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This thesis is in the area of unconstrained Global Optimization (GO). Specifically, the problem is to find a global minimum for an unconstrained continuous function (Dixon & Szegö, 1978; Törn & Žilinskas, 1989; Kan & Timmer, 1989; Horst & Tuy, 1990). Such problems are ubiquitous in many fields of science, engineering and management domains. Data fitting problems across disciplines, including regression, multidimensional scaling, clustering, etc. (Go e, Ferrier, & Rogers, 1994; Groenen & Heiser, 1996; Go e, 1997; Jerrell & Campione, 2001), neural network learning (Hassoun, 1995), molecular cluster problems in computational chemistry (Wales, Doye, Miller, Mortenson, & Walsh, 2000), and finding the equilibrium point in an economy (Wu & Wang, 1998) are some of the examples of

Funnel functions are an important class of such unconstrained GO problems. Of late, there is growing interest on f

2004; Iwamatsu & Okabe, 2004; Cheng, Cai, & Shao, 2005).

This thesis proposes e cient metaheuristics for stochastic global optimization of unconstrained funnel functions. We explore the possibility of using simplex based search procedure for funnel functions. Specifically, we use the Nelder-Mead (NM) algorithm (Nelder & Mead, 1965; Olsson & Nelson, 1975), which is still a popular direct search method. It was invented for function minimization as an alternative to descent-based local minimization. In this thesis, we use NM on the

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Extensive empirical investigations were carried out on the four algorithms: NMLS, NMLS-S, MBH and LOS. The experiments were categorized as *systematic* and *exploratory* sets. Detailed experiments on popular benchmark functions are presented under the systematic set . Scoping experiments on problems of special interest are categorized under the exploratory set.

Results of the systematic set have clearly demonstrated the superiority of the NMLS and NMLS-S algorithms over the competing (or existing) algorithms MBH and LOS for low level functions. The strengths of the proposed algorithms have been observed in their robustness in finding the global minima as well as in the e ciency of the search. NMLS and NMLS-S uniformly outperformed MBH and LOS with respect to all performance metrics, across various complexities of each benchmark function tested. All these algorithms deteriorate in their performance with increasing complexity of the objective function[4]. However, the deterioration is slower for NMLS and NMLS-S compared to MBH and LOS, as asymmetries are introduced in the size of the level sets. Further, NMLS and NMLS-S are found to be much less sensitive to the choice of tunable parameters[5]. Between NMLS and NMLS-S, the latter has been found to work better.

The exploratory set of experiments are still in a preliminary stage to make any conclusive observations. We have tried to explore in a few directions and documented the initial findings. Cases of mixing of complexities of the objective function, multifunnel functions[6] and Lennard-Jones clusters were the problems tried. The algorithms proposed in the thesis were able to find the putative global

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3

optimum for many configurations of LJ clusters. This fact is encouraging, but the probe need to be made much deeper.

E orts to make NMLS and NMLS-S more e cient on multifunnel functions, performance of these algorithms on real life problems, finding new applications of funnel functions, especially in the broad discipline of management, work on the theoretical characterizations of funnel functions and study of the relation of the funnel functions to the "globally convex" functions are some of the natural extensions of the thesis work.

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L : Funnel functions and multilevel funnels in unconstrained global optimization have been discussed with the help of a directed graph representation since no clear definition of funnel or funnel-like functions has been found in the literature which is widely accepted. However, one definition of funnel found in the literature has been used to argue that there could be multiple categories (some not so trivial) of single funnel functions in dimensions more than one.

: Two simple hybrids based on Nelder Mead

LOS for funnel functions (which is subsequently substantiated by empirical study).

E [illegible]**:** Based on the results on a systematic set of experiments the following observations were made on the performance of NMLS and NMLS-S with respect to MBH and LOS. Note that observations 2 and 3 involve the following complexities of objective function – amplitude, perturbation, asymmetry in local searches and function values of local minima . **F** [illegible] ff [illegible].

- [illegible] **1:** Performance of NMLS & NMLS-S are uniformly better than that of MBH & LOS.
- [illegible] **2:** Performance of each of the four algorithms generally deteriorates with increasing complexity of the objective function.
- [illegible] **3:** NMLS & NMLS-S are less sensitive to asymmetry in the size of the local minimum basins compared to MBH & LOS. For other complexities of the objective function the relative behaviour is in favour of NMLS & NMLS-S.
- [illegible] **4:** NMLS & NMLS-S are robust to side-length (of the simplex) whereas MBH & LOS are too sensitive to radius (of the neighbourhood hypersphere). Both NMLS and NMLS-S work for any side-length above a minimum threshold.
- [illegible] **5:** NMLS & NMLS-S are robust to the number of iterations in the stopping phase, whereas MBH & LOS are not so.
- [illegible] **6:** Performance of NMLS-S is better than that of NMLS.

7

E: An exploratory set of experiments were conducted to study the performance of the algorithms on problems of special interest. These experiments are still in a preliminary stage to make any conclusive observations. We have tried to explore in the following directions and documented the initial findings:

- Mixing of complexities of the objective function.
- Multifunnel functions
- LJ cluster

K: Unconstrained function minimization, Funnel functions, Local minimum mapping, Monotonic Basin Hopping, Local Optima Smoothing, Simplex Based Search, Nelder Mead Local Search, NMLS-Shrink variant

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