Chapter 0

Introduction and Summary

0.1. Introduction -

Monte Carlo is a small town in Monaco near Italy. The name 'Monte Carlo Methods' is associated with games of chance those played in the famous casinos of Monte Carlo. Monte Carlo methods have been used for centuries, but this method is systematically developed after 1944. The name 'Monte Carlo' was coined by Stan Slaw Ulam during the Manhattan project of second war. The method is named as 'Monte Carlo Method', because of the similarity between game of chance and gambling in Monte Carlo town. It is also called as method of statistical trials. Now, Monte Carlo method is used routinely in several computational sciences.

Basically, Monte Carlo method is a numerical method which uses random numbers to compute quantities of interest. This method provides approximate solutions to ~~a~~ various mathematical problems by performing simulations on a computer. Hence, it is also described as statistical simulation method. Statistical simulation is a general term, which utilizes sequence of random numbers.

Monte Carlo method is one of the fundamental tools in computational Statistics. Random number generation is the central part of the Monte Carlo method. In many applications of Monte Carlo method the only requirement is that the system be described by probability density functions or probability mass functions. Once the probability distribution is known, simulation can be proceeded by random sampling and desired result is obtained.

It is important to note that, this method is used to solve the numerical problems which are impractical or impossible to solve by traditional methods.

0.2. Importance –

Monte Carlo methods are used when mathematical problems are complicated to solve analytically. It gives approximate numeric solution to such problems. Monte Carlo methods are used widely in different branches of science like Physics, Chemistry, Kinetics etc. Computation of complex integral is one of the major applications of Monte Carlo method. Suppose we have to compute normal CDF $I(t) = \int_{-\infty}^{t} \frac{1}{\sqrt{2\pi}} e^{-x^2/2}\, dx$. This integral can not be solved analytically. In such cases, we switch to numerical techniques for solving integral. This integral can be evaluated by using independently identically distributed (i.i.d.) variables. To do the same generate $X_1, X_2, \ldots\ldots, X_n$ i.i.d. N(0, 1) and the value of integral is approximated as

$$\hat{I}(t) = \frac{1}{n}\sum_{i=1}^{n} I_{X_i \le t} \quad \text{where, } I_{X_i \le t} = \begin{cases} 1 & X_i \le t \\ 0 & \text{otherwise} \end{cases}$$

We note that, $\hat{I}(t)$ is an unbiased estimator of $I(t)$. It is obvious that $\hat{I}(t)$ is not exactly equal to value of $I(t)$. However, sound statistical theory supports to the fact that as n increases $\hat{I}(t)$ approaches to $I(t)$. Now – a - days high speed computing facility is available. Therefore there is no problem to choose 'n' large enough. Thus, using random samples generated from various known distribution, it is possible to answer many problems which otherwise are difficult to attempt analytically.

Monte Carlo method is also used in computing various mathematical equations. Monte Carlo tests are used when distributions of the test statistic under null hypothesis is unknown.

Markov Chain Monte Carlo (MCMC) is an effective technique to simulate from distributions, which are not easy by routine method. It is useful to generate random samples from multivariate as well as mixture of the distributions. Generation from a non-standard distribution is a tedious job, but MCMC method does this job easily. Suppose we have to generate G(α, β), when α is not an integer. Here, we can not use inversion or transformation methods to generate random sample from G(α, β) distribution. Notably, MCMC methods give better result in generating from this complex density and have major applications in Bayesian inference.

Thus, Monte Carlo statistical methods based on i.i.d. random variables or based on Markov Chain have now become one of the standard set of techniques used by statisticians. These methods have found number of applications in the area of statistical inference, reliability, design of experiments and many such areas. In fact, it will be not an exaggeration to state that Monte Carlo methods have occupied the whole world of Statistics. In the following, we report review of literature survey related to Monte Carlo methods.

0.3. Literature Survey -

Survey of Literature is classified in three classes as : generation of random sample, Expectation – Maximization (EM) algorithm and Markov Chain Monte Carlo (MCMC) method. Many scholars studied these methods and gave various applications in their literature.

Box and Muller (1958) have discussed a formula for generation of normal variates. Kennedy and Gentle (1980) have described generation of uniform random samples as well as generation of variates of specific distributions like normal, gamma, beta, chi-square, F, t, binomial, Poisson etc.

Devroye's (1986) book 'Non – Uniform Random Generation' is devoted to generation of random samples from various distributions. It is worth to mention that the book was available online. (http://cg.scs.carleton.ca/~luc/rnbookindex.html). He gives very useful information about generation of random samples. The book can be one of the most useful resources on the random number generation.

Another good reference is due to Rubinstein (1981). Also Rubinstein (1982) covers generating random vectors. Gentle (1998) has discussed generation from univariate and multivariate distributions. He also covers Monte Carlo method of integration and variance reduction methods.

Dempster, Laird and Rubin (1977) introduced EM algorithm. They presented maximum likelihood estimation for incomplete data.

Here, Dempster used EM algorithm effectively. Mclachlan and Krishnan (1997) gave more details about EM algorithm. Little and Rubin (2002) have discussed EM algorithm for exponential family of distributions. Casella and Berger (2002) gave EM algorithm with examples.

Lange (2003) discusses EM algorithm in simple way. He also gives better examples which are helpful to understand EM algorithm. In Handbook of Computational Statistics by Gentle (2004), the author presents generalized EM algorithm and its rate of convergence. In the same book, Siddartha Chib discussed concept of MCMC technique. He describes Markov Chain, Metropolis–Hastings (M-H) algorithm and Gibbs Sampler.

Various applications of Monte Carlo methods are studied by Bauer (1958). He discusses applications like computing integral, inverse of matrix and solving differential equations. Casella and George (1992) wrote an excellent article on Gibbs sampler. He illustrated Gibbs sampler by providing some examples. He also gave simple proof of convergence of Gibbs sampler and examples on it.

Chib and Greenberg (1995) have studied very good examples of M–H algorithm. Gamerman (1997) has presented stochastic simulation and Markov chain. He discussed Gibbs sampling and M –

H algorithm. Gilks (1998) explained M–H algorithm for generating N(0,1) samples by various proposed distributions. He compared these samples diagrammatically. Brooks (1998) described updating schemes in MCMC methods. He concentrated on M–H algorithm and Gibbs sampler.

Robert and Casella (1999) wrote excellent book namely 'Monte Carlo Statistical Methods'. The book covers most of the branches of Monte Carlo methods. Generation of random samples, Monte Carlo integration, Markov chain, Monte Carlo optimization methods, various M–H algorithms and Gibbs sampler are described in the book.

Gelfand (2000) described, how Gibbs sampler works? Describe the way Gibbs sampler works. Billera and Diaconis (2001) discussed a geometric interpretation of the M–H algorithm. Yang (2002) studied a Monte Carlo method of integration. He discussed Riemann integrals and complicated boundaries integrals.

Chakraborty (2002a, 2002b) studied Markov chain and MCMC by simple examples. Athreya, Delampady, and Krishnan (2003) wrote good series of four articles. Athreya *et al.* (2003a) described Monte Carlo methods in i.i.d case. Athreya *et al.* (2003b) discussed Monte Carlo methods in Markov chain case. He they presented M – H algorithm, Gibbs sampler and used Gibbs sampler for generation from bivariate normal.

Athreya *et al.* (2003c) have described some statistical concepts and Athreya *et al.* (2003d) discusse~~s~~d applications of M – H algorithm. They use M – H algorithm for generation from gamma distribution having non – integer shape parameter. Recently, Roberts and Polson (2007) have described geometric convergence of the Gibbs sampler in finite and continuous case.

In the present study, we focus on the following.

a) Generation of random samples for standard discrete and continuous distributions.
b) Monte Carlo integration and E-M algorithm.
c) Methopolis - Hastings algorithm and application.
d) Gibb sampler and application.

In the following we report summary of the dissertation.

0.4. Chapter wise Summary -

Chapter 1 contains generation of random samples from several probability distributions. In order to use Monte Carlo method, the basic requirement is a random sample from a suitable distribution. Therefore, it is necessary to study the methods of generating random samples from such distributions. Here, we discuss various methods of generation of non - uniform random numbers. Section 1.1 is introductory and gives description about generation of random numbers.

Section 1.2 presents generation of random samples from discrete distributions. In this section, we discuss generation of samples from a discrete distribution with countable support, Bernoulli distribution, Binomial distribution, Hyper geometric distribution, discrete uniform distribution, Geometric distribution, Negative Binomial distribution and Poisson distribution.

Section 1.3 contains generation of random samples from continuous distributions using inversion method. That is by inverting cumulative distribution function (CDF) of a continuous distribution. Here, we discuss generation of random samples from continuous uniform distribution, Exponential distribution and Cauchy distribution by computing inverse of the CDF. Here, we also cover the generation of random sample from Gamma distribution with integer valued shape parameter.

In Section 1.4, we describe transformation method for generation of random samples from continuous distribution namely; Normal distribution, Chi-square distribution, F distribution, Student's t distribution, Beta distribution, Cauchy distribution, Log-Normal distribution and Double Exponential (Laplace) distribution. Further, we explain the generation from discrete uniform distribution and mixture of the distributions. Results also have been reported to generate samples from various interrelated distributions.

Section 1.5 is devoted to Accept - Reject method of generating observations. In this section, we prove the related result. It is used to generate random samples from Normal distribution. Additionally, we compare Central limit theorem, Box - Muller formula and Accept – Reject method in case of generation of random samples from Normal distribution.

Chapter 2 presents Monte Carlo techniques related to applications of i.i.d. Monte Carlo methods. Section 2.1 is introductory. In Section 2.2, we discuss Monte Carlo methods used in statistical inference. Section 2.3 presents evaluation of integrals by Monte Carlo method. We use uniform density to estimate π. We obtain estimates of π for different sample size.

In Section 2.4, we present concept of importance sampling and use this concept to evaluate the integral. To evaluate the integral, we use various probability distributions. Section 2.5 deals with Expectation – Maximization (EM) Algorithm. In this section, we describe basic idea of EM Algorithm. Further the necessity of EM

Algorithm is discussed in this section. Several examples on EM Algorithm are provided in the same section.

Chapter 3 deals with Markov Chain Monte Carlo (MCMC) method. Section 3.1 is introductory. In section 3.2, we present concept of Markov chain. Here, we discuss various types of chains and classification of states of chain.

Section 3.3 describes generation of Markov chain and law of large numbers for Markov chain. In this section, we introduce Markov Chain Monte Carlo (MCMC) method. Section 3.4 is devoted to Metropolis- Hastings (M- H) algorithm. In this section, we discuss M – H algorithm for independent case and random walk case. We generate samples from non – integer gamma distribution and bivariate normal distribution by using M-H algorithm. To this end, we compare M-H algorithm method with other methods.

Chapter 4 covers Gibbs sampling. Section 4.1 is expository. Section 4.2 and section 4.3 describe concept of Gibbs sampling in multivariate and bivariate case respectively. In section 4.3, we discuss Gibbs Sampler as special case of the M– H algorithm. Further, convergence of Gibbs Sampler is discussed in section 4.4. In this section, we solve some examples on Gibbs sampling. Finally, we discuss areas of future research on Markov Chain Monte Carlo (MCMC) methods.

Silent features of the work reported here are as follows:

(i) Basic results related to generation of random numbers from various discrete and continuous distributions have been provided. Some important algorithms are also presented.

(ii) Standard techniques like inversion . method, transformation method, Accept-Reject method have been illustrated with good number of examples.

(iii) Applications of i.i.d. Monte Carlo methods are discussed and illustrated with variety of problems.

(iv) Markov Chain Monte Carlo Methods; namely M-H algorithm and Gibbs Sampler have been discussed and illustrated with examples.

(v) Computer programs in 'C' have been used to implement some of the important algorithms.

(vi) Use of SYSTAT has been done in addition to the programs developed for M-H algorithm and Gibbs Sampler.