

## Chapter 2

# OPTIMALITY, RELAXATION AND GENERAL SOLUTION PROCEDURES

In this chapter, we discuss some fundamental concepts and basic solution frameworks for the following general nonlinear integer programming problem:

$$\begin{aligned} (P) \quad & \min f(x) \\ & \text{s.t. } g_i(x) \leq b_i, \quad i = 1, \dots, m, \\ & \quad h_k(x) = c_k, \quad k = 1, \dots, l, \\ & \quad x \in X \subseteq \mathbb{Z}^n, \end{aligned}$$

where all  $f, g_i$ 's and  $h_k$ 's are real-valued functions defined on  $\mathbb{R}^n$  and  $\mathbb{Z}^n$  is the set of integer points in  $\mathbb{R}^n$ .

A solution  $\tilde{x} \in X$  is said to be a *feasible* solution of  $(P)$  if  $g_i(\tilde{x}) \leq b_i$ , for all  $i = 1, \dots, m$ , and  $h_k(\tilde{x}) = c_k$ , for all  $k = 1, \dots, l$ . A feasible solution  $x^*$  is said to be an *optimal* solution of  $(P)$  if  $f(x^*) \leq f(x)$  for any feasible solution  $x$  of  $(P)$ .

This chapter is organized as follows: We introduce the concept of an optimality condition using bounds in Section 2.1. In Section 2.2, we present a general framework of partial enumeration methods, first a general branch-and-bound method, then a backtrack partial enumeration method for 0-1 programming and its implementation in 0-1 linear integer programming. In Section 2.3, we introduce the concept of relaxation and discuss the relationship between Lagrangian relaxation and continuous relaxation. We study the relationship between continuous and integer optimal solutions of nonlinear integer programming problems in Section 2.4. In Section 2.5, we discuss how to convert a general constrained nonlinear integer programming problem into an unconstrained one by using an exact penalty function. Finally, we present in Section 2.6 optimality conditions for binary quadratic problems.

## 2.1 Optimality Condition via Bounds

An essential task in designing any solution algorithm for  $(P)$  is to derive an optimal condition or a stopping criterion to terminate the algorithm, i.e., to judge if the current solution is optimal to  $(P)$  or to conclude that there is no feasible solution to  $(P)$ . Except for very few special cases, such as unconstrained quadratic binary problems (see Section 2.6), it is difficult to obtain an explicit optimality condition for problem  $(P)$ . As in linear integer program and other discrete optimization problems, however, optimality of the nonlinear integer programming problem  $(P)$  can be verified through the convergence of a sequence of upper bounds and a sequence of lower bounds of the objective function. Let  $f^*$  be the optimal value of  $(P)$ . Suppose that an algorithm generates a nonincreasing sequence of upper bounds

$$\bar{f}_1 \geq \bar{f}_2 \geq \cdots \geq \bar{f}_k \geq \cdots \geq f^*$$

and a nondecreasing sequence of lower bounds

$$\underline{f}_1 \leq \underline{f}_2 \leq \cdots \leq \underline{f}_k \leq \cdots \leq f^*,$$

where  $\underline{f}_k$  and  $\bar{f}_k$  are the lower and upper bounds of  $f^*$  generated at the  $k$ -th iteration, respectively. If  $\bar{f}_k - \underline{f}_k \leq \epsilon$  holds for some small  $\epsilon \geq 0$  at the  $k$ -th iteration, then the following is evident:

$$f^* - \epsilon \leq \underline{f}_k \leq f^*.$$

Notice that an upper bound of  $f^*$  is often associated with a feasible solution  $x^k$  to  $(P)$ , since  $f(x^k) \geq f^*$ . A lower bound of  $f^*$  is usually achieved by solving a relaxation problem of  $(P)$  which we will discuss in later sections of this chapter. A feasible solution  $x^k$  is called an  $\epsilon$ -approximate solution to  $(P)$  when  $f(x^k) = \bar{f}_k$  and  $\bar{f}_k - \underline{f}_k \leq \epsilon > 0$ .

We have the following theorem.

**THEOREM 2.1** *Suppose that  $\{\bar{f}_k\}$  and  $\{\underline{f}_k\}$  are the sequences of upper bounds and lower bounds of  $f^*$ , respectively. If  $\bar{f}_k - \underline{f}_k = 0$  for some  $k$  and  $x^k$  is a feasible solution to  $(P)$  with  $f(x^k) = \bar{f}_k$ , then  $x^k$  is an optimal solution to  $(P)$ .*

The key question is how to generate two converging sequences of upper and lower bounds of  $f^*$  in a solution process. Continuous relaxation, Lagrangian relaxation (Chapter 3) and surrogate relaxation (Chapter 4) are three typical ways of getting a lower bound of an integer programming problem. The upper bound of  $f^*$  is usually obtained via feasible solutions of problem  $(P)$ .

## 2.2 Partial Enumeration

Although the approach of total enumeration is infeasible for large-scale integer programming problems, the idea of partial enumeration is still attractive

if there is a guarantee of identifying an optimal solution of  $(P)$  without checking explicitly all the points in  $X$ . The efficiency of any partial enumeration scheme can be measured by the average reduction of the search space of integer solutions to be examined in the execution of the solution algorithm. The branch-and-bound method is one of the most widely used partial enumeration schemes.

### 2.2.1 Outline of the general branch-and-bound method

The branch-and-bound method has been widely adopted as a basic partial enumeration strategy for discrete optimization. In particular, it is a successful and robust method for linear integer programming when combined with linear programming techniques. The basic idea behind the branch-and-bound method is an implicit enumeration scheme that systematically discards non-promising points in  $X$  that are hopeless in achieving optimality for  $(P)$ . The same idea can be applied to nonlinear integer programming problem  $(P)$ . To partition the search space, we divide the integer set  $X$  into  $p$  ( $\geq 2$ ) subsets:  $X_1, \dots, X_p$ . A *subproblem* at node  $i$ ,  $(P(X_i))$ ,  $i = 1, \dots, p$ , is formed from  $(P)$  by replacing  $X$  with  $X_i$ . One or more subproblems are selected from the subproblem list. For each selected node, a lower bound  $LB_i$  of the optimal value of subproblem  $(P(X_i))$  is estimated. If  $LB_i$  is greater than or equal to the function value of the *incumbent*, the best feasible solution found, then the subproblem  $(P(X_i))$  is removed or *fathomed* from further consideration. Otherwise, problem  $(P(X_i))$  is kept in the subproblem list. The incumbent is updated whenever a better feasible solution is found. One of the unfathomed nodes,  $(P(X_i))$ , is selected and  $X_i$  is further divided or *branched* into smaller subsets. The process is repeated until there is no subproblem left in the list. It is convenient to use a node-tree structure to describe a branch-and-bound method in which a *node* stores the information necessary for describing and solving the corresponding subproblem. We describe the general branch-and-bound method in details as follows.

ALGORITHM 2.1 (GENERAL BRANCH-AND-BOUND METHOD FOR  $(P)$ )

**Step 0** (Initialization). Set the subproblem list  $L = \{P(X)\}$ . Set an initial feasible solution as the incumbent  $x^*$  and  $v^* = f(x^*)$ . If there is no feasible solution available, then set  $v^* = +\infty$ .

**Step 1** (Node Selection). If  $L = \emptyset$ , stop and  $x^*$  is the optimal solution to  $(P)$ . Otherwise, choose one or more nodes from  $L$ . Denote the set of  $k$  selected nodes by  $L^s = \{P(X_1), \dots, P(X_k)\}$ . Let  $L := L \setminus L^s$ . Set  $i = 1$ .

**Step 2** (Bounding). Compute a lower bound  $LB_i$  of subproblem  $(P(X_i))$ . Set  $LB_i = +\infty$  if  $(P(X_i))$  is infeasible. If  $LB_i \geq v^*$ , go to Step 5.

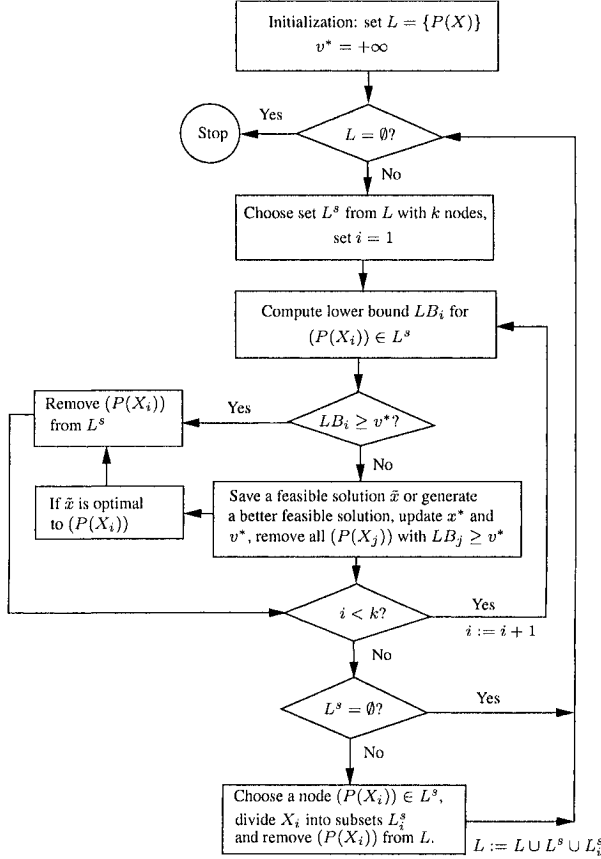


Figure 2.1. Diagram of the general branch-and-bound method.

**Step 3** (Feasible solution). Save the best feasible solution found in Step 2 or generate a better feasible solution when possible by certain heuristic method. Update the incumbent  $x^*$  and  $v^*$  when needed. Remove from  $L^s$  all  $(P(X_j))$  satisfying  $LB_j \geq v^*$ ,  $1 \leq j \leq i$ . If  $i < k$ , set  $i := i + 1$  and return to Step 2. Otherwise, go to Step 4.

**Step 4** (Branching). If  $L^s = \emptyset$ , go to Step 1. Otherwise, choose a node  $(P(X_i))$  from  $L^s$ . Further divide  $X_i$  into smaller subsets:  $L_i^s = \{X_i^1, \dots, X_i^p\}$ . Remove  $(P(X_i))$  from  $L^s$  and set  $L := L \cup L^s \cup L_i^s$ . Go to Step 1.

**Step 5** (Fathoming). Remove  $(P(X_i))$  from  $L^s$ . If  $i < k$ , set  $i := i + 1$  and return to Step 2. Otherwise, go to Step 4.

Figure 2.1 illustrates the diagram of Algorithm 2.1.

**THEOREM 2.2** *Algorithm 2.1 stops at an optimal solution to  $(P)$  within a finite number of iterations.*

**Proof.** Note that the fathoming procedure, either in Step 3 or Step 5 of the algorithm, will not remove any feasible solution of  $(P)$  better than the incumbent. Notice that  $X$  is finite. Thus only a finite number of branching steps can be executed. At an extreme, when  $X_i$  is a singleton, either  $(P(X_i))$  is infeasible or an optimal solution to  $(P(X_i))$  can be found, thus  $(P(X_i))$  being fathomed in Step 5. Within a finite number of iterations,  $L$  will become empty and the optimality of the incumbent is evident.  $\square$

One key issue to develop an efficient branch-and-bound method is to get a good (high) lower bound  $LB_i$  generated by the bounding procedure in Step 2. The better the lower bound, the more subproblems can be fathomed in Steps 3 and 5 and the faster the algorithm converges. There is a trade-off, however, between the quality of the lower bounds and the associated computational efforts. For nonlinear integer programming problem  $(P)$ , *continuous relaxation* and *Lagrangian relaxation* are two commonly used methods for generating lower bounds in Step 2.

### 2.2.2 The back-track scheme

The back-track scheme was proposed originally as a systematic way to thread a maze. Known by its different names, the back-track scheme was rediscovered from time to time in different fields. Especially, it was adopted as an efficient procedure for implicit enumeration in solving many kinds of combinatorial problems. We discuss the back-track scheme in this subsection as a powerful partial enumeration scheme for 0-1 programming problems.

Let's consider the following general nonlinear 0-1 integer programming problem:

$$\begin{aligned} (0-1P) \quad & \min f(x) \\ & \text{s.t. } g_i(x) \leq b_i, \quad i = 1, 2, \dots, m, \\ & \quad x \in X = \{0, 1\}^n, \end{aligned}$$

where  $f$  is assumed to be monotonically increasing, i.e.,  $f(x) \geq f(y)$  if  $x \geq y$ . It is clear that there are at most  $2^n$  possible candidates to be considered for achieving an optimality of problem  $(0-1P)$ . However, an efficient solution algorithm should be devised such that, in most situations, only a significantly small portion of the  $2^n$  possible solutions needs to be explicitly enumerated. These possible solutions should rather be implicitly enumerated group by group.

To group the  $2^n$  solutions, we define a *partial solution* to be an assignment of binary values to a subset of the  $n$  decision variables. Let  $N = \{1, \dots, n\}$ .

At iteration  $t$ , let  $J_t = \{j \text{ or } -j \mid j \in I_t \subseteq N\}$  denote the partial solution with  $x_j = 1$  when  $j \in J_t$  and  $x_j = 0$  when  $-j \in J_t$ , where  $I_t$  is the index set of  $J_t$ . Only one of  $j$  or  $-j$  could be included in  $J_t$ . Any variable  $x_j$  whose index  $j$  is not included in  $I_t$  is defined to be *free*. A completion of  $J_t$  is defined as a solution determined by  $J_t$  together with a binary specification of the free variables. It is clear that a  $k$ -element partial solution could determine  $2^{n-k}$  different completions as a group. When all free variables are set to be zero, the completion is termed *typical*. Since the objective function  $f$  in problem  $(0-1P)$  is monotonically increasing, the typical completion of  $J_t$  has the minimum objective function value among all completions of  $J_t$ . For example,  $J_t = \{3, 5, -2\}$  with  $n = 5$  specifies a partial solution of  $x_3 = 1$ ,  $x_5 = 1$  and  $x_2 = 0$ .  $J_t$  has two free variables ( $x_1$  and  $x_4$ ) and four possible completions, among which the one with  $x_1 = x_4 = 0$  is the typical completion.

After a partial solution  $J_t$  is generated at iteration  $t$ , we need to determine if its corresponding solution group (completions) could include an optimal solution to  $(P)$ . In the following two situations,  $J_t$  can be *fathomed*.

Case (i): If the typical completion of  $J_t$  is feasible in  $(0-1P)$ ,  $J_t$  can be fathomed in this case (after updating the incumbent if the typical completion of  $J_t$  has an objective value less than the one of the incumbent), since no other completion of  $J_t$  could generate an objective value of  $(0-1P)$  smaller than the objective value of the typical completion as  $f$  is monotonically increasing.

Case (ii): If the typical completion of  $J_t$  has an objective value larger than or equal to the one of the incumbent,  $J_t$  can be fathomed in this case since no other completion of  $J_t$ , including the typical completion, could do better than the incumbent.

There is only one remaining situation which fits neither Case (i) nor Case (ii): the typical completion of  $J_t$  is infeasible in  $(0-1P)$  and has an objective value less than that of the incumbent. In this situation, we augment  $J_t$  by assigning values to some free variables of  $J_t$  according to some rules such that a new partial solution is generated for further fathoming.

The back-track scheme, as a systematic method, is designed to implicitly enumerate all solutions without generating any redundant partial solutions. To ensure having a new non-redundant partial solution when a partial solution is fathomed, at least one element of the partial solution has to be changed to its complement. When the chosen element is replaced by its complement, it is marked by an underline in order to prevent a turning back in the solution process. This process repeats and terminates when there is no non-underlined component in the partial solution, which implies that all possible solutions are implicitly enumerated. In the back-track procedure, we always locate in a partial solution the right-most element which is not underlined. We replace this right-most non-underlined element by its underlined complement and delete all elements to its right. If no non-underlined element exists in the partial solution,

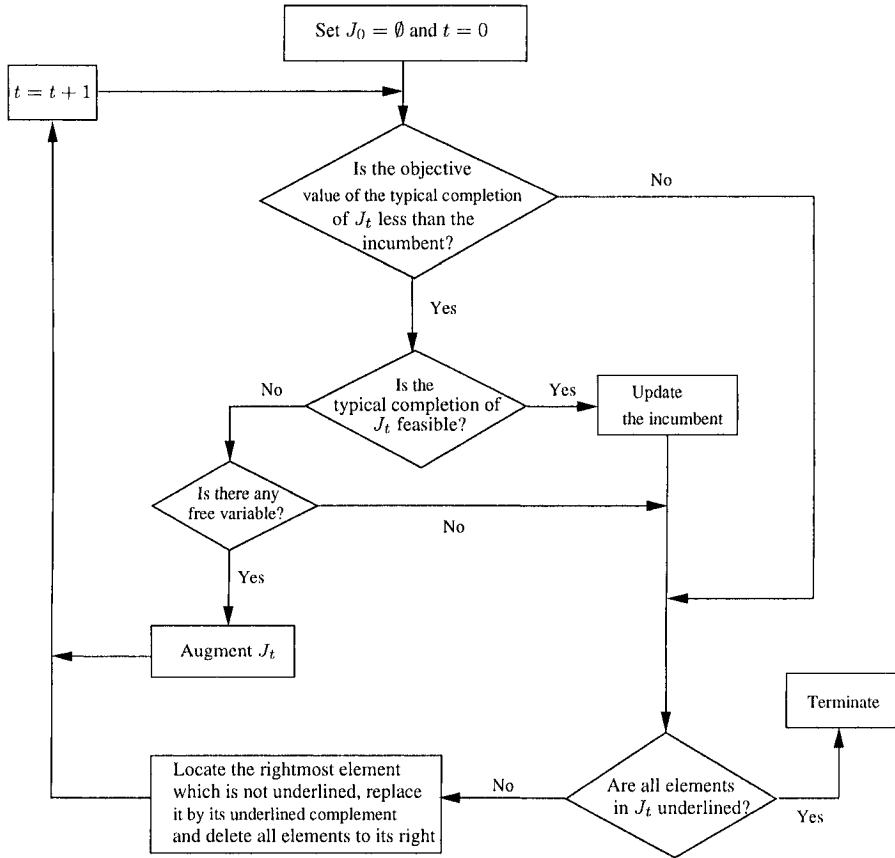


Figure 2.2. Diagram of the back-track scheme.

we can claim that all  $2^n$  solutions have been implicitly enumerated and the solution procedure terminates. For example, if  $J_t = \{3, 5, \underline{-2}\}$  is fathomed at iteration  $t$ , the new partial solution  $J_{t+1}$  is  $\{3, \underline{-5}\}$  in the back-track procedure.

A diagram of the general solution framework for the back-track scheme is given in Figure 2.2. Notice that for different types of 0-1 programming problems, such as 0-1 linear programming problems and polynomial 0-1 programming problems, different fathoming and augmenting rules could be designed to explore special structures of the problems.

**THEOREM 2.3** *The back-track scheme leads to a non-redundant sequence of partial solutions which terminates only when all  $2^n$  solutions have been (implicitly) enumerated.*

Theorem 2.3 indicates that the back-track scheme is a finite algorithm. If (0-1P) is feasible, the optimal solution will be in store of the incumbent at termination of the procedure.

Although we start with  $J_0 = \emptyset$  in Figure 2.2,  $J_0$  could essentially be any other partial solution without an underlined element. In addition, in the process of augmentation, we can augment more than one free variable on the right of  $J_t$ .

### 2.2.2.1 The additive algorithm for solving linear 0-1 programming problems

In 1965, Balas proposed an implicit enumeration method to directly solve linear zero-one programming problems [7]. Due to the fact that only addition is required as an arithmetic operation in the solution procedure, the solution procedure is called as the additive algorithm. One advantage of the additive algorithm is that there is no roundoff error. The additive algorithm is considered to be fundamental for the later development of various implicit enumeration methods for integer programming problems.

In this subsection we consider the following linear zero-one programming problem:

$$\begin{aligned}
 (0-1LP) \quad & \min f(x) = \sum_{j=1}^n c_j x_j, \\
 \text{s.t.} \quad & g_i(x) = \sum_{j=1}^n a_{ij} x_j \leq b_i, \quad i \in M = \{1, 2, \dots, m\}, \\
 & x_j \in \{0, 1\}, \quad j \in N = \{1, 2, \dots, n\}.
 \end{aligned}$$

Without loss of generality, we assume that  $c_j \geq 0$  for all  $j \in N$ . By introducing  $m$  slack variables, problem (0-1LP) can be rewritten as follows,

$$\begin{aligned}
 (0-1LP_s) \quad & \min f(x) = \sum_{j=1}^n c_j x_j, \\
 \text{s.t.} \quad & g_i(x) = \sum_{j=1}^n a_{ij} x_j + y_i = b_i, \quad i \in M, \\
 & x_j \in \{0, 1\}, \quad j \in N, \\
 & y_i \geq 0, \quad i \in M,
 \end{aligned}$$

where  $y_i, i \in M$ , are nonnegative slack variables.

The additive algorithm starts with a partial solution  $J_0 = \emptyset$  and an upper bound of the minimum value of the objective function,  $f^* = \sum_{j=1}^n c_j$ . At iteration  $t$ ,



the partial solution is  $J_t$ . Let  $x^t$  be the typical completion of  $J_t$  and  $y^t \in \mathbb{R}^m$  be the corresponding vector of slack variables.

When  $f(x^t) \geq f^*$ , the partial solution  $J_t$  can be fathomed, no matter if  $x^t$  is feasible or not in (0-1LP), since no completion of  $J_t$  will give an objective value less than  $f^*$ . The algorithm proceeds then to the back-track procedure.

When  $f(x^t) < f^*$  and  $y^t \geq 0$ ,  $x^t$  is a better feasible solution. We update the incumbent by setting  $f^* = f(x^t)$ . The partial solution  $J_t$  can be fathomed, since no other completions of  $J_t$  can yield an objective value less than  $f(x^t)$ . The algorithm proceeds then to the back-track procedure.

When  $f(x^t) < f^*$  and  $y^t \not\geq 0$ , the typical completion of  $J_t$ ,  $x^t$ , is infeasible in (0-1LP) and we need to augment  $J_t$  with at least one free variable (if any). The principle of augmentation is to pursue a reduction in both the objective value and the degree of infeasibility. To identify a candidate of augmentation from among all free variables, a set  $T^t$  is constructed as follows,

$$T^t = \{j \in N \setminus I_t \mid f(x^t) + c_j < f^* \text{ and there exists } i \in M \text{ such that } a_{ij} < 0 \text{ and } y_i^t < 0\}.$$

It is clear that only those  $x_j$ 's with  $j$  in  $T^t$  need to be considered as candidates to augment  $J_t$  on the right because assigning 1 to some free variable not in  $T^t$  would either lead to a larger lower objective value than  $f^*$  or increase the degree of the infeasibility of  $x^t$ . If  $T^t$  is empty, we know that there does not exist a feasible completion of  $J_t$  which can do better than the incumbent, and  $J_t$  is thus fathomed.

When  $T^t$  is not empty, we check further the following inequality for those  $i \in M$  with  $y_i^t < 0$ :

$$y_i^t - \sum_{j \in T^t} \min\{0, a_{ij}\} \geq 0. \quad (2.2.1)$$

If (2.2.1) does not hold for any  $i \in M$  with  $y_i^t < 0$ , then the slack variable of the  $i$ -th constraint will remain negative for whatever solution augmented from  $J_t$  by assigning 1 to some variables in  $T^t$ . In other words, it is impossible for  $J_t$  to have a feasible completion which can be adopted to improve the current incumbent value and thereby  $J_t$  is fathomed.

If (2.2.1) holds for all  $i \in M$  with  $y_i^t < 0$ , we could augment  $J_t$  on the right. A suitable criterion in selecting a free variable from  $T^t$  is to use the following formulation:

$$j^t = \arg \max_{j \in T^t} \sum_{i=1}^m \min\{y_i^t - a_{ij}, 0\}. \quad (2.2.2)$$

If  $j^t$  is chosen according to the above formulation,  $J_{t+1} = J_t \cup \{j^t\}$  has the "least" degree of the violation of the constraints.

The back-track scheme can be used to clearly interpret the additive algorithm of Balas and has been adopted to simplify the additive algorithm of Balas such that not only the solution logic in the algorithm becomes much clearer, but also the memory requirement of computation is significantly reduced. Based on the back-track scheme, the additive algorithm of Balas can be explained via the following flow chart in Figure 2.3.

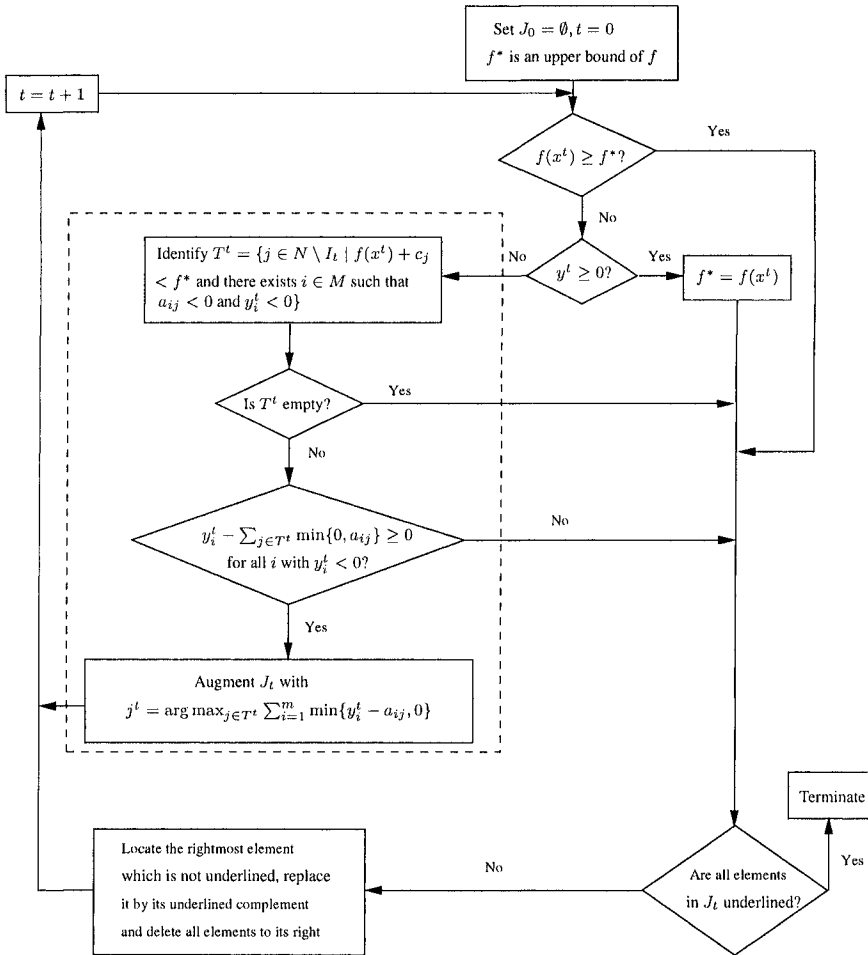


Figure 2.3. Diagram of the additive algorithm of Balas.

The following linear 0-1 programming problem serves as an example to illustrate the back-track scheme in the additive algorithm.

**EXAMPLE 2.1**

$$\begin{aligned}
& \min 5x_1 + 7x_2 + 10x_3 + 3x_4 + x_5 \\
& \text{s.t. } -x_1 + 3x_2 - 5x_3 - x_4 + 4x_5 \leq -2, \\
& \quad 2x_1 - 6x_2 + 3x_3 + 2x_4 - 2x_5 \leq 0, \\
& \quad x_2 - 2x_3 + x_4 + x_5 \leq -1, \\
& \quad x_1, x_2, x_3, x_4, x_5 \in \{0, 1\}.
\end{aligned}$$

Adding slack variables yields the following standard formulation,

$$\begin{aligned}
& \min 5x_1 + 7x_2 + 10x_3 + 3x_4 + x_5 \\
& \text{s.t. } -x_1 + 3x_2 - 5x_3 - x_4 + 4x_5 + y_1 = -2, \\
& \quad 2x_1 - 6x_2 + 3x_3 + 2x_4 - 2x_5 + y_2 = 0, \\
& \quad x_2 - 2x_3 + x_4 + x_5 + y_3 = -1, \\
& \quad x_1, x_2, x_3, x_4, x_5 \in \{0, 1\}, y_1, y_2, y_3 \geq 0.
\end{aligned}$$

**Initial Iteration**

*Step 0.* Set  $J_0 = \emptyset$  and  $f^* = \sum_{j=1}^5 c_j = 26$ .

**Iteration 1** ( $t = 0$ )

*Step 1.*  $x^0 = (0, 0, 0, 0, 0)^T$ ,  $f(x^0) = 0 < f^* = 26$  and  $y^0 = (-2, 0, -1)^T \not\geq 0 \Rightarrow$  Augmenting  $J_0$ .

*Step 2.* Notice that all  $x_1, x_2, x_3, x_4, x_5$  are free variables and  $T^0 = \{1, 3, 4\}$ .

*Step 3.* For  $i = 1$ ,  $y_1^0 - \sum_{j \in T^0} \min\{0, a_{1j}\} = -2 - (-1 - 5 - 1) = 5 \geq 0$ ;  
For  $i = 3$ ,  $y_3^0 - \sum_{j \in T^0} \min\{0, a_{3j}\} = -1 - (-2) = 1 \geq 0$ .

*Step 4.*  $j^0 = \arg \max_{j \in T^0} \{\sum_{i=1}^3 \min(y_i^0 - a_{ij}, 0)\} = \arg \max\{-1 - 2 - 1, -3, -1 - 2 - 2\} = 3 \Rightarrow J_1 = \{3\}$ .

**Iteration 2** ( $t = 1$ )

*Step 1.*  $x^1 = (0, 0, 1, 0, 0)^T$ ,  $f(x^1) = 10 < f^* = 26$  and  $y^1 = (3, -3, 1)^T \not\geq 0 \Rightarrow$  Augmenting  $J_1$ .

*Step 2.* Notice  $x_1, x_2, x_4, x_5$  are free variables and  $T^1 = \{2, 5\}$ .

*Step 3.* For  $i = 2$ ,  $y_2^1 - \sum_{j \in T^1} \min(0, a_{2j}) = -3 - (-6 - 2) = 5 \geq 0$ .

*Step 4.*  $j^1 = \arg \max_{j \in T^1} \{\sum_{i=1}^3 \min(y_i^1 - a_{ij}, 0)\} = \arg \max\{0, -1 - 1\} = 2$ . Thus  $J_2 = \{3, 2\}$ .

**Iteration 3** ( $t = 2$ )

*Step 1.*  $x^2 = (0, 1, 1, 0, 0)^T$ ,  $f(x^2) = 17 < f^* = 26$  and  $y^2 = (0, 3, 0)^T \not\geq 0$   
 $\Rightarrow$  Record  $x^* = \{0, 1, 1, 0, 0\}$ , set  $f^* = 17$  and  $J_2$  is fathomed.

*Step 2.* Back track and get  $J_3 = \{3, \underline{-2}\}$ .

#### Iteration 4 ( $t = 3$ )

*Step 1.*  $x^3 = (0, 0, 1, 0, 0)^T$ ,  $f(x^3) = 10 < f^* = 17$  and  $y^3 = (3, -3, 1)^T \not\geq 0$   
 $\Rightarrow$  Augmenting  $J_3$ .

*Step 2.* Notice that  $x_1, x_4, x_5$  are free variables and  $T^3 = \{5\}$ .

*Step 3.* For  $i = 2$ ,  $y_2^3 - \sum_{j \in T^3} \min(0, a_{2j}) = -3 - (-2) = -1 < 0 \Rightarrow$   
 $J_3$  is fathomed.

*Step 4.* Back track and get  $J_4 = \{\underline{-3}\}$ .

#### Iteration 5 ( $t = 4$ )

*Step 1.*  $x^4 = (0, 0, 0, 0, 0)^T$ ,  $f(x^4) = 0 < f^* = 17$  and  $y^4 = (-2, 0, -1)^T \not\geq 0$   
 $\Rightarrow$  Augmenting  $J_4$ .

*Step 2.* Notice that  $x_1, x_2, x_4, x_5$  are free variables and  $T^4 = \{1, 4\}$ .

*Step 3.* For  $i = 3$ ,  $y_3^4 - \sum_{j \in T^4} \min(0, a_{3j}) = -1 - (0) = -1 < 0 \Rightarrow J_4$   
is fathomed.

*Step 4.* No element in  $J_4$  is not underlined.  $\Rightarrow$  The algorithm terminates  
with an optimal solution  $x^* = \{0, 1, 1, 0, 0\}$  and  $f^* = 17$ .

## 2.3 Continuous Relaxation and Lagrangian Relaxation

Let  $v(Q)$  denote the optimal value of problem  $(Q)$ . A problem  $(R(\xi))$  with a parameter  $\xi$  is called a relaxation of the primal problem  $(P)$  if  $v(R(\xi)) \leq v(P)$  holds for all possible values of  $\xi$ . In other words, solving a relaxation problem offers a lower bound of the optimal value of the primal problem. The dual problem,  $(D)$ , is formulated to search for an optimal parameter,  $\xi^*$ , such that the duality gap of  $v(P) - v(R(\xi))$  is minimized at  $\xi = \xi^*$ . The quality of a relaxation should be thus judged by two measures. The first measure is how easier the relaxation problem can be solved when compared to the primal problem. The second measure is how tight the lower bound can be, in other words, how small the duality gap can be reduced to.

### 2.3.1 Continuous relaxation

The continuous relaxation of  $(P)$  can be expressed as follows:

$$\begin{aligned}
 (\overline{P}) \quad & \min f(x) \\
 \text{s.t.} \quad & g_i(x) \leq b_i, \quad i = 1, \dots, m, \\
 & h_k(x) = c_k, \quad k = 1, \dots, l, \\
 & x \in \text{conv}(X),
 \end{aligned}$$

where  $\text{conv}(X)$  is the convex hull of the integer set  $X$ . Problem  $(\bar{P})$  is a general constrained nonlinear programming problem. Since  $X \subset \text{conv}(X)$ , it holds  $v(\bar{P}) \leq f^*$ . Generally speaking, a continuous relaxation problem is easier to solve than the primal nonlinear integer programming problem.

When all  $f$  and  $g_i$ 's are convex and all  $h_k$ 's are linear in  $(\bar{P})$ , the continuous relaxation problem is convex. For continuous convex minimization problems, many efficient solution methods have been developed over the last four decades. Below is a list of some of the well-known solution methods for convex constrained optimization (see e.g. [13][58][148]):

- Penalty Methods;
- Successive Quadratic Programming (SQP) methods;
- Feasible Direction Methods:
  - Wolfe's Reduced Gradient Method for linearly constrained problems;
  - The Generalized Reduced Gradient Method for nonlinearly constrained problems;
  - Rosen's Gradient Projection Methods.
- Trust Region Methods.

There does not exist a general-purpose solution method, however, for searching for a global solution for nonconvex constrained optimization problems. Nevertheless, there are several solution algorithms developed in *global optimization* for nonconvex problems with certain special structures, for example, outer approximation methods for concave minimization with linear constraints ([105] [174]) and convexification methods for monotone optimization problems ([136] [207]).

### 2.3.2 Lagrangian relaxation

Define the following Lagrangian function of  $(P)$  for  $\lambda \in \mathbb{R}_+^m$  and  $\mu \in \mathbb{R}^l$ :

$$L(x, \lambda, \mu) = f(x) + \sum_{i=1}^m \lambda_i (g_i(x) - b_i) + \sum_{k=1}^l \mu_k (h_k(x) - c_k).$$

The Lagrangian relaxation problem of  $(P)$  is posted as follows:

$$(L_{\lambda, \mu}) \quad d(\lambda, \mu) = \min_{x \in X} L(x, \lambda, \mu). \quad (2.3.1)$$

Denote the feasible region of  $(P)$  by

$$S = \{x \in X \mid g_i(x) \leq b_i, i = 1, \dots, m, h_k(x) = c_k, k = 1, \dots, l\}.$$

The following *weak duality* relation will be derived in the next chapter:

$$d(\lambda, \mu) \leq f(x), \quad \forall \lambda \in \mathbb{R}_+^m, \mu \in \mathbb{R}^l, x \in S. \quad (2.3.2)$$

This ensures that solving  $(L_{\lambda, \mu})$  gives a lower bound of  $f^*$ , the optimal value of  $(P)$ . The dual problem of  $(P)$  is to search for the best lower bound provided by the Lagrangian relaxation:

$$(D) \quad \max_{\lambda \in \mathbb{R}_+^m, \mu \in \mathbb{R}^l} d(\lambda, \mu). \quad (2.3.3)$$

### 2.3.3 Continuous bound versus Lagrangian bound

We first establish a relationship between the continuous bound and the Lagrangian bound in convex cases of  $(P)$ . We need the following assumption.

**ASSUMPTION 2.1** *Functions  $f$  and  $g_i$  ( $i = 1, \dots, m$ ) are convex, functions  $h_k$  ( $k = 1, \dots, l$ ) are linear, and certain constraint qualification holds for  $(\bar{P})$ .*

One sufficient condition to ensure the satisfaction of the constraint qualification in Assumption 2.1 is that the gradients of the active inequality constraints and that of the equality constraints at the optimal solution to  $(\bar{P})$  are linearly independent.

The following theorem shows that the Lagrangian bound for convex integer programming problem  $(P)$  is at least as good as the bound obtained by the continuous relaxation.

**THEOREM 2.4** *Under Assumption 2.1, it holds  $v(D) \geq v(\bar{P})$ .*

**Proof.** Since  $X \subseteq \text{conv}(X)$ , we have

$$\begin{aligned} v(D) &= \max_{\lambda \in \mathbb{R}_+^m, \mu \in \mathbb{R}^l} \min_{x \in X} L(x, \lambda, \mu) \\ &\geq \max_{\lambda \in \mathbb{R}_+^m, \mu \in \mathbb{R}^l} \min_{x \in \text{conv}(X)} L(x, \lambda, \mu) \\ &= v(\bar{P}). \end{aligned}$$

The last equality is due to the strong duality theorem of convex programming under Assumption 2.1.  $\square$

The tightness of the Lagrangian bound has been also witnessed in many combinatorial optimization problems. In the case of nonlinear integer programming, to compute the Lagrangian bound  $v(D)$ , one has to solve the Lagrangian relaxation problem (2.3.1). When all functions  $f$ ,  $g_i$ 's and  $h_k$ 's and set  $X$  are separable, the Lagrangian relaxation problem (2.3.1) can be solved efficiently

via decomposition which we are going to discuss in Chapter 3. When some of the functions  $f$ ,  $g_i$ 's and  $h_k$ 's are nonseparable, problem (2.3.1) is not easier to solve than the original problem  $(P)$ . Nevertheless, the Lagrangian bound of a quadratic 0-1 programming problem can still be computed efficiently (see Chapter 11). Lagrangian bounds for linearly constrained convex integer programming problems can also be computed via certain decomposition schemes (see Chapter 3).

Next, we compare the continuous bound with the Lagrangian bound for a nonconvex case of  $(P)$ , more specifically, the following linearly constrained concave integer programming problem:

$$\begin{aligned} (P_v) \quad & \min f(x) \\ & \text{s.t. } Ax \leq b, \\ & \quad Bx = d, \\ & \quad x \in X = \{x \in \mathbb{Z}^n \mid l_j \leq x_j \leq u_j, j = 1, \dots, n\}, \end{aligned}$$

where  $f(x)$  is a concave function,  $A$  is an  $m \times n$  matrix,  $B$  is an  $l \times n$  matrix,  $b \in \mathbb{R}^m$ ,  $d \in \mathbb{R}^l$ ,  $l_j$  and  $u_j$  are integer lower bound and upper bound of  $x_j$ , respectively. Let  $(\bar{P}_v)$  denote the continuous relaxation problem of  $(P_v)$ .

The Lagrangian dual problem of  $(P_v)$  is:

$$(D_v) \quad \max_{\lambda \in \mathbb{R}_+^m, \mu \in \mathbb{R}^l} d_v(\lambda, \mu),$$

where

$$d_v(\lambda, \mu) = \min_{x \in X} [f(x) + \lambda^T(Ax - b) + \mu^T(Bx - d)],$$

for  $\lambda \in \mathbb{R}_+^m$  and  $\mu \in \mathbb{R}^l$ .

The following result shows that, on the contrary to the convex case of  $(P)$ , the continuous relaxation of  $(P_v)$  always generates a lower bound of  $(P_v)$  at least as good as that by the Lagrangian dual.

**THEOREM 2.5** *Assume that  $f$  is a concave function on  $X$  in  $(P_v)$ . Then  $v(D_v) \leq v(\bar{P}_v)$ .*

**Proof.** Let  $\Omega$  denote the set of extreme points of  $\text{conv}(X)$ :

$$\Omega = \{x^i \mid i = 1, \dots, K\},$$

where  $K = 2^n$ . Consider the following convex envelope of  $f$  over  $\text{conv}(X)$ :

$$\phi(x) = \min \left\{ \sum_{i=1}^K \gamma_i f(x^i) \mid \sum_{i=1}^K \gamma_i x^i = x, \gamma \in \Lambda \right\}, \quad (2.3.4)$$

where  $\Lambda = \{\gamma \in \mathbb{R}^K \mid \sum_{i=1}^K \gamma_i = 1, \gamma_i \geq 0, i = 1, \dots, K\}$ . It is clear that  $\phi$  is a piecewise linear convex function on  $\text{conv}(X)$ . By the concavity of  $f$ , we have

$$f(x) \geq \phi(x), \quad \forall x \in \text{conv}(X) \quad (2.3.5)$$

and  $f(x) = \phi(x)$  for all  $x \in \Omega$ . Recall that  $f(x)$  and  $\phi(x)$  have the same global optimal value over  $\text{conv}(X)$  (see [182]). Notice that a concave function always achieves its minimum over a polyhedron at one of the extreme points. Also, the extreme points of  $\text{conv}(X)$  are integer points. Thus, we have

$$\begin{aligned} v(D_v) &= \max_{\lambda \in \mathbb{R}_+^m, \mu \in \mathbb{R}^l} \min_{x \in X} [f(x) + \lambda^T(Ax - b) + \mu^T(Bx - d)] \\ &= \max_{\lambda \in \mathbb{R}_+^m, \mu \in \mathbb{R}^l} \min_{x \in \text{conv}(X)} [f(x) + \lambda^T(Ax - b) + \mu^T(Bx - d)] \\ &= \max_{\lambda \in \mathbb{R}_+^m, \mu \in \mathbb{R}^l} \min_{x \in \text{conv}(X)} [\phi(x) + \lambda^T(Ax - b) + \mu^T(Bx - d)] \\ &= \min_{x \in \text{conv}(X)} \max_{\lambda \in \mathbb{R}_+^m, \mu \in \mathbb{R}^l} [\phi(x) + \lambda^T(Ax - b) + \mu^T(Bx - d)] \\ &= \min_{x \in \text{conv}(X)} \{\phi(x) \mid Ax \leq b, Bx = d\} \\ &\leq \min_{x \in \text{conv}(X)} \{f(x) \mid Ax \leq b, Bx = d\} \\ &= v(\overline{P}_v). \end{aligned}$$

The fourth equation in the above derivation is due to the strong duality theorem for piecewise linear programming.  $\square$

Combining Theorems 2.4 and 2.5 gives rise to the well-known result in classical linear integer programming theory: The Lagrangian dual bound is identical to the continuous bound for linear integer programming.

**COROLLARY 2.1** *If  $f$  is a linear function in  $(P_v)$ , then  $v(D_v) = v(\overline{P}_v)$ .*

## 2.4 Proximity between Continuous Solution and Integer Solution

A natural and simple way to solve  $(P)$  is to relax the integrality of  $x$  and to solve the continuous version of  $(P)$  as a nonlinear programming problem. The optimal solution to the continuous relaxation is then rounded to its nearest integer point in  $X$  which sometimes happens to be a good sub-optimal feasible solution to  $(P)$ . In many situations, however, the idea of rounding the continuous solution may result in an integer solution that is not only far away from the optimal solution of  $(P)$  but also infeasible. Thus, it is important to study the relationship between the integer and continuous solutions in mathematical programming problems.



### 2.4.1 Linear integer program

Consider a linear integer program

$$\begin{aligned} \min \quad & c^T x \\ \text{s.t.} \quad & Ax \leq b, \\ & x \in \mathbb{Z}^n, \end{aligned} \tag{2.4.1}$$

and its continuous relaxation:

$$\begin{aligned} \min \quad & c^T x \\ \text{s.t.} \quad & Ax \leq b, \\ & x \in \mathbb{R}^n, \end{aligned} \tag{2.4.2}$$

where  $A$  is an integer  $m \times n$  matrix and  $c \in \mathbb{R}^n$  and  $b \in \mathbb{R}^m$ . Denote by  $\Delta(A)$  the maximum among the absolute values of all sub-determinants of matrix  $A$ .

**THEOREM 2.6** *Assume that the optimal solutions of problems (2.4.1) and (2.4.2) both exist. Then:*

(i) *For each optimal solution  $\bar{x}$  to (2.4.2), there exists an optimal solution  $z^*$  to (2.4.1) such that*

$$\|\bar{x} - z^*\|_\infty \leq n\Delta(A). \tag{2.4.3}$$

(ii) *For each optimal solution  $\bar{z}$  to (2.4.1), there exists an optimal solution  $x^*$  to (2.4.2) such that*

$$\|x^* - \bar{z}\|_\infty \leq n\Delta(A). \tag{2.4.4}$$

**Proof.** Let  $\bar{x}$  and  $\bar{z}$  be optimal solutions to (2.4.2) and (2.4.1), respectively. Partition  $A$  into  $A^T = [A_1^T, A_2^T]$ , where  $A_1\bar{x} \geq A_1\bar{z}$  and  $A_2\bar{x} < A_2\bar{z}$ , and partition  $b$  into  $b^1$  and  $b^2$  accordingly. Note that  $A_2\bar{x} < A_2\bar{z} \leq b^2$ . Let  $\bar{\lambda}_1 \geq 0$  and  $\bar{\lambda}_2 \geq 0$  be optimal dual variables corresponding to  $A_1$  and  $A_2$ , respectively, for (2.4.2). By the complementary slackness condition,  $\bar{\lambda}_2 = 0$  and thus we have  $A_1^T \bar{\lambda}_1 = -c$ . Consider the following cone:

$$C = \{x \mid A_1x \geq 0, A_2x \leq 0\}.$$

Obviously,  $\bar{x} - \bar{z} \in C$ . Furthermore  $c^T x \leq 0$  for all  $x \in C$ , since  $c^T x = -\bar{\lambda}_1^T A_1 x \leq 0$  for all  $x \in C$ . By Carathéodory's theorem, there exist  $t$  ( $t \leq n$ ) integer vectors  $d^i \in C$ ,  $i = 1, \dots, t$ , and  $\mu_i \geq 0$ ,  $i = 1, \dots, t$ , such that

$$\bar{x} - \bar{z} = \mu_1 d^1 + \dots + \mu_t d^t. \tag{2.4.5}$$

By Cramer's rule, we can assume that  $\|d^i\|_\infty \leq \Delta(A)$ ,  $i = 1, \dots, t$ .

Let

$$z^* = \bar{z} + \lfloor \mu_1 \rfloor d^1 + \cdots + \lfloor \mu_t \rfloor d^t. \quad (2.4.6)$$

where  $\lfloor x \rfloor$  is the maximum integer number less than or equal to  $x$ . By (2.4.5), we have

$$z^* = \bar{x} + (\lfloor \mu_1 \rfloor - \mu_1) d^1 + \cdots + (\lfloor \mu_t \rfloor - \mu_t) d^t. \quad (2.4.7)$$

Thus,

$$\begin{aligned} A_1 z^* &= A_1 \bar{x} + (\lfloor \mu_1 \rfloor - \mu_1) A_1 d^1 + \cdots + (\lfloor \mu_t \rfloor - \mu_t) A_1 d^t \leq A_1 \bar{x} \leq b^1, \\ A_2 z^* &= A_2 \bar{z} + \lfloor \mu_1 \rfloor A_2 d^1 + \cdots + \lfloor \mu_t \rfloor A_2 d^t \leq A_2 \bar{z} \leq b^2. \end{aligned}$$

So  $Az^* \leq b$ . Moreover, since  $c^T d^i = -\bar{\lambda}_1^T A_1 d^i \leq 0$  for all  $i = 1, \dots, t$ , we imply from (2.4.6) that  $c^T z^* \leq c^T \bar{z}$ . Therefore,  $z^*$  is an optimal solution to (2.4.1) and by (2.4.7), we get

$$\|z^* - \bar{x}\|_\infty \leq \|d^1\|_\infty + \cdots + \|d^t\|_\infty \leq n\Delta(A),$$

which is (2.4.3). Moreover, combining  $c^T z^* \leq c^T \bar{z}$  with the optimality of  $\bar{z}$  and (2.4.6) leads to  $c^T d^i = 0$  for  $i$  with  $\mu_i \geq 1$ .

Now, let

$$x^* = \bar{x} - \lfloor \mu_1 \rfloor d^1 - \cdots - \lfloor \mu_t \rfloor d^t. \quad (2.4.8)$$

Then,

$$A_1 x^* = A_1 \bar{x} - \lfloor \mu_1 \rfloor A_1 d^1 - \cdots - \lfloor \mu_t \rfloor A_1 d^t \leq A_1 \bar{x} \leq b^1. \quad (2.4.9)$$

Also, by (2.4.5), it holds

$$x^* = \bar{z} + (\mu_1 - \lfloor \mu_1 \rfloor) d^1 + \cdots + (\mu_t - \lfloor \mu_t \rfloor) d^t.$$

Thus, we obtain  $\|x^* - \bar{z}\|_\infty \leq n\Delta(A)$  using the similar arguments as in part (i). Moreover, we have

$$A_2 x^* = A_2 \bar{z} + (\mu_1 - \lfloor \mu_1 \rfloor) A_2 d^1 + \cdots + (\mu_t - \lfloor \mu_t \rfloor) A_2 d^t \leq A_2 \bar{z} \leq b^2. \quad (2.4.10)$$

Combining (2.4.9) with (2.4.10) gives rise to  $Ax^* \leq b$ . Since  $c^T d^i = 0$  for  $i$  with  $\mu_i \geq 1$  and  $\lfloor \mu_i \rfloor = 0$  for  $i$  with  $0 \leq \mu_i < 1$ , we obtain from (2.4.8) that  $c^T x^* = c^T \bar{x}$ . Thus,  $x^*$  is an optimal solution to (2.4.2).  $\square$

## 2.4.2 Linearly constrained separable convex integer program

The proximity results in the previous subsection can be extended to separable convex programming problems. Consider the following problems:

$$\begin{aligned} \min f(x) &= \sum_{j=1}^n f_j(x_j) \\ \text{s.t. } Ax &\leq b, \\ x &\in \mathbb{Z}^n, \end{aligned} \quad (2.4.11)$$

and its continuous relaxation:

$$\begin{aligned} \min f(x) &= \sum_{j=1}^n f_j(x_j) \\ \text{s.t. } Ax &\leq b, \\ x &\in \mathbb{R}^n, \end{aligned} \quad (2.4.12)$$

where  $f_j(x_j)$ ,  $j = 1, \dots, n$ , are all convex functions on  $\mathbb{R}$ ,  $A$  is an integer  $m \times n$  matrix and  $b \in \mathbb{R}^m$ . The following result generalizes Theorem 2.6.

**THEOREM 2.7** *Assume that the optimal solutions of problems (2.4.11) and (2.4.12) both exist. Then:*

(i) *For each optimal solution  $\bar{x}$  to (2.4.12), there exists an optimal solution  $z^*$  to (2.4.11) such that*

$$\|\bar{x} - z^*\|_\infty \leq n\Delta(A). \quad (2.4.13)$$

(ii) *For each optimal solution  $\bar{z}$  to (2.4.11), there exists an optimal solution  $x^*$  to (2.4.12) such that*

$$\|x^* - \bar{z}\|_\infty \leq n\Delta(A). \quad (2.4.14)$$

**Proof.** Let  $\bar{x}$  and  $\bar{z}$  be optimal solutions to (2.4.12) and (2.4.11), respectively. Let  $S^*$  be the intersection of the feasible region of (2.4.12) with the minimal box that contains  $\bar{x}$  and  $\bar{z}$ . Let

$$A^* = \begin{bmatrix} A \\ I_{n \times n} \\ -I_{n \times n} \end{bmatrix}, \quad b^* = \begin{bmatrix} b \\ \max(\bar{x}, \bar{z}) \\ -\min(\bar{x}, \bar{z}) \end{bmatrix}. \quad (2.4.15)$$

Then  $S^*$  can be expressed as  $\{x \in \mathbb{R}^n \mid A^*x \leq b^*\}$ . Now, consider the linear over-estimation of  $f_j(x_j)$ . Let  $c_j^* = (f_j(\bar{x}_j) - f_j(\bar{z}_j))/(\bar{x}_j - \bar{z}_j)$ . Without loss of generality, we can assume that  $\bar{z}_j = f_j(\bar{z}_j) = 0$ . So  $f_j(\bar{x}_j) = c_j^* \bar{x}_j$ .

Moreover, by the convexity of  $f_j$ , we have  $f_j(x_j) \leq c_j^* x_j$  for all  $j = 1, \dots, n$  and  $x \in S^*$ . Consider the following linear program:

$$\begin{aligned} \min \quad & (c^*)^T x \\ \text{s.t.} \quad & A^* x \leq b^*, \\ & x \in \mathbb{R}^n. \end{aligned} \tag{2.4.16}$$

Since  $(c^*)^T \bar{x} = f(\bar{x}) \leq f(x) \leq (c^*)^T x$  for all  $x \in S^*$ ,  $\bar{x}$  is also an optimal solution to (2.4.16). Note that the upper bound of the absolute values of subdeterminants of  $A^*$  remains  $\Delta(A)$ .

By Theorem 2.6, there exists an integer  $z^* \in S^*$  such that  $\|\bar{x} - z^*\|_\infty \leq n\Delta(A)$  and  $(c^*)^T z^* \leq (c^*)^T z$  for all integer  $z \in S^*$ . Note that  $f(z^*) \leq (c^*)^T z^* \leq (c^*)^T \bar{z} = f(\bar{z})$ . It follows that  $z^*$  is an optimal solution to (2.4.11). This proves part (i) of the theorem. Part (ii) can be proved similarly.  $\square$

### 2.4.3 Unconstrained convex integer program

In this subsection, we establish some proximity results for general unconstrained convex integer programs which are not necessarily separable. For a separable convex function the distance (in  $\infty$ -norm) between its integer and real minimizers is bounded by 1. This is simply because the distance between the integer and real minimizers of a univariate convex function is always dominated by 1. Thus, we first concentrate in this subsection on a proximity bound for nonseparable quadratic functions and then extend it to strictly convex functions. We further discuss an extension to mixed-integer cases.

Let  $Q$  be an  $n \times n$  symmetric positive definite matrix. Define

$$q(x) = (x - x_0)^T Q (x - x_0).$$

Consider

$$\min\{q(x) \mid x \in \mathbb{R}^n\} \tag{2.4.17}$$

and

$$\min\{q(x) \mid x \in \mathbb{Z}^n\}. \tag{2.4.18}$$

Obviously,  $x_0$  is the unique minimizer of (2.4.17). For any  $n \times n$  real symmetric matrix  $P$ , denote by  $\lambda_{\max}(P)$  and  $\lambda_{\min}(P)$  its largest and smallest eigenvalues, respectively.

**THEOREM 2.8** *For any optimal solution  $\bar{x}$  to (2.4.18), it holds*

$$\|\bar{x} - x_0\|_2 \leq \frac{1}{2} \sqrt{n\kappa}, \tag{2.4.19}$$

where  $\kappa = \lambda_{\max}(Q)/\lambda_{\min}(Q)$  is the condition number of  $Q$ .

Proof. Let

$$q(\bar{x}) = (\bar{x} - x_0)^T Q(\bar{x} - x_0) = r. \quad (2.4.20)$$

We assume without loss of generality that  $\bar{x} \neq x_0$  and thus  $r > 0$ . By the optimality of  $\bar{x}$ , no integer point is contained in the interior of the following ellipsoid:

$$E = \{x \in \mathbb{R}^n \mid (x - x_0)^T Q(x - x_0) \leq r\}.$$

Since the diameter of the circumscribed sphere of a unit cube in  $\mathbb{R}^n$  is  $\sqrt{n}$ , the interior of a ball in  $\mathbb{R}^n$  with diameter greater than  $\sqrt{n}$  must contain at least one integer point. It is clear that ellipsoid  $E$  contains the ball centered at  $x_0$  with diameter  $2\sqrt{r\lambda_{\min}(Q^{-1})}$ . Hence, we have

$$2\sqrt{r\lambda_{\min}(Q^{-1})} \leq \sqrt{n}. \quad (2.4.21)$$

Notice also that ellipsoid  $E$  is enclosed in the ball centered at  $x_0$  with diameter  $2\sqrt{r\lambda_{\max}(Q^{-1})}$ . We therefore find from (2.4.20) and (2.4.21) that

$$\begin{aligned} \|\bar{x} - x_0\|_2 &\leq \sqrt{r\lambda_{\max}(Q^{-1})} \\ &\leq \frac{1}{2} \sqrt{\frac{n\lambda_{\max}(Q^{-1})}{\lambda_{\min}(Q^{-1})}} \\ &= \frac{1}{2} \sqrt{\frac{n\lambda_{\max}(Q)}{\lambda_{\min}(Q)}} \\ &= \frac{1}{2} \sqrt{n\kappa}. \end{aligned}$$

□

Let  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  be a twice differentiable convex function satisfying the following strong convexity condition:

$$0 < m \leq \lambda_{\min}(\nabla^2 f(x)) \leq \lambda_{\max}(\nabla^2 f(x)) \leq M, \quad \forall x \in \mathbb{R}^n. \quad (2.4.22)$$

Consider

$$\min\{f(x) \mid x \in \mathbb{R}^n\} \quad (2.4.23)$$

and

$$\min\{f(x) \mid x \in \mathbb{Z}^n\}. \quad (2.4.24)$$

**THEOREM 2.9** *Let  $x_0$  be the unique optimal solution to (2.4.23). Then for any optimal solution  $\bar{x}$  to (2.4.24), it holds*

$$\|\bar{x} - x_0\|_2 \leq \frac{1}{2}\sqrt{n\kappa_1},$$

where  $\kappa_1 = M/m$ .

**Proof.** Note that the condition (2.4.22) and Taylor's Theorem imply

$$\frac{1}{2}m\|x - x_0\|_2^2 \leq f(x) - f(x_0) \leq \frac{1}{2}M\|x - x_0\|_2^2, \quad \forall x \in \mathbb{R}^n. \quad (2.4.25)$$

Let  $r = f(\bar{x}) - f(x_0)$ . By (2.4.25), the convex level set  $\{x \in \mathbb{R}^n \mid f(x) - f(x_0) \leq r\}$  contains a sphere with diameter  $2\sqrt{2rM^{-1}}$  and is enclosed in a sphere with diameter  $2\sqrt{2rm^{-1}}$ . The theorem then follows by using the same arguments as in the proof of Theorem 2.8.  $\square$

Now we consider the mixed-integer convex program:

$$\min\{f(x) \mid x = (y, z)^T, y \in \mathbb{Z}^l, z \in \mathbb{R}^k\}, \quad (2.4.26)$$

where  $l > 0, k > 0, l + k = n$  and  $f(x)$  satisfies condition (2.4.22).

**THEOREM 2.10** *Let  $x_0$  be the unique optimal solution to (2.4.23). Then for any optimal solution  $\bar{x}$  of (2.4.26), it holds*

$$\|\bar{x} - x_0\|_2 \leq \frac{1}{2}\sqrt{n\kappa_1},$$

where  $\kappa_1 = M/m$ .

**Proof.** Note that every sphere in  $\mathbb{R}^n$  with diameter  $\sqrt{n}$  has a nonempty intersection with a  $k$ -dimensional hyperplane  $\{x \in \mathbb{R}^n \mid x = (y, z)^T, y = a\}$  for some integer  $a \in \mathbb{Z}^l$ . The theorem can then be proved along the same line as in the proof of Theorem 2.8.  $\square$

One promising application of the above proximity results is their usage in reducing the set of feasible solutions in integer programming problems.

**EXAMPLE 2.2** Consider the following unconstrained quadratic integer program:

$$\begin{aligned} \min \quad & q(x) = 27x_1^2 - 18x_1x_2 + 4x_2^2 - 3x_2 \\ \text{s.t.} \quad & x \in \mathbb{Z}^2. \end{aligned}$$

The optimal solution of the continuous relaxation of this example is  $x_0 = (0.5, 1.5)^T$  with  $q(x_0) = -2.25$ . Theorem 2.8 can be used to reduce the

feasible region by setting the bounds for the integer variables. It is easy to verify that  $\kappa = 33.5627$ . From (2.4.19) we have  $\|\bar{x} - x_0\|_2 \leq (1/2)\sqrt{2\kappa} = 4.0965$ . We can thus attach a box constraint  $-3 \leq x_1 \leq 4$ ,  $-2 \leq x_2 \leq 5$  to Example 2.2. This significant reduction in the feasible region may help the solution process when a branch-and-bound algorithm is used as a solution scheme. Applying a branch-and-bound procedure to Example 2.2 with the box constraint yields an optimal solution  $\bar{x} = (1, 3)^T$  with  $q(\bar{x}) = 0$ . We note that  $\bar{x}$  cannot be obtained by rounding the continuous optimal solution  $x_0$  since  $q((0, 1)^T) = q((1, 2)^T) = 1$ ,  $q((1, 1)^T) = q((0, 2)^T) = 10$ .

The following example shows that the bound in (2.4.19) can be achieved in some situations.

EXAMPLE 2.3 Consider the following problem:

$$\min\left\{\sum_{i=1}^n \left(x_i - \frac{1}{2}\right)^2 \mid x \in \mathbb{Z}^n\right\}.$$

It is easy to see that all vertices of the unit cube  $[0, 1]^n$  are the optimal integer solutions of this problem. Since  $x_0 = (1/2, 1/2, \dots, 1/2)^T$ , we get  $\|\bar{x} - x_0\|_2 = \sqrt{n}/2$ . On the other hand, since  $Q = I$ , we have  $\kappa = 1$  and  $\sqrt{n\kappa}/2 = \sqrt{n}/2$ .

Now, we give another example in which the strict inequality in (2.4.19) holds while both  $\|\bar{x} - x_0\|_2$  and  $\kappa$  tend to infinity simultaneously. As a by-product, we can get a method in constructing nonseparable quadratic test problems where the distance between the continuous and integer solutions can be predetermined.

Let  $v_1 = (\cos \theta, \sin \theta)^T$ ,  $v_2 = (-\sin \theta, \cos \theta)^T$ . Then  $v_1$  and  $v_2$  are orthonormal and the angle between  $v_1$  and  $x_1$ -axis is  $\theta$ . For  $\lambda_1 \geq \lambda_2 > 0$ , let

$$\begin{aligned} P &= \lambda_1 v_1 v_1^T + \lambda_2 v_2 v_2^T \\ &= \begin{pmatrix} \lambda_1 \cos^2 \theta + \lambda_2 \sin^2 \theta & (\lambda_1 - \lambda_2) \sin \theta \cos \theta \\ (\lambda_1 - \lambda_2) \sin \theta \cos \theta & \lambda_1 \sin^2 \theta + \lambda_2 \cos^2 \theta \end{pmatrix}. \end{aligned} \quad (2.4.27)$$

It follows that  $P$  is a  $2 \times 2$  symmetric positive definite matrix and it has eigenvalues  $\lambda_1$  and  $\lambda_2$  with corresponding eigenvectors  $v_1$  and  $v_2$ , respectively.

EXAMPLE 2.4 Consider the following problem:

$$\min\{q(x) := (x - x_0)^T P^{-1} (x - x_0) \mid x \in \mathbb{Z}^2\}, \quad (2.4.28)$$

where  $P$  is defined by (2.4.27),  $x_0 = (0, 1/2)^T$  and  $\lambda_2 \in (0, 1/4)$ .

For any positive integer  $m > 0$  and  $\lambda_2 \in (0, 1/4)$ , we can determine the values of  $\theta$  and  $\lambda_1$  such that axis  $x_2 = 0$  supports ellipsoid  $E(x_0, P^{-1}) = \{x \in$

$\mathbb{R}^2 \mid (x - x_0)^T P^{-1}(x - x_0) \leq 1\}$  at  $(-m, 0)$ . For  $t \in \mathbb{R}$ , consider equation  $q((t, 0)^T) = 1$ . From (2.4.27) and (2.4.28), this equation is equivalent to

$$a_1 t^2 + a_2 t + a_3 = 0, \quad (2.4.29)$$

where

$$\begin{aligned} a_1 &= \lambda_1 \sin^2 \theta + \lambda_2 \cos^2 \theta, \\ a_2 &= (\lambda_1 - \lambda_2) \sin \theta \cos \theta, \\ a_3 &= \frac{1}{4} \lambda_1 \cos^2 \theta + \frac{1}{4} \lambda_2 \sin^2 \theta - \lambda_1 \lambda_2. \end{aligned}$$

Note that

$$a_2^2 - 4a_1 a_3 = -\lambda_1 \lambda_2 + 4\lambda_1 \lambda_2 (\lambda_1 \sin^2 \theta + \lambda_2 \cos^2 \theta).$$

Therefore, equation (2.4.29) has a unique real root if and only if

$$\lambda_1 \sin^2 \theta + \lambda_2 \cos^2 \theta = \frac{1}{4}. \quad (2.4.30)$$

If condition (2.4.30) holds,  $a_1 = \frac{1}{4}$  and the root of equation (2.4.29) is

$$t = -\frac{a_2}{2a_1} = -2(\lambda_1 - \lambda_2) \sin \theta \cos \theta. \quad (2.4.31)$$

Setting  $t = -m$  in (2.4.31), we get

$$(\lambda_1 - \lambda_2) \sin(2\theta) = m. \quad (2.4.32)$$

Equations (2.4.30) and (2.4.32) uniquely determine the values of  $\theta \in (0, \pi/2)$  and  $\lambda_1 > 1/4$  for which  $(-m, 0)^T$  is the unique intersection point of ellipsoid  $E(x_0, P^{-1})$  and  $x_1$ -axis. By the symmetry of the ellipsoid,  $(m, 1)^T$  is the unique intersection point of  $E(x_0, P^{-1})$  and the line  $x_2 = 1$ . Since no integer point other than  $(-m, 0)^T$  and  $(m, 1)^T$  lies in  $E(x_0, P^{-1})$ ,  $\bar{x}_1(m) = (-m, 0)^T$  and  $\bar{x}_2(m) = (m, 1)^T$  are the optimal solutions of (2.4.28).

Now, we set  $\lambda_2 = 1/5$ . For any positive integer  $m$ , let  $\theta(m)$  and  $\lambda_1(m)$  be determined from (2.4.30) and (2.4.32). Denote  $\kappa(m) = \lambda_1(m)/\lambda_2 = 5\lambda_1(m)$ .



By (2.4.30) and (2.4.32), we have

$$\begin{aligned}
 & \|\bar{x}_1(m) - x_0\|_2 = \|\bar{x}_2(m) - x_0\|_2 \\
 &= \sqrt{m^2 + \frac{1}{4}} \\
 &= \sqrt{4(\lambda_1(m) - 1/5)^2 \sin^2[\theta(m)](1 - \sin^2[\theta(m)]) + \frac{1}{4}} \\
 &= \sqrt{4(\lambda_1(m) - 1/5)^2 \left( \frac{1/4 - 1/5}{\lambda_1(m) - 1/5} \right) \left( 1 - \frac{1/4 - 1/5}{\lambda_1(m) - 1/5} \right) + \frac{1}{4}} \\
 &= \sqrt{\frac{1}{5} \lambda_1(m) + \frac{1}{5}} \\
 &= \sqrt{\frac{1}{25} \kappa(m) + \frac{1}{5}}.
 \end{aligned}$$

Thus,  $\|\bar{x}_1(m) - x_0\|_2 = \|\bar{x}_2(m) - x_0\|_2 \rightarrow \infty$  and  $\kappa(m) \rightarrow \infty$  when  $m \rightarrow \infty$ . Moreover, since  $\kappa(m) > 1$ , we have

$$\|\bar{x}_1(m) - x_0\|_2 = \sqrt{\frac{1}{25} \kappa(m) + \frac{1}{5}} < \frac{1}{2} \sqrt{2\kappa(m)}.$$

## 2.5 Penalty Function Approach

Generally speaking, an unconstrained integer programming problem is easier to solve than a constrained one. We discuss in this section how to convert a general constrained integer programming problem into an unconstrained one by using an exact penalty method. Consider the following problem:

$$\begin{aligned}
 (P) \quad & \min f(x) \\
 & \text{s.t. } g_i(x) \leq 0, \quad i = 1, \dots, m, \\
 & \quad h_j(x) = 0, \quad j = 1, \dots, l, \\
 & \quad x \in X,
 \end{aligned}$$

where  $f, g_i(x)$  ( $i = 1, \dots, m$ ) and  $h_j(x)$  ( $j = 1, \dots, l$ ) are continuous functions, and  $X$  is a finite set in  $\mathbb{Z}^n$ . Let

$$S = \{x \in X \mid g_i(x) \leq 0, \quad i = 1, \dots, m, \quad h_j(x) = 0, \quad j = 1, \dots, l\}.$$

Define a penalty function  $P(x)$  such that:  $P(x) = 0$  for  $x \in S$  and  $P(x) \geq \epsilon > 0$  for  $x \notin S$ . A typical penalty function for (P) is

$$P(x) = \sum_{i=1}^m \max(g_i(x), 0) + \sum_{j=1}^l h_j^2(x). \quad (2.5.1)$$

Define the penalty problem of  $(P)$  as follows:

$$(PEN) \quad \min_{x \in X} T(x, \mu) = f(x) + \mu P(x), \quad \mu > 0.$$

Since  $T(x, \mu) = f(x)$  for  $x \in S$  and  $S \subseteq X$ , we have  $v(P) \geq v(PEN)$ .

**THEOREM 2.11** *Let  $\underline{f}$  be a lower bound of  $\min_{x \in X} f(x)$  and  $\gamma > 0$  be a lower bound of  $\min_{x \in X \setminus S} P(x)$ . Suppose that  $X \setminus S \neq \emptyset$ . Then, there exists a  $\mu_0$  such that for any  $\mu > \mu_0$ , any solution  $x^*$  that solves  $(PEN)$  also solves  $(P)$  and  $v(PEN) = v(P)$ .*

*Proof.* Let

$$\mu_0 = \frac{v(P) - \underline{f}}{\gamma}. \quad (2.5.2)$$

For any  $x \in X \setminus S$  and any  $\mu > \mu_0$ ,

$$\begin{aligned} T(x, \mu) &= f(x) + \mu P(x) \\ &> f(x) + \mu_0 P(x) \\ &\geq f(x) + (v(P) - \underline{f}) \\ &\geq v(P). \end{aligned}$$

Therefore, the minimum of  $T(x, \mu)$  over  $X$  must be achieved in  $S$ . Since  $T(x, \mu) = f(x)$  for any  $x \in S$ , we conclude that  $x^*$  solves  $(P)$  and  $v(PEN) = T(x^*, \mu) = f(x^*) = v(P)$ .  $\square$

**COROLLARY 2.2** *Let  $\bar{f}$  be an upper bound of  $v(P)$ . If  $m = 0$  and  $h_j$  ( $j = 1, \dots, l$ ) are integer-valued functions on  $X$ , then for any  $\mu \geq \mu_0 = \bar{f} - \underline{f}$ , any solution  $x^*$  solves  $(PEN)$  also solves  $(P)$ , where  $P(x) = \sum_{j=1}^l h_j^2(x)$  in problem  $(PEN)$ .*

*Proof.* Since  $h_j$  is integer-valued, we deduce that  $P(x) \geq 1$  for any  $x \in X \setminus S$  and hence  $\gamma$  can be taken as 1. Moreover,  $v(P) \geq \underline{f}$ , thus, by (2.5.2),  $\mu_0 \leq \bar{f} - \underline{f}$ . The conclusion then follows from Theorem 2.11.  $\square$

If  $h_j(x) \geq 0$  for any  $x \in X$ ,  $j = 1, \dots, l$ , then  $P(x)$  in Corollary 2.2 can be taken as  $P(x) = \sum_{j=1}^l h_j(x)$ .

## 2.6 Optimality Conditions for Unconstrained Binary Quadratic Problems

### 2.6.1 General case

We consider the following unconstrained binary quadratic optimization problem:

$$(BQ) \quad \min_{x \in \{-1, 1\}^n} q(x) = \frac{1}{2} x^T Q x + b^T x,$$

where  $Q$  is a symmetric matrix in  $\mathbb{R}^{n \times n}$  and  $b \in \mathbb{R}^n$ . Notice that any binary quadratic problem with  $y_i \in \{l_i, u_i\}$ ,  $i = 1, \dots, n$ , can be transformed into the form of  $(BQ)$  by the linear transformation:  $y_i = l_i + (u_i - l_i)(x_i + 1)/2$ ,  $i = 1, \dots, n$ . It is clear that  $(BQ)$  is equivalent to the following continuous quadratic problem:

$$(CQ) \quad \min q(x) = \frac{1}{2}x^T Qx + b^T x, \\ \text{s.t. } x_i^2 = 1, \quad i = 1, \dots, n.$$

Problem  $(CQ)$  is essentially a nonconvex continuous optimization problem even if matrix  $Q$  is positive semidefinite. Thus, problem  $(CQ)$  is the same as hard as the primal problem  $(BQ)$ .

To motivate the derivation of the global optimality conditions, let's consider the relationship between the solutions of the following two scalar optimization problems with  $a > 0$ :

$$(SQ) \quad \min \left\{ \frac{1}{2}ax^2 + bx \mid x \in \{-1, 1\} \right\}$$

and

$$(\overline{SQ}) \quad \min \left\{ \frac{1}{2}ax^2 + bx \mid -1 \leq x \leq 1 \right\}.$$

We are interested in conditions under which  $v(SQ) = v(\overline{SQ})$ , and furthermore  $(SQ)$  and  $(\overline{SQ})$  have the same optimal solution. Note that we can rewrite  $\frac{1}{2}ax^2 + bx$  as  $\frac{1}{2}a(x + \frac{b}{a})^2 - \frac{b^2}{2a}$ . It can be verified that when  $a \leq |b|$  and  $b > 0$ ,  $x^* = -1$  solves both  $(SQ)$  and  $(\overline{SQ})$  and when  $a \leq |b|$  and  $b < 0$ ,  $x^* = 1$  solves both  $(SQ)$  and  $(\overline{SQ})$ . In summary,  $a \leq |b|$  is both a necessary and sufficient condition for generating an optimal solution of the integer optimization problem  $(SQ)$  by its continuous optimization problem  $(\overline{SQ})$ .

Consider the following Lagrangian relaxation of problem  $(CQ)$ :

$$\min_{x \in \mathbb{R}^n} L(x, y) = q(x) + \sum_{i=1}^n y_i(x_i^2 - 1),$$

where  $y_i \in \mathbb{R}$  is the Lagrangian multiplier for constraint  $x_i^2 = 1$ ,  $i = 1, \dots, n$ . Define two  $n \times n$  diagonal matrices  $X = \text{diag}(x)$  and  $Y = \text{diag}(y)$ . The Lagrangian relaxation problem of  $(CQ)$  can be expressed as

$$(LCQ) \quad h(y) = \min_{x \in \mathbb{R}^n} \left[ \frac{1}{2}x^T(Q + 2Y)x + b^T x - e^T y \right],$$

where  $e$  is an  $n$  dimensional vector with all components equal to 1. The dual problem of  $(CQ)$  is then given as

$$(DQ) \quad \max_{y \in \text{dom } h} h(y),$$

where

$$\text{dom } h = \{y \in \mathbb{R}^n \mid h(y) > -\infty\}.$$

Note that the necessary and sufficient conditions for  $h(y) > -\infty$  are:

- (i) There exists an  $x$  such that  $(Q + 2Y)x + b = 0$ ;
- (ii) The matrix  $Q + 2Y$  is positive semidefinite.

Although problem  $(CQ)$  is nonconvex, if we are lucky enough to find out an  $\bar{x}$  that is feasible in  $(CQ)$  and  $\bar{y} \in \text{dom } h$  such that  $q(\bar{x}) = h(\bar{y})$ , then  $\bar{x}$  must be a global optimal solution to  $(CQ)$ .

**THEOREM 2.12** *Let  $\bar{x} = \bar{X}e$  be feasible in  $(CQ)$ . If*

$$\bar{X}Q\bar{X}e + \bar{X}b \leq \lambda_{\min}(Q)e, \quad (2.6.1)$$

*where  $\lambda_{\min}(Q)$  is the minimum eigenvalue of matrix  $Q$ , then  $\bar{x}$  is a global optimal solution of  $(CQ)$  or  $(BQ)$ .*

**Proof.** Let

$$\bar{y} = -\frac{1}{2}(\bar{X}Q\bar{X}e + \bar{X}b). \quad (2.6.2)$$

Let  $\bar{Y} = \text{diag}(\bar{y})$ . Then

$$\begin{aligned} (Q + 2\bar{Y})\bar{x} + b &= Q\bar{X}e + 2\bar{Y}\bar{X}e + b \\ &= Q\bar{X}e + 2\bar{X}\bar{y} + b \\ &= Q\bar{X}e - \bar{X}^2Q\bar{X}e - \bar{X}^2b + b \\ &= 0, \end{aligned}$$

where the last equality is due to  $\bar{X}^2 = I$  when  $\bar{x}$  is feasible to  $(CQ)$ . This implies that  $\bar{x}$  is a solution to  $(LCQ)$  with  $y = \bar{y}$  when  $Q + 2\bar{Y}$  is positive semidefinite.

From (2.6.1) and (2.6.2), we have

$$\lambda_{\min}(2\bar{Y}) = \min_{1 \leq i \leq n} (-\bar{X}Q\bar{X}e - \bar{X}b)_i \geq -\lambda_{\min}(Q).$$

Thus,

$$\lambda_{\min}(Q + 2\bar{Y}) \geq \lambda_{\min}(Q) + \lambda_{\min}(2\bar{Y}) \geq 0.$$

We can conclude that matrix  $Q + 2\bar{Y}$  is positive semidefinite. Thus  $\bar{y}$  defined in (2.6.2) belongs to  $\text{dom } h$ . The remaining task in deriving the sufficient global optimality condition is to prove that the dual value  $h(\bar{y})$  attains the objective

value of the feasible solution  $\bar{x}$ ,

$$\begin{aligned}
 h(\bar{y}) &= \min_{x \in \mathbb{R}^n} \left\{ \frac{1}{2} x^T (Q + 2\bar{Y}) x + b^T x - e^T \bar{y} \right\} \\
 &= -\frac{1}{2} \bar{x}^T (Q + 2\bar{Y}) \bar{x} - e^T \bar{y} \\
 &= -\frac{1}{2} e^T \bar{X} (Q + 2\bar{Y}) \bar{X} e - e^T \bar{y} \\
 &= -\frac{1}{2} e^T \bar{X} Q \bar{X} e - 2e^T \bar{y} \\
 &= \frac{1}{2} e^T \bar{X} Q \bar{X} e + b^T \bar{X} e \\
 &= q(\bar{x}),
 \end{aligned}$$

where the fact of  $\bar{X} \bar{Y} \bar{X} e = \bar{X}^2 \bar{Y} e = \bar{Y} e$  is used in the fourth equality and (2.6.2) is applied in the fifth equality.  $\square$

The next theorem gives a necessary global optimality condition for  $(CQ)$  or  $(BQ)$ .

**THEOREM 2.13** *If  $x^* = X^* e$  is a global optimal solution to  $(CQ)$ , then*

$$X^* Q X^* e + X^* b \leq \text{diag}(Q) e, \quad (2.6.3)$$

where  $\text{diag}(Q)$  is a diagonal matrix formed from matrix  $Q$  by setting all its nondiagonal elements at zero.

**Proof.** Let  $e_i$  be the  $i$ -th unit vector in  $\mathbb{R}^n$ . If  $x^*$  is optimal to  $(CQ)$ , then  $q(x^*) \leq q(z)$  for every feasible  $z$  to  $(CQ)$ . Especially, setting  $z = x^* - 2x_i^* e_i$  in the above relation yields

$$x_i^* e_i^T Q x^* + x_i^* b^T e_i \leq q_{ii}, \quad i = 1, \dots, n,$$

where  $q_{ii}$  is the  $i$ -th diagonal element of  $Q$ .  $\square$

The above derived sufficient and necessary global optimality conditions for the unconstrained binary quadratic problem  $(BQ)$  can be rewritten in the following form where the two bear a resemblance,

$$\text{Sufficient Condition for } (BQ) : \quad X(Q - \lambda_{\min}(Q)I)X e \leq -Xb,$$

$$\text{Necessary Condition for } (BQ) : \quad X(Q - \text{diag}(Q)I)X e \leq -Xb.$$

Note that  $q_{ii} \geq \lambda_{\min}(Q)$  for all  $i = 1, \dots, n$ . Thus,  $\text{diag}(Q)e \geq \lambda_{\min}(Q)e$ . Obviously, sufficient condition (2.6.1) implies necessary condition (2.6.3).

### 2.6.2 Convex case

We now consider a special case of  $(BQ)$  where matrix  $Q$  is positive semi-definite. Consider the following relaxation of  $(BQ)$ :

$$\begin{aligned} (\overline{BQ}) \quad \min \quad & q(x) = \frac{1}{2}x^T Q x + b^T x, \\ \text{s.t.} \quad & x_i^2 \leq 1, \quad i = 1, \dots, n. \end{aligned}$$

It is clear that  $(\overline{BQ})$  is a continuous convex minimization problem when  $q$  is convex. It is also obvious that if  $x \in \{-1, 1\}^n$  is optimal to  $(\overline{BQ})$ , then  $x$  is also optimal to problem  $(BQ)$ . On the other hand, if  $x^* \in \{-1, 1\}^n$  is optimal to problem  $(BQ)$ , then  $v(\overline{BQ}) \leq q(x^*)$ .

**THEOREM 2.14** *Assume that  $Q$  is positive semidefinite. Then  $x^* \in \{-1, 1\}^n$  is an optimal solution to both  $(BQ)$  and  $(\overline{BQ})$  if and only if*

$$X^* Q X^* e + X^* b \leq 0, \quad (2.6.4)$$

where  $X^* = \text{diag}(x^*)$  and  $e = (1, \dots, 1)^T$ .

**Proof.** Assume that  $x^*$  satisfies (2.6.4). For any  $y \in \mathbb{R}_+^n$ , consider the Lagrangian relaxation of problem  $(\overline{BQ})$ :

$$h(y) = \min_{x \in \mathbb{R}^n} L(x, y) = q(x) + \sum_{i=1}^n y_i (x_i^2 - 1). \quad (2.6.5)$$

Let

$$y^* = -\frac{1}{2}(X^* Q X^* e + X^* b),$$

which is nonnegative according to the assumption in (2.6.4). Furthermore, matrix  $(Q + 2Y^*)$  is positive semidefinite, where  $Y^* = \text{diag}(y^*)$ . As the same as in proving Theorem 2.12, we can prove that  $x^*$  solves problem (2.6.5) and  $h(y^*) = q(x^*)$ . Thus,  $x^* \in \{-1, 1\}^n$  is optimal to  $(\overline{BQ})$ , thus an optimal solution to  $(BQ)$ .

To prove the converse, assume that  $x^* \in \{-1, 1\}^n$  solves both  $(\overline{BQ})$  and  $(BQ)$ . Then from the KKT conditions for  $(\overline{BQ})$ , there exists a  $\bar{y} \in \mathbb{R}_+^n$  such that  $(Q + 2\bar{Y})x^* + b = 0$ , where  $\bar{Y} = \text{diag}(\bar{y})$ . Thus,

$$\begin{aligned} X^* Q X^* e + X^* b &= X^*(Q x^* + b) \\ &= -2X^* \bar{Y} x^* \\ &= -2\bar{Y} e \leq 0. \end{aligned}$$

□

Notice that problem  $(\overline{BQ})$  is a box constrained convex quadratic programming problem and hence is much easier to solve than  $(BQ)$ . Solving  $(\overline{BQ})$ , however, in general only yields a real solution. The next result gives a sufficient condition for getting a nearby integer optimal solution to  $(BQ)$  based on a real optimal solution to  $(\overline{BQ})$ .

**THEOREM 2.15** *Assume that  $Q$  is a real positive semidefinite matrix and  $x^*$  is an optimal solution to  $(\overline{BQ})$ . If  $z^* \in \{-1, 1\}^n$  satisfies the following conditions:*

- (i)  $z_i^* = x_i^*$  for  $x_i^* \in \{-1, 1\}$ , and
- (ii)  $Z^*Q(z^* - x^*) \leq \lambda_{\min}(Q)e$ , where  $Z^* = \text{diag}(z^*)$  and  $\lambda_{\min}(Q)$  is the minimum eigenvalue of  $Q$ ,

*then  $z^*$  is an optimal solution to  $(BQ)$ .*

**Proof.** There exists Lagrangian multiplier vector  $y \in \mathbb{R}_+^n$  such that  $x^*$  satisfies the following KKT conditions for  $(\overline{BQ})$ :

$$\begin{aligned} (Q + 2Y)x^* + b &= 0, \\ y_i[(x_i^*)^2 - 1] &= 0, \quad i = 1, \dots, n, \end{aligned}$$

where  $Y = \text{diag}(y)$ . Let  $\delta = z^* - x^*$  and  $\Delta = \text{diag}(\delta)$ . It can be verified that  $y_i\delta_i = 0, i = 1, \dots, n$ . Thus  $\Delta Y = 0$ . We have

$$\begin{aligned} Z^*QZ^*e + Z^*b &= Z^*Qz^* + Z^*b \\ &= Z^*[Q(x^* + \delta) + b] \\ &= Z^*(-2Yx^* + Q\delta) \\ &= (X^* + \Delta)(-2Yx^* + Q\delta) \\ &= -2y + Z^*Q\delta - 2\Delta Yx^* \\ &= -2y + Z^*Q(z^* - x^*) \\ &\leq Z^*Q(z^* - x^*). \end{aligned}$$

Thus  $Z^*Q(z^* - x^*) \leq \lambda_{\min}(Q)e$  implies  $Z^*QZ^*e + Z^*b \leq \lambda_{\min}(Q)e$ . Applying Theorem 2.12 concludes that  $z^*$  is optimal to  $(BQ)$ .  $\square$

The above theorem can be used to check the global optimality of an integer solution by rounding off a continuous solution.

**EXAMPLE 2.5** Consider problem  $(BQ)$  with

$$Q = \begin{pmatrix} 4 & 2 & 0 & 2 \\ 2 & 4 & 0 & 2 \\ 0 & 0 & 4 & 2 \\ 2 & 2 & 2 & 4 \end{pmatrix}, \quad b = (4, 4, 3, 3)^T.$$

For this problem, we have  $\lambda_{\min}(Q) = 1.0376$  and the optimal solution to  $(\overline{BQ})$  is  $x^* = (-0.875, -0.875, -1, 0.625)^T$ . Rounding  $x^*$  to its nearest integer point in  $\{-1, 1\}^n$ , we obtain  $z^* = (-1, -1, -1, 1)^T$ . It can be verified that  $Z^*Q(z^* - x^*) = (0, 0, -0.75, 1)^T \leq 1.0376 \times e = \lambda_{\min}(Q)e$  is satisfied. Thus, by Theorem 2.15,  $z^*$  is an optimal solution to  $(BQ)$ .

## 2.7 Notes

The concept of relaxation in integer programming was first formally presented in [76]. The framework of the branch-and-bound method for integer programming was first presented in [124]. More about implicit enumeration techniques can be found in [176].

In 1965, Glover first introduced the back-track scheme in his algorithm for solving linear 0-1 programming problems [77]. Based on Glover's previous work, Geoffrion [73] proposed a framework for implicit enumeration using the concept of the back-tracking scheme which was used later to simplify the well-known additive algorithm of Balas [7] for linear 0-1 programming problems. Both Glover [77] and Geoffrion [73] proved Theorem 2.3 separately using induction.

The relationship between the integer and continuous solutions in mathematical programming problems has been an interesting and challenging topic discussed in the literature. Proximity results were first established in [43] (see also [28][191]) for linear integer programming and then extended to linearly constrained convex separable integer programming problems in [102][225] (see also [11]). The proximity results for nonseparable convex function were obtained in [204].

There is almost no optimality condition derived in the literature for nonlinear integer programming problems. The binary quadratic optimization problem may be the only exception for which optimality conditions were investigated (see e.g., [15][179]).





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