Randomness Characterization in Computing and Stochastic Simulations

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Introduction

- Physics: classical (deterministic) → modern (quantum physics)
- Mathematics: Lebesgue measures → probabilistic measures
- Computations: deterministic → pseudo random and stochastic
- Simulations: computations → Monte Carlo and stochastic
- Predictions: simulations → stochastic and probabilistic
- Practical considerations
  - exact rigorous computations are not always possible
  - stochastic simulations often offer practical solutions
  - reproducibility often restricted to confidence levels
- Applications to direct and inverse problems

Randomness

- Mathematics

  Randomness applies only to processes
  'Lawlessness' ≈ algorithmic incompressibility
  Axiomatization in terms of non-deterministic processes

- Physics

  Unpredictable chaotic random processes
  Unpredictable quantum random processes
  Natural unpredictable processes

- Computational Science

  Unreproducible computations
  Algorithmic probabilistic entropy
  Computer code of shortest description

Distributional Aspects

Randomness in data sequences does not obviously imply low discrepancy nor a uniform distribution as can easily be seen in sample spatial and spectral plots.

Spatial plots of random numbers show clumping effects in places and open gaps in other places. Such spatial discrepancies are usually unrelated to the distributional properties of the sequences. Some quasi random sequences are especially designed to have low discrepancy characteristics (without necessarily being random).

Well known procedures can be used to transform a random variate y with a distribution p(y) into another variate x with distribution p(x). The transformation follows the usual approach with Jacobians in integrals:

$$p(y)dy = p(x)\left|\frac{\partial x}{\partial y}\right|dy$$

which can obviously be simplified with uniform distributions.

Gibbs Sampler

A Gibbs sampler is a technique for generating random variables indirectly from some (marginal) distribution without calculating the density.

In conventional Monte Carlo applications, random variables are required with some assumed distribution often derived somehow from other random variables having known distributional characteristics. Most random number generators are designed to produce a uniform distribution of random numbers over the unit interval (0, 1).

In practice, it really depends on the application context to decide on the most appropriate Gibbs sampler. For example, in digital image restoration, the Gibbs sampler is often based on immediate pixel neighborhoods for the Markov random field (see e.g. Geman & Geman, 1984).

True Random Number Sequences

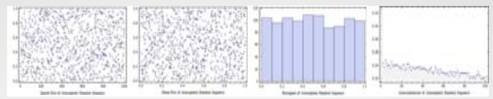
Basis: physical phenomena 'known' to be random

Examples:

HotBits service based on radioactive decay
www.fourmilab.ch

Quantis generated by quantum mechanical process
www.idquantique.com

Random generated by atmospheric noise (radio static)
www.random.org

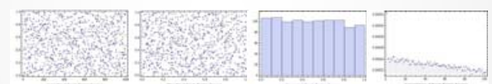


Pseudo Random Number Sequences

Basis: computational rounding-off or related errors

Common Methodology:

most often using some linear congruential model applied recursively such as
$x_n \equiv c \odot x_{n-1}$ modulo ρ (for large prime ρ and constant c)
or lagged Fibonacci congruential sequence, such as
$x_n \equiv x_{n-p} \odot x_{n-q}$ modulo ρ (for large primes ρ and p, q)
in which ⊙ usually stands for ordinary multiplication



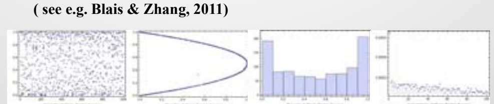
Chaotic Random Number Sequences

Basis: computational chaotic processes

Common Methodology:

Using the Logistic equation (with parameter equal to four)
$x_n = 4\, x_{n-1}\,(1 - x_{n-1})$ for n = 1, 2, 3, …
using some random seed x_0 in (0, 1), which exhibits randomness with a density
$\rho(x) = 1 / \pi\, [x\,(1 - x)]^{1/2}$ (not uniform distribution)

Other similar procedures given in the literature
(see e.g. Blais & Zhang, 2011)



Quasi Random Number Sequences

Basis: computational sequences of low discrepancy

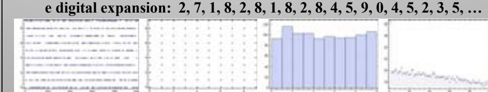
Varied Methodology:

Van der Corput (binary) sequences:
1, 10, 11, 100, 101, 111, … ⇒ 0.1, 0.01, 0.11, 0.001, 0.101, 0.111,…

Halton (binary) sequences:
½, ¼, ¾, 1/8, 5/8, 3/8, 7/8, 1/16, ….

π digital expansion: 3, 1, 4, 1, 5, 9, 2, 6, 5, 3, 5, 8, 9, 7, 9, 3, 2, 3, 8, …

e digital expansion: 2, 7, 1, 8, 2, 8, 1, 8, 2, 8, 4, 5, 9, 0, 4, 5, 2, 3, 5, …



Expected Variances in Monte Carlo Simulations

Numerical Recipes state:

$$\int_V f\, dV \approx V\langle f\rangle \pm \sqrt{\left(\langle f^2\rangle - \langle f\rangle^2\right)/N} \qquad \text{implying a variance } O(1/N)$$

In general, then with N data values,
True Random Numbers ⇒ O(1/N) error variance
Pseudo Random Numbers ⇒ O(1/N) error variance
Chaotic Random Numbers ⇒ O(1/N) error variance
but
Quasi Random Numbers ⇒ $O((\ln N)^{2s}/N^2)$ error variance
for spatial dimension s, and apparently under the so-called 'superefficiency conditions with dynamical correlations for large N'
Chaotic Random Numbers ⇒ $O(1/N^2)$ error variance
(See e.g. Umeno 2000, 1999, 1998 and Blais & Zhang, 2011)

Adaptive and Recursive Monte Carlo Strategies

- Importance Sampling

  Essentially by analyzing the nature of the integrand
  Variable of integration may be transformed for better results
  Significant improvements are possible with complex problems

- Stratified Sampling

  Largely by analyzing the characteristics of the integration domain
  Segmenting the domain may be considered for different sampling
  Small sample means often contribute to better overall results

- Mixed/Adaptive Strategies

  Both importance and stratified sampling can often be combined into optimal mixed and/or adaptive implementations, especially in high-dimensional applications

Markov Chain Monte Carlo Modeling

Sequences of Monte Carlo simulations can be modeled as Markov chains with appropriate transition probabilities. Explicitly, considering a sequence of such simulations $\{S_0, S_1, S_2, S_3, \ldots, S_{k-1}, S_k, S_{k+1}, \ldots\}$, then

$$E[S_k \mid S_{k-1}, S_{k-2}, S_{k-3}, \ldots] = E[S_k \mid S_{k-1}] \quad \text{for all } k=1, 2, 3, \ldots$$

The Markovian properties imply that only the immediate past transition probabilities need to be considered in current simulations. This greatly simplifies the modeling and the analysis.

The transition probabilities are often modeled in terms of decreasing 'temperatures' to simulate annealing processes converging to some appropriate uniform distribution. This is described as 'stochastic relaxation' in digital image and similar restoration.

Applications and Conclusions

In Monte Carlo volume estimation and stochastic simulations, the randomness requirements can be quite different:

In the former, randomness is often secondary to the distributional aspects of the data sequences. In fact, quasi random numbers of the deterministic type can give the best results , essentially $O(1/N^2)$ with N data values.

In the latter, however, randomness can be critical for the probabilistic aspects of the simulations. For instance, in digital image restoration, the equivalence of the Gibbs distribution and the Markov random field is explicitly used in the stochastic modeling and restoration.

Applications abound in geomatics, geoscience and elsewhere (see e.g. Blais & Zhang, 2011; Blais, 2010; Blais, 2009; Blais et al, 2008)