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CONTENTS

Sr. No.	Author	Title of the Paper	Page No.
1	Chiya Parvizpur &	The Unconscious Criticality of	
	Fazel Asadi Amjad	Wright's Native Son to Capitalism	
2	B.A. Tina Zahel &	Ageing Workers in SMEs and the	12
	Prof. Dr. Franz Josef Gellert	Influence on Corporate's	
		Internationalization	
3	Mimita Sachdeva	Life Skills and the Autistic Child	26
4	Talluri Mathew Bhaskar	The Fire and the Rain: A Myth	29
	C A	Retold	
5	Dr. Ankita Khanna	Assessments beyond Writing: An	44
		Attempt to Provide a Fair Chance	
		to the Learners	
6	Dr. Meetakshi Pant	Total Factor Productivity and	49
		Financial Structure of Steel	
		Industry	
7	Ashish Kumar	Carelessness of Man's Mind: a	62
		Study of Albert Camus's the	
		Stranger	
8	Dr. Manju Lalwani Pathak	Debunking the image of Sindhis as	68
		Refugees	
9	Rita Malache	Approaches of tribal development:	72
		A critical Perspective	
10	Prof. Dr. Patil Vijaykumar	Wendy Wasserstein's An American	82
	Ambadasrao	Daughter: An Analysis	

11	Dr. Khandekar Surendra Sakha	Portrayal of Relations and	89
		Globalization in Kiran Desai's	
		Novel 'The Inheritance of Loss'	
12	Dr. Rakseh Rai	A Study of Social Intelligence	95
		among College Students of Tura	
		(West Garo Hills) in Meghalaya	
13	Prof. Vijay D. Songire	Male Sufferers in Toni Morrison's	109
		The Bluest Eye, Sula and Arundhati	
		Roy's The God of Small Things	
14	Prof. R.Y. Shinde &	Vijay Tendulkar's His Fifth	116
	Dr. Archana Durgesh	Woman: A Brief Introduction	
15	Prof. (Dr) Mala Tandon	Alternate Schooling and Teacher	122
		Education: Issues, Challenges and	
	A	Priorities	
16	Dr. J. Thirumaran	A study on three leading stochastic	130
		Optimization methods in simulation	
17	Dr Tanu Tandon	Media and Education: Pathways to	135
	Mr. Durgesh Pathak	End Women Violence	
18	K. Ravi Sankar &	The Inner Awareness of the Human	139
	Dr. V. B. Chithra	Soul: A Study of the Apprentice	
19	Dr. Vitthal V. Parab	A Socio-Literary Perspective in the	147
		Novels of Jhumpa Lahiri & Bharati	
	スン	Mukherjee	

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A study on three leading stochastic Optimization methods in simulation

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Abstract

Many investigators have studied the problem of numerically optimizing an objective function. One approach is stochastic optimization. In many different applications settings, it is of interest to numerically optimize a system over a set of decision variables. While Monte Carlo simulationbased methods have been successfully used for stochastic optimization problems with deterministic constraints, there is a growing body of work on its use for problems with stochastic constraints. We consider is to maximize or minimize the objective function. When the system contains uncertainty, it often is the case that either the objective function to be minimized and/or the constraints on the set of feasible decision variables will involve expectations of random variables. In this paper we review three leading stochastic optimization methods-simulated annealing (SA), genetic algorithms (GA), and table search (TS). Another possible approach to numerical optimization is to generate a random sample from which one can effectively create a global approximation to the objective function and constraints, and to numerically optimize the approximating surface using conventional optimization methods. This approach is known as "sample-average approximation" (SAA). This "random search" approach has properties quite different. In this paper, we will discuss and contrast the performance of these two different families of algorithms, in the setting in which the sample size and/or the number of points sampled is large. Also the paper pointed out the key role that smoothness of the objective function in the decision variable plays in these algorithms. This paper is intended to provide an overview of these two topics.

Key Words: Stochastic programming; Monte Carlo simulation; simulated annealing, genetic algorithms, and table search, simple-average approximation

Introduction

Computer simulations are used extensively as models of real systems to evaluate output responses. Applications of simulation are widely found in many areas including supply chain management, finance, manufacturing, engineering design and medical treatment. The choice of optimal simulation parameters can lead to improved operation, but configuring them well remains a challenging problem. Historically, the parameters are chosen by selecting the best from a set of candidate parameter settings.

Stochastic optimization: In the past 50 years, since the development of digital computers, many investigators have studied the problem of numerically optimizing an objective function. One approach is stochastic optimization, in which the search

for the optimal solution involves randomness in some constructive way. Stochastic approximation is an iterative technique, which can often be used to solve optimization problems from both real systems and computer simulations of real systems. The category of stochastic approximation algorithms can be used in situations where loss function extreme are desired and only noisy loss function measurements are available. We will review two types of stochastic approximation algorithms, Simultaneous perturbation stochastic approximation (SPSA) and finite differences stochastic approximation (FDSA).

Review of Literature: An algorithm like the well-known local search (LS), which only accepts moves with higher values of the objective function than the previous move, will not perform well in this situation, since it is likely that the search will get stuck in a local optimum [1]. It is often difficult to isolate small region of good design that can be accurately represented by a low-order polynomial response surface model [2].There are multiple ways to use Monte Carlo methods in problem (SP) [3]. A generic way of describing them is to construct an approximating problem [4]. The idea is similar to that of the sample-path optimization method, except that of Bayesian inference tools in a novel fashion to compute variable numbers of replications for different points [5]. The idea of Response Surface Methodology (RSM) is to construct one (or multiple) mathematical model A, which is called a surrogate model, to approximate the underlying function f, so

that it is can be easily and cheaply evaluated at each parameter point. We focus on a particular approach to such problems, which is based on simulation (Monte Carlo) techniques, and apply it to a specific class of problems [6]. This method draws on insights from solving inverse problems using simulated annealing and shows how sequential Monte Carlo methods overcome the curse of dimensionality [7].Conceptually the idea of two-stage programming with recourse can be readily extended to *multistage* programming with recourse [8].

Heuristic methods: Heuristic methods have proven to be practically useful in many realworld applications. We will briefly introduce the three most popular methods: genetic algorithms, table search and simulated annealing.

Genetic algorithms are inspired from the process of biological evolution. The algorithm is initialized with a finite set of potential solutions called the population. Each potential solution, referred to as an individual, be coded as a binary string or a real-coded integer or taken from a fixed alphabet of characters. These solutions are evaluated by a fitness function (normally the objective function) and the fit individuals are assigned a high probability to "reproduce" in the next generation of solutions, a sort of survival of the fittest scheme. Table search is a Met heuristic based on the local search method, which iteratively moves the current iterate to a neighbour solution, until certain criteria are satisfied. The algorithm allows a move to a neighbour solution that has a worse objective value.

Simulated annealing searches local moves randomly from list of candidates neighbour points. If a better neighbour point is encountered, it replaces the current iterate with probability one, or if a worse point is found, it replaces the iterate with a probability value strictly less than one. The appropriate probability value is determined by the difference of the objective values. For the algorithm to converge, the probability of moving towards a worse point should decrease along the iterations according to the decrement of a certain 'temperature' value, which changes based on a *cooling schedule*.

All of the three algorithms are considered as global optimization method since they are able to move iterates out of regions where locally optimal

Derivative-free optimization methods: Derivative-free optimization methods are a class of methods that do not try to utilize or directly estimate the gradient value, thus are a good fit for the optimization problem. Compared stochastic approximation to algorithms, the derivative-free methods avoid the gradient estimation step, which is sensitive and crucial to the convergence of these algorithms. In many practical examples, we find that the gradient estimation tools often become incorrect and problematic when the gradient value gets close to zero (i.e., when near a local solution).

There are two categories of derivative-free methods: the so-called model based approach and the pattern or geometry-based approach. The model-based approach typically constructs a chain of local models that approximate the objective function and the algorithm proceeds based on model predictions; an alternative to the modelbased approach is the pattern-based approach, which directly uses the functional output at locations specified by geometric arguments, such as the pattern search method.

Simulated Annealing (SA): Let p(x, y, T)be the probability of accepting a candidate move to y given the present configuration. This probability is controlled by the temperature T, a choice of terminology made by analogy to the physical cooling process described above. Typically the temperature values are chosen independently of the current value of the objective function as a fixed sequence *Tt* indexed by time *t*, the cooling schedule. In SA Algorithm, moves away from the current configuration are chosen according to a proposal distribution, such as the uniform distribution on the neighbourhood. The algorithm is very general and a number of decisions must be made in order to implement it for the solution of particular problem.

Genetic Algorithms (GA): The genetic algorithm (GA) was first introduced by Holland (1975), and since then has become popular method for solving large optimization problems with multiple local optima. Many researchers have claimed success for GA in a broad spectrum of applications. The phrase "genetic algorithm" is more aptly used in the plural, because of the wealth of variations on the basic idea that has grown up since the 1970s; here we use the abbreviation GA to stand for any of these variations.

Table Search (TS): *Table search* (TS) is a "higher-level" heuristic procedure for solving optimization problems, designed to escape the trap of local optima.

Discussion: The literature comparing the performance of stochastic optimization methods such as simulated annealing (SA), genetic algorithms (GA), and table search (TS) has grown considerably in recent years. Many authors working in different problem areas have recently made detailed compare sons of SA and GA:) in image analysis, in problems involving the use of a sample to minimize the expectation of a random variable, and in scheduling jobs in a permutation flow shop to minimize the total time. These comparisons yield a somewhat complex picture:

(1) We find that "GAs are not adept at handling problems involving a great many variables of roughly equal influence" and

(2) That a GA-SA hybrid outperforms either method individually in the problem they examine; and we demonstrate the superiority of SA over GA in their class of problems;

(3) And find that a hybrid genetic descent algorithm performs best in their flow-shop context.

(4) we compared GA and TS in problems of flexible molecular docking, concluding that GA "performs best in terms of the median energy of the solutions located" but that TS "shows a better performance in terms of locating solutions close to the crystallographic lig and conformation",

(5) We suggested that a GA-TS hybrid might outperform either method. Compared SA, GA, and TS in problems involving the reconfiguration of radial distribution electric power networks and find that TS performs best in this class of problems.

(6) Finally, We compared SA, GA, and TS in problems involving the minimization of assembly time in printed wiring assembly, service restoration in electricity distribution systems, graph partitioning, structural engineering optimization, balancing hydraulic turbine runners, and the floorplanning of very large scale integrated (VLSI) circuits, respectively, in many cases without identifying any clear winners.

Conclusion: Two basic themes emerge from this paper: (a) the winning optimization method is highly context-specific, and (b) hybridization of competing algorithms often narrows the performance gap between methods, and sometimes yields an approach that is superior to any of the algorithms being hybridized. What has not yet emerged from this paper is an unambiguous identification of regions in the space of optimization problems in which one method clearly dominates the others and an intuitive explanation for such dominance when it can be found.

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