



QPPAL: A Two-phase Proximal Augmented Lagrangian Method for High-dimensional Convex Quadratic Programming Problems

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In this article, we aim to solve high-dimensional convex quadratic programming (QP) problems with a large number of quadratic terms, linear equality, and inequality constraints. To solve the targeted QP problem to a desired accuracy efficiently, we consider the restricted-Wolfe dual problem and develop a two-phase Proximal Augmented Lagrangian method (QPPAL), with Phase I to generate a reasonably good initial point to warm start Phase II to obtain an accurate solution efficiently. More specifically, in Phase I, based on the recently developed symmetric Gauss-Seidel (sGS) decomposition technique, we design a novel sGS-based semi-proximal augmented Lagrangian method for the purpose of finding a solution of low to medium accuracy. Then, in Phase II, a proximal augmented Lagrangian algorithm is proposed to obtain a more accurate solution efficiently. Extensive numerical results evaluating the performance of QPPAL against existing state-of-the-art solvers Gurobi, OSQP, and QPALM are presented to demonstrate the high efficiency and robustness of our proposed algorithm for solving various classes of large-scale convex QP problems. The MATLAB implementation of the software package QPPAL is available at <https://blog.nus.edu.sg/mattohkc/software/qppal/>.

CCS Concepts: • **Theory of computation** → **Quadratic programming**; • **Mathematics of computing** → **Solvers**;

Additional Key Words and Phrases: Convex quadratic programming, restricted-Wolfe dual, symmetric Gauss-Seidel, augmented Lagrangian method

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1 INTRODUCTION

We begin with some notation that will be used throughout the article. Let \mathcal{S}_+^n be the cone of $n \times n$ symmetric and positive semidefinite matrices in the space of $n \times n$ symmetric matrices \mathcal{S}^n endowed with the standard trace inner product $\langle \cdot, \cdot \rangle$ and the Frobenius norm $\| \cdot \|$. The range space of a matrix $Q \in \mathcal{S}^n$ is denoted by $\text{Range}(Q)$. Let \mathcal{X} be any real finite-dimensional Euclidean space and $\mathcal{M} : \mathcal{X} \rightarrow \mathcal{X}$ be any self-adjoint positive semidefinite linear operator, denote $\|x\|_{\mathcal{M}} = \sqrt{\langle x, \mathcal{M}x \rangle}$ and $\text{dist}_{\mathcal{M}}(x, C) = \inf_{x' \in C} \|x' - x\|_{\mathcal{M}}$ for any $x \in \mathcal{X}$ and any set $C \subseteq \mathcal{X}$. For a given closed proper convex function $\theta : \mathbb{R}^n \rightarrow (-\infty, +\infty]$, the effective domain of θ is defined by $\text{dom } \theta = \{x \in \mathbb{R}^n : \theta(x) < \infty\}$, the subdifferential of θ at $x \in \text{dom } \theta$ is defined by $\partial\theta(x) = \{v \in \mathbb{R}^n : \theta(y) \geq \theta(x) + \langle v, y - x \rangle, \forall y \in \mathbb{R}^n\}$ and the convex conjugate function $\theta^* : \mathbb{R}^n \rightarrow (-\infty, +\infty]$ of θ is defined by $\theta^*(y) := \sup\{\langle y, x \rangle - \theta(x) : x \in \mathbb{R}^n\}$. In particular, for a given closed convex set $C \subseteq \mathcal{X}$, we use $\delta_C(\cdot)$ to denote the indicator function of C with $\delta_C^*(\cdot)$ being its convex conjugate function. Moreover, the relative interior of C is denoted by $\text{ri}(C)$. For more details on convex sets and convex functions, we recommend the monograph [Rockafellar 1997].

Consider the high-dimensional convex **quadratic programming (QP)** problem in the following standard form:

$$(P) \quad \min_{x \in \mathbb{R}^n} \left\{ \frac{1}{2} \langle x, Qx \rangle + \langle c, x \rangle \mid Ax = b, x \in C \right\},$$

where $c \in \mathbb{R}^n$, $Q \in \mathcal{S}_+^n$, $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$, $C = \{x \in \mathbb{R}^n : l \leq x \leq u\}$ with the given vectors $\ell, u \in \mathbb{R}^n$ satisfying $-\infty \leq l \leq u \leq +\infty$. Note that (P) covers convex QP problems with linear inequality constraints by adding slack variables. However, we only consider (P) in the theoretical development for the purpose of notational simplicity. Moreover, we assume for the rest of this article that problem (P) satisfies the Slater's condition.

In this article, we are interested in the case where the dimensions n and/or m are extremely large. Since n is huge, one generally cannot expect an explicitly matrix representation for Q . Even if it is available, one may encounter severe memory issues when trying to store a large-scale and dense matrix Q . Hence, in this article, we only assume that Q is defined as a linear operator on \mathbb{R}^n , and its matrix representation is not needed explicitly, i.e., for any given $x \in \mathbb{R}^n$, Qx can be obtained at a reasonable cost but the matrix representation of Q with respect to the standard basis in \mathbb{R}^n may not be available.

The restricted-Wolfe dual [Li et al. 2018] of (P) can be written in the form of

$$(D) \quad \max_{(z, w, y) \in \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^m} \left\{ -\delta_C^*(-z) - \frac{1}{2} \langle w, Qw \rangle + \langle b, y \rangle \mid z - Qw + A^*y = c, w \in \mathcal{W} \right\},$$

where \mathcal{W} is any subspace of \mathbb{R}^n containing $\text{Range}(Q)$. In this article, we fix $\mathcal{W} = \text{Range}(Q)$. We will see in the subsequent analysis that this choice in fact plays an important role in the design of our algorithms. Problem (D) belongs to a general class of multi-block convex composite quadratic optimization problems of the form

$$\min_{y_i \in \mathcal{Y}_i, i=1, \dots, p} \left\{ \theta(y_1) + f(y_1, y_2, \dots, y_p) \mid \mathcal{A}_1^*y_1 + \mathcal{A}_2^*y_2 + \dots + \mathcal{A}_p^*y_p = c \right\}, \quad (1)$$

where p is a given positive integer, $\theta : \mathcal{Y}_1 \rightarrow (-\infty, +\infty]$ is a closed proper convex function whose proximal mapping is assumed to be computable at a moderate cost, $f : \mathcal{Y}_1 \times \mathcal{Y}_2 \times \dots \times \mathcal{Y}_p \rightarrow \mathbb{R}$ is a convex quadratic function (not necessarily separable), $\mathcal{A}_i : \mathcal{X} \rightarrow \mathcal{Y}_i$, $i = 1, \dots, p$ are linear maps, $\mathcal{Y}_1, \dots, \mathcal{Y}_p$ and \mathcal{X} are all real finite-dimensional Euclidean spaces each equipped with an inner product $\langle \cdot, \cdot \rangle$ and its induced norm $\|\cdot\|$. For notational convenience, we let $\mathcal{Y} := \mathcal{Y}_1 \times \mathcal{Y}_2 \times \dots \times \mathcal{Y}_p$, and write $y := (y_1, y_2, \dots, y_p) \in \mathcal{Y}$. Moreover, define the linear map $\mathcal{A} : \mathcal{X} \rightarrow \mathcal{Y}$ whose adjoint map is given by $\mathcal{A}^*y = \sum_{i=1}^p \mathcal{A}_i^*y_i$, $\forall y \in \mathcal{Y}$.

Convex QP has been extensively studied for the last few decades, see, for example the influential works [Cottle 1963, 1964; Dantzig 1961, 1963; Gould 1985; Gould et al. 2001; Gould and Toint 2000; Stellato et al. 2020; Sun 1993; Wright and Nocedal 2006; Ye 1998] and references therein. One may also refer to the QP webpage¹ for more information. To the best of our knowledge, all the major software packages for solving convex QP problems are based on active set methods [Wright and Nocedal 2006, Chapter 16.4], interior point methods [Nesterov and Nemirovskii 1994], operator splitting methods [Stellato et al. 2020] or primal-based (proximal) augmented Lagrangian methods [Hermans et al. 2019, 2020]. Among these methods, active set methods have the appealing feature to drop many of the inactive constraints to make the problem smaller in scale and hence much easier to solve. However, the worst-case iteration complexity of active set methods can be exponentially large with respect to the problem size and they may take a long time to solve the problem when the active sets are not estimated correctly. Achieving great progress over the past few decades, interior point method-based solvers are perhaps the most notable ones for solving large-scale convex QPs problems. For example, as a representative interior point method-based solver, Gurobi [2021]² is a highly optimized state-of-the-art solver for large-scale convex QP problems and is often used as a computational backbone of many real world applications. However, for solving high-dimensional convex QP problems with a large number of constraints, interior point method-based solvers (e.g., Gurobi) may encounter inherent numerical difficulties. Indeed, the computational costs of these methods become prohibitively expensive when the systems of linear equations to be solved are fully dense or when the corresponding sparse Cholesky factors are dense. Unlike interior point methods, which are generally considered as second-order methods, first-order methods such as operator splitting methods (including alternating direction methods of multipliers) have been at the forefront of the recent progress in solving convex optimization problems. For example, a well-known operator splitting algorithm for solving convex QP problems is the open source solver OSQP studied in Stellato et al. [2020]. First-order methods have the appealing feature that the per-iteration cost is quite cheap and hence they are highly scalable. However, these methods generally can only return approximate solutions with low to medium accuracy and they often stagnate even before delivering a crude approximate solution. Therefore, if more accurate solutions are needed, first order methods may not be sufficient. Recently, a highly optimized and efficient solver, named QPALM, was developed by applying the proximal ALM method to the primal problem (P); see Hermans et al. [2019, 2020]. QPALM is demonstrated to be quite efficient for solving many sparse QP problems. However, based on our experience gained from many numerical tests, QPALM is observed to be much less efficient under the high-dimensional settings considered in the present article. Last, as far as we are aware of, the major solvers just mentioned and their variants all require an explicit matrix representation of Q . Thus, there is clearly a need to design an algorithm that can handle high-dimensional convex QP problems beyond the scope covered by highly optimized solvers such as Gurobi, OSQP and QPALM.

¹<http://www.numerical.rl.ac.uk/people/nimg/qp/qp.html>.

²Based on the results presented in <http://plato.asu.edu/ftp/barrier.html>.

We shall next raise the following question: Can we design a highly efficient, scalable, and robust algorithm for solving convex QP problems having the following three characteristics? (a) the matrix representation of Q may not be available; (b) Q does not have a favourable sparsity pattern; (c) the number of linear constraints is extremely large or there are many dense linear constraints. We try to provide a positive answer to the above question by embracing the influential (dual-based) **augmented Lagrangian method (ALM)** for solving the more general problem (1). In our opinion, the (dual-based) ALM is perhaps the most promising algorithm for problem (1), which has some of or all the three characteristics just mentioned. To briefly explain the idea of ALM, let $\sigma > 0$ be a given parameter and the augmented Lagrangian function associated with (1) is defined by

$$\mathcal{L}_\sigma(y; x) := \theta(y_1) + f(y) + \langle x, \mathcal{A}^*y - c \rangle + \frac{\sigma}{2} \|\mathcal{A}^*y - c\|^2, \quad (x, y) \in \mathcal{X} \times \mathcal{Y}.$$

Starting with any initial points $y^0 \in \text{dom}(\theta) \times \mathcal{Y}_2 \times \cdots \times \mathcal{Y}_p$ and $x^0 \in \mathcal{X}$, ALM performs the following steps iteratively:

$$y^{k+1} = \operatorname{argmin}_{y \in \mathcal{Y}} \mathcal{L}_\sigma(y; x^k), \quad (2)$$

$$x^{k+1} = x^k + \tau \sigma (\mathcal{A}^*y^{k+1} - c), \quad (3)$$

where $\tau \in (0, 2)$ guarantees the convergence. However, in the high-dimensional setting, the non-separable quadratic terms and the composite structure in the inner subproblem (2) make the task of computing y^{k+1} exactly or with high accuracy extremely difficult and expensive. Fortunately, this difficulty could be alleviated if a good initial point is provided for the ALM, in light of the experience gained from a series of works [Li et al. 2018, 2020; Yang et al. 2015; Zhao et al. 2010] on developing elegant theoretical properties and efficient implementation of the (proximal) ALM for solving several classes of optimization problems. In fact, the ALM equipped with a semismooth Newton method for solving the ALM inner subproblems is shown to be a highly efficient approach for solving Equation (1) to a high accuracy, if the initial iterate lies in the fast convergence region of the semismooth Newton method. In this article, by further exploring the idea in the Schur complement-based semi-proximal **alternating direction method of multipliers (ADMM)** proposed in the recent papers [Li et al. 2016a, b], we are able to propose a symmetric Gauss-Seidel-based semi-proximal ALM to efficiently solve the non-separable convex composite optimization problem (1) to low or medium accuracy. Therefore, we shall use this algorithm as a warm-starting scheme to provide a reasonably good initial point for the ALM. Using this initial point, we then propose a proximal ALM to compute a highly accurate solution efficiently. Consequently, we come up with a two-phase algorithm. As we shall see later in the numerical experiments, the proposed algorithmic framework is shown to be more suitable for large-scale convex QP problems having the aforementioned characteristics compared to interior point methods, operator splitting algorithms and the primal-based ALM. Indeed, we observe that applying the proximal ALM to the (restricted-Wolfe) dual problem (D) appears to be more effective.

The remaining parts of this article are organized as follows. In Section 2, we first propose an **inexact semi-proximal augmented Lagrangian method (isPALM)** and establish its convergence. Then, as our phase I algorithm for solving the convex composite quadratic programming model (1), a symmetric Gauss-Seidel-based inexact semi-proximal augmented Lagrangian method (sGS-isPALM) is designed via incorporating the sGS decomposition technique with the aforementioned isPALM algorithm. In Section 3, we propose our two-phase algorithm QPPAL. In QPPAL Phase I, the sGS-isPALM is directly applied to solve the convex quadratic programming problem (D). Then, in QPPAL Phase II, a proximal ALM, with the semismooth Newton method for solving the inner minimization problems, is proposed and the convergence are also established. In Section 5, we discuss key implementation issues and present numerical experiments to evaluate

our QPPAL in solving some classes of large-scale convex QP problems. We conclude our article in Section 6.

2 AN INEXACT SEMI-PROXIMAL AUGMENTED LAGRANGIAN METHOD

In this section, by revisiting the convergence of the inexact semi-proximal ALM and applying the **symmetric Gauss-Seidel (sGS)** decomposition technique to the convex composite quadratic programming model (1), we shall propose an sGS-based inexact semi-proximal ALM method with convergence guarantees. These theoretical results have been analyzed extensively in the recent work [Chen et al. 2021] and references therein. In this work, we focus on the detailed numerical implementation of the methods for solving convex QPs. Hence, we refrain from adding too much theoretical detail on the algorithm.

To begin, we first consider the following linearly constrained convex optimization problem

$$\min_{v \in \mathcal{V}} \{g(v) \mid \mathcal{G}^*v = c\}, \quad (4)$$

where $g : \mathcal{V} \rightarrow (-\infty, +\infty]$ is a closed proper convex function, $\mathcal{G} : \mathcal{X} \rightarrow \mathcal{V}$ is a given linear map and \mathcal{V} is a real finite-dimensional Euclidean space. We make the following standard solvability assumption for Equation (4).

Assumption 2.1. The solution set to the following KKT system of Equation (4)

$$0 \in \partial g(\bar{v}) + \mathcal{G}\bar{x}, \quad \mathcal{G}^*\bar{v} = c, \quad (\bar{x}, \bar{v}) \in \mathcal{X} \times \mathcal{V} \quad (5)$$

is nonempty.

Let $\sigma > 0$ be a given parameter. The augmented Lagrangian function associated with Equation (4) is given as follows:

$$\mathcal{L}_\sigma(v; x) = g(v) + \langle x, \mathcal{G}^*v - c \rangle + \frac{\sigma}{2} \|\mathcal{G}^*v - c\|^2, \quad (v, x) \in \mathcal{V} \times \mathcal{X}.$$

Let ∂g be the subdifferential mapping of g . Then ∂g is a maximally monotone operator. Hence, there exists a self adjoint positive semidefinite linear operator Σ_g such that for all $v, \tilde{v} \in \text{dom}(g)$, $\zeta \in \partial g(v)$, and $\tilde{\zeta} \in \partial g(\tilde{v})$, it holds that (see, e.g., Theorem 12.17 in Rockafellar and Wets [2009])

$$\langle \zeta - \tilde{\zeta}, v - \tilde{v} \rangle \geq \|v - \tilde{v}\|_{\Sigma_g}^2. \quad (6)$$

The isPALM for solving Equation (4) is described in Figure 1.

The global convergence result for Algorithm isPALM under certain technical assumptions is presented as follows whose proof can be taken directly from the Theorem 3.1 in Chen et al. [2021].

THEOREM 2.1. Assume that Assumption 2.1 holds and that $\Sigma_g + \mathcal{T} + \sigma \mathcal{G}\mathcal{G}^* > 0$. Let $\{(v^k, x^k)\}$ be generated from Algorithm isPALM. Then the following results hold:

- (a) the sequence $\{(v^k, x^k)\}$ is bounded;
- (b) any accumulation point of the sequence $\{(v^k, x^k)\}$ solve the KKT system of Equation (4);
- (c) the whole sequence $\{(v^k, x^k)\}$ converges to a solution to the KKT system of Equation (4).

2.1 A Symmetric Gauss-Seidel-based Inexact Semi-proximal ALM

In the remaining part of this section, we focus on the convex composite quadratic programming model (1), where the convex quadratic function $f : \mathcal{Y} \rightarrow \mathbb{R}$ is defined by $f(y) = \frac{1}{2} \langle y, \mathcal{P}y \rangle - \langle b, y \rangle$, with $b \in \mathcal{Y}$ and \mathcal{P} being a self-adjoint positive semidefinite linear operator defined on \mathcal{Y} .

Algorithm isPALM: An inexact semi-proximal augmented Lagrangian method for Equation (4).

Let $\sigma > 0$ and $\tau \in (0, 2)$ be given parameters, $\{\varepsilon_k\}_{k \geq 0}$ be a nonnegative summable sequence. Let \mathcal{T} be a given self-adjoint positive semidefinite linear operator defined on \mathcal{V} such that $\mathcal{N} := \Sigma_g + \mathcal{T} + \sigma \mathcal{G} \mathcal{G}^* > 0$. Choose $(v^0, x^0) \in \text{dom}(g) \times \mathcal{X}$. Perform the following steps in each iteration for $k = 0, 1, 2, \dots$.

Step 1. Compute

$$v^{k+1} \approx \tilde{v}^{k+1} := \underset{v \in \mathcal{V}}{\operatorname{argmin}} \mathcal{L}_\sigma(v; x^k) + \frac{1}{2} \|v - v^k\|_{\mathcal{T}}^2 \quad (7)$$

such that there exists d_k satisfying $\|\mathcal{N}^{-1/2} d^k\| \leq \varepsilon_k$ and

$$d^k \in \partial_v \mathcal{L}_\sigma(v^{k+1}; x^k) + \mathcal{T}(v^{k+1} - v^k). \quad (8)$$

Step 2. Compute $x^{k+1} = x^k + \tau \sigma (\mathcal{G}^* v^{k+1} - c)$.

Fig. 1. Algorithm isPALM.

For later discussions, we consider the following decomposition for \mathcal{P} :

$$\mathcal{P}y \equiv \begin{pmatrix} \mathcal{P}_{11} & \mathcal{P}_{12} & \cdots & \mathcal{P}_{1p} \\ \mathcal{P}_{12}^* & \mathcal{P}_{22} & \cdots & \mathcal{P}_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{P}_{1p}^* & \mathcal{P}_{2p}^* & \cdots & \mathcal{P}_{pp} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_p \end{pmatrix},$$

where $\mathcal{P}_{ij} : \mathcal{Y}_j \rightarrow \mathcal{Y}_i$, $i = 1, \dots, p$, $j \leq i$ are linear maps.

We first introduce a self-adjoint semidefinite linear operator \mathcal{S}_1 defined on \mathcal{Y}_1 to handle the convex, possibly nonsmooth, functions $\theta(y_1)$, such that

$$\mathcal{E}_{11} := \mathcal{P}_{11} + \mathcal{S}_1 + \sigma \mathcal{A}_1 \mathcal{A}_1^* > 0, \quad (9)$$

and the well-defined optimization problem

$$\min_{y_1} \left\{ \theta(y_1) + \frac{1}{2} \|y_1 - \bar{y}_1\|_{\mathcal{E}_{11}}^2 \mid y_1 \in \mathcal{Y}_1 \right\}$$

can easily be solved for any $\bar{y}_1 \in \mathcal{Y}_1$. Then, for $i = 2, \dots, p$, let \mathcal{S}_i be a self-adjoint positive semidefinite linear operator on \mathcal{Y}_i such that

$$\mathcal{E}_{ii} := \mathcal{P}_{ii} + \sigma \mathcal{A}_i \mathcal{A}_i^* + \mathcal{S}_i > 0. \quad (10)$$

In practice, we would choose \mathcal{S}_i in such a way that the inverse of \mathcal{E}_{ii} can be computed at a moderate cost. But note that for the algorithm under consideration to be efficient, we need \mathcal{S}_i to be as small as possible for each $i = 1, \dots, p$.

Now, we are ready to present our **symmetric Gauss-Seidel-based inexact semi-proximal augmented Lagrangian (sGS-isPALM)** algorithm for solving Equation (1) in Figure 2.

To prove the convergence of Algorithm sGS-isPALM for solving Equation (1), we shall study the relationship between Algorithm sGS-isPALM and Algorithm isPALM. To this end, let $\mathcal{S} := \text{Diag}(\mathcal{S}_1, \dots, \mathcal{S}_p)$ and define the following linear operators:

$$\mathcal{E} := \mathcal{P} + \sigma \mathcal{A} \mathcal{A}^* + \mathcal{S} = \mathcal{E}_u^* + \mathcal{E}_d + \mathcal{E}_u, \quad \text{sGS}(\mathcal{E}) = \mathcal{E}_u \mathcal{E}_d^{-1} \mathcal{E}_u^*, \quad (11)$$

where $\mathcal{E}_d = \text{Diag}(\mathcal{E}_{11}, \dots, \mathcal{E}_{pp})$ and

$$\mathcal{E}_u := \begin{pmatrix} \mathbf{0} & \mathcal{P}_{12} + \sigma \mathcal{A}_1 \mathcal{A}_2^* & \cdots & \mathcal{P}_{1p} + \sigma \mathcal{A}_1 \mathcal{A}_p^* \\ & \ddots & \cdots & \vdots \\ & & \mathbf{0} & \mathcal{P}_{(p-1)p} + \sigma \mathcal{A}_{p-1} \mathcal{A}_p^* \\ & & & \mathbf{0} \end{pmatrix}.$$

Algorithm sGS-isPALM: A symmetric Gauss-Seidel based inexact semi-proximal augmented Lagrangian method for solving Equation (1).

Let $\sigma > 0$ and $\tau \in (0, 2)$ be given parameters, $\{\epsilon_k\}_{k \geq 0}$ be a nonnegative summable sequence. Choose $(y^0, x^0) \in \text{dom}(\theta_1) \times \mathcal{Y}_2 \times \dots \times \mathcal{Y}_p \times \mathcal{X}$. Perform the following steps in each iteration.

Step 1. (Backward GS sweep) Compute for $i = p, \dots, 2$,

$$\bar{y}_i^k \approx \underset{y_i \in \mathcal{Y}_i}{\operatorname{argmin}} \mathcal{L}_\sigma((y_{<i}^k, y_i, \bar{y}_{>i}^k); x^k) + \frac{1}{2} \|y_i - y_i^k\|_{S_i}^2$$

such that there exists δ_i^k satisfying $\|\delta_i^k\| \leq \epsilon_k$ and

$$\delta_i^k \in \partial \mathcal{L}_\sigma((y_{<i}^k, \bar{y}_i^k, \bar{y}_{>i}^k); x^k) + S_i(\bar{y}_i^k - y_i^k).$$

Step 2. (Forward GS sweep) Compute for $i = 1, \dots, p$,

$$y_i^{k+1} \approx \underset{y_i \in \mathcal{Y}_i}{\operatorname{argmin}} \mathcal{L}_\sigma((y_{<i}^{k+1}, y_i, \bar{y}_{>i}^k); x^k) + \frac{1}{2} \|y_i - y_i^k\|_{S_i}^2$$

such that there exists $\hat{\delta}_i^k$ satisfying $\|\hat{\delta}_i^k\| \leq \epsilon_k$ and

$$\hat{\delta}_i^k \in \partial \mathcal{L}_\sigma((y_{<i}^{k+1}, y_i^{k+1}, \bar{y}_{>i}^k); x^k) + S_i(y_i^{k+1} - y_i^k).$$

Step 3. Compute $x^{k+1} = x^k + \tau \sigma (\mathcal{A}^* y^{k+1} - c)$.

Fig. 2. Algorithm sGS-isPALM.

For $k \geq 0$, let $\delta_1^k = \hat{\delta}_1^k$, $\delta^k := (\delta_1^k, \dots, \delta_p^k)$, and $\hat{\delta}^k := (\hat{\delta}_1^k, \dots, \hat{\delta}_p^k)$. Then, we have the following result, which establishes the relationship between Algorithm sGS-isPALM and Algorithm isPALM. We refer the readers to Appendix A.1.

PROPOSITION 2.1. *It holds that $\widehat{\mathcal{E}} = \mathcal{E} + \text{sGS}(\mathcal{E}) > 0$. For any $k \geq 0$, the point (y^{k+1}, x^{k+1}) obtained by Algorithm sGS-isPALM for solving problem (1) can be generated exactly according to the following iteration:*

$$\begin{cases} y^{k+1} = \underset{y \in \mathcal{Y}}{\operatorname{argmin}} \mathcal{L}_\sigma(y; x^k) + \frac{1}{2} \|y - y^k\|_{S + \text{sGS}(\mathcal{E})}^2 - \langle d^k, y \rangle, \\ x^{k+1} = x^k + \tau \sigma (\mathcal{A}^* y^{k+1} - c), \end{cases} \quad (12)$$

where $d^k = \hat{\delta}^k + \mathcal{E}_u \mathcal{E}_d^{-1} (\hat{\delta}^k - \delta^k)$. Moreover, it holds that

$$\|\widehat{\mathcal{E}}^{-1/2} d^k\| \leq ((2p-1)\|\mathcal{E}_d^{-1/2}\| + p\|\widehat{\mathcal{E}}^{-1/2}\|)\epsilon_k, \quad \forall k \geq 0.$$

By combining Theorem 2.1 with Proposition 2.1, we can finally state our main convergence theorem under suitable assumptions.

THEOREM 2.2. *Suppose that the solution set of problem (1) is nonempty and that there exists $\hat{y} \in \text{ri}(\text{dom } \theta) \times \mathcal{Y}_2 \times \dots \times \mathcal{Y}_p$ such that $\mathcal{A}^* \hat{y} = c$. Let $\{(y^k, x^k)\}$ be generated from Algorithm sGS-isPALM with $\tau \in (0, 2)$. Then, the sequence $\{y^k\}$ converges to an optimal solution to problem (1) and $\{x^k\}$ converges to an optimal solution of the dual of problem (1).*

Remark 2.1. We can also establish the nonergodic iteration complexity for the sequence generated by Algorithm sGS-isPALM. For more details on this topic, we refer the readers to Theorem 4.4 in Chen et al. [2021].

3 A TWO-PHASE PROXIMAL ALM FOR SOLVING CONVEX QP PROBLEMS

In this section, we shall present a two-phase proximal ALM for solving convex quadratic programming problems (D) to high accuracy efficiently. For simplicity, we call our algorithm QPPAL. We will discuss the implementation detail for the algorithm in Section 4.

Algorithm QPPAL-Phase-I: An sGS-isPALM method for (D).

Select an initial point (z^0, w^0, y^0) with $-z^0 \in \text{dom}(\delta_C^*)$, $(w^0, y^0) \in \mathcal{W} \times \mathcal{R}^m$. Let $\{\epsilon_k\}$ be a summable sequence of nonnegative numbers, $\sigma > 0$ and $\tau \in (0, 2)$ be given parameters. Set $k = 0$. Iterate the following steps.

Step 1. Compute

$$\begin{aligned}\bar{y}^k &= \operatorname{argmin}_y \left\{ L_\sigma(z^k, w^k, y; x^k) - \langle \delta_E^k, y \rangle \mid y \in \mathcal{R}^m \right\}, \\ \bar{w}^k &= \operatorname{argmin}_w \left\{ L_\sigma(z^k, w, \bar{y}^k; x^k) - \langle \delta_Q^k, w \rangle \mid w \in \mathcal{W} \right\}, \\ z^{k+1} &= \operatorname{argmin}_z \left\{ L_\sigma(z, \bar{w}^k, \bar{y}^k; x^k) \mid z \in \mathcal{R}^n \right\}, \\ w^{k+1} &= \operatorname{argmin}_w \left\{ L_\sigma(z^{k+1}, w, \bar{y}^k; x^k) - \langle \delta_Q^k, w \rangle \mid w \in \mathcal{W} \right\}, \\ y^{k+1} &= \operatorname{argmin}_y \left\{ L_\sigma(z^{k+1}, w^{k+1}, y; x^k) - \langle \delta_E^k, y \rangle \mid y \in \mathcal{R}^m \right\},\end{aligned}$$

where $\delta_E^k, \hat{\delta}_E^k \in \mathcal{R}^m$, $\delta_Q^k, \hat{\delta}_Q^k \in \mathcal{W}$ are error vectors such that

$$\max\{\|\delta_E^k\|, \|\hat{\delta}_E^k\|, \|\delta_Q^k\|, \|\hat{\delta}_Q^k\|\} \leq \epsilon_k.$$

Step 2. Compute $x^{k+1} = x^k + \tau\sigma(z^{k+1} - Qw^{k+1} + A^*y^{k+1} - c)$.

Fig. 3. Algorithm QPPAL-Phase-I.

3.1 QPPAL Phase I

In Phase I, we shall apply Algorithm sGS-isPALM directly to solve (D). Given $\sigma > 0$, let $L_\sigma(z, w, y; x)$ be the augmented Lagrangian function associated with problem (D) (here, we reformulate (D) as a minimization problem), i.e., for any $(z, w, y, x) \in \mathcal{R}^n \times \mathcal{W} \times \mathcal{R}^m \times \mathcal{R}^n$,

$$L_\sigma(z, w, y; x) = \delta_C^*(-z) + \frac{1}{2} \langle w, Qw \rangle - \langle b, y \rangle + \frac{\sigma}{2} \|z - Qw + A^*y - c + \sigma^{-1}x\|^2 - \frac{1}{2\sigma} \|x\|^2. \quad (13)$$

Then, the detailed steps of our Phase I algorithm for convex quadratic programming are given in Figure 3.

The convergence of the Phase I algorithm follows from Theorems 2.1 and 2.2 without much difficulty.

THEOREM 3.1. *Suppose that the solution set of (P) is nonempty and A has full row rank. Let $\{(z^k, w^k, y^k, x^k)\}$ be the sequence generated by Algorithm QPPAL-Phase-I. Then, the sequence $\{(z^k, w^k, y^k)\}$ converges to an optimal solution of (D) and $\{x^k\}$ converges to an optimal solution of (P).*

We note that there are two choices on the order of updating the dual variables (z, w, y) in **Step 1**. Specifically, one may choose either one of the two following orders: (1) $\bar{y}^k \rightarrow \bar{w}^k \rightarrow z^{k+1} \rightarrow w^{k+1} \rightarrow y^{k+1}$; (2) $\bar{w}^k \rightarrow \bar{y}^k \rightarrow z^{k+1} \rightarrow y^{k+1} \rightarrow w^{k+1}$. In fact, we observe that both updating rules have similar practical performance.

3.2 QPPAL Phase II

In the second part of this section, we discuss our Phase II algorithm for solving the convex quadratic programming (D). The purpose of this phase is to obtain highly accurate solutions efficiently, with warm-starting by the Phase-I algorithm. As we shall see in the numerical experiments, the Phase II algorithm is indeed necessary and important for obtaining accurate solutions.

To proceed, we first note that problem (D) has the following equivalent minimization form:

$$- \min_{(w, y) \in \mathcal{W} \times \mathcal{R}^m} \left\{ h(w, y) := \delta_C^*(-Qw + A^*y - c) + \frac{1}{2} \langle w, Qw \rangle - \langle b, y \rangle \right\}. \quad (14)$$

Algorithm QPPAL-Phase-II: An inexact proximal ALM for solving (D)

Let $\sigma_0, \sigma_\infty > 0$ be given parameters, and $\{\tau_k\}_{k=0}^\infty$ be a given nonincreasing sequence such that $\tau_k > 0$ for all $k \geq 0$. Choose $(w^0, y^0) \in \mathcal{W} \times \mathcal{R}^m$ and $x^0 \in \mathbb{R}^n$. Set $k = 0$. Iterate the following steps.

Step 1. Compute

$$(w^{k+1}, y^{k+1}) \approx \operatorname{argmin} \left\{ \begin{array}{l} \Psi_k(w, y) := \tilde{L}_{\sigma_k}(w, y; x^k) + \frac{\tau_k}{2\sigma_k} (\|w - w^k\|_Q^2) \\ + \|y - y^k\|^2 \mid w \in \mathcal{W}, y \in \mathcal{R}^m \end{array} \right\}. \quad (15)$$

Step 2. Compute

$$x^{k+1} = \Pi_C \left(x^k + \sigma_k (-Qw^{k+1} + A^*y^{k+1} - c) \right), \quad z^{k+1} = \frac{1}{\sigma_k} \left(x^{k+1} - \left(x^k + \sigma_k (-Qw^{k+1} + A^*y^{k+1} - c) \right) \right).$$

Step 3. Update $\sigma_{k+1} \uparrow \sigma_\infty \leq \infty$.

Fig. 4. Algorithm QPPAL-Phase-II.

Then, we identify Equation (14) with the problem of minimizing $h(w, y) = \tilde{h}(w, y, 0)$ over $\mathcal{W} \times \mathcal{R}^m$, where

$$\tilde{h}(w, y, \xi) = \delta_C^*(-Qw + A^*y - c + \xi) + \frac{1}{2} \langle w, Qw \rangle - \langle b, y \rangle, \quad (w, y, \xi) \in \mathcal{W} \times \mathcal{R}^m \times \mathbb{R}^n.$$

Since \tilde{h} is jointly convex in (w, y, ξ) , we are able to write down the Lagrangian function $\tilde{l} : \mathcal{W} \times \mathcal{R}^m \rightarrow \mathbb{R}$ through partial dualization (see, for instance, Examples 11.46 and 11.57 in Rockafellar and Wets [2009]) as follows:

$$\tilde{l}(w, y; x) := \inf_{\xi} \left\{ \tilde{h}(w, y, \xi) - \langle x, \xi \rangle \right\} = \frac{1}{2} \langle w, Qw \rangle - \langle b, y \rangle - \langle x, Qw - A^*y + c \rangle - \delta_C(x).$$

Given $\sigma > 0$, the augmented Lagrangian function corresponding to Equation (14) in variables y, w and x can be obtained as follows:

$$\begin{aligned} \tilde{L}_\sigma(w, y; x) &:= \sup_{s \in \mathcal{R}^n} \left\{ \tilde{l}(w, y; s) - \frac{1}{2\sigma} \|s - x\|^2 \right\} \\ &= - \inf_{s \in \mathcal{R}^n} \left\{ \langle s, Qw - A^*y + c \rangle + \delta_C(s) + \frac{1}{2\sigma} \|s - x\|^2 \right\} + \frac{1}{2} \langle w, Qw \rangle - \langle b, y \rangle \\ &= - \langle Qw - A^*y + c, \Pi_C[x - \sigma(Qw - A^*y + c)] \rangle \\ &\quad - \frac{1}{2\sigma} \|\Pi_C[x - \sigma(Qw - A^*y + c)] - x\|^2 + \frac{1}{2} \langle w, Qw \rangle - \langle b, y \rangle, \end{aligned}$$

where $\Pi_C(\cdot)$ is the metric projector onto C , i.e., $\Pi_C(x) := \operatorname{argmin}_{z \in \mathcal{R}^n} \{\|x - z\| \mid z \in C\}$.

We then propose to solve (D) via an inexact proximal ALM. Its template is described in Figure 4.

We next analyze the convergence of the algorithm QPPAL-Phase-II via establishing the connection between the proposed inexact proximal ALM and the preconditioned PPA studied in Li et al. [2020], which extends the influential results in Luque [1984] and Rockafellar [1976a, b]. To briefly explain the idea, let $\mathcal{X} := \mathcal{W} \times \mathcal{R}^m \times \mathcal{R}^n$, and for $k \geq 0$ and any given $(\bar{w}, \bar{y}, \bar{x})$, define the function

$$P_k(\bar{w}, \bar{y}, \bar{x}) := \operatorname{argminimax}_{(w, y, x) \in \mathcal{X}} \left\{ \hat{l}(w, y, x) := \tilde{l}(w, y, x) + \frac{\tau_k}{2\sigma_k} (\|y - \bar{y}\|^2 + \|w - \bar{w}\|_Q^2) - \frac{1}{2\sigma_k} \|x - \bar{x}\|^2 \right\}, \quad (16)$$

i.e., $P_k(\bar{w}, \bar{y}, \bar{x})$ is obtained by minimizing and maximizing $\hat{l}(w, y, x)$ with respect to (w, y) and x , respectively. For the closed proper convex-concave function \hat{l} , define the maximal monotone

operator $\mathcal{T}_{\tilde{l}}$ by

$$\begin{aligned}\mathcal{T}_{\tilde{l}}(w, y, x) &:= \left\{ (w', y', x') \mid (w', y', -x') \in \partial \tilde{l}(w, y, x) \right\} \\ &= \left\{ (w', y', x') \mid w' = Q(w - x), y' = -b + Ax, x' \in Qw - A^*y + c + \partial \delta_C(x) \right\}.\end{aligned}$$

Notice that since C is polyhedral, $\mathcal{T}_{\tilde{l}}$ is a polyhedral set-valued mapping. Furthermore, since $\mathcal{T}_{\tilde{l}}$ is a maximal monotone operator [Minty 1962], its inverse exists and is given by

$$\mathcal{T}_{\tilde{l}}^{-1}(w', y', x') := \operatorname{argminimax}_{(w, y, x) \in \mathcal{X}} \left\{ \tilde{l}(w, y, x) - \langle w', w \rangle - \langle y', y \rangle + \langle x', x \rangle \right\}. \quad (17)$$

Then, the next lemma characterizes the optimal solution set in Equation (16) whose proof can be found in Appendix A.2.

LEMMA 3.2. *For all $k \geq 0$, let $\Lambda_k := \operatorname{Diag}(\tau_k Q, \tau_k I_m, I_n)$, which is positive definite on \mathcal{X} , and for any $(w, y, x) \in \mathcal{X}$, denote $\Lambda_k(w, y, x) = (\tau_k Qw, \tau_k y, x) \in \mathcal{X}$. Then it holds that*

$$P_k(\bar{w}, \bar{y}, \bar{x}) = (\Lambda_k + \sigma_k \mathcal{T}_{\tilde{l}})^{-1} \Lambda_k(\bar{w}, \bar{y}, \bar{x}), \quad \forall (\bar{w}, \bar{y}, \bar{x}) \in \mathcal{W} \times \mathbb{R}^m \times \mathbb{R}^n. \quad (18)$$

Moreover, $P_k(w^*, y^*, x^*) = (w^*, y^*, x^*)$ if and only if $(w^*, y^*, x^*) \in \mathcal{T}_{\tilde{l}}^{-1}(0)$.

Using Lemma 3.2, the next proposition (see a proof in Appendix A.3) allows us to propose a practical inexact rule (which implies the criteria used in Section 2 in Li et al. [2020]) for the inexact computation in Equation (15) via estimating the norm of the gradient of the function $\Psi_k(\cdot)$ (see Equation (15)) that is given by

$$\nabla \Psi_k(w, y) = \begin{bmatrix} Qw - Q\Pi_C[x^k - \sigma_k(Qw - A^*y + c)] + \frac{\tau_k}{\sigma_k} Q(w - w^k) \\ -b + A\Pi_C[x^k - \sigma_k(Qw - A^*y + c)] + \frac{\tau_k}{\sigma_k} (y - y^k) \end{bmatrix}.$$

PROPOSITION 3.1. *For any $k = 0, 1, \dots$, it holds that*

$$\|(w^{k+1}, y^{k+1}, x^{k+1}) - P_k(w^k, y^k, x^k)\|_{\Lambda_k} \leq \frac{\sigma_k}{\min\{1, \sqrt{\tau_k}, \sqrt{\tau_k \lambda_+(Q)}\}} \|\nabla \Psi_k(w^{k+1}, y^{k+1})\|, \quad (19)$$

where $\lambda_+(Q) > 0$ denotes the smallest positive eigenvalue of Q .

Based on Proposition 3.1, we then propose the following stopping criteria for the inexact computation in Equation (15):

$$\begin{aligned}(\text{A}) \quad & \|\nabla \Psi_k(w^{k+1}, y^{k+1})\| \leq \frac{\min\{1, \sqrt{\tau_k}, \sqrt{\tau_k \lambda_+(Q)}\}}{\sigma_k} \epsilon_k, \\ (\text{B}) \quad & \|\nabla \Psi_k(w^{k+1}, y^{k+1})\| \leq \frac{\delta_k \min\{1, \sqrt{\tau_k}, \sqrt{\tau_k \lambda_+(Q)}\}}{\sigma_k} \|(w^{k+1}, y^{k+1}, x^{k+1}) - (w^k, y^k, x^k)\|_{\Lambda_k},\end{aligned}$$

where $\{\epsilon_k\}$ and $\{\delta_k\}$ are given nonnegative sequences such that $\sum_{k=0}^{\infty} \epsilon_k < \infty$, and $\delta_k < 1$, $\sum_{k=0}^{\infty} \delta_k < \infty$. Thus, we can directly present the convergence properties of the proposed algorithm in the following theorem, which combines the results of Theorems 1 and 2 in Li et al. [2020] by observing that Algorithm QPPAL-Phase-II actually computes $(w^{k+1}, y^{k+1}, x^{k+1}) \approx P_k(w^k, y^k, x^k) = (\Lambda_k + \sigma_k \mathcal{T}_{\tilde{l}})^{-1} \Lambda_k(w^k, y^k, x^k)$. We omit the proof here, since it can be done exactly the same way as in Li et al. [2020].

THEOREM 3.3. *Suppose that the solution set of (P) and (D) is nonempty, A has full row rank, and the positive sequence $\{\tau_k\}$ is non-increasing and bounded away from zero, i.e., $\tau_k \downarrow \tau_{\infty} > 0$. Let $\{(w^k, y^k, x^k)\}$ be the sequence generated by Algorithm QPPAL-Phase-II.*

Algorithm QPPAL: A two-phase algorithm for (D).

Input. Stopping tolerances tol_1 and tol_2 , and maximum number of iterations MaxIter_1 and MaxIter_2 .

Step 1. Run Algorithm QPPAL-Phase-I and terminate it when either one of the following two conditions is met:

(1) Optimality and feasibility measure is less than tol_1 ; (2) The number of iterations reaches MaxIter_1 .

Step 2. Run Algorithm QPPAL-Phase-II with the initial point given in **Step 1**, and terminate it when either one of the following two conditions is met:

(1) Optimality and feasibility measure is less than tol_2 ; (2) The number of iterations reaches MaxIter_2 .

Fig. 5. Algorithm QPPAL.

- (1) If the algorithm is executed under the inexactness condition (A), then the sequence $\{(w^k, y^k, x^k)\}$ is bounded. Furthermore, $\{x_k\}$ converges to an optimal solution of (P) and $\{(w^k, y^k)\}$ converges to an optimal solution of (D).
- (2) Let $r > \sum_{k=0}^{\infty} \epsilon_k$ be any positive constant and $\kappa > 0$ be the corresponding error bound constant³ such that

$$\text{dist}((w, y, x), \mathcal{T}_i^{-1}(0)) \leq \kappa \text{dist}(0, \mathcal{T}_i(w, y, x)), \quad \forall (w, y, x) \text{ s.t. } \text{dist}((w, y, x), \mathcal{T}_i^{-1}(0)) \leq r.$$

Moreover, suppose that the initial point (w^0, y^0, x^0) satisfies $\text{dist}((w^0, y^0, x^0), \mathcal{T}_i^{-1}(0)) \leq r - \sum_{k=0}^{\infty} \epsilon_k$ and the proposed algorithm is executed under both conditions (A) and (B). Then, for all $k \geq 0$, it holds that

$$\text{dist}_{\Lambda_k}((w^{k+1}, y^{k+1}, x^{k+1}), \mathcal{T}_i^{-1}(0)) \leq \mu_k \text{dist}_{\Lambda_k}((w^k, y^k, x^k), \mathcal{T}_i^{-1}(0)), \quad (20)$$

where $\mu_k = (1 - \delta_k)^{-1} \left(\delta_k + (1 + \delta_k) \kappa \gamma_k / \sqrt{\sigma_k^2 + \kappa^2 \gamma_k^2} \right)$ with $\gamma_k := \max\{1, \tau_k, \tau_k \|Q\|_2\}$ and

$$\limsup_{k \rightarrow \infty} \mu_k = \mu_{\infty} = \frac{\kappa \gamma_{\infty}}{\sqrt{\sigma_{\infty}^2 + \kappa^2 \gamma_{\infty}^2}} < 1, \quad (\mu_{\infty} := 0 \text{ if } \sigma_{\infty} = \infty),$$

with $\gamma_{\infty} = \max\{1, \tau_{\infty}, \tau_{\infty} \|Q\|_2\}$.

Since $0 < \inf_k \min\{\tau_k \lambda_+(Q), \tau_k, 1\} \leq \sup_k \max\{\tau_k \|Q\|_2, \tau_k, 1\} < \infty$, the distance induced by Λ_k can be replaced by the Euclidean distance without much difficulty. Moreover, the above theorem shows that the linear rate μ_k can be arbitrarily small if σ_k is sufficiently large, i.e., the linear convergence of the algorithm can be “arbitrarily fast.” However, in practice, it is not advisable to choose σ_k to be extremely large for the purpose of numerical stability. Therefore, given that $\sigma_k \leq \sigma_{\infty} < \infty$, a smaller τ_k will lead to a better linear convergence rate, i.e., a smaller μ_k . So for better theoretical performance, one prefers to choose a smaller τ_k . In fact, Theorem 3.3 indicates that ideally we would choose $\tau_k \leq \min\{1, \|Q\|_2^{-1}\}$ for better convergence rate.

To summarize, we shall present our conceptual two-phase algorithm QPPAL in Figure 5. Readers may refer to Section 5 for the termination rules with respect to a given tolerance of our algorithms. Note that tol_1 and MaxIter_1 may be chosen differently for different problems to achieve greater efficiency.

3.3 A Semismooth Newton Method for Solving Equation (15)

In this subsection, we discuss how to solve the subproblem in Equation (15) efficiently. To this end, for given $(\hat{w}, \hat{y}, \hat{x}) \in \mathcal{W} \times \mathcal{R}^m \times \mathcal{R}^n$, $\tau > 0$ and $\sigma > 0$, we define the function

$$\varphi(w, y) := \tilde{L}_{\sigma}(w, y; \hat{x}) + \frac{\tau}{2\sigma} \left(\|w - \hat{w}\|_Q^2 + \|y - \hat{y}\|^2 \right), \quad \forall (w, y) \in \mathcal{W} \times \mathcal{R}^m,$$

³The existence of such r and κ associated with the polyhedral multifunction \mathcal{T}_i [Sun 1993] can be derived from the classic error bound result in Robinson [1981]. See, for example, Lemma 2.4 in Li et al. [2020].

whose gradient is given by

$$\nabla\varphi(w, y) = \begin{bmatrix} Qw - Q\Pi_C(z(w, y)) + \frac{\tau}{\sigma}Q(w - \hat{w}) \\ -b + A\Pi_C(z(w, y)) + \frac{\tau}{\sigma}(y - \hat{y}) \end{bmatrix}, \quad (w, y) \in \mathcal{W} \times \mathcal{R}^m,$$

where $z(w, y) := \hat{x} - \sigma(Qw - A^*y + c)$. Note that solving the minimization problem

$$\min_{w, y} \left\{ \varphi(w, y) \mid (w, y) \in \mathcal{W} \times \mathcal{R}^m \right\} \quad (21)$$

is equivalent to solving the following system of nonlinear equations:

$$\nabla\varphi(w, y) = 0, \quad (w, y) \in \mathcal{W} \times \mathcal{R}^m. \quad (22)$$

Since C is a polyhedral set, $\Pi_C(\cdot)$ is piecewise linear and hence strongly semismooth. Thus, we can design a **semismooth Newton (SSN)** method to solve Equation (22) and could expect a superlinear or even quadratic convergence rate. For any $(w, y) \in \mathcal{W} \times \mathcal{R}^m$, define

$$\hat{\partial}^2\varphi(w, y) := \begin{bmatrix} Q & 0 \\ 0 & 0 \end{bmatrix} + \sigma \begin{bmatrix} Q \\ -A \end{bmatrix} \partial\Pi_C(z(w, y)) \begin{bmatrix} Q \\ -A \end{bmatrix}^* + \frac{\tau}{\sigma} \begin{bmatrix} Q & 0 \\ 0 & I \end{bmatrix},$$

where $\partial\Pi_C(z(w, y))$ is the Clarke subdifferential [Clarke 1990] of $\Pi_C(\cdot)$ at $z(w, y)$. Note that from Hiriart-Urruty et al. [1984], we know that

$$\hat{\partial}^2\varphi(w, y)(d_w; d_y) = \partial^2\varphi(w, y)(d_w; d_y), \quad \forall (d_w; d_y) \in \mathcal{W} \times \mathcal{R}^m, \quad (23)$$

where $\partial^2\varphi(w, y)$ denotes the generalized Hessian of φ at (w, y) , i.e., the Clarke generalized Jacobian of $\nabla\varphi$ at (w, y) . Given $(w, y) \in \mathcal{W} \times \mathcal{R}^m$, let $U \in \partial\Pi_C(z(w, y))$ and

$$V = \begin{bmatrix} Q & 0 \\ 0 & 0 \end{bmatrix} + \sigma \begin{bmatrix} Q \\ -A \end{bmatrix} U \begin{bmatrix} Q \\ -A \end{bmatrix}^* + \frac{\tau}{\sigma} \begin{bmatrix} Q & 0 \\ 0 & I \end{bmatrix}. \quad (24)$$

Then, we have $V \in \hat{\partial}^2\varphi(w, y)$.

After all the preparations, we can design a semismooth Newton method (see Figure 6) as in Zhao et al. [2010] to solve Equation (22).

The convergence results for the above SSN algorithm are stated in Theorem 3.4.

THEOREM 3.4. *Let the sequence $\{(w^j, y^j)\}$ be generated by Algorithm SSN. Suppose at each step $j \geq 0$, the tolerance η_j is achieved, i.e.,*

$$\|V_j(d_w; d_y) + \nabla\varphi(w^j, y^j)\| \leq \eta_j.$$

Algorithm SSN: A semismooth Newton algorithm.

Given $\bar{\eta} \in (0, 1)$, $\nu \in (0, 1]$, $\delta \in (0, 1)$ and $\rho \in (0, 1/2)$. Choose $(w^0, y^0) \in \mathcal{W} \times \mathcal{R}^m$. Iterate the following steps for $j = 0, 1, \dots$.

Step 1. Find an approximate solution $(d_w^j; d_y^j) \in \mathcal{W} \times \mathcal{R}^m$ to

$$V_j(d_w; d_y) = -\nabla\varphi(w^j, y^j) \quad (25)$$

such that

$$\|V_j(d_w^j; d_y^j) + \nabla\varphi(w^j, y^j)\| \leq \eta_j := \min(\bar{\eta}, \|\nabla\varphi(w^j, y^j)\|^{1+\nu}),$$

where $V_j \in \hat{\partial}^2\varphi(w^j, y^j)$ is defined as in (24) with $U_j \in \partial\Pi_C(z(w^j, y^j))$.

Step 2. Set $\alpha_j = \delta^{m_j}$, where m_j is the first nonnegative integer m for which

$$\varphi(w^j + \delta^m d_w^j, y^j + \delta^m d_y^j) \leq \varphi(w^j, y^j) + \rho \delta^m \langle \nabla\varphi(w^j, y^j), (d_w^j; d_y^j) \rangle. \quad (26)$$

Step 3. Set $w^{j+1} = w^j + \alpha_j d_w^j$ and $y^{j+1} = y^j + \alpha_j d_y^j$.

Fig. 6. Algorithm SSN.

Then the sequence $\{(w^j, y^j)\}$ converges to the unique optimal solution, say (\bar{w}, \bar{y}) , of the optimization problem in Equation (21) and

$$\|(w^{j+1}, y^{j+1}) - (\bar{w}, \bar{y})\| = O(\|(w^j, y^j) - (\bar{w}, \bar{y})\|^{1+\nu}). \quad (27)$$

PROOF. Note that $\Pi_C(\cdot)$ is strongly semismooth. Since $\varphi(w, y)$ is a strongly convex function defined on $\mathcal{W} \times \mathcal{R}^n$, problem (21) then has a unique solution (\bar{w}, \bar{y}) and the level set $\{(w, y) \in \mathcal{W} \times \mathcal{R}^n \mid \varphi(w, y) \leq \varphi(w^0, y^0)\}$ is compact. Therefore, the sequence generated by SSN is bounded as (d_w^j, d_y^j) is a descent direction [Zhao et al. 2010, Proposition 3.3]. Note that for all $(w, y) \in \mathcal{W} \times \mathcal{R}^n$, every $V \in \hat{\partial}^2 \varphi(w, y)$ is self-adjoint and positive definite on $\mathcal{W} \times \mathcal{R}^n$. Thus, the desired convergence can be easily obtained by combining Theorems 3.4 and 3.5 in Zhao et al. [2010]. \square

In Theorem 3.4, it is clear that V_j in the Newton system (25) in the form of Equation (24) is guaranteed to be positive definite as a positive definite proximal term is added. Indeed, adding the proximal term in our algorithmic design relieves the need of requiring additional conditions, such as the constraint nondegenerate condition (see, e.g., Zhao et al. [2010]), to ensure the nonsingularity of V_j in Equation (25). Moreover, to improve the condition number of the corresponding coefficient matrix, we would prefer a larger τ_k . However, to obtain better convergence rate for Algorithm QPPAL-Phase-II, we want a smaller τ_k . The two opposing effects imply that in the implementation of the algorithm we need to choose the parameter τ_k appropriately to balance the efficiency and robustness of the proposed algorithm.

4 IMPLEMENTATION OF QPPAL

In this section, we provide implementation details for our proposed QPPAL. Note that in both phase one and phase two algorithms, the main difficulty is to solve several types of linear systems. Thus, our main focus in this section is on how to solve such linear systems efficiently. Moreover, since choosing the parameters τ_k and σ_k plays an important role in the numerical implementation of the QPPAL-Phase-II algorithm, we also describe at the end of this section on how to adjust these parameters dynamically based on the optimality and infeasibility measures that will be defined later.

4.1 Implementation of QPPAL-Phase-I

We first discuss how to perform **Step 1** in Algorithm QPPAL-Phase-I efficiently. First, to obtain \bar{y}^k , a system of linear equations of the following form is solved:

$$-(b + \delta_E^k) + \sigma A(z^k - Qw^k + A^*y - c + \sigma^{-1}x^k) = 0.$$

By simple calculations, we derive that

$$(\sigma AA^*) \bar{y}^k = g^k + \delta_E^k,$$

where $g^k = (b - Ax^k) - \sigma A(z^k - Qw^k - c)$. Similarly, y^{k+1} is computed as follows:

$$(\sigma AA^*) y^{k+1} = g^{k+1} + \hat{\delta}_E^k,$$

where $g^{k+1} = (b - Ax^k) - \sigma A(z^{k+1} - Qw^{k+1} - c)$. Note that both δ_E^k and $\hat{\delta}_E^k$ should be interpreted as the residual vectors obtained by solving the above linear systems without these terms on the right-hand-sides. Observe that when the sparse Cholesky factorization of AA^* (which only need to be computed once) can be obtained at a moderate cost, we can solve these two linear systems by backward-forward substitutions cheaply in each iteration of QPPAL-Phase-I. In the event when solving the linear systems directly is too costly or not possible due to the memory constraint, one may use an iterative solver, such as a preconditioned **minimum residual method**

(MINRES) [Paige and Saunders 1975] or a **preconditioned symmetric quasi-minimal residual method (PSQMR)** [Freund and Nachtigal 1994], to solve the target linear systems. In the latter situation, the residual vectors just need to satisfy the conditions that

$$\|\delta_E^k\| \leq \epsilon_k, \quad \|\hat{\delta}_E^k\| \leq \epsilon_k,$$

where $\{\epsilon_k\}$ is a given nonnegative summable sequence, for example, one may choose $\epsilon_k = \min\{10^{-2}, 1/k^{1.1}\}$ for all $k \geq 1$. Observe that the accuracy requirement on the residual norm is actually quite mild, since for the previous choice, $\epsilon_k \approx 4 \times 10^{-5}$ even when k is as large as 10,000.

To obtain \tilde{w}^k and w^{k+1} , we need to solve a system of linear equations of the form

$$(Q + \sigma Q^2)w \approx Qh, \quad w \in \mathcal{W}, \quad (28)$$

where $h \in \mathbb{R}^n$ is a given vector. In particular, when computing \tilde{w}^k , $h := \sigma(z^k - A^* \bar{y}^k - c) + x^k$, and when computing w^{k+1} , $h := \sigma(z^{k+1} - A^* \bar{y}^k - c) + x^k$. Typically, we can only afford to solve the linear system (28) by an iterative solver inexactly. In this case, we require the residual vector δ_Q corresponding to a computed solution \hat{w} to satisfy the condition that

$$\|\delta_Q\| = \|Qh - (Q + \sigma Q^2)\hat{w}\| \leq \epsilon_k. \quad (29)$$

Note that there is a unique solution that solves Equation (28) exactly, since Q is positive definite on the subspace \mathcal{W} . Under the high-dimensional setting where n is huge and the matrix representation of Q may not be available, Equation (28) can only be solved inexactly by an iterative method. Indeed, based on our numerical experiments for solving QP relaxations for certain classes of integer programming problems and the QP problems arising from portfolio optimization, matrices Q in these problems are usually fully dense and large-scale. Hence, a direct solver may not be sufficiently efficient. Moreover, due to the presence of the subspace constraint $w \in \mathcal{W}$, it is apparently difficult to solve Equation (28) if $\mathcal{W} \neq \mathbb{R}^n$. Fortunately, we are able to propose the following strategy to rectify this difficulty. Instead of solving Equation (28), we propose to solve the following simpler linear system:

$$(I + \sigma Q)w \approx h, \quad (30)$$

with the residual norm of a computed solution \hat{w} satisfying

$$\|h - (I + \sigma Q)\hat{w}\| \leq \frac{\epsilon_k}{\|Q\|_2}. \quad (31)$$

The following simple spectral analysis will show that the coefficient matrix in Equation (30) generally would have a much better conditioning than that of Equation (28). Suppose $\lambda_1, \lambda_n, \lambda_n^+$ denote the largest, smallest, and smallest positive, eigenvalue of Q , respectively. Based on standard convergence analysis of an iterative method such as MINRES, we know that its convergence rate for solving Equation (28) is determined by the condition number $\kappa_1 = \frac{\lambda_1}{\lambda_n^+} \frac{1+\sigma\lambda_1}{1+\sigma\lambda_n^+}$, whereas the convergence rate for solving Equation (30) is determined by $\kappa_2 = \frac{1+\sigma\lambda_1}{1+\sigma\lambda_n}$. For the case that $\lambda_n^+ = \lambda_n$, i.e., Q is positive definite, it is clear that $\kappa_2 = \frac{\lambda_n}{\lambda_1} \kappa_1 \leq \kappa_1$. For the case where $\lambda_n^+ > \lambda_n = 0$, i.e., Q is singular, it is clear that κ_2 would be smaller than κ_1 if $\lambda_n^+(1 + \sigma\lambda_n^+) < \lambda_1$, or equivalently $\lambda_n^+ < \frac{1}{2}(\sqrt{\sigma^2 + 4\lambda_1} - \sigma)$. One would expect the latter condition to hold for most matrices Q unless λ_n^+ is large.

We can apply an iterative method (e.g., PSQMR, MINRES) to solve Equation (30) to obtain an approximate solution \hat{w} such that Equation (31) holds for \hat{w} . Then

$$\|\delta_Q\| = \|Q(h - (I + \sigma Q)\hat{w})\| \leq \|Q\|_2 \|h - (I + \sigma Q)\hat{w}\| \leq \|Q\|_2 \frac{\epsilon_k}{\|Q\|_2} = \epsilon_k.$$

Thus, we have that $w^* = \Pi_{\mathcal{W}}(\hat{w}) \in \mathcal{W}$ solves Equation (28) with the corresponding residual satisfying Equation (29). Surprisingly, much to our delight, it is not necessary for us to compute w^*

explicitly, since to update the iterations in Algorithm QPPAL-Phase-I, we only need to compute Qw^* , which is easily shown to be equal to $Q\hat{w}$. Hence, we only need to solve the linear system Equation (30) to obtain an approximate solution \hat{w} and then compute $Q\hat{w}$.

4.2 Implementation of QPPAL-Phase-II

We next illustrate how to solve the linear system (25) at each iteration of SSN efficiently. Notice that for a given $\sigma > 0$, $\hat{x} \in \mathbb{R}^n$ and $z(w, y) = \hat{x} - \sigma(Qw - A^*y + c)$, we can choose $U \in \partial\Pi_C(z(w, y))$ to be a diagonal matrix of order n whose diagonal entries are given as follows:

$$U_{ii} = \begin{cases} 1 & l_i < (z(w, y))_i < u_i \\ 0 & \text{otherwise} \end{cases}, \quad 1 \leq i \leq n.$$

Thus, the $(n + m) \times (n + m)$ coefficient matrix is given by

$$V = \begin{bmatrix} (1 + \frac{\tau}{\sigma})Q + \sigma QUQ & -\sigma QUA^* \\ -\sigma AUQ & \frac{\tau}{\sigma}I_m + \sigma AUA^* \end{bmatrix}, \quad (32)$$

for a given $\tau > 0$. Recall that V is positive definite on $\mathcal{W} \times \mathbb{R}^m$ and hence for any $r \in \mathcal{W} \times \mathbb{R}^m$, the linear system

$$V(d_w; d_y) = r, \quad (d_w; d_y) \in \mathcal{W} \times \mathbb{R}^m, \quad (33)$$

has a unique solution. In the following discussion, we always take

$$r := \begin{bmatrix} Qr_1 \\ r_2 \end{bmatrix} := - \begin{bmatrix} Q(w - \Pi_C(z(w, y)) + \frac{\tau}{\sigma}(w - \hat{w})) \\ -b + A\Pi_C(z(w, y)) + \frac{\tau}{\sigma}(y - \hat{y}) \end{bmatrix} = -\nabla\varphi(w, y).$$

Since Q is possibly a large dimensional and dense matrix, applying a direct method to solve Equation (33) may not be practical. Moreover, matrix-vector multiplications involving Q could be expensive. Therefore, iterative solvers such as PSQMR for solving Equation (33) may also be expensive. To resolve this issue, instead of solving Equation (33) directly, we solve a simpler linear system to compute Qd_w approximately via solving a nonsymmetric linear system. In particular, we shall use the BICGSTAB method studied in Saad [2003] to solve the new system. The next proposition (see Proposition 4.1 in Li et al. [2018]) demonstrates this approach and further implies that only one matrix-vector multiplication with respect to Q is required in each BICGSTAB iteration. This indeed reduces the computational cost compared with using V directly (especially when Q is dense), since the latter requires two such matrix-vector multiplications in each PSQMR iteration.

PROPOSITION 4.1. *Let the matrix V be given by Equation (32), and denote*

$$\hat{V} := \begin{bmatrix} (1 + \frac{\tau}{\sigma})I_n + \sigma UQ & -\sigma UA^* \\ -\sigma AUQ & \frac{\tau}{\sigma}I_m + \sigma AUA^* \end{bmatrix}. \quad (34)$$

Suppose $(\hat{d}_w; \hat{d}_y)$ is an approximate solution to the following system:

$$\hat{V}(\hat{d}_w; \hat{d}_y) \approx (r_1; r_2), \quad (35)$$

with the residual satisfying

$$\|\hat{V}(\hat{d}_w; \hat{d}_y) - (r_1; r_2)\| \leq \frac{\epsilon}{\max\{\|Q\|_2, 1\}}.$$

Let $d_w := \Pi_{\mathcal{W}}(\hat{d}_w) \in \mathcal{W}$. Then $(d_w, \hat{d}_y) \in \mathcal{W} \times \mathbb{R}^m$ solves Equation (33) with the residual norm satisfying

$$\|V(d_w; \hat{d}_y) - (Qr_1; r_2)\| \leq \epsilon.$$

Moreover,

$$Qd_w = Q\hat{d}_w, \quad \langle d_w, Qd_w \rangle = \langle \hat{d}_w, Q\hat{d}_w \rangle.$$

Again, similar to the case in Algorithm QPPAL-Phase-I, when updating the variable w , we do not need to compute d_w explicitly, since we can safely excute the algorithm by only updating Qw , namely, computing Qd_w . The fact that one can replace Equation (33) by the simpler linear system (35) is a powerful feature of our proposed algorithm.

Finally, we can further reduce the size of the linear system in Equation (34) by exploiting the special structure of the diagonal matrix U . To this end, we assume without loss of generality that U has the following representation:

$$U = \begin{bmatrix} I_p & 0 \\ 0 & 0 \end{bmatrix} \in \mathbb{R}^{n \times n}, \quad I_p \in \mathbb{R}^{p \times p}, \quad 0 \leq p \leq n.$$

Based on the above representation, we can then partition the vectors \hat{d}_w and r_1 , the matrices A and Q accordingly as follows:

$$\hat{d}_w = \begin{bmatrix} \hat{d}_w^P \\ \hat{d}_w^Z \end{bmatrix}, \quad r_1 = \begin{bmatrix} r_1^P \\ r_1^Z \end{bmatrix}, \quad A = \begin{bmatrix} A_P & A_Z \end{bmatrix}, \quad Q = \begin{bmatrix} Q_{PP} & Q_{PZ} \\ Q_{PZ}^T & Q_{ZZ} \end{bmatrix},$$

where $\hat{d}_w^P \in \mathbb{R}^p$, $\hat{d}_w^Z \in \mathbb{R}^{n-p}$, $r_1^P \in \mathbb{R}^p$, $r_1^Z \in \mathbb{R}^{n-p}$, $A_P \in \mathbb{R}^{m \times p}$, $A_Z \in \mathbb{R}^{m \times (n-p)}$, $Q_{PP} \in \mathbb{R}^{p \times p}$, $Q_{PZ} \in \mathbb{R}^{p \times (n-p)}$, and $Q_{ZZ} \in \mathbb{R}^{(n-p) \times (n-p)}$. Moreover, simple calculations show that

$$UQ = \begin{bmatrix} Q_{PP} & Q_{PZ} \\ 0 & 0 \end{bmatrix}, \quad UA^* = \begin{bmatrix} A_P^* \\ 0 \end{bmatrix}, \quad AUA^* = A_PA_P^*.$$

For notational simplicity, we denote $v := \sigma^{-1}\tau$. Based on the aforementioned partitions, we rewrite the linear system (35) as follows:

$$\begin{aligned} (1+v)\hat{d}_w^Z &= r_1^Z, \\ ((1+v)I_p + \sigma Q_{PP})\hat{d}_w^P - \sigma A_P^* \hat{d}_y &= r_1^P - \sigma Q_{PZ} \hat{d}_w^Z = r_1^P - \sigma(1+v)^{-1}Q_{PZ}r_1^Z =: \bar{r}_1, \\ -\sigma A_P Q_{PP} \hat{d}_w^P + (vI_m + \sigma A_P A_P^*)\hat{d}_y &= r_2 + \sigma A_P Q_{PZ} \hat{d}_w^Z = r_2 + \sigma(1+v)^{-1}A_P Q_{PZ}r_1^Z =: \bar{r}_2. \end{aligned}$$

Now, by writing the third equation as

$$-A_P((1+v)I_p + \sigma Q_{PP})\hat{d}_w^P + (1+v)A_P \hat{d}_w^P + (vI_m + \sigma A_P A_P^*)\hat{d}_y = \bar{r}_2$$

and making use of the second equation, we get after some simple manipulations that

$$\hat{d}_y = v^{-1} \left(A_P \bar{r}_1 + \bar{r}_2 - (1+v)A_P \hat{d}_w^P \right). \quad (36)$$

By using the above expression of \hat{d}_y in the second equation, we get

$$((1+v)I_p + \sigma Q_{PP} + v^{-1}(1+v)\sigma A_P^* A_P)\hat{d}_w^P = \bar{r}_1 + v^{-1}\sigma A_P^* (A_P \bar{r}_1 + \bar{r}_2). \quad (37)$$

It is obvious that the new target linear system (37) has a symmetric positive definite coefficient matrix of size $p \leq n$. Therefore, we can apply a direct solver to solve Equation (37) via computing the Cholesky factorization of the coefficient matrix when $p \ll n$ or an iterative solver such as PSQMR when $p \approx n$. Observe that by exploiting the active-set structure in U , we only need to solve a smaller-scale problem of dimension $p \times p$ instead of the $(n+m)$ -dimensional problem (35).

As a conclusion, instead of solving the non-symmetric linear system (35), we can solve the smaller symmetric positive definite linear system (37) for \hat{d}_w^P . Once that is computed, we can obtain \hat{d}_y from Equation (36). We should mention that while Equation (37) appears to be more appealing than Equation (35), the former can be much more ill-conditioned than the latter when σ is large. Thus, when Equation (37) itself is large-scale and requires an iterative solver, it would be more efficient to apply the BICGSTAB solver to Equation (35) directly when σ is large.

4.3 Updating Rules for τ_k and σ_k

Before describing the updating rule for τ_k and σ_k , we shall define the optimality and infeasibility measures of an approximate optimal solution $(x^k, z^k, w^k, y^k) \in \mathbb{R}^n \times \mathbb{R}^n \times \mathcal{W} \times \mathbb{R}^m$ for problems (P) and (D) at the k -th iteration of QPPAL-Phase-II algorithm. In particular, we define the following relative KKT residuals:

$$\eta_p^k := \frac{\|Ax^k - b\|}{1 + \|b\|}, \quad \eta_d^k := \frac{\|z^k - Qw^k + A^*y^k - c\|}{1 + \|c\|}, \quad \eta_Q^k := \frac{\|Qx^k - Qw^k\|}{1 + \|Qx^k\| + \|Qw^k\|}, \quad \eta_C^k := \frac{\|x^k - \Pi_C(x^k - z^k)\|}{1 + \|x^k\| + \|z^k\|}.$$

Then, starting from $\sigma_0 > 0$ and $\tau_0 > 0$, we update σ_k as follows:

$$\sigma_k = \begin{cases} \frac{5}{4}\sigma_{k-1} & \text{if } \max\{\eta_p^k, \eta_Q^k, \eta_C^k\} < \frac{3}{4}\eta_d^k, \\ \frac{4}{5}\sigma_{k-1} & \text{if } \eta_d^k < \frac{3}{4}\max\{\eta_p^k, \eta_Q^k, \eta_C^k\}, \\ \sigma_{k-1} & \text{otherwise,} \end{cases} \quad \forall k \geq 1.$$

Moreover, we update τ_k such that $\frac{\tau_k}{\sigma_k} = \max\{10^{-12}, \kappa \cdot k^{-2.5}\}$, for $k \geq 1$, where $\kappa > 0$ is a given constant that depends on the problems to be solved. Typically, κ is chosen to be in the range $[10^{-4}, 10^2]$.

5 NUMERICAL EXPERIMENTS

Consider the following more general QP problem with both linear equality and inequality constraints:

$$\min_{x' \in \mathbb{R}^N} \left\{ \frac{1}{2} \langle x', Q'x' \rangle + \langle c', x' \rangle \mid A_E x' = b_E, A_I x' \leq b_I, x' \in C' \right\}, \quad (38)$$

where $Q' \in \mathbb{S}_+^N$, $c' \in \mathbb{R}^N$, $A_E : \mathbb{R}^N \rightarrow \mathbb{R}^{m_E}$, $A_I : \mathbb{R}^N \rightarrow \mathbb{R}^{m_I}$ are two linear maps, $b_E \in \mathbb{R}^{m_E}$, $b_I \in \mathbb{R}^{m_I}$ and $C' := \{x' \in \mathbb{R}^N \mid -\infty \leq \ell' \leq x' \leq u' \leq \infty\}$. By adding a slack variable $s \in \mathbb{R}^{m_I}$, we can rewrite Equation (38) into the following form:

$$\min_{x' \in \mathbb{R}^n, s \in \mathbb{R}^{m_I}} \left\{ \frac{1}{2} \langle x', Q'x' \rangle + \langle c', x' \rangle \mid A_E x' = b_E, A_I x' + s = b_I, x' \in C', s \geq 0 \right\}. \quad (39)$$

By taking $n = N + m_I$, $x = (x'; s) \in \mathbb{R}^n$, $C := \{x = (x'; s) \in \mathbb{R}^n \mid x' \in C, s \geq 0\}$, and

$$Q := \begin{pmatrix} Q' & 0 \\ 0 & 0 \end{pmatrix} \in \mathbb{S}_+^n, \quad c := \begin{pmatrix} c' \\ 0 \end{pmatrix} \in \mathbb{R}^n, \quad A := \begin{pmatrix} A_E & 0 \\ A_I & I \end{pmatrix} \in \mathbb{R}^{m \times n}, \quad b := \begin{pmatrix} b_E \\ b_I \end{pmatrix} \in \mathbb{R}^m,$$

it is readily seen that problem (39) is of the form (P) and hence QPPAL can be applied to it directly.

In our numerical experiments, we measure the accuracy of an approximate optimal solution $(x^k, z^k, w^k, y^k) \in \mathbb{R}^n \times \mathbb{R}^n \times \mathcal{W} \times \mathbb{R}^m$ for QP (39) and its dual problem by using the same relative KKT residuals, i.e., $\eta_p^k, \eta_d^k, \eta_Q^k$ and η_C^k , as defined in Section 4.3. Additionally, we compute the relative gap by

$$\eta_g^k = \frac{\text{obj}_P - \text{obj}_D}{1 + |\text{obj}_P| + |\text{obj}_D|},$$

where $\text{obj}_P := \frac{1}{2} \langle x^k, Qx^k \rangle + \langle c, x^k \rangle$ and $\text{obj}_D := -\delta_C^*(-z^k) - \frac{1}{2} \langle w^k, Qw^k \rangle + \langle b, y^k \rangle$. For any given tolerance $\text{tol} \geq 0$, we terminate the algorithm if the following condition holds:

$$\eta^k := \max\{\eta_p^k, \eta_d^k, \eta_Q^k, \eta_C^k, |\eta_g^k|\} \leq \text{tol}.$$

Table 1. Settings for Each Solver

Solvers	Settings
GUROBI	FeasibilityTol = OptimalityTol = 1e-6, TimeLimit = 10800
OSQP	eps_abs = eps_rel = eps_prim_inf = eps_dual_inf = 1e-6, max_iter = 10000
QPALM	delta = 100, proximal = true, scaling = 2, eps_abs = eps_rel = 1e-6, max_iter = 1000
sGS-isPALM	tol = 1e-6, MaxIter = 10000
QPPAL	tol ₁ = 1e-4, MaxIter ₁ = 10000, tol ₂ = 1e-6, MaxIter ₂ = 1000

5.1 Benchmark

We compare our Algorithm QPPAL (implemented in MATLAB, version R2021a) with the state-of-the-art solvers,⁴ Gurobi, OSQP [Stellato et al. 2020], and QPALM [Hermans et al. 2019] for solving various classes of QP problems (38) (see Section 5.2) whose matrix representations for Q are available, since the latter three solvers all explicitly require Q to be a matrix. Moreover, since we use sGS-isPALM as our Phase I algorithm, we also present the numerical results obtained by running sGS-isPALM alone for the purpose of demonstrating the power and importance of our two-phase framework for solving difficult QP problems.

All our numerical experiments are conducted on a Linux machine (note that QPALM is only available for Unix machines) with Intel Xeon E5-2650 processors. The following table describes the settings for the termination conditions of each solver in our benchmark. For detailed descriptions on the meaning of the settings in Table 1 for Gurobi, OSQP and QPALM, we refer readers to their documentations.

Notice that each solver uses its own stopping criteria, so we decide to evaluate the accuracy of the computed solutions using the relative KKT residuals presented previously. We next explain how we conduct our comparisons. Note that all the solvers generate primal and dual solutions of the QP problems. Thus, we can readily extract the solutions $(x^k, z^k, w^k, y^k) \in \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^m$ from their outputs. Specifically, for Gurobi, OSQP, and QPALM, we always take $w^k = x^k$. Then, we can compute their corresponding relative KKT residuals and objective values, i.e., $\eta_p^k, \eta_d^k, \eta_Q^k, \eta_C^k, \eta_g^k, \text{obj}_P$ and obj_D , respectively. It is clear that for Gurobi, OSQP, and QPALM, it always holds that $\eta_Q^k = 0$.

To compare the robustness of each solver, we give our definition of “failure” in terms of the KKT residuals, primal and dual objective values. In particular, we say that a solver fails in terms of primal feasibility if it returns a solution with $\eta_p^k > 5 \times 10^{-6}$. Similar definition applies to η_d^k, η_Q^k , and η_C^k . For the comparison of objective function values, a solver with obj_P and obj_D is considered as a failure in terms of primal and dual objective values if

$$\text{err}_P := \frac{|\text{obj}_P - \text{obj}_{P,\text{best}}|}{1 + |\text{obj}_{P,\text{best}}|} > 5 \times 10^{-5} \quad \text{and} \quad \text{err}_D := \frac{|\text{obj}_D - \text{obj}_{D,\text{best}}|}{1 + |\text{obj}_{D,\text{best}}|} > 5 \times 10^{-5},$$

respectively, where $\text{obj}_{P,\text{best}}, \text{obj}_{D,\text{best}}$ are the primal and dual objective values of the solver having the smallest KKT residual η^k . We then compute the total number of problems that are marked as failures based on the above definition for four problem classes in the next subsection. Obviously a solver with a smaller number of failures is considered to be more robust.

For comparing the efficiency in terms of computation times, we adopt the Dolan-Moré performance profile [Dolan and Moré 2002].⁵ In particular, suppose that we are benchmarking S solvers on P problems. Let $t_{i,j}$ denote the time required by solver i to solve problem j . Then the

⁴These solvers are implemented in C/C++, and we call their MATLAB interfaces in our numerical tests.

⁵We use the script provided by <https://www.mcs.anl.gov/~more/cops/> to create performance profiles.

performance ratio of solver i for problem j is defined as

$$r_{i,j} = t_{i,j} / \min_i \{t_{i,j} : 1 \leq i \leq S\}, \quad 1 \leq i \leq S, \quad 1 \leq j \leq P.$$

In the performance profile, one plots the following functions for each solver i :

$$f_s(\tau) := \frac{1}{P} \sum_{1 \leq j \leq P} f_\tau(r_{i,j}), \quad 1 \leq i \leq S, \quad \forall \tau \in \mathbb{R}_{++},$$

where the function $f_\tau(\cdot) : \mathbb{R} \rightarrow [0, 1]$ is defined as

$$f_\tau(r) := \begin{cases} 1 & \text{if } r \leq \tau, \\ 0 & \text{otherwise,} \end{cases} \quad \forall r \in \mathbb{R}.$$

It is not difficult to observe that the value of $f_s(\tau)$ represents the fraction of problems that are solved within τ times of the best solver. Hence, the higher the plotted curve is, the better the performance of the corresponding solver has. Finally, note that the performance profile is meaningful only if all the solvers are able to solve the problems successfully. Hence, failures on a given problem (in the sense that $\eta_{kkt}^k := \max\{\eta_p^k, \eta_d^k, \eta_Q^k, \eta_C^k\} > 5 \times 10^{-6}$) are represented by “NaN” (i.e., “Not a Number”) when we prepare the performance profiles.

As argued in Gould and Scott [2016], the performance profiles plots may cause issues when more than two algorithms are compared at the same time. For this reason and for compactness, we also provide the **normalized shifted geometric mean (nSGM)** of the computational time. In particular, for each problem set consisting of P testing instances, we compute

$$\bar{t}_i = \left(\prod_{1 \leq j \leq P} (t_{i,j} + \zeta) \right)^{\frac{1}{P}} - \zeta = \exp\left(\frac{1}{P} \sum_{1 \leq j \leq P} \ln(t_{i,j} + \zeta)\right) - \zeta, \quad 1 \leq i \leq S.$$

Then the nSGM for the solver i is computed as $\tilde{t}_i := \bar{t}_i / \min\{\bar{t}_i : 1 \leq i \leq S\}$. In this article, a shift of $\zeta = 1$ is applied. Note that a smaller value of the nSGM indicates a better performance.

5.2 Some Classes of QP Problems

We next list four classes of QP problems arising from different scenarios with some brief descriptions.

Example 5.1 (QPs Arising from Relaxations of QAP Problems). Given matrices $A, B \in \mathcal{S}^d$, the **quadratic assignment problem (QAP)** is given by

$$\min_{X \in \mathbb{R}^{d \times d}} \{ \langle \text{vec}(X), (B \otimes A) \text{vec}(X) \rangle \mid Xe = e = X^T e, X \geq 0, X \in \{0, 1\}^{d \times d} \},$$

where \otimes denotes the Kronecker product, $\text{vec}(X)$ is the vectorization of the matrix X , i.e.,

$$\text{vec}(X) = [x_{1,1}, \dots, x_{d,1}, x_{1,2}, \dots, x_{d,2}, \dots, x_{1,d}, \dots, x_{d,d}]^T \in \mathbb{R}^{d^2}.$$

It has been shown in Anstreicher and Brixius [2001] that a reasonably good lower bound for the above QAP can often be obtained by solving the following convex QP relaxation:

$$\min_{\text{vec}(X) \in \mathbb{R}^{d^2}} \{ \langle \text{vec}(X), Q \text{vec}(X) \rangle \mid (e^T \otimes I) \text{vec}(X) = e = (I \otimes e^T) \text{vec}(X), \text{vec}(X) \geq 0 \}, \quad (40)$$

where $Q = B \otimes A - I \otimes S - T \otimes I$, and $S, T \in \mathcal{S}^d$ are given as follows. Consider the eigenvalue decompositions, $A = V_A D_A V_A^T$, $B = V_B D_B V_B^T$, where V_A and $D_A = \text{Diag}(\alpha_1, \dots, \alpha_d)$ correspond to the eigenvectors and eigenvalues of A , and V_B and $D_B = \text{Diag}(\beta_1, \dots, \beta_d)$ correspond to the eigenvectors and eigenvalues of B , respectively. We assume that $\alpha_1 \geq \dots \geq \alpha_d$ and $\beta_1 \leq \dots \leq \beta_d$. Let (\bar{s}, \bar{t}) be an optimal solution to the LP: $\max\{e^T s + e^T t \mid s_i + t_j \leq \alpha_i \beta_j, i, j = 1, \dots, d\}$, whose

solution can be computed analytically as shown in Anstreicher and Brixius [2001]. Then, $S = V_A \text{Diag}(\bar{s}) V_A^T$ and $T = V_B \text{Diag}(\bar{t}) V_B^T$. The data for the QAPs are obtained from QAPLIB [Burkard et al. 1997].

Example 5.2 (QP Relaxations of Quartic Optimization with Binary Constraints). Consider the following binary constrained quartic optimization problem:

$$\min_{x \in \mathbb{R}^d} \left\{ (\langle x, Qx \rangle)^2 \mid x \in \{0, 1\}^d, \|x\|_0 \geq \beta \right\},$$

where $Q \in \mathcal{S}^d$, and $\beta > 0$ is a given constant. The presence of the cardinality constraint $\|x\|_0 \geq \beta$ is to avoid the trivial case when $x = 0$ is an optimal solution. Let $\lambda_{\max}(Q)$ and $\lambda_{\min}(Q)$ denote the maximal and minimal eigenvalue of Q , respectively. It holds that the minimal eigenvalue of $Q \otimes Q$ is given as follows:

$$\lambda_{\min}(Q \otimes Q) = \begin{cases} \lambda_{\min}(Q)^2 & \text{if } \lambda_{\min}(Q) \geq 0, \\ \lambda_{\max}(Q)^2 & \text{if } \lambda_{\max}(Q) \leq 0, \\ \lambda_{\min}(Q) \cdot \lambda_{\max}(Q) & \text{otherwise.} \end{cases}$$

Notice that the $(\langle x, Qx \rangle)^2 = \langle \text{vec}(xx^T), (Q \otimes Q) \text{vec}(xx^T) \rangle$. Then, a direct QP relaxation for the above optimization problem is given as follows:

$$\min_{X \in \mathcal{S}^d, x \in \mathbb{R}^d} \left\{ \langle \text{svec}(X), \tilde{Q} \text{svec}(X) \rangle + \lambda_0 \langle e_d, x \rangle \mid (X, x) \in \mathcal{F}_{BIQ} \right\},$$

where $\lambda_0 := \min\{0, \lambda_{\min}(Q \otimes Q)\}$, $e_d \in \mathbb{R}^d$ is the vector of all ones, $\tilde{Q} \in \mathcal{S}_+^{d(d+1)/2}$ satisfies

$$\langle \text{vec}(X), [(Q \otimes Q) - \lambda_0 I_{d^2}] \text{vec}(X) \rangle = \langle \text{svec}(X), \tilde{Q} \text{svec}(X) \rangle,$$

for any $X \in \mathcal{S}^d$, and

$$\mathcal{F}_{BIQ} := \left\{ (X, x) \in \mathcal{S}^d \times \mathbb{R}^d \mid \begin{array}{l} \text{diag}(X) = x, \langle e_d, x \rangle \geq \beta, -X_{ij} + x_j \geq 0, -X_{ij} + x_i \geq 0, \\ X_{ij} - x_i - x_j \geq -1, 1 \leq i < j \leq d, X \geq 0, x \geq 0 \end{array} \right\}.$$

Note that in the above, $\text{svec}(X)$ denotes the vector obtained by stacking the upper triangular part of X , column by column sequentially. Moreover, the off-diagonal elements of X are scaled by $\sqrt{2}$.

In our numerical experiments, the tested matrices Q are selected from the BIQM MAC library [Wiegele 2007], and we take $\beta = d/5$.

Example 5.3 (QPs Selected from Maros-Mészáros Collection). In this example, we compare the performance of all the solvers on the QP instances that are selected from the Maros-Mészáros collections [Maros and Mészáros 1999]. The QP problems from this collection are often used to benchmark QP solvers, since this collection contains many large-scale and very difficult (ill-conditioned) QP problems. Thus, they are quite challenging to solve. Since we focus on solving large-scale QP problems in this article, we only select those problems such that the sum of linear equality and inequality constraints and the number of decision variables is at least 1,000.

Example 5.4 (QPs Arising from Portfolio Optimization). Portfolio optimization [Perold 1984; Takehara 1993] employed by the investment community seeks to allocate assets in a way that optimizes the risk adjusted return. In this example, we consider a simplified version of portfolio optimization, which is in fact a convex QP given as follows:

$$\min_{x \in \mathbb{R}^n} \{ \gamma \langle x, \Sigma x \rangle - \langle \mu, x \rangle \mid \langle e_n, x \rangle = 1, x \geq 0 \},$$

where $x \in \mathbb{R}^n$ is the decision variable, and the data matrix $\Sigma \in \mathcal{S}^n$ is symmetric positive semidefinite, $\mu \in \mathbb{R}^n$, $\gamma > 0$ and $e_n \in \mathbb{R}^n$ is the vector of all ones. We generate our test data randomly via the following MATLAB script as follows:

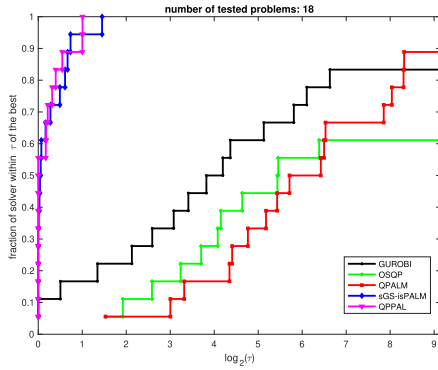


Fig. 7. Performance comparison for Example 5.1. **Left:** Performance profile. **Right:** Statistics for each solver.

```
n = 1000*k; p = 10*k; % k = 1:10
F = sprandn(n, p, 0.1); D = sparse(diag(sqrt(p)*rand(n,1)));
Sigma = cov(F') + D;
mu = randn(n,1); gamma = 1.0;
```

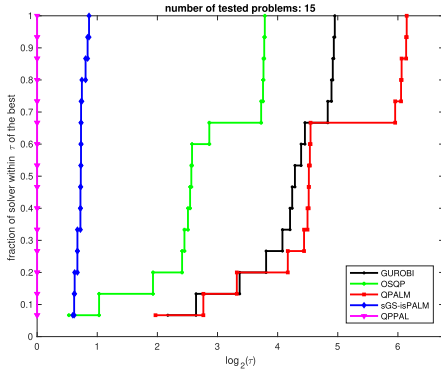
5.3 Numerical Results

We are now ready to present our numerical results by showing the performance profiles, the failure rates, and the nSGM of the five solvers on the four previous examples. The detailed computational results are available in the Supplementary Material.

Figures 7 and 8 present the computational results for Examples 5.1 and 5.2, respectively. We observe from the performance profiles that our proposed algorithms are indeed much more efficient than the existing state-of-the-art solvers. In particular, QPPAL is shown to be substantially more efficient than other solvers. While OSQP performs better than Gurobi on Example 5.2, the former is slightly less efficient than the latter on Example 5.1. For both examples, QPALM turns out to be less efficient than the other solvers. This observation supports our claim that for solving large-scale dense QP problems, applying the proximal ALM method to the (restricted-Wolfe) dual problem (D) is more effective. For the comparison on the failure numbers of each solver, we see that QPPAL and sGS-isPALM are able to solve all the instances successfully for both examples, whereas OSQP and QPALM can solve all the instances in Example 5.2 but fail on quite a few instances in Example 5.1. Gurobi is also quite robust as it can solve all the instances in both examples except for three instances with bad η_C in Example 5.1. Overall, we see that QPPAL and sGS-isPALM are quite efficient and robust for solving large-scale and dense QP problems.

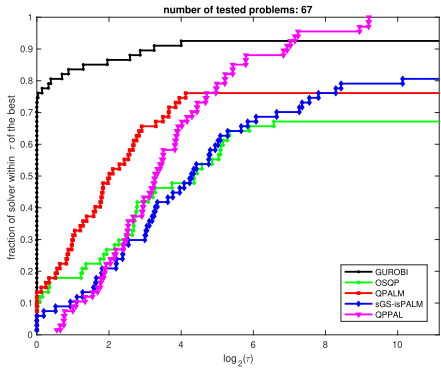
Figure 9 shows the comparison results for solving QPs in Example 5.3. Recall that these QP problems are highly sparse and are quite challenging to solve because of degeneracy such as the nonexistence of a strictly feasible point for either the primal or dual problem. It is commonly accepted that interior point methods would be both efficient and robust for solving degenerate problems. The numerical results for Gurobi that we have presented support this argument.

Note that though the focus of this article is to design scalable and robust algorithms for solving large-scale QP problems having some or all the three characteristics mentioned in Section 1, our purpose of presenting the results for those QP problems in the Maros-Mészáros collection is to evaluate the robustness of our proposed algorithm. Indeed the presented results show that our proposed QPPAL is robust even for difficult sparse QPs. More specifically, the results show the need of our Phase II algorithm, since one can easily observe that there are numerous problems in the collection for which the first-order algorithms OSQP and sGS-isPALM cannot deliver accurate



Solver	GUROBI	OSQP	QPALM	sGS-isPALM	QPPAL
η_p	0	0	0	0	0
η_d	0	0	0	0	0
η_Q	0	0	0	0	0
η_C	0	0	0	0	0
obj_p	0	0	0	0	0
obj_d	0	0	0	0	0
η_{kkt}	0	0	0	0	0
Failure rate[%]	0.00	0.00	0.00	0.00	0.00
nSGM	17.51	6.84	24.74	1.64	1.00

Fig. 8. Performance comparison for Example 5.2. **Left:** Performance profile. **Right:** Statistics for each solver.

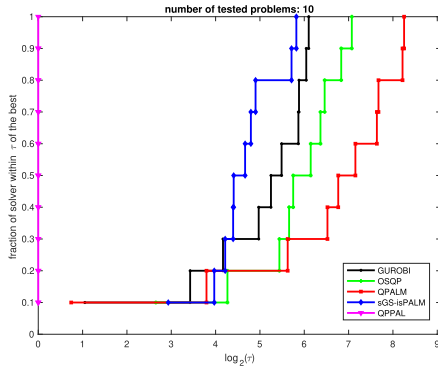


Solver	GUROBI	OSQP	QPALM	sGS-isPALM	QPPAL
η_p	0	7	10	2	0
η_d	0	20	7	13	0
η_Q	0	0	1	10	0
η_C	5	12	4	9	0
obj_p	0	24	16	24	14
obj_d	0	24	16	25	14
η_{kkt}	5	22	16	13	0
Failure rate[%]	7.46	32.84	23.88	19.40	0.00
nSGM	1.00	6.26	3.61	11.58	7.82

Fig. 9. Performance comparison for Example 5.3. **Left:** Performance profile. **Right:** Statistics for each solver.

approximate solutions. However, our two-phase algorithm QPPAL is able to obtain solutions with the desired accuracy. As a second-order algorithm, QPALM is also demonstrated to be more robust than OSQP and sGS-isPALM. However, it is less robust than Gurobi and QPPAL. For the comparison between OSQP and sGS-isPALM, we observe that both algorithms have similar performance in terms of robustness.

For the comparison on efficiency, it is clear that Gurobi is the most powerful solver that outperforms all the other solvers in terms of the computational time on the successful instances. Moreover, QPALM is generally more efficient than OSQP and our solvers in this collection. We also observe that the numerical performance of Gurobi, OSQP, and QPALM showed in this article coincides the one presented in Section 7.3 of Hermans et al. [2020]. In addition, given the fact that QPALM and OSQP are less robust than Gurobi, it may take more computational effort for QPALM and OSQP to compute more accurate solutions. Therefore, we would recommend Gurobi for solving sparse and difficult QP problems if one wants to obtain highly accurate solutions efficiently. However, QPPAL is less efficient than QPALM, but it has comparable performance as OSQP and it is more efficient than sGS-isPALM. The latter observation together with the comparison of robustness between QPPAL and sGS-isPALM again shows that the second phase of QPPAL is indeed necessary and further supports our motivation to design a two-phase algorithm. For the comparison between OSQP and sGS-isPALM, one sees that OSQP usually requires less computational time, especially for the small-scale problems.



Solver	GUROBI	OSQP	QPALM	sGS-isPALM	QPPAL
η_p	0	0	0	0	0
η_d	0	0	0	0	0
η_Q	0	0	0	0	0
η_C	0	0	0	0	0
obj_p	0	10	10	0	0
obj_d	0	10	10	0	0
η_{kkt}	0	0	0	0	0
Failure rate[%]	0.00	0.00	0.00	0.00	0.00
nSGM	25.69	42.62	69.38	19.85	1.00

Fig. 10. Performance comparison for Example 5.4. **Left:** Performance profile. **Right:** Statistics for each solver.

Figure 10 presents the computational results for Example 5.4. From the presented results, we can see that QPPAL outperforms the other solvers in terms of the computational time. In fact, QPPAL is at least ten times faster than the other solvers when the problem size is large, say when the dimension of the decision variable is larger than 2000. One can also observe that both OSQP and QPALM require much longer computational times and the objective values returned by OSQP and QPALM are obviously worse than Gurobi, sGS-isPALM, and QPPAL. One possible reason is that the matrix Q in these problems are fully dense and applying a direct solver for solving linear systems involving Q may not be a wise choice. However, OSQP and QPALM currently only support direct solvers.

We finish this subsection with some final comments on the computational results. Obviously, Gurobi and QPALM have the best performance for convex QP problems whose matrices Q and A are highly sparse and with special structures. However, QPALM is demonstrated to be less robust than Gurobi. On the contrary, for dense and large-scale problems, Gurobi and QPALM may no longer be a good option, since they require too much computational effort. As ADMM-type algorithms, both OSQP and sGS-isPALM are highly efficient for well-conditioned problems such as convex QP relaxations of QAP and quartic polynomial minimization problems. However, our numerical results show that sGS-isPALM is more likely to outperform OSQP in terms of efficiency and accuracy for large-scale QP problems. However, for small-scale QP problems, sGS-isPALM is demonstrated to have comparable performance as OSQP in terms of robustness. Finally, the computational results for those difficult problems that sGS-isPALM cannot solve efficiently indicate that the design of our two-phase algorithm QPPAL is indeed useful and important. Overall, the above numerical results demonstrate that the proposed QPPAL is highly efficient and robust for solving large-scale and dense convex QP problems.

5.4 Computational Results on Matrices Q Without Matrix Representations

In this subsection, we consider QP problems arising in Section 5.2 for which the matrix representations for Q may not be available. The test problems are selected from QP relaxations for QAP problems with $d \geq 100$ and BIQ problems with $n \geq 150$. For these problems, the matrices Q are usually fully dense. Moreover, even if the matrix representations for Q are available, storing them would require a large amount of memory. Thus, we can only use iterative solvers (such as PSQMR) to solve the underlying linear systems, and Gurobi, QPALM, and OSQP are not able to cope with these large scale QPs, since they currently only support direct solvers for solving linear systems.

The computational results are presented in Table 2. In the table, the three integers below the name of the problem represent the sizes of the underlying QP problem. For instance,

Table 2. Numerical Results for QP Problems in Examples 5.1 and 5.2 Having No Matrix Representation of Q

Name	Solver	Iter	Time	η_p	η_d	η_Q	η_C	obj _P	obj _D	η_g
tai100a (200, 0, 10,000)	sGS-isPALM	567	2.577	7e-13	1e-06	3e-07	7e-07	4.5239e-01	4.5239e-01	-1e-07
	QPPAL	8(278)	2.122	6e-16	7e-07	3e-08	6e-08	4.5239e-01	4.5239e-01	-1e-07
tai100b (200, 0, 10,000)	sGS-isPALM	1,870	16.619	6e-13	1e-06	2e-07	9e-07	2.7470e-01	2.7470e-01	-3e-07
	QPPAL	11(237)	5.727	6e-16	8e-07	4e-08	8e-08	2.7470e-01	2.7470e-01	-3e-07
tai256c (512, 0, 65,536)	sGS-isPALM	280	4.096	3e-07	1e-06	8e-08	2e-08	8.4942e-02	8.4942e-02	6e-08
	QPPAL	8(185)	5.139	6e-16	3e-07	2e-09	7e-12	8.4942e-02	8.4942e-02	4e-10
tai150b (300, 0, 22,500)	sGS-isPALM	2,183	44.252	6e-13	9e-07	2e-07	9e-07	2.7753e-01	2.7753e-01	-3e-07
	QPPAL	19(307)	23.315	7e-16	8e-07	2e-09	2e-10	2.7753e-01	2.7753e-01	-2e-07
tho150 (300, 0, 22,500)	sGS-isPALM	2,316	44.249	6e-13	1e-06	2e-07	7e-07	3.7766e-01	3.7766e-01	-2e-07
	QPPAL	21(320)	24.713	7e-16	9e-07	3e-09	5e-10	3.7766e-01	3.7766e-01	-2e-07
wil100 (200, 0, 10,000)	sGS-isPALM	2,630	19.507	8e-13	9e-07	2e-07	1e-06	5.2368e-01	5.2368e-01	-2e-07
	QPPAL	14(299)	8.132	9e-16	7e-07	5e-08	5e-08	5.2368e-01	5.2368e-01	-2e-07
esc128 (256, 0, 16,384)	sGS-isPALM	244	1.398	1e-06	7e-07	5e-07	1e-08	1.2167e-01	1.2167e-01	3e-08
	QPPAL	3(154)	1.033	4e-16	1e-07	3e-07	5e-11	1.2167e-01	1.2167e-01	2e-11
be150.3.1 (150, 33,526, 11,475)	sGS-isPALM	266	25.502	8e-08	3e-07	1e-06	3e-11	2.8738e+06	2.8738e+06	-3e-07
	QPPAL	11(176)	16.459	8e-07	8e-07	2e-07	6e-16	2.8738e+06	2.8738e+06	1e-07
be150.8.1 (150, 33,526, 11,475)	sGS-isPALM	266	41.347	8e-08	3e-07	1e-06	1e-11	7.2801e+06	7.2801e+06	-3e-07
	QPPAL	11(176)	26.238	8e-07	7e-07	3e-07	2e-16	7.2801e+06	7.2801e+06	1e-07
be200.3.1 (200, 59,701, 20,300)	sGS-isPALM	266	47.742	6e-08	3e-07	1e-06	2e-11	5.1907e+06	5.1907e+06	-7e-08
	QPPAL	14(176)	32.482	6e-07	1e-07	2e-07	7e-16	5.1907e+06	5.1907e+06	5e-08
be250.1 (250, 93,376, 31,625)	sGS-isPALM	270	52.404	5e-08	4e-07	9e-07	5e-11	3.1315e+06	3.1315e+06	1e-07
	QPPAL	16(177)	38.030	1e-07	6e-07	2e-07	2e-15	3.1315e+06	3.1315e+06	-8e-07
bqp250-1 (250, 93,376, 31,625)	sGS-isPALM	270	53.029	5e-08	4e-07	1e-06	1e-11	1.0644e+07	1.0644e+07	9e-08
	QPPAL	16(177)	38.077	9e-08	6e-07	9e-08	7e-16	1.0644e+07	1.0644e+07	-7e-07
bqp500-1 (500, 37,4251, 125,750)	sGS-isPALM	440	488.023	3e-09	1e-06	1e-06	6e-12	4.0835e+07	4.0835e+07	-3e-07
	QPPAL	18(195)	274.971	4e-07	3e-08	2e-07	1e-15	4.0835e+07	4.0835e+07	-1e-06

(200, 0, 10, 000) under the first column indicates that the QP problem has 200 linear equality constraints, no linear inequality constraint, and 10,000 decision variables. The columns Iter and Time represent the iteration number and computational time, respectively. In particular, 5(280) means that QPPAL takes 5 phase II iterations with 280 phase I iterations for warm-starting. The meanings of the remaining columns in the table are clear from the context and we omit the description for simplicity.

From Table 2, we observe that for very large-scale and dense QP problems, our QPPAL is still able to solve them efficiently and robustly. In particular, for the last instance in the table, QPPAL is able to solve the QP with more than 374,000 constraints and 125,000 variables in under 5 min. This shows that our proposed algorithm is indeed scalable, robust and highly efficient for convex QP problems having the three characteristics mentioned in Section 1. Moreover, QPPAL is empirically more efficient than sGS-isPALM. This again supports our motivation of developing QPPAL in this article.

6 CONCLUSIONS

In this article, we have proposed a two-phase proximal augmented Lagrangian method (QPPAL) for solving convex quadratic programming problems based on their restricted-Wolfe dual problems. In the first phase of QPPAL, we applied a symmetric Gauss-Seidel-based semi-proximal augmented Lagrangian method for the purpose of generating a good starting point. In the second phase of QPPAL, a proximal augmented Lagrangian method of multipliers with elegant convergence properties developed recent by Li et al. [2020] was applied. To solve the corresponding inner subproblems efficiently, a semismooth Newton method with a fast local convergence rate was adopted. With

well-developed theoretical results, we then conducted extensive numerical experiments to evaluate the performance of the proposed algorithm against the highly powerful commercial solver Gurobi, the operator splitting-based solver OSQP, and the primal-based augmented Lagrangian method (QPALM). Promising numerical results demonstrated that the proposed QPPAL is highly efficient and robust for solving large-scale and dense problems. Last, for further efficiency, we plan to implement our proposed algorithms by using C/C++ in our future work.

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A APPENDIX

A.1 Proof of Proposition 2.1

Before proving the theorem, we need the following lemma that provides an estimation of the distance between v^{k+1} and \bar{v}^{k+1} in the Algorithm isPALM.

LEMMA A.1. *Let $\{(v^k, x^k)\}$ be the sequence generated by the Algorithm isPALM and $\{\bar{v}^k\}$ be defined by Equation (7). Then,*

$$\|v^{k+1} - \bar{v}^{k+1}\|_N \leq \|N^{-1/2}d^k\| \leq \varepsilon_k, \quad \forall k \geq 0.$$

PROOF. From Equations (7) and (8), we have for all $k \geq 0$,

$$\begin{aligned} 0 &\in \partial g(\bar{v}^{k+1}) + \mathcal{G}x^k + \sigma\mathcal{G}(\mathcal{G}^*\bar{v}^{k+1} - c) + \mathcal{T}(\bar{v}^{k+1} - v^k), \\ d^k &\in \partial g(v^{k+1}) + \mathcal{G}x^k + \sigma\mathcal{G}(\mathcal{G}^*v^{k+1} - c) + \mathcal{T}(v^{k+1} - v^k). \end{aligned}$$

Then, by Equation (6), we know that

$$\langle d^k + (\mathcal{T} + \sigma\mathcal{G}\mathcal{G}^*)(v^{k+1} - \bar{v}^{k+1}), \bar{v}^{k+1} - v^{k+1} \rangle \geq \|\bar{v}^{k+1} - v^{k+1}\|_{\Sigma_g}^2.$$

By simple calculations, we can obtain that

$$\|\bar{v}^{k+1} - v^{k+1}\|_{\Sigma_g + \mathcal{T} + \sigma\mathcal{G}\mathcal{G}^*}^2 \leq \langle d^k, \bar{v}^{k+1} - v^{k+1} \rangle,$$

i.e.,

$$\|\bar{v}^{k+1} - v^{k+1}\|_N^2 \leq \langle N^{-1/2}d^k, N^{1/2}(\bar{v}^{k+1} - v^{k+1}) \rangle \leq \|N^{-1/2}d^k\| \|\bar{v}^{k+1} - v^{k+1}\|_N.$$

From here, the required result follows directly. \square

PROOF OF PROPOSITION 2.1. The positive definiteness of $\widehat{\mathcal{E}}$ and the equivalence follows directly from Theorem 4.1 in Chen et al. [2021]. By Lemma A.1, we know that for $k \geq 0$

$$\|\widehat{\mathcal{E}}^{-1/2}d^k\| \leq \|\mathcal{E}_d^{-1/2}\| \|\hat{\delta}^k - \delta^k\| + \|\widehat{\mathcal{E}}^{-1/2}\| \|\delta^k\| \leq ((2p-1)\|\mathcal{E}_d^{-1/2}\| + p\|\widehat{\mathcal{E}}^{-1/2}\|)\varepsilon_k,$$

which completes the proof. \square

A.2 Proof of Lemma 3.2

PROOF. By the first optimality conditions for the minimax problem in Equation (16), we derive that, for any $(w, y, x) \in P_k(\bar{w}, \bar{y}, \bar{x})$

$$\begin{aligned} 0 &= Q(w - x) + \frac{\tau_k}{\sigma_k} Q(w - \bar{w}), \\ 0 &= -b + Ax + \frac{\tau_k}{\sigma_k} (y - \bar{y}), \\ 0 &\in Qw - A^*y + c + \partial\delta_C(x) + \frac{1}{\sigma_k} (x - \bar{x}). \end{aligned}$$

By the definition of \mathcal{T}_i , the above conditions can be written as

$$\left(\mathcal{T}_i + \frac{1}{\sigma_k} \Lambda_k \right) (w, y, x) - \frac{1}{\sigma_k} \Lambda_k(\bar{w}, \bar{y}, \bar{x}) = 0, \quad \forall (w, y, x) \in P_k(\bar{w}, \bar{y}, \bar{x}).$$

This establishes Equation (18). The last statement in the lemma follows easily by Equation (18). This completes the proof. \square

A.3 Proof of Proposition 3.1

PROOF. It is not difficult to show that

$$(w^{k+1}, y^{k+1}, x^{k+1}) = (\Lambda_k + \sigma_k \mathcal{T}_i)^{-1} \Lambda_k \left(\Lambda_k^{-1} (\sigma_k \nabla \Psi_k(w^{k+1}, y^{k+1}), 0) + (w^k, y^k, x^k) \right).$$

Note here that Λ_k^{-1} is well-defined, since $(\sigma_k \nabla \Psi_k(w^{k+1}, y^{k+1}), 0) \in \mathcal{X}$ and Λ_k is positive definite over \mathcal{X} . Then, by Lemma 3.2, we have

$$\begin{aligned} &\|(w^{k+1}, y^{k+1}, x^{k+1}) - P_k(w^k, y^k, x^k)\|_{\Lambda_k} \\ &= \|(\Lambda_k + \sigma_k \mathcal{T}_i)^{-1} \Lambda_k \left(\Lambda_k^{-1} (\sigma_k \nabla \Psi_k(w^{k+1}, y^{k+1}), 0) + (w^k, y^k, x^k) - (w^k, y^k, x^k) \right)\|_{\Lambda_k} \\ &\leq \|\Lambda_k^{-1} (\sigma_k \nabla \Psi_k(w^{k+1}, y^{k+1}), 0)\|_{\Lambda_k} \quad (\text{since } P_k \text{ is non-expansive}) \\ &\leq \frac{\sigma_k}{\min\{1, \sqrt{\tau_k}, \sqrt{\tau_k \lambda_+(Q)}\}} \|\nabla \Psi_k(w^{k+1}, y^{k+1})\|, \end{aligned}$$

as desired. \square

REFERENCES

- K. M. Anstreicher and N. W. Brixius. 2001. A new bound for the quadratic assignment problem based on convex quadratic programming. *Math. Program.* 89, 3 (Feb. 2001), 341–357.
- R. E. Burkard, S. E. Karisch, and F. Rendl. 1997. QAPLIB—A quadratic assignment problem library. *J. Global Optim.* 10, 4 (June 1997), 391–403. Retrieved from <http://anjos.mgi.polymtl.ca/qaplib/inst.html>.
- L. Chen, X. Li, D. Sun, and K.-C. Toh. 2021. On the equivalence of inexact proximal ALM and ADMM for a class of convex composite programming. *Math. Program.* 185, 1 (Jan. 2021), 111–161.
- F. H. Clarke. 1990. *Optimization and Nonsmooth Analysis*. Society for Industrial and Applied Mathematics.
- R. W. Cottle. 1963. Symmetric dual quadratic programs. *Q. Appl. Math.* 21, 3 (1963), 237–243.
- R. W. Cottle. 1964. Note on a fundamental theorem in quadratic programming. *J. Soc. Ind. Appl. Math.* 12, 3 (Sept. 1964), 663–665.
- G. B. Dantzig. 1961. *Quadratic programming: A variant of the Wolfe-Markowitz algorithm*. Technical Report. California University Berkeley Operations Research Center.
- G. B. Dantzig. 1963. *Linear Programming and Extensions*. Princeton University Press, Princeton, NJ. ch. 24-4, 490–497.
- E. D. Dolan and J. J. Moré. 2002. Benchmarking optimization software with performance profiles. *Math. Program.* 91, 2 (2002), 201–213.
- R. W. Freund and N. M. Nachtigal. 1994. *A new Krylov-subspace method for symmetric indefinite linear systems*. Technical Report. Oak Ridge National Laboratory, Oak Ridge, TN.
- N. I. M. Gould and J. Scott. 2016. A note on performance profiles for benchmarking software. *ACM Trans. Math. Softw.* 43, 2 (2016), 1–5.

- N. I. M. Gould. 1985. On practical conditions for the existence and uniqueness of solutions to the general quality quadratic programming problem. *Math. Program.* 32, 1 (May 1985), 90–99.
- N. I. M. Gould, M. E. Hribar, and J. Nocedal. 2001. On the solution of equality constrained quadratic programming problems arising in optimization. *SIAM J. Sci. Comput.* 23, 4 (Jan. 2001), 1376–1395.
- N. I. M. Gould and P. L. Toint. 2000. A quadratic programming bibliography. *Numer. Anal. Group Intern. Rep.* 1 (2000), 32.
- Gurobi. 2021. Gurobi Optimizer Reference Manual.
- B. Hermans, A. Themelis, and P. Patrinos. 2019. QPALM: A Newton-type proximal augmented Lagrangian method for quadratic programs. In *Proceedings of the 58th IEEE Conference on Decision and Control*.
- B. Hermans, A. Themelis, and P. Patrinos. 2020. QPALM: A proximal augmented Lagrangian method for nonconvex quadratic programs. Retrieved from <https://arXiv:2010.02653>.
- J. B. Hiriart-Urruty, J. J. Strodiot, and V. H. Nguyen. 1984. Generalized Hessian matrix and second-order optimality conditions for problems with $C^{1,1}$ data. *Appl. Math. Optim.* 11, 1 (Feb. 1984), 43–56.
- M. Li, D. Sun, and K.-C. Toh. 2016a. A majorized ADMM with indefinite proximal terms for linearly constrained convex composite optimization. *SIAM J. Optim.* 26, 2 (Jan. 2016), 922–950.
- X. Li, D. Sun, and K.-C. Toh. 2016b. A Schur complement based semi-proximal ADMM for convex quadratic conic programming and extensions. *Math. Program.* 155, 1 (Jan. 2016), 333–373.
- X. Li, D. Sun, and K.-C. Toh. 2018. QSDPNAL: A two-phase augmented Lagrangian method for convex quadratic semidefinite programming. *Math. Prog. Comp.* 10, 4 (Dec. 2018), 703–743.
- X. Li, D. Sun, and K.-C. Toh. 2020. An asymptotically superlinearly convergent semismooth Newton augmented Lagrangian method for linear programming. *SIAM J. Optim.* 30, 3 (Jan. 2020), 2410–2440.
- F. J. Luque. 1984. Asymptotic convergence analysis of the proximal point algorithm. *SIAM J. Control Optim.* 22, 2 (Mar. 1984), 277–293.
- I. Maros and C. Mészáros. 1999. A repository of convex quadratic programming problems. *Optim. Methods Softw.* 11, 1–4 (1999), 671–681. Retrieved from www.cuter.rl.ac.uk/Problems/marmes.shtml.
- G. J. Minty. 1962. Monotone nonlinear operators in Hilbert space. *Duke Math. J.* 29, 3 (1962), 341–346.
- Y. Nesterov and A. Nemirovskii. 1994. *Interior-point Polynomial Algorithms in Convex Programming*. Society for Industrial and Applied Mathematics.
- C. C. Paige and M. A. Saunders. 1975. Solution of sparse indefinite systems of linear equations. *SIAM J. Numer. Anal.* 12 (1975), 617–629.
- A. F. Perold. 1984. Large-scale portfolio optimization. *Manag. Sci.* 30, 10 (1984), 1143–1160.
- S. M. Robinson. 1981. Some continuity properties of polyhedral multifunctions. In *Mathematical Programming at Oberwolfach*. Springer, 206–214.
- R. T. Rockafellar. 1976a. Augmented Lagrangians and applications of the proximal point algorithm in convex programming. *Math. Oper. Res.* 1, 2 (1976), 97–116.
- R. T. Rockafellar. 1976b. Monotone operators and the proximal point algorithm. *SIAM J. Control Optim.* 14, 5 (1976), 877–898.
- R. T. Rockafellar. 1997. *Convex Analysis*. Vol. 36. Princeton University Press.
- R. T. Rockafellar and R. J. B. Wets. 2009. *Variational analysis*. Vol. 317. Springer Science & Business Media.
- Y. Saad. 2003. *Iterative Methods for Sparse Linear Systems*. Society for Industrial and Applied Mathematics.
- B. Stellato, G. Banjac, P. Goulart, A. Bemporad, and S. Boyd. 2020. OSQP: An operator splitting solver for quadratic programs. *Math. Program. Comput.* (2020), 1–36.
- J. Sun. 1993. A convergence proof for an affine-scaling algorithm for convex quadratic programming without nondegeneracy assumptions. *Math. Program.* 60, 1 (1993), 69–79.
- H. Takehara. 1993. An interior point algorithm for large scale portfolio optimization. *Ann. Oper. Res.* 45, 1 (1993), 373–386.
- A. Wiegele. 2007. Biq Mac library—A collection of Max-Cut and quadratic 0-1 programming instances of medium size. *Preprint* 51 (2007). Retrieved from <http://www.biqmac.uni-klu.ac.at/biqmaclib.html>.
- S. Wright and J. Nocedal. 2006. *Numerical Optimization*. Springer Science & Business Media.
- L. Yang, D. Sun, and K.-C. Toh. 2015. SDPNAL+: A majorized semismooth Newton-CG augmented Lagrangian method for semidefinite programming with nonnegative constraints. *Math. Program. Comput.* 7, 3 (2015), 331–366.
- Y. Ye. 1998. On the complexity of approximating a KKT point of quadratic programming. *Math. Program.* 80, 2 (1998), 195–211.
- X. Zhao, D. Sun, and K.-C. Toh. 2010. A Newton-CG augmented Lagrangian method for semidefinite programming. *SIAM J. Optim.* 20, 4 (2010), 1737–1765.

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