Chapter 16

Theorems Supporting r-flip Search for Pseudo-Boolean Optimization

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ABSTRACT

Modern metaheuristic methodologies rely on well defined neighborhood structures and efficient means for evaluating potential moves within these structures. Move mechanisms range in complexity from simple 1-flip procedures where binary variables are “flipped” one at a time, to more expensive, but more powerful, r-flip approaches where “r” variables are simultaneously flipped. These multi-exchange neighborhood search strategies have proven to be effective approaches for solving a variety of combinatorial optimization problems. In this paper, we present a series of theorems based on partial derivatives that can be readily adopted to form the essential part of r-flip heuristic search methods for Pseudo-Boolean optimization. To illustrate the use of these results, we present preliminary results obtained from four simple heuristics designed to solve a set of Max 3-SAT problems.

INTRODUCTION

Pseudo Boolean formulations are widely known for their ability to represent a rich variety of important discrete problems. While special cases exist for which provably optimal solutions can be found in reasonable time, often the problems are NP-hard and heuristic methods must be employed to produce solutions in a reasonable amount of computer time. In their important early work (Hammer & Rudeanu, 1968), Hammer and Rudeanu discussed Pseudo-Boolean optimization and gave a dynamic programming procedure for solving certain problems. Furthermore, they gave
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a definition of a first-order derivative and indicated its use in solving discrete Pseudo-Boolean optimization problems. Specifically they gave the necessary and sufficient results for any local optimal solution of the problem when one element of $x$ is changed at a time (1-flip move, or 1-move, defined later in the paper). More recently, excellent surveys of Pseudo-Boolean optimization are given by Boros and Hammer (2002) and Crama and Hammer (2007). These sources provide extensive discussions of key topics as well as comprehensive bibliographies.

In this paper we extend this notion of first order derivatives by defining higher-order derivatives for discrete Pseudo-Boolean optimization. Moreover, in the context of changing $r$ elements of $x$ at a time (the so-called $r$-flip moves for $r=2,3$), we present closed-form formulas that allow ‘efficient’ implementation of such compound moves. Then, for the important special cases of quadratic and cubic optimization, we define a general $r$-flip move that allows efficient implementation of multi-exchange neighborhood search process for solving such problems. Finally, we illustrate the use of such moves by applying variants of simple search processes based on $r$-flip moves (with $r = 1$ and 2) to a test bed of max 3-sat problems. The paper then concludes with summary and a look ahead to future research.

We note that the use of simple exchange procedures such as $r$-opt for binary optimization have been reported by several authors (Ahuja, Ergun, Orlin, & Punnen, 2002; Ahuja, Orlin, Pallottino, Scaparra, & Scutellà, 2004; Deineko & Woeginger, 2000; Frangioni, Necciari, & Scutellà, 2004; Glover, 1996; Li & Alidaee, 2002; Magazine, Polak, & Sharma, 2002; Vredeveld & Lenstra, 2003; Yaguiura & Ibaraki, 1999; Yaguiura & Ibaraki, 2001). However, in all such applications the method presented are highly problem specific. The $r$-flip rules we present in this paper are quite general and can be applied to a variety of problem classes.

**PSEUDO-BOOLEAN OPTIMIZATION**

Let $R$ be the set of reals, $Z$ the set of integers, and $B = \{0,1\}$. For a positive integer $n$ let $V = \{1,2,\ldots,n\}$. Let $x = (x_1,\ldots,x_n) \in B^n$ be a binary vector and $\overline{x}_i = 1 - x_i$ complement of $x_i$ for $i \in V$. Define the set of literals to be $L = \{x_1, \overline{x}_1, \ldots, x_n, \overline{x}_n\}$. Mappings $f : B^n \rightarrow \mathbb{R}$ are called Pseudo-Boolean functions. Since there is a one-to-one correspondence between subsets of $V$ and the set of binary vectors $B^n$, these functions are set functions. All Pseudo-Boolean functions can be uniquely represented as multi-linear polynomials of the form given below (see (Boros & Hammer, 2002) for a comprehensive discussion) where $q_s$ is a weight associated with the set $S \subseteq V$:

$$f(x_1,\ldots,x_n) = \sum_{S \subseteq V} q_S \prod_{j \in S} x_j$$

The Pseudo-Boolean optimization problem can be stated as $\text{Max } f(x)$.

**Definition 1:** Hammer and Rudeanu (1968) defined the first derivative of $f$ with respect to $x_i$ as,

$$\Delta_i (x) = \frac{\partial f(x)}{\partial x_i} =$$

$$f(x_1,\ldots,x_{i-1},1,x_{i+1},\ldots,x_n) - f(x_1,\ldots,x_{i-1},0,x_{i+1},\ldots,x_n) \quad \forall i \in V$$

**Definition 2:** For a given $x = (x_1,\ldots,x_{i-1},x_i,x_{i+1},\ldots,x_n)$, define $x' = (x_1,\ldots,x_{i-1},\overline{x}_i,x_{i+1},\ldots,x_n)$ to be 1-flip move with respect to the $i$th position of $x$.

Based on Definition 2 an 1-flip local search process can be defined as follows:
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