A Quadratic Simplex Algorithm for Primal Optimization over Zero-One Polytopes (Extended Abstract)

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1 Introduction

We consider (implicitly binary) quadratic programming problems of the form

$$\inf \left\{ f(x) := \frac{1}{2} x^\intercal Q x + c^\intercal x : x \in \text{ext}(P) \right\} \tag{1}$$

where $Q \in \mathbb{R}^{n \times n}$ is symmetric, $c \in \mathbb{R}^n$, and $P := \{x \in \mathbb{R}^n : x \geq 0, Ax = b\}$ with $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$ is assumed to define a 0-1-polytope whose vertices (extreme points) we refer to by $\text{ext}(P)$. This special case covers in particular Unconstrained Binary Quadratic Programs (UBQPs), the Quadratic Assignment Problem (QAP), and further 0-1 problems where $Ax = b$ is total dual integral [4].

Interestingly, while the linear simplex algorithm [3] applied to P implicitly delivers a sequence of improving integer feasible solutions from $\text{ext}(P)$, there appears to be no prescribed access to such a sequence in the quadratic case. In particular, the quadratic simplex algorithm (e.g. [1, 2, 5]) (for convex f) cannot provide one since it is supposed to find $\inf \{f(x) : x \in P\}$ which is not necessarily attained at a vertex of P.

Yet, and although global optimality cannot be guaranteed (even if f is convex), sequences of f-improving vertices of P are still of practical interest. Providing these, the presented primal simplex algorithm generalizes on local improvement heuristics for e.g. UBQPs and the QAP. It may particularly serve to improve vertex solutions obtained from other contexts (such as branch-and-bound), ideally an incumbent feasible basis by simply switching pivoting rules.

2 A Primal Quadratic Simplex Algorithm

As is common, we assume that the description of P in (1) satisfies $n \geq m$ and $\text{rank}(A) = m$. To simplify presentation, we further assume that potential upper bounds on the variables x (such as $x \leq 1$) are either implied by or part of the system $Ax = b$. For a set $S \subseteq \{1, \ldots, n\}$, we denote by A_S the submatrix of A consisting of the columns indexed by S, and by x_S we denote the vector consisting of the components of x indexed by S (for singletons, the index is used).

In particular, for certain $B \subseteq \{1, \ldots, n\}$ with $|B| = m$, and the corresponding $N \coloneqq \{1, \ldots, n\} \setminus B$, we will refer to x_B and x_N as the *basic* and *non-basic variables*, respectively. In addition, we denote with Q_{iB} (Q_{Bi}) the i-th row (column) of Q w.r.t. the columns (rows) associated with B, and accordingly, with Q_{BB} the symmetric matrix consisting of the rows and columns indexed by B.

Let some initial partition (B,N) of a basic feasible solution $(x_B, x_N)^\mathsf{T}$ to (1) be given (e.g. from an incumbent solution of a branch-and-bound search) or derived (e.g. via a phase-I linear simplex algorithm) provided that one exists. Recall that if some variable x_r, $r \in N$, is to enter the basis then we are about to move to a solution of $A_B x_B + A_r x_r = b$, i.e., we will turn x_B into $x'_B = A_B^{-1} b - A_B^{-1} A_r x'_r$. Thus, $d = A_B^{-1} A_r$ is the direction of change w.r.t. x_B, and feasibility requests that $x'_B = x_B - d x'_r \geq 0$ which imposes a limit on the increase of x'_r only if $d_i > 0$ for at least one $i \in \{1, \ldots, m\}$ (ratio test). In the here considered case of a 0-1-polytope, this is guaranteed (and $d_i \in \{-1, 0, 1\}$). Hence, the mentioned limit or primal step length $\theta_P \coloneqq \max\{t \in \mathbb{R} : x_B - td \geq 0\}$ is well defined and predetermined, and so is the new solution:

$$\begin{pmatrix} x'_B \\ x'_r \end{pmatrix} = \begin{pmatrix} x_B - \theta_P d \\ \theta_P \end{pmatrix} \text{ and } x'_k = 0 \text{ for all } k \in \{1, \ldots, n\} \setminus (B \cup \{r\}) \tag{2}$$

Moreover, referring to the i-th index in B by $B(i)$, any $i \in \{1, \ldots, m\}$ with $x_{B(i)} - \theta_P d_i = 0$ gives a candidate variable $x_{B(i)}$ to leave the basis and thus to define a new unique basic feasible solution.

To decide whether a basis exchange involving x_r as the entering variable is worthwhile (i.e., leads to a decrease in the objective), we outline in this extended abstract a short-hand rationale. It does not exploit dual solution information (such as reduced costs) which may reduce computational efforts for deciding on candidates to enter the basis (pricing) especially but not only in the case of convex f. Fortunately, one can still exploit that the change of $f(x) = c_B x_B + \frac{1}{2} x_B^\mathsf{T} Q_{BB} x_B$ to $f(x')$ as of (2) only depends on x_B, x_r, and θ_P. Indeed, by defining

$$\eta \coloneqq Q_{BB}(-d) + Q_{Br} \text{ as well as } \gamma \coloneqq -d^\mathsf{T}\eta - d^\mathsf{T} Q_{Br} + Q_{rr},$$

we find after substituting and resolving that

$$\begin{aligned} f(x') &= c_r\theta_P + c_B^\mathsf{T}(x_B - \theta_P d) + \frac{1}{2}\left[(x_B - \theta_P d)\ \theta_P\right] \begin{bmatrix} Q_{BB} & Q_{Br} \\ Q_{Br}^\mathsf{T} & Q_{rr} \end{bmatrix} \begin{bmatrix} (x_B - \theta_P d) \\ \theta_P \end{bmatrix} \\ &= f(x) + \underbrace{\theta_P(c_r - c_B^\mathsf{T} d + x_B^\mathsf{T}\eta) + \frac{1}{2}\theta_P^2\gamma}_{=: \Delta_r} \end{aligned}$$

while Δ_r further simplifies for our problem (1) as $\theta_P \in \{0, 1\}$.

A straightforward employment of this rationale to determine whether a strict improvement is possible for the current basic feasible solution, i.e. to check explicitly whether $\theta_P = 1$ and $\Delta_r < 0$ for at least one non-basic variable x_r, is displayed as Algorithm 1. It terminates only if this is not the case, i.e., if the current basis is locally optimal which is guaranteed to happen since P is bounded.

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1  Solve the system $A_B x_B = b$;
2  repeat
3      forall $r \in N$ do
4          Solve the system $A_B d = A_{\cdot r}$;
5          $\theta_P \leftarrow \min \left\{ \frac{x_{B(i)}}{d_i} : d_i > 0,\ i \in \{1, \ldots, m\} \right\}$;
6          if $\theta_P > 0$ then
7              $\eta \leftarrow Q_{BB}(-d) + Q_{Br}$;
8              $\gamma \leftarrow Q_{rr} - d^\top \eta - d^\top Q_{Br}$;
9              $\Delta_r \leftarrow c_r - c_B^\top d + x_B^\top \eta + \frac{1}{2}\gamma$;
10             if $\Delta_r < 0$ then
11                 $x_B \leftarrow x_B - \theta_P d$;
12                 $x_r \leftarrow \theta_P$;
13                 Choose $i \in \{1, \ldots, m\} : d_i > 0, \frac{x_{B(i)}}{d_i} = \theta_P$;
14                 $B \leftarrow (B \setminus \{i\}) \cup \{r\}$;
15                 $N \leftarrow (N \setminus \{r\}) \cup \{i\}$;
16                 Go to line 3;
17     return $x$;
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Algorithm 1: A Primal Quadratic Simplex Algorithm for 0-1 Polytopes

Theorem 1. *Started with an initial partition (B,N) of a basic feasible solution $x = (x_B, x_N)^\top$, Algorithm 1 terminates in a finite number of steps with a locally optimum basic feasible solution $x^* = (x^*_{B^*}, x^*_{N^*})^\top$ such that $f(x^*) \leq f(x)$.*

Remark 1. By the restriction to strictly improving pivots, cycling is impossible. On the other hand, (ignored) pivots with $\theta_P = 0$ may exist such that the objective value could be strictly decreased *after* that pivot. Thus, a locally optimum basic feasible solution but not necessarily a locally optimum vertex is computed.

Naturally, the initial basis and the applied pivoting rule impact the performance of Algorithm 1. While a competitiveness to problem-specific and multi-start heuristics cannot be expected, experiments with established QAP, UBQP, and Maximum Cut instances reveal moderate iteration counts and sometimes strong quality improvements.

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