuth vol II)



Summary

– Deneration of random numbers has over 60-years of history
  - Tested and known generators well available
  - Dont try to do it yourself
  - Do not use unknown and undocumented generator (details, references missing) without testing (vs the ”secret” generator of IBM PC:s Basic language)
  - You have to understand the generator to make controlled replications