

PROBABILITY ESTIMATION AND ITS
APPLICATIONS

by

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I. Introduction

This thesis is about the estimation of probabilities according to multivariate distributions and its applications. Approximation of multivariate probability integral is a hard problem in general. However, if the domain of probability integral is the multidimensional interval, then the problem reduces to the approximation of multivariate probability distribution function values. The evaluation of probabilities according to multivariate distribution is an important problem in many applications of statistics and related fields. Over the years, several methods have been proposed for the computation of probabilities according to multivariate distributions which can be classified into broad categories, numerical integration, numerical approximations, bounding techniques and simulation. Only a few paper is dealing with the computation of Dirichlet probabilities. Yassae ([48], [49], [50]) computes the probability integral of Dirichlet distribution by computing the probability integral of inverted Dirichlet distribution, Szántai ([44], [45]), used variance reduction simulation techniques to estimate the probability of Dirichlet distribution.

The Dirichlet distribution is one of the important multivariate distributions that appears in many applications, in order statistics, probabilistic constrained programming models, delivery problems. Such applications may be found in Prékopa and Kelle ([33]), Prékopa ([35]), Tiao and Guttman ([46]), Johnson ([20]), Sobel and Uppuluri ([43]), Phillips ([32]), Fabius ([11]), James ([19]), Chotikapanich and Griffiths ([5]) and Goodman and Nguyen ([13]). Another application is the modeling of consumer purchasing behavior for non durable items such as foods and toiletries (Narayanan ([31]) and Chatfield and Goodhardt ([3])). A model for multibrand purchasing behavior is given for the use of multivariate beta distribution for the independent case. Suppose this is a product field with k brands and let the random variables Z_i represent the average rate of purchase of brand i let $W = \sum_{i=1}^k Z_i$ represent a consumer's rate of buying of the product field as a whole. Then the joint distribution of $(X_1, X_2, \dots, X_{k-1})$ follows a Dirichlet distribution where $X_i = \frac{Z_i}{W}$ represents the proportion of a consumer's total purchases devoted to brand i . Another application would be modeling the activity times in a PERT (Program Evaluation and Review Technique) network. A PERT network has a collection

of activities and each activity is usually modeled as a random variable following a beta distribution. A Dirichlet distribution for the entire network follows directly since each marginal distribution of Dirichlet is a beta. Using the properties of the Dirichlet distribution we can see that any subnetwork will follow a Dirichlet distribution. Monhor ([28], [29]) uses the Dirichlet distribution for modeling the activity times of a PERT network and derive's an upper bound for the completion time of the project. More details about the applications of Dirichlet distribution can be found in Kotz, Balakrishnan and Johnson ([23]).

Stochastic simulation has proven itself in practice; it is commonly used for accurate estimations in many problems. However, there are some limitations to the standard stochastic simulation method in many cases. An important class of problems that cannot be efficiently solved using standard simulation is that involving rare events. Since these rare events occur so seldom in a standard simulation the simplest method to estimate the rare event probability is the Crude Monte-Carlo (CMC) simulation method but it needs a very large sample size, what need too much CPU time. This is why different methods and techniques have been developed to estimate rare event probabilities starting at the last decade. Lieber, Rubinstein and Elmakis ([26]) developed the Cross Entropy (CE) method as an adaptive technique for the estimation of reference parameters applied in Importance Sampling (IS) method.

The rare event probability estimation problem is hard to do with CMC simulation when the desired probability, which we will call, is extremely small. In this case the CMC simulation method is very inefficient and simulation takes a very long time. The CMC method consists of simulating the system without making any changes to its stochastic behavior; as a consequence, very few samples will actually hit the rare event. Let we have a sample of size n (X_1, \dots, X_n), say, random observations in which the rare event A may occur; let $P(A) = l$ and the value of a random variable X_i equals one when the rare event is seen in the i -th attempt, and equals zero otherwise. The CMC estimator is simply $\hat{l} = \frac{1}{n} \sum_{i=1}^n X_i$, and the variance of a CMC estimator using n samples is equal to $Var(\hat{l}) = \frac{l(1-l)}{n}$.

Importance sampling is typically presented as a method for reducing the variance of the estimate of an expectation by carefully choosing a sampling distribution (Rubinstein ([37])). For example, the most direct method for evaluating $E_g[f(\eta)] = \int f(x) g(x) dx$ is to sample independent identical distribution $x_i \sim g(x)$ and use $\frac{1}{n} \sum_i f(x_i)$ as the estimate. However, by choosing a different distribution $q(x)$ which has higher density in the places where $|f(x)|$ is larger, we can get a new estimate which is still unbiased and has lower variance. In particular, we can draw $x_i \sim q(x)$ and use $\frac{1}{n} \sum_i f(x_i) \frac{g(x_i)}{q(x_i)}$ which is like approximating $\int f(x) \frac{g(x)}{q(x)} q(x) dx$ with samples drawn from $q(x)$. If $q(x)$ is chosen properly, our new estimate has lower variance. It is always unbiased provided that the support of $g(x)$ and $q(x)$ are the same. In this thesis we always have the same support. The density function $q(x)$ will be chosen from the parametric family of $g(x)$ and $q(x)$ to reduce variance, the CE method will be used to estimate the reference parameters of $q(x)$ which will achieve minimal variance.

Rubinstein ([38]) and Lieber, Rubinstein and Elmakis ([26]) developed the CE method as an adaptive technique for the estimation of reference parameters applied in IS variance reduction technique. The CE method can be viewed as a model-based optimization technique, which involves two phases. (1) Generation of a sample of random vectors according to a specified random mechanism. (2) Updating the parameters of the random mechanism, on the basis of the data, in order to produce a better sample in the next iteration. The significance of the CE method is that it defines a precise mathematical framework for deriving fast, and in some sense "optimal" updating rules, based on advanced simulation theory. Estimation of the probability of rare events is essential for guaranteeing that the performance of engineering systems is adequate. For example, consider a telecommunication system that accepts calls from many customers. Under normal operating conditions each client may be rejected with a very small probability. In order to estimate this small probability the system should be simulated under normal operating conditions for a long time. A better way to estimate this probability is to use IS, in which the system is simulated under a different set of parameters, so as to make the occurrence of the rare event more likely. A major drawback of the IS technique is that the optimal reference parameters to be used in IS are usually very difficult to

obtain. The advantage of the CE method is that it provides a simple adaptive procedure for estimating the near optimal reference parameters, and the CE method enables simulating the system under irregular conditions and estimating the rejection probability for normal conditions. Moreover, the CE method also enjoys asymptotic convergence properties.

The original PERT technique, developed by Malcolm et al. ([27]), is a technique to approximate the expected duration of the project. PERT networks have been used extensively in the business world. Analysis of PERT networks, also known as stochastic activity networks, has received considerable attention in the literature (Elmaghraby, [9]). PERT is based on the concept that a project is divided into a number of activities which are arranged in some order according to the job requirements. A PERT network consists of a set of nodes and arcs, where a node represents the beginning or completion of one or more activities and an activity is represented by an arc (arrow) connecting two nodes in activity-on-arrow (AOA) representation. Activity-on-node (AON) representations have also been used. We use the AOA representation in this thesis. The project starts at the initial node and ends at the terminal node. A path is a set of nodes connected by arrows which begin at the initial node and end at the terminal node. This collection of arcs, nodes and paths is collectively called an activity network. A project is deemed complete if work along all paths is complete. After the development of the network, the next major planning step is the estimation of activity and project times. Typical methods for estimating activity times have been to use point estimates or some sort of ranges or distributions. The type of method used depends on the situation facing the project manager. Hershauer and Nabielsky ([16]) categorize the situations into three major categories, viz., certainty, risk and uncertainty. They further subdivide these categories based on availability of knowledge regarding the mode, range and distribution on the time estimates. They then map the situation and estimations to the appropriate methods to be adopted. If activity times are deterministic, the duration of the project completion time is determined by the length of the longest path in the network. For a stochastic activity network, Kulkarni and Adlakha ([25]) have identified three important measures of performance: (a) Distribution of the project completion time. (b) The probability that a

given path is critical, also known as the "path criticality index". (c) The probability that a given activity belongs to a critical path, also known as the "activity criticality index". Performance measures derived from (a) are the most commonly used; measures and most studies have concentrated on the properties of the completion time of the project Dodin and Sirvanci ([7]), Kamburowski ([21]), Sculli ([39]) among others. Determination of the exact distribution of the completion time of the project is complicated by the fact that different paths are correlated and also because of the need to find the maximum of a set of random variables, as we shall see later. Hence one cannot easily determine the exact distribution of the completion time of the project. The research has branched off primarily in three directions: (1) Exact methods, Martin ([30]), Dodin ([6]), Fisher et al. ([12]), Hagstrom ([15]) and Kulkarni and Adlakha ([25]) are some of the papers that deal with these methods. Most of their results are limited in that they make quite restrictive assumptions. For example Martin ([30]) assumes that the arc duration density functions are polynomial. Hagstrom ([15]) assumes task durations have discrete distributions. (2) Approximating and bounding approaches. These have been the most abundant in the literature. Malcolm et al. ([27]), Sculli ([39]) Golenko-Ginzburg [14]), Dodin ([8]), Sculli and Wong ([40]), and Dodin and Sirvanci ([7]) determine approximations for the distribution and moments of the completion time of the project. Kamburowski ([22]), Shogan ([41]), Kleindorfer ([24]) and Robillard and Trahan ([36]), on the other hand, try to find upper and lower bounds for the distributions and moments of the completion time of the project and Prékopa, Long and Szántai ([34]) describe new bounds and approximations for the probability distribution of the length of the critical path. (3) Simulation methods. These methods have been discussed in the literature by Van Slyke ([47]), Burt and Garman ([2]) and Sigal et al.([42]). Simulation provides a powerful methodology to obtain desired statistics for any network with specified distribution of activities. To obtain reliable results, however, it may be necessary to repeat the experiments several times. Main drawback of the traditional PERT modeling is that the probabilistic characteristics determined for the finishing time of the project are only valid when it is supposed that any activity can be started promptly after finishing all of its predecessor activities. This is possible in the case of scheduling computer tasks, however it is impossible in the case

of architectural project planning what is the most important application area of PERT modeling. We shall introduce a new PERT modeling technique to solve this problem.

The aim of the thesis is to compute the cumulative distribution function values of Dirichlet distribution by using several algorithms and estimate the probability in network models via cross entropy method and completion time estimation in PERT network.

II. Estimation of Probabilities According to Dirichlet Distribution.

The main numerical difficulty in probabilistic constrained stochastic programming problems is the calculation of the probability values according to the underlying multivariate probability distributions. From point of view of the nonlinear programming algorithms to be applied it is preferable to be able to calculate the first and second order partial derivatives of these probability functions according to the decision variables. In this thesis there will be given a solution to the above problems in the case of Dirichlet distribution. The estimation of probabilities according to Dirichlet distribution will be described. A recursive algorithm for the calculation of Dirichlet probability distribution function values up to 7 dimensions will be developed. This procedure is based on a generalization of Szántai's result published in his dissertation for candidate degree of HAS and the Lauricella series expansion. This gives the possibility of application all algorithms for bounding and estimating multivariate normal probability distribution function values developed before by J. Bukszár, A. Prékopa and T. Szántai. In stochastic programming applications one need the gradient vector and Hessian matrix of the multivariate probability distribution function, too. A new algorithm for the Hessian matrix calculation will be given. All these estimations are most effective when the estimated probability value is close to one. However many times one need to estimate small probability values, too. These are called rare event probabilities in the literature, the Sequential Conditioned Sampling (SCS) and Sequential Conditioned Importance Sampling (SCIS) algorithms will be developed to estimate the rare event probabilities of Dirichlet distribution. On the base of an interesting property of the Dirichlet distribution new versions of the SCS and SCIS algorithms will be developed, called SCSA, SCSB, SCISA and SCISB, respectively and modified algorithms need more CPU time but they result

significant variance reduction. Their resultant efficiency will be compared to the simple "hit-or-miss Monte Carlo" simulation method with conventional sampling of the Dirichlet distributed random vectors what we call Crude Monte Carlo (CMC) simulation method.

III. Probability Estimation in Network Models

In the first part, we describe the estimation of rare event probabilities in stochastic networks. The well known variance reduction technique, called Importance Sampling(IS) is an effective tool for doing this. The main idea of IS is to simulate the random system under a modified set of parameters, so as to make the occurrence of the rare event more likely. The major problem of the IS technique is that the optimal modified parameters, called reference parameters to be used in IS are usually very difficult to obtain. Rubinstein ([38]) developed the CE method for the solution of this problem of IS technique and then he and his collaborators applied this for estimation of rare event probabilities in stochastic networks with exponential distribution (see De Boer, Kroese, Mannor and Rubinstein ([1]) . In this thesis we test this simulation technique also for medium sized stochastic networks and compare its effectiveness to the simple crude Monte Carlo (CMC) simulation. The effectiveness of a variance reduction simulation algorithm is measured in the following way. We calculate the product of the necessary CPU time and the estimated variance of the estimation. This product is compared to the same for the simple Crude Monte Carlo simulation. This was originally used for comparison of different variance reduction techniques by Hammersley and Handscombe ([17]). The main result of the first part is the extension of CE method for estimation of rare event probabilities in stochastic networks with normal and beta distributions. In the second case the calculation of reference parameters of the importance sampling distribution requires numerical solution of a nonlinear equation system. This is done by applying a Newton–Raphson iteration scheme. In this case the CPU time spent for calculation of the reference parameter values can not be neglected. The basic CE algorithm will be specialized for the shortest path problem with exponential, beta and normal distributed activity duration times. We will discuss two modifications of the basic CE algorithm for rare event simulation. The first modification is new result, the second was published by

Homem-de Mello and Rubinstein ([18]). Numerical results will also be presented.

In the second part, a stochastic programming based PERT modeling will be introduced. This modeling will produce deterministic earliest starting times for the activities of the project. These deterministic starting times will be attainable with prescribed probability. So we also get an estimated finishing time of the project what is realizable with the same prescribed probability. As the random activity duration times in PERT are supposed to be independent and beta distributed, the application of the multivariate Dirichlet distribution is plausible in this context. The code developed for Dirichlet probability calculations can be incorporated into the AMPL modeling language environment. Moderate sized numerical examples will be given for comparing the traditional and the newly introduced PERT modeling techniques.

IV. New scientific results in the thesis

1. A recursive algorithm for the calculation of Dirichlet probability distribution function values up to 7 dimensions was developed.
2. The hypermultitree bounding algorithm and a variance reduction simulation procedure based on these bounds for the calculation of higher dimensions of Dirichlet probability distribution function values was developed.
3. A new algorithm to calculate the Hessian matrix of Dirichlet probability distribution function values and the formulae for the calculation of the first and second order partial derivatives were developed.
4. New sampling techniques as Sequential Conditioned Sampling (SCS), the Sequential Conditioned Importance Sampling (SCIS) algorithms and modified versions called SCISA, SCSB, SCISA and SCISB algorithms to calculate of Dirichlet probability distribution function values were introduced.
5. The application of the basic CE algorithm for the shortest path problem with normal and beta distributed activity duration times was developed.
6. Development of a modification of the basic CE algorithm for rare event simulation.

7. A new stochastic programming approach and the application of the multivariate Dirichlet distribution to PERT modeling was developed.
8. The traditional and the newly developed PERT modeling techniques were compared on larger sized numerical examples than it was published before.

List of Publications

- [1] GOUDA, A. and SZÁNTAI, T., New sampling techniques for calculation of Dirichlet probabilities, *The Central European Journal of Operations Research*. **12 No.4** (2004) 389–403.
- [2] GOUDA, A. and SZÁNTAI, T., On Numerical calculation of probabilities according to Dirichlet distribution, *Annals of Operations Research*, (submitted).
- [3] GOUDA, A. and SZÁNTAI, T., Estimation of Rare event probabilities in stochastic networks, *Mathematical and Computer Modeling*, (submitted)
- [4] GOUDA, A. and SZÁNTAI, T., Estimation of Rare event probabilities in stochastic networks with exponential and beta distribution. RESIM/COP'04, Proceeding of 5th International Workshop on Rare Event Simulation and Related Combinatorial Optimization Problems, Budapest, Hungary, September, 1–24, 2004.
- [5] GOUDA, A., MONHOR, M. and SZÁNTAI, T., A New stochastic programming model of PERT, *Alkalmazott Matematikai Lapok*, (accepted).
- [6] GOUDA, A., MONHOR, M. and SZÁNTAI, T., A New stochastic programming model of PERT, in: The IFIP/IIASA/GAMM/–Workshop on Coping with Uncertainty, held at the International Institute for Applied Systems Analysis – IIASA, Laxenburg/Vienna, Austria, December 13-16, 2004,(abstract), Special Volume to Springer-Verlag, Berlin, (2005) (submitted).

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