STATISTICAL SIMULATION AND NUMERICAL PROCEDURES

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Contents

1. Introduction
2. Random Number Generation
   2.1. Linear Congruential Generators
   2.2. Other Sources of Uniform Random Numbers
3. Non Uniform Random Variate Generation
   3.1. General Methods
      3.1.1. The Inverse Method
      3.1.2. The Composition (Mixture) Method
      3.1.3. The Acceptance-Rejection Method
   3.2. Other Methods
      3.2.1. Ratio-of-uniform Method
      3.2.2. Simulation of some Particular Distributions
      3.2.3. Simulation of Some Multivariate Distributions
4. The Use of Simulation in Statistics
   4.1. Estimation of Parameters via Simulation
   4.2. Use of Simulation in Hypotheses Testing
   4.3. The Bootstrap Technique
5. Use of Simulation in Numerical Calculation
   5.1. Generalities on the Monte Carlo Method
   5.2. Evaluating an Integral
      5.2.1. Crude Monte Carlo
      5.3. Variance Reduction Techniques
         5.3.1. Importance Sampling
         5.3.2. Antithetic Variates
         5.3.3. Control Variates
      5.4. Solving Operatorial Equations
         5.4.1. Solving Systems of Linear Equations
         5.4.2. Solving Integral Equations
   5.5. Monte Carlo Optimization
   5.6. Markov Chain Monte Carlo

Glossary
Bibliography
Biographical Sketch

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Summary

The paper presents in short the main questions related to the use of simulation in studying statistical problems and solving some classes of numerical problems. First, methods for simulating various types of statistical distributions are presented. Then, some applications of simulation in statistics, including bootstrap techniques, are also discussed. A special attention is paid to Monte Carlo techniques and the Markov Chain Monte Carlo method. References contain only some of the representative or recent publications.

1. Introduction

The term simulation represents today science of a wide class of problems, solved or analyzed via computers. There are many ways to define and understand simulation but all of them assume the use of random numbers to perform a computer experiment for solving some mathematical or practical problem. In this article, the word simulation is also associated with terms like Monte Carlo techniques and resampling techniques, the last one involving statistical problems.

Random numbers are sampling values on the uniform distribution over \((0, 1)\) which has the probability density function (pdf)

\[
f(u) = \begin{cases} 
1, & \text{if } u \in (0,1) \\
0, & \text{otherwise.}
\end{cases}
\]

(Note that it makes no difference if we consider the interval \((0,1)\) as being open or closed at any of its limits).

The following proposition (due to Khintchine) plays a great role in simulating non-uniform random variates.

**Theorem 1:** If \(X\) is a random variable having the cumulative distribution function (cdf) \(F(x)\), \(x \in \mathbb{R}\), and \(U\) denotes the random variable uniformly distributed over \((0,1)\), then the random variable \(F^{-1}(U)\) (with \(F^{-1}\)-the inverse of \(F\)), has the cdf \(F\).

In other words, this theorem gives a general method for simulating a sampling value \(x\) of the random variable \(X\) when we have a sampling value \(u\) of \(U\), namely, \(x = F^{-1}(u)\). That is why the next chapter will be dedicated to simulating random numbers. The same theorem suggests that there could be various methods which transform sequences of random numbers into non-uniform variates. Thus, another chapter will discuss these methods.

Since one purpose of this paper is to discuss the use of simulation in solving statistical problems, one section is devoted to the bootstrap method and some applications. The Monte Carlo method for solving various numerical problems is introduced in another
chapter. Some applications of the so-called Markov Chain Monte Carlo are also presented.

2. Random Number Generation

Random numbers, i.e. sampling values on the random variable $U$ uniformly distributed over $(0,1)$ (denoted $U \sim (0,1)$), are very important for the problems to be treated in this paper.

The aim of this chapter is to present in short some methods for generating with the computer sampling values on the random variable $U$, which are independent and uniformly distributed over $[0,1)$. As Knuth and other authors have shown, the computer calculations necessary to produce good random numbers, require first to generate uniformly distributed integers over some interval $[0,m)$, and then to divide this by $m$ in order to obtain the required random number. The calculations needed to produce uniformly distributed integers in $[0,m)$ must be simple. In other words, the generation algorithm must have a low complexity, both regarding computing time and memory complexities. Details on random number generation are found in many books (see for instance Devroye-1986, Ermakov-1971, Gentle-1998, Ripley-1986 and Ross-1997).

2.3. Linear Congruential Generators

A linear congruential generator is of the form

$$x_n = \left(\sum_{i=1}^{k} a_i x_{n-i} + c\right) \mod m, \quad x_n \in \mathbb{N},$$  \hspace{1cm} (1)

where $m$ is a large positive integer, $k \leq n$, and $a_i, x_i, i = 1, \ldots, k, c$ are given constants, all chosen such that the produced numbers $x_n, n > k$ are integers uniformly distributed over the interval $[0, m-1)$ and $\mathbb{N}$ is the set of natural numbers. Then the uniform $U[0,1)$ random numbers are obtained as

$$u_n = \frac{x_n}{m}. \hspace{1cm} (1a)$$

The usual linear (mixed) congruential generator is the one with $k = 1$, i.e. $x_{n+1} = (a x_n + c) \mod m$. If $a$, $c$ and $m$ are properly chosen, then, in this case, $u_n$ "look like" they are randomly and uniformly distributed between 0 and 1. Even if this linear congruential generator has a low complexity, the most used is the multiplicative congruential generator

$$x_{n+1} = (a x_n) \mod m. \hspace{1cm} (2)$$

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If \( x_0 \neq 0 \) is prime with \( m \), and \( a \) is a primitive root \( \mod m \), close to \( \sqrt{m} \), then the numbers \( u_n \), produced by this generator have a large period \( \lambda \), (defined as the minimum \( \lambda \) such as \( x_n = x_{n+\lambda} \)), they are approximately uniform \((0,1)\) distributed and have a small serial correlation coefficient \( \rho = \text{corr}(u_n, u_{n+1}) \forall n \) (i.e. are almost independent). Of course, the modulus \( m \) must be very large (usually close to the computer word, i.e. close to \( 2^{31} \)).

In simulation we use sequences of random numbers \( u_1, u_2, \ldots, u_n \) produced by a random number generator. These numbers must pass any test which assumes that they are uniformly distributed and stochastically independent. It is obvious that a random number generator cannot produce "pure" random numbers to pass the mentioned tests. Therefore we call them pseudo-random numbers. A "good" random number generator must produce sequences close to pure random numbers. A linear congruential generator cannot produce good random numbers. It can be used when there is no need to perform very accurate calculations or to obtain exact solutions to the problems.

One trouble with using pseudorandom numbers produced by a linear congruential generator is that pairs \( (u_i, u_{i+1}) \) or triplets \( (u_i, u_{i+1}, u_{i+2}) \) are lying on lines or planes (i.e. have a lattice structure). This means that these generators must be used with care in numerical calculations. In order to obtain "better" random numbers from a uniform pseudo-random number generator, the numbers produced by the generator must be transformed. If we consider the binary representation of the numbers \( u_i \), then one way to obtain better numbers is to use the bit stripping, i.e. to obtain the new numbers by selecting some bits from the sequences of bits representing previous given numbers (e.g. odd bits or even bits, etc).

### 2.4. Other Sources of Uniform Random Numbers

Note that if in (2) we take \( a^k \) instead of \( a \) and start with \( x_s \), then the sequence of pseudo-random numbers obtained is \( x_s + x_{s+k} + x_{s+2k}, \ldots \) and therefore, for various values of \( s \), the corresponding stream can be used by one processor in a parallel architecture.

**Shuffling random numbers**: A way of improving the quality of a uniform pseudo-random number generator is to define the new number \( y \) by mixing (or shuffling) two generators \( G_1, G_2 \). One mixing algorithm (due to MacLaren and Marsaglia) is:

Take an array (i.e. a table) \( \begin{array}{c} T[1 \ldots k], k = \text{fixed} \end{array} \) and initialize (fill in) it using \( G_1 \);
generate with \( G_2 \) a random index \( j \in \{1, 2, \ldots, k\} \); take \( y \leftarrow T[j] \); generate \( x \) with \( G_1 \), and put \( T[k] = x \).

(The expression \( a := b \) means that \( b \) is assigned to \( a \)). The better generated number is \( y \). This mixed generator can have a larger period and can break up the lattice structure.
of the generated sequence \( \{ y_i \} \). If instead of two generators we use only one, 
\( G = G_1 = G_2 \), then the above algorithm (called Bays-Durham shuffling of random 
numbers) can be easily changed by generating only one \( x \) in the initial step and 
determining \( j \) by the "bit stripping" procedure mentioned before.

**Lagged Fibonacci sequences:** Apart from linear congruential generators, another way 
of generating random numbers is to use the *lagged Fibonacci generator*, defined as

\[
x_i = (x_{i+j} + x_{i-k}) \pmod{m}
\]

which, when \( m \) is prime and \( k > j \), gives a period close to \( m^k - 1 \).

**Inversive congruential generators:** This method produces uniform integers over 
\([0, m-1]\) by the relation

\[
x_i = \left( ax_{i-1}^{-1} + c \right) \pmod{m}
\]

where \( x^{-1} \) denotes the multiplicative inverse modulo \( m \) if it exists, or else is 0. Even if 
these inverting generators imply computational difficulties, they promise to give high 
quality random sequences.

**Matrix congruential generators:** Such a generator is of the form

\[
x_i = (A x_{i-1} + C) \pmod{m}
\]

where \( x_i \) are vectors of dimension \( d \) and \( A \) and \( C \) are \( d \times d \) matrices. This kind of 
generators are important when parallel computers are used to produce correlated 
random vectors.

**Feedback shift register generators:** Such a generator takes into consideration the 
binary representation of integers in registers of the computer. If \( a_i, i = 1, \ldots, p \), denote 
the binary digits of the random number, and \( c_i \) are given (not all zero) binary digits, 
then the digits \( a_i \) of the new generated number are produced by

\[
a_i = (c_p a_{i-p} + c_{p-1} a_{i-p+1} + \ldots + c_1 a_{i-1}) \pmod{2}.
\]

This generator was introduced by Tausworthe. In practice it has the form

\[
a_i = (a_{i-p} + a_{i-p+q}) \pmod{2}
\]

or, if we denote \( \oplus \), the *binary exclusive-or operation*, as addition of 0's and 1's modulo 
2, equation (5a) becomes
\[ a_i = a_{i-p} \oplus a_{i-p+q}. \] (5b)

Note that this recurrence of bits \( a_i \)'s is the same as the recurrence of random numbers, (interpreted as \( l \)–tuples of bits), namely,

\[ x_i = x_{i-p} \oplus x_{i-p+q}. \] (6)

If the random number has \( l \) binary digits \((l \leq p)\), and \( l \) is relatively prime to \( 2^p - 1 \), then the period of the \( l \)–tuples (i.e. of the sequence of generated numbers) is \( 2^p - 1 \). A variation of the Tausworthe generator, called generalized feedback shift register \((GFSR)\), is obtained if we use a bit-generator in the form \((5a)\) to obtain an \( l \)–bit binary number and next bit-positions are obtained from the same bit-positions but with delay (by shifting usually to the left). A particular GFSR is

\[ x_i = x_{i-3p} \oplus x_{i-3q}, \quad p = 521, \quad q = 32 \quad \text{which gives a period } 2^{521} - 1. \]

Another generator of this kind is the so-called twisted GFSR generator, which recurrently defines the random integers \( x_i \) as

\[ x_i = x_{i-p} \oplus A x_{i-p+q} \] (6a)

where \( A \) is a properly chosen \( p \times p \) matrix.

**A practical remark:** Apart from shuffling random numbers as mentioned above, some other simple combinations could be used to produce "good" random numbers. Thus, if we use the following three generators

\[ x_i = 171x_{i-1} \pmod{30269}, \quad y_i = 172y_{i-1} \pmod{30307}, \quad z_i = 170z_{i-1} \pmod{30323} \]

with positive initializations (seeds) \((x_0, y_0, z_0)\) and take uniform \((0, 1)\) numbers such as

\[ u_i = \left( \frac{x_i}{30269} + \frac{y_i}{30307} + \frac{z_i}{30323} \right) \pmod{1} \]

it can be shown that the sequence of \( u_i \)'s has a period of order \( 10^{12} \).

### 3. Non Uniform Random Variate Generation

In this chapter we assume that a uniform \((0, 1)\) random number generator called \texttt{rnd} is given. The aim of this chapter is to present methods and algorithms which transform sequences of random numbers \( u_1, u_2, \ldots, u_n, n \geq 1 \) into a sampling value of a given random variable \( X \) which has a cdf \( F(x) \). (For further information see Devroye-1986, Gentle-1998 and Ross-1997).
3.3. General Methods

3.3.1. The Inverse Method

Theorem 1 leads to the following algorithm (the inverse method):

generate $u$ with \texttt{rnd}; take $x := F^{-1}(u)$.

The following list gives some examples of the inverse method:

<table>
<thead>
<tr>
<th>Distribution</th>
<th>cdf</th>
<th>Inverse</th>
</tr>
</thead>
<tbody>
<tr>
<td>exp($\lambda$)</td>
<td>$F(x) = 1 - e^{-\lambda x}, x &gt; 0, \lambda &gt; 0$</td>
<td>$x := -\ln(u)$</td>
</tr>
<tr>
<td>Weib$(0,1,\nu)$</td>
<td>$F(x) = 1 - e^{-x^\nu}, \nu &gt; 0$</td>
<td>$x := (-\ln(u))^{1/\nu}$</td>
</tr>
<tr>
<td>Cauch</td>
<td>$F(x) = \frac{1}{\pi} \arctan \left( x + \frac{\pi}{2} \right), x \in \mathbb{R}$</td>
<td>$x = \tan \pi (u - \frac{1}{2})$</td>
</tr>
<tr>
<td>Pears XI</td>
<td>$F(x) = 1 - \left(\frac{1}{1 + \alpha x^\nu}\right)^\nu, x &gt; 0, \nu &gt; 0$</td>
<td>$x = \frac{1}{u^{1/\nu}}$</td>
</tr>
</tbody>
</table>

(The abbreviations are: exp for exponential; Weib for Weibull; Cauch for Cauchy; Pears XI for Pearson type XI).

In the multivariate case, there is a generalization of Theorem 1 which gives a similar algorithm for simulating a sampling value $x = (x_1, x_2, \ldots, x_k)'$ of the $k$-dimensional random vector $X$ which has the cdf $F(x)$. Let us denote

$F_i(x_i) = P(X_i < x_i), F_j(x_j) = P(X_j < x_j | X_{j-1} = x_{j-1}, \ldots, X_1 = x_1), 1 < j \leq k.$

The algorithm is (the multivariate inverse method):

generate $u$ with \texttt{rnd};
take $x_1 = F_1^{-1}(u)$
for $i := 2$ to $k$ do
begin
Generate $u$ with \texttt{rnd}; take $x_i = F_i^{-1}(u)$;
end.

An inverse algorithm for simulating a finite discrete random variate having probability distribution
\[ X = \left( \begin{array}{cccc}
   a_1 & a_2 & \ldots & a_n \\
   p_1 & p_2 & \ldots & p_n 
\end{array} \right) \]

is:

calculate \( F_i = \sum_{\alpha=1}^{i} p_{\alpha} \), \( 1 \leq i \leq n \); take \( i := 0 \);

generate \( u \) with \texttt{rnd};

\textbf{repeat}

\( i := i + 1 \);

\textbf{until} \( u < F_i \);

take \( x := a_i \).

The loop in the algorithm searches for the value of index \( i \); this can be better done by using the \textit{binary search} technique.

\begin{itemize}
  \item 
  \item 
  \item 
\end{itemize}

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\begin{itemize}
  \item \textbf{Bibliography}
\end{itemize}


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**Biographical Sketch**

**Ion Văduva** is a professor of Faculty of Mathematics at the University of Bucharest, Romania. He was born on November 25, 1936 in Romania and graduated in Mathematics from the University of Bucharest in 1960. He received Ph.D. in Mathematical Statistics in 1968, from the Center of Mathematical Statistics of the Romanian Academy and M.Sc. in Automatic Computation in 1969, from the University of Manchester, Institute of Science and Technology (UMIST).

His research interests and activities are in the areas of Computer Simulation and Modeling, Mathematical Statistics and Data Analysis, Operation Research, Computation. He teaching experience spans the following subject: Computer Simulation and Monte Carlo Methods (for under-graduates), Software Reliability (for undergraduates), Computerized Stochastic Models (for M.Sc. students), Multivariate Statistical Analysis (for postgraduates and undergraduates), Background of Computer Science (for undergraduates). Since 1971 he has been supervising research work of scholars for Ph.D. He published more than 90 papers in various Romanian or International journals and 18 books or textbooks (all in Romanian). He received the "Simion Stoilow" Prize of the Romanian Academy in 1977. He is Associate Chief Editor of "Analele Universitatii Bucuresti Matematica-Informatica". He was a Visiting Researcher at the following places GMD-Bonn (1974,1976), Sheffield Hallam University (1972), TH-Darmstadt (1993), Alborg University (1998).

Professor Văduva is a Member of Biometric Society, International Association of Statistical Computing (IASC) and American Mathematical Society (AMS).